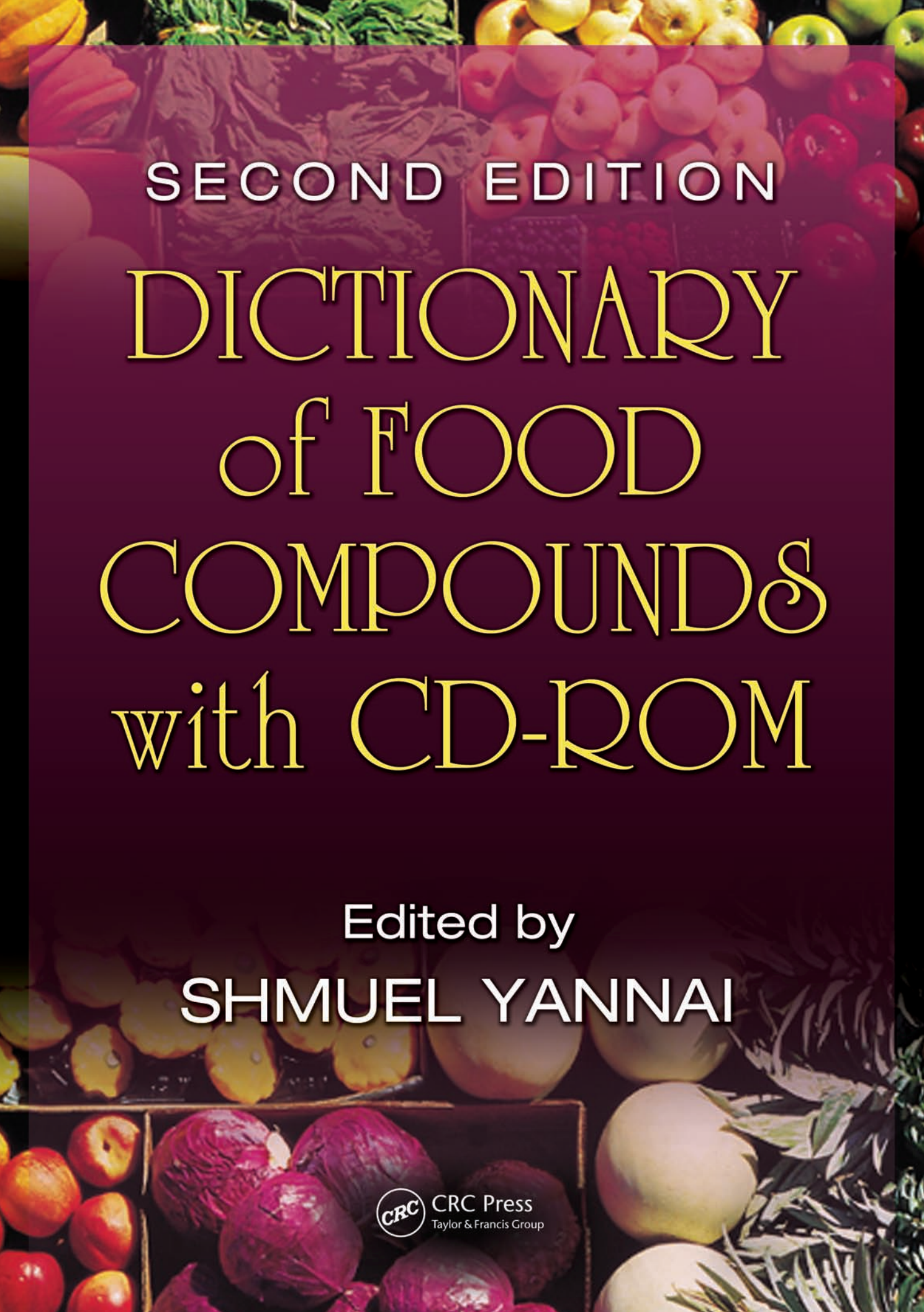
SECOND EDITION
DICTIONARY of FOOD COMPOUNDS with CD-ROM
Edited by
SHMUEL YANNAI
CRC Press
Taylor & Francis Group

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Taylor & Francis Group
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Preface from the first edition

For some years, those involved in food chemistry and technology have felt the need for a comprehensive and well-organised reference source documenting the whole range of substances on which they may need information during their day-to-day work. Whilst there are many valuable compilations and tabulations of particular areas, for example permitted food additives or natural flavourings, there has been nothing available that is truly comprehensive. In addition, the existing reference works have mostly evolved as traditional books, with their associated shortcomings in terms of indexing and expense of updating.

With the increasing and sometimes contradictory demands of the consumer market today, the need for the best up-to-date and accurate information has never been greater. This is perhaps not the place to digress into the debate on 'Chemicals in Food'; anyone in the position of reading this preface will be quite aware of most of the issues involved, and will have his or her own views. What is certain, however, is that from whatever direction one approaches the debate, it is a sterile and unproductive one unless there is good information about the true state of the science. And that science is of course by no means limited to food technology. Any participant in the debate who is ignorant about the effects of the natural products in the foods we eat is seriously misinformed.

CRC Press in their role as chemical information specialists are uniquely able to provide a technology capable of aiding the compilation and publication of such a comprehensive reference source. Their experience of database publishing in chemistry goes back to the late 1970s when compilation of the first electronic edition of the *Dictionary of Organic Compounds* was begun. Since that time, a series of high quality searchable data compilations has appeared at regular intervals. In due course, it only remained to put this technical expertise together with the specialist knowledge of an experienced international Editorial Board with overall responsibility for content, and a team of contributors with knowledge of particular areas of food components. The resulting *Dictionary of Food Compounds* is available both in hard copy and electronically, as a CD-ROM product. Each has its own advantages. There is nothing to rival the ease of consulting a book version for quick queries and for browsing to get an overall view of the whole field. On the other hand, the electronic version is searchable by chemical substructure as well as text and, for obvious reasons, is much more easily updated so that the user can get a very rapid summary of new developments in the science. The *Dictionary* is aimed not only at food scientists and technologists, but at the wide range of people whose work brings them into contact with the regulatory aspects of food supply and monitoring.

The book and CD-ROM versions are complementary. The important thing for the user to be assured of is that the *Dictionary of Food Compounds* is an ongoing project which the Publishers hope and expect will become a central feature of the information needs of everyone involved in food.

Every effort has been taken to ensure the accuracy of the information contained in DFC. Any errors or omissions should be communicated to the Publishers, who will also be pleased to receive any comments about the coverage, and especially suggestions for its expansion.

Supplementary Resources Disclaimer

Additional resources were previously made available for this title on CD. However, as CD has become a less accessible format, all resources have been moved to a more convenient online download option.

You can find these resources available here: www.routledge.com/9781420083514

Please note: Where this title mentions the associated disc, please use the downloadable resources instead.

Editorial Board

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Foreword

RATIONAL EXPLOITATION OF FOOD RESOURCES

The growing demand of the increasing world population for palatable, nutritious, and safe food, competition for arable land, pasture, and rich fishing grounds as well as the environmental and sustainability concerns make it necessary to exploit in a sustainable way the available plant and animal resources of the planet for human consumption. This may be achieved, e.g., by:

- increasing the direct use as food of legumes that are mainly produced for feeding animals,
- breeding and market introduction of various small grain cereals including those of wild species,
- diversification in fish aquaculture by introducing rapidly growing species of high consumers' acceptability,
- rational exploitation of marine resources, including the open-sea small pelagic fish and Antarctic krill,
- increasing the productivity and quality of slaughter animals,
- preventing the waste of food in a global scale caused by lack of knowledge, management, storage facilities, and proper processing,
- improving the education of the population in matters of food hygiene, properties, and nutrition.

In searching for better use of the available resources, numerous factors must be considered. Because of sustainability concerns the negative impact of some aspects of food production and use related to wastage as well as to energy and water consumption are also of utmost importance.

HEALTH HAZARDS RELATED TO FOOD

Globalization of the food market increases the hazards associated with transfer and spread of harmful organisms present in plant and animal raw materials as well as in the environment. Applying proper diagnostic procedures, processing treatments, and international regulations must counteract the risk caused by parasitic infestation of numerous seafoods and slaughter animals. Furthermore, diseases of livestock occur in new locations. They have a significant effect on animal health, as well as on the economy of food production and trade. This results in economic losses in plant production and animal breeding and in serious health hazards to the consumers.

Pathogenic microorganisms and their toxins in foods are the most important risk factor and call for adequate control systems. Bacterial food poisoning can be to a large extent prevented mainly by low temperature handling and storage, practicing severe hygienic principles in the industry and at home, and applying proper parameters of sterilization. On the other hand, the hazards associated with mycotoxins in cereal grains, rice, peanuts, and other agricultural commodities depend predominantly on the conditions of harvest and post-harvest treatment of the crop.

Numerous natural toxic compounds of plant origin including the dangerous mushroom toxins, fish and shellfish toxins, and biogenic amines in fish and fermented products must also be considered in evaluating the safety of foods. Further health hazards are associated with environmental pollution by, e.g., heavy metals, dioxins, polychlorinated biphenyls, polycyclic aromatic hydrocarbons, and pesticide residues. Several compounds generated in food processing, e.g., acrylamide, mutagenic/carcinogenic heterocyclic amines in heated products, nitrite and N-nitrosamines in cured meats and fish meal, or unnatural amino acids like lysinoalanine and lanthionine are reasons for concern. The threat for the consumers' health caused by some of these compounds in various foods should be carefully evaluated in order to prevent any prejudice toward products manufactured in conditions complying with current international safety regulations.

DESIRABLE EFFECTS OF PROCESSING

Changes in food components due to post-harvest enzyme activity and industrial processing affect positively several quality aspects of the products. Postmortem tenderization improves the texture of beef; enzyme treatments and physical processing serve in producing different food commodities and enhance the functional properties of various protein isolates and preparations. Properly applied heating inactivates the antinutritional factors in, e.g., legumes and eliminates the hazard of bacterial poisoning associated with many products, predominantly milk and canned foods. Heating as applied in bakery and cookery leads to color changes due to the Maillard reaction and to generation of volatile aroma compounds, although it may also decrease somewhat

the nutritional value of the products. Fermentation processes result in formation of desirable flavors of wine, cheeses, and bread. Due to lipid hydrolysis and oxidation, both pleasant and rancid flavors are formed.

In order to increase the shelf life of foods and to improve various sensory attributes of the products, e.g., color, flavor, taste, and texture, numerous additives, both natural and synthetic, are used in the industry. Their application is limited by appropriate international regulations. Furthermore, the risks and benefits should be evaluated in considering whether or not certain additives should be used. The general rule is that an additive may be applied only if the intended technological effect cannot be achieved by other means. Nevertheless, some consumers regard the presence of such compounds as harmful, regardless that strict control of their safety and conditions of use is obligatory. In response to consumer preferences, some companies replace artificial colors, flavors, and preservatives in their products by natural ingredients.

FOOD–HUMAN HEALTH RELATION

The biological role of individual food components and of the whole human diet is actually in the forefront of research and industrial projects. The awareness of the role of the diet as an important risk factor for cancer, obesity, allergy, inflammatory bowel diseases, diabetes, hypertension, coronary heart diseases, strokes, depression, and many other illnesses is increasing. The beneficial action of certain food compounds, e.g., vitamins, n-3 fatty acids, mineral components, dietary fiber, natural antioxidants, prebiotics, various food additives, and different non-nutrient phytochemicals is also taken into consideration both by nutritionists and food producers. Responding to the market demands the food industry is eager to develop new products, basing on sound information on the contents of various components in available raw materials displaying specific biological and functional properties. Numerous assortments of tailor-made products targeted to special groups of customers are manufactured, e.g., light, sugar-free, low-salt, gluten-free, rich in fiber, free of most food allergens, and high in n-3 polyenoic fatty acids, as well as some esoteric foods.

CONTROL OF FOOD QUALITY

Although in recent decades the overall quality and shelf life of food offered on the market has improved very significantly, there is still concern about safety in situations of unexpected microbiological hazard outbreaks or environmental contaminations. Increasing attention is given to the authenticity of many commodities. The consumer requires that the product offered on the market has the specific characteristics declared on the label regarding its origin, species or variety, contents of nutrients, absence/presence of additives and genetically modified constituents, method of production, and processing treatments, e.g., solvent extraction, freeze-drying, frying, canning, freezing, or irradiation. There is a need for global harmonization of food standards and creation of tools to precisely detect fraud and assure that foods match the information declared on the label.

To cope with safety and quality demands, various research programs are under way that aim at developing practical solutions for controlling the spread of pests and pathogens and eliminating the hazards caused by environmental contamination and undesirable effects of processing. Numerous compounds originally present in food raw materials or generated due to post-harvest changes and reactions induced by processing have an important diagnostic role. They serve as indicators in conventional sensory assessment of quality. They may also be applied in various sensors used for real-time monitoring of the environment, as well as in on-line or in-line control of quality and safety attributes in quality management systems like good manufacturing practice or hazard analysis and critical control points.

ROLE OF CHEMICAL ANALYSIS

The unprecedented, rapid developments in methods of diagnostics and analytical equipment contribute to assuring safety and quality along the food chain. Different chromatographic procedures are used for determining a variety of individual food constituents — lipids, amino acids, saccharides, veterinary drug and antibiotic residues, additives, and pollutants or characterization of the entire profile of components in metabolomic studies. New molecular diagnostic tools for pathogen assays, detection of genetically modified foods and feed, and procedures for food/feed traceability have been developed. Ultrasound techniques can be applied for texture evaluation, grading of beef carcasses, density and particle size measurements, and detection of foreign bodies. Nuclear magnetic resonance has been used for food traceability and in analysis of vegetable and fish oils. DNA-based techniques are effective in microbiological analyses and for detecting genetically modified food ingredients. Immunoassays are useful for control of food authenticy/adulteration, detection of food-borne pathogens,

microbial toxins, pesticides, and allergens. The developments in this field are being presented in numerous monographs, e.g., in the CRC book *Methods of Analysis of Food Components and Additives. Second Edition*, edited by Semih Ötles.

The use of modern analytical techniques makes it possible to determine trace quantities of harmful analytes in various foods. The limit of detection of *Clostridium botulinum* neurotoxins by immuno-polymerase chain reaction is 5 pg/cm^3, while that of CH_3Hg and inorganic Hg, using electrothermal vaporization with inductively coupled plasma mass spectrometry, about 2 and 6 ng/g, respectively.

The results of chemical experiments and analyses of food samples are often scattered, mainly due to the natural variability of the biological material. Therefore, their interpretation may be difficult; Theodore Labuza pointed to it years ago in his limerick:

"There was a young chemist from Lata
who could not interpret his data.
So he drew a straight line.
Now everything is fine,
except for the damnable scatter".

However, thanks to the developments in chemometrics and metabolomics this difficulty can now be overcome.

NON-FOOD USE OF RESOURCES

Food plants and animal resources are a rich source of compounds, which have various industrial applications, e.g., enzymes, pharmaceuticals, cosmetics, surfactants, pigments, and flavoring agents. Numerous valuable products can be obtained by utilization of inedible parts of plant and animal raw materials separated during processing. One example of such resources is the Antarctic krill, rich in very active hydrolytic enzymes and a source of chitin, which can be transformed into chitosan by chemical and enzymatic treatments. Various derivatives of chitin and chitosan are used in chemical analysis, water treatment, medicine, veterinary medicine, textile industry, and as antimicrobial agents.

THE ROLE OF *THE DICTIONARY OF FOOD COMPOUNDS*

The properties and reactions of the main food components, predominantly water, proteins, saccharides, lipids, and many other compounds constituting the bulk of most foods have been expertly presented in leading food chemistry textbooks, like the *Lehrbuch der Lebensmittelchemie* by Belitz, Grosch, and Schieberle (Springer), *Fennema's Food Chemistry* edited by Damodaran, Parkin, and Fennema (CRC), and *Chemie Potravin* by Davidek, Janiček, and Pokorny (SNTL). Valuable information on food additives can still be found in the old *Handbook of Food Additives*, edited by Furia (CRC). The constantly accumulating new knowledge regarding these compounds is being reviewed in numerous monographs, e.g., the *Advances in Food and Nutrition Research* (Elsevier) and the CRC series *Chemical and Functional Properties of Food Components*. However, to cope with the large range of tasks related to food availability, safety, nutritional value, sensory properties, processing, storage, quality assessment and assurance, and distribution, it is necessary to have access to a collection of sound information on almost all compounds found in foods, since even those present in minute concentrations may exert very serious desirable or negative effects. The *Dictionary of Food Compounds, Second Edition* is such a source, essential in libraries, to be used by food chemists, technologists, and nutritionists. It has been published in a user-friendly form available as a hard copy and on a CD-ROM. It contains entries describing natural components of food raw materials and products, as well as compounds added to foods or formed in the course of storage or processing. Each entry contains the name of the component, the chemical and physical characteristics, description of functional properties related to food use, and nutritional and toxicological data. More detailed information about any particular compound can be obtained by consulting the cited literature.

The idea of preparing the *Dictionary of Food Compounds* was supported by the Division of Food Chemistry of the European Federation of Chemical Societies. The book has been edited by Dr. Shmuel Yannai, Professor (Emeritus since 2006) at Technion - Israel Institute of Technology. Professor Yannai is a world authority in food chemistry, especially as regards metabolic transformation and elimination of toxic, mutagenic, and carcinogenic compounds in biological systems, anticarcinogenic effects of some compounds, elimination of toxic metals from

certain foods and drinking water, disinfection of agricultural produce by treatment with ozone, characterization and inactivation of food allergens, and effect of chromium on carbohydrate metabolism in healthy and diabetic patients. Thanks to his extensive research and teaching experience Professor Yannai was able to succeed in directing the work of the team who prepared the book which will serve people interested in many areas of food chemistry.

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Department of Food Chemistry, Technology, and Biotechnology

Introduction

Users interested in more detailed factual information on topics outlined below are referred to the *Organic Chemist's Desk Reference, Second Edition* (Cooper, C., CRC Press, 2011).

1. USING THE DICTIONARY OF FOOD COMPOUNDS

The arrangement of entries is alphabetical by name. The criteria governing the choice of entry name are described below. Many compounds in the Dictionary are present as derivatives of a parent. The CD-ROM version can be searched by all names given throughout the dictionary, whether entry names, synonyms or derivative names.

Every entry is assigned a dictionary number to assist ready location. The dictionary number consists of a letter of the alphabet followed by a number, e.g., A-124. All index entries refer to the dictionary number.

2. COMPOUND SELECTION AND PRESENTATION

The selection of compounds for the Dictionary is broad. Included are all compounds or group of compounds of interest or potential interest to the food industry in its widest connotation. Compounds need not have been exactly defined structurally to be included.

A full description of the scope of compounds included can be gained by perusing the headings in the Type of Compound Index on the CD-ROM, since virtually every compound or group of compounds included is listed under at least one of the headings.

The printed Dictionary contains a number of derivatives that are not of direct food interest, but are included because they have been used for chemical characterisation of the main entry compound. However, the number of these is strictly limited. In contrast, the version of an entry on the CD-ROM, where space is not a limitation, is the full version as present on the Chemical Database and may include many more derivatives not thought to be of current food interest. When using the CD-ROM, the possibilities for flexible searching are such that the portion of the entry most relevant to food science can rapidly be homed in on.

The Dictionary contains many natural products known to occur in food plants for which no specific food-related information, such as flavour or toxicity, appears to be available. In such cases, the decision to include them has been based on the species information given in the entry. If one or more of the species recorded is a food plant or other food source, the compound has been selected for inclusion in the dictionary dataset. The label 'food plant' is broadly defined and includes edible wild foods as well as established crop foods, also toxic plants of potential interest to nutritionists. Where there is some doubt about whether a particular plant is of food significance, it has generally been included. The sources used to validate food plant information include the CropSEARCH database (www.hort.purdue.edu/newcrop/, Purdue University, USA) and the titles: *World Economic Plants – A Standard Reference* (Wiersema, J.H. and León, B., CRC Press, 1999); *Fenaroli's Handbook of Flavor Ingredients* (6^{th} edn., Burdock, G.A., CRC Press, 2010); *Encyclopedia of Food and Color Additives* (Burdock, G.A., CRC Press, 1996); *Handbook of Nutraceuticals & Functional Foods* (Wildman, R.E.C., CRC Press, 2000).

3. THE TYPE OF COMPOUND INDEX

This is a most important feature of the Dictionary. Every compound of food interest included in the dictionary is indexed under at least one heading; usually two or more. The headings are of five types.

Structural headings (WA) classify naturally occurring food constituents under one of 30 headings according to their chemical structure, such as

WA1100 Natural food colourants (betalaines)
WA5100 Food sugars (disaccharides)

Deliberate food additive headings (WC) refer to the various functions performed by such additives, such as

WC0700 Antioxidants
WC2100 Curing agents

Food flavour and odour headings (WE) are self-explanatory and may refer to natural, nature-identical or synthetic odours and flavours.

Food contaminant headings (WG) classify all undesirable/unintended compounds present in foods, such as

WG1000 Animal feed contaminants
WG3500 Food allergens

Food Source headings (WI) classify food compounds, both natural and processing-derived, by their food source. Examples are

WI1000 Cereals and bakery products
WI6000 Dairy products

Food function headings (WK) are self-explanatory and include for example

WK1500 Antimutagenic agents
WK6500 Nutraceuticals

Once again, compounds classified under these headings may be natural, synthetic or nature-identical.

On the CD-ROM, a combination of these headings with other types of compound codes provides powerful search possibilities.

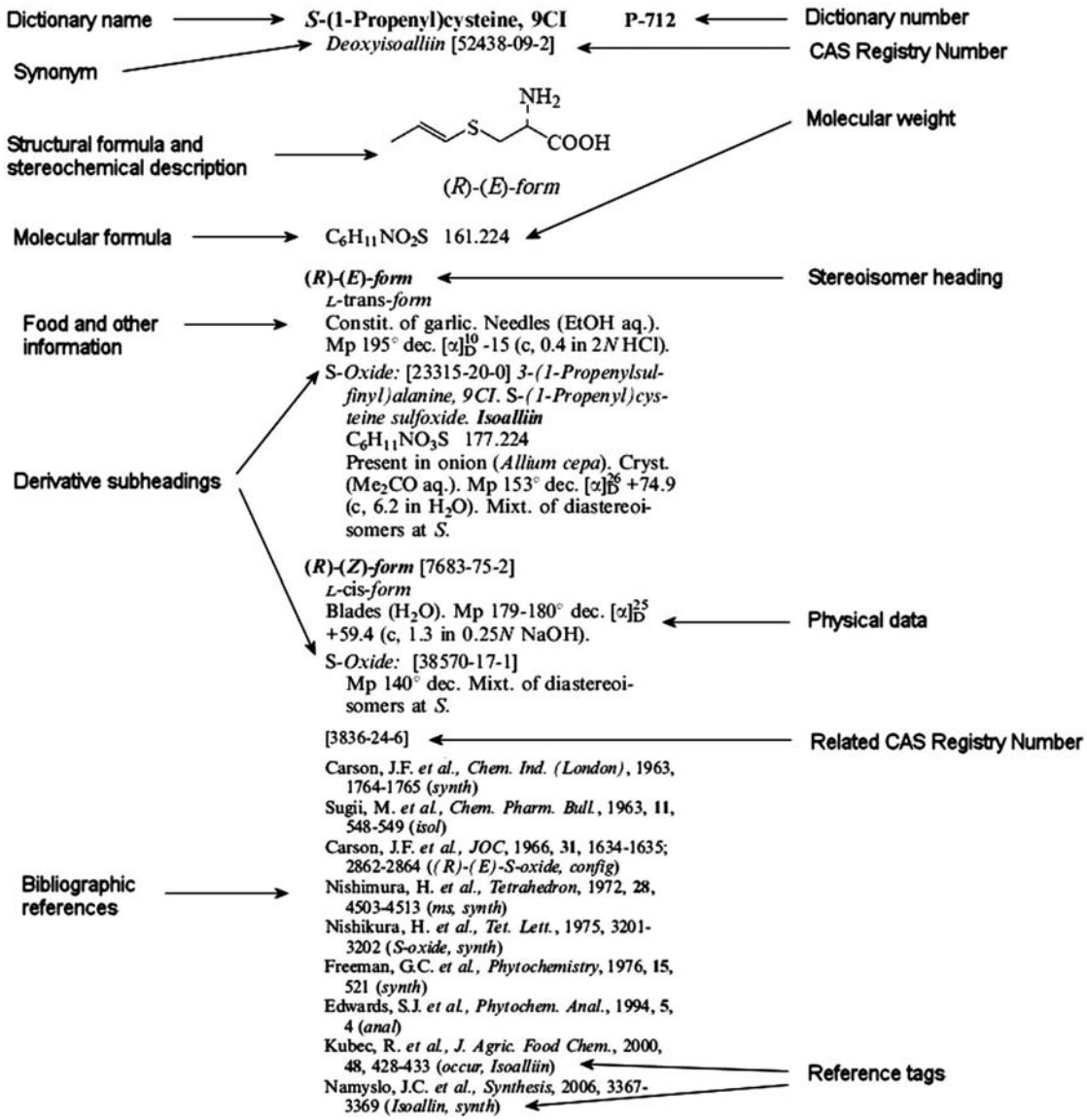


FIG.1 The format of a typical entry in the Dictionary of Food Compounds

4. LITERATURE COVERAGE

In compiling this edition the primary literature has been surveyed to 2011.

5. ORGANISATION OF ENTRIES

Fig. 1 illustrates the format of a typical entry within which the individual types of data have been labelled.

5.1 Chemical Names and Synonyms

5.1.1 The Entry name

The Entry name is that chosen to head each entry and is that which, in the opinion of the Editors, is the one most likely to be known by, and of use to, most readers.

The American spelling sulf- is used throughout in preference to the British sulph-.

The Dictionary does not seek to establish standards of nomenclature, and the adoption of a particular name as entry name does not imply endorsement in any way. However, the Dictionary dataset was carefully reviewed before publication in order to give a high degree of internal consistency in the choice of entry names.

Users interested in a fuller explanation of nomenclature policy and nomenclature rules in general are referred to the *Organic Chemist's Desk Reference, Second Edition.*

5.1.2 Synonyms

Nearly all entries and derivatives are accompanied by various synonyms. These come from a variety of sources:

Chemical Abstracts Services (CAS) names. CAS assigns a unique name to every chemical substance. Because of the necessity to employ strict nomenclature rules to arrive at such a unique name, CAS names are often cumbersome, and in addition, many CAS parent names are relatively unfamiliar to many potential Dictionary users (for example, benzenamine for aniline and 1-methylethyl for isopropyl). If the CAS name is not the entry name, the Dictionary will often give it as a synonym if it is not too cumbersome for effective use.

The names in use by CAS for organic compounds have been largely unchanged since the beginning of the 9th collective index period in 1972 and are followed by the suffix **9CI**. This suffix means that the name is one in use by CAS since 1972, and does not necessarily mean that the compound can be found in the 9th collective index of CAS, which covers 1972-1976 only.

Names in use by CAS before 1972 may also be given. Names from the 8th collective index period (1967-71) are usually suffixed **8CI**, but names used before 1967 are not specially labelled.

Other chemical names not corresponding to any found in CAS may also be given; these have either been found in the chemical/food literature or have been added editorially for consistency or clarity. Some compounds, particularly natural products, possess trivial names. A favoured trivial name will appear in boldface.

Trade names, generic names and names allocated by regulatory bodies are invariably given. Their names may be invented names, e.g., for pesticides, or may be serial numbers, e.g., the E numbers. Examples of such bodies are the Flavor and Extract Manufacturers' Association (FEMA) and the EU Commission (E numbers). Also included are those recommended by the British Pharmaceutical Commission as British Approved Names (BAN), the United States Adopted Name Review Board (USAN), the British Standards Institute (BSI) or the World Health Organisation as an International Nonproprietary Name (INN). No distinction is made between International Nonproprietary Names which are currently proposed (pINN) and those which are recommended (rINN).

Names which are known to be duplicated within the chemical literature are marked with the symbol ‡.

5.2 CAS Registry Numbers

CAS numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by CAS since 1965 (plus some retrospective allocation of numbers by CAS to compounds from earlier index periods). The numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature. They are extensively used for exchanging information between individuals and databases. The numbers take the form NNNNNN-NN-R, where the total number of digits is five or more and R is a check digit.

For practical purposes, CAS numbers have certain shortcomings arising from their free allocation, resulting in one substance having more than one potential number. Duplication may arise for one of several reasons to do

with the detailed chemistry of the substance, for example tautomerism, solvent formation, partially unspecified stereochemistry. There are also replaced numbers. For this reason, the Dictionary entries will often contain one or more *Additional CAS numbers* which may help the user to obtain further information about the substance, especially by online searching.

Some entries in the Dictionary refer to families of compounds, especially natural products. An example is the entry for the group of peptide hormones, Relaxins. Here, general information is given that applies to all the species variants, plus a significant number of additional CAS numbers which may refer to additional members of the group that are less well documented or characterised.

Clearly, the additional CAS numbers given in the Dictionary have to be used with care. Their inclusion in the entry is the result of an editorial decision by the Dictionary contributor that they refer to what is essentially the same substance, but this decision may be a subjective one. Care has been taken to ensure that the main CAS number given in the Dictionary for each substance is the correct one.

Further information on CAS number allocation policy can be obtained from CAS indexes or the *Organic Chemist's Desk Reference, Second Edition.*

5.3 Structural Formulae

Every attempt has been made to present the structures of chemical substances as accurately as possible according to best current practice and recommendations of IUPAC (The International Union of Pure and Applied Chemistry). As much consistency as possible has been aimed at between closely-related structures. For example, all sugars are shown as Haworth formulae, and whenever possible in complex structures the rings are oriented in the standard Haworth convention so that structural comparisons can be quickly made.

5.4 Molecular Formula and Molecular weight

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or more strictly, molar masses in daltons) and are rounded to three places in decimals. In the case of some high molecular mass substances, such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

5.5 Food Information

The information given on the food uses of many of the substances included in the Dictionary is of key importance and has, as far as possible, been based on critical sources. However in the case of compounds that have become of interest only recently, or for which little information is available, the information may be based on journal references only, in which case the reference will normally be given.

In a few cases, the only information that can be found that a compound is of food-related significance is the fact that the compound has been included in a database such as EAFUS Food Additive Database, and there appears to be no published literature supporting that inclusion. This fact will normally be noted in the entry.

The Dictionary also contains much information on the non-food uses of compounds. This information is of obvious potential use when it is identified for example as a food contaminant.

5.6 Physical Data

The Dictionary gives the following physical characteristics of substances, when available; appearance, melting point, boiling point, optical rotation, density, refractive index, solubility, pKa. All of these fields are searchable by numerical value (including range searching) in the CD-ROM version of the Dictionary.

5.6.1 Appearance

Organic compounds are considered to be colourless unless otherwise stated. Where the compound contains a chromophore which would be expected to lead to visible colour, but no colour is mentioned in the literature, the Dictionary entry will mention this fact if it has been noticed by the contributor. An indication of crystal form and of recrystallisation solvent is often given but these are imprecise items of data; most compounds can be crystallised from several solvent systems and the crystal form often varies. In the case of the small number of

compounds where crystal behaviour has been intensively studied (e.g. pharmaceuticals), it is found that polymorphism is a very common phenomenon and there is no reason to believe that it is not widespread among organic compounds generally.

5.6.2 Melting Points and Boiling Points

The policy followed in the case of conflicting data is as follows:

(a) Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted
(b) Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus Mp 139° (134-135°)
(c) Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus Mp 142°, Mp 205-206°
(d) Known cases of polymorphism or double melting points are noted

Boiling point determination is less precise than that of melting points and conflicting boiling point data is not usually reported except when there appears to be a serious discrepancy between the different authors.

5.6.3 Optical Rotations

These are given wherever possible, and normally refer to what the Dictionary contributor believes to be the best characterised sample of highest chemical and optical purity. Where available an indication of the optical purity (op) or enantiomeric excess (ee) of the sample measured follows the specific rotation value.

Specific rotations are dimensionless numbers and the degree sign which was formerly universal in the literature has been discontinued.

5.6.4 Densities and Refractive indexes

Densities and refractive indexes are now of less importance for the identification of liquids than has been the case in the past, but are quoted for common or industrially important substances such as solvents, or where no boiling point can be found in the literature.

Densities and refractive indexes are not quoted where the determination appears to refer to an undefined mixture of stereoisomers.

5.6.5 Solubilities

Solubilities are given only where the solubility is unusual for a compound. Typical organic compounds are soluble in the usual organic solvents such as ether and chloroform, and virtually insoluble in water. The presence of polar groups (OH, NH_2, and especially COOH, SO_3H and NR_3^+) increases water solubility.

5.6.6 pK_a Values

pK_a values are given for both acids and bases. The pK_b of a base can be obtained by subtracting its pK_a from 14.17 (at 20°) or from 14.00 (at 25°).

5.7 Spectroscopic Data

Many dictionary entries include ultraviolet spectra which are presented in the format:

[neutral] λ_{max} 198 (log ε 1.55); 224 (sh) (log ε 0.61); 241 (sh) (log ε 0.55) (H_2O) (Berdy)

where ε is the absorption coefficient for a given UV maxima value (λ_{max}). A description of the solvent conditions used, if reported in the literature, is listed at the beginning and end of the UV data in parentheses. All peak absorptions cited are maxima unless otherwise described, e.g., shoulder/inflection (sh) and end absorption (end). In addition, UV data may be followed by the term 'Berdy' or 'DEREP' indicating from which database the data originated. The absence of either of these terms implies that the data was abstracted from the primary literature.

On the CD-ROM, all the λ_{max} values are indexed in the UV Maxima field and can be searched for numerically including range searching. Similarly, the solvent data associated with the UV data are indexed in the UV Solvent field.

5.8 Hazard and Toxicity Information

5.8.1 General

Toxicity and hazard information is highlighted by the symbol ▶ and has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

Physical, ***reactive*** and ***toxic*** properties all contribute to the hazard associated with a particular chemical. As part of the ***physical data***, flash points, explosive limits and autoignition temperatures have been included where appropriate. Flammable classifications, which are based on flash point measurements and boiling points, are also mentioned, and the opportunity has been taken to include UK occupational exposure limits, or for some compounds threshold limit values published by the American Conference of Governmental Industrial Hygienists (ACGIH). For the ***reactive*** hazards, a brief comment is made on any explosive (or violent polymerisation) properties and aspects of the chemical reactivity of a substance which are of concern. These include the potential for peroxidation, oxidising/reducing properties and incompatibility with commonly available chemicals. ***Toxicity*** information has been chosen to show hazardous effects from short-term or long-term exposure. Observations from human exposure are summarised if available (including possible adverse effects of drugs), otherwise experimental (exp.) tests are quoted. Included in the toxicity data are the results of irritancy tests, acute lethality data, target organ toxicity, and carcinogenic and reproductive properties where appropriate. Those chemicals which have been classified by the International Agency for Research on Cancer (IARC) as *human carcinogens*, *probable human carcinogens* or *possible human carcinogens* have been identified in the Dictionary accordingly.

The Publishers cannot be held responsible for any inaccuracies in the reported information, neither does the omission of hazard data in the *Dictionary* imply an absence of this data from the literature. Widely recognised hazards are included however, and where possible key toxicity reviews are identified in the references. Further advice on the storage, handling and disposal of chemicals is given in the *Organic Chemist's Desk Reference, Second Edition*.

Finally, it should be emphasised that any chemical has the potential for harm if it is carelessly used.

5.8.2 RTECS® Accession Numbers*

Many entries in the dictionary contain one or more RTECS® Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH *Registry of Toxic Effects of Chemical Substances*, which is a compendium of toxicity data extracted from the scientific literature.

For each Accession Number the RTECS® database provides the following data when available: substance prime name and synonyms; data when the substance record was last updated; CAS Registry Number; molecular weight and formula; reproductive, tumorigenic, and toxic dose data; and citations to aquatic toxicity ratings, IARC reviews, ACGIH Threshold Limit Values, toxicological reviews, existing Federal standards, the NIOSH criteria document program for recommended standards, the NIOSH current intelligence program, the NCI Carcinogenesis Testing Program, and the EPA Toxic Substance Control Act inventory. Each data line and citation is referenced to the source from which the information was extracted.

5.9 Bibliographic References

The selection of references is made with the aim of facilitating entry into the chemical and food literature for the user who wishes to locate more detailed information about a particular compound. The contents of most references are indicated by reference tags (suffixes) indicating their content and in particular the stereoisomers and derivatives of the parent compound which they document. The number of references cited does not indicate the relative importance of a compound; one key recent citation may supersede a number of older ones.

Journal abbreviations generally follow the practice of the Chemical Abstracts Service Source Index (CASSI), except for a short list of very well known journals where the Dictionary gives shorter abbreviations to save space (e.g. *JACS* instead of *J. Am. Chem. Soc.*)

5.9.1 Further References

Further useful information on a variety of topics concerned with the structure, description, stereochemistry and nomenclature of organic compounds can be found in the *Organic Chemist's Desk Reference, Second Edition.*

6. ABBREVIATIONS

The following is a selection of the most common Database abbreviations used:

Abbreviation	**Name**
[α]	specific rotation
abs config	absolute configuration
Ac	acetyl
acc	according
AcOH	acetic acid
Ac_2O	acetic anhydride
ACGIH	American Conference of Governmental Industrial Hygienists
ADI	Acceptable Daily Intake
alk	alkaline
amorph	amorphous
amt	amount
anal	analytical applications, analysis of detection
anhyd	anhydrous
aq	aqueous
BAN	British Approved Name
bibl	bibliography
biosynth	biosynthesis
Bp	boiling point
c	concentration
ca	(*circa*) about
cd	circular dichroism
CAS	Chemical Abstracts Service
chromatog	chromatography
cmr	carbon (^{13}C) nuclear magnetic resonance
CNS	central nervous system
col	colour, coloration
coml	commercial(ly)
compd	compound
conc	concentrated
config	configuration
conformn	conformation
constit	constituent
cryst struct	X-ray crystal structure determination
d	density
dck	duck
dec	decomposes, decomposition
degradn	degradation
deriv(s)	derivative(s)
detn	detection, determination
dil	dilute, dilution
dimorph	dimorphic
diss	dissolves, dissolved

dist(n)	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
epr	electron paramagnetic (spin) resonance
equilib	equilibrium
esp	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq	aqueous ethanol
exp	experimental
FEMA	Flavor and Extract Manufacturers' Association
fl p	flash point
fluor	fluoresces, fluorescence
formn	formation
Fp	freezing point
g	gram
glc	gas liquid chromatography
Glc	β-D-glucopyranosyl
GRAS	Generally Recognised As Safe
ham	hamster
haz	hazard
hplc	high performance liquid chromatography
hydrol	hydrolyses, hydrolysed, hydrolysis
ihl	inhalation
ims	intramuscular
INN	International Nonproprietary Name
intermed	intermediate
ipr	intraperitoneal
ir	infra-red spectrum
isol(n)	isolation, isolated
isom	isomerism, isomers, isomerises
ivn	intravenous
JAN	Japanese Accepted Name
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
LC	lethal concentration
LD	lethal dose: LD_{50}, a dose which is lethal to 50% of the animals tested
M	molecular weight (formula weight)
manuf	manufacturer, manufactured
max	maximum
Me	methyl
MeOH	methanol
Me_2CO	acetone
MEL	maximum exposure limit
metab	metabolite, metabolism
misc	miscible
mixt	mixture
mod	moderately
Mp	melting point
ms	mass spectrum
mus	mouse
n	index of refraction, e.g. n_D^{20} for 20° and sodium light
nmr	nuclear magnetic resonance spectrum (general)
obt	obtained
oc	open cup

occup	occupational
OES	Occupational Exposure Standard
op	optical purity
ord	optical rotatory dispersion
orl	oral
Ph	phenyl (C_6H_5)
pharmacol	pharmacology
pmr	proton (^1H) nuclear magnetic resonance
polarog	polarography
polym	polymerises, polymer
ppd	precipitated
ppm	parts per million
props	properties
purifn	purification
Py	pyridine
rbt	rabbit
ref	reference
resoln	resolution
rev	review
rt	room temperature
scu	subcutaneous
sepn	separation
skn	skin
sl	slightly
sol	soluble
soln	solution
solv	solvent
sp	species (singular)
spar	sparingly
spp	species (plural)
ssp	subspecies
subl	sublimation, sublimes
synth	synthesis
tautom	tautomerism
THF	tetrahydrofuran
tlc	thin layer chromatography
TLV	Threshold Limit Value
tox	toxicity
unsatd	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v	very
var	variety
vis	visible
vol	volume

6.1 Reference Tags

The following is a selection of the most common Reference Tag abbreviations used:

Abbreviation	**Name**
abs config	absolute configuration
anal	analysis
bibl	bibliography
biosynth	biosynthesis

cd	circular dichroism
chromatog	chromatography
cmr	^{13}C nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination
deriv(s)	derivative(s)
detn	determination, detection
dsc	differential scanning calorimetry
dta	differential thermal analysis
ed	electron diffraction
electrochem	electrochemistry, cyclic voltammetry
em	electron microscopy
epr	electron paramagnetic (spin) resonance spectrum
esca	electron spectroscopy for chemical analysis
exafs	extended X-ray diffraction fine structure
glc	gas-liquid chromatography
haz	hazard
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
manuf	manufacture
metab	metabolism
mineral	mineralogy
ms	mass spectrum
nmr	nuclear magnetic resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pe	photoelectron spectroscopy
pharmacol	pharmacology
photol	photolysis
pmr	proton (^{1}H) nuclear magnetic resonance spectrum
polarog	polarography
powder struct	X-ray powder structure determination
props	properties (chemical or physical)
Raman	Raman spectrum
resoln	resolution
rev	review
sepn	separation
soly	solubility
spectra	
struct	structure
synonyms	
synth	synthesis
tautom	tautomerism
tga	thermogravimetric analysis
theory	MO calculations etc.
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
use(s)	
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum

7. THE DICTIONARY OF FOOD COMPOUNDS ON CD-ROM

The *Dictionary of Food Compounds* is published together with a fully searchable CD-ROM. Space considerations have precluded the inclusion of indexes other than the Name Index in the hard-copy version. By contrast, the CD-ROM contains searchable indexes on the following 35 fields:

Accurate Mass	Dissociation Constant	Molecular Weight	Reference Year
All Entries	Food Information	Optical Rotation	Refractive Index
All Text	Hazard & Toxicity	Partition Coefficient (Calc.)	Rotation Conditions
Boiling Point	Hazard Flag	Percent Composition	RTECS Accession No.
Boiling Point Pressure	Ion Charge	Reference Author	Supplier
CAS Registry Number	Melting Point	Reference Patentee	Type of Compound
Chemical Name	Molecular Formula	Reference Tag	Type of Compound Words
CRC Number	Molecular Formula	Reference Title	UV Maxima
Density	by Element	Reference Volume	UV Solvent

Once installed, a User Guide providing additional information on data content and guide to searching is available from the CRC Press_Dictionary of Food Compounds on CD folder in the Start Menu and from the Help menu on the CD-ROM.

When accessing the *Dictionary of Food Compounds on CD-ROM* the first screen that is obtained is the Search Form window (**Fig.2**).

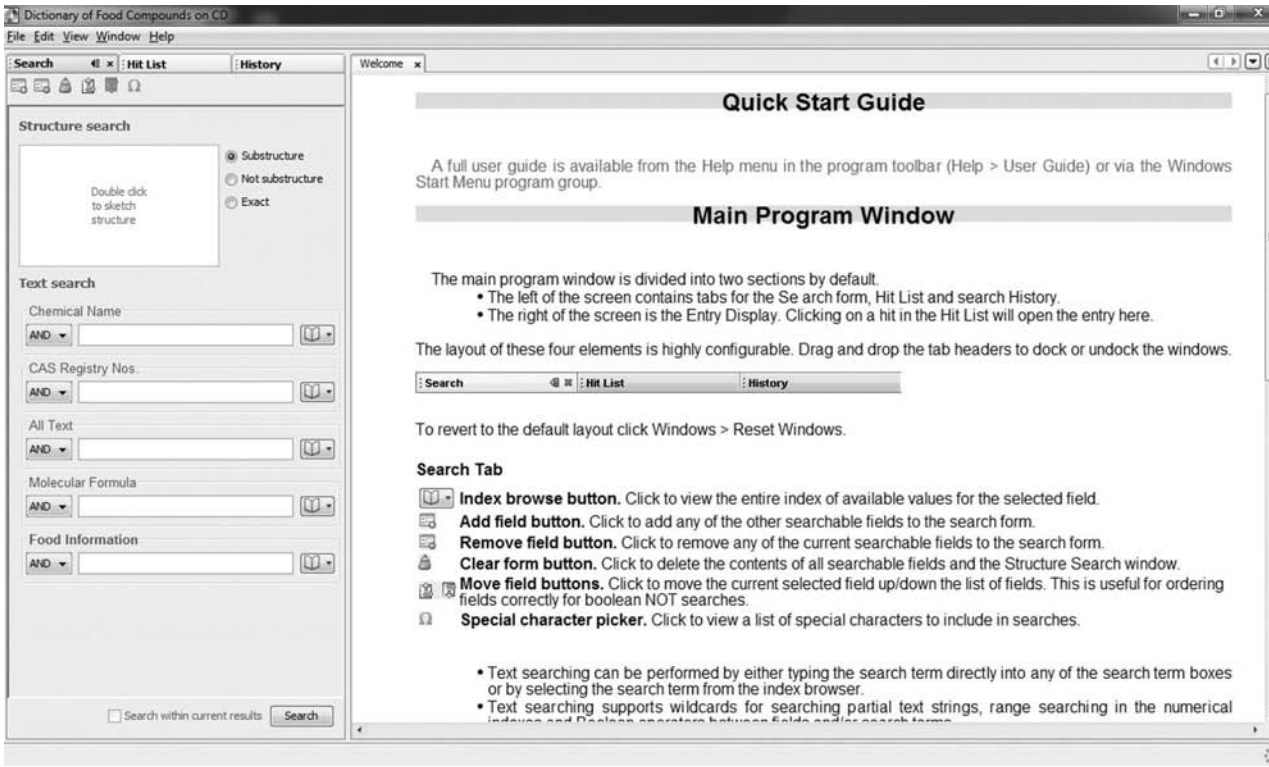


FIG.2 Search Form Window

The Search Form window consists of two parts:

1. Structure Search – allowing structure and substructure searching
2. Text search – search from one or more of the 35 available data/text fields

From the Search Form window design your search profile using text, structure or text/structure searching. Once your search has been performed the resultant hits are listed alphabetically by chemical name in the Hit List screen. Clicking on any one of the hits in the Hit List screen will result in that entry being displayed in the Entry Display screen (**Fig.3**).

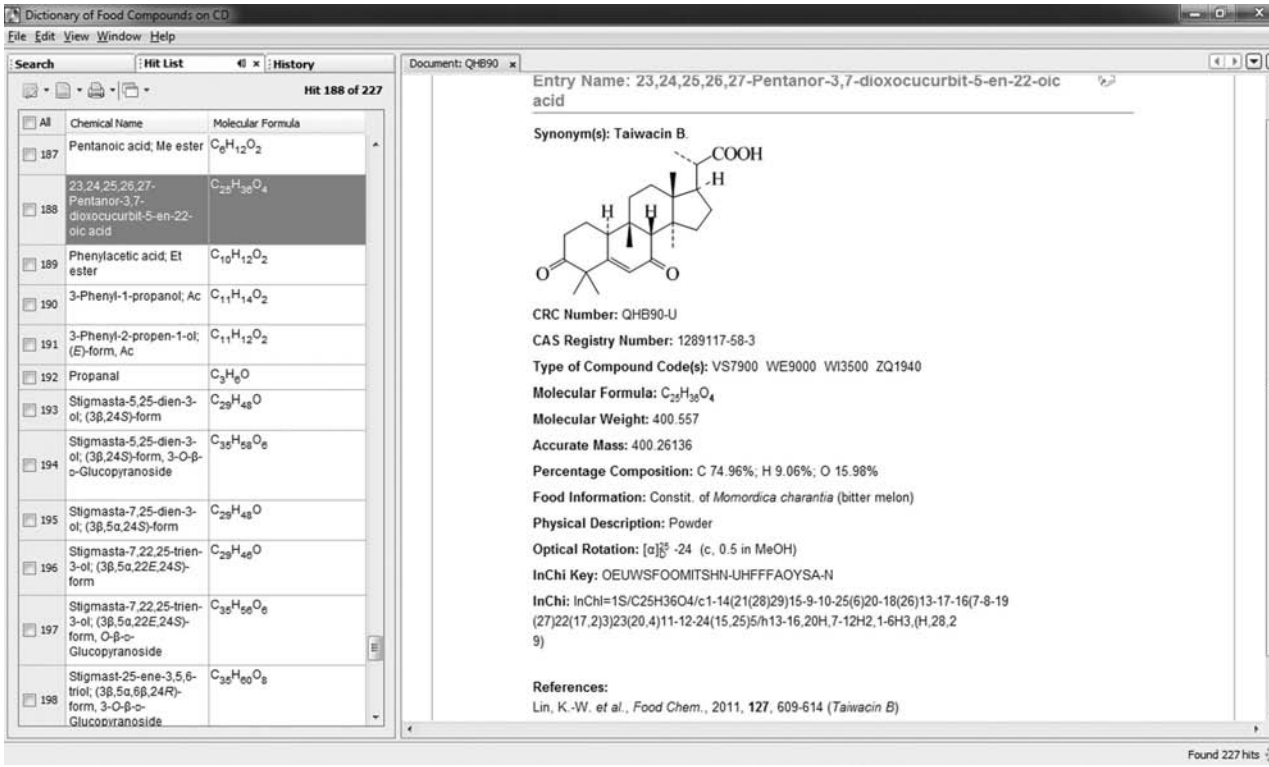


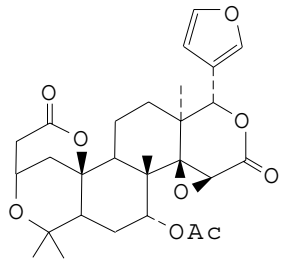
FIG.3 Hit List and Entry Display screens

Any comments and suggestions for inclusion may be sent to:

The Editors, Dictionary of Food Compounds
CRC Press/Taylor & Francis Group
Albert House, 3rd Floor
1-4 Singer Street
London EC2A 4BQ

Email: steve.walford@informa.com

1(10 →19)-Abeo-7-acetoxyisoobacun-3,10-olide A-1

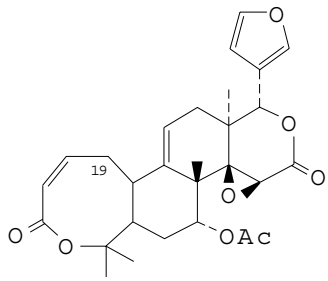


$C_{28}H_{34}O_9$ 514.571

(7α,10β)-*form* [85643-98-7]
Constit. of the fruits of a *Citrus-Poncirus* hybrid.
Cryst. (MeOH).
Mp 271-274°.

Bennett, R.D. *et al., Phytochemistry*, 1982, **21**, 2349-2354 (*isol, pmr, cmr*)

1(10 →19)-Abeo-7-acetoxyobacun-9(11)-ene A-2



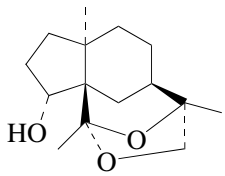
$C_{28}H_{32}O_8$ 496.556

7α-*form* [85643-97-6]
Constit. of the fruits of a *Citrus-Poncirus* hybrid.

Bennett, R.D. *et al., Phytochemistry*, 1982, **21**, 2349-2354 (*isol, pmr, cmr*)

3(4 →5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol A-3

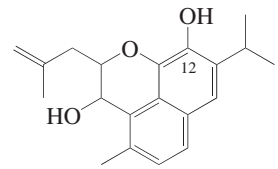
[210106-16-4]



$C_{15}H_{24}O_3$ 252.353
Constit. of *Cyperus rotundus* (nutgrass). Oil. $[\alpha]_D^{21}$ +15 (c, 0.04 in $CHCl_3$).

Ohira, S. *et al., Phytochemistry*, 1998, **47**, 1577-1581

20(10 →5)-Abeo-2,11-epoxy-4,5-seco-4(18),5,7,9,11,13-abietahexaene-1,12-diol A-5

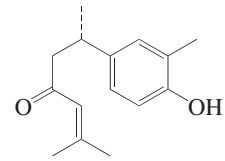


$C_{20}H_{24}O_3$ 312.408

12-Me ether: [1234681-29-8] *20(10 →5)-Abeo-2,11-epoxy-12-methoxy-4,5-seco-4(18),5,7,9,11,13-abietahexaen-1-ol*
$C_{21}H_{26}O_3$ 326.435
Constit. of *Salvia sclarea* (clary sage).

Yamasaki, A. *et al., J. Essent. Oil Res.*, 2009, **21**, 528-530 (*Salvia sclarea constit*)

15(3 →2)-Abeo-3-hydroxy-1,3,5,10-bisabolatetraen-9-one A-6

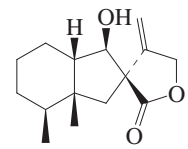


$C_{15}H_{20}O_2$ 232.322

(*S*)-*form* [949081-05-4]
Constit. of *Curcuma longa* (turmeric).
Oil. $[\alpha]_D^{25}$ +51.1 (c, 0.9 in MeOH).

Zeng, Y.C. *et al., Chem. Pharm. Bull.*, 2007, **55**, 940-943 (*Curcuma longa constit*)

7(8 →9)-Abeo-9-hydroxy-11(13)-eremophilen-8,12-olide A-7



$C_{15}H_{22}O_3$ 250.337

(7β,9β,10β)-*form* [226711-43-9]
Bakkenolide S. *9-Hydroxyfukinanolide*
Oil. $[\alpha]_D$ -87 (c, 0.037 in MeOH).

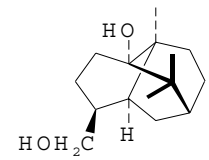
Ac: [35945-70-1] ***9-Acetoxyfukinanolide***
$C_{17}H_{24}O_4$ 292.374
Constit. of *Petasites japonicus* (sweet coltsfoot). Cryst. Mp 96-97°. $[\alpha]_D^{25}$ -28.5 (c, 1 in $CHCl_3$).

2-Methylpropanoyl: [226711-33-7] ***Bakkenolide I***
$C_{19}H_{28}O_4$ 320.428
Oil. $[\alpha]_D$ -32 (c, 0.079 in MeOH).

3-Methylbutanoyl: [226711-34-8] ***Bakkenolide J***
$C_{20}H_{30}O_4$ 334.455
Oil. $[\alpha]_D$ -140 (c, 0.013 in MeOH).

Hamelin, O. *et al., Nat. Prod. Lett.*, 1997, **10**, 99-103 (*9-Acetoxyfukinanolide, synth*)
Wu, T.-S. *et al., Chem. Pharm. Bull.*, 1999, **47**, 375-382 (*Bakkenolides*)
Brocksom, T.J. *et al., JACS*, 2002, **124**, 15313-15325 (*synth*)
Phillips, E.M. *et al., Org. Lett.*, 2010, **12**, 2830-2833 (*synth*)

5(1 →10)-Abeo-1,12-patchoulanediol A-8

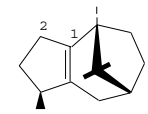


$C_{15}H_{26}O_2$ 238.369
Constit. of *Pogostemon cablin* (patchouli). Cryst. (hexane/C_6H_6). Mp 132.5-133°.

Trifilieff, E. *et al., Phytochemistry*, 1980, **19**, 2467 (*isol, struct*)
Niwa, H. *et al., Tet. Lett.*, 1984, **25**, 2797 (*synth*)

11(1 →10)-Abeo-1(5)-patchoulene A-9

1,2,3,4,5,6,7,8-Octahydro-1,4,9,9-tetramethyl-4,7-methanoazulene, 9CI. ***β-Patchoulene*** [514-51-2]

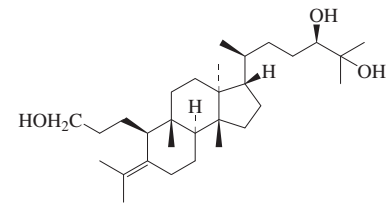


$C_{15}H_{24}$ 204.355
Constit. of guaiac wood oil (*Bulnesia sarmienti*). Oil. $Bp_{0.6}$ 66.8°. $[\alpha]_D^{30}$ -42.6 (c, 10.5 in $CHCl_3$). n_D^{25} 1.4978.

$\Delta^{1,2}$-Isomer: [53823-16-8] *11(1 →10)-Abeo-1-patchoulene.* ***δ-Patchoulene***
$C_{15}H_{24}$ 204.355
Constit. of *Pogostemon cablin* (patchouli). Oil. $[\alpha]_D^{25}$ -61.7 (EtOH).

Büchi, G. *et al., JACS*, 1961, **83**, 927 (*isol, struct*)
Bates, R.B. *et al., JACS*, 1962, **84**, 1307 (*synth*)
Narayanan, C.S. *et al., Tetrahedron*, 1964, **20**, 963 (*isol*)
Mookherjee, B.D. *et al., J. Agric. Food Chem.*, 1974, **22**, 771 (*δ-Patchoulene*)
Akhita, A. *et al., Phytochemistry*, 1987, **26**, 2705 (*biosynth*)

19(10 →9)-Abeo-3,4-secotirucall-4-ene-3,24,25-triol A-10



$C_{30}H_{54}O_3$ 462.755

(24*R*)-*form* [527743-15-3]
Gum.

3-Octanoyl: [527743-08-4]
$C_{38}H_{68}O_4$ 588.953
Constit. of sunflower pollen (*Helianthus annuus*). Gum. $[\alpha]_D$ +13.2 (c, 0.4 in $CHCl_3$).

4,5α-Epoxide: [527743-20-0] ***19(10→9)-Abeo-4,5-epoxy-3,4-secotirucallane-3,24,25-triol***
$C_{30}H_{54}O_4$ 478.754
Gum.

4,5α-Epoxide, 3-octanoyl: [527743-13-1]
$C_{38}H_{68}O_5$ 604.952
Constit. of sunflower pollen (*Helianthus annuus*). Gum. $[\alpha]_D$ +3.1 (c, 0.3 in $CHCl_3$).

(24*S*)-*form* [527743-14-2]
Gum.

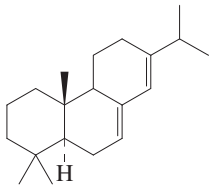
3-Octanoyl: [527743-07-3]
$C_{38}H_{68}O_4$ 588.953
Constit. of sunflower pollen (*Helianthus annuus*). Gum. $[\alpha]_D$ +1 (c, 0.8 in $CHCl_3$).

4,5α-Epoxide: [527743-19-7]
$C_{30}H_{54}O_4$ 478.754
Gum.

4,5α-Epoxide, 3-octanoyl: [527743-12-0]
$C_{38}H_{68}O_5$ 604.952
Constit. of sunflower pollen (*Helianthus annuus*). Gum. $[\alpha]_D$ -3.6 (c, 0.2 in $CHCl_3$).

Ukiya, M. *et al., J. Agric. Food Chem.*, 2003, **51**, 2949-2957 (*isol, pmr, cmr*)

7,13-Abietadiene A-11



5α-*form*

$C_{20}H_{32}$ 272.473

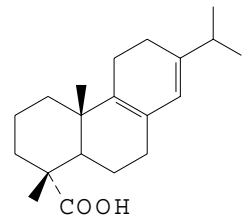
5α-*form* [35241-40-8]
Constit. of various sources incl. *Pinus* spp. Oil. $[\alpha]_D^{20}$ -121 (c, 0.8 in $CHCl_3$).

ent*-5α-*form [42895-82-9]
Oil. $[\alpha]_D^{24}$ +127 (c, 2 in $CHCl_3$).

Norin, T. *et al., Phytochemistry*, 1971, **10**, 2818-2821 (*Cedrus constit*)
Anthonsen, T. *et al., Acta Chem. Scand.*, 1973, **27**, 1073-1082 (*Solidago missouriensis constit*)
Bohlmann, F. *et al., Phytochemistry*, 1980, **19**, 869-871 (*Helichrysum chionosphaerum constit*)
San Feliciano, A. *et al., Magn. Reson. Chem.*, 1993, **31**, 841-844 (*cmr*)
Ravn, M.M. *et al., Chem. Comm.*, 1998, 21-22 (*biosynth*)
Ravn, M.M. *et al., Org. Lett.*, 2000, **2**, 573-576 (*biosynth*)
Lee, H.-J. *et al., Tetrahedron*, 2001, **57**, 6155-6167 (*synth, bibl*)
Ravn, M.M. *et al., JACS*, 2002, **124**, 6998-7006 (*biosynth*)

8,13-Abietadien-18-oic acid A-12

Palustric acid [1945-53-5]



$C_{20}H_{30}O_2$ 302.456
Constit. of *Pinus palustris* (pitch pine). Cryst. (MeOH). Mp 162-167°. $[\alpha]_D$ +71.6 (EtOH). λ_{max} 265 (NaOH) (Berdy).

18-Alcohol: [21414-53-9] *8,13-Abietadien-18-ol.* ***Palustrol****. Palustrinol*
$C_{20}H_{32}O$ 288.472
Constit. of *Pinus koraiensis* (Korean pine).

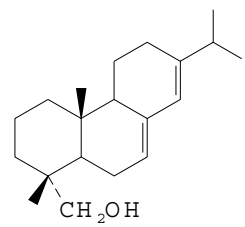
18-Aldehyde: [13508-03-7] *8,13-Abietadien-18-al.* ***Palustral***
$C_{20}H_{30}O$ 286.456
Isol. from *Pinus koraiensis* (Korean pine) and other conifers. Cryst. (EtOH). $[\alpha]_D^{20}$ +59 (c, 4.24 in $CHCl_3$).

8α,9α:13α,14α-Diepoxide: ***8,9:13,14-Diepoxy-18-abietanoic acid***
$C_{20}H_{30}O_4$ 334.455
Cryst. (diisopropyl ether) (as Me ester). Mp 130-132° (Me ester).

Wenkert, E. *et al., JACS*, 1964, **86**, 2038
Radulgin, V.A. *et al., Khim. Prir. Soedin.*, 1974, **10**, 674; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 696 (*Palustral*)
Khan, V.A. *et al., Khim. Prir. Soedin.*, 1984, **20**, 115-116 (*Palustrol*)
Delgado, G. *et al., Phytochemistry*, 1994, **37**, 1119 (*diepoxide*)

7,13-Abietadien-18-ol A-13

Abietinol [666-84-2]



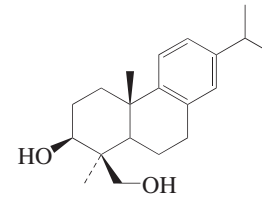
$C_{20}H_{32}O$ 288.472
Isol. from *Pinus sylvestris* (Scotch pine). Cryst. or oil. Mp 85.5-87°. $[\alpha]_D$ -132.5 (c, 2 in EtOH). $[\alpha]_D$ -73 ($CHCl_3$).

18-Tigloyl:
$C_{25}H_{38}O_2$ 370.574
Gum.

18-Aldehyde: [6704-50-3] *7,13-Abietadien-18-al.* ***Abietinal***
$C_{20}H_{30}O$ 286.456
Constit. of *Pinus sylvestris* (Scotch pine). Cryst. or oil. Mp 45-48°. $[\alpha]_D$ -116 ($CHCl_3$).

Erdtman, H. *et al., Acta Chem. Scand.*, 1963, **17**, 1826
Chirkova, M.A. *et al., Khim. Prir. Soedin.*, 1966, **2**, 99; *Chem. Nat. Compd. (Engl. Transl.)*, 1966, **2**, 77
Caputo, R. *et al., Gazz. Chim. Ital.*, 1974, **104**, 491
Caputo, R. *et al., Phytochemistry*, 1974, **13**, 471
San Feliciano, A. *et al., Magn. Reson. Chem.*, 1993, **31**, 841 (*cmr*)
Lu, T. *et al., Phytochemistry*, 1995, **38**, 451 (*isol, pmr, cmr*)

8,11,13-Abietatriene-3,19-diol A-14



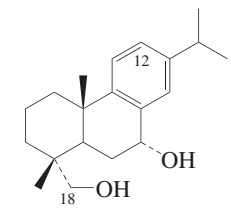
$C_{20}H_{30}O_2$ 302.456

3β-*form* [251340-91-7]
Triptobenzene L
Amorph. powder. $[\alpha]_D$ +30.4 (c, 0.5 in MeOH). λ_{max} 238 (log ϵ 3.79); 267 (log ϵ 2.87) (MeOH).

15,16-Didehydro, 19-carboxylic acid: [1202270-05-0] ***3-Hydroxy-8,11,13,15-abietatetraen-19-oic acid***
$C_{20}H_{26}O_3$ 314.424
Constit. of *Callicarpa japonica* (Japanese beautyberry).
Amorph. powder. $[\alpha]_D^{25}$ +131.7 (c, 1.8 in Py).

Duan, H. *et al., J. Nat. Prod.*, 1999, **62**, 1522-1525 (*Triptobenzene L*)
Ono, M. *et al., J. Nat. Med. (Tokyo)*, 2009, **63**, 318-322 (*Callicarpa japonica constit*)

8,11,13-Abietatriene-7,18-diol A-15



$C_{20}H_{30}O_2$ 302.456

7α-*form* [26920-04-7]
Needles (Me_2CO). Mp 89°. $[\alpha]_D^{20}$ -3.3 (c, 0.46 in EtOH).

18-O-*(3-Carboxypropanoyl):* [1210347-46-8] ***Abiesadine F***
$C_{24}H_{34}O_5$ 402.53
Amorph. powder. $[\alpha]_D^{20}$ -1.3 (c, 0.5 in MeOH).

18-O-*(3-Methoxycarbonylpropanoyl):* [1210347-48-0] ***Abiesadine H***
$C_{25}H_{36}O_5$ 416.556
Amorph. powder. $[\alpha]_D^{20}$ +3 (c, 0.41 in MeOH).

7-Me ether, 18-O-*(carboxypropanoyl):* [1210347-47-9] ***Abiesadine G***
$C_{25}H_{36}O_5$ 416.556
Amorph. powder. $[\alpha]_D^{20}$ +8.9 (c, 0.52 in MeOH).

7-Ketone: 18-Hydroxy-8,11,13-abietatrien-7-one

7-Ketone, 18-Ac: [33980-73-3] ***Pomiferin G***
$C_{22}H_{30}O_3$ 342.477
Amorph.

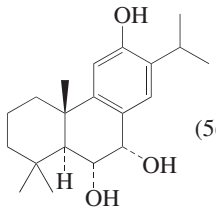
7-Ketone, 18-hexadecanoyl: [1004979-06-9]
$C_{36}H_{58}O_3$ 538.852
Oil.

7-Ketone, 18-O-*(3-carboxypropanoyl):* [369364-79-4] ***Abiesadine Q***
$C_{24}H_{32}O_5$ 400.514
Amorph. powder. $[\alpha]_D^{20}$ +0.3 (c, 0.5 in MeOH).

12-Hydroxy, 18-aldehyde, 7-ketone: [96888-45-8] ***12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al***. ***Suginal***
$C_{20}H_{26}O_3$ 314.424
Constit. of *Salvia sclarea* (clary sage). Cryst. Mp 227° dec. $[\alpha]_D^{15}$ -100.5 (c, 1 in $CHCl_3$).

Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1987, **35**, 229-234 (*Cedrus deodara constit*)
Kuo, Y.-H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 3195-3201 (*Suginal*)
Barrero, A.F. *et al., Phytochemistry*, 1992, **31**, 615-620 (*Abies marocana constit*)
Topcu, G. *et al., Phytochemistry*, 1994, **36**, 743-745 (*Pomiferin G*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971-974 (*12-Hydroxy-7-oxo-8,11,13-abietatrien-18-al*)
Seca, A.M.L. *et al., Phytochemistry*, 2008, **69**, 498-505 (*Juniperus brevifolia constit*)
Yang, X.-W. *et al., Bioorg. Med. Chem.*, 2010, **18**, 744-754 (*Abiesadines F,G,H,Q*)

8,11,13-Abietatriene-6,7,12-triol A-16



(5α,6α,7α)-*form*

$C_{20}H_{30}O_3$ 318.455

(5α,6α,7α)-*form*

7-Me ether: [956473-74-8] *7-Methoxy-8,11,13-abietatriene-6,12-diol*. ***Taxodistin B***
$C_{21}H_{32}O_3$ 332.482
$[\alpha]_D^{22}$ +63 (c, 0.5 in $CHCl_3$).

(5α,6α,7β)-*form* [111197-59-2] ***6,7-Dihydroxyferruginol***

6-Ac: [886448-93-7] ***Sugikurojin E***
$C_{22}H_{32}O_4$ 360.492
Solid. $[\alpha]_D^{25}$ +30 (c, 1.2 in $CHCl_3$). λ_{max} 210 (log ε 4.66); 280 (log ε 3.65) (MeOH).

6,12-Di-Ac: [1034371-30-6] ***Fortunin B***
$C_{24}H_{34}O_5$ 402.53
Amorph. powder. $[\alpha]_D^{20}$ +72 (c, 0.17 in $CHCl_3$). λ_{max} 267 (log ε 5.15); 275 (log ε 5.1) (MeOH).

7-Ketone: [55898-07-2] *6,12-Dihydroxy-8,11,13-abietatrien-7-one*. ***6-Hydroxysugiol***
$C_{20}H_{28}O_3$ 316.439
Cryst. Mp 207-208°. $[\alpha]_D^{25}$ +35.3 (c, 0.5 in $CHCl_3$).

6,7-Diketone: [119817-27-5] *12-Hydroxy-8,11,13-abietatriene-6,7-dione*. ***Prexanthoperol***. *Hypargenin C*
Minor constit. of *Juniperus communis* (juniper). Yellow cryst. or orange amorph. solid. Mp 207-210°. Identity of Prexanthoperol and Hypargenin C not definitely establ. λ_{max} 218 (ε 3150); 320 (ε 12500); 333 (ε 15800); 403 (ε 5000) (MeOH) (Berdy).

(5α,7ξ)-*form*

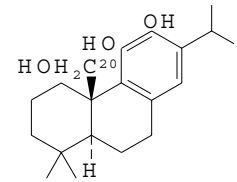
6-Ketone: [128741-29-7] *7,12-Dihydroxy-8,11,13-abietatrien-6-one*. ***Trilobinone***
Constit. of *Salvia triloba* (Greek sage). Light yellow powder.

5β-*form*

6,7-Diketone: [564-23-8] ***Xanthoperol***
Constit. of *Juniperus communis* (juniper). Yellow cryst. (C_6H_6). Mp 255-270° dec. $[\alpha]_D^{20}$ +132.5 (c, 1.2 in EtOH).

Brendenberg, J.B. *et al., Acta Chem. Scand.*, 1956, **10**, 1511 (*Xanthoperol, Prexanthoperol*)
Nasipuri, D. *et al., JCS*, 1962, 4248 (*synth*)
Kondo, Y. *et al., Chem. Pharm. Bull.*, 1963, **11**, 678 (*Xanthoperol, struct*)
Lin, Y.-T. *et al., J. Chin. Chem. Soc. (Peking)*, 1975, **22**, 331 (*6-Hydroxysugiol*)
Ulubelen, A. *et al., J. Nat. Prod.*, 1988, **51**, 1178 (*Hypargenin C*)
Ulubelen, A. *et al., Planta Med.*, 1990, **56**, 82 (*Trilobinone*)
Ghosal, M. *et al., Indian J. Chem., Sect. B*, 1992, **31**, 524 (*synth*)
Su, W.-C. *et al., Phytochemistry*, 1994, **35**, 1279 (*6-Hydroxysugiol*)
Nagahama, S. *et al., Mokuzai Gakkaishi*, 2002, **48**, 380-386 (*6,7-Dihydroxyferruginol*)
Yoshikawa, K. *et al., Chem. Pharm. Bull.*, 2006, **54**, 315-319 (*Sugikurojin E*)
Hirasawa, Y. *et al., Bioorg. Med. Chem. Lett.*, 2007, **17**, 5868-5871 (*Taxodistin B*)
Yao, S. *et al., J. Nat. Prod.*, 2008, **71**, 1242-1246 (*Fortunin B*)

8,11,13-Abietatriene-11,12,20-triol A-17



$C_{20}H_{30}O_3$ 318.455
Amorph. solid.

20-Carboxylic acid: [3650-09-7] *11,12-Dihydroxy-8,11,13-abietatrien-20-oic acid*. ***Carnosic acid***. *Deoxypicrosalvinic acid. Salvin*†
$C_{20}H_{28}O_4$ 332.439
Isol. from *Salvia officinalis* (sage) and *Rosamarinus officinalis* (rosemary). Cryst. (hexane). Sol. Et_2O, MeOH, bases, $CHCl_3$; poorly sol. H_2O. Mp 185-190° dec. $[\alpha]_D^{23}$ +191 (c, 1.07 in MeOH). λ_{max} 212 (ε 21500); 233 (ε 9650); 284 (ε 1690) (EtOH) (Berdy).

20-Carboxylic acid, di-Ac:
Needles (hexane). Mp 212-217° (196-215° dec.). $[\alpha]_D^{22}$ +139 (c, 1.15 in $CHCl_3$).

20-Carboxylic acid, 11-Me ether: [313050-47-4] ***12-Hydroxy-11-methoxy-8,11,13-abietatrien-20-oic acid***
$C_{21}H_{30}O_4$ 346.466
Constit. of *Citrus* roots infected by nematode *Tylenchulus semipenetrans.* Amorph. solid. Mp 140-141°. $[\alpha]_D^{20}$ +12.1 (c, 0.28 in $CHCl_3$).

20-Carboxylic acid, 12-Me ether: [62201-71-2] *12-Methoxycarnosic acid (incorr.)*
$C_{21}H_{30}O_4$ 346.466
Isol. from rosemary. Cryst. $[\alpha]_D^{21}$ +250 (c, 0.04 in MeOH). λ_{max} 226 (log ε 3.39); 276 (log ε 1.71) (MeOH).

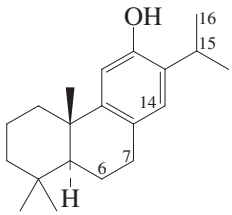
20→11 Lactone, 20-carboxylic acid, 12-Me ether. ***12-Methoxy-8,11,13-abietatrien-20,11-olide***
$C_{21}H_{28}O_3$ 328.45
Constit. of *Salvia officinalis* (sage). Cryst. (petrol). Mp 112-114°.

10-Epimer, 20-carboxylic acid, 12-Me ether: [827611-91-6]
$C_{21}H_{30}O_4$ 346.466
Isol. from rosemary. Cryst. $[\alpha]_D^{21}$ +50 (c, 0.06 in MeOH). λ_{max} 224 (log ε 3.3); 277 (log ε 0.8) (MeOH).

Linde, H. *et al., Helv. Chim. Acta*, 1964, **47**, 1234 (*isol, uv, ir, pmr*)
Wenkert, E. *et al., JOC*, 1965, **30**, 2931 (*isol, ir, pmr, config*)
Narayanan, C.R. *et al., Tet. Lett.*, 1965, 3647 (*struct*)
Meyer, W.L. *et al., Tet. Lett.*, 1966, 4261 (*synth*)
Dentali, S.J. *et al., Phytochemistry*, 1990, **29**, 993 (*isol*)
González, A.G. *et al., Phytochemistry*, 1991, **30**, 4067 (*isol, pmr, cmr*)
Djarmati, Z. *et al., Phytochemistry*, 1992, **31**, 1307 (*isol, pmr, cmr, cryst struct*)

Luis, J.G. *et al., Nat. Prod. Lett.*, 2000, **14**, 379-385 (*20-acid-11-Me ether*)
Oluwatuyi, M. *et al., Phytochemistry*, 2004, **65**, 3249-3254 (*20-acid-12-Me ethers*)
Tada, M. *et al., Chem. Pharm. Bull.*, 2010, **58**, 27-29 (*synth*)

8,11,13-Abietatrien-12-ol A-18



5α-*form*

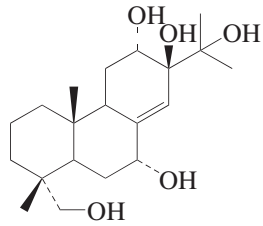
$C_{20}H_{30}O$ 286.456

5α-*form* [514-62-5]
Ferruginol†
Oil. $Bp_{0.3}$ 175°. $[\alpha]_D^{16}$ +40.6 (EtOH).

6,7-Didehydro: [34539-84-9] *6,8,11,13-Abietatetraen-12-ol.* ***Δ⁶-Dehydroferruginol***. *6,7-Didehydroferruginol*
$C_{20}H_{28}O$ 284.441
Isol. from woods of *Juniperus communis* (juniper). Light yellow solid. $[\alpha]_D^{20}$ -60 (EtOH).

Briggs, L.H. *et al., Tetrahedron*, 1959, **7**, 270-276 (*Dehydroferruginol*)
González, A.G. *et al., Phytochemistry*, 1992, **31**, 1691-1695 (*6,7-Didehydroferruginol*)

8(14)-Abietene-7,12,13,15,18-pentol A-19



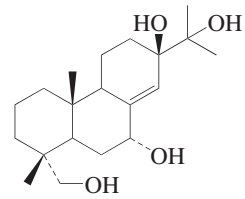
$C_{20}H_{34}O_5$ 354.486

(7α,12α,13β)-*form* [262356-04-7]
Powder (MeOH aq.). Mp >300°. $[\alpha]_D$ -23 (c, 0.2 in $CHCl_3$/MeOH).

18-Carboxylic acid, 7-ketone: [1073175-19-5] *12,13,15-Trihydroxy-7-oxo-8(14)-abieten-18-oic acid.* ***Pinkornocid B***. *PK-B*
$C_{20}H_{30}O_6$ 366.453
Constit. of *Pinus koraiensis* (Korean pine). Cryst. (MeOH). Mp 291°. $[\alpha]_D^{25}$ +1.6 (c, 0.4 in MeOH). λ_{max} 244 (log ϵ 4.02) (MeOH).

Ohtsu, H. *et al., Can. J. Chem.*, 2000, **78**, 31-40 (*Larix kaempferi constit*)
Yang, X. *et al., Fitoterapia*, 2008, **79**, 179-181 (*Pinkornocid B*)

8(14)-Abietene-7,13,15,18-tetrol A-20



(7α,13β)-*form*

$C_{20}H_{34}O_4$ 338.486

(7α,13β)-*form* [262355-97-5]
Needles (MeOH aq.). Mp 221-222°. $[\alpha]_D^{23}$ -25.8 (c, 0.57 in EtOH).

7-Ketone: [262356-00-3] ***13,15,18-Trihydroxy-8(14)-abieten-7-one***
$C_{20}H_{32}O_4$ 336.47
Oil. $[\alpha]_D$ -8.3 (c, 0.29 in EtOH).

18-Carboxylic acid: ***7,13,15-Trihydroxy-8(14)-abieten-18-oic acid***
$C_{20}H_{32}O_5$ 352.47
Plates (MeOH aq.). Mp 215-216°. $[\alpha]_D^{23}$ -8.6 (c, 0.64 in EtOH).

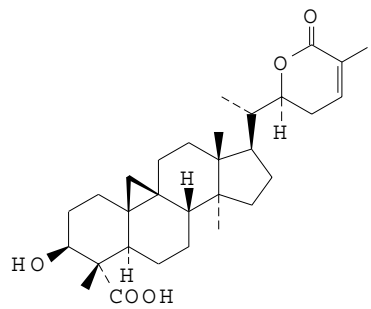
18-Carboxylic acid, 7-ketone: [959118-98-0] *13,15-Dihydroxy-7-oxo-8(14)-abieten-18-oic acid.* ***Pinkornocid A***. *PK-A*
$C_{20}H_{30}O_5$ 350.454
Constit. of *Pinus koraiensis* (Korean pine). Cryst. (MeOH). Mp 287°. $[\alpha]_D^{25}$ +12.9 (c, 0.35 in MeOH). λ_{max} 240 (log ϵ 4.23) (MeOH).

(*ent*-7α,13ξ)-*form*

18-Carboxylic acid: [162613-95-8]
Powder.

Lu, T. *et al., Phytochemistry*, 1995, **38**, 451-456 (*Solidago rugosa constit*)
Ohtsu, H. *et al., Can. J. Chem.*, 2000, **78**, 31-40 (*Larix kaempferi constits, cryst struct*)
Yang, X. *et al., Fitoterapia*, 2008, **79**, 179-181 (*Pinkornocid A*)

Abrusogenin A-21



$C_{30}H_{44}O_5$ 484.675
Mp 278-280°. $[\alpha]_D$ +37 (c, 0.1 in $CHCl_3$/MeOH).

3-O-β-D-Glucopyranoside: [124962-06-7] ***Abrusoside A***
$C_{36}H_{54}O_{10}$ 646.817
Natural sweetener. Cryst. Mp 278-280°. $[\alpha]_D$ +11.2 (c, 0.31 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-6-methylglucuronopyranoside]: [125002-98-4] ***Abrusoside B***
$C_{43}H_{64}O_{16}$ 836.969
Natural sweetener. Cryst. Mp 243-245°. $[\alpha]_D$ +5.8 (c, 0.35 in Py).

3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucopyranoside]: [125002-99-5] ***Abrusoside C***
$C_{42}H_{64}O_{15}$ 808.959
Natural sweetener. Cryst. Mp 260-262°. $[\alpha]_D$ +31.4 (c, 0.34 in Py).

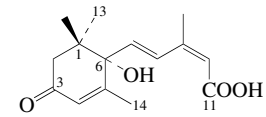
3-O-[β-D-Glucopyranosyl-(1→2)-β-D-glucuronopyranoside]: [125003-00-1] ***Abrusoside D***
$C_{42}H_{62}O_{16}$ 822.942
Natural sweetener. Cryst. Mp 237-239°. $[\alpha]_D$ +9.9 (c, 0.31 in Py).

3-O-[β-D-Glucuronopyranosyl-(1→2)-β-D-glucopyranoside]: ***Abrusoside E***
$C_{42}H_{62}O_{16}$ 822.942
Natural sweetener. Amorph. powder. Mp 265° dec. $[\alpha]_D$ +2 (c, 0.2 in Py).

Choi, Y.-H. *et al., J. Nat. Prod.*, 1989, **52**, 1118 (*isol, pmr, cmr, cryst struct*)
Kennelly, E.J. *et al., Phytochemistry*, 1996, **41**, 1381 (*Abrusoside E*)
Kinghorn, A.D. *et al., Pure Appl. Chem.*, 2002, **74**, 1169-1179 (*Abrusosides, sweetener*)

Abscisic acid A-22

5-(1-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-2,4-pentadienoic acid, 9CI. Abscisin II. Dormin [7773-56-0] [52392-36-6, 2228-72-0]



(*S*)-*form*

$C_{15}H_{20}O_4$ 264.321
Terpenoid (cyclofarnesane) numbering shown. Other schemes freq. encountered. Used to regulate ripening of fruit. λ_{max} 252 (ϵ 25200) (no solvent reported) (Derep). λ_{max} 244 (ϵ 25000) (EtOH/NaOH) (Derep). λ_{max} 245 (sh); 260 (ϵ 21300) (EtOH) (Derep).
▶ RZ2475100

(*S*)-*form* [21293-29-8]
[72029-68-6, 72029-69-7]
Constit. of cabbage, potato, lemon etc. Cryst. ($CHCl_3$/petrol). Mp 160-161°. $[\alpha]_D$ +430. pK_a 4.61. The incorrect abs. config. was formerly assigned.

▶ LD_{50} (rat, orl) >5000mg/kg.

β-D-Glucopyranosyl ester: [21414-42-6] ***Abscisyl β-D-glucopyranoside***
$C_{21}H_{30}O_9$ 426.463
Mp 114°. $[\alpha]_D^{17}$ +180 (c, 0.35 in EtOH).

11-Aldehyde: [41944-86-9] ***Abscisic aldehyde***
$C_{15}H_{20}O_3$ 248.321
Cryst. (CH_2Cl_2/hexane). Mp 127-128°. $[\alpha]_D^{20}$ +450.5 (c,1 in EtOH).

3α-Alcohol: [84026-26-6] ***4′-Dihydroabscisic acid***
$C_{15}H_{22}O_4$ 266.336

Isol. from immature seeds of broad bean (*Vicia faba*).

3β-Alcohol: [85718-96-3]
$C_{15}H_{22}O_4$ 266.336
λ_{max} 265 (EtOH) (Berdy).

13-Hydroxy: [25841-53-6] *13-Hydroxyabscisic acid*
$C_{15}H_{20}O_5$ 280.32
Constit. of cowpea (*Vigna unguiculata*) fruits.

13-Hydroxy, 13-O-*β*-D-*glucopyranoside:* [711029-32-2]
$C_{21}H_{30}O_{10}$ 442.462
Constit. of avocado seeds (*Persea americana*). Gum. $[\alpha]_D$ +196.5 (c, 0.13 in MeOH).

13-Hydroxy, 13-O-*(3-hydroxy-3-methylglutaroyl) (3*S-*):* [69790-31-4] ***9′-(3-Hydroxy-3-methylglutaroyloxy)abscisic acid***. *β-Hydroxy-β-methylglutarylhydroxyabscisic acid. HMG-HOABA* [69790-32-5]
$C_{21}H_{28}O_9$ 424.447
Gum. $[\alpha]_D^{20}$ +560 (c, 0.013 in EtOH).

13-Hydroxy, 13-O-*(3-hydroxy-3-methylglutaroyl) (3*S-*), 5′-Me ester:* [111672-32-3] ***MeHMG-HOABA***
$C_{22}H_{30}O_9$ 438.474
$[\alpha]_D^{15}$ +243 (c, 0.15 in MeOH).

13-Hydroxy, 3-alcohol: Pisumic acid
$C_{15}H_{22}O_5$ 282.336
Isol. from peas (*Pisum sativum*) irrigated with (±)-abscisic acid. Tentative struct.

14-Hydroxy: [91897-25-5] ***Nigellic acid***
$C_{15}H_{20}O_5$ 280.32
Isol. from leaves of *Vicia faba*. Mp 185-187°.

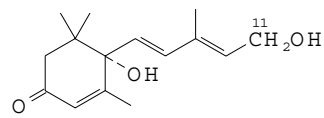
(±)-*form* [14375-45-2]
Mp 188-190°.

[79199-48-7, 97806-70-7, 14674-85-2, 78340-30-4, 14398-53-9, 58801-55-1, 69350-43-2, 40331-02-0, 69350-44-3, 6755-41-5, 6735-04-2]

Cornforth, J. *et al., Nature (London)*, 1965, **206**, 715 (*synth*)
Koreeda, M. *et al., JACS*, 1973, **95**, 239-240 (*synth*)
Milborrow, B.V. *et al., Phytochemistry*, 1975, **14**, 2403-2405 (*biosynth*)
Shibasaki, M. *et al., Chem. Pharm. Bull.*, 1976, **24**, 315-322 (*synth*)
Mayer, H.J. *et al., Helv. Chim. Acta*, 1976, **59**, 1424-1427 (*synth, uv, pmr, ms*)
Burden, R.S. *et al., Pure Appl. Chem.*, 1976, **47**, 203 (*rev*)
Ueda, H. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 1506-1509 (*cryst struct*)
Kienzle, F. *et al., Helv. Chim. Acta*, 1978, **61**, 2616-2627 (*synth, aldehyde*)
Hirai, N. *et al., Phytochemistry*, 1978, **17**, 1625-1627; 1981, **20**, 1867-1869 (*HMG-HOABA*)
Adesomoju, A.A. *et al., Phytochemistry*, 1980, **19**, 223-225 (*13-Hydroxyabscisic acid*)
Norman, S.M. *et al., Phytochemistry*, 1981, **20**, 2343-2344 (*biosynth*)
Neill, S.J. *et al., Phytochemistry*, 1982, **21**, 61-65; 1983, **22**, 2469 (*biosynth*)
Dathe, W. *et al., Phytochemistry*, 1982, **21**, 1798-1799 (*4′-Dihydroabscisic acid*)
Lehmann, H. *et al., Phytochemistry*, 1983, **22**, 1277-1278; 1988, **27**, 677-678 (*Nigellic acid*)
Takeda, N. *et al., Agric. Biol. Chem.*, 1984, **48**, 685-694; 1986, **50**, 2295-2230; 1987, **51**, 2351-2357 (*HMG-HOABA, MeHMG-HOABA*)
Bennet, R.D. *et al., Phytochemistry*, 1984, **23**, 1913-1915; 1990, **29**, 3473-3477 (*biosynth*)
Oritani, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 245-249 (*biosynth*)
Tietz, D. *et al., Physiol. Plant.*, 1985, **65**, 171-176 (*Pisumic acid*)
Constantino, M.G. *et al., JOC*, 1986, **51**, 253-254 (*synth, ir, pmr, ms*)
Boyer, G.L. *et al., Phytochemistry*, 1986, **25**, 1103-1105 (*Nigellic acid*)
Hirai, N. *et al., Phytochemistry*, 1986, **25**, 1865-1868 (*biosynth*)
Southwick, S.M. *et al., Plant Physiol.*, 1986, **81**, 323-325 (*glucopyranosyl ester*)
Okamoto, M. *et al., Phytochemistry*, 1987, **26**, 1269-1271; 1988, **27**, 2099-2103 (*3β-alcohol, biosynth*)
Soukup, M. *et al., Helv. Chim. Acta*, 1989, **72**, 361-364 (*synth*)
Willows, R.D. *et al., Phytochemistry*, 1989, **28**, 2641-2642; 1992, **31**, 2649-2653; 1993, **34**, 233-237 (*biosynth, pmr, Abscisic aldehyde*)
Abrams, S.R. *et al., Phytochemistry*, 1989, **28**, 2885-2889 (*pmr*)
Parry, A.D. *et al., Phytochemistry*, 1991, **30**, 815-821 (*biosynth*)
Cornforth, J. *et al., Aust. J. Chem.*, 1992, **45**, 179-185 (*synth*)
Hampson, C.R. *et al., Phytochemistry*, 1992, **31**, 2645-2648 (*13-Hydroxyabscisic acid*)
Sakai, K. *et al., Tetrahedron*, 1992, **48**, 8229-8238 (*synth*)
Yamamoto, H. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 992-993 (*synth*)
Yamauchi, S. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 1968 (*glucopyranosyl ester*)
Milborrow, B.V. *et al., Phytochemistry*, 1997, **45**, 257-260 (*biosynth*)
Hirai, N. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1448-1458 (*biosynth*)
Yamamoto, H. *et al., Tennen Yuki Kagobutsu Toronkai Koen Yoshishu*, 2000, **42**, 271-276 (*biosynth*)
Jadulco, R. *et al., J. Nat. Prod.*, 2002, **65**, 730-733 (*Niphates olemda constit*)
Hanson, J.R. *et al., J. Chem. Res., Synop.*, 2003, 426-427 (*synth*)
Schwartz, S.H. *et al., Plant Physiol.*, 2003, **131**, 1591-1601 (*biosynth*)
Del Refugio Ramos, M. *et al., Phytochemistry*, 2004, **65**, 955-962 (*Persea americana constit*)
Kamo, T. *et al., Phytochemistry*, 2004, **65**, 2517-2520 (*HMG-HOABA, abs config*)
Inomata, M. *et al., Phytochemistry*, 2004, **65**, 2667-2678 (*biosynth*)
Smith, T.R. *et al., Org. Biomol. Chem.*, 2006, **4**, 4186-4192 (*synth*)
Pesticide Manual, 15th edn., 2009, No. 2

Abscisic alcohol A-23

[113472-20-1]



$C_{15}H_{22}O_3$ 250.337
Constit. of quince (*Cydonia oblonga*) fruit.

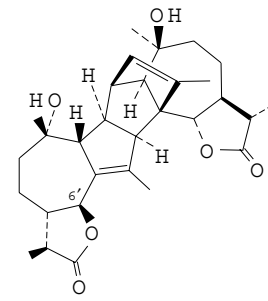
11-O-*β*-D-*Glucopyranoside:* [145153-00-0]
$C_{21}H_{32}O_8$ 412.479
Constit. of quince (*Cydonia oblonga*) fruit.

9,10-Dihydro: ***9,10-Dihydroabscisic alcohol***. *2,3-Dihydroabscisic alcohol*
$C_{15}H_{24}O_3$ 252.353
Constit. of starfruit *Averrhoa carambola*. $[\alpha]_D$ +49.7 (c, 0.0018 in EtOH).

Lutz, A. *et al., J. Agric. Food Chem.*, 1992, **40**, 116 (*isol, pmr, cmr*)
Lutz, A. *et al., Phytochemistry*, 1993, **32**, 57; 1994, **36**, 811 (*isol, pmr, cmr, cd*)

Absinthin A-24

[1362-42-1]



$C_{30}H_{40}O_6$ 496.642
Constit. of *Artemisia absinthium* (wormwood). Orange-yellow needles. Mp 182-183° dec. $[\alpha]_D$ +180.

6′-Epimer: [11029-90-6] ***Isoabsinthin***
$C_{30}H_{40}O_6$ 496.642
Constit. of *Artemisia absinthium* (wormwood). Cryst. (MeOH). Mp 172-174°.

11-Epimer: ***11-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +159 (c, 0.34 in $CHCl_3$).

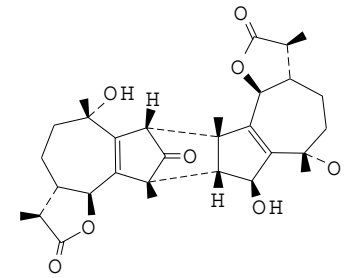
10′,11′-Diepimer: ***10′,11′-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +107 (c, 0.62 in $CHCl_3$).

10′,11,11′-Triepimer: ***10′,11,11′-Epiabsinthin***
$C_{30}H_{40}O_6$ 496.642
Oil. $[\alpha]_D^{24}$ +46 (c, 0.35 in $CHCl_3$).

Kasymov, Sh.Z. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1979, 430-435 (*isol*)
Beauhaire, J. *et al., Tet. Lett.*, 1980, **21**, 3191; 1981, **22**, 2269 (*isol, struct*)
Bohlmann, F. *et al., Phytochemistry*, 1985, **24**, 1009 (*isol, derivs*)
Ma, C.-M. *et al., J. Nat. Prod.*, 2000, **63**, 1626-1629 (*activity*)
Zhang, W. *et al., JACS*, 2005, **127**, 18-19 (*synth*)

Absintholide A-25

[91997-90-9]



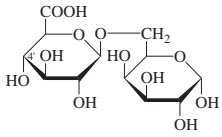
$C_{30}H_{38}O_8$ 526.625

Constit. of *Artemisia absinthium* (wormwood). Cryst. (C_6H_6). Mp 227-228°. $[\alpha]_D^{25}$ +127 (c, 1.3 in $CHCl_3$).

Beauhaire, J. *et al., Tet. Lett.*, 1984, **25**, 2751

Acaciabiuronic acid A-26

6-O-β-D-Glucopyranuronosyl-D-galactose, 9CI, 8CI [7264-19-9]



α-Pyranose-*form*

$C_{12}H_{20}O_{12}$ 356.283

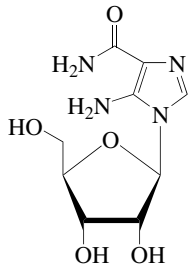
Probably the commonest aldobiouronic acid present as a structural unit in plant gums. Isol. from partial acid hydrolysates from the following plants: *Prunus domestica* (egg plum), *Prunus amygdalus* (almond), *Prunus persica* (peach) and *Ferula* spp. Also isol. from wheat straw. Mp 118-119° (hydrate). $[\alpha]_D$ +11.6 → -8.6 (H_2O).

[1693-80-7, 5566-99-4]

Hotchkiss, R.D. *et al., J. Biol. Chem.*, 1936, **115**, 285 (*deriv*)
Goebel, W.F. *et al., J. Biol. Chem.*, 1938, **124**, 207 (*isol*)
Aspinall, G.O. *et al., JCS*, 1955, 1160; 1961, 3461 (*isol*)
Mukherjee, S. *et al., JACS*, 1958, **80**, 2536 (*isol*)
Jones, J.K.N. *et al., Can. J. Chem.*, 1961, **39**, 162 (*isol*)
Bailey, R.W. *et al., Oligosaccharides*, Pergamon Press, London, 1965, **4**, 134 (*occur*)
Peciar, C. *et al., Chem. Zvesti*, 1974, **28**, 83 (*config, pmr*)
Di Fabio, J.L. *et al., Carbohydr. Res.*, 1982, **99**, 41 (*isol*)

Acadesine, BAN, INN, USAN A-27

*5-Amino-1-ribofuranosyl-1*H*-imidazole-4-carboxamide, 9CI. AICA-Riboside. Acadra. AICAR. GP 1-110* [2627-69-2]



$C_9H_{14}N_4O_5$ 258.233

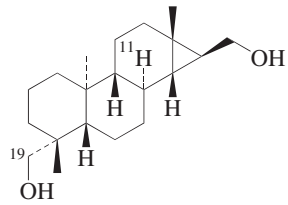
Pink rosettes (EtOH). Sol. H_2O. Mp 215-216° dec. $[\alpha]_D^{27}$ -62.4 (c, 0.5 in H_2O). Log P -2.97 (calc).

5′-Phosphate: [3031-94-5]
$C_9H_{15}N_4O_8P$ 338.213
Produced by the action of brewer's yeast on the riboside. The 5′-phosphate and its nontoxic salts are potent flavour enhancers of soups, canned foods, beverages, etc. Converted by Bratton-Marshall reagents to a purple dye with λ_{max} 540 nm. λ_{max} 268 (ε 12800) (H_2O).

Greenberg, G.R. *et al., J. Biol. Chem.*, 1956, **219**, 411; 423 (*isol*)
Burrows, I.E. *et al., JCS(C)*, 1967, 1088 (*synth, phosphate*)
US Pat., 1967, 3 355 301 (*use*)
Panzica, R.P. *et al., JOC*, 1971, **36**, 1594 (*synth*)
Panzica, R.P. *et al., J. Het. Chem.*, 1972, **9**, 623 (*synth, tri-Ac, tetra-Ac*)
Ivanovics, G.A. *et al., JOC*, 1974, **39**, 3651 (*synth*)
Adamiak, D.A. *et al., Acta Cryst. B*, 1979, **35**, 924 (*cryst struct*)
Sabina, R.L. *et al., J. Biol. Chem.*, 1982, **257**, 10178 (*metab*)
Ferris, J.P. *et al., JOC*, 1985, **50**, 747 (*synth, uv, pmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1329

Acasiane A A-28

[1187656-73-0]



$C_{20}H_{34}O_2$ 306.487

Constit. of *Acacia farnesiana* (sweet acacia). Cryst. (MeOH). $[\alpha]_D^{24}$ -53.5 (c, 0.2 in MeOH).

19-Deoxy, 11β-hydroxy: [1187656-74-1]
Acasiane B
$C_{20}H_{34}O_2$ 306.487
Constit. of *Acacia farnesiana* (sweet acacia). Oil. $[\alpha]_D^{24}$ -7.9 (c, 0.42 in MeOH).

Lin, A.-S. *et al., Planta Med.*, 2009, **75**, 256-261 (*Acasianes A,B, cryst struct*)

Acemannan, INN, USAN A-29

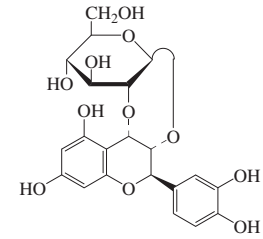
Carrisyn. Polymannoacetate [110042-95-0]

Long chain polymer consisting of linear (1→4)-D-mannopyranosyl units, randomly acetylated (0.8 Ac per monomer) MW >10000 Dalton. Constit. of leaf juice of *Aloe barbadensis*. Used in flavouring. Fluffy amorph. powder.

Pat. Coop. Treaty (WIPO), 1987, (*Carrington Lab*)0 052 (*extraction*)
Womble, D. *et al., Int. J. Immunopharmacol.*, 1988, **10**, 967 (*activity*)
Pat. Coop. Treaty (WIPO), 1990, (*Carrington Lab*)01 253 (*prep, activity*)
Fogleman, R.W. *et al., Vet. Hum. Toxicol.*, 1992, **34**, 144; 201 tox
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 536
Rodriguez, E.R. *et al., Crit. Rev. Food Sci. Nutr.*, 2010, **50**, 305-326 (*Aloe vera constit*)

Aceronidin A-30

[894078-20-7]



Absolute Configuration

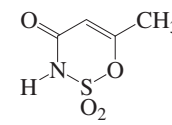
$C_{21}H_{22}O_{11}$ 450.398

Constit. of green mature acerola (*Malpighia emarginata*). Cryst. $[\alpha]_D^{20}$ +46.9 (c, 1 in MeOH). λ_{max} 278 (MeOH).

Kawaguchi, M. *et al., Biosci., Biotechnol., Biochem.*, 2007, **71**, 1130-1135 (*isol, cd, pmr, cmr, ms*)

Acesulfame, BAN, INN A-31

*6-Methyl-1,2,3-oxathiazin-4(3*H*)-one 2,2-dioxide, 9CI. 3,4-Dihydro-6-methyl-1,2,3-oxathiazin-4-one 2,2-dioxide* [33665-90-6]



$C_4H_5NO_4S$ 163.154

Non-nutritive sweetener. Needles ($CHCl_3$ or C_6H_6). Mp 123-123.5°.

K salt: [55589-62-3] *Acesulfame K. E950. Hoe 095K. H 733293*
ADI 15 mg/kg (1991). Intense-type sweetener permitted at 300-5500 ppm in foods. Sweetness approx. 200 × sucrose. Polymorphic cryst. Sol. H_2O. Mp 225° dec. (on slow heating).

Ger. Pat., 1971, 2 001 017-1193 (*synth, ir*)
Paulus, E.F. *et al., Acta Cryst. B*, 1975, **31**, 1191-1993 (*cryst struct*)
Clauss, K. *et al., Z. Lebensm.-Unters. -Forsch.*, 1976, **162**, 37-40 (*synth, use*)
Von Rymon Lipinski, G.-W. *et al., Chem. Ind. (London)*, 1983, 427-432 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AAF900
Mayer, D.G. *et al., Acesulfame-K*, M. Dekker, New York, 1991, (*book*)
Von Rymon Lipinski, G.-W. *et al., Food Sci. Technol.*, 1991, **48**, 11-28 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 3-4
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1353
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Klug, C. *et al., Alternative Sweeteners*, 4th edn., (ed. O'Brien-Nabors, L.), CRC Press, 2011, 13-30 (*use, rev*)
Velaga, S.P. *et al., Chem. Comm.*, 2012, 3562-3564 (*polymorphism*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAF900

Acetal R A-32

Acetaldehyde phenethyl propyl acetal. Propyl phenethyl acetal. Pepital. [2-(1-Propoxyethoxy)ethyl]benzene, 9CI. FEMA 2004 [7493-57-4]

$PhCH_2CH_2OCH(CH_3)OCH_2CH_2CH_3$

$C_{13}H_{20}O_2$ 208.3

(±)-*form*

Flavouring ingredient with a green pepper taste; useful in vegetable as fruit flavours. Liq. with powerful leafy odour. d_{25}^{25} 0.95. n_D^{20} 1.4800.

Arctander, S. *et al., Perfume and Flavor Chemicals*, Steffen Arctander, 1969, **1**, (*rev*)
Ford, R.A. *et al., Food Chem. Toxicol.*, 1992, **30**, 109S (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 10-11 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 9-10 (*use*)

Acetaldehyde, 9CI A-33

Ethanal. FEMA 2003 [75-07-0]

H_3CCHO

C_2H_4O 44.053

For enol form see Ethenol, E-391. Flavouring agent and adjuvant used to impart orange, apple and butter flavours; component of food flavourings added to milk products, baked goods, fruit juices, candy, desserts and soft drinks. Liq. with a pungent fruity odour. Misc. H_2O, org. solvs. d_4^{20} 0.78. Mp -121°. Bp 21°. n_D^{20} 1.3316. pK_{a1} 13.57 (25°,hydrate). Vp 900 mmHg (25°). Readily polymerises. At low temps., cationic or anionic polym. gives poly(acetaldehyde). At higher temps. cyclisation to the cyclic trimer, paraldehyde, and the cyclic tetramer, metaldehyde, occurs. The trimer may be formed on standing; redistn. regenerates acetaldehyde. Ceiling temp. for polym. T_c-39° (pure liq.). Crit. point 181.5°/63.2 atm.

▶ Extremely flammable, fl. p.-38°, autoignition temp. 140/175°. Reacts violently with a range of organic and inorganic substances. Possible human carcinogen (IARC 2B). Skin and severe eye irritant. A systemic irritant by inhalation. High vapour conc. narcotic preceded by sore throat and headache. Exp. carcinogen and teratogen. Exp. reprod. effects. AB1925000

Di-Me acetal: [534-15-6] *1,1-Dimethoxyethane, 9CI. FEMA 3426*
$C_4H_{10}O_2$ 90.122
Flavouring ingredient. Sol. H_2O, EtOH, Et_2O, Me_2CO, $CHCl_3$. Mp -113.2°. Bp 64.5°. n_D^{20} 1.3668.

▶ Highly flammable, fl. p. 1°. AB2825000

Et, isopropyl acetal: [25334-93-4] *2-(1-Ethoxyethoxy)propane. 1-Ethoxy-1-(2-propoxy)ethane. Acetaldehyde ethyl isopropyl acetal. FEMA 4432*
$C_7H_{16}O_2$ 132.202
Flavouring ingredient. Liq. Bp 124-125° (estimated).

Et, 2-methylpropyl acetal: [6986-51-2] *1-(1-Ethoxyethoxy)-2-methylpropane. Acetaldehyde ethyl isobutyl acetal. FEMA 4528*
$C_8H_{18}O_2$ 146.229
Flavouring agent. Detected in rum. Liq. Bp 155°.

Dipropyl acetal: [105-82-8] *1,1′-[Ethylidenebis(oxy)]bispropane, 9CI. 1,1-Dipropoxyethane. FEMA 4688*
$C_8H_{18}O_2$ 146.229
Flavour and fragrance ingredient. Reported in rum, wine and tomato. Liq. d_4^{20} 0.83. Bp 147-148°. n_D^{20} 1.3971.

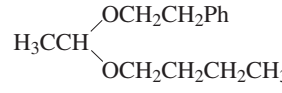
Bis(2-methylpropyl) acetal: [5669-09-0] *1,1′-[Ethylidenebis(oxy)]bis[2-methylpropane], CAS. 1,1-Bis(2-methylpropoxy)ethane. Acetaldehyde diisobutyl acetal. FEMA 4527*
$C_{10}H_{22}O_2$ 174.283
Flavouring ingredient. Detected in rum and cider. Liq. Bp 171°.

[1019-57-4, 25473-09-0, 631-59-4, 1632-89-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 214A; 465B; **2**, 921A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 348C; 727A; **3**, 487A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 551A; 1577A (*ir*)
Wertheim, E. *et al., JACS*, 1922, **44**, 2658 (*synth*)
Kalinowski, H.O. *et al., Org. Magn. Reson.*, 1974, **6**, 305 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AAG250
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 94 (*rev*)
Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 3; 171
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 9-10; 841-842
The Good Scents Company, www.thegoodscentscompany.com/search.html, (*acetal derivs, use, occur*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 47
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0776
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 2
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAG250; AAH250; DOO600
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 283 (*tox, rev*)
IARC Monogr. (Web), http://monographs.iarc.fr

Acetaldehyde butyl phenethyl acetal A-34

[2-(1-Butoxyethoxy)ethyl]benzene, 9CI. FEMA 3125 [64577-91-9]



$C_{14}H_{22}O_2$ 222.327
Flavour ingredient with a green pepper taste; useful in vegetable as fruit flavours. Liq.

Zyryanova, N.Ya. *et al., CA*, 1978, **89**, 117528g (*synth, use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 10 (*use*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 4 (*use, props*)

Acetamide, 9CI A-35

Ethanamide. Methanecarboxamide. FEMA 4251 [60-35-5]

H_3CCONH_2

C_2H_5NO 59.068
Food contact component of sealing gaskets for food containers. Deliquescent, hexagonal cryst. Odourless when pure but usually has characteristic "mouse" odour. V. sol. H_2O, EtOH; sol. $CHCl_3$; prac. insol. Et_2O. Mp 82-83°. Bp 222° Bp_5 92°. pK_{a1} -1.4 (25°). Tribuluminescent.

▶ Fl. p. >104°. Possible human carcinogen (IARC 2B). Irritant. Exp. carcinogen (v. large dose). Exp. reprod. and teratogenic effects (large doses). AB4025000

N-*(13-Methyltetradecyl):* [64317-66-4] ***Capsiamide***
$C_{17}H_{35}NO$ 269.47
Constit. of fruit of hot pepper varieties of *Capsicum annuum*.

Takahashi, M. *et al., Yakugaku Zasshi*, 1977, **97**, 758 (*Capsiamide*)
The Good Scents Company, www.thegoodscentscompany.com/search.html, (*use*)

2-Acetamidobenzoic acid A-36

2-(Acetylamino)benzoic acid, 9CI. N-*Acetylanthranilic acid. Lappaconitic acid* [89-52-1]

$C_9H_9NO_3$ 179.175
Needles (AcOH). Mp 185°. pK_a 5.64.

▶ LD_{50} (mus, orl) 1114 mg/kg. CB2455000

Me ester: [2719-08-6] *FEMA 4170*
$C_{10}H_{11}NO_3$ 193.202
Flavour and fragrance agent. Needles (EtOH). Mp 101°.

Et ester: [20628-20-0]
$C_{11}H_{13}NO_3$ 207.229
Needles (EtOH). Mp 64-65°.

Amide: [33809-77-7] *2-Acetamidobenzamide. 2-(Acetylamino)benzamide.* ***Antibiotic NP 101A***. *NP 101A*
$C_9H_{10}N_2O_2$ 178.19
Needles (EtOH). Sol. MeOH, EtOH, EtOAc, C_6H_6, DMSO, Py; poorly sol. H_2O. Mp 179-180° (α-form) Mp 189-190° (β-form). Exists in two cryst. forms, accounting for unreliable melting point determinations. λ_{max} 219 (log ϵ 3.56); 252 (log ϵ 3.31); 299 (log ϵ 2.72) (MeOH). λ_{max} 219 (ϵ 3630); 252 (ϵ 2042); 299 (ϵ 550) (MeOH) (Berdy).

▶ CU8702020

Nitrile: [25116-00-1]
$C_9H_8N_2O$ 160.175
Cryst. (Et_2O). Mp 134-135°.

N-*Ac: Diacetylanthranilic acid*
$C_{11}H_{11}NO_4$ 221.212
Prisms (EtOH). Mp 180°.
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 356D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1362B (*nmr*)
Matsuo, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 990 (*nmr*)
Erikson, J. *et al., J. Chem. Educ.*, 1972, **49**, 688 (*synth*)
Matsuda, V. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 430 (*synth*)
Ger. Pat., 1976, 2 556 590 (*synth*)
Errede, L.A. *et al., JCS Perkin 2*, 1981, 233-238 (*2-Acetamidobenzamide*)
Banasik, M. *et al., J. Biol. Chem.*, 1992, **267**, 1569-1575 (*2-Acetamidobenzamide, activity*)
Phay, N. *et al., J. Antibiot.*, 1996, **49**, 703-705 (*NP 101A*)
Shaaban, M. *et al., Dissertation*, Univ. of Göttingen, 2004, (*Cytophaga marinoflava isol*)
Kelleher, J.M. *et al., ARKIVOC*, 2007, **xvi**, 209-226 (*Acetamidobenzamide, powder struct, polymorphism*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*Me ester, use*)

Acetic acid, 9CI, USAN A-37

Ethanoic acid. Methanecarboxylic acid. E260. FEMA 2006 [64-19-7]

H_3CCOOH
$C_2H_4O_2$ 60.052
Many esters (acetates) are known apart from those cross-referenced below. Most are recorded as Ac derivs. of the relevant alcohols. Salts are included in the *Dictionary of Inorganic Compounds*. Has been used as a food preservative since antiquity. Used in - and contributes to - the flavour of pickles, sauces, mayonnaise and salad dressings. Acts synergistically with lactic and sorbic acid, and is more effective against yeasts and bacteria than against moulds. Used in food processing as a flavour enhancer, flavouring agent, pH control agent, pickling agent, solvent and formulation aid. Liq. or cryst. with pungent vinegar odour. Misc. H_2O, EtOH, Et_2O; sol. most org. solvs.; insol. CS_2. d_4^{20} 1.05. Mp 16.7°. Bp_{31} 30° Bp 118°. n_D^{20} 1.3718. n_D^{25} 1.3696. pK_a 4.76 (20°,H_2O). pK_a 4.78 (25°). Vp 15.5 mmHg (25°). Molecular Fp depression 39, molecular Bp elevation 29.9. Dissolves elemental S.
▶ Flammable, fl. p. 39°, autoignition temp. 463°. Reacts violently with some oxidants. Corrosive and irritating to all tissues. Exp. reprod. effects. OES: long-term 10 ppm; short-term 15 ppm. AF1340000

Me ester: see Methyl acetate, M-378
Et ester: see Ethyl acetate, E-405
Vinyl ester: see Ethenol, E-391
Isopropyl ester: see Isopropyl acetate, I-155
Benzyl ester: see Benzyl acetate, B-63
Ph ester: see Phenyl acetate, P-342
Hydrazide: [1068-57-1] *Acethydrazide. Acetylhydrazide. Acetylhydrazine. Ethanoylhydrazine*
$C_2H_6N_2O$ 74.082
Needles (EtOH). Sol. H_2O, EtOH, Et_2O. Mp 67°. Bp_{18} 127°. pK_{a1} 3.24; pK_{a2} 13.04 (25°,NH). Reduces $NH_3.AgNO_3$.
▶ AI1225000
Anhydride: see Acetic anhydride, A-38

[71-50-1, 758-12-3, 1186-52-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 481B; 768B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 751A; 1254C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 573B (*ir*)
Kolbe, H. *et al., Ann. Chim. Farm.*, 1845, **54**, 145 (*synth*)
Thompson, C.D. *et al., Anal. Chem.*, 1970, **42**, 1474 (*detn, H_2O*)
Perrin, D.D. *et al., Masking and Demasking of Chemical Reactions*, Interscience, New York, 1970,
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 682 (*occur*)
Lowry, R.P. *et al., Hydrocarbon Process.*, 1974, **53**, 103 (*rev, bibl*)
Michael, R.P. *et al., Science (Washington, D.C.)*, 1974, 1217
Preti, G. *et al., J. Chem. Ecol.*, 1975, **1**, 361
Couperus, P.A. *et al., Org. Magn. Reson.*, 1978, **11**, 590 (*cmr*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 121 (*rev, bibl*)
Acetic Acid and its Derivatives, (eds. Agreda, V.H. *et al*), M. Dekker, N.Y., 1993, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1329
Encyclopedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 11-13 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 13-17
Zhou, B.-H. *et al., Acta Cryst. E*, 2009, **65**, o2821 (*hydrazide, cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 12-13 (*use*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4909
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 47
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0781
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 5; 11
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAT250; ACM750

Acetic anhydride, 9CI A-38

[108-24-7]

$H_3CCO–O–COCH_3$
$C_4H_6O_3$ 102.09
Esterification agent for use in prepn. of modified food starch and for acetylation of monoglycerides. Liq. with pungent, irritating odour. Spar. sol. H_2O, sol. org. solvs. d_4^{15} 1.09. Mp -73°. Bp 139.55° Bp_{15} 44°. Aq. soln. reacts neutral and is very slowly hyd. to acetic acid.
▶ Flammable, fl. p. 49°, autoignition temp. 316/390°. Reacts violently with some oxidants. Acid-catalysed hydrolysis can be violent. Vapour is a severe irritant of eyes, mucous membranes and skin. Contact with liq. causes burns and blisters of the skin, and can damage eyes. OES: short-term 5 ppm. AK1925000

[16649-49-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 711A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1165A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 760C (*ir*)
Orshansky, J. *et al., Chem. Ind. (London)*, 1944, 382 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 1 (*use*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 142 (*rev, bibl*)
Encyclopedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 13-21 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 17-18
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 13 (*use, occur*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 48
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1437
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 6
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AAX500

Acetoacetyl-CoA hydrolase A-39

E.C. 3.1.2.11. Acetoacyl CoA deacylase [37288-10-1]

Thioester hydrolase enzyme. Isol. from cow, rabbit. Ox enzyme activity range pH 6.7-9.0.
Drummond, G.I. *et al., J. Biol. Chem.*, 1960, **235**, 318-325 (*ox*)
Baird, G.D. *et al., Biochem. J.*, 1969, **115**, 49; 1970, **117**, 703-709 (*ox*)
Rous, S. *et al., Biochem. Biophys. Res. Commun.*, 1976, **69**, 74-78 (*human*)
Zammit, V.A. *et al., FEBS Lett.*, 1979, **103**, 212-215 (*mouse, rat, rabbit*)
Aragon, J.J. *et al., J. Biol. Chem.*, 1983, **258**, 4725-4733 (*rat*)

Acetone A-40

2-Propanone, 9CI. Dimethyl ketone. FEMA 3326 [67-64-1]

H_3CCOCH_3
C_3H_6O 58.08
Solvent used in food processing as a colour diluent, flavour ingredient, etc. Volatile liq. Misc. H_2O, org. solvs. d_{25}^{25} 0.79. Mp -94°. Bp 56.2°. n_D^{20} 1.3588. Crit. temp. 246.1°.

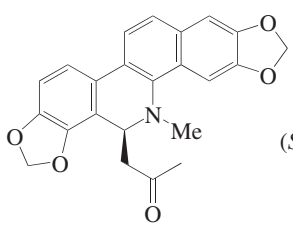
▶ Highly flammable, fl. p. -19°, autoignition temp. 538°. Reacts vigorously with $CHCl_3$ in presence of base. Liquid is severe eye irritant and defats skin. High vapour conc. irritate respiratory tract. Inhalation of vapour initially causes excitement followed by CNS depression with headache, restlessness and fatigue. Coma may result. Exp. reprod. effects by inhalation. OES: long-term 750 ppm; short-term 1500 ppm. AL3150000

[666-52-4, 43022-03-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 219D; 220A; 405A; **2**, 921B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 351C; 352A; 631A; **3**, 487B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 289A; 487A; 1577B (*ir*)
Org. Synth., 1970, **50**, 3 (*synth*)
Ullmann's Encycl. Ind. Chem., 5th edn., VCH-Weinheim, 1985, **A1**, 79 (*rev*)
Kamar, A. *et al., Can. J. Chem.*, 1986, **64**, 1979 (*ms*)
Nyquist, R.A. *et al., Appl. Spectrosc.*, 1990, **44**, 433 (*ir*)
Hayashi, S. *et al., Anal. Sci.*, 1991, **7**, 955 (*pmr, cmr*)
O'Toole, L. *et al., J. Chem. Soc., Faraday Trans.*, 1991, **87**, 3343 (*uv*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **1**, 176 (*rev, bibl*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1099
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 20-22
Allan, D.R. *et al., Chem. Comm.*, 1999, 751-752 (*cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 16 (*use*)
Chemical Hazards of the Workplace, 2nd edn., (eds. Proctor, N.H. et al), J.B. Lippincott, 1988, 49
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1146
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 7
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABC750; ABF000; TFQ250; ABD250; DOM400
Patty's Ind. Hyg. Toxicol., 4th edn., Vol. 2, Wiley, 1993, 149 (*tox, rev*)

8-Acetonyldihydrosanguinarine A-41

6-Acetonylsanguinarine. 6-Acetonyldihydrosanguinarine [37687-34-6]



(*S*)-*form*

$C_{23}H_{19}NO_5$ 389.407

(*S*)-*form*

Needles ($CHCl_3$/EtOH). Mp 209-210°. $[\alpha]_D^{20}$ +25.3 (c, 0.02 in $CHCl_3$). λ_{max} 232 (log ϵ 4.4); 282 (log ϵ 4.6); 323 (log ϵ 4.8) ($CHCl_3$).

(ξ)-*form*

Alkaloid from *Papaver somniferum* (opium poppy). Pale yellow needles (MeOH/$CHCl_3$). Mp 194-195.5°.

Furuya, T. *et al., Phytochemistry*, 1972, **11**, 3041-3044 (*isol, uv, ir, pmr, ms, struct, synth*)
Döpke, W. *et al., Z. Chem.*, 1976, **16**, 54-55 (*occur, uv, ir, pmr, ms, struct*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533-536 (*occur*)
Koul, S. *et al., Planta Med.*, 2002, **68**, 262-265 (*isol, pmr, cmr, ms*)

Acetophenone, 8CI A-42

1-Phenylethanone, 9CI. Methyl phenyl ketone. Hypnone. Acetylbenzene. FEMA 2099 [98-86-2]

$PhCOCH_3$

C_8H_8O 120.151

Flavouring ingredient used in fruit flavours; leavening agent. Reported in cocoa, beef, peas, raspberry and grapes. Plates (freq. obt. as liq.) with penetrating sweet odour. Sol. EtOH, Et_2O; insol. H_2O. d_4^{20} 1.03. Mp 20°. Bp 202° Bp_5 67°. n_D^{20} 1.5342. pK_{a1} -6.4 (25°, H_2SO_4 aq.).

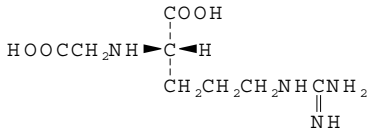
▶ Fl. p. 77°, autoignition temp. 570°. Skin and severe eye irritant. LD_{50} (rat, orl) 815 mg/kg. AM5250000

[59130-82-4, 19547-00-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 8B
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 802A
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1228B (*ir*)
Registry of Mass Spectral Data, Wiley-Interscience, 180 (*ms*)
Sadtler Standard C-13 NMR Spectra, 550 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 953 (*uv*)
Org. Synth., Coll. Vol., 1, 1932, 109 (*synth*)
Adv. Chem. Ser., 1955, **15**, 353 (***props***)
Jordanov, N. *et al., Talanta*, 1968, **15**, 850 (*use*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 99 (*rev, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1974, **4**, 5 (*use*)
Taylor, R. *et al., JCS Perkin 2*, 1988, 737 (*synth, pmr*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 23-24
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 16 (*use, occur*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 9
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABH000

Acetopine A-43

N^2-*(Carboxymethyl)arginine, 9CI. Demethyloctopine*



$C_8H_{16}N_4O_4$ 232.239

(*S*)-*form* [18416-86-9]

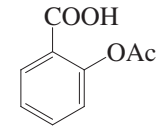
L-form

Isol. from calluses of soybean plant and cotton (*Gossypium hirsutum*). Cryst. (EtOH aq.). Mp 281-282°. $[\alpha]_D^{24}$ +24 (c, 2.5 in H_2O).

Herbst, R.M. *et al., JOC*, 1946, **11**, 368 (*synth*)
Christou, P. *et al., Plant Physiol.*, 1986, **82**, 218 (*isol*)

2-Acetoxybenzoic acid A-44

2-Acetyloxybenzoic acid, 9CI. Salicylic acid acetate, 8CI. Acetylsalicylic acid. ***Aspirin, BAN, USAN*** [50-78-2]



$C_9H_8O_4$ 180.16

Constit. of *Glycyrrhiza glabra* var. *typica* (licorice) roots. Cryst. Mp 135° (rapid heat) Fp 118. pK_a 3.38 (25°, 1*M* KCl). Log P 1.02 (calc). Ca salt used in combination with urea as Carbaspirin calcium, USAN.

▶ Dust explosion haz. Irritant. Main adverse effects are gastrointestinal, with other dose dependent systemic effects. LD_{50} (rat, orl) 200 mg/kg. Exp. teratogenic effects. OES: long-term 5 mg m^{-3}. VO0700000

Me ester: [580-02-9]
$C_{10}H_{10}O_4$ 194.187
Cryst. (petrol). Mp 49°.

Et ester: [529-68-0]
$C_{11}H_{12}O_4$ 208.213
Liq. Bp 289° Bp 272°.

Propyl ester: [60310-03-4]
$C_{12}H_{14}O_4$ 222.24
Light yellow liq. Bp 289° Bp_{10} 162-164°.

Butyl ester: [52602-16-1]
$C_{13}H_{16}O_4$ 236.267
Liq. Bp_1 128-130°.

Ph ester: [134-55-4] *Acetylsalol. Phennin. Spiroform. Vesipyrin*
$C_{15}H_{12}O_4$ 256.257
Cryst. (EtOH). Mp 97°. Bp_{11} 197-198°. Log P 3.15 (calc).

Chloride: [5538-51-2]
$C_9H_7ClO_3$ 198.605
Solid. Mp 43-46°. $Bp_{0.01}$ 86°.

Azide: [31385-27-0]
$C_9H_7N_3O_2$ 189.173
Waxy solid. Mp 65° dec.

Nitrile: [5715-02-6]
$C_9H_7NO_2$ 161.16
Liq. Bp_{17} 140°.

Anhydride: [1466-82-6]
$C_{18}H_{14}O_7$ 342.304
Mp 85°.

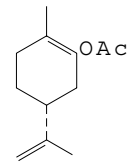
▶ VO0710000

[5749-67-7, 493-53-8, 37933-78-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 315D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1293B (*nmr*)
Ciusa, R. *et al., Chem. Zentralbl.*, 1943, **2**, 615 (*synth*)
Libermann, S. *et al., Bull. Soc. Chim. Fr.*, 1958, 185 (*synth, nitrile*)
Campini, G. *et al., Ann. Chim. (Rome)*, 1964, **54**, 975 (*synth, anhydride*)
Henriques, H.P. *et al., Mikrochim. Acta*, 1971, 807 (*detn, Mn*)
Scott, K. *et al., J. Magn. Reson.*, 1972, **6**, 55 (*nmr*)
Rüchardt, C. *et al., Annalen*, 1974, 15 (*chloride*)
Ali, S.L. *et al., Pharm. Ztg.*, 1976, **121**, 621 (*esters, synth, ir, pmr*)
Florey, K. *et al., Anal. Profiles Drug Subst.*, 1979, **8**, 1 (*rev*)
Mitscher, L.A. *et al., J. Nat. Prod.*, 1980, **43**, 259 (*occur*)
Byrn, S.R. *et al., J. Pharm. Sci.*, 1981, **70**, 280 (*cryst struct, anhydride*)
Barnett, H.J.M. *et al., Acetylsalicylic Acid*, Raven Press, N.Y., 1982, (*book*)
Collier, H.O.J. *et al., Discoveries Pharmacol.*, 1984, **2**, 555 (*rev, pharmacol*)
Hallam, J. *et al., Int. Congr. Symp. Ser. R. Soc. Med.*, 1984, (*rev*)
Kim, Y. *et al., Chem. Pharm. Bull.*, 1985, **33**, 2641 (*cryst struct*)
Chang, C.J. *et al., Magn. Reson. Chem.*, 1986, **24**, 768 (*cmr*)
Pelz, J. *et al., Pharmazie*, 1986, **41**, 733 (*history*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1120 (*synonyms*)
Bundgaard, H. *et al., J. Med. Chem.*, 1989, **32**, 727 (*esters, synth, props*)
Vane, J.R. *et al., Aspirin and Other Salicylates*, Ed., Chapman and Hall, 1992, (*book*)
Liebeskind, L.S. *et al., JOC*, 1993, **58**, 3543 (*chloride*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 3
Benefic. Toxic Eff. Aspirin, (ed., Feinman, S.E.), CRC Press, 1994,
Randi, M.L. *et al., Clin. Appl. Thromb. Hemost.*, 1999, **5**, 131-135 (*pharmacol*)
Wilson, C.C. *et al., New J. Chem.*, 2002, **26**, 1733-1739 (*cryst struct*)
Bond, A.D. *et al., Angew. Chem., Int. Ed.*, 2007, **46**, 615-617; 618-622 (*polymorphism*)
Ray, S. *et al., Synth. Commun.*, 2010, **40**, 2377-2388 (*azide*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2937
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 17
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADA725

2-Acetoxy-*p*-mentha-1,8-diene A-45

[1134-96-9]



$C_{12}H_{18}O_2$ 194.273
Enol acetate of *p*-Menth-8-en-2-one, M-245.

(R)-form
Isol. from grapefruit oil. Oil. $[\alpha]_D^{24}$ +77.

Fairlie, J.C. *et al., Chem. Comm.*, 1969, 1196 (*synth*)
Moshonas, M.G. *et al., J. Agric. Food Chem.*, 1971, **19**, 769 (*isol*)

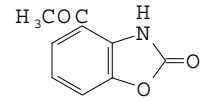
Acetylalkylglycerol acetylhydrolase A-46

E.C. 3.1.1.71. 2-Acetyl-1-alkyl-sn-*glycerol acetylhydrolase. Alkylacetylglycerol acetylhydrolase*
Carboxylic ester hydrolase enzyme. Isol. from rabbit.

Blank, M.L. *et al., Biochem. Biophys. Res. Commun.*, 1984, **124**, 156-163 (*rabbit*)
Blank, M.L. *et al., Biochim. Biophys. Acta*, 1990, **1042**, 153-158 (*mouse*)

4-Acetyl-2(3*H*)-benzoxazolone, 9CI A-47

4-Acetylbenzoxazolin-2-one [70735-79-4]

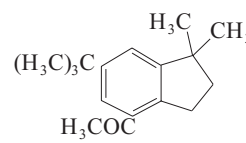


$C_9H_7NO_3$ 177.159
Found in kernels of *Zea mays* (sweet corn). Needles (Me_2CO aq.). Mp 217-218°. λ_{max} 250 (ϵ 9777); 320 (ϵ 5128) (MeOH) (Berdy). λ_{max} 268 (ϵ 8912); 351 (ϵ 7413) (MeOH/NaOH) (Berdy).

Fielder, D.A. *et al., Tet. Lett.*, 1994, **35**, 521-524 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Fielder, D.A. *et al., J. Nat. Prod.*, 1995, **58**, 456-458 (*synth*)
Escobar, C.A. *et al., J. Het. Chem.*, 1997, **34**, 1407-1414 (*synth*)
Kluge, M. *et al., J. Nat. Prod.*, 1998, **61**, 821-822 (*synth*)

4-Acetyl-6-*tert*-butyl-1,1-dimethylindane A-48

*1-[6-(1,1-Dimethylethyl)-2,3-dihydro-1,1-dimethyl-1*H*-inden-4-yl]ethanone, 9CI. 6-*tert*-Butyl-1,1-dimethyl-4-indanyl methyl ketone, 8CI. Celestolide. Chrysolide. Musk celestolide. Esperone. FEMA 3653* [13171-00-1]



$C_{17}H_{24}O$ 244.376
Flavouring ingredient. Reported in cooked asparagus. Cryst. (MeOH). Mp 77.2-77.9°.

Semicarbazone:
Cryst. (EtOH). Mp 168-168.6°.

2,4-Dinitrophenylhydrazone:
Cryst. (MeOH). Mp 180-181°.

Beets, M.G.J. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1958, **77**, 854-871 (*synth, struct*)
Ferrero, C. *et al., Helv. Chim. Acta*, 1959, **42**, 2111-2121 (*synth*)
US Pat., 1959, 2 899 358 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, Suppl., 1976, **14**, 669 (*rev, tox*)
De Ridder, D.J.A. *et al., Acta Cryst. C*, 1992, **48**, 140-142 (*cryst struct*)
Kagabu, S. *et al., J. Chem. Educ.*, 1992, **69**, 420-421 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 27
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 22 (*use, occur*)

Acetylcholine(1+) A-49

2-Acetyloxy-N,N,N-*trimethylethanaminium, 9CI. Choline acetate* [51-84-3]

$Me_3N^{\oplus}CH_2CH_2OAc$
$C_7H_{16}NO_2^{\oplus}$ 146.209
Occurs in *Capsella bursa-pastoris* (shepherd's purse). Easily hyd. by alkalis, and *in vivo* by cholinesterases.

▶ FZ9700000

Chloride: [60-31-1] ***Acetylcholine chloride, BAN, INN, USAN.*** *Miochol. Ovisot*
$C_7H_{16}ClNO_2$ 181.662
V. deliquescent cryst. powder. Sol. H_2O. Mp 149-152°.

▶ LD_{50} (rat, orl) 2500 mg/kg. LD_{50} (rat, ivn) 22 mg/kg. FZ9800000

Bromide: [66-23-9]
$C_7H_{16}BrNO_2$ 226.113
Deliquescent prisms (EtOH). Mp 143°.

▶ FZ9680000

Iodide: [2260-50-6]
$C_7H_{16}INO_2$ 273.113
Mp 161°.

▶ KH3300000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 678C; 678D; 679A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1078A (*nmr*)
Renshaw, R.R. *et al., JACS*, 1926, **48**, 1726-1732 (*bromide, synth*)
Dudley, H.W. *et al., Biochem. J.*, 1929, **23**, 1064-1074 (*Acetylcholine, synth, bibl*)
Marquardt, P. *et al., Arzneim.-Forsch.*, 1956, **6**, 168-173; 309-322 (*Acetylcholine, biosynth*)
Culvenor, C.C.J. *et al., Chem. Comm.*, 1966, 537-539 (*Acetylcholine, pmr, conformn*)
Beveridge, D.L. *et al., JACS*, 1971, **93**, 3759 (*Acetylcholine, struct, conformn*)
Micelson, M.J. *et al., Acetylcholine; Approach of Mol. Mech. of Action*, Pergamon, 1974,
Hanin, I. *et al., Choline Acetylcholine: Handb. Chem. Assay Methods*, Raven Press, NY, 1974, (*anal*)
Svinning, T. *et al., Acta Cryst. B*, 1975, **31**, 1581-1586 (*bromide, cryst struct*)
Sax, M. *et al., Acta Cryst. B*, 1976, **32**, 1953-1956 (*Acetylcholine, conformn*)
Jagner, S. *et al., Acta Cryst. B*, 1977, **33**, 2757-2762 (*iodide, cryst struct*)

Takasuka, M. *et al., JCS Perkin 2*, 1982, 585-592 (*Acetylcholine, ir*)
Anjaneyulu, B. *et al., J. Labelled Compd. Radiopharm.*, 1985, **22**, 745-750 (*radiolabelled iodide deriv, synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1112
Al-Badr, A.A. *et al., Anal. Profiles Drug Subst.*, 2004, **31**, 3-115 (*chloride, rev*)
Zelder, F.H. *et al., Chem. Comm.*, 2006, 753-754 (*chloride, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 11th edn., J. Wiley*, 2004, ABO000; CMF250

Acetylcholinesterase A-50

E.C. 3.1.1.7. Acetylcholine acetylhydrolase. Choline esterase I. Cholinesterase†*. True cholinesterase. Acetylcholine hydrolase* [9000-81-1]

Carboxylic ester hydrolase enzyme. Isol. from cow, chicken, rabbit and garden pea. Acts on a variety of acetic esters and catalyses some transacetylations. Rat enzyme activity range pH 7.8-8.4; at 4°, shows complete loss of activity but stable up to a month at -20°.

Dudai, Y. *et al., Methods Enzymol.*, 1974, **34**, 571-580 (*rev*)
Tunnicliff, G. *et al., J. Biochem. (Tokyo)*, 1976, **54**, 389-392 (*rat*)
Kasturi, R. *et al., Phytochemistry*, 1976, **15**, 1345-1347 (*Pisum sativum*)
Sine, J.P. *et al., Biochim. Biophys. Acta*, 1985, **817**, 190-192 (*rabbit*)
Ott, P. *et al., Biochim. Biophys. Acta*, 1985, **822**, 375-392 (*human, rat, ox, chicken*)
Ralston, J.S. *et al., J. Biol. Chem.*, 1985, **260**, 4312-4318 (*ox*)
Bourne, Y. *et al., J. Biol. Chem.*, 1999, **274**, 2963-2970 (*cryst struct, mouse*)

Acetyl-CoA *C*-acetyltransferase A-51

E.C. 2.3.1.9. Acetyl-CoA:acetyl-CoA C-*acetyltransferase. Acetoacetyl-CoA thiolase. Thiolase II* [9027-46-7]

Enzyme. Isol. from ox liver and pig heart.

Stern, J.R. *et al., Methods Enzymol.*, 1955, **1**, 573-585 (*pig heart*)
Stern, J.R. *et al., J. Biol. Chem.*, 1960, **235**, 313-317 (*ox liver*)
Huth, W. *et al., Eur. J. Biochem.*, 1975, **59**, 475-489 (*ox liver*)
Feigenbaum, J. *et al., J. Bacteriol.*, 1975, **122**, 407-411 (*Escherichia coli*)

Acetyl-CoA *C*-acyltransferase A-52

E.C. 2.3.1.16. Acyl-CoA:acetyl-CoA C-*acyltransferase. 3-Ketoacyl-CoA thiolase. 3-Ketothiolase. Thiolase I* [9029-97-4]

Enzyme. Widespread in nature, e.g. from beef liver, pig heart muscle, baker's yeast and sunflower.

Goldman, D.S. *et al., J. Biol. Chem.*, 1954, **208**, 345-357 (*beef liver*)
Berndt, H. *et al., Arch. Microbiol.*, 1975, **103**, 21-30 (*Clostridium pasteurianum*)
Nishimura, T. *et al., Arch. Microbiol.*, 1978, **116**, 21-27 (*Zoogloea ramigera*)
Miyazawa, S. *et al., J. Biochem. (Tokyo)*, 1981, **90**, 511-519 (*rat liver*)
Schulz, H. *et al., Methods Enzymol.*, 1981, **71**, 398-403 (*pig heart muscle*)
Mathieu, M. *et al., Structure (London)*, 1994, **2**, 797-808 (*Saccharomyces cerevisiae, cryst struct*)
Erdmann, R. *et al., Yeast*, 1994, **10**, 1173-1186 (*Saccharomyces cerevisiae*)
Oeljeklaus, S. *et al., Planta*, 2002, **21**, 597-607 (*Helianthus annuus*)

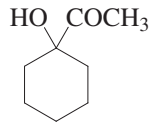
Acetyl-CoA hydrolase A-53

E.C. 3.1.2.1. Acetyl-CoA acylase. Acetyl-CoA deacylase [9027-54-7]

Thioester hydrolyse enzyme. Isol. from mammals, e.g. cow, pig; also from plants, e.g. potato, pea, castor bean, maize. Rat enzyme activity range pH 6.5-8.5. At 4°, can be stored for 4 months.

Gergely, J. *et al., J. Biol. Chem.*, 1952, **198**, 323-334 (*pig*)
Robinson, J.B. *et al., Biochem. Biophys. Res. Commun.*, 1976, **71**, 959-965 (*rat*)
Klein, R.A. *et al., Biochem. Soc. Trans.*, 1976, **4**, 285-287 (*Trypanosoma*)
Prass, R.L. *et al., J. Biol. Chem.*, 1980, **255**, 5215-5223 (*ox, guinea pig, rat*)
Namboodiri, M.A.A. *et al., J. Biol. Chem.*, 1982, **257**, 10030-10032 (*rat*)
Zeiher, C.A. *et al., Plant Physiol.*, 1990, **94**, 20-27 (*maize, pea, potato, castor*)

1-Acetylcyclohexanol A-54



$C_8H_{14}O_2$ 142.197

Ac: [52789-73-8] *1-[1-(Acetyloxy)-1-cyclohexyl]ethanone, 9CI. 1-Acetylcyclohexyl acetate. FEMA 3701*
$C_{10}H_{16}O_3$ 184.235
Flavourant for food and tobacco. Oily liq. with sweet, fruity/floral odour. Bp_2 105° (Kugelrohr).

US Pat., 1982, 4 327 749 (*synth, use*)
Fukuda, Y. *et al., JOC*, 1991, **56**, 3729-3731 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1208 (*use*)

N-Acetylcysteine A-55

2-Acetamido-3-mercaptopropanoic acid. ***Acetylcysteine, BAN, INN, USAN****. Mercapturic acid. Acetadote*

$C_5H_9NO_3S$ 163.197
Log P -0.64 (calc).

▶ Adverse effects reported when used therapeutically. LD_{50} (rat, orl) 5050 mg/kg. HA1660000

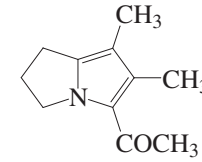
(*R*)-*form* [616-91-1]
L-form. Airbron. Fabrol. Mucomyst. Parvolex. Respaire. Fluimucil. NSC 111180
Effective inhibitor of enzymic browning in foods. Cryst. (H_2O). Mp 109-110°. $[\alpha]_D$ +5 (c, 3 in H_2O). Pharmacol. active isomer.

(±)-*form*
Cryst. (EtOH). Mp 124.5-125.5°. pK_a 9.52 (30°,SH, 0.3*M* KCl).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 786D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1282B (*nmr*)
Smith, H.A. *et al., JOC*, 1961, **26**, 820 (*synth*)
US Pat., 1965, 3 184 505 (*synth*)
Ohta, G. *et al., Chem. Pharm. Bull.*, 1967, **15**, 644 (*synth*)
Martin, T.A. *et al., J. Med. Chem.*, 1968, **11**, 625 (*synth*)
Suzuki, N. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3155 (*synth*)
McKinney, G.R. *et al., Pharmacol. Biochem. Prop. Drug Subst.*, 1979, **2**, 479 (*rev, pharmacol*)
Hopkins, S.J. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 41 (*rev*)
Takusagawa, F. *et al., Acta Cryst. B*, 1981, **37**, 1591 (*cryst struct*)
Naulet, N. *et al., Org. Magn. Reson.*, 1983, **21**, 564 (*N-15 nmr*)
Van der Kuy, A. *et al., Pharm. Weekbl.*, 1986, 121; 646; 649; 663 (*pharmacol, rev*)
De Vries, N. *et al., J. Cell Biochem.*, (Suppl. 17F), 1993, 270 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 741
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACH000

5-Acetyl-2,3-dihydro-6,7-dimethyl-1*H*-pyrrolizine A-56

*1-(2,3-Dihydro-6,7-dimethyl-1*H*-pyrrolizin-5-yl)ethanone* [97073-03-5]



$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Debrauwer, L. *et al., Bull. Soc. Chim. Fr.*, 1991, 244-254 (*occur*)

7-Acetyl-2,3-dihydro-5,6-dimethyl-1*H*-pyrrolizine A-57

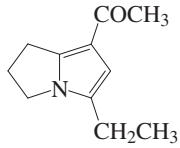
*1-(2,3-Dihydro-5,6-dimethyl-1*H*-pyrrolizin-7-yl)ethanone*

$C_{11}H_{15}NO$ 177.246
Proline- or lysine-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

7-Acetyl-2,3-dihydro-5-ethyl-1*H*-pyrrolizine A-58

*1-(2,3-Dihydro-5-ethyl-1*H*-pyrrolizin-7-yl)ethanone* [97073-13-7]

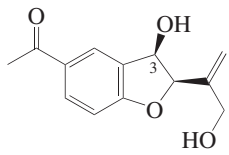


$C_{11}H_{15}NO$ 177.246
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

5-Acetyl-2,3-dihydro-3-hydroxy-2-[1-(hydroxymethyl)ethenyl]-benzofuran A-59

10-Hydroxytoxol



(2*R* ,3*R*)-*form*

$C_{13}H_{14}O_4$ 234.251

(2*R*,3*R*)-*form*
cis-*form*

*2′-*O*-β-D-Glucopyranoside:*
$C_{19}H_{24}O_9$ 396.393
Amorph. powder. $[\alpha]_D$ -5 (c, 0.1 in MeOH). λ_{max} 222; 274 (MeOH).

2′-Ac: [75680-15-8] ***10-Acetoxytoxol***
$C_{15}H_{16}O_5$ 276.288
Constit. of *Helichrysum italicum* (curry plant). Needles ($CHCl_3$/Et_2O). Mp 110°. λ_{max} 275 (log ϵ 4.09) ($CHCl_3$).

Di-Ac:
$C_{17}H_{18}O_6$ 318.326
Gum.

(2*R,3*S**)-*form***
trans-*form*

*3-*O*-β-D-Glucopyranoside:*
$C_{19}H_{24}O_9$ 396.393
Cryst. Mp 130° dec. $[\alpha]_D^{20}$ +55 (c, 0.002 in MeOH).

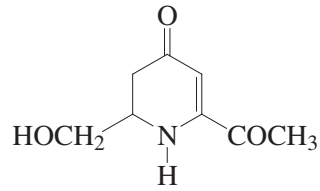
3-Angeloyl:
$C_{18}H_{20}O_5$ 316.353

(2ξ,3ξ)-*form*

2′-Ac: [1084819-03-3]
$C_{15}H_{16}O_5$ 276.288
Haensel, R. *et al., Phytochemistry*, 1980, **19**, 639-644 (*2′-Ac*)
De Guttierrez, A.N. *et al., Phytochemistry*, 1995, **39**, 795-800 (*isol, pmr, ms*)
De Lampasona, M.E.P. *et al., Phytochemistry*, 1997, **46**, 1077-1080 (*di-Ac*)
Gongora, L. *et al., Phytochemistry*, 2002, **59**, 857-860 (*Phagnalon glucoside*)
Dobner, M.J. *et al., Helv. Chim. Acta*, 2003, **86**, 733-738 (*3-glucoside*)
Wollenweber, E. *et al., Z. Naturforsch., C*, 2008, **63**, 731-739 (*Ozothamnus 2′-Ac*)

6-Acetyl-2,3-dihydro-2-(hydroxymethyl)-4(1*H*)-pyridinone, 9CI A-60

[214218-63-0]

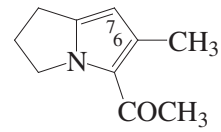


$C_8H_{11}NO_3$ 169.18
Minor product from the Maillard reaction of xylose and glycine. Pale yellow solid.

Ames, J.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 438-443 (*formn, pmr, cmr, ms*)

5-Acetyl-2,3-dihydro-6-methyl-1*H*-pyrrolizine A-61

*1-(2,3-Dihydro-6-methyl-1*H*-pyrrolizin-5-yl)ethanone, 9CI* [55041-86-6]



$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Constit. of beer and malt aroma. Characterised spectroscopically.

Shigematsu, H. *et al., J. Agric. Food Chem.*, 1975, **23**, 233-237 (*occur, ms, pmr*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923; 1993, **41**, 547-553 (*occur, ms, pmr*)

5-Acetyl-2,3-dihydro-7-methyl-1*H*-pyrrolizine A-62

*1-(2,3-Dihydro-7-methyl-1*H*-pyrrolizin-5-yl)ethanone* [80933-77-3]

$C_{10}H_{13}NO$ 163.219
Proline- or lysine-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923; 1993, **41**, 547-553 (*occur, ms*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

7-Acetyl-2,3-dihydro-5-methyl-1*H*-pyrrolizine A-63

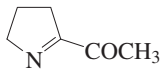
*1-(2,3-Dihydro-5-methyl-1*H*-pyrrolizin-7-yl)ethanone* [97073-06-8]

$C_{10}H_{13}NO$ 163.219
Proline-derived Maillard product. Characterised spectroscopically.

Tressl, R. *et al., J. Agric. Food Chem.*, 1985, **33**, 919-923 (*occur, ms, pmr*)

5-Acetyl-3,4-dihydro-2*H*-pyrrole A-64

*1-(3,4-Dihydro-2*H*-pyrrol-5-yl)ethanone, 9CI. 2-Acetyl-1-pyrroline. FEMA 4249* [85213-22-5]

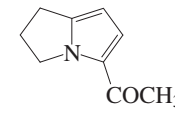


C_6H_9NO 111.143
Key flavour/aroma component of cooked rice, wheatbread crust, popcorn, sweetcorn, roasted sesame and ham. Responsible for 'mousy' off-flavour in wine. Flavouring agent. Liq. with popcorn odour. Mp 19°. Bp 182-183° Bp_{15} 26-28°. Unstable. Odour threshold of 0.02ng/L in air.

Buttery, R.G. *et al., Chem. Ind. (London)*, 1982, 958; 1983, 478 (*isol, synth*)
Favino, T.F. *et al., JOC*, 1996, **61**, 8975-8979 (*synth, pmr, bibl*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (***synth, ms, bibl***)
Wongpornchai, S. *et al., J. Agric. Food Chem.*, 2003, **51**, 457-462 (*isol*)
Harrison, T.J. *et al., JOC*, 2005, **70**, 10872-10874 (*synth*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)
Snowdon, E.M. *et al., J. Agric. Food Chem.*, 2006, **54**, 6465-6474 (*rev*)
Fuganti, C. *et al., Tetrahedron*, 2007, **63**, 4762-4767 (*synth*)
Song, H. *et al., J. Food Sci.*, 2008, **73**, C29-C35 (*detn, ham*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use, props*)

5-Acetyl-2,3-dihydro-1*H*-pyrrolizine A-65

*1-(2,3-Dihydro-1*H*-pyrrolizin-5-yl)ethanone, 9CI* [55041-85-5]

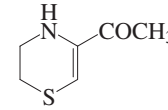


$C_9H_{11}NO$ 149.192
Proline-derived Maillard product. Constit. of popcorn, beer and cooked asparagus aroma. Mp 45.5°.

Shigematsu, H. *et al., J. Agric. Food Chem.*, 1975, **23**, 233-237 (*occur, synth, uv, ms*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1997, **45**, 837-843 (*occur, ms*)
Chen, W.C. *et al., J. Agric. Food Chem.*, 1997, **45**, 2996-2999 (*occur, ms*)
Miranda, L.D. *et al., Tet. Lett.*, 2000, **41**, 3035-3038 (*synth, ir, pmr*)

5-Acetyl-2,3-dihydro-1,4-thiazine A-66

*1-(3,4-Dihydro-2*H*-1,4-thiazin-5-yl)ethanone, 9CI* [164524-93-0]



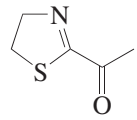
C_6H_9NOS 143.209

Formed by thermal treatment of cysteine and ribose mixtures. Liq. with intense roasty, popcorn-like odour. Mp 171-172° (as hydrochloride). Odour threshold 0.06 ng/L in air.

Hofman, T. *et al., J. Agric. Food Chem.*, 1995, **43**, 2187-2194 (*occur*)
De Kimpe, N.G. *et al., J. Agric. Food Chem.*, 1998, **46**, 2278-2281 (*synth, pmr, cmr*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)

2-Acetyl-4,5-dihydrothiazole A-67

1-(4,5-Dihydro-2-thiazolyl)ethanone, 9CI. Methyl 2-thiazolin-2-yl ketone, 8CI. 2-Acetyl-2-thiazoline. FEMA 3817 [29926-41-8]



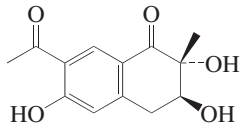
C_5H_7NOS 129.182
Reported in beef broth, roast beef, Camembert cheese and overpasteurised beer. Roasted meat-like flavour ingredient. Oil or cryst. with onion/grassy odour. Mp 25-26°. Bp_{11} 94°. n_D^{20} 1.5294.

Oxime: [37112-89-3]
$C_5H_8N_2OS$ 144.197
Cryst. (CCl_4). Mp 178-179° dec.

Doornbos, T. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1972, **91**, 711 (*synth, oxime, ir, pmr, uv, ms*)
US Pat., 1973, 3 778 518 (*props*)
Sakaguchi, M. *et al., J. Agric. Food Chem.*, 1978, **26**, 1179-1183 (*occur*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1995, **43**, 2946-2950 (*occur*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)
Fuganti, C. *et al., Tetrahedron*, 2007, **63**, 4762-4767 (*synth, pmr, cmr*)
Sourabié, A.M. *et al., J. Agric. Food Chem.*, 2008, **56**, 4974-4680 (*detn*)

7-Acetyl-3,4-dihydro-2,3,6-trihydroxy-2-methyl-1(2*H*)-naphthalenone A-68

7-Acetyl-2,3,6-trihydroxy-2-methyl-1-tetralone

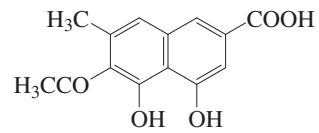


$C_{13}H_{14}O_5$ 250.251

(2*RS*,3*SR*)-*form* [1262840-98-1]
Monaspurpurone
Isol. from *Monascus purpureus* BCRC 38113 on red mould rice (koji). Yellowish oil. λ_{max} 210 (log ϵ 4.55); 256 (log ϵ 4.16); 292 (log ϵ 3.72) (MeOH).

Cheng, M.-J. *et al., Nat. Prod. Res.*, 2010, **24**, 1719-1725 (*Monaspurpurone*)

6-Acetyl-4,5-dihydroxy-7-methyl-2-naphthalenecarboxylic acid A-69



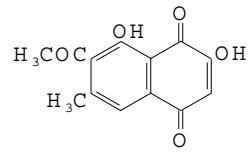
$C_{14}H_{12}O_5$ 260.246

4-O-β-D-Glucopyranoside: ***Rumexoside***
$C_{20}H_{22}O_{10}$ 422.388
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. λ_{max} 224; 260; 301; 334 (MeOH).

Demirezer, O. *et al., Phytochemistry*, 2001, **56**, 399-402

7-Acetyl-2,8-dihydroxy-6-methyl-1,4-naphthoquinone A-70

[80597-54-2]



$C_{13}H_{10}O_5$ 246.219
Yellow solid. Mp 206-209° dec.

2-Me ether: [64756-97-4] *7-Acetyl-8-hydroxy-2-methoxy-6-methyl-1,4-naphthoquinone.* ***Orientalone***
$C_{14}H_{12}O_5$ 260.246
Constit. of *Prunus cerasoides* (wild Himalayan cherry). Yellow-orange cryst. (C_6H_6/petrol). Mp 191-192°.

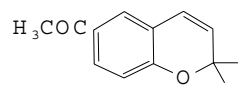
8-Me ether: [95455-42-8] *7-Acetyl-2-hydroxy-8-methoxy-6-methyl-1,4-naphthoquinone*
$C_{14}H_{12}O_5$ 260.246
Yellow solid. Mp 173-177° dec.

Di-Me ether: [80597-53-1] *7-Acetyl-2,8-dimethoxy-6-methyl-1,4-naphthoquinone*
$C_{15}H_{14}O_5$ 274.273
Yellow solid. Mp 182-184°.

Sharma, M. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 544; 1978, **16**, 289 (*Orientalone*)
Jung, M.E. *et al., Tetrahedron*, 1984, **40**, 4751 (*synth, pmr, cmr*)
Garg, M. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1985, **55**, 95 (*Orientalone*)

6-Acetyl-2,2-dimethyl-2*H*-1-benzopyran A-71

*1-(2,2-Dimethyl-2*H*-1-benzopyran-6-yl)ethanone, 9CI. 6-Acetyl-2,2-dimethyl-3-chromene. Demethoxyencecalin* [19013-07-1]



$C_{13}H_{14}O_2$ 202.252
Constit. of *Helianthus annuus* (sunflower). Oil. $Bp_{0.05}$ 95°.

2,4-Dinitrophenylhydrazone: [26932-01-4] Mp 230-232° dec.

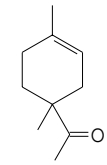
3,4-Dihydro: [32333-31-6] *6-Acetyl-3,4-dihydro-2,2-dimethyl-2*H*-1-benzopyran. 6-Acetyl-2,2-dimethylchroman*
$C_{13}H_{16}O_2$ 204.268
Mp 90-91°.

1′-Alcohol: [71822-00-9] *6-(1-Hydroxyethyl)-2,2-dimethyl-2*H*-1-benzopyran. α,2,2-Trimethyl-2*H*-1-benzopyran-6-methanol, 9CI. Demethoxyencecalinol*
$C_{13}H_{16}O_2$ 204.268
Constit. of *Helianthus annuus* (sunflower). Oil.

Arnone, A. *et al., Tet. Lett.*, 1967, **8**, 4201-4206 (*pmr, struct*)
Bohlmann, F. *et al., Chem. Ber.*, 1970, **103**, 90-96; 1972, **105**, 863-873 (*isol, pmr, synth*)
Naidu, M.V. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 73 (*synth, pmr, deriv*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 281-286 (*Demethoxyencecalinol*)
Yamaguchi, S. *et al., Bull. Chem. Soc. Jpn.*, 1984, **57**, 442-445 (*synth, pmr*)
Varga, E. *et al., Fitoterapia*, 1984, **55**, 307 (*isol*)
Ahluwalia, V.K. *et al., Indian J. Chem., Sect. B*, 1984, **23**, 1124 (*synth, pmr*)
Satoh, A. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 664-665 (*isol, activity*)

4-Acetyl-1,4-dimethyl-1-cyclohexene A-72

1-(1,4-Dimethyl-3-cyclohexenyl)ethanone. FEMA 3449 [43219-68-7]

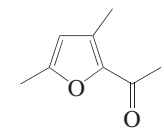


$C_{10}H_{16}O$ 152.236
Occurs in origanum and juniper oil. Flavouring ingredient. Oil. Bp 208-211°. $[\alpha]_D^{20}$ +2.1 (c, 1 in CCl_4).

Thomas, A.F. *et al., Helv. Chim. Acta*, 1973, **56**, 1800 (*isol*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1974, **57**, 164 (*synth*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 932 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 845
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 455 (*use, occur*)

2-Acetyl-3,5-dimethylfuran A-73

1-(3,5-Dimethyl-2-furanyl)ethanone, 9CI. FEMA 4071 [22940-86-9]



$C_8H_{10}O_2$ 138.166
Flavouring ingredient with sweet, balsamic taste. d_4^{20} 1.04. Mp 18°. Bp 195° Bp_4 64°. n_D^{20} 1.4962.

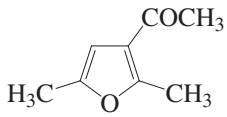
Oxime:
$C_8H_{11}NO_2$ 153.18
Cryst. (EtOH aq.). Mp 82°.

*2,4-Dinitrophenylhydrazone(*E-*):* [92494-90-1]
Mp 216°.

Balaban, A.T. *et al., Chem. Ber.*, 1960, **93**, 599-602 (*synth*)
Shuikin, N.I. *et al., Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1962, 452-454 (*synth*)
Balaban, A.T. *et al., Spectrochim. Acta*, 1963, **19**, 367-378 (*synth, oxime*)
Balaban, A.T. *et al., Org. Prep. Proced. Int.*, 1969, **1**, 63-66 (*synth*)
Balaban, A.T. *et al., Synthesis*, 1980, 136-138 (*pmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 23-26 (*use, props*)

3-Acetyl-2,5-dimethylfuran A-74

1-(2,5-Dimethyl-3-furanyl)ethanone, 9CI. 2,5-Dimethyl-3-furyl methyl ketone, 8CI. FEMA 3391 [10599-70-9]



$C_8H_{10}O_2$ 138.166
Flavouring ingredient. Present in coffee. d_4^{25} 1.03. $Bp_{0.25}$ 62°. n_D^{20} 1.4850.

Oxime:
$C_8H_{11}NO_2$ 153.18
Cryst. (EtOH aq.). Mp 78°.

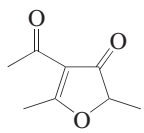
Phenylhydrazone:
Cryst. (EtOH aq.). Mp 137°.

2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 194-195°.

Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223 (*ms*)
Yanami, T. *et al., JCS Perkin 1*, 1978, 1144 (*synth, pmr, uv*)
Kretchmer, R.H. *et al., JOC*, 1978, **43**, 4596 (*synth*)
Baciocchi, E. *et al., Synth. Commun.*, 1988, **18**, 1841 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 27-28
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 24-25 (*use, props, occur*)

4-Acetyl-2,5-dimethyl-3(2*H*)-furanone, CAS A-75

FEMA 4070 [36871-78-0]

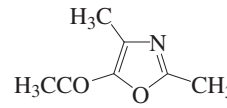


$C_8H_{10}O_3$ 154.165
Caramellic flavouring agent. Mp 34° Mp 54°. λ_{max} 230 (ϵ 12200); 265 (ϵ 13500) (EtOH).

Gelin, S. *et al., C. R. Seances Acad. Sci., Ser. C*, 1972, **275**, 897-900 (*FEMA 4070, synth, uv*)
The Good Scents Company, (*FEMA 4070, use, props*)

5-Acetyl-2,4-dimethyloxazole A-76

1-(2,4-Dimethyl-5-oxazolyl)ethanone, 9CI [23012-25-1]



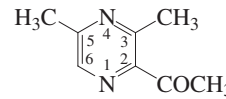
$C_7H_9NO_2$ 139.154
Constit. of Arabica coffee and baked potato aromas. Orange cryst. Mp 61°.

2,4-Dinitrophenylhydrazone:
Red cryst. (Me_2CO/DMF). Mp 204-205°.

Vitzthum, O.G. *et al., J. Food Sci.*, 1974, **39**, 1210-1215 (*isol, ms, coffee*)
Padwa, A. *et al., JACS*, 1975, **97**, 6484-6491 (*synth, pmr, uv, ir*)
Coleman, E.C. *et al., J. Agric. Food Chem.*, 1981, **29**, 42-48 (*isol, potato*)
Sauers, R.R. *et al., JOC*, 1990, **55**, 4011-4019 (*synth, pmr*)
Valgimigli, L. *et al., Chem. Eur. J.*, 2003, **9**, 4997-5010 (*synth*)

2-Acetyl-3,5-dimethylpyrazine A-77

1-(3,5-Dimethylpyrazinyl)ethanone, 9CI [54300-08-2]



$C_8H_{10}N_2O$ 150.18
Constit. of wood smoke and coffee aroma. Bp_7 70°. Normally obt. as a mixt. with 2-Acetyl-3,6-dimethylpyrazine, A-78 to which the Bp and FEMA 3327 refer.

Vitzthum, O.G. *et al., Z. Lebensm.-Unters. - Forsch.*, 1974, **156**, 300-307 (*occur*)
Wolt, J. *et al., JOC*, 1975, **40**, 1178-1179 (*synth*)
Maga, J.A. *et al., Flavour Fragrance J.*, 1985, **1**, 37-42 (*occur*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 26 (*FEMA 3327*)

2-Acetyl-3,6-dimethylpyrazine A-78

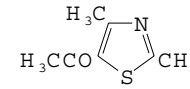
1-(3,6-Dimethylpyrazinyl)ethanone, 9CI [54300-09-3]

$C_8H_{10}N_2O$ 150.18
Component of coffee aroma. Normally obt. as a mixt. with 2-Acetyl-3,5-dimethylpyrazine, A-77 as FEMA 3327.

Vitzthum, O.G. *et al., Z. Lebensm.-Unters. - Forsch.*, 1974, **156**, 300-307 (*occur*)
Sakamoto, T. *et al., Synthesis*, 1984, 245-247 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 26 (*FEMA 3327*)

5-Acetyl-2,4-dimethylthiazole A-79

1-(2,4-Dimethyl-5-thiazolyl)ethanone, 9CI. 2,4-Dimethyl-5-thiazolyl methyl ketone. FEMA 3267 [38205-60-6]



C_7H_9NOS 155.22
Flavouring ingredient. Bp 228-230°. n_D^{20} 1.5436.

Hydrochloride: [88323-87-9]
Cryst. (EtOH aq.). Mp 180°.

Picrate: Mp 184-185°.

Oxime: [40236-03-1]
$C_7H_{10}N_2OS$ 170.235
Cryst. (EtOH aq. or C_6H_6). Mp 134°.

Semicarbazone: Mp 230°.

Ganapathi, K. *et al., Proc. - Indian Acad. Sci., Sect. A*, 1945, **22**, 343 (*synth*)
Beraud, J. *et al., Bull. Soc. Chim. Fr.*, 1962, 2072 (*synth*)
Pittet, A.O. *et al., J. Agric. Food Chem.*, 1974, **22**, 264 (*ms*)
Mane, R.A. *et al., Indian J. Chem., Sect. B*, 1983, **22**, 690 (*oxime*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 844-845
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 456 (*use*)

3-Acetyl-2,5-dimethylthiophene A-80

1-(2,5-Dimethyl-3-thienyl)ethanone, 9CI. 2,5-Dimethyl-3-thienyl methyl ketone, 8CI. FEMA 3527 [2530-10-1]

$C_8H_{10}OS$ 154.232
Flavouring ingredient. Reported in cooked beef. Liq. with burnt-roasted nutty odour. Bp_{15} 105-108°. n_D^{20} 1.5440.

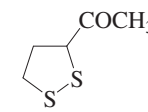
▶ OB2888000

S,S-*Dioxide:*
$C_8H_{10}O_3S$ 186.231
Cryst. Mp 124°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1473D; **2**, 597C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 54C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1473D (*ir*)
Glaze, A.P. *et al., JCS Perkin 1*, 1985, 957 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 28-29
Rozen, S. *et al., JOC*, 1997, **62**, 1457-1462 (*dioxide, synth, ir, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 27 (*use, occur*)

3-Acetyl-1,2-dithiolane A-81

1-(1,2-Dithian-3-yl)ethanone [89712-89-0]



$C_5H_8OS_2$ 148.25
Produced by thermal degradation of thiamine and by Maillard reaction of cysteine. Component of model meat aroma systems. Characterised spectroscopically.

Schmidt, U. *et al., Annalen*, 1963, **670**, 157-168 (*synth, uv*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, synth, pmr, ms*)
Zhang, Y. *et al., J. Agric. Food Chem.*, 1991, **39**, 760-763 (*occur*)

Acetylesterase A-82

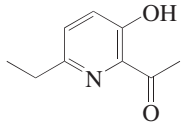
E.C. 3.1.1.6. Acetic ester acetylhydrolase. Acetic ester hydrolase. C-esterase (in animal tissues) [9000-82-2]

Carboxylic ester hydrolase enzyme. Isol. from orange, chicory, cow. *Nocardia* Enzyme stable for several months at 4°.

Eubanks, E.F. *et al., J. Bacteriol.*, 1974, **120**, 1133-1143 (*Nocardia*)
Arav, R. *et al., Biochim. Biophys. Acta*, 1987, **916**, 313-320 (*ox*)
Biely, P. *et al., Methods Enzymol.*, 1988, **160**, 700-707 (*Schizophyllum commune*)
Kormelink, F.J.M. *et al., J. Biotechnol.*, 1993, **27**, 267-282 (*Aspergillus niger*)
Gerber, K. *et al., Acta Cryst. D*, 2004, **60**, 531-533 (*cryst struct, Escherichia coli*)
Pasta, P. *et al., Biocatal. Biotransform.*, 2004, **22**, 221-224 (*orange*)
Thonar, C. *et al., J. Exp. Bot.*, 2006, **57**, 81-89 (*chicory*)

2-Acetyl-6-ethyl-3-hydroxypyridine A-83

1-(6-Ethyl-3-hydroxy-2-pyridinyl)ethanone, 9CI [1038399-41-5]

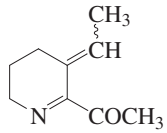


$C_9H_{11}NO_2$ 165.191
Constit. of *Abelmoschus moschatus* (ambrette) seeds. No phys. props. reported.

Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*isol, pmr, cmr, ms*)

2-Acetyl-3-ethylidene-3,4,5,6-tetrahydropyridine A-84

1-(3-Ethylidene-3,4,5,6-tetrahydro-2-pyridinyl)ethanone [118355-72-9]

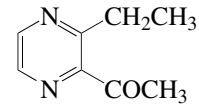


$C_9H_{13}NO$ 151.208
Proline or lysine-derived Maillard product. Characterised spectroscopically.

Helak, B. *et al., J. Agric. Food Chem.*, 1989, **37**, 400-404 (*occur, ms, pmr*)
Hill, V.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 3675-3681 (*occur*)

2-Acetyl-3-ethylpyrazine A-85

1-(3-Ethylpyrazinyl)ethanone, 9CI. FEMA 3250 [32974-92-8]

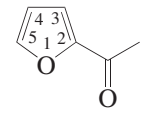


$C_8H_{10}N_2O$ 150.18
Flavouring ingredient. Found in pork liver and cocoa. Liq. Bp_6 77°. n_D 1.5142.

Ger. Pat., 1971, 2 166 323 (*synth*)
Mookherjee, B.D. *et al., JOC*, 1972, **37**, 511 (*synth, ir, pmr, ms*)
Wolt, J. *et al., JOC*, 1975, **40**, 1178
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 29-30
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 28 (*use, occur*)

2-Acetylfuran A-86

1-(2-Furanyl)ethanone, 9CI. 2-Acetofurone. α-Furyl methyl ketone. FEMA 3163 [1192-62-7]



$C_6H_6O_2$ 110.112
Present in cooked apple, morello cherry, wine grapes, peach, strawberry, plum, rabbiteye blueberry, asparagus, kohlrabi, baked potato, pineapple, bread products, rice, yoghurt, wines, soybean, black tea and calamus (European origin). Contributes to aroma of many foods and beverages. Used in flavour compositions. Liq. or cryst. with sweet balsamic odour. Mp 33°. Bp 173° Bp_{10} 67°. n_D^{20} 1.5042 (1.5014).

▶OB3870000

Oxime (E-):
$C_6H_7NO_2$ 125.127
Prisms (Et_2O/petrol). Mp 104°.

Oxime (Z-):
Cryst. (H_2O). Mp 74°.

Phenylhydrazone: [61726-90-7]
Yellow plates (EtOH aq.). Mp 86.5°.

Semicarbazone:
Plates (MeOH). Mp 150°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 583B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 23A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1457A (*ir*)
Hartough, H. *et al., JACS*, 1947, **69**, 1012 (*synth*)
Dullien, F. *et al., Can. J. Chem.*, 1957, **35**, 1366-1374 (*oximes*)
Dorofeenko, G.N. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1962, **32**, 2997 (*synth*)
Heyns, K. *et al., Tetrahedron*, 1966, **22**, 2223-2235 (*ms*)
Arlinger, L. *et al., Acta Chem. Scand.*, 1970, **24**, 662-671 (*pmr, conformn*)
Angelelli, J.M. *et al., Tetrahedron*, 1972, **28**, 2037 (*ir*)
Forsyth, D.A. *et al., JACS*, 1979, **101**, 5309-5316 (*cmr*)
Milstein, D. *et al., JOC*, 1979, **44**, 1613 (*synth*)
Okubo, J. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 2067 (*uv*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1153-1154 (*use, occur*)
Tranchida, P.Q. *et al., J. Chromatogr., A*, 2009, **1216**, 7301-7306 (*food anal*)
Singh, V. *et al., Synth. Commun.*, 2010, **40**, 1280-1291 (*synth, ir, pmr, cmr*)

N-Acetylgalactosamine-4-sulfatase A-87

E.C. 3.1.6.12. N-*Acetyl-D-galactosamine-4-sulfate 4-sulfohydrolase. Arylsulfatase B. Chondroitinase*† *Chondroitinsulfatase*† [55354-43-3]

Sulfuric ester hydrolase enzyme. Isol. from chicken, cow. Also acts on *N*-acetylglucosamine 4-sulfate. Human enzyme activity range pH 3.9-6.1. Chicken enzyme stable for 6 months at -20°.

Nicholls, R.G. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1971, **5**, 21-41 (*human, ox, kangaroo*)
Tsuii, M. *et al., Biochim. Biophys. Acta*, 1980, **612**, 373-383 (*chicken, stability*)
Wojczyk, B.S. *et al., Int. J. Biochem.*, 1992, **24**, 1561-1571 (*rat*)
Bradford, T.M. *et al., Biochemistry*, 2002, **41**, 4962-4971 (*human, activity*)
Balbaa, M. *et al., J. Enzyme Inhib. Med. Chem.*, 2006, **21**, 81-85 (*mouse*)

α-*N*-Acetylgalactosaminidase A-88

E.C. 3.2.1.49. α-N-*Acetyl-D-galactosaminide* N-*acetylgalactosaminohydrolase. α-Galactosidase B. α-NAGA* [9075-63-2]

Glycosidase enzyme. Isol. from chicken, cow, pig. Human enzyme activity range pH 3.0-8.0. Lyophilised enzyme stable for several years at -20°.

Weissmann, B. *et al., Biochemistry*, 1969, **8**, 2034-2043 (*pig, ox*)
Sweeley, C.C. *et al., Arch. Biochem. Biophys.*, 1983, **223**, 158-165 (*human, stability*)
Williams, A.G. *et al., Curr. Microbiol.*, 1984, **10**, 287-294 (*rumen bacteria, protozoa*)
Hata, J. *et al., Biochem. Int.*, 1992, **28**, 77-86 (*chicken*)
Matsuura, T. *et al., Int. J. Oncol.*, 2004, **24**, 521-528 (*human, activity*)

β-*N*-Acetylgalactosaminidase A-89

E.C. 3.2.1.53. β-N-*Acetyl-D-galactosaminide* N-*acetylgalactosaminohydrolase* [9054-43-7]

Glycosidase enzyme. Isol. from cow. Ox enzyme most active at pH 6.0 and not active below pH 4.0. At -20°, inactivated after several weeks.

Frohwein, Y.Z. *et al., Biochemistry*, 1967, **6**, 2775-2782 (*ox*)
Izumi, T. *et al., J. Biol. Chem.*, 1983, **258**, 6991-6999 (*rat*)
Tanaka, A. *et al., J. Biochem. (Tokyo)*, 1997, **122**, 330-336 (*Bacillus*)

α-*N*-Acetylgalactosaminide α-2,6-sialyltransferase A-90

*E.C. 2.4.99.3. CMP-*N*-acetylneuraminate:glycano-1,3-(*N*-acetyl-α-D-galactosaminyl)-glycoprotein α-2,6-*N*-acetylneuraminyltransferase* [71124-50-0]

Glycosyltransferase enzyme. Isol. from submaxillary glands and from foetal calf liver.

Carlson, D.M. *et al., Methods Enzymol.*, 1966, **8**, 361-365 (*sheep submaxillary gland*)
Sadler, J.E. *et al., J. Biol. Chem.*, 1979, **254**, 5934-5941 (*porcine submaxillary gland*)
Bergh, M.L. *et al., J. Biol. Chem.*, 1983, **258**, 7430-7436 (*foetal calf liver*)

***N*-Acetylglucosamine kinase** A-91

*E.C. 2.7.1.59. ATP:*N*-acetyl-D-glucosamine 6-phosphotransferase. Acetylaminodeoxyglucokinase. ATP:2-acetylamino-2-deoxy-D-glucose 6-phosphotransferase. GlcNAc kinase* [9027-48-9]

Phosphotransferase enzyme with alcohol acceptor. Isol. from pig. Bacterial enzyme also acts on D-glucose. Rat and *Candida* enzymes inhibited by sulfhydryl reagents. Rat enzyme rel. stable at pH 6.2 but rapidly loses activity >pH 8.5; at -10°, stable for several months. Human enzyme loses 50% activity within 2 mins at pH 5; at -20°, stable for 6 months; stable for 3 days at 4°.

Barkulis, S.S. *et al., Methods Enzymol.*, 1966, **9**, 415-420 (*Streptococcus pyogenes*)
Asensio, C. *et al., Methods Enzymol.*, 1966, **9**, 421-425 (*Escherichia coli*)
Datta, A. *et al., Biochim. Biophys. Acta*, 1970, **220**, 51-60 (*pig*)
Datta, A. *et al., Methods Enzymol.*, 1975, **42C**, 58-62 (*pig*)
Rai, Y.P. *et al., Biochim. Biophys. Acta*, 1980, **614**, 350-356 (*Candida albicans*)
Hinderlich, S. *et al., Eur. J. Biochem.*, 1998, **252**, 133-139 (*rat*)
Hinderlich, S. *et al., Eur. J. Biochem.*, 2000, **267**, 3301-3308 (*human, mouse*)
Yamada-Okabe, T. *et al., Eur. J. Biochem.*, 2001, **268**, 2498-2505 (*human, Candida albicans*)
Uehara, T. *et al., J. Bacteriol.*, 2004, **186**, 7273-7279 (*Escherichia coli*)

***N*-Acetylglucosamine-1-phosphodiester α-*N*-acetylglucosaminidase** A-92

E.C. 3.1.4.45. Glycoprotein N*-acetyl-D-glucosaminyl-phospho-D-mannose* N*-acetyl-D-glucosaminylphosphohydrolase.* α-N*-Acetylglucosaminyl phosphodiesterase. Lysosomal* α-N*-acetylglucosaminidase* [75788-84-0]

Phosphoric diester hydrolase enzyme. Isol. from cow. Constitutes second step in synth. of the mannose 6-phosphate determinant. Human enzyme activity range pH 6.0-9.5. At 4°, stable for 1 month.

Waheed, A. *et al., J. Biol. Chem.*, 1981, **256**, 4150-4152; 5717-5721 (*human, rat*)
Gheesling, M. *et al., J. Biol. Chem.*, 1994, **269**, 1718-1726; 1727-1733 (*human, mouse, ox*)
Lee, J.K. *et al., Arch. Biochem. Biophys.*, 1995, **319**, 413-425 (*human, hamster, activity*)
Page, T. *et al., Glycobiology*, 1996, **6**, 619-626 (*human, stability*)
Wei, Y. *et al., Glycoconjugate J.*, 2005, **22**, 13-19 (*human*)

***N*-Acetylglucosamine-6-sulfatase** A-93

E.C. 3.1.6.14. N*-Acetyl-D-glucosamine-6-sulfate 6-sulfohydrolase. Chondroitinsulfatase*†*. Glucosamine-6-sulfatase* [65666-34-4]
[60320-99-2]

Sulfuric ester hydrolase enzyme. Isol. from cow. May be identical with Disulfoglucosamine-6-sulfatase, D-1331. Ox enzyme activity range pH 4.0-9.0. At 4°, pH 5.5 in 0.02% NaN_3, stable for 1 month; at -80° under similar conditions, stable for several months.

Freeman, C. *et al., Biochem. J.*, 1987, **246**, 347-354; 355-365 (*human, ox, rat*)
Shilatifard, A. *et al., Biochemistry*, 1994, **33**, 4273-4282 (*ox, activity, stability*)
Litjens, T. *et al., Biochem. J.*, 1997, **327**, 89-94 (*goat*)
Xu, S. *et al., Biochem. J.*, 2005, **387**, 841-847 (*human*)

α-*N*-Acetylglucosaminidase A-94

E.C. 3.2.1.50. α-N*-Acetyl-D-glucosaminide* N*-acetylglucosaminohydrolase.* α-D*-2-Acetamido-2-deoxyglucosidase. NAG* [37288-40-7]

Glycosidase enzyme. Isol. from mammals, e.g. pig, rabbit. Human enzyme activity range pH 3.5-6.5. Stable for 1 year at 4° in 10*mM* sodium phosphate buffer, pH 7.2, with 150*mM* NaCl.

Weissmann, B. *et al., Biochemistry*, 1967, **6**, 207-214 (*rat, pig*)
Von Figura, K. *et al., Eur. J. Biochem.*, 1977, **80**, 525-533; 535-542 (*human, activity*)
Hook, G.E.R. *et al., J. Biol. Chem.*, 1982, **257**, 9211-9220 (*rabbit*)
Sasaki, T. *et al., J. Biochem. (Tokyo)*, 1991, **110**, 842-846 (*human*)
Zhao, K.W. *et al., Protein Expr. Purif.*, 2000, **19**, 202-211 (*human, stability*)

***N*-Acetylglucosaminyldiphosphodolichol *N*-acetylglucosaminyltransferase** A-95

*E.C. 2.4.1.141. UDP-*N*-acetyl-D-glucosamine:*N*-acetyl-D-glucosaminyl-diphosphodolichol* N*-acetyl-D-glucosaminyltransferase* [75536-54-8]

Hexosyltransferase enzyme. Isol. from mammalian tissues, e.g. pig liver. Key enzyme in the dolichol pathway for synth. of *N*-linked glycoproteins.

Turco, S.J. *et al., J. Biol. Chem.*, 1977, **252**, 2918-2928 (*rat lung*)
Sharma, C.B. *et al., Eur. J. Biochem.*, 1982, **126**, 319-325 (*yeast*)
Tai, V.W. *et al., Bioorg. Med. Chem.*, 2001, **9**, 1133-1140 (*pig liver*)

β-*N*-Acetylglucosaminyl-glycopeptide β-1,4-galactosyltransferase A-96

*E.C. 2.4.1.38. UDP-galactose:*N*-acetyl-β-D-glucosaminylglycopeptide β-1,4-galactosyltransferase. UDP-galactose:glycoprotein galactosyltransferase. Glycoprotein 4-β-galactosyltransferase* [37237-43-7]

Hexosyltransferase enzyme. Present in mammalian tissues, e.g. calf thymus. Terminal *N*-acetyl-β-D-glucosaminylglycopeptide residues in polysaccharides, glycoproteins and glycopeptides can act as acceptors.

Fraser, I.H. *et al., Biochem. J.*, 1976, **156**, 347-355 (*rat liver, rat serum*)
Bella, A. *et al., Biochem. J.*, 1977, **167**, 621-628 (*human plasma*)
Beyer, T.A. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1981, **52**, 23-175 (*rev*)
Blanken, W.M. *et al., J. Biol. Chem.*, 1985, **260**, 12927-12934 (*calf thymus*)

***N*-Acetylglucosaminyl-proteoglycan 4-β-D-glucuronosyltransferase** A-97

E.C. 2.4.1.225. Heparan glucuronyltransferase II

Hexosyltransferase enzyme. Isol. from bovine serum.

Lind, T. *et al., J. Biol. Chem.*, 1998, **273**, 26265-26268

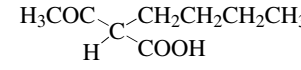
Acetylglutamate kinase A-98

*E.C. 2.7.2.8. ATP:*N*-acetyl-L-glutamate 5-phosphotransferase. Acetylglutamate phosphokinase.* N*-Acetylglutamic 5-phosphotransferase* [9027-58-1]

Phosphotransferase enzyme with carboxy acceptor. Isol. from pea and rice. *Chlamydomonas reinhardtii* Enzyme exhibits 75% maximal activity at pH 4.6 and 60% at pH 7.0. *Pseudomonas aeruginosa* Enzyme is stable at 4° in 0.1*M* phosphate buffer, and at -20° is stable over extended periods.

Baich, A. *et al., Biochem. Biophys. Res. Commun.*, 1962, **7**, 491-496 (*Escherichia coli*)
Farago, A. *et al., Biochim. Biophys. Acta*, 1967, **136**, 6-18 (*purifn, props, Chlamydomonas reinhardtii*)
Vogel, H.J. *et al., Methods Enzymol.*, 1970, **17A**, 251-255 (*Escherichia coli*)
Haas, D. *et al., Eur. J. Biochem.*, 1975, **52**, 365-375; 377-383 (*Pseudomonas aeruginosa*)
McKay, G. *et al., Biochem. J.*, 1981, **195**, 71-81 (*pea*)
Fernandez-Murga, M.L. *et al., Acta Cryst. D*, 2002, **58**, 1045-1047 (*cryst struct, Pseudomonas aeruginosa*)
Sugiyama, K. *et al., Plant Cell Physiol.*, 1984, **45**, 1768-1778 (*rice*)
Ferrario-Mery, S. *et al., FEBS Lett.*, 2006, **580**, 2015-2020 (*thale cress*)

2-Acetylhexanoic acid A-99



$C_8H_{14}O_3$ 158.197

(±)-*form*

Et ester: [1540-29-0] *Ethyl 2-acetylhexanoate. FEMA 4452*
$C_{10}H_{18}O_3$ 186.25
Flavour and fragrance ingredient. d_4^{20} 0.95. Bp_{16} 112-117° Bp 218-220°. n_D 1.4301.

Org. Synth., Coll. Vol., 1, 1932, 248-250 (*Et ester, synth*)
Ceuterick, P. *et al., Bull. Soc. Chim. Belg.*, 1936, **45**, 545-564 (*Et ester, synth*)
Zaugg, H.E. *et al., JOC*, 1961, **26**, 644-651 (*Et ester, synth*)
Wamhoff, H. *et al., Annalen*, 1969, **722**, 12-20 (*Et ester, tautom*)
Brandaenge, S. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 740-744 (*Et ester, synth, cmr*)
Deng, R. *et al., Synth. Commun.*, 1994, **24**, 111-115 (*Et ester, synth*)
The Good Scents Company, (*Et ester, use*)

β-*N*-Acetylhexosaminidase A-100

E.C. 3.2.1.52. β-N-*Acetyl-D-hexosaminide* N-*acetylhexosaminohydrolase. Hexosaminidase.* N-*Acetyl-β-glucosaminidase. E.C. 3.2.1.29 (incorporated). E.C. 3.2.1.30 (incorporated)* [9012-33-3]

Glycosidase enzyme. Isol. from mammals, e.g. cow; also from plants, e.g. mango, papaya, tomato, chilli pepper. Acts on *N*-acetylglucosides and *N*-acetylgalactosides. Toad enzyme activity range pH 3.0-6.5. At 0-4°, stable for several days.

Sarber, R.L. *et al., Methods Enzymol.*, 1978, **50**, 520-523 (*ox*)
Trimble, R.B. *et al., Methods Enzymol.*, 1982, **83**, 603-610 (*Streptomyces*)
Kinoshita, K. *et al., J. Biochem. (Tokyo)*, 1988, **104**, 827-831 (*human*)
Martinez, M.L. *et al., Mol. Reprod. Dev.*, 2000, **57**, 194-203 (*toad, activity, stability*)
Jagadeesh, B.H. *et al., Phytochemistry*, 2002, **61**, 295-300 (*mango, chilli pepper, tomato, papaya*)
Lemieux, M.J. *et al., J. Mol. Biol.*, 2006, **359**, 913-929 (*cryst struct, human*)

O-Acetylhomoserine aminocarboxypropyltransferase A-101

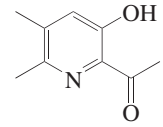
E.C. 2.5.1.49. O-*Acetyl-L-homoserine:-methanethiol 3-amino-3-carboxypropyltransferase.* O-*Acetylhomoserine (thiol)-lyase.* O-*Acetylhomoserine sulfhydrolase. E.C. 4.2.99.10 (transferred)* [37290-90-7]

Alkyltransferase enzyme. Isol. from baker's yeast. Also reacts with other thiols and H_2S giving homocysteine and thioethers.

Kerr, D. *et al., Methods Enzymol., Part B*, 1971, **17**, 446-450 (*Neurospora crassa*)
Yamagata, S. *et al., J. Biochem. (Tokyo)*, 1974, **75**, 1221-1229; 1976, **80**, 777-785; 787-797 (*yeast*)
Yamagata, S. *et al., Methods Enzymol.*, 1987, **143**, 478-483 (*yeast*)

2-Acetyl-3-hydroxy-5,6-dimethylpyridine A-102

1-(3-Hydroxy-5,6-dimethyl-2-pyridinyl)ethanone, 9CI [1038399-43-7]

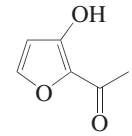


$C_9H_{11}NO_2$ 165.191
Constit. of *Abelmoschus moschatus* (ambrette) seeds. No phys. props. reported.

Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*isol, pmr, cmr, ms*)

2-Acetyl-3-hydroxyfuran A-103

1-(3-Hydroxy-2-furanyl)ethanone, 8CI. Isomaltol [3420-59-5]



$C_6H_6O_3$ 126.112
Cryst. (H_2O or Et_2O). Mp 98-103°. Subl.18 115. pK_a 5.7.

O-α-D-*Glucopyranoside:* [85559-61-1] *Glucosylisomaltol*
$C_{12}H_{16}O_8$ 288.254
Browning product produced during bread and cereal baking. Constit. of the roots of *Eleutherococcus senticosus* (Siberian ginseng). Solid. Mp 158-160°. $[\alpha]_D^{20}$ +60 (c, 1 in H_2O).

O-β-D-*Galactopyranoside:* [82756-28-3]
$C_{12}H_{16}O_8$ 288.254
Browning product produced during bread baking. Solid. Mp 200-201.5°. $[\alpha]_D^{20}$ -4.8 (c, 2 in H_2O).

Benzoyl: [38986-03-7]
$C_{13}H_{10}O_4$ 230.22
Mp 100-101°.

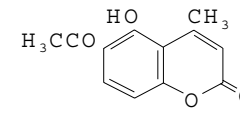
Me ether: [3420-58-4]
$C_7H_8O_3$ 140.138
Prisms (Et_2O). Mp 101-102°.

Me ether, oxime: [89776-76-1]
$C_7H_9NO_3$ 155.153
Mp 124-125°.

Hodge, J.E. *et al., Cereal Chem.*, 1961, **38**, 207-221 (*synth, ir, uv, benzoyl*)
Fisher, B.E. *et al., JOC*, 1964, **29**, 776-781 (*Me ether oxime*)
Weeks, P.D. *et al., JOC*, 1980, **45**, 1109-1113 (*use*)
Goodwin, J.C. *et al., Carbohydr. Res.*, 1983, **115**, 281-287 (*glucoside, galactoside*)
Bartulin, J. *et al., J. Het. Chem.*, 1992, **29**, 1017-1029 (*synth, ir*)
Fox, R.C. *et al., Synth. Commun.*, 1999, **29**, 989-1001 (*synth, pmr, cmr*)
Li, X.-C. *et al., Planta Med.*, 2001, **67**, 776-778 (*glucoside*)
Guerra-Hernández, E. *et al., J. Agric. Food Chem.*, 2002, **50**, 7282-7287 (*glucoside, isol*)
Vermeulen, C. *et al., J. Agric. Food Chem.*, 2006, **54**, 5061-5068 (*ms*)

6-Acetyl-5-hydroxy-4-methyl-2*H*-1-benzopyran-2-one, 9CI A-104

6-Acetyl-5-hydroxy-4-methylcoumarin. ***Liqcoumarin*** [36695-19-9]



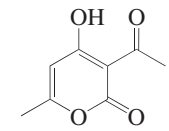
$C_{12}H_{10}O_4$ 218.209
Isol. from *Glycyrrhiza glabra* (licorice). Cryst. Mp 165-166°.

O-*Benzoyl:*
Cryst. Mp 115-116°.

Wadodkar, P.N. *et al., Indian J. Chem.*, 1972, **10**, 145
Bhardwaj, D.K. *et al., Phytochemistry*, 1976, **15**, 1182 (*isol*)

3-Acetyl-4-hydroxy-6-methyl-2*H*-pyran-2-one, 9CI A-105

Dehydroacetic acid. Dehydracetic acid [771-03-9]
[520-45-6]



$C_8H_8O_4$ 168.149
Fungicide used against moulds on fresh and dried fruit. Now superseded. Rhombic needles or plates (EtOH). Sol. H_2O, EtOH, Me_2CO, Et_2O. Mp 109°. Bp 270° Bp_5 132-133°. pK_a 5.12 (25°). λ_{max} 223; 308 (MeOH) (Berdy).

▶ LD_{50} (rat, orl) 500 mg/kg.

Na salt: [4418-26-2]
Used as a preservative for cut or peeled squash. Mp 284-287°.

▶ UP8225000

Oxime:
$C_8H_9NO_4$ 183.163
Mp 153-154°.

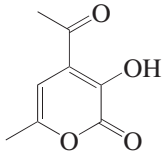
Anilide:
$C_{14}H_{13}NO_3$ 243.262
Mp 115°.

Berson, J.A. *et al., JACS*, 1952, **74**, 5172-5175 (*uv*)
Kiang, A.K. *et al., JCS*, 1965, 2283-2284 (*synth*)
Royals, E.E. *et al., JOC*, 1965, **30**, 1255-1256 (*uv, ir, pmr, struct*)
Manku, G.S. *et al., Talanta*, 1971, **18**, 1079-1082 (*use*)
Rivera, C. *et al., Experientia*, 1976, **32**, 1490 (*Solandra nitida constit*)
Ohta, S. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2762-2768 (*synth, ir, pmr*)
Tan, S.-F. *et al., JCS Perkin 2*, 1982, 513-521; 1984, 1317-1321 (*ir, pmr, uv, cmr, tautom*)
Hyatt, J.A. *et al., JOC*, 1984, **49**, 5105-5108 (*synth*)
Freiermuth, B. *et al., JOC*, 1991, **56**, 2286-2289 (*synth*)
Pesticide Manual, 9th edn., 1991, No. 3870
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 788-789; 2549-2550

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 11th edn., J. Wiley*, 2004, MFW500; SGD000

4-Acetyl-3-hydroxy-6-methyl-2*H*-pyran-2-one A-106

Passiflactone [1130942-01-6]

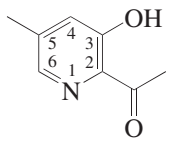


$C_8H_8O_4$ 168.149
Constit. of the juice of *Passiflora edulis* (passion fruit).

Lu, Q. *et al., Yunnan Zhiwu Yanjiu*, 2007, **29**, 375-376

2-Acetyl-3-hydroxy-5-methylpyridine A-107

1-(3-Hydroxy-5-methyl-2-pyridinyl)ethanone, 9CI [1038399-47-1]



$C_8H_9NO_2$ 151.165
Constit. of *Abelmoschus moschatus* (ambrette) seeds. No phys. props. reported.

Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*isol, pmr, cmr, ms*)

2-Acetyl-3-hydroxy-6-methylpyridine A-108

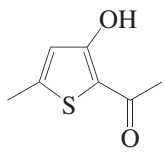
1-(3-Hydroxy-6-methyl-2-pyridinyl)ethanone, 9CI [1038399-45-9]

$C_8H_9NO_2$ 151.165
Constit. of *Abelmoschus moschatus* (ambrette) seeds. No phys. props. reported.

Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*isol, pmr, cmr, ms*)

2-Acetyl-3-hydroxy-5-methylthiophene A-109

1-(3-Hydroxy-5-methyl-2-thienyl)ethanone, CAS. FEMA 4142 [133860-42-1]

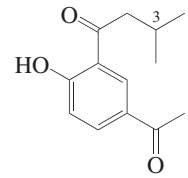


$C_7H_8O_2S$ 156.205
Savoury flavouring agent. Mp 73-76°. Bp 268-269°.

The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4142, use, props*)

1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone, 9CI A-110

4′-Hydroxy-3′-isovalerylacetophenone [62458-64-4]



$C_{13}H_{16}O_3$ 220.268
Constit. of *Polymnia sonchifolia* (yacon). Cryst. Mp 94.5-96°.
λ_{max} 242 (ϵ 15200); 271 (ϵ 5800) (MeOH).

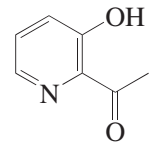
Me ether: [51995-98-3] *1-(5-Acetyl-2-methoxyphenyl)-3-methyl-1-butanone, 9CI. 3-Isovaleroyl-4-methoxyacetophenone.* ***Espeletone***
$C_{14}H_{18}O_3$ 234.294
Oil.

3-Hydroxy, 2′-Me ether: [246247-86-9] *1-(5-Acetyl-2-methoxyphenyl)-3-hydroxy-3-methyl-1-butanone*
$C_{14}H_{18}O_4$ 250.294
Amorph. yellow powder.
λ_{max} 208 (log ϵ 4.02); 240 (log ϵ 4.27); 268 (log ϵ 4.09) (MeOH).

Bohlmann, F. *et al., Chem. Ber.*, 1973, **106**, 3035-3038; 1977, **110**, 295-300; 1980, **113**, 261-266 (*isol, ms, ir, pmr, synth*)
Takasugi, M. *et al., Phytochemistry*, 1996, **43**, 1019 (*isol, uv, ir, pmr, cmr, ms*)
Fan, X. *et al., J. Nat. Prod.*, 2009, **72**, 1184-1190 (*Heteroplexis constit*)

2-Acetyl-3-hydroxypyridine A-111

1-(3-Hydroxy-2-pyridinyl)ethanone, 9CI [13210-29-2]



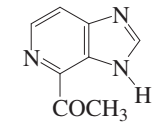
$C_7H_7NO_2$ 137.138
Constit. of *Abelmoschus moschatus* (ambrette) seeds. Cryst. (hexane). Mp 58-60°. $Bp_{0.3}$ 110-130° (bath).

Et ether: [81376-88-7] *2-Acetyl-3-ethoxypyridine*
$C_9H_{11}NO_2$ 165.191
$Bp_{0.5}$ 120° (bath).

Yamazaki, T. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1150-1154 (*synth, ir, pmr*)
Shiotani, S. *et al., J. Het. Chem.*, 1986, **23**, 665-668 (*synth, Et ether*)
Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*occur, pmr, cmr, ms*)

4-Acetylimidazo[4,5-*c*]pyridine A-112

*1-(1*H*-Imidazo[4,5-*c*]pyridin-4-yl)ethanone, 9CI. 2-Acetylpyrido[3,4-*d*]imidazole (incorr.)* [146874-38-6]

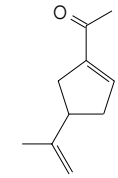


$C_8H_7N_3O$ 161.163
3*H*-form shown. Maillard prod. derived from histidine and glucose. Solid. Characterised spectroscopically.

Gi, U.-S. *et al., J. Agric. Food Chem.*, 1993, **41**, 644-646; 1995, **43**, 2226-2230 (*isol, ms, pmr, ir*)

1-Acetyl-4-isopropenylcyclopentene A-113

1-[4-(1-Methylethenyl)-1-cyclopenten-1-yl]ethanone, 9CI [2704-76-9]



$C_{10}H_{14}O$ 150.22
Isol. from oil of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Bp_{738} 225-225.5° $Bp_{1.5}$ 67-68°. $n_D^{24.5}$ 1.4965.

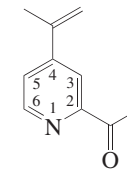
2,4-Dinitrophenylhydrazone:
Red plates (EtOH). Mp 178-180°.

Semicarbazone:
Cryst. (MeOH). Mp 195-196°.

Schmidt, H. *et al., Chem. Ber.*, 1947, **80**, 528; 533 (*isol*)
Wolinsky, J. *et al., JACS*, 1960, **82**, 636 (*struct, synth*)
Conia, J.M. *et al., Bull. Soc. Chim. Fr.*, 1964, 1963 (*synth, uv, ir, pmr*)
Vig, P. *et al., Indian J. Chem.*, 1968, **6**, 564 (*synth*)

2-Acetyl-4-isopropenylpyridine A-114

1-[4-(1-Methylethenyl)-2-pyridinyl]ethanone, CAS. FEMA 4636 [142896-11-5]



$C_{10}H_{11}NO$ 161.203
Constit. of *Mentha gentilis* (spearmint) oil. Flavouring ingredient. Oil.

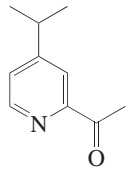
Ishihara, M. *et al., J. Agric. Food Chem.*, 1992, **40**, 1647-1655 (*Mentha gentilis constit*)
US Pat., 1993, 5 214 027 (*FEMA 4636, synth, use, pmr, ms, ir*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4636, use*)

4-Acetyl-2-isopropenylpyridine **A-115**
1-[2-(1-Methylethenyl)-4-pyridinyl]ethanone, CAS. FEMA 4637 [142896-12-6]

$C_{10}H_{11}NO$ 161.203
Constit. of *Mentha gentilis* (spearmint) oil. Flavouring ingredient. Oil.

Ishihara, M. *et al., J. Agric. Food Chem.*, 1992, **40**, 1647-1655 (*Mentha gentilis constit*)
US Pat., 1993, 5 214 027 (*FEMA 4637, synth, use, pmr, ms, ir*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4637, use*)

2-Acetyl-4-isopropylpyridine **A-116**
1-[4-(1-Methylethyl)-2-pyridinyl]ethanone, CAS. FEMA 4638 [142896-09-1]



$C_{10}H_{13}NO$ 163.219
Constit. of *Mentha gentilis* (spearmint) oil. Flavour and fragrance ingredient. Oil.

Ishihara, M. *et al., J. Agric. Food Chem.*, 1992, **40**, 1647-1655 (*Mentha gentilis constit*)
US Pat., 1993, 5 214 027 (*FEMA 4638, synth, use, pmr, ms, ir*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4638, use*)

***N*-Acetyllactosamine synthase** **A-117**
*E.C. 2.4.1.90. UDP-galactose:*N-*acetyl-D-glucosamine 4-β-D-galactosyltransferase. β-1,4-Galactosyltransferase. E.C. 2.4.1.98 (incorporated)* [9054-94-8]

Hexosyltransferase enzyme. Isol. from cow's milk. Acts on either free *N*-acetyl-D-galactose or on the non-reducing terminal monosaccharide of a carbohydrate chain of a glycoprotein or glycolipid.

Helting, T. *et al., Biochim. Biophys. Acta*, 1973, **293**, 94-104 (*mouse mastocytoma*)
Deshmukh, D.S. *et al., Biochim. Biophys. Acta*, 1978, **542**, 284-295 (*rat brain*)
Schachter, H. *et al., Methods Enzymol.*, 1983, **98**, 98-134 (*bovine milk*)
Ramakrishnan, B. *et al., Biochem. Biophys. Res. Commun.*, 2002, **291**, 1113-1118 (*rev*)
Ramakrishnan, B. *et al., Curr. Opin. Struct. Biol.*, 2004, **14**, 593-600 (*rev*)

***N*-Acetyllactosaminide *N*-acetylglucosaminyltransferases** **A-118**
Hexosyltransferase enzymes.

***N*-Acetyllactosaminide β-1,3-*N*-acetylglucosaminyltransferase** [85638-39-7]
*E.C. 2.4.1.149. Poly-*N-*acetyllactosamine extension enzyme*
Present in calf serum. R represents the remainder of an asialo-α^1-acid glycoprotein.

***N*-Acetyllactosaminide β-1,6-*N*-acetylglucosaminyltransferase** [85638-40-0]
E.C. 2.4.1.150

Van den Eijnden, D.H. *et al., J. Biol. Chem.*, 1983, **258**, 3435-3437; 1988, **263**, 12461-12471 (*Novikoff ascites tumour cells*)
Piller, F. *et al., J. Biol. Chem.*, 1983, **258**, 12293-12299 (*E.C. 2.4.1.149, human serum*)
Hosumi, A. *et al., J. Biochem. (Tokyo)*, 1984, **95**, 1655-1659 (*E.C. 2.4.1.149, human serum*)
Kawashima, H. *et al., J. Biol. Chem.*, 1993, **268**, 27118-27126 (*E.C. 2.4.1.149, calf serum*)

***N*-Acetyllactosaminide 3-α-galactosyltransferase** **A-119**
*E.C. 2.4.1.87. UDP-galactose:*N-*acetyllactosaminide 3-α-D-galactosyltransferase. α-1,3-Galactosyltransferase. E.C. 2.4.1.124 (incorporated). E.C. 2.4.1.151 (incorporated)* [128449-51-4]

Hexosyltransferase enzyme. Isol. from rabbit and cow. Acts on glycoproteins and on *N*-acetyllactosamine.

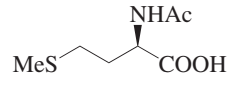
Basu, M. *et al., J. Biol. Chem.*, 1973, **248**, 1700-1706 (*rabbit bone marrow*)
Betteridge, A. *et al., Eur. J. Biochem.*, 1983, **132**, 29-35 (*rabbit stomach mucosa*)
Blanken, W.M. *et al., J. Biol. Chem.*, 1985, **260**, 12927-12934 (*calf thymus*)

***N*-Acetyllactosaminide α-2,3-sialyltransferase** **A-120**
*E.C. 2.4.99.6. CMP-*N-*acetylneuraminate:β-D-galactosyl-1,4-*N-*acetyl-D-glucosaminyl-glycoprotein α-2,3-*N-*acetylneuraminyltransferase* [77537-85-0]

Glycosyltransferase enzyme. Present in foetal calf liver and embryonic chicken brain.

Van den Eijnden, D.H. *et al., J. Biol. Chem.*, 1981, **256**, 3159-3162 (*isol*)
Nemansky, M. *et al., Glycoconjugate J.*, 1993, **10**, 99-108 (*human placenta*)

***N*-Acetylmethionine, 9CI** **A-121**
2-(Acetylamino)-4-(methylthio)butanoic acid. Aminotylon. Methionamine. Thiomedon-Amp



(*R*)-*form*

$C_7H_{13}NO_3S$ 191.251

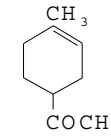
(*R*)-*form* [1509-92-8]
Cryst. (EtOAc or H_2O). Mp 104-105°. $[\alpha]_D^{25}$ +20.3 (c, 4 in H_2O).

(*S*)-*form* [65-82-7]
Nutrient supplement used as a source of L-methionine. Mp 104°. $[\alpha]_D^{25}$ -20.3.
▶PD0480000

(±)-*form* [1115-47-5]
Cryst. (H_2O). Mp 114-115°.
▶PD0500000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 784D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1280A (*nmr*)
Wheeler, G.P. *et al., JACS*, 1951, **73**, 4604 (*synth*)
US Pat., 1962, 3 028 395 (*resoln*)
Heyns, K. *et al., Annalen*, 1963, **667**, 194 (*ms*)
UK Pat., 1967, 1 072 876 (*resoln*)
Jung, G. *et al., Eur. J. Biochem.*, 1973, **35**, 436 (*cd*)
Rotruck, J.T. *et al., J. Nutr.*, 1975, **105**, 331 (*metab*)
Hawkes, G.E. *et al., Nature (London)*, 1975, **257**, 767 (*N-15 nmr*)
Boggs, R.W. *et al., Adv. Exp. Med. Biol.*, 1978, **105**, 571 (*props*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982,
Ponnuswamy, M.N. *et al., Acta Cryst. C*, 1985, **41**, 917 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 30-31
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ACQ275

4-Acetyl-1-methylcyclohexene **A-122**
*1-(4-Methyl-3-cyclohexen-1-yl)ethanone, 9CI. 1′,2′,3′,6′-Tetrahydro-4′-methylacetophenone. Tetrahydro-*p-*acetyltoluene*
[6090-09-1]

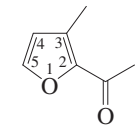


$C_9H_{14}O$ 138.209
Flavouring ingredient. Isol. from the famine food *Santalum album* (sandalwood). Oil. Bp 205-206°.

[70286-20-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **3**, 530D (*ir*)
Thomas, A.F. *et al., Helv. Chim. Acta*, 1973, **56**, 1800 (*synth, struct*)
Demole, E. *et al., Helv. Chim. Acta*, 1976, **59**, 737 (*synth*)

2-Acetyl-3-methylfuran **A-123**
1-(3-Methyl-2-furanyl)ethanone, 9CI. Methyl (3-methyl-2-furyl) ketone, 8CI
[13101-45-6]



$C_7H_8O_2$ 124.139
Present in oils of *Perilla frutescens* and *Elsholtzia ciliata* and sesame oil. Bp_{20} 116-119° Bp_{10} 60°.

Oxime:
$C_7H_9NO_2$ 139.154
Mp 62-63°.

2,4-Dinitrophenylhydrazone: Mp 192-193° (180°).

[119363-99-4]

Ueda, T. *et al., Nippon Kagaku Zasshi*, 1960, **81**, 1756 (*isol*)

Fujita, Y. *et al., Nippon Kagaku Zasshi*, 1966, **87**, 1361 (*isol*)
Kutney, J.P. *et al., Tetrahedron*, 1971, **27**, 3323 (*synth, ir, uv, pmr*)

2-Acetyl-5-methylfuran A-124

1-(5-Methyl-2-furanyl)ethanone, 9CI. Methyl (5-methyl-2-furyl) ketone, 8CI. FEMA 3069 [1193-79-9]

$C_7H_8O_2$ 124.139
Isol. from raisins, roasted onion, French fried potato, tomato, smoked fatty fish, cooked beef, fried cured pork, beer, spirits, black tea, wild rice, squid and coffee aroma. Organoleptic and flavouring agent. d_4^{20} 1.07. Bp_{10} 80°. n_D^{20} 1.5138.

► LT8528000

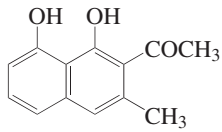
Semicarbazone: Mp 190.5-191.5°.

[73750-15-9]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 23C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1457C (*ir*)
Farrer, M.W. *et al., JACS*, 1950, **72**, 3695 (*synth*)
Morizur, J.P. *et al., Bull. Soc. Chim. Fr.*, 1966, 2296 (*pmr*)
Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)
Ferretti, A. *et al., J. Agric. Food Chem.*, 1970, **18**, 13 (*isol*)
Scholz, S. *et al., Annalen*, 1985, 1935 (*synth, pmr, cmr, ir*)
Boykin, D.W. *et al., J. Het. Chem.*, 1988, **25**, 643 (*O-17 nmr*)
Farmer, L.J. *et al., J. Sci. Food Agric.*, 1989, **49**, 347
Baig, M.A. *et al., JCS Perkin 2*, 1989, 1981 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 32-33 (*use, occur*)

2-Acetyl-3-methyl-1,8-naphthalenediol A-125

*1-(1,8-Dihydroxy-3-methyl-2-naphthalenyl)ethanone, 9CI. 2-Acetyl-1,8-dihydroxy-3-methylnaphthalene. **Musizin**. Dianellidin. Nepodin* [3785-24-8]



$C_{13}H_{12}O_3$ 216.236
Yellow needles (EtOH or petrol/C_6H_6). Mp 164-165° (evac. tube).

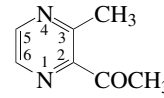
8-O-[β-D-Glucopyranosyl-(1→3)-β-D-glucopyranoside]: ***Orientaloside***
$C_{25}H_{32}O_{13}$ 540.52
Constit. of the roots of *Rumex patientia* (patience dock). Amorph. λ_{max} 225; 260; 301; 333; 345 (MeOH).

4-Chloro, 8-O-β-D-glucopyranoside: [349636-06-2] ***Patientoside A***
$C_{19}H_{21}ClO_8$ 412.823
Constit. of the roots of *Rumex patientia* (patience dock). Pale yellow powder. $[\alpha]_D^{20}$ -109.7 (c, 0.75 in MeOH). λ_{max} 234 (log ϵ 3.97); 312 (log ϵ 3.73); 339 (log ϵ 3.69) (MeOH).

Kuruuzum, A. *et al., J. Nat. Prod.*, 2001, **64**, 688-690 (*Patientoside A*)
Demirezer, O. *et al., Phytochemistry*, 2001, **56**, 399-402 (*Orientaloside*)

2-Acetyl-3-methylpyrazine A-126

1-(3-Methylpyrazinyl)ethanone, 9CI. Methyl (3-methylpyrazinyl) ketone, 8CI [23787-80-6]

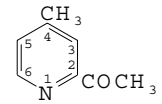


$C_7H_8N_2O$ 136.153
Aroma constit. of spiny lobster (*Panulirus argus*) and roasted sesame seed. Liq. with burnt, popcorn-like odour. d 1.11. $Bp_{0.5}$ 56°. n_D^{20} 1.5216. Odour threshold 2 x 10^{-2} ppm in H_2O.

Mookherjee, B.D. *et al., JOC*, 1972, **37**, 511-513 (*synth, ir, pmr, ms*)
Wolt, J. *et al., JOC*, 1975, **40**, 1178-1179 (*synth, pmr, ms*)
Mihara, S. *et al., J. Agric. Food Chem.*, 1988, **36**, 1242-1247 (*props*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*glc, occur*)
Cadwallader, K.R. *et al., J. Agric. Food Chem.*, 1995, **43**, 2432-2437 (*detn, occur*)

2-Acetyl-4-methylpyridine A-127

1-(4-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 4-methyl-2-pyridyl ketone, 8CI. 2-Acetyl-4-picoline [59576-26-0]



C_8H_9NO 135.165
Component of fig leaf absolute (*Ficus carica*). Cryst. (petrol). Sol. EtOH. Mp 33-34°. Bp_{15} 95-97°.

*Oxime (*E-*):* [23089-35-2]
$C_8H_{10}N_2O$ 150.18
Cryst. (C_6H_6/petrol). Mp 98-99° Mp 125-128°.

Semicarbazone:
Solid. Mp 195-198°.

[18103-84-9]

Case, F.H. *et al., JACS*, 1956, **78**, 5842 (*synth*)
Nishimoto, N. *et al., Yakugaku Zasshi*, 1961, **81**, 88 (*synth*)
Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Co, Cu, Fe*)

2-Acetyl-5-methylpyridine A-128

1-(5-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 5-methyl-2-pyridyl ketone, 8CI. 2-Acetyl-5-picoline [5308-63-4]

C_8H_9NO 135.165
Component of roasting coffee aroma. Liq. $Bp_{0.1}$ 60-70°.

Crabb, T.A. *et al., Org. Magn. Reson.*, 1982, **20**, 242 (*synth*)
US Pat., 1986, 4 574 125 (*synth*)

2-Acetyl-6-methylpyridine A-129

1-(6-Methyl-2-pyridinyl)ethanone, 9CI. Methyl 6-methyl-2-pyridyl ketone, 8CI. 6-Acetyl-2-picoline [6940-57-4]

C_8H_9NO 135.165
Minor component of rum. Flavour modifying agent for coffee. Constit. of *Abelmoschus moschatus* (ambrette) seed. Liq. Bp_1 46°.

*Oxime (*E-*):* [23089-39-6]
$C_8H_{10}N_2O$ 150.18
Cryst. (petrol). Sol. EtOH. Mp 49-50°.

Dimethylhydrazone: [33785-80-7]
$C_{10}H_{15}N_3O$ 193.248
Liq. $Bp_{0.1}$ 53-54°. n_D^{26} 1.5370.

[18103-88-3]

Case, F.H. *et al., J. Het. Chem.*, 1968, **5**, 161 (*synth, oxime*)
Schilt, A. *et al., Talanta*, 1969, **16**, 448 (*detn, Cu*)
Newkome, G.R. *et al., JOC*, 1972, **37**, 1329 (*deriv*)
Zanger, M. *et al., Anal. Chem.*, 1974, **46**, 2042 (*pmr*)
Amin, H.B. *et al., JCS Perkin 2*, 1979, 624 (*synth*)
Du, Z. *et al., J. Agric. Food Chem.*, 2008, **56**, 7388-7392 (*detn*)

4-Acetyl-2-methylpyridine A-130

1-(2-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 2-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-2-picoline [2732-28-7]

C_8H_9NO 135.165
Component of roasting coffee aroma. Liq. Bp_{10} 120-124° Bp_4 130°.

Picrate: [31931-61-0]
Solid (EtOH). Mp 174-175°.

[80882-67-3]

Suzuki, Y. *et al., Yakugaku Zasshi*, 1961, **81**, 795 (*synth*)
Eilhauer, H.D. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1965, **298**, 131 (*synth*)
Govindachari, T.R. *et al., Indian J. Chem.*, 1966, **4**, 398 (*synth*)

4-Acetyl-3-methylpyridine A-131

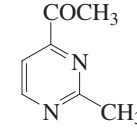
1-(3-Methyl-4-pyridinyl)ethanone, 9CI. Methyl 3-methyl-4-pyridyl ketone, 8CI. 4-Acetyl-3-picoline [82352-00-9]

C_8H_9NO 135.165
Component of roasting coffee aroma. Bp_1 93-95°.

Hibino, S. *et al., J. Het. Chem.*, 1990, **27**, 1751 (*synth, pmr, ms*)

4-Acetyl-2-methylpyrimidine A-132

1-(2-Methyl-4-pyrimidinyl)ethanone, 9CI. FEMA 3654 [67860-38-2]

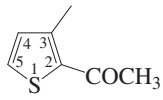


$C_7H_8N_2O$ 136.153
Flavouring ingredient. Present in cooked meats. Liq. d_4^{20} 1.1. Bp_{10} 85-90°. n_D^{20} 1.5039.

Ger. Pat., 1977, 2 800 443 (*synth, use*)
Sakamoto, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 4554-4560 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 32 (*use, occur*)

2-Acetyl-3-methylthiophene A-133

1-(3-Methyl-2-thienyl)ethanone, 9CI. Methyl 3-methyl-2-thienyl ketone, 8CI [13679-72-6]



C_7H_8OS 140.206
Flavouring ingredient with a honey-like flavour. Bp 216° Bp_{14} 98-99°. n_D^{20} 1.5620.

Oxime:
C_7H_9NOS 155.22
Mp 85-86°.

Demuth, R. *et al., Ber.*, 1885, **18**, 3026 (*synth*)
Von Gerlach, M. *et al., Annalen*, 1892, **267**, 153 (*synth, oxime*)
Campaigne, E. *et al., JOC*, 1963, **28**, 914 (*synth*)

2-Acetyl-5-methylthiophene A-134

1-(5-Methyl-2-thienyl)ethanone, 9CI. Methyl 5-methyl-2-thienyl ketone. FEMA 4643 [13679-74-8]

C_7H_8OS 140.206
Organoleptic. Constit. of coffee aroma, cooked meats and krill. Mp 25°. Bp 232-233° Bp_8 98-100°.

► OB4972000

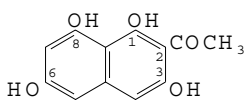
Oxime: [1956-44-1]
C_7H_9NOS 155.22
Mp 125°.

Semicarbazone: Mp 215-217° dec.

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*isol*)
Kaper, L. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1970, **81**, 825 (*uv*)
Bagli, J. *et al., J. Med. Chem.*, 1976, **19**, 876 (*synth*)
Drage, J.S. *et al., Organometallics*, 1985, **4**, 389 (*synth, pmr*)
Spinelli, D. *et al., Acta Chem. Scand.*, 1993, **47**, 160 (*cmr, O-17 nmr*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use, occur*)

2-Acetyl-1,3,6,8-naphthalenetetrol A-135

2-Acetyl-1,3,6,8-tetrahydroxynaphthalene. Acetyl-T4HN



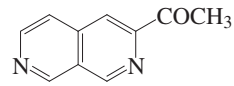
$C_{12}H_{10}O_5$ 234.208

1,6-Di-Me ether, 3-O-β-D-apiofuranoside, 8-O-β-D-glucopyranoside: [170384-73-3] ***Cassitoroside***
$C_{25}H_{32}O_{14}$ 556.519
Constit. of the seeds of *Cassia tora* (charota). Pale yellow needles. Mp 234-236°. λ_{max} 231 (log ε 5.12); 276 (log ε 5.03); 314 (log ε 4.44); 396 (log ε 4.32) (MeOH).

Choi, J.S. *et al., Phytochemistry*, 1995, **40**, 997-999 (*Cassitoroside*)
Wheeler, M.H. *et al., Eukaryotic Cell*, 2008, **7**, 1699-1711 (*biosynth*)

3-Acetyl-2,7-naphthyridine A-136

1-(2,7-Naphthyridin-3-yl)ethanone, 9CI [73607-00-8]



$C_{10}H_8N_2O$ 172.186
Alkaloid from *Valeriana officinalis* (valerian).

Janot, M.M. *et al., Ann. Pharm. Fr.*, 1979, **37**, 413-420 (*isol, cryst struct*)
Barbu, E. *et al., Heterocycl. Commun.*, 2000, **6**, 25-28 (*synth*)

N-Acetylneuraminate acetyltransferases† A-137

Sialate acetyltransferase
Enzymes. Isol. from bovine and equine salivary glands.

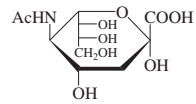
***N*-Acetylneuraminate 4-*O*-acetyltransferase** [51004-25-2]
*E.C. 2.3.1.44. Acetyl-CoA:*N-*acetylneuraminate 4*-O-*acetyltransferase*

***N*-Acetylneuraminate 7-*O*(*or* 9-*O*)-acetyltransferase** [9054-50-6]
*E.C. 2.3.1.45. Acetyl-CoA:*N-*acetylneuraminate 7*-O-(or 9-O)-*acetyltransferase*

Schauer, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1970, **351**, 559-602; 749-758 (*bovine salivary gland, horse salivary gland*)
Schauer, R. *et al., Methods Enzymol.*, 1978, **50**, 381-386 (*bovine salivary gland*)
Diaz, S. *et al., Methods Enzymol.*, 1989, **179**, 416-422 (*rat liver golgi vessels*)
Iwersen, M. *et al., Biol. Chem.*, 2003, **384**, 1035-1047 (*guinea pig liver*)

N-Acetylneuraminic acid A-138

5-(Acetylamino)-3,5-dideoxy-D-glycero-D-galacto-2-nonulosonic acid, 9CI. O-*Sialic acid.* ***Aceneuramic acid, INN.*** *Lactaminic acid. Gynaminic acid. Serolactaminic acid. KI 111. NANA. Neu5Ac. Neu5NAc* [131-48-6]



α-D-Pyranose-*form*

$C_{11}H_{19}NO_9$ 309.272
Isol. from eggs, milk and colostrum by acid or enzymic hydrol. of the constit. sialoproteins and oligosaccharides. Most abundant source is the nest cementing glycoprotein of the Chinese swiftlet used in birdsnest soup. Mp 185-187° dec. $[\alpha]_D^{22}$ -32 (H_2O). The only sialic acid formed in human tissues. Store below 0° in the dark.

[19342-33-7, 126934-33-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 758C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1239A (*nmr*)
Gottschalk, A. *et al., The Chemistry and Biology of Sialic Acids and Related Substances*, Cambridge Univ. Press, London, 1960, (*book*)
Blix, G. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 246-250 (*isol*)
O'Connell, A.M. *et al., Acta Cryst. B*, 1973, **29**, 2320-2328 (*cryst struct*)
Codington, J.F. *et al., Methods Carbohydr. Chem.*, 1976, **7**, 226-232 (*isol, detn*)
Martin, J.E. *et al., Carbohydr. Res.*, 1977, **56**, 423-425 (*isol*)
Jaques, L.W. *et al., J. Biol. Chem.*, 1977, **252**, 4533-4538 (*cmr*)
Czarniecki, M.F. *et al., JACS*, 1977, **99**, 8273-8279 (*isol, cmr*)
Benzing-Nguyen, L. *et al., JOC*, 1978, **43**, 551-554 (*synth, cmr*)
Friebolin, H. *et al., Angew. Chem., Int. Ed.*, 1980, **19**, 208-209 (*equilib*)
Schauer, R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1982, **40**, 131-234 (*rev*)
Sialic Acids: Chem. Metab. and Function, (Ed. Schauer, R.), Springer-Verlag, Vienna, 1982, 5 (*rev*)
Csuk, R. *et al., Helv. Chim. Acta*, 1988, **71**, 609-618 (*synth*)
Prytulla, A. *et al., Magn. Reson. Chem.*, 1990, **28**, 888-901 (*cmr, pmr*)
Kragl, U. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 827-828 (*enzymic synth*)
DeNinno, M.P. *et al., Synthesis*, 1991, 583-593 (*synth, gly, rev*)
Bodenmüller, A. *et al., Annalen*, 1994, 541-548 (*synth*)
Kragl, U. *et al., Ann. N.Y. Acad. Sci.*, 1995, **750**, 300-305 (***synth***)
Chan, T.H. *et al., JOC*, 1995, **60**, 4228-4232 (*synth*)
Maru, I. *et al., Carbohydr. Res.*, 1998, **306**, 575-578 (***synth***)
Banwell, M. *et al., JCS Perkin 1*, 1998, 2251-2252 (*synth*)
Ooi, H.C. *et al., Aust. J. Chem.*, 1999, **52**, 937-940 (*synth*)

(α-*N*-Acetylneuraminyl-2,3-β-galactosyl-1,3)-*N*-acetylgalactosaminide 6-α-sialyltransferase A-139

*E.C. 2.4.99.7. CMP-*N-*acetylneuraminate:(*α-N-*acetylneuraminyl-2,3-β-D-galactosyl-1,3)-*N-*acetyl-D-galactosaminide α-2,6-*N-*acetylneuraminyltransferase* [129924-24-9]

Glycosyltransferase enzyme. Present in foetal calf liver. R may be a protein or *p*-nitrophenol.

Bergh, M.L. *et al., J. Biol. Chem.*, 1983, **258**, 7430-7436

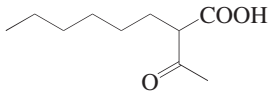
N-Acetylneuraminylgalactosylglucosylceramide β-1,4-*N*-acetylgalactosaminyltransferase A-140

E.C. 2.4.1.165 [109136-50-7]

Hexosyltransferase enzyme. Isol. from embryonic chicken brain. Requires $Mn^{2\oplus}$.

Chien, J.L. *et al., J. Biol. Chem.*, 1973, **248**, 1778-1785 (*embryonic chicken brain*)
Piller, F. *et al., Carbohydr. Res.*, 1986, **149**, 171-184 (*human kidney*)
Takeya, A. *et al., J. Biochem. (Tokyo)*, 1987, **101**, 251-259 (*human blood plasma*)

2-Acetyloctanoic acid A-141



$C_{10}H_{18}O_3$ 186.25

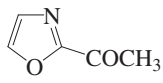
(±)-*form*

Et ester: [29214-60-6] *Ethyl 2-acetyloctanoate. Jasmin acetoacetate. FEMA 4459*
$C_{12}H_{22}O_3$ 214.304
Flavour and fragrance ingredient. Liq. with floral odour. Bp 253° Bp_{25} 148-149°.

Wallingford, V.H. *et al., JACS*, 1942, **64**, 580-582 (*Et ester*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*Et ester, use*)

2-Acetyloxazole A-142

1-(2-Oxazolyl)ethanone, 9CI [77311-07-0]

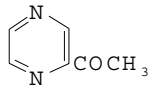


$C_5H_5NO_2$ 111.1
Constit. of roasted peanuts and cocoa beans. No synth. reported. Identification of the food product was by ms only with no indication of whether a reference sample was available.

Ho, C.-T. *et al., J. Food Sci.*, 1981, **47**, 127-133 (*occur, ms*)
Carlin, J.T. *et al., J. Am. Oil Chem. Soc.*, 1986, **63**, 1031-1036 (*occur*)

2-Acetylpyrazine A-143

Methyl pyrazinyl ketone. 1-Pyrazinylethanone. FEMA 3126 [22047-25-2]



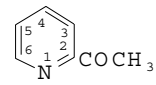
$C_6H_6N_2O$ 122.126
Flavouring ingredient. Present in bread, cooked meats, roasted cereals, roasted nuts, cocoa, popcorn, guava and black tea. Cream cryst. with popcorn-like flavour. Mp 75-77°. Bp 188°.

2-Thiazolylhydrazone: [73568-92-0]
$C_9H_9N_5S$ 219.27
Cryst. (EtOH). Sol. common org. solvs. Mp 210°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 844A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 407C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1562B (*ir*)
Kushner, S. *et al., JACS*, 1952, **74**, 3617-3621 (*synth, deriv*)
Schilt, A.A. *et al., Talanta*, 1980, **27**, 55-58 (*thiazolylhydrazone, use*)
Easmon, J. *et al., J. Med. Chem.*, 1992, **35**, 3288-3296 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 34
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 32 (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADA350

2-Acetylpyridine A-144

1-(2-Pyridinyl)ethanone, 9CI. Methyl 2-pyridyl ketone. 2-Acetopyridine. FEMA 3251 [1122-62-9]



C_7H_7NO 121.138
Organoleptic. Flavouring agent. Present in wheat bread, cooked beef, roast lamb, grape brandies, roast peanut, roast filbert, beer, cocoa, black tea, coriander seed and other foodstuffs. Liq. with roasted odour. Bp 192°. n_D^{20} 1.5203. pK_a 2.64 (25°). Turns yellow in air.

Hydrochloride: Mp 183-185° dec.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 779A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 310A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1542B (*ir*)
Miyajama, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Lesman, T. *et al., Org. Mass Spectrom.*, 1973, **7**, 1321 (*ms*)
Seth-Paul, W.A. *et al., Spectrochim. Acta A*, 1974, **30**, 1817 (*ir*)
Reimann, E. *et al., Annalen*, 1976, 1351 (*synth*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 35 (*occur*)
Girardot, M. *et al., JOC*, 1998, **63**, 10063-10068 (*synth*)

3-Acetylpyridine A-145

1-(3-Pyridinyl)ethanone, 9CI. Methyl 3-pyridyl ketone. 3-Acetopyridine. FEMA 3424 [350-03-8]

C_7H_7NO 121.138
Organoleptic, flavouring ingredient. Liq. Sol. H_2O. Bp 220° Bp_{12} 106°. pK_a 3.26 (25°). Yellows in air.

▶OB5425000

Hydrochloride: Mp 80° dec.

N-*Oxide:* [14188-94-4]
$C_7H_7NO_2$ 137.138
Mp 140-141°.

Oxime: [5973-83-1]
$C_7H_8N_2O$ 136.153
Mp 130.5°.

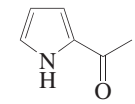
▶OB5600000

Phenylhydrazone: Mp 137°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 780C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 312B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1543A (*ir*)
Scott, F.L. *et al., JOC*, 1957, **22**, 1568 (*synth*)
Katritzky, A.R. *et al., JCS*, 1958, 3165 (*uv*)
Kavalewski, V.J. *et al., J. Chem. Phys.*, 1962, **36**, 266 (*pmr*)
Miyajama, G. *et al., Chem. Pharm. Bull.*, 1972, **20**, 429 (*cmr*)
Lesman, T. *et al., Org. Mass Spectrom.*, 1973, **7**, 1321 (*ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 35-36; *Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press*, 1995, **2**, 15
Balicki, R. *et al., Synth. Commun.*, 2000, **30**, 1529-1534 (*N-oxide*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABI000

2-Acetylpyrrole A-146

1-(1H-Pyrrol-2-yl)ethanone, 9CI. Methyl 2-pyrrolyl ketone. 2-Acetopyrrole. Pseudoacetylpyrrole. FEMA 3202 [1072-83-9]



C_6H_7NO 109.127
Organoleptic which contributes to many aromas, including roasted filbert. Present in cooked apple, asparagus, wheat bread, tea, roasted peanut, popcorn, potato chips, licorice, Chinese boxthorn and other foodstuffs. Cryst. (petrol) with bread-like odour. Sol. H_2O. Mp 90°. Bp 220°. λ_{max} 247; 287 (MeOH) (Berdy).

N-*Me:* [932-16-1] *2-Acetyl-1-methylpyrrole. FEMA 3184*
C_7H_9NO 123.154
Flavouring ingredient. Constit. of coffee aroma, asparagus, crispbread, cooked beef, black tea, okra and clam. Bp 200-202°. n_D^{20} 1.5420.

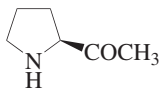
N-*Et:* [39741-41-8] *2-Acetyl-1-ethylpyrrole. FEMA 3147*
$C_8H_{11}NO$ 137.181
Flavouring ingredient. Constit. of coffee and green tea. Bp_{12} 82°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 567D; 568A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 5B; 5C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1447B; 1447C (*ir*)
Cionga, E. *et al., C. R. Hebd. Seances Acad. Sci.*, 1935, **200**, 780 (*isol*)
Sugisawa, H. *et al., Chem. Ind. (London)*, 1958, 887 (*synth*)
Budzikiewicz, H. *et al., JCS*, 1964, 1949 (*ms*)
Abraham, R.J. *et al., JCS Perkin 2*, 1974, 1004 (*cmr*)
Sannai, A. *et al., Agric. Biol. Chem.*, 1983, **47**, 2397 (*isol*)
Miyayawa, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2925; 1984, **48**, 2847 (*isol*)
Kakushima, M. *et al., JOC*, 1983, **48**, 3214 (*synth*)
Garrido, D.O.A. *et al., JOC*, 1984, **49**, 2619 (*synth*)
Anderson, H.J. *et al., Can. J. Chem.*, 1985, **63**, 896 (*synth*)
Eyley, S.C. *et al., Tet. Lett.*, 1985, **26**, 4649 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ADA 375

Pindur, H. *et al., J. Het. Chem.*, 1989, **26**, 1563 (*ir*)
Kuroda, Y. *et al., Tet. Lett.*, 1989, **30**, 2411 (*synth*)
Ito, M. *et al., Agric. Biol. Chem.*, 1991, **55**, 2117 (*isol, props*)
Goldberg, Yu. *et al., Synth. Commun.*, 1991, **21**, 557 (*N-alkyl derivs, synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 944; 1709; 1853-1854 (*occur, props, use*)
Camarillo, C.A. *et al., Acta Cryst. E*, 2007, **63**, o2593-o2594 (*cryst struct*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 564; 1209; 1382 (*use, N-Me, N-Et*)
Laurila, M.L. *et al., Org. Process Res. Dev.*, 2009, **13**, 1199-1201 (*N-Me*)

2-Acetylpyrrolidine A-147

1-(2-Pyrrolidinyl)ethanone, 9CI [60026-20-2]



(*S*)-*form*

$C_6H_{11}NO$ 113.159
Aroma constit. of wheat bread crust. Proposed precursor of the roasty-popcorn flavour material 5-Acetyl-3,4-dihydro-2*H*-pyrrole, A-64 formed in food processing. Undergoes ready air oxidn. to 5-Acetyl-3,4-dihydro-2*H*-pyrrole, A-64.

(*S*)-*form* [120966-82-7]
[90427-71-7] $[\alpha]_D^{25}$ -2.4 (c, 3 in 2*M* HCl).

N-tert-*Butyloxycarbonyl:*
$C_{11}H_{19}NO_3$ 213.276
Cryst. (pentane). Mp 38°. $[\alpha]_D^{25}$ -57.8 (c, 4.3 in $CHCl_3$).

N-*Benzyl:*
$C_{13}H_{17}NO$ 203.283
$Bp_{0.01}$ 85° (bulb). $[\alpha]_D^{25}$ -81.2 (c, 1.04 in EtOH).

(±)-*form*

N-*Me:* [54969-35-6] *2-Acetyl-1-methylpyrrolidine*
$C_7H_{13}NO$ 127.186
Bp_{14} 58-59°.

N-*Benzyl:* [901279-60-5]
Oil.

Duhamel, L. *et al., C. R. Seances Acad. Sci., Ser. C*, 1974, **279**, 1159-1161 (*N-Me*)
Fittkau, S. *et al., J. Prakt. Chem.*, 1986, **328**, 529-538 (*S-form, synth*)
Goldstein, S.W. *et al., JOC*, 1992, **57**, 1179-1190 (*S-form, Boc, N-benzyl*)
Hofmann, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619 (*synth, ms*)
Zhao, S. *et al., Tetrahedron*, 2006, **62**, 6361-6369 (*N-benzyl*)

Acetylsalicylate deacetylase A-148

E.C. 3.1.1.55. Acetylsalicylate O-*acetylhydrolase. Aspirin esterase. Aspirin hydrolase. Acetylsalicylic acid esterase* [87348-04-7]

Carboxylic ester hydrolase enzyme. Isol. from mammals, e.g. cow, sheep, goat. Acts on a number of acetyl esters of aryl alcohols as well as thioesters. The microsomal enzyme hydrolyses some other negatively-charged esters. Guinea pig enzyme activity range pH 5.5-9.0. Rat enzyme at -20°, pH 6.8, shows 7% loss of activity per month.

White, K.N. *et al., Biochim. Biophys. Acta*, 1984, **785**, 138-147 (*guinea pig*)
Kim, D.H. *et al., Biochem. Pharmacol.*, 1990, **40**, 481-487 (*rat*)
Benedito, M.A. *et al., J. Pharm. Pharmacol.*, 1997, **49**, 273-276 (*assay, mouse, rat*)
Singh, S. *et al., Int. J. Clin. Pharmacol. Ther.*, 2000, **38**, 315-319 (*human*)
Al-Qarawi, A.A. *et al., J. Vet. Med., Ser. A*, 2003, **50**, 201-203 (*ox, camel, sheep, goat*)

Acetylserotonin *O*-methyltransferase A-149

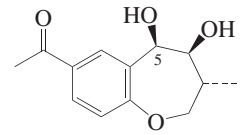
E.C. 2.1.1.4. S-*Adenosyl-L-methionine:*N-*acetylserotonin* O-*methyltransferase. Hydroxyindole methyltransferase. HIOMT* [9029-77-0]

Methyltransferase enzyme. Isol. from cow and chicken pineal glands. Other hydroxyindoles can act as acceptors, but more slowly.

Axelrod, J. *et al., J. Biol. Chem.*, 1961, **236**, 211-213 (*bovine pineal*)
Axelrod, J. *et al., Methods Enzymol., Part B*, 1971, **17**, 764-766 (*bovine pineal*)
Kuwano, R. *et al., J. Neurochem.*, 1978, **31**, 815-824 (*bovine pineal*)
Nakane, M. *et al., J. Neurochem.*, 1983, **40**, 790-796 (*bovine pineal, chicken pineal*)
Sugden, D. *et al., J. Pineal Res.*, 1986, **3**, 389-395 (*rat pineal*)

7-Acetyl-2,3,4,5-tetrahydro-4,5-dihydroxy-3-methyl-1-benzoxepin A-150

1-(2,3,4,5-Tetrahydro-4,5-dihydroxy-3-methyl-1-benzoxepin-7-yl)ethanone



$C_{13}H_{16}O_4$ 236.267

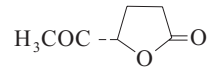
(3*R*,4*S*,5*R*)-*form*

5-O-*β-D-Glucopyranoside:* [296789-07-6]
$C_{19}H_{26}O_9$ 398.409
Constit. of the roots of *Helianthus annuus* (sunflower).

Nishikawa, K. *et al., Nat. Med. (Tokyo)*, 2000, **54**, 93-96 (*isol*)

5-Acetyltetrahydro-2(3*H*)-furanone, 9CI A-151

5-Oxo-4-hexanolide. ***Solerone*** [29393-32-6]



(*S*)–*form*

$C_6H_8O_3$ 128.127

(*S*)-*form* [61262-92-8]
$Bp_{0.2}$ 83°. $[\alpha]_D^{25}$ +13.4 (c, 0.25 in MeOH).

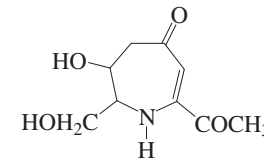
(±)-*form* [69308-41-4]
$Bp_{1.2}$ 102-104°.

(ξ)-*form*
Aroma constit. of wine esp. sherry. Formed during fermentation. Isol. from dried figs.

Augustyn, D.P.H. *et al., J. Agric. Food Chem.*, 1971, **19**, 1128 (*synth, struct*)
Yanrad, S.-I. *et al., Tet. Lett.*, 1976, 2557 (*synth*)
Jensen, J.E. *et al., Acta Chem. Scand., Ser. B*, 1978, **32**, 457 (*synth, ir, pmr*)
Näf, R. *et al., Flavour Fragrance J.*, 1995, **10**, 243-247 (*figs, isol*)
Häring, D. *et al., J. Agric. Food Chem.*, 1997, **45**, 369-372 (*sherry, isol, synth*)

2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4*H*-azepine-4-one A-152

[220662-49-7, 220662-48-6]

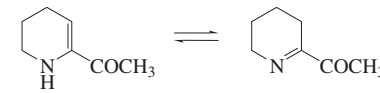


$C_9H_{13}NO_4$ 199.206
Minor product from the Maillard reaction of xylose and glycine. Yellow solid. Isol. as *cis*/*trans*- mixt.

Ames, J.M. *et al., J. Agric. Food Chem.*, 1999, **47**, 438-443 (*formn, pmr, cmr, ms*)

6-Acetyl-1,2,3,4-tetrahydropyridine A-153

Methyl 3,4,5,6-tetrahydro-2-pyridyl ketone, 8CI. 2-Acetyl-3,4,5,6-tetrahydropyridine. 2-Acetyl-Δ¹-piperideine. 2-Acetyl-Δ²-piperideine. 1-(1,4,5,6-Tetrahydro-2-pyridinyl)ethanone, 9CI [27300-27-2]



1*H*-*form* 3*H*-*form*

$C_7H_{11}NO$ 125.17
Tautomeric, 1*H*-form predominates *ca.* 2:1. Responsible for mousy taint in wines. Constit. of wheat, popcorn and bread aroma. Unstable liq. Bp_3 65-67°. Odour threshold 0.06 ng/L in air.

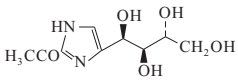
Hydrochloride: Mp 112-119°.

Hunter, I.R. *et al., Cereal Chem.*, 1969, **46**, 189 (*isol*)
Büchi, G. *et al., JOC*, 1971, **36**, 609 (*ir, uv, pmr, ms, synth*)
Strauss, C.R. *et al., Chem. Ind. (London)*, 1984, 109 (*isol*)
De Kimpe, N. *et al., JOC*, 1993, **58**, 2904 (*synth, pmr, cmr, ms*)
De Kimpe, N. *et al., Tetrahedron*, 1995, **51**, 2387 (*synth*)
Hofman, T. *et al., J. Agric. Food Chem.*, 1998, **46**, 616-619; 2270-2277 (*synth, ms, bibl*)
Naef, R. *et al., J. Agric. Food Chem.*, 2005, **53**, 9161-9164 (*isol, pmr, ms*)
Harrison, T.J. *et al., JOC*, 2005, **70**, 10872-10874 (*synth*)
Adams, A. *et al., Chem. Rev.*, 2006, **106**, 2299-2319 (*rev*)

Snowdon, E.M. *et al., J. Agric. Food Chem.*, 2006, **54**, 6465-6474 (*rev*)
Fuganti, C. *et al., Tetrahedron*, 2007, **63**, 4762-4767 (*synth*)

2-Acetyl-4(5)-(1,2,3,4-tetrahydroxybutyl)imidazole A-154

1-[4-(1,2,3,4-Tetrahydroxybutyl)-1H-imidazol-2-yl]ethanone, 9CI [95120-07-3]



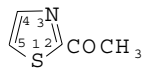
(1*R*,2*S*,3*R*)-*form*

$C_9H_{14}N_2O_5$ 230.22

(1*R*,2*S*,3*R*)-*form* [94944-70-4]
Minor component of Caramel Colour III. Cryst. (H_2O). Mp 232-233°. $[\alpha]_D^{25}$ -12 (c, 1.17 in 1M HCl).
Kröplien, U. *et al., JOC*, 1985, **50**, 1131 (*isol, struct*)
Halweg, K.M. *et al., JOC*, 1985, **50**, 1133 (*synth, uv, pmr, cmr, ir*)
Sweeny, J.G. *et al., JOC*, 1985, **50**, 1133 (*synth, pmr, uv, ir, cmr, abs config*)

2-Acetylthiazole A-155

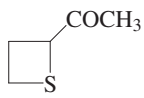
1-(2-Thiazolyl)ethanone, 9CI. Methyl 2-thiazolyl ketone, 8CI. FEMA 3328 [24295-03-2]



C_5H_5NOS 127.167
Important flavour component; antioxidant. Present in asparagus, kohlrabi, cooked potatoes, roast turkey, raw chicken, cooked beef, pork liver, beer, whisky, heated beans, various mushrooms, rice bran and maize. Mp 64.5-65.5°. Bp_{15} 98-102°.
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1494D (*ir*)
Hartman, G.J. *et al., J. Agric. Food Chem.*, 1983, **31**, 1030 (*isol*)
Medici, A. *et al., Tet. Lett.*, 1983, **24**, 2901 (*synth*)
Dondoni, A. *et al., JOC*, 1991, **56**, 5294 (*synth, ir, pmr, cmr*)
Thiel, V. *et al., Org. Biomol. Chem.*, 2010, 234-246 (*Oceanibulbus indolifex constit*)

2-Acetylthietane A-156

1-(2-Thietanyl)ethanone, 9CI [119209-96-0]



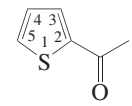
C_5H_8OS 116.184

(±)-*form*
Bp_7 49°.

(ξ)-*form*
Thiamine thermal degradation product formed in meat aroma model systems.
Yonemoto, H. *et al., Yakugaku Zasshi*, 1957, **77**, 1128-1132 (*synth*)
Guentert, M. *et al., J. Agric. Food Chem.*, 1990, **38**, 2027-2041 (*occur, pmr, ms*)

2-Acetylthiophene A-157

1-(2-Thienyl)ethanone, 9CI. Methyl 2-thienyl ketone. 2-Acetothienone [88-15-3]



C_6H_6OS 126.179
Organoleptic which contributes to several aromas. Liq. d^{24} 1.17. Mp 9°. Bp 213-214° Bp_{13} 94.5-96.5°. n_D^{20} 1.5668.
▶ LD_{50} (mus, ipr) 40 mg/kg. OB6300000
Oxime (E-): [92313-54-7]
C_6H_7NOS 141.193
Cryst. (EtOAc/hexane). Mp 113-114°.
Oxime (Z-): [92313-45-6]
C_6H_7NOS 141.193
Cryst. (EtOAc/hexane). Mp 84-85°.
Phenylhydrazone: [55968-17-7]
Yellow cryst. (EtOH). Mp 96°.
Semicarbazone: [3771-70-8]
Plates (C_6H_6). Mp 190-191°.
Di-Et acetal: 2-(1,1-Diethoxyethyl)thiophene
$C_{10}H_{16}O_2S$ 200.301
Bp_{10} 85-89°.
[39709-34-7]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 596C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 53A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1472C (*ir*)
Hartough, H.D. *et al., JACS*, 1947, **69**, 1012 (*synth*)
Goldfarb, Ya.L. *et al., Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1960, 2071 (*di-Et acetal*)
Bohlmann, F. *et al., Chem. Ber.*, 1964, **97**, 2135; 1967, **100**, 107 (*isol, ir, uv, pmr, synth*)
Nishiwaki, T. *et al., Tetrahedron*, 1967, **23**, 2979 (*ms*)
Fringuelli, F. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 175-184 (*pmr*)
Zeisberg, R. *et al., Chem. Ber.*, 1975, **108**, 1040 (*cmr, struct*)
Galli, C. *et al., Synthesis*, 1979, 303-304 (*synth*)
Conde, S. *et al., J. Het. Chem.*, 1985, **22**, 301 (*oximes, config, pmr*)
Keumi, T. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 455 (*synth*)
Goda, H. *et al., Synthesis*, 1992, 849 (*synth*)
Spinelli, D. *et al., Acta Chem. Scand.*, 1993, **47**, 160 (*cmr, O-17 nmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ABI500

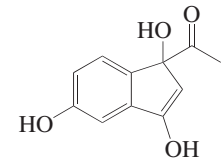
3-Acetylthiophene A-158

1-(3-Thienyl)ethanone, 9CI. Methyl 3-thienyl ketone. 3-Acetothienone [1468-83-3]

C_6H_6OS 126.179
Maillard product; organoleptic. Mp 61-62°. Bp_5 78-79°.
Phenylhydrazone: Mp 114°.
Semicarbazone: Mp 173-174°.
[39709-34-7]
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 597B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 54B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1473C (*ir*)
Macdowell, D.W.H. *et al., J. Het. Chem.*, 1965, **2**, 44 (*synth*)
Stoffelsma, J. *et al., J. Agric. Food Chem.*, 1968, **16**, 1000-1004 (*ir, ms*)
Gronowitz, S. *et al., Chem. Scr.*, 1975, **7**, 76 (*cmr*)
Clarke, J.A. *et al., Tet. Lett.*, 1975, 4705 (*synth*)
Macco, A.A. *et al., JOC*, 1978, **43**, 1591 (*synth, pmr*)
Collins, S. *et al., JOC*, 1990, **55**, 3565 (*synth*)

1-Acetyl-1,3,5-trihydroxy-1*H*-indene A-159

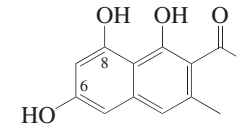
1-Acetyl-1H-indene-1,3,5-triol, 9CI



$C_{11}H_{10}O_4$ 206.198
3,5-Di-Me ether: [151466-74-9] *1-Acetyl-1-hydroxy-3,5-dimethoxy-1H-indene.* ***Coixinden B***
$C_{13}H_{14}O_4$ 234.251
Constit. of *Coix lacrima-jobi* var. *mayuen*.
Ishiguro, Y. *et al., Chem. Lett.*, 1993, 1139 (*isol, activity*)

2-Acetyl-1,6,8-trihydroxy-3-methylnaphthalene A-160

1-(1,6,8-Trihydroxy-3-methyl-2-naphthalenyl)ethanone, 9CI. 1′,6′,8′-Trihydroxy-3′-methyl-2′-acetonaphthone, 8CI. 7-Acetyl-6-methyl-1,3,8-naphthalenetriol. ***6-Hydroxymusizin*** [23520-25-4]



$C_{13}H_{12}O_4$ 232.235
Yellow powder. Mp 198.4-204° dec. λ_{max} 233 (log ϵ 4.46); 271 (log ϵ 4.5); 389 (log ϵ 4.03) (EtOH).
8-O-β-D-Glucopyranoside: [23566-96-3]
$C_{19}H_{22}O_9$ 394.377
Isol. from the rhubarb Rhei rhizoma. Needles (EtOAc). Mp 214-215° (207°).
6-Me ether: [22649-04-3] *2-Acetyl-1,8-dihydroxy-6-methoxy-3-methylnaphthalene.* ***Torachrysone.*** *Nakahalene*
$C_{14}H_{14}O_4$ 246.262
Isol. from seeds of *Cassia tora* (charota). Yellow needles (C_6H_6). Mp 214-215° dec. (207-208°).
6-Me ether, 8-O-β-D-glucopyranoside: [64032-49-1] ***Torachrysone 8-glucoside***
$C_{20}H_{24}O_9$ 408.404
Isol. from Rhei rhizoma, rhubarb. Needles + $1H_2O$ (MeOH). Mp 150-152°. $[\alpha]_D^{21}$ -109 (c, 0.5 in MeOH).

*6-Me ether, 8-*O*-(6-*O*-oxalyl-β-D-glucopyranoside):* [64078-76-8] ***Torachrysone 8-(6-oxalylglucoside)***
$C_{22}H_{24}O_{12}$ 480.424
Constit. of a Rhei sp., rhubarb. Pale yellow powder. $[\alpha]_D^{18}$ -102 (c, 0.25 in H_2O).

*6-Me ether, 8-*O*-[β-D-xylopyranosyl-(1→6)-β-D- glucopyranoside]:* [150566-02-2]
$C_{25}H_{32}O_{13}$ 540.52
Orange needles ($CHCl_3$/MeOH). Mp 252-253°.

*6-Me ether, 8-*O*-[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [245724-11-2] ***Torachrysone 8-(2-apiosylglucoside)***
$C_{25}H_{32}O_{13}$ 540.52
Constit. of the seeds of *Cassia tora* (charota). Pale yellow powder. $[\alpha]_D$ -23.4 (c, 0.1 in Py). λ_{max} 233 (log ε 4.41); 262 (log ε 4.09); 306 (log ε 3.58); 323 (log ε 3.59); 337 (log ε 3.64) (MeOH).

*6-Me ether, 8-*O*-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [245724-09-8] ***Torachrysone 8-β-gentiobioside***
$C_{26}H_{34}O_{14}$ 570.546
Constit. of the seeds of *Cassia tora* (charota). Needles (MeOH). Mp 221°. $[\alpha]_D$ -18.7 (c, 0.1 in MeOH). λ_{max} 236 (log ε 4.38); 263 (log ε 4.19); 310 (log ε 3.59); 324 (log ε 3.59); 339 (log ε 3.59) (MeOH).

*6-Me ether, 8-*O*-[β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [1002727-58-3]
$C_{32}H_{44}O_{19}$ 732.688
Constit. of the seeds of *Cassia tora* (charota). Yellow needles (MeOH). Mp 249-251°. $[\alpha]_D^{25}$ -38.5 (c, 0.32 in MeOH). λ_{max} 240 (log ε 4.95); 265 (log ε 4.61); 310 (log ε 4.12); 324 (log ε 4.11); 340 (log ε 4.12) (MeOH).

*6-Me ether, 8-*O*-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→3)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [245724-10-1]
$C_{38}H_{54}O_{24}$ 894.83
Constit. of the seeds of *Cassia tora* (charota). Pale yellow powder. $[\alpha]_D$ -9 (c, 0.1 in Py). λ_{max} 236 (log ε 4.48); 262 (log ε 4.24); 312 (log ε 3.64); 325 (log ε 3.65); 340 (log ε 3.65) (MeOH).

6-Me ether, di-Ac: [22649-05-4]
Plates (EtOH). Mp 181-182°.

8-Me ether: [173867-28-2] *2-Acetyl-1,6-dihydroxy-8-methoxy-3-methylnaphthalene. Tinnevellin.* ***Isotorachrysone***
$C_{14}H_{14}O_4$ 246.262
Yellow needles ($CHCl_3$/MeOH). Mp 219°.

*8-Me ether, 6-*O*-α-D-ribofuranoside:* [1084953-65-0] *Isotorachrysone 6-α-D-ribofuranoside*
$C_{19}H_{22}O_8$ 378.378
Yellow needles (MeOH). Mp 174-176°. $[\alpha]_D^{20}$ +178.6 (c, 0.11 in MeOH). λ_{max} 245 (log ε 3.41); 308 (log ε 3.33); 337 (log ε 3.29) (MeOH).

*8-Me ether, 6-*O*-β-D-glucopyranoside:* [80358-06-1]
$C_{20}H_{24}O_9$ 408.404
Pale yellow powder. Mp 175°.

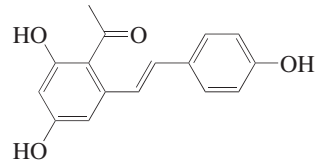
6,8-Di-Me ether: [22699-07-6] *2-Acetyl-1-hydroxy-6,8-dimethoxy-3-methylnaphthalene. 1-(1-Hydroxy-6,8-dimethoxy-3-methyl-2-naphthaleny-l)ethanone, 9CI. 2-Acetyl-6,8-dimethoxy-3-methyl-1-naphthol*
$C_{15}H_{16}O_4$ 260.289
Needles. Mp 98-99°.

Tri-Me ether: [22649-03-2]
Tiny plates (MeOH aq.). Mp 63-64°.

Shibata, S. *et al., Chem. Pharm. Bull.*, 1969, **17**, 454-475 (*Torachrysone, isol*)
Brown, K.S. *et al., Tet. Lett.*, 1969, 471-476 (*8-glucoside, isol*)
Harris, T.M. *et al., JACS*, 1975, **97**, 3270-3271 (*synth*)
Dreyer, D.L. *et al., JACS*, 1975, **97**, 4985-4990 (*3,8-di-Me ether, isol*)
Tsuboi, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 2708-2712 (*6-Me 8-glucosides*)
Yamasaki, K. *et al., Tet. Lett.*, 1977, 1231-1234 (*cmr, glucosides*)
Lemli, J. *et al., Planta Med.*, 1981, **43**, 11-17 (*Tinnevellin glucoside*)
Gill, M. *et al., Prog. Chem. Org. Nat. Prod.*, 1987, **51**, 121-122 (*3,8-di-Me ether, occur*)
Wei, B.-L. *et al., J. Nat. Prod.*, 1992, **55**, 967-969 (*Nakahalene*)
Lin, C.N. *et al., Phytochemistry*, 1993, **33**, 905-908 (*6-Me ether, 8-xylosylglucoside*)
Lin, C.-N. *et al., J. Nat. Prod.*, 1995, **58**, 1934-1940 (*Isotorachrysone*)
Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*Torachrysone glycosides, activity*)
Horikawa, M. *et al., Tetrahedron*, 2004, **60**, 1229-1234 (*6-Hydroxymusizin*)
El-Halawany, A.M. *et al., Chem. Pharm. Bull.*, 2007, **55**, 1476-1482 (*Torachrysone triglucoside*)
Du, L. *et al., J. Nat. Prod.*, 2008, **71**, 1837-1842 (*Isotorachrysone 6-riboside*)

2-Acetyl-3,4′,5-trihydroxystilbene A-161

1-(2-Acetyl-3,5-dihydroxyphenyl)-2-(4-hydroxyphenyl)ethylene. ***2-Acetylresveratrol***



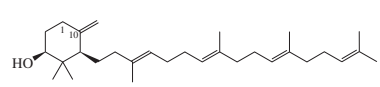
$C_{16}H_{14}O_4$ 270.284

(E)-form [1184663-64-6]
Isol. from the stilbene synthase of *Pinus sylvestris* (Scots pine).

Li, T.-L. *et al., ChemBioChem*, 2009, **10**, 896-901 (*isol, pmr, cmr*)

Achilleol A A-162

[125287-06-1]



$C_{30}H_{50}O$ 426.724
$[\alpha]_D$ -10.9 (c, 0.9 in $CHCl_3$).

Dodecanoyl: [213007-57-9]
$C_{42}H_{72}O_2$ 609.03

Tetradecanoyl: [213007-39-7]
$C_{44}H_{76}O_2$ 637.083

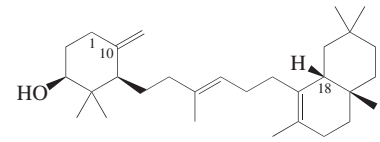
Hexadecanoyl: [213007-45-5]
$C_{46}H_{80}O_2$ 665.137

$\Delta^{1(10)}$-Isomer: [220359-76-2] ***Camelliol C***
$C_{30}H_{50}O$ 426.724
Constit. of sasanqua oil (*Camellia sasanqua*). Gum. $[\alpha]_D^{25}$ -12.9 (c, 0.2 in $CHCl_3$).

Barrero, A.F. *et al., Tet. Lett.*, 1989, **30**, 3351-3352 (*Achilleol A*)
Barrero, A.F. *et al., Phytochemistry*, 1998, **48**, 1237-1240 (*esters*)
Akihisa, T. *et al., J. Nat. Prod.*, 1999, **62**, 265-268 (*Camelliol C*)
Joubert, B.M. *et al., Org. Lett.*, 2000, **2**, 339-341 (*biosynth*)
Kolesnikova, M.D. *et al., Org. Lett.*, 2007, **9**, 5223-5226 (*biosynth*)

Achilleol B A-163

[132922-73-7]



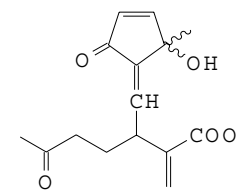
$C_{30}H_{50}O$ 426.724
C-18 Stereochem. revised in 2008. Viscous oil. $[\alpha]_D$ -8.1 (c, 1 in $CHCl_3$).

$\Delta^{1(10)}$-Isomer: [220359-69-3] ***Camelliol A***
$C_{30}H_{50}O$ 426.724
Constit. of Sasanqua oil (*Camellia sasanqua*). Gum. $[\alpha]_D^{25}$ +4 (c, 0.2 in $CHCl_3$).

Barrero, A.F. *et al., Tetrahedron*, 1990, **46**, 8161-8168 (*isol, ir, pmr, cmr, ms*)
Akihisa, T. *et al., J. Nat. Prod.*, 1999, **62**, 265-268 (*Camelliol A*)
Arteaga, J.F. *et al., Org. Lett.*, 2008, **10**, 1723-1726 (*synth, config*)
Smith, S.G. *et al., JACS*, 2010, **132**, 12946-12959 (*pmr, cmr, struct*)
Ito, R. *et al., Org. Lett.*, 2011, **13**, 2678-2681 (*biosynth*)

Achimilic acid A-164

3-[(2-Hydroxy-2-methyl-5-oxo-3-cyclopenten-1-ylidene)methyl]-2-methylene-6-oxoheptanoic acid, 9CI [110732-04-2]



$C_{15}H_{18}O_5$ 278.304
Isol. from *Achillea millefolium* (yarrow). Obt. as mixture of diastereoisomers.

Me ester:
$C_{16}H_{20}O_5$ 292.331
Cryst. (Et_2O/pentane). Mp 76-77°. $[\alpha]_D$ -23.6 ($CHCl_3$).

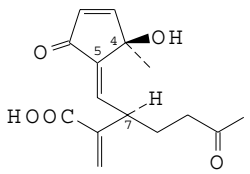
Me ester, stereoisomer (1): Achimilic acid B methyl ester
$C_{16}H_{20}O_5$ 292.331
Oil. $[\alpha]_D$ -78.2 ($CHCl_3$).

Me ester, stereoisomer (2): Achimilic acid C methyl ester
$C_{16}H_{20}O_5$ 292.331
Oil. $[\alpha]_D$ -87.3 ($CHCl_3$).

Japan. Pat., 1987, 87 81 349 (*isol, cmr, ir, uv, ms*)

Achimillic acid A A-165

[157184-04-8]



$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Needles (as Me ester). Mp 76-77° (Me ester). $[\alpha]_D$ -23.6 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (EtOH) (Derep).

5Z-Isomer: [157184-05-9] ***Achimillic acid B***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Oil (as Me ester). $[\alpha]_D$ -78.2 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (EtOH) (Derep).

4-Epimer: [157184-06-0] ***Achimillic acid C***
$C_{15}H_{18}O_5$ 278.304
Constit. of *Achillea millefolium* (yarrow). Oil (as Me ester). $[\alpha]_D$ -87.3 (c, 1 in $CHCl_3$) (Me ester). λ_{max} 245 (EtOH) (Derep).

Tozyo, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1096 (*isol, pmr, cmr, cryst struct*)

Acid phosphatase A-166

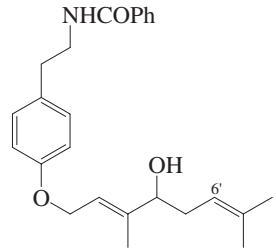
E.C. 3.1.3.2. Phosphate-monoester phosphohydrolase (acid optimum). Acid phosphomonoesterase. Phosphomonoesterase†. *Glycerophosphatase*† [9001-77-8]

Phosphoric monoester hydrolase enzyme. Isol. from mammals, e.g. cow, pig, rabbit; from plants, e.g. soybean, kidney bean, wheatgerm, black mustard; and from baker's yeast. Wide specificity. Catalyses transphosphorylations. Human enzyme activity range pH 4.0-7.0. At -25°, pH 6.0, stable for years.

Joyce, B.K. *et al., J. Biol. Chem.*, 1960, **235**, 2278-2281 (*wheatgerm*)
Hollander, V.P. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1971, **4**, 449-498 (*mammals, yeast, bacteria, tobacco*)
Ullah, A.H.J. *et al., Arch. Biochem. Biophys.*, 1988, **260**, 514-520 (*soybean*)
Himeno, M. *et al., J. Biochem. (Tokyo)*, 1989, **105**, 449-456 (*rat*)
Duff, S.M.G. *et al., Arch. Biochem. Biophys.*, 1991, **286**, 226-232 (*black mustard*)
Naseri, J.I. *et al., Arch. Biochem. Biophys.*, 2004, **432**, 25-36 (*pig*)
Tanaka, M. *et al., FEBS Lett.*, 2004, **571**, 197-204 (*human*)
Tejera Garcia, N.A. *et al., Plant Physiol. Biochem. (Paris)*, 2004, **42**, 585-591 (*kidney bean*)

Acidissiminol A-167

[126006-00-6]



$C_{25}H_{31}NO_3$ 393.525
Alkaloid from the fruit of *Limonia acidissima* (wood apple). Cryst. (EtOAc/hexane). Mp 85-87°.

O-*Ac:* [33055-26-4] **N-*Benzoyl-4-(4-acetoxyneryloxy)phenethylamine***
$C_{27}H_{33}NO_4$ 435.562
Cryst. (EtOAc/hexane). V. sol. MeOH. Mp 64-65°. Opt. inactive.

O-*Octadecanoyl:* [126005-91-2] ***Acidissiminin***
$C_{43}H_{65}NO_4$ 659.991
Alkaloid from the fruits of *Limonia acidissima* (wood apple). Amorph. solid (EtOAc/hexane). Mp 65°. $[\alpha]_D$ 0 ($CHCl_3$). λ_{max} 225; 277 (sh); 286 (MeOH) (Derep).

6′,7′-Epoxide: [139165-01-8] ***Acidissiminol epoxide***. *Severine*†
[33055-25-3]
$C_{25}H_{31}NO_4$ 409.524
Alkaloid from fruits of *Limonia acidissima* (wood apple). Cryst. (MeOH). Mp 146-149° (141-143°). Severine originally considered to be a diol with formula $C_{25}H_{33}NO_4$. Identity of Acidissiminol epoxide and Severine not confirmed; stereochem. not established.

6′,7′-Epoxide, O-*octadecanoyl:* [139083-09-3] ***Acidissiminin epoxide***. *Severine palmitate*
$C_{43}H_{65}NO_5$ 675.99
Alkaloid from the fruit of *Limonia acidissima* (wood apple). Cryst. (C_6H_6/hexane). Mp 105-106° Mp 113-114°. Identity of Acidissiminin epoxide and Severin palmitate not definitely establ. Mps are similar.

*6′*R,*7′-Epoxide,* O-*(9*E*-octadecenoyl):* [1203465-68-2] ***9″,10″-Didehydroacidissiminin epoxide***
$C_{43}H_{63}NO_5$ 673.974
Alkaloid from the bark of *Limonia acidissima* (wood apple). Gum. $[\alpha]_D^{25}$ +39.3 (c, 0.15 in MeOH). λ_{max} 225 (log ϵ 4.25); 283 (log ϵ 1.42); 298 (log ϵ 1.4) (MeOH).

6′,7′-Dihydro, 6′,7′-dihydroxy: [160387-10-0] ***Dihydroxyacidissiminol***
$C_{25}H_{33}NO_5$ 427.539
Alkaloid from fruits of *Limonia acidissima* (wood apple). Amorph. semisolid.

*6′,7′-Dihydro, 6′*R,*7′-dihydroxy, 4′-*O-*octadecanoyl:* [1203465-66-0] ***Dihydroxyacidissiminin***
$C_{43}H_{67}NO_6$ 694.005
Alkaloid from the bark of *Limonia acidissima* (wood apple). Gum. $[\alpha]_D^{25}$ +72.5 (c, 0.2 in MeOH). Possesses 4′*R*-config. λ_{max} 225 (log ϵ 4.27); 283 (log ϵ 1.42); 298 (log ϵ 1.38) (MeOH).

*6′,7′-Dihydro, 6′*R,*7′-dihydroxy, 4′-*O-*(9*E*-octadecenoyl):* [1203465-67-1] ***9″,10″-Didehydrodihydroxyacidissiminin***
$C_{43}H_{65}NO_6$ 691.99
Alkaloid from the bark of *Limonia acidissima* (wood apple). Gum. $[\alpha]_D^{25}$ +97 (c, 0.22 in MeOH). Possesses 4′*R*-config. λ_{max} 225 (log ϵ 4.23); 282 (log ϵ 1.44); 298 (log ϵ 1.38) (MeOH).

Dreyer, D.L. *et al., Tetrahedron*, 1967, **23**, 4613-4622; 1970, **26**, 5745-5751; 1980, **36**, 827-829 (*Severine, Severine palmitate, N-Benzoyl-4-(4-acetoxyneryloxy)phenethylamine*)
Ghosh, P. *et al., J. Nat. Prod.*, 1989, **52**, 1323-1326; 1991, **54**, 1389-1393 (*Acidissiminol, Acidissiminin*)
Ghosh, P. *et al., Phytochemistry*, 1994, **37**, 757-760 (*Dihydroxyacidissiminol, Acidissiminol epoxide*)
Kim, K.H. *et al., Planta Med.*, 2009, **75**, 1146-1151 (*Dihydroxyacidissiminin, Didehydroacidissiminins*)

Acidocin A-168

Peptide bacteriocins. Bacteriocins with possible food uses.

Acidocin A [165170-19-4]
Prod. by *Lactobacillus acidophilus* TK 9201.

Acidocin B [155462-64-9]
Prod. by *Lactobacillus acidophilus* M46. Comprises 59 amino acid residues.

Acidocin CH5 [175644-54-9]
Prod. by *Lactobacillus acidophilus* CH5.

Acidocin J1132 [174394-56-0]
Prod. by *Lactobacillus acidophilus* JCM 1132. Comprises 2 components, α and β; β has an additional Gly residue.

Acidocin J1229 [185915-27-9]
Prod. by *Lactobacillus acidophilus* JCM 1229.

Acidocin 8912 [142106-05-6]
Prod. by *Lactobacillus acidophilus* TK 8912.

Tahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1992, **56**, 1212-1215 (*Acidocin 8912*)
Ten Brink, B. *et al., J. Appl. Bacteriol.*, 1994, **77**, 140-148 (*Acidocin B*)
Kanatani, K. *et al., Appl. Environ. Microbiol.*, 1995, **61**, 1061-1067 (*Acidocin A*)
Chumchalova, J. *et al., Chem. Mikrobiol. Technol. Lebensm.*, 1995, **17**, 145-150 (*Acidocin CH5*)
Leer, R.J. *et al., Microbiology (Reading, U.K.)*, 1995, **141**, 1629-1635 (*Acidocin B, struct*)
Tahara, T. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 892-897 (*Acidocin J1132*)
Tahara, T. *et al., J. Appl. Bacteriol.*, 1996, **81**, 669-677 (*Acidocin J1229*)
Tahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 884-886 (*Acidocins J1229,J1132, partial struct*)

Acidocin CH5 A-169

Peptide. Prod. by *Lactobacillus acidophilus* CH5 isol. from a dairy starter culture.

Chumchalova, J. *et al., J. Appl. Microbiol.*, 2004, **96**, 1082-1089 (*Acidocin CH5*)

Acidocin D20079 A-170

Peptide. Prod. by *Lactobacillus acidophilus* DSM 20079.

Deraz, S.F. *et al., J. Biotechnol.*, 2005, **117**, 343-354 (*Acidocin D20079*)

Acidophilin 801 A-171

[265656-95-9]

Proteinaceous, MW <6.5 kDa. Prod. by *Lactobacillus acidophilus* IBB 801.

Zamfir, M. *et al., J. Appl. Microbiol.*, 1999, **87**, 923-931 (*isol*)

Acidophilucin A A-172

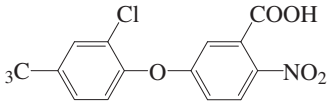
[137699-22-0]

Prod. by *Lactobacillus acidophilus* LAPT 1060. Bacteriocin.

Toba, T. *et al., Lett. Appl. Microbiol.*, 1991, **12**, 106-108 (*isol*)

Acifluorfen, ANSI, BSI, ISO, WSSA A-173

5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid, 9CI. Tackle 25 [50594-66-6]



$C_{14}H_7ClF_3NO_5$ 361.661

Selective pre- and post-emergence herbicide. Used on soybeans and peanuts. Off-white solid. Mp 151.5-157° (140-150°) Mp 240°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 2025 mg/kg. DG5643070

Na salt: [62476-59-9] *Acifluorfen sodium. Blazer. Scifluorfen. RH 6201*
Powder. Mp 124-125°.

▶ DG5643200

Me ester: [50594-67-7] *Acifluorfen methyl*
$C_{15}H_9ClF_3NO_5$ 375.688

Carboxymethyl ester: [77501-60-1] ***Fluoroglycofen, ANSI, BSI***. O-*[5-(2-Chloro-α,α,α-trifluoro*-p-*tolyloxy)-2-nitrobenzoyl]glycolic acid*

2-Ethoxy-2-oxoethyl ester: [77501-90-7] ***Fluoroglycofen-ethyl***
$C_{18}H_{13}ClF_3NO_7$ 447.751
Dark amber solid. d^{25} 1.01. Mp 65°.

▶ LD_{50} (rat, orl) 1500 mg/kg. DG5643100

Nitrile: [50594-65-5]
Cryst. Mp 95-103°.

Ger. Pat., 1973, 2 311 638 (*synth*)
Johnson, W.O. *et al., J. Agric. Food Chem.*, 1978, **26**, 285 (*synth, props*)
Eur. Pat., 1980, 20 052 (*synth, activity, Fluoroglycofen*)
Orr, G.L. *et al., ACS Symp. Ser.*, 1982, **181**, 131 (*rev*)
Lee, G.H. *et al., J. Agric. Food Chem.*, 1985, **33**, 499 (*pmr, cmr*)
Kennard, C.H.L. *et al., Aust. J. Chem.*, 1987, **40**, 1131 (*cryst struct*)
Teasdale, J.R. *et al., Weed Technol.*, 1987, **1**, 165 (*activity, Fluoroglycofen*)
Maigrot, P.H. *et al., Proc. Br. Crop Prot. Conf. Weeds*, 1989, 47 (*activity, Fluoroglycofen-Et*)
Pesticide Manual, 9th edn., 1991, No. 40; No. 6565
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A788

Acireductone synthase A-174

E.C. 3.1.3.77. 5-(Methylthio)-2,3-dioxopentyl-phosphate phosphohydrolase (isomerising). E-1 enolase phosphatase
Phosphoric monoester hydrolase enzyme. Involved in methionine metab. *Klebsiella oxytoca* Enzyme can be stored at -80° in 50% glycerol.

Myers, R.W. *et al., J. Biol. Chem.*, 1993, **268**, 24785-24791 (*Klebsiella pneumoniae*)
Balakrishnan, R. *et al., J. Biol. Chem.*, 1993, **268**, 24792-24795 (*Klebsiella*)
Wray, J.W. *et al., J. Biol. Chem.*, 1995, **270**, 3147-3153 (*Klebsiella pneumoniae*)

Aconitate methyltransferases A-175

Methyltransferase enzymes.

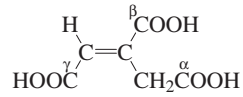
***trans*-Aconitate 2-methyltransferase**
E.C. 2.1.1.144. S-*Adenosyl-L-methionine:(E)-1-propene-1,2,3-tricarboxylate 2′-O-methyltransferase*
[235107-12-7]

***trans*-Aconitate 3-methyltransferase**
E.C. 2.1.1.145. S-*Adenosyl-L-methionine:(E)-1-propene-1,2,3-tricarboxylate 3′-O-methyltransferase*
[235107-12-7]
Isol. from *Saccharomyces cerevisiae* (baker's yeast).

Cai, H. *et al., J. Biol. Chem.*, 1999, **274**, 13470-13479 (*E.C. 2.1.1.144, isol*)
Cai, H. *et al., Biochemistry*, 2001, **40**, 2210-2219 (*isol*)

Aconitic acid A-176

1-Propene-1,2,3-tricarboxylic acid, 9CI. Achilleaic acid. Citridinic acid. Equisetic acid. Pyrocitric acid. 3-Carboxy-2-pentenedioic acid. FEMA 2010 [499-12-7]



(*E*)-*form*

$C_6H_6O_6$ 174.11

▶ UD2380000

Mixed Et esters: Ethyl aconitate. FEMA 2417
$C_8H_{10}O_6$ 202.163
Flavouring ingredient. Prepd. as mixt. of mono-, di- and triesters by acid-catalysed esterification of aconitic acid with EtOH or by heating #HJD17-G. Oily liq. with sweet, fruity odour and flavour. Mp 260°.

(*E*)-*form* [4023-65-8]
Isol. from *Asarum europaeum*, from cane-sugar molasses, roasted chicory root, roasted malt barley, passion fruit, sorghum root and sugar beet. Flavouring agent used in fruit flavours and alcoholic beverages. Leaflets (H_2O). Sol. H_2O, EtOH. Mp 194-195° dec. pK_{a1} 2.8; pK_{a2} 4.46 (25°). Decarboxylates at Mp to Methylenebutanedioic acid, M-529. Mp variable with rate of heating.

Tri-Et ester: [68077-28-1]
[5349-99-5]
$C_{12}H_{18}O_6$ 258.271
Bp_{18} 172°.

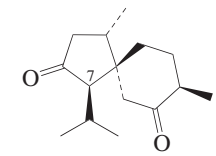
(*Z*)-*form* [585-84-2]
Present in apple fruits, maple syrup and passion fruit juice. Mp 125°. Gives (*E*)-form on heating.

[1321-30-8, 5349-99-5, 65629-33-6, 20820-77-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 505D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 789B; 789C (*nmr*)
Malachowski, R. *et al., Ber.*, 1928, **61**, 2521 (*synth, props*)
Org. Synth., Coll. Vol., 2, 1943, 12 (*synth*)
Miller, R.E. *et al., Adv. Carbohydr. Chem.*, 1951, **6**, 231 (*rev*)
Klostergaard, H. *et al., JOC*, 1958, **23**, 108-110 (*tri-Et ester*)
Krogh, A. *et al., Acta Chem. Scand.*, 1969, **23**, 2932 (*isol*)
Bartos, J. *et al., Pure Appl. Chem.*, 1984, **56**, 467 (*use*)
Barlianto, H. *et al., Z. Lebensm.-Unters. - Forsch.*, 1994, **198**, 215-222 (*occur, glc, ms*)
Nagel, N. *et al., Acta Cryst. C*, 1996, **52**, 2912-2915 (*cryst struct, Z-form*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 38; 944-945 (*mixed Et esters*)
Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.), Vol. 2, Wiley, 1980, 4974
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ADH000

3,8-Acoranedione A-177

Acorone [10121-28-5]



$C_{15}H_{24}O_2$ 236.353

Constit. of *Acorus calamus* (sweet flag). Cryst. (heptane). Mp 100°. $[\alpha]_D^{15}$ +139.5 (EtOH).

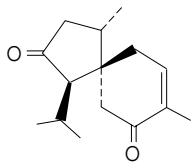
7-Epimer: ***Epiacorone***
$C_{15}H_{24}O_2$ 236.353
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -53.9 (c, 0.54 in MeOH).

McEachan, C.E. *et al., JCS(C)*, 1966, 579 (*cryst struct*)
Andersen, N.H. *et al., Tet. Lett.*, 1972, 899 (*abs config*)
Marx, J.N. *et al., JOC*, 1975, **40**, 1602 (*synth*)
McCrae, D.A. *et al., JOC*, 1977, **42**, 1607 (*synth*)
Ackroyd, J. *et al., Helv. Chim. Acta*, 1985, **68**, 338 (*synth*)
Rao, G.S.R.S. *et al., Indian J. Chem., Sect. B*, 1986, **25**, 783 (*synth*)

Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175 (*isol, pmr, cmr*)
Srikrishna, A. *et al., Tet. Lett.*, 1996, **37**, 1683 (*synth*)
Biju, P.J. *et al., Tet. Lett.*, 1999, **40**, 2405-2406 (*synth*)
Srikrishna, A. *et al., Tetrahedron*, 2000, **56**, 8189-8195 (*synth*)

4-Acorene-3,8-dione A-178

Acoronene [33983-45-8]



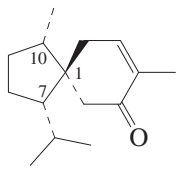
$C_{15}H_{22}O_2$ 234.338
Constit. of *Acorus calamus* (sweet flag). Cryst. (hexane). Mp 69°. $[\alpha]_D$ +66.8 (c, 1 in dioxan). $[\alpha]_D$ -104 (c, 0.12 in MeOH).

7-Epimer: ***Epiacoronene***
$C_{15}H_{22}O_2$ 234.338
Constit. of *Acorus calamus* (sweet flag). Oil. $[\alpha]_D$ -96 (c, 0.12 in MeOH). λ_{max} 238 (ε 3640) (MeOH).

Minato, H. *et al., Chem. Pharm. Bull.*, 1971, **19**, 638
Nawamaki, K. *et al., Phytochemistry*, 1996, **43**, 1175 (*isol, pmr, cmr*)

4-Acoren-3-one A-179

Acorenone [5956-05-8]



$C_{15}H_{24}O$ 220.354
Constit. of carrot (*Daucus carota*) and *Acorus calamus* (sweet flag). Oil. $Bp_{0.1}$ 61°. $[\alpha]_D^{20}$ -22.3. n_D^{20} 1.5039.

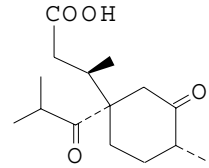
1-Epimer: [21653-33-8] *3-Acoren-5-one.* ***Acorenone B***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D$ +12.3 (c, 0.25 in $CHCl_3$).

1,7-Diepimer: [311350-99-9] ***10-Epi-3-acoren-5-one***
$C_{15}H_{24}O$ 220.354

McClure, R.J. *et al., Chem. Comm.*, 1968, 1135 (*cryst struct*)
Trost, B.M. *et al., JACS*, 1975, **97**, 5873 (*synth*)
Oppolzer, W. *et al., Helv. Chim. Acta*, 1977, **60**, 2388 (*synth*)
Lange, G.L. *et al., Tet. Lett.*, 1977, 4479 (*synth*)
Rascher, W. *et al., Tetrahedron*, 1977, **33**, 575 (*synth*)
Naegeli, P. *et al., Tet. Lett.*, 1978, 2127 (*synth*)
White, J.D. *et al., JACS*, 1981, **103**, 1813 (*synth*)
Baldwin, S.W. *et al., Tet. Lett.*, 1982, **23**, 1235 (*synth*)
Iwata, C. *et al., Chem. Comm.*, 1984, 781 (*synth*)
Nagumo, S. *et al., Chem. Comm.*, 1990, 1778 (*synth*)
Kido, F. *et al., JCS Perkin 1*, 1992, 229 (*synth, bibl*)
Wu, C.-L. *et al., J. Chin. Chem. Soc. (Taipei)*, 1995, **42**, 597 (*isol, pmr, cmr*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 2000, **15**, 61-83 (*1,7-diepimer*)
Kim, H. *et al., Nat. Prod. Sci.*, 2000, **6**, 36-39 (*activity*)
Brock, N.L. *et al., Eur. J. Org. Chem.*, 2011, 5167-5175 (*synth, abs config*)

Acoric acid A-180

[5956-06-9]



$C_{15}H_{24}O_4$ 268.352
Constit. of *Acorus calamus* (sweet flag). Cryst. (Et_2O/petrol). Mp 166-168°. $[\alpha]_D^{25}$ +27 (c, 1 in $CHCl_3$). Log P 1.53 (calc).

Birch, A.J. *et al., JCS*, 1964, 2923 (*isol*)
Birch, A.J. *et al., JCS Perkin 1*, 1972, 1186 (*synth*)
Rao, G.S.R.S. *et al., Indian J. Chem., Sect. B*, 1981, **20**, 1089 (*synth*)
Ramanathan, H. *et al., Indian J. Chem., Sect. B*, 1991, **30**, 901 (*synth*)

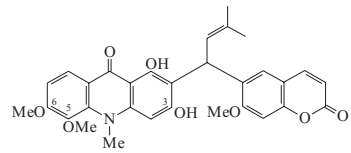
Acridone synthase A-181

*E.C. 2.3.1.159. Malonyl-CoA:*N*-methylanthraniloyl-CoA malonyltransferase (cyclising)* [99085-53-7]

Enzyme. Isol. from *Ruta graveolens* (rue).
Baumert, A. *et al., Z. Naturforsch., C*, 1994, **49**, 26-32

Acrimarine A A-182

[119152-47-5]



$C_{31}H_{29}NO_8$ 543.572
Pale yellow oil. $[\alpha]_D$ -9.76 (c, 0.082 in $CHCl_3$).

3-Me ether: ***Acrimarine N***
$C_{32}H_{31}NO_8$ 557.599
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisi*) x Dancy tangerine (*Citrus tangerina*)]. Yellow oil. Opt. inactive.

3-Me ether, N*-de-Me:* [119152-48-6] ***Acrimarine B***
$C_{31}H_{29}NO_8$ 543.572
Yellow prisms (Me_2CO). Mp 288-290°. $[\alpha]_D$ -7.14 (c, 0.056 in $CHCl_3$).

O^6*-De-Me:* [147395-91-3] ***Acrimarine K***
$C_{30}H_{27}NO_8$ 529.545
Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.0695 in $CHCl_3$).

O^6*-De-Me, 3-Me ether:* [129722-89-0] ***Acrimarine F***
$C_{31}H_{29}NO_8$ 543.572
Pale yellow powder.

O^6*-De-Me, 3-Me ether,* N^6*-de-Me:* [129722-88-9] ***Acrimarine E***
$C_{30}H_{27}NO_8$ 529.545
Pale yellow prisms (Me_2CO). Mp 274-276°. $[\alpha]_D$ +20.1 (c, 0.05 in Me_2CO).

6-Demethoxy, O^5*-de-Me:* [129722-97-0] ***Acrimarine G***
$C_{29}H_{25}NO_7$ 499.519
Yellow oil. $[\alpha]_D$ +8 (c, 0.075 in $CHCl_3$).

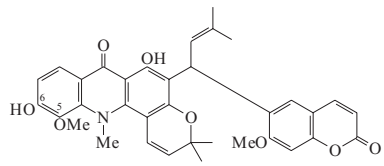
6-Demethoxy, O^5*-de-Me, 3-Me ether:* [132185-44-5] ***Acrimarine H***
$C_{30}H_{27}NO_7$ 513.546
Alkaloid from roots of *Citrus* spp. Yellow oil. $[\alpha]_D$ 0 (Me_2CO).

Bis(demethoxy): [147513-68-6] ***Acrimarine M***
$C_{29}H_{25}NO_6$ 483.52
Yellow oil. $[\alpha]_D^{25}$ 0 (c, 0.052 in $CHCl_3$).

Ito, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2586 (*Acrimarine H*)
Furukawa, H. *et al., JCS Perkin 1*, 1990, 1593 (*isol, pmr, cmr, struct*)
Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*Acrimarine K, Acrimarine M*)
Takemura, Y. *et al., Heterocycles*, 1994, **38**, 1937 (*Acrimarine N*)

Acrimarine J A-183

[147395-90-2]

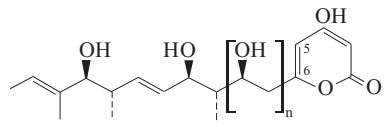


$C_{35}H_{33}NO_8$ 595.648
Alkaloid from roots of Yalaha [several hybrid seedlings resulting from a cross of Duncan grapefruit (*Citrus paradisii*) × Dancy tangerine (*Citrus tangerina*)]. Yellow oil. $[\alpha]_D^{28}$ 0 (c, 0.106 in $CHCl_3$).

6-Deoxy, O^5*-de-Me:* [147395-89-9] ***Acrimarine I***
$C_{34}H_{31}NO_7$ 565.621
Alkaloid from roots of Yalaha. Yellow oil. $[\alpha]_D^{26}$ +27.8 (c, 0.036 in $CHCl_3$).

Takemura, Y. *et al., Heterocycles*, 1992, **34**, 2363 (*isol, uv, ir, pmr, cmr, ms, struct*)

ACRL Toxins II-IV A-184



Toxin II, n = 0
Toxin III, n= 1
Toxin IV, n = 2

ACRL Toxin II [101951-84-2]

$C_{17}H_{24}O_5$ 308.374
Prod. by the fungus *Alternaria citri* on rough lemon. Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 67-68°. $[\alpha]_D$ +5 (c, 0.25 in MeOH). λ_{max} 277 (ϵ 4100) (MeOH) (Berdy). λ_{max} 285 (MeOH-HCl) (Berdy).

ACRL Toxin III [101951-97-7]
$C_{19}H_{28}O_6$ 352.427
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 142-145°. $[\alpha]_D$ -17 (c, 0.60 in MeOH). λ_{max} 280 (MeOH) (Berdy).

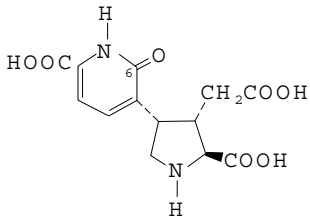
5,6-Dihydro: [98353-41-4] ***ACRL Toxin I***
$C_{19}H_{30}O_6$ 354.442
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 192-196°. Major phytotoxic component. λ_{max} 245 (ϵ 9500) (MeOH) (Berdy). λ_{max} 236 (MeOH-HCl) (Berdy).

ACRL toxin IV [101951-98-8]
$C_{21}H_{32}O_7$ 396.48
Sol. MeOH, EtOAc; poorly sol. H_2O, hexane. Mp 102-105°. $[\alpha]_D$ -11 (c, 0.30 in MeOH). λ_{max} 280 (MeOH) (Berdy).

Gardner, J.M. *et al., Phytochemistry*, 1985, **24**, 2861; 1986, **25**, 69 (*isol, ACRL Toxin I*)
Kono, Y. *et al., Phytochemistry*, 1985, **24**, 2869; 1986, **25**, 69 (*isol, struct, abs config*)
Lichtenthaler, F.W. *et al., Angew. Chem., Int. Ed.*, 1991, **30**, 1339 (*synth*)
Mulzer, J. *et al., Angew. Chem., Int. Ed.*, 1993, **32**, 1452 (*synth*)
Munchhof, M.J. *et al., JOC*, 1994, **59**, 7566 (*synth*)
Paterson, I. *et al., Synthesis*, 1998, 639-652 (*synth*)

Acromelic acid A A-185

5-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. ***Acromelinic acid A*** [86630-09-3]



$C_{13}H_{14}N_2O_7$ 310.263
Isol. from the mushroom *Clitocybe acromelalga*. Cryst. Sol. H_2O; poorly sol. Me_2CO, hexane. Mp 310°. $[\alpha]_D$ +27.8 (c, 0.35 in H_2O). Struct. established by synth. Phys. props. are of synthetic material. λ_{max} 240 (ϵ 4370); 315 (ϵ 8910) (pH 2). λ_{max} 241 (ϵ 5130); 312 (ϵ 9120) (pH 12) (Derep). λ_{max} 243 (ϵ 5500); 315 (ϵ 9550) (H_2O pH 7) (Derep).

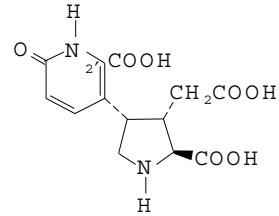
6-Deoxo, 5,6-didehydro: [102329-71-5] ***Acromelic acid D***
$C_{13}H_{14}N_2O_6$ 294.263
Sol. H_2O. $[\alpha]_D$ +17.6 (c, 0.07 in H_2O). λ_{max} 221; 269 (H_2O) (Berdy).

6-Deoxo, 5,6-didehydro, 4-decarboxy, 6-carboxy: [145237-01-0] ***Acromelic acid E***
$C_{13}H_{14}N_2O_6$ 294.263
Sol. H_2O. λ_{max} 266 (H_2O) (Berdy).

Konno, K. *et al., Tetrahedron*, 1982, **38**, 3281-3284 (*Clitocybe acromelalga constits*)
Konno, K. *et al., Phytochemistry*, 1984, **23**, 1003-1006 (*Clitocybe acromelalga constit*)
Hashimoto, K. *et al., Chem. Lett.*, 1986, 1399-1400 (*Clitocybe acromelalga constits*)
Takano, S. *et al., JACS*, 1987, **109**, 5523-5524 (*synth*)
Konno, K. *et al., JACS*, 1988, **110**, 4807-4815 (*isol, synth, ir, uv, pmr*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473-1476 (*synth, bibl*)
Fushiya, S. *et al., Heterocycles*, 1992, **34**, 1277-1280 (*isol, pmr, cd, struct*)
Barco, A. *et al., Gazz. Chim. Ital.*, 1993, **123**, 185-188 (*synth*)
Baldwin, J.E. *et al., Tetrahedron*, 1998, **54**, 7465-7484 (*synth*)
Itadani, S. *et al., Tet. Lett.*, 2002, **43**, 7777-7780 (*Acromelic acids, synth*)

Acromelic acid B A-186

3-[5-Carboxy-4-(carboxymethyl)-3-pyrrolidinyl]-1,6-dihydro-6-oxo-2-pyridinecarboxylic acid, 9CI. Acromelinic acid B [86630-10-6]



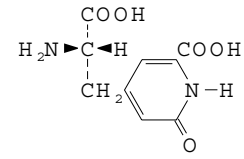
$C_{13}H_{14}N_2O_7$ 310.263
Isol. from the mushroom *Clitocybe acromelalga*. Amorph. powder. Sol. H_2O; poorly sol. Me_2CO, hexane. $[\alpha]_D$ +50.1 (c, 0.45 in H_2O). Struct. established by synth. Phys. props. are of synthetic material. λ_{max} 231; 308 (pH 2). λ_{max} 241; 311 (pH 12). λ_{max} 236 (ϵ 6320); 302 (ϵ 2920) (MeOH) (Berdy).

2′-Decarboxy: [133740-47-3] ***Acromelic acid C***
$C_{12}H_{14}N_2O_5$ 266.253
Powder. $[\alpha]_D$ +31.9 (c, 0.23 in H_2O). λ_{max} 230 (ϵ 11000); 302 (ϵ 6150) (MeOH) (Derep). λ_{max} 230 (ϵ 10592); 301 (ϵ 6150) (H_2O) (Berdy).
▶ LD_{50} (mus, ipr) 10 mg/kg.

Hashimoto, K. *et al., Chem. Lett.*, 1986, 1399-1400 (*synth, uv, ir, cd, abs config*)
Konno, K. *et al., JACS*, 1988, **110**, 4807-4815 (*isol, uv, pmr, synth, struct*)
Takano, S. *et al., Heterocycles*, 1989, **29**, 1473-1476 (*synth, bibl*)
Fushiya, S. *et al., Tet. Lett.*, 1990, **31**, 3901-3904 (*Acromelic acid C, toxicity*)
Horikawa, M. *et al., Heterocycles*, 1995, **40**, 1009-1014 (*synth*)
Hashimoto, K. *et al., JOC*, 1996, **61**, 4685-4692 (*stereochem*)
Wood, M.E. *et al., Adv. Nitrogen Heterocycl.*, 1998, **3**, 159-218 (*Acromelic acid C, synth*)
Baldwin, J.E. *et al., Tetrahedron*, 1998, **54**, 7465-7484 (*synth*)

Acromelobic acid A-187

α-Amino-6-carboxy-1,2-dihydro-2-oxo-4-pyridinepropanoic acid. 3-(2-Carboxy-6-oxo-4-pyridinyl)alanine [158703-45-8]



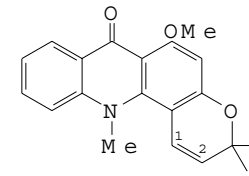
$C_9H_{10}N_2O_5$ 226.188
Isol. from the mushroom *Clitocybe acromelalga*.

(*S*)-*form* [142179-90-6]
L-form
Pale yellow solid. Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. $[\alpha]_D^{23}$ -133.1 (c, 0.05 in H_2O). λ_{max} 230 (log ϵ 3.22); 310 (log ϵ 3.09) (H_2O).

Yamano, K. *et al., Heterocycles*, 1992, **34**, 445-448 (*isol*)
Yamano, K. *et al., Tetrahedron*, 1993, **49**, 2427-2436 (*isol, uv, pmr*)
Baldwin, J.E. *et al., Tet. Lett.*, 1994, **35**, 6575-6576 (*synth*)
Adamcyzk, M. *et al., Tetrahedron*, 2002, **58**, 6943-6950 (*synth, pmr, cmr*)
Wild, N. *et al., Eur. J. Org. Chem.*, 2003, 4445-4449 (*synth, pmr, cmr*)

Acronycine A-188

3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano[2,3-c]acridin-7-one, 9CI, 8CI. ***Acronine, INN, USAN****. NSC 403169. Compound 42339* [7008-42-6]



$C_{20}H_{19}NO_3$ 321.375
Yellow needles (EtOH). Mp 175-176°. Log P 3.7 (calc). λ_{max} 280 (ϵ 39800); 291 (ϵ 34700); 304 (ϵ 19100); 392 (ϵ 6920) (EtOH) (Derep). λ_{max} 224 (ϵ 24500); 281 (ϵ 48000); 293 (ϵ 43500); 308 (ϵ 40700); 380 (ϵ 10250) (MeOH) (Berdy).
▶ LD_{50} (mus, orl) 522 mg/kg. Exp. carcinogenic data. UQ0330000

11-Methoxy, O*-de-Me:* [51179-68-1] ***5-Methoxynoracronycine****. Baiyumine A*
$C_{20}H_{19}NO_4$ 337.374
Alkaloid from the bark of *Citrus junos* (yuzu). Light yellow prisms, or orange needles (Me_2CO/hexane), or orange plates (Et_2O). Mp 146-148° Mp 160-161° (155-157°).

Ju-ichi, M. *et al., Heterocycles*, 1986, **24**, 1595 (*5-Methoxynoracronycine*)
Wu, T.S. *et al., Phytochemistry*, 1987, **26**, 871 (*Baiyumine A*)

Acrosin A-189

E.C. 3.4.21.10. Acrosomal proteinase. Acrosin amidase. Acrozonase [9068-57-9]

Serine endopeptidase enzyme. Isol. from pig, cow, chicken. Enzyme is glycosylated and consists of light and heavy chains held together by disulfide bonds. Formed from proacrosin by limited proteolysis. Human enzyme activity range pH 6.0-

10.5. Stable for weeks at 4°, pH 3.2, 0.5*M* KCl.

Gilboa, E. *et al., Eur. J. Biochem.*, 1973, **39**, 85-92 (*human, activity, stability*)
Elce, J.S. *et al., Can. J. Biochem.*, 1981, **60**, 8-14 (*human, cow*)
Mueller-Esterl, W. *et al., Methods Enzymol.*, 1981, **80**, 621-632 (*pig*)
Froman, D.P. *et al., Poultry Sci.*, 1990, **69**, 812-817 (*chicken*)
Raterman, D. *et al., Mol. Reprod. Dev.*, 2008, **75**, 1196-1207 (*animals*)

Actinchinin A-190

Protein. Isol. from the gold kiwi fruit.

Xia, L. *et al., Peptides (N.Y.)*, 2004, **25**, 1093-1098 (*isol*)

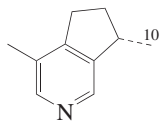
Actinidain A-191

E.C. 3.4.22.14. Actinidia *Anionic protease. Actinidin* [39279-27-1]

Cysteine endopeptidase enzyme. Isol. from *Actinidia chinensis* (kiwifruit). Activity range pH 3.5-8.8. At 4°, crystalline enzyme resuspended in dialysis buffer at pH 4.0 is stable for several months.

McDowall, M.A. *et al., Eur. J. Biochem.*, 1970, **14**, 214-221 (*Actinidia chinensis, activity, stability*)
Baker, E.N. *et al., J. Mol. Biol.*, 1973, **74**, 411-412; 1976, **101**, 185-196; 1977, **115**, 263-277; 1980, **141**, 441-484 (*Actinidia chinensis, cryst struct*)
Tello-Solis, S.R. *et al., Plant Sci. (Shannon, Irel.)*, 1995, **106**, 227-232 (*Actinidia chinensis*)
Sugiyama, S. *et al., Biosci., Biotechnol., Biochem.*, 1996, **60**, 1994-2000 (*Actinidia chinensis*)

Actinidine A-192



(*S*)-*form*

$C_{10}H_{13}N$ 147.219

(*R*)-*form* [15524-81-9]
Liq. Bp_{10} 92-94°. $[\alpha]_D^{20}$ +10.8 (c, 0.36 in $CHCl_3$).

Picrate: Mp 146-147°.

(*S*)-*form* [524-03-8]
Alkaloid from *Actinidia arguta* (taravine) and *Valeriana officinalis* (valerian). Oil. Bp_9 100-103°. $[\alpha]_D^{11}$ -7.2 ($CHCl_3$).

Picrate: Mp 143°.

N-*[2-(4-Hydroxyphenyl)ethyl]:* [15794-92-0] **N-(p-*Hydroxyphenethyl)actinidine***
$C_{18}H_{22}NO^{\oplus}$ 268.378
Quaternary alkaloid from the roots of *Valeriana officinalis* (valerian). Mp 201-203° dec. (as chloride). $[\alpha]_D^{22}$ +50.5 (MeOH).

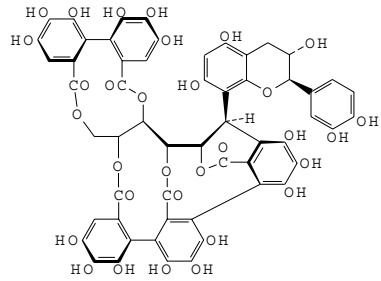
10-Acetoxy: ***10-Acetoxyactinidine***
$C_{12}H_{15}NO_2$ 205.256
Amorph. solid. Stereochem. not certain.

(±)-*form* [79254-93-6]
Oil. Mp 146-146.5° (as picrate). Bp_9 100-103°.

Sakan, T. *et al., Bull. Chem. Soc. Jpn.*, 1959, **32**, 315; 1155; 1960, **33**, 712 (*uv, ir, isol, struct, synth*)
Djerassi, C. *et al., Chem. Ind. (London)*, 1961, 210 (*pmr*)
Torssell, K. *et al., Acta Chem. Scand.*, 1967, **21**, 53 (*N-4-Hydroxyphenethylactinidine*)
Cavill, G.W.K. *et al., Aust. J. Chem.*, 1967, **20**, 349 (*synth, uv, pmr*)
Johnson, R.D. *et al., Phytochemistry*, 1971, **10**, 3334 (*isol, ms*)
Wuest, J.D. *et al., JOC*, 1977, **42**, 2111 (*synth*)
Nitta, M. *et al., Chem. Lett.*, 1981, 933 (*synth*)
Davies, L.B. *et al., JCS Perkin 1*, 1981, 1909 (*synth, uv, ir, pmr, ms*)
Tomalski, M.D. *et al., J. Chem. Ecol.*, 1987, **13**, 253-263 (*isol, ms*)
Cossy, J. *et al., Tet. Lett.*, 1988, **29**, 6113 (*synth*)
Ranarivelo, Y. *et al., Heterocycles*, 1990, **31**, 1727-1731 (*(S)-form, synth*)
Huth, A. *et al., J. Chem. Ecol.*, 1990, **16**, 2691-2711 (*isol*)
Cossy, J. *et al., JOC*, 1993, **58**, 2351 (*synth*)
Shiao, M.J. *et al., JOC*, 1993, **58**, 3162 (*synth*)
Stepanov, A.V. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 1998, **47**, 2286-2291 (*synth*)
Jones, K. *et al., Tetrahedron*, 1998, **54**, 2275-2280 (*synth*)
Bianco, A. *et al., Nat. Prod. Lett.*, 2002, **16**, 77-80 (*10-Acetoxyactinidine*)
Becket, J.S. *et al., Org. Lett.*, 2010, **12**, 1408-1411 (*synth*)

Acutissimin A A-193

[108906-66-7]



$C_{56}H_{38}O_{31}$ 1206.898
Isol. from *Castanea crenata* (Japanese chestnut). Off-white amorph. powder + 3½ or $5H_2O$. $[\alpha]_D^{32}$ -74 (c, 1.2 in Me_2CO). λ_{max} 225 (ϵ 85100); 275 (ϵ 28800) (MeOH) (Berdy).

Ishimaru, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 602 (*isol, uv, cd, pmr, cmr*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2151 (*struct*)

Acyl-[acyl-carrier-protein] desaturase A-194

E.C. 1.14.19.2. Acyl-[acyl-carrier-protein], hydrogen-donor:oxygen oxidoreductase. Stearyl-ACP desaturase. E.C. 1.14.99.6 (transferred) [37256-86-3]

Ferredoxin-dependent oxidoreductase enzyme. Isol. from safflower and castor oil.

McKeon, T.A. *et al., J. Biol. Chem.*, 1968, **243**, 12141-12147 (*safflower seeds*)
Jaworski, J.G. *et al., Arch. Biochem. Biophys.*, 1974, **162**, 158-165 (*safflower seeds*)
McKeon, T. *et al., Methods Enzymol.*, 1981, **71**, 275-281 (*safflower seeds*)
Lindquist, H. *et al., EMBO J.*, 1996, **15**, 4081-4092 (*castor seeds*)
Cahoon, E.B. *et al., Plant Mol. Biol.*, 1997, **33**, 1105-1110 (*milkweed seeds*)

Acylaminoacyl peptidase A-195

E.C. 3.4.19.1. Acylamino acid-releasing enzyme. N-*Acylpeptide hydrolase. E.C. 3.4.14.3 (transferred)* [73562-30-8]

Omega peptidase enzyme. Isol. from pig, rabbit, cucumber. Several variants of the enzyme exist. Human erythrocyte enzyme is relatively specific for removal of *N*-acetylalanine from peptides. Human enzyme activity range pH 7.0-9.0. Rabbit enzyme in 0.05*M* sodium phosphate, pH 6.9, with 2*mM* $MgCl_2$, 1*mM* EDTA is stable over several months at -20°.

Schoenberger, O.L. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1981, **362**, 865-873 (*human, activity*)
Radhakrishna, G. *et al., J. Biol. Chem.*, 1989, **264**, 11076-11081 (*rabbit, stability*)
Jones, W.M. *et al., Methods Enzymol.*, 1994, **244**, 227-231 (*human*)
Yamauchi, Y. *et al., J. Biochem. (Tokyo)*, 2003, **134**, 251-257 (*cucumber, thale cress*)
Wright, H. *et al., Acta Cryst. F*, 2005, **61**, 942-944 (*cryst struct, pig*)

[Acyl-carrier-protein] *S*-acetyltransferase A-196

E.C. 2.3.1.38. Acetyl-CoA:[acyl-carrier-protein] S-*acetyltransferase* [37257-16-2]

Enzyme. Isol. from spinach leaves.

Williamson, I.P. *et al., J. Biol. Chem.*, 1966, **241**, 2326-2332 (*Escherichia coli*)
Alberts, A.W. *et al., Methods Enzymol.*, 1969, **14**, 50-53 (*Escherichia coli*)
Shimakata, T. *et al., J. Biol. Chem.*, 1983, **258**, 3592-3598 (*spinach leaves*)
Shimakata, T. *et al., Methods Enzymol.*, 1986, **122**, 53-59 (*spinach leaves*)
Lowe, P.N. *et al., Biochem. J.*, 1988, **250**, 789-796 (*Escherichia coli*)

[Acyl-carrier-protein] *S*-malonyltransferase A-197

E.C. 2.3.1.39. Malonyl-CoA:[acyl-carrier-protein] S-*malonyltransferase* [37257-17-3]

Enzyme. Present in soybean. Participates in fatty acid biosynth.

Williamson, I.P. *et al., J. Biol. Chem.*, 1966, **241**, 2326-2332 (*Escherichia coli*)
Alberts, A.W. *et al., Methods Enzymol.*, 1969, **14**, 53-56 (*Escherichia coli*)
Guerra, D.I. *et al., Arch. Biochem. Biophys.*, 1986, **246**, 274-285 (*soybean*)
Chohnan, S. *et al., FEMS Microbiol. Lett.*, 1998, **169**, 37-43 (*Pseudomonas putida*)
White, S.W. *et al., Annu. Rev. Biochem.*, 2005, **74**, 791-831 (*rev*)

[Acyl-carrier-protein] phosphodiesterase A-198

E.C. 3.1.4.14. Holo-[acyl-carrier protein] 4′-pantetheine-phosphohydrolase. ACP hydrolase. ACP phosphodiesterase [37288-21-4]

Phosphoric diester hydrolase enzyme. Isol. from pig. Rat enzyme stable for several months at -20° in dithiothreitol.

Kim, M. *et al., Arch. Biochem. Biophys.*, 1977, **181**, 580-590 (*pig*)
Burton, D.N. *et al., Methods Enzymol.*, 1979, **62**, 249-262 (*rat, stability*)
Fischl, A.S. *et al., J. Bacteriol.*, 1990, **172**, 5445-5449 (*Escherichia coli*)
Thomas, J. *et al., J. Biol. Chem.*, 2005, **280**, 34675-34683 (*Escherichia coli*)

Acyl-CoA hydrolase **A-199**
E.C. 3.1.2.20. Acyl-CoA thioesterase [37270-64-7]

Thioester hydrolase enzyme. Isol. from cow, pig, rabbit and garden pea. Broad specificity for medium- to long-chain acyl CoA derivs. Insensitive to $NAD^{\oplus}$ Rat enzyme activity range pH 7.5-9.0. At -20°, stable for over 1 month.

Lee, K.Y. *et al., J. Biol. Chem.*, 1979, **254**, 4516-4523 (*pig*)
Murphy, D.J. *et al., Eur. J. Biochem.*, 1984, **142**, 43-48 (*Pisum sativum*)
Alexson, S.E.H. *et al., Biochim. Biophys. Acta*, 1989, **1005**, 13-19 (*rat*)
Swenson, L. *et al., J. Mol. Biol.*, 1994, **236**, 660-662 (*cryst struct*)
Yamada, J. *et al., Arch. Biochem. Biophys.*, 1996, **326**, 106-114 (*human, rabbit, pig, ox, hamster*)
Yamada, J. *et al., J. Biochem. (Tokyo)*, 1999, **126**, 1013-1019 (*human*)
Tilton, G. *et al., Biochem. Soc. Trans.*, 2000, **28**, 946-947 (*Arabidopsis thaliana*)

Acylglycerol lipase **A-200**
E.C. 3.1.1.23. Glycerol ester acylhydrolase. Monoacylglycerol lipase. Monoglyceride lipase [9040-75-9]

Carboxylic ester hydrolase enzyme. Isol. from cow, chicken. Rat enzyme activity range pH 5.0-9.5. Stable for 2 weeks at 0°.

Ikeda, Y. *et al., Biochim. Biophys. Acta*, 1977, **488**, 128-139 (*rat, activity, stability*)
Khoo, J.C. *et al., Methods Enzymol.*, 1981, **71**, 627-636 (*chicken*)
Farooqui, A.A. *et al., Biochem. Biophys. Res. Commun.*, 1984, **122**, 1241-1246 (*ox*)
Somma-Delpero, C. *et al., Biochem. J.*, 1995, **312**, 519-525 (*human*)
Imamura, S. *et al., J. Biochem. (Tokyo)*, 2000, **127**, 419-425 (*Bacillus*)
Karlsson, M. *et al., Protein Expr. Purif.*, 2000, **18**, 286-292 (*mouse*)
Yoneda, K. *et al., Acta Cryst. D*, 2002, **58**, 1232-1233 (*cryst struct*)

1-Acylglycerol-3-phosphate *O*-acyltransferase **A-201**
E.C. 2.3.1.51. Acyl-CoA:1-acyl-sn-*glycerol-3-phosphate 2*-O-*acyltransferase. Lysophosphatidic acid acyltransferase* [51901-16-7]

Enzyme. Widespread in nature. Occurs in plants, e.g. pea and spinach chloroplasts.

Yamashita, S. *et al., Eur. J. Biochem.*, 1973, **38**, 25-31 (*rat liver*)
Yamashita, S. *et al., Methods Enzymol.*, 1981, **71**, 528-536 (*rat liver*)
Kessels, J.M. *et al., Biochim. Biophys. Acta*, 1983, **753**, 227-235 (*Escherichia coli*)
Frentzen, M. *et al., Eur. J. Biochem.*, 1983, **129**, 629-636 (*pea, spinach chloroplasts*)
Dircks, L. *et al., Prog. Lipid Res.*, 1999, **36**, 461-479 (*rev*)

1-Acylglycerophosphocholine *O*-acyltransferase **A-202**
E.C. 2.3.1.23. Acyl-CoA:1-acyl-sn-*glycero-3-phosphocholine* O-*acyltransferase. Lysolecithin acyltransferase. Lysophosphatidylcholine acyltransferase* [9027-64-9]

Enzyme. Isol. from bovine heart.

Van Den Bosch, H. *et al., Biochim. Biophys. Acta*, 1967, **144**, 613-623 (*rat liver*)
Miki, Y. *et al., Eur. J. Biochem.*, 1977, **81**, 433-441 (*rat liver*)
Bell, R.M. *et al., Annu. Rev. Biochem.*, 1980, **49**, 459-487 (*rev*)
Hasegawa-Sasaki, H. *et al., Biochim. Biophys. Acta*, 1980, **617**, 205-217 (*rat liver*)
Yamashita, S. *et al., Methods Enzymol.*, 1981, **71**, 528-536 (*rat liver*)
Gavino, V.G. *et al., J. Bioenerg. Biomembr.*, 1982, **14**, 513-526 (*rat liver*)
Sanjanwala, M. *et al., Arch. Biochem. Biophys.*, 1988, **265**, 476-483 (*bovine heart*)
Yamashita, A. *et al., J. Biochem. (Tokyo)*, 1997, **122**, 1-16 (*rev*)

***N*-Acylneuraminate cytidylyltransferase** **A-203**
*E.C. 2.7.7.43. CTP:*N-*acylneuraminate cytidylyltransferase. CMP sialate pyrophosphorylase. CMP sialate synthase. Cytidine 5′-monophosphosialic acid synthetase. CMP* N-*acetylneuraminic acid synthase. Many other names* [9067-82-7]

Nucleotidyltransferase enzyme. Isol. from cow and pig. Also acts on *N*-acetyl and *N*-glycolyl derivs. Rat enzyme activity range pH 7-10. At -20°, shows 50% loss of activity in 2 weeks.

Kean, E.L. *et al., J. Biol. Chem.*, 1966, **241**, 5643-5650 (*human, cow, pig*)
Kean, E.L. *et al., Methods Enzymol.*, 1966, **8**, 208-215; 1972, **28**, 413-421 (*rev*)
Schauer, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1973, **354**, 1405-1414; 1980, **361**, 641-648 (*pig, horse, frog*)
Rodriguez-Aparicio, L.B. *et al., J. Biol. Chem.*, 1992, **267**, 9257-9263 (*rat*)
Vionnet, J. *et al., Glycobiology*, 1999, **9**, 481-487 (*cow*)
Fujita, A. *et al., Anal. Biochem.*, 2005, **337**, 12-21 (*assay, mouse*)

***N*-Acylneuraminate 9-phosphate synthase** **A-204**
*E.C. 2.5.1.57. Phosphoenolpyruvate:*N-*acyl-*D-*mannosamine-6-phosphate 1-(2-carboxy-2-oxoethyl)transferase. Sialic acid 9-phosphate synthase. E.C. 4.1.3.20 (transferred)* [9031-58-7]

Alkyltransferase enzyme. Isol. from pig. Involved in biosynth. of *N*-Acetylneuraminic acid, A-138.

Watson, D.R. *et al., J. Biol. Chem.*, 1966, **241**, 5627-5636 (*hog submaxillary gland*)
Chen, H. *et al., Glycobiology*, 2002, **12**, 65-71 (*rat liver*)
Tanner, M.E. *et al., Bioorg. Chem.*, 2005, **33**, 216-218 (*rev*)

Acyloxyacyl hydrolase **A-205**
E.C. 3.1.1.77. AOAH [110277-64-0]

Carboxylic ester hydrolase enzyme. Isol. from cow. The substrate is lipid A on the reducing end of the toxic lipopolysaccharide of *Salmonella typhimurium* and related organisms. Human enzyme activity range pH 4.5-5.5.

Munford, R.S. *et al., J. Biol. Chem.*, 1989, **264**, 15613-15619; 1992, **267**, 10116-10121 (*human*)
Erwin, A.L. *et al., J. Biol. Chem.*, 1990, **265**, 16444-16449 (*human*)
McDermott, C.M. *et al., Infect. Immun.*, 1991, **59**, 485-487 (*human, ox*)
Munford, R.S. *et al., Methods Enzymol.*, 1992, **209**, 485-492 (*human*)
Feulner, J.A. *et al., Infect. Immun.*, 2004, **72**, 3171-3178 (*mouse*)

Acylsucroses **A-206**
Naturally occurring acyl derivs. of Sucrose, S-379. See that entry for synthetic acyl derivs. of sucrose, e.g. acetates, Sucrapans.

6-O-*(3-Methylbutanoyl):* [70284-38-7]
$C_{17}H_{30}O_{12}$ 426.417
Constit. of green coffee beans (*Coffea arabica*).

1′-O-*(3,4,5-Trihydroxybenzoyl):* [115713-45-6] ***1′*-O-*Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
A tannin isol. from commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +47 (c, 0.84 in MeOH).

2-O-*(3,4,5-Trihydroxybenzoyl):* [115713-46-7] ***2*-O-*Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Isol. from the commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $2H_2O$. $[\alpha]_D^{27}$ +67.1 (c, 0.79 in MeOH).

4′-O-*(3,4,5-Trihydroxybenzoyl):* [115713-44-5] ***4′*-O-*Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Tannin constit. of commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +14.9 (c, 0.72 in MeOH).

6-O-*(3,4,5-Trihydroxybenzoyl):* [115731-15-2] ***6*-O-*Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Isol. from commercial Chinese rhubarb (*Rheum* spp.). Amorph. powder + $1H_2O$. $[\alpha]_D^{27}$ +48 (c, 0.65 in MeOH).

6′-O-*(3,4,5-Trihydroxybenzoyl):* [115713-43-4] ***6′*-O-*Galloylsucrose***
$C_{19}H_{26}O_{15}$ 494.405
Isol. from commercial Chinese rhubarb (*Rheum* spp.). Needles + $2H_2O$ (H_2O). Mp 149-151°. $[\alpha]_D^{28}$ +88.6 (c, 0.74 in MeOH).

6-O-*(4-Hydroxy-3-methoxybenzoyl):* [412029-01-7] ***6*-O-*Vanilloylsucrose***
$C_{20}H_{28}O_{14}$ 492.433
Constit. of cane sugar. λ_{max} 208; 220; 263; 291 (MeOH).

6-O-*(4-Hydroxy-3,5-dimethoxybenzoyl):* [412029-02-8] ***6*-O-*Syringoylsucrose***
$C_{21}H_{30}O_{15}$ 522.459
Constit. of cane sugar. λ_{max} 217; 276 (MeOH).

6′-O-*(4-Hydroxy*-E-*cinnamoyl), 1′,3,4,6-tetra-Ac:* [457640-04-9] ***Prunose II***
$C_{29}H_{36}O_{17}$ 656.593
Constit. of the flowers of *Prunus mume* (Japanese apricot). Powder. $[\alpha]_D^{28}$ +18.7

(c, 1 in MeOH). λ_{max} 228 (log ϵ 3.84); 315 (log ϵ 4.12) (MeOH).

6′-O-*(4-Hydroxy*-E-*cinnamoyl), 3,4,4′,6-tetra-Ac:* [500995-02-8] ***Prunose III***
$C_{29}H_{36}O_{17}$ 656.593
Constit. of the flowers of *Prunus mume* (Japanese apricot). Powder. $[\alpha]_D^{26}$ +27.8 (c, 0.9 in MeOH). λ_{max} 228 (log ϵ 3.96); 314 (log ϵ 4.24) (MeOH).

6′-O-*(4-Hydroxy*-E-*cinnamoyl), 1′,3,4,4′,6-penta-Ac:* [457639-62-2] ***Prunose I***
$C_{31}H_{38}O_{18}$ 698.63
Constit. of the flowers of *Prunus mume* (Japanese apricot). Powder. $[\alpha]_D^{27}$ +26.9 (c, 1 in MeOH). λ_{max} 229 (log ϵ 4.1); 316 (log ϵ 4.41) (MeOH).

3′,6′-Bis-O-*(4-hydroxy*-E-*cinnamoyl), 6-Ac:* [761447-92-1] ***6-Acetyl-3′,6′-di*-p-*coumaroylsucrose***
$C_{32}H_{36}O_{16}$ 676.627
Constit. of the rhizomes of *Canna edulis* (arrowroot). Light yellow amorph. solid. $[\alpha]_D^{23}$ +23.4 (c, 0.25 in MeOH). λ_{max} 316 (log ϵ 4.76) (MeOH).

6-O-*(3,4-Dihydroxy*-E-*cinnamoyl):* [223261-29-8] *6-Caffeoylsucrose*
$C_{21}H_{28}O_{14}$ 504.444
Constit. of *Salvia officinalis* (sage). Cryst. (MeOH). Mp 210-212°. $[\alpha]_D^{23}$ +27.2 (c, 0.13 in MeOH).

6-O-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl):* [137941-45-8] *6*-O-*Feruloylsucrose.* ***Arillatose B***
$C_{22}H_{30}O_{14}$ 518.471
Constit. of brown rice. Amorph. powder. $[\alpha]_D^{27}$ +15.8 (c, 0.13 in MeOH). λ_{max} 235 (log ϵ 3.73); 295 (log ϵ 3.66); 326 (log ϵ 3.76) (MeOH).

6′-O-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl), 3′*-O-*(4-hydroxy*-E-*cinnamoyl), 6-Ac:* [761447-91-0]
$C_{33}H_{38}O_{17}$ 706.653
Constit. of the rhizomes of *Canna edulis* (arrowroot). Light yellow amorph. solid. λ_{max} 319 (log ϵ 4.84) (MeOH).

3′-O-*(4-Hydroxy-3,5-dimethoxy*-E-*cinnamoyl), 6*-O-*(4-hydroxy-3-methoxy*-E-*cinnamoyl):* [291767-08-3] ***6-Feruloyl-3′-sinapoylsucrose***
$C_{33}H_{40}O_{18}$ 724.668
Constit. of *Ruta graveolens* (rue). Yellow powder. $[\alpha]_D^{25}$ -69.1 (c, 0.34 in MeOH). λ_{max} 202 (log ϵ 4.53); 238 (log ϵ 4.32); 328 (log ϵ 4.43) (MeOH).

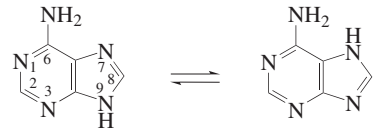
6-O-*(4-Hydroxy-3,5-dimethoxycinnamoyl):* [139726-40-2] *6-Sinapoylsucrose. Arillanin C.* ***Neohancoside D.*** *Sibiricose A_1*
$C_{23}H_{32}O_{15}$ 548.497
Constit. of brown rice. Needles ($CHCl_3$) (as per-Ac). Mp 138-140° (per-Ac). $[\alpha]_D^{23}$ +18 (c, 4.4 in MeOH). λ_{max} 224 (sh) (log ϵ 4.1); 239 (log ϵ 4.13); 328 (log ϵ 4.18) (MeOH).

3′,6-Bis-O-*(4-hydroxy-3,5-dimethoxycinnamoyl):* [139891-98-8] ***3′,6-Disinapoylsucrose***
$C_{34}H_{42}O_{19}$ 754.694
Constit. of radish (*Raphanus sativus*). Yellow powder. Mp 138-141°. $[\alpha]_D$ -94 (c, 0.2 in MeOH).

Kashiwada, Y. *et al., Phytochemistry*, 1988, **27**, 1469-1472 (*gallates*)
Wang, M. *et al., J. Nat. Prod.*, 1999, **62**, 454-456 (*6-Caffeoylsucrose*)
Chen, C.-C. *et al., J. Nat. Prod.*, 2001, **64**, 990-992 (*6-Feruloyl-3′-sinapoylsucrose*)
Takara, K. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 29-35 (*6-Syringoylsucrose, 6-Vanilloylsucrose*)
Yoshikawa, M. *et al., J. Nat. Prod.*, 2002, **65**, 1151-1155 (*Prunoses I,II*)
Weckerle, B. *et al., Phytochemistry*, 2002, **60**, 409-414 (*3-methylbutanoyl ester*)
Matsuda, H. *et al., Chem. Pharm. Bull.*, 2003, **51**, 440-443 (*Prunose III*)
Tian, S. *et al., J. Agric. Food Chem.*, 2004, **52**, 4808-4813 (*6-Feruloylsucrose, 6-Sinapoylsucrose, isol, pmr, cmr, uv*)
Yun, Y.S. *et al., Phytochemistry*, 2004, **65**, 2167-2171 (*Canna edulis derivs*)

Adenine, JAN, USAN A-207

*1*H-*Purin-6-amine, 9CI. 6-Aminopurine. Vitamin B_4. Angustmycin B* [73-24-5]



9H-form *7H-form*

$C_5H_5N_5$ 135.128

9*H*-form is favoured in free base. CAS refers mainly to 1*H* struct. which is not in reality a favoured tautomer. Widespread throughout animal and plant tissue, purine components of DNA, RNA, and coenzymes. Vitamin. Needles + $3H_2O$ (H_2O). Mp 360-365° (anhyd.) dec. pK_{a1} 4.12; pK_{a2} 9.83 (25°).

▶ Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 745 mg/kg. AU6125000

Hydrochloride: [2922-28-3]
Cryst. + $0.5H_2O$. Mp 285°.

Sulfate: [321-30-2] [6509-19-9]
Mp 285° dec.

▶ AU7140000

6-N-*Benzyl:* [1214-39-7] N-*Benzyladenine, 8CI. 6-Benzylaminopurine.* ***Cytokinin B.*** *BAP*
$C_{12}H_{11}N_5$ 225.252
Cryst. (C_6H_6). Mp 229°.

▶ AU6252200

6-N-*(2-Hydroxybenzyl):* [20366-83-0] *6*-N-*(2-Hydroxybenzyl)adenine.* **ortho-*Topolin***
$C_{12}H_{11}N_5O$ 241.252
Isol. from coconut water (*Cocos nucifera*).

[6055-72-7, 2312-73-4]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 589C; 589D; 590C (*pmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 708A; 713C; 713D; 714D (*ir*)
Traube, W. *et al., Annalen*, 1904, **331**, 64-88 (*synth*)
Skinner, C.G. *et al., JACS*, 1955, **77**, 6692-6693 (*Cytokinin B*)
Ge, L. *et al., Electrophoresis*, 2005, **26**, 1768-1777 (*ortho-Topolin, isol*)

Adenine phosphoribosyltransferase A-208

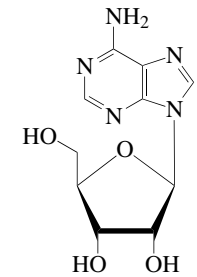
E.C. 2.4.2.7. AMP:diphosphate phospho-D-ribosyltransferase. AMP pyrophosphorylase [9027-80-9]

Pentosyltransferase enzyme. Isol. from a wide variety of yeast, plant and animal tissues. For example, from *Saccharomyces cerevisiae*, *Brassica juncea* (Abyssinian cabbage) and beef liver.

Flaks, J.G. *et al., Methods Enzymol.*, 1963, **6**, 136-158 (*Saccharomyces cerevisiae, beef liver*)
Hochstadt, J. *et al., Methods Enzymol.*, 1978, **51**, 558-567 (*Escherichia coli*)
Arnold, W.J. *et al., Methods Enzymol.*, 1978, **51**, 568-574 (*human erythrocytes*)
Groth, D.P. *et al., Methods Enzymol.*, 1978, **51**, 574-580 (*rat liver*)
Hershey, H.V. *et al., Prep. Biochem.*, 1978, **8**, 453-462 (*rat liver*)
Holden, J.A. *et al., J. Biol. Chem.*, 1979, **254**, 6951-6955 (*human erythrocytes*)
Moffatt, B.A. *et al., Arch. Biochem. Biophys.*, 1990, **283**, 484-490 (*Brassica juncea leaves*)
Alfonso, J.D. *et al., Biochim. Biophys. Acta*, 1997, **1341**, 173-182 (*Saccharomyces cerevisiae*)
Craig, S.P. *et al., J. Biol. Chem.*, 2000, **275**, 20231-20234 (*rev*)
Silva, M. *et al., Biochim. Biophys. Acta*, 2004, **1696**, 31-39 (*Leishmania tarentolae*)

Adenosine, 9CI, 8CI, BAN, USAN A-209

*9-β-D-Ribofuranosyl-9*H-*purin-6-amine, 9CI. 9-β-D-Ribofuranosyladenine, 8CI. 6-Amino-9-β-D-ribofuranosyl-9*H-*purine. Adenocard. Adenocor. Adenoscan. SR 96225* [58-61-7]



$C_{10}H_{13}N_5O_4$ 267.244
Cryst. (H_2O). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. Mp 234-236°. $[\alpha]_D^{11}$ -61.7 (c, 0.7 in H_2O). pK_{a1} 3.6; pK_{a2} 12.4 (25°). Log P -2.88 (calc). Component of numerous preparations. λ_{max} 259 (ϵ 15400) (H_2O). λ_{max} 260 (ϵ 15100) (H_2O) (Berdy).

▶ LD_{50} (mus, ipr) 500 mg/kg. AU7175000

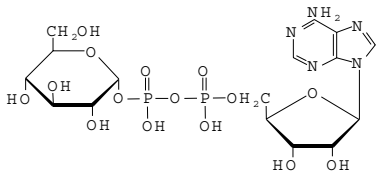
5′-O-*(4-Hydroxy*-E-*cinnamoyl):* [903574-32-3] *5′*-O-trans-p-*Coumaroyladenosine.* ***Amaricin***
$C_{19}H_{19}N_5O_6$ 413.389
Constit. of *Amaranthus spinosus* (spiny amaranth).

[3080-29-3]

Azhar-ul-Haq, *et al., Pol. J. Chem. (Rocz. Chem.)*, 2006, **80**, 259-263 (*Amaricin*)

Adenosine diphosphate glucose A-210

Adenosine 5′-(trihydrogen diphosphate) mono-α-D-glucopyranosyl ester, 9CI. ADPG [2140-58-1]



$C_{16}H_{25}N_5O_{15}P_2$ 589.345

Present in ripening cereal grains. λ_{max} 257 nm (pH 2). λ_{max} 259 (ϵ 15400) (H_2O) (as di-K salt). λ_{max} 257 (dil. acid) (pH2).

Roseman, S. *et al., JACS*, 1961, **83**, 659
Murata, T. *et al., Arch. Biochem. Biophys.*, 1964, **106**, 371 (*isol, synth*)
Frydman, R.B. *et al., Biochim. Biophys. Acta*, 1966, **113**, 620 (*occur*)
Krauss, G. *et al., J. Chromatogr.*, 1973, **76**, 248 (*chromatog*)
Sarma, R.H. *et al., FEBS Lett.*, 1973, **36**, 157 (*nmr*)
Lee, C.H. *et al., Biochemistry*, 1976, **15**, 697 (*conformn, pmr*)

Adenosine kinase A-211

E.C. 2.7.1.20. ATP:adenosine 5′-phosphotransferase [9027-72-9]

Phosphotransferase enzyme with alcohol acceptor. Isol. from cow, baker's yeast, wheat and spinach.

Kornberg, A. *et al., J. Biol. Chem.*, 1951, **193**, 481-495 (*metab*)
Lindberg, B. *et al., J. Biol. Chem.*, 1967, **242**, 350-356 (*mammals*)
Leibach, T.K. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1971, **352**, 328-344 (*Saccharomyces cerevisiae*)
Chen, C.M. *et al., Plant Physiol.*, 1977, **59**, 443-447 (*Triticum aestivum, Nicotiana tabacum*)
Rudolph, F.B. *et al., Methods Enzymol.*, 1979, **63**, 22-42 (*assay*)
Yamada, Y. *et al., Biochim. Biophys. Acta*, 1981, **660**, 36-43 (*human*)
Eckstein, F. *et al., Methods Enzymol.*, 1982, **87**, 192-212 (*stereochem*)
Rotllan, P. *et al., Eur. J. Biochem.*, 1985, **151**, 365-371 (*cow*)
Long, M.C. *et al., J. Bacteriol.*, 2003, **185**, 6548-6555 (*Mycobacterium tuberculosis*)
Schoor, S. *et al., Front. Biosci.*, 2004, **9**, 1771-1781 (*plants*)
Reddy, M.C. *et al., J. Biol. Chem.*, 2007, **282**, 27334-27342 (*Mycobacterium tuberculosis*)
Park, J. *et al., Cell. Mol. Life Sci.*, 2008, **65**, 2875-2896 (*plants*)

Adenosine nucleosidase A-212

E.C. 3.2.2.7. Adenosine ribohydrolase. Adenosine hydrolase. Adenosinase [9075-41-6]

N-Glycosyl hydrolase enzyme. Isol. from plants, e.g. barley, Jerusalem artichoke, wheat, tea, coffee. *Helianthus tuberosus* Enzyme activity range pH 5.0-7.0. Wheat enzyme stored at -20° retains 95% activity after 1 month.

Guranowski, A. *et al., Biochim. Biophys. Acta*, 1977, **482**, 145-158 (*barley*)
Imagawa, H. *et al., Agric. Biol. Chem.*, 1979, **43**, 2337-2342 (*tea*)
Le Floc'h, F. *et al., Phytochemistry*, 1981, **20**, 2127-2129 (*Helianthus tuberosus, activity*)
Chen, C.M. *et al., Plant Physiol.*, 1981, **68**, 1020-1023 (*wheat, stability*)
Campos, A. *et al., Phytochemistry*, 2005, **66**, 147-151 (*coffee*)

Adenosylhomocysteinase A-213

E.C. 3.3.1.1. S-*Adenosyl-L-homocysteine hydrolase.* S-*Adenosylhomocysteine synthase. AdoHcyase. SAHase* [9025-54-1]

Ether hydrolase enzyme. Isol. from rabbit, chicken, spinach and cereals, e.g. barley, maize. Human enzyme activity range pH 6.0-8.0. Storage at -70°, 1-2 mg enzyme/ml, results in 10% loss of activity over 6 months.

Walker, R.D. *et al., Can. J. Biochem.*, 1975, **53**, 312-319 (*animals, spinach, barley, maize*)
Shimizu, S. *et al., Eur. J. Biochem.*, 1984, **141**, 385-392 (*prokaryotes*)
Hershfield, M.S. *et al., Biochem. J.*, 1985, **230**, 43-52 (*human, stability*)
Guranowski, A. *et al., Methods Enzymol.*, 1987, **143**, 430-434 (*Lupinus luteus*)
Nakanishi, M. *et al., J. Biochem. (Tokyo)*, 2001, **129**, 101-105 (*human, activity*)
Tanaka, N. *et al., J. Mol. Biol.*, 2004, **343**, 1007-1017 (*cryst struct, Plasmodium*)

Adenosylmethionine cyclotransferase A-214

E.C. 2.5.1.4. S-*Adenosyl-L-methionine alkyltransferase (cyclising). Adenosylmethioninase* [9030-34-6]

Alkyltransferase enzyme. Isol. from baker's yeast.

Mudd, S.H. *et al., J. Biol. Chem.*, 1959, **234**, 87-92; 1784-1786 (*isol*)

Adenosylmethionine hydrolase A-215

E.C. 3.3.1.2. S-*Adenosyl-L-methionine hydrolase. Methylmethionine sulfonium salt hydrolase.* S-*Adenosylmethionine cleaving enzyme. Adenosylmethionine lyase* [37288-62-3]

Ether hydrolase enzyme. Isol. from cabbage. *Corynebacterium* Enzyme activity range pH 6.0-8.0. Stable for 3 months at -10°.

Mazelis, M. *et al., Biochim. Biophys. Acta*, 1965, **105**, 106-114 (*Corynebacterium, activity, stability*)
Gefter, M.L. *et al., Methods Enzymol., Part B*, 1971, **17**, 406-411 (*rev, Escherichia coli*)
Spoerel, N. *et al., Eur. J. Biochem.*, 1979, **95**, 227-233 (*Bacteriophage T3*)
Hughes, J.A. *et al., J. Bacteriol.*, 1987, **169**, 3625-3632 (*Bacteriophage T3*)
Takigawa, S. *et al., Acta Horticult.*, 2000, **517**, 457-462 (*cabbage*)

Adenylate kinase A-216

E.C. 2.7.4.3. ATP:AMP phosphotransferase. Myokinase. 5′-AMP kinase. Adenylic kinase. Adenylokinase [9013-02-9]

Phosphotransferase enzyme with phosphate acceptor. Isol. from cow, pig, rabbit, maize, wheat and lemon. Inorganic triphosphate, dATP and dAMP can also act as substrates. Human enzyme exhibits approx. 50% maximal activity at pH 6.5 and pH 8.2. At -20°, stable for several weeks, but at -20° in ammonium sulfate soln. stable for a prolonged period.

Noda, L. *et al., The Enzymes*, 2nd edn., (eds. Boyer, P.D. *et al*), Academic Press, 1962, **6**, 139-149 (*mammals, plants*)
Khoo, J.C. *et al., Biochim. Biophys. Acta*, 1972, **268**, 98-101 (*human, rabbit*)
Noda, L. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1973, **8**, 279-305 (*mammals, plants*)
Itakura, T. *et al., Eur. J. Biochem.*, 1978, **82**, 431-437 (*pig*)
Criss, W.E. *et al., Methods Enzymol.*, 1978, **51**, 459-467 (*rat*)
Kuby, S.A. *et al., J. Biol. Chem.*, 1983, **258**, 1901-1907 (*human, cow*)
Hall, S.W. *et al., Eur. J. Biochem.*, 1986, **161**, 551-556 (*cow*)
Kleczkowski, L.A. *et al., Plant Physiol.*, 1986, **81**, 1110-1114 (*maize*)
Kleczkowski, L.A. *et al., Z. Naturforsch., C*, 1990, **45**, 607-613 (*maize*)
Ren, H. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2005, **102**, 303-308 (*cryst struct, human*)

Adenylyl sulfate kinase A-217

E.C. 2.7.1.25. ATP:adenylyl sulfate 3′-phosphotransferase. Adenosine phosphosulfokinase. Adenosine 5′-phosphosulfate 3′-phosphokinase. APS kinase [9012-38-8]

Phosphotransferase enzyme with alcohol acceptor. Isol. from baker's yeast. In humans, the phosphoadenosine-phosphosulfate synthase (PAPS) system is a bifunctional enzyme. By contrast, in bacteria, fungi and plants formn. of PAPS is carried out by two individual polypeptides, E.C. 2.7.1.25 and Sulfate adenylyltransferase, S-398.

Robbins, P.W. *et al., J. Biol. Chem.*, 1957, **229**, 837-851 (*isol*)
Schriek, U. *et al., Arch. Microbiol.*, 1986, **145**, 32-38 (*Escherichia coli, Saccharomyces cerevisiae*)
Hommes, F.A. *et al., Biochim. Biophys. Acta*, 1987, **924**, 270-275 (*rat*)
Venkatachalam, K.V. *et al., J. Biol. Chem.*, 1998, **273**, 19311-19320 (*human, bifunctional enzyme*)
MacRae, I.J. *et al., Biochemistry*, 2000, **39**, 1613-1621 (*Penicillium chrysogenum*)
Harjes, S. *et al., Acta Cryst. D*, 2004, **60**, 350-352 (*human, cryst struct*)
Yu, Z. *et al., J. Mol. Biol.*, 2007, **365**, 732-745 (*Aquifex aeolicus, cryst struct*)

Adenylylsulfate ammonia adenylyltransferase A-218

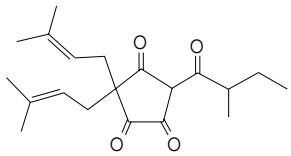
E.C. 2.7.7.51. Adenylyl sulfate:ammonia adenylyltransferase. APSAT [79121-94-1]

Nucleotidyltransferase enzyme. Isol. from barley and spinach.

Frankhauser, H. *et al., Plant Physiol.*, 1979, **63S**, 162 (*microorganisms, plants*)
Frankhauser, H. *et al., Plant Physiol.*, 1979, **65S**, 17 (*Chlorella*)
Frankhauser, H. *et al., Biochem. J.*, 1981, **195**, 545-560 (*Escherichia coli, barley, spinach, Dictyostelium discoideum*)

Frankhauser, H. *et al., Methods Enzymol.*, 1987, **143**, 354-361 (*Escherichia coli, barley, spinach, Dictyostelium discoideum*)

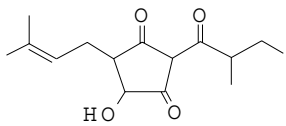
Adhulupone A-219



$C_{20}H_{28}O_4$ 332.439
Minor constit. of hops. Oil. $Bp_{0.007}$ 130°.

Brown, P.M. *et al., JCS*, 1964, 4774 (*struct*)
Gienapp, E. *et al., Food/Nahrung*, 1975, **19**, 697 (*struct*)

Adhumulinic acid A-220

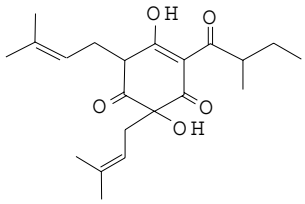


$C_{15}H_{22}O_4$ 266.336
Constit. of hops. Cryst. (petrol). Mp 83°.

Rigby, F.L. *et al., JACS*, 1955, **77**, 2828

Adhumulone A-221

[28374-89-2]



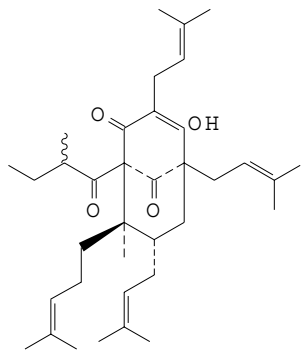
$C_{21}H_{30}O_5$ 362.465
Tautomeric. Constit. of hops. Viscous oil. Sol. MeOH, Et_2O; fairly sol. H_2O. $[\alpha]_D$ -187 (MeOH). λ_{max} 236; 288; 323 (HCl) (Berdy). λ_{max} 325; 360 (NaOH) (Berdy).

[31769-65-0, 71800-99-2]

Molyneux, R.J. *et al., J. Agric. Food Chem.*, 1975, **23**, 1201

Adhyperforin A-222

[143183-63-5]

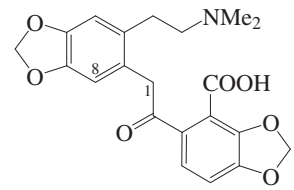


$C_{36}H_{54}O_4$ 550.82
Constit. of *Hypericum perforatum* (St Johns Wort). λ_{max} 292 (ϵ 9450) (MeOH). λ_{max} 275 (ϵ 8150) (MeOH/HCl). λ_{max} 297 (ϵ 11200) (MeOH/NaOH).

Maisenbacher, P. *et al., Planta Med.*, 1992, **58**, 291-293 (*Adhyperforin*)
Bilia, A.R. *et al., J. Agric. Food Chem.*, 2001, **49**, 2115-2124 (*pmr, cmr*)
Jensen, A.G. *et al., Life Sci.*, 2001, **68**, 1593-1605 (*activity*)
Sleno, L. *et al., Rapid Commun. Mass Spectrom.*, 2006, **20**, 2641-2648 (*ms*)
Karppinen, K. *et al., Phytochemistry*, 2007, **68**, 1038-1045 (*biosynth*)

Adlumidiceine A-223

5-[[6-[2-(Dimethylamino)ethyl]-1,3-benzodioxol-5-yl]acetyl]-1,3-benzodioxole-4-carboxylic acid, 9CI [51059-65-5]



$C_{21}H_{21}NO_7$ 399.399
Alkaloid from *Papaver rhoeas* (corn poppy). Cryst. (MeOH). Mp 244-246°. λ_{max} 232 (sh) (log ϵ 4.14); 294 (log ϵ 3.87); 306 (sh) (log ϵ 3.75) (EtOH).

1-Hydroxy: [116368-95-7] ***Narceimicine***
$C_{21}H_{21}NO_8$ 415.399
Pale yellow granules (MeOH aq.). Mp 242-246° dec. Shown in the paper as the enediol tautomer.

1-Hydroxy, Me ester: [169626-17-9] ***Paprafumine***
$C_{22}H_{23}NO_8$ 429.426
Amorph. solid. Shown in the paper as the enediol tautomer.

1-Oxo: [59443-00-4] ***Narceimine****. Bicuculline. Alkaloid F45*
$C_{21}H_{19}NO_8$ 413.383
Mp 268° (259-260°). λ_{max} 228 (log ϵ 4.1); 300 (log ϵ 4.38); 310 (sh) (log ϵ 4.18); 330 (log ϵ 4.42) (MeOH).

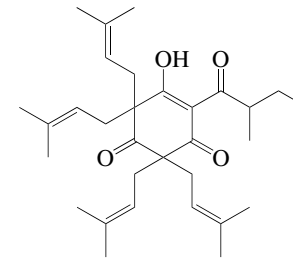
1-Oxo, Me ester: Mp 188°.

1-Oxo, N-*Me:* [777007-71-3] **N-*Methylnarceimine***. N-*Methylnarceimicine (incorr.)*
$C_{22}H_{22}NO_8^{\oplus}$ 428.418
Yellow cryst. (MeOH). Mp 194-196°. Counterion not specified. λ_{max} 207 (log ϵ 4.48); 331 (log ϵ 4.02) (MeOH).

Preininger, V. *et al., Phytochemistry*, 1973, **12**, 2513-2515 (*ir, uv, pmr, ms, struct*)
Preininger, V. *et al., Coll. Czech. Chem. Comm.*, 1975, **40**, 699-704 (*ir, uv, pmr, ms, struct*)
Rodrigo, R.G.A. *et al., Can. J. Chem.*, 1976, **54**, 471-472 (*isol, ir, pmr, cmr, ms, struct, Narceimine*)
Seth, K.K. *et al., Chem. Ind. (London)*, 1979, 744-745 (*ir, uv, pmr, ms, struct, Narceimine*)
Popova, M.E. *et al., Planta Med.*, 1982, **45**, 120-122 (*isol*)
Tripathi, Y.C. *et al., Phytochemistry*, 1988, **27**, 1918-1919 (*Narceimicine, isol, ir, uv, pmr, ms, struct*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1995, **40**, 593-596 (*Parafumine*)
Wu, Y.-R. *et al., Planta Med.*, 2007, **73**, 787-791 (*N-Methylnarceimine*)

Adlupone A-224

[16595-43-0]

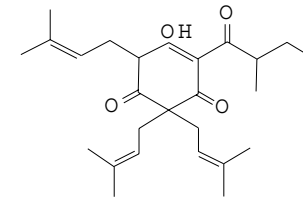


$C_{31}H_{46}O_4$ 482.702
Constit. of hops. Mp 45°. $Bp_{0.002}$ 150-155° (bath).

Laws, D.R.J. *et al., JCS*, 1965, 6542-6543 (*synth*)

Adlupulone A-225

[28374-71-2]

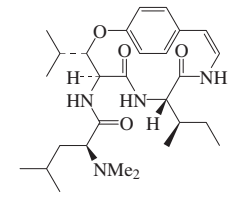


$C_{26}H_{38}O_4$ 414.584
Constit. of hops. Cryst. (MeOH). Sol. MeOH, Et_2O; fairly sol. H_2O. Mp 82-83°.

Howard, G.A. *et al., JCS*, 1955, 174 (*struct*)
Brown, P.M. *et al., JCS*, 1964, 4774 (*synth*)
Kowaka, M. *et al., Proc. Conv. - Inst. Brew. (Aust. N.Z. Sect.)*, 1970, **11**, 35 (*isol*)

Adouetine X A-226

Ceanothamine B [19542-37-1]



Absolute Configuration

$C_{28}H_{44}N_4O_4$ 500.68
Alkaloid from *Ceanothus americanus* (New Jersey tea) and *Zizyphus jujuba* var. *inermis*. Needles (MeOH or CH_2Cl_2/EtOAc). Mp 279-280.5°. $[\alpha]_D^{25}$ -370 (c, 0.205 in $CHCl_3$).

N-*De-Me:* [96562-84-4] ***Discarine F***. N-*Demethyladouetine X*
$C_{27}H_{42}N_4O_4$ 486.653
Mp 264°. $[\alpha]_D^{20}$ -191 ($CHCl_3$).

Païs, M. *et al., Ann. Pharm. Fr.*, 1963, **21**, 139-146 (*isol, ir, pmr*)

Warnhoff, E.W. *et al., Can. J. Chem.*, 1965, **43**, 2594-2602 (*isol, uv, ms, pmr*)
Païs, M. *et al., Bull. Soc. Chim. Fr.*, 1968, 1145-1148 (*uv, ir, pmr, ms, struct*)
Servis, R.E. *et al., JACS*, 1969, **91**, 5619-5624 (*isol, ms*)
Branch, G.B. *et al., Aust. J. Chem.*, 1972, **25**, 2209-2216 (*isol*)
Otsuka, H. *et al., Phytochemistry*, 1974, **13**, 2016 (*isol, ir, pmr, ms*)
Morel, A. *et al., Z. Naturforsch., B*, 1984, **39**, 1825 (*Discarine F*)

ADP-phosphoglycerate phosphatase A-227

E.C. 3.1.3.28. 3-(ADP)-2-phosphoglycerate phosphohydrolase [37288-12-3]

Phosphoric monoester hydrolase enzyme. Isol. from rabbit muscle. Also acts on 2,3-bisphosphoglycerate. Rabbit enzyme activity range pH 5.0-9.0.

Zancan, G.T. *et al., Biochim. Biophys. Acta*, 1964, **92**, 125-131 (*rabbit*)

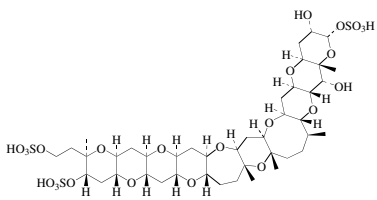
β-Adrenergic-receptor kinase A-228

E.C. 2.7.11.15. ATP:[β-adrenergic receptor] phosphotransferase. β-Receptor kinase. β-AR kinase. E.C. 2.7.1.126 (transferred) [102925-39-3]

Phosphotransferase enzyme. Isol. from cow. Requires G-protein for activation. Inhibited by $Zn^{2\oplus}$ and digitonin. Crude ox enzyme is stable for several months at 4°; purified enzyme has $t_{1/2}$ 5-10 days.

Benovic, J.L. *et al., J. Biol. Chem.*, 1987, **262**, 9026-9032; 17251-17253 (*cow*)
Benovic, J.L. *et al., FEBS Lett.*, 1991, **283**, 122-126 (*human*)
Benovic, J.L. *et al., Methods Enzymol.*, 1991, **200**, 351-362 (*cow*)
Penn, R.B. *et al., J. Biol. Chem.*, 1994, **269**, 14924-14930 (*human*)
Inglese, J. *et al., Methods Enzymol.*, 1995, **250**, 149-158 (*rev*)
Jaber, M. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1996, **93**, 12974-12979 (*mouse*)
Laugwitz, K.L. *et al., Cardiovasc. Res.*, 1997, **35**, 324-333 (*rat, hamster*)
Lodowski, D.T. *et al., Acta Cryst. D*, 2003, **59**, 936-939 (*cow, cryst struct*)

Adriatoxin A-229

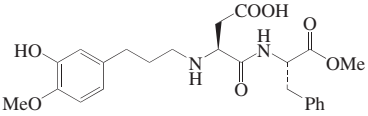


$C_{42}H_{66}O_{24}S_3$ 1051.167
Toxic constit. of the mussel *Mytilus galloprovincialis* from northern Adriatic Sea. λ_{max} 230 (MeOH) (Berdy).

Ciminiello, P. *et al., Tet. Lett.*, 1998, **39**, 8897-8900 (*isol, pmr*)
Briggs, L.R. *et al., J. Agric. Food Chem.*, 2004, **52**, 5836-5842 (*detn*)

Advantame A-230

N-*[N-[3-(3-Hydroxy-4-methoxyphenyl)-propyl]-α-aspartyl]phenylalanine methyl ester. 4-[(1-Benzyl-2-methoxy-2-oxoethyl)amino]-3-[3-(3-hydroxy-4-methoxyphenyl)propylamino]-4-oxobutanoic acid. FEMA 4716. ANS 9801* [714229-20-6]



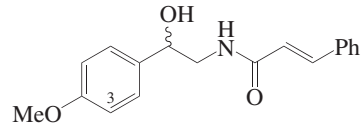
Absolute Configuration

$C_{24}H_{30}N_2O_7$ 458.51
High intensity sweetener, >20,000 x sucrose. Solid.

US Pat., 2003, (*Ajinomoto*)6 652 901 (*FEMA 4716, synth, use, pmr*)
Amino, Y. *et al., ACS Symp. Ser.*, 2008, **979**, 463-480 (*synth*)
Bishay, I.E. *et al., Alternative Sweeteners*, 4th edn. (ed. O'Brien-Nabors, L.), CRC Press, 2011, 31-45 (*rev*)
Renwick, A. *et al., Food Chem. Toxicol.*, Suppl.1, 2011, **49**, S1-S84 (*rev*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4716, use*)

Aegeline A-231

N-*[2-Hydroxy-2-(4-methoxyphenyl)ethyl]-3-phenyl-2-propenamide, 9CI. N-β-Hydroxy-β-*p*-methoxyphenethylcinnamamide. N-Cinnamoyl-2-hydroxy-2-(4-methoxyphenyl)ethylamine. Cinnamic acid 2-hydroxy-2-(*p*-methoxyphenyl)ethylamide. Egeline* [456-12-2]



$C_{18}H_{19}NO_3$ 297.353
Originally assigned the formula $C_{18}H_{18}O_4$.

(+)-form [15298-36-9]
Cryst. (EtOH). Mp 196-197°. $[\alpha]_D^{22}$ +36 (c, 0.4 in $CHCl_3$). $[\alpha]_D^{21}$ -48.1 (c, 0.5 in EtOH).

(-)-form [15298-37-0]
Cryst. (EtOH). Mp 196-197°. $[\alpha]_D$ -35.1 ($CHCl_3$). $[\alpha]_D$ +47.5 (c, 0.5 in EtOH).

(±)-form [37791-13-2]
Alkaloid from the leaves of *Aegle marmelos* (bael). Cryst. (EtOH/EtOAc). Mp 176° (173-175°).

Ac:
$C_{20}H_{21}NO_4$ 339.39
Plates (EtOAc). Mp 124°.

Me ether: [70546-93-9] N-*[2-Methoxy-2-(4-methoxyphenyl)ethyl]cinnamide. 7-O-Methylaegeline*
$C_{19}H_{21}NO_3$ 311.38
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 135°. Artifact.

Et ether: [70546-94-0] N-*[2-Ethoxy-2-(4-methoxyphenyl)ethyl]cinnamide*
$C_{20}H_{23}NO_3$ 325.407
Isol. from *Aegle marmelos* (bael). Cryst. (C_6H_6/hexane). Mp 99-100°. Artifact.

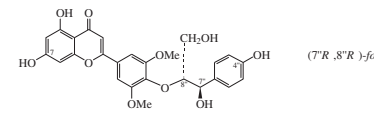
3-Methoxy: ***3-Methoxyaegeline***
$C_{19}H_{21}NO_4$ 327.379
Cryst. (EtOAc/MeOH). Mp 138-139°. λ_{max} 218 (log ϵ 4.37); 225 (log ϵ 4.57); 278 (log ϵ 4.65) (MeOH).

3-Methoxy, Ac: ***7-O-Acetyl-3-methoxyaegeline***
$C_{21}H_{23}NO_5$ 369.416
Pale yellow powder. λ_{max} 242 (log ϵ 4.82); 252 (log ϵ 4.67); 282 (log ϵ 4.98) (MeOH).

Chatterjee, A. *et al., JOC*, 1959, **24**, 687 (*isol, uv, ir, struct, synth*)
Albónico, S.M. *et al., JCS(C)*, 1967, 1327 (*synth*)
Della Casa de Marcano, D. *et al., Phytochemistry*, 1972, **11**, 1531 (*isol*)
Manandhar, M.D. *et al., Phytochemistry*, 1978, **17**, 1814 (*derivs*)
Patra, A. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 385 (*isol, uv, ir*)
Swinehart, J. *et al., Phytochemistry*, 1980, **19**, 1219 (*isol*)
Patra, A. *et al., Org. Magn. Reson.*, 1981, **16**, 65 (*cmr*)
Sharma, B.R. *et al., Phytochemistry*, 1981, **20**, 2606 (*isol*)
Somanathan, R. *et al., Synth. Commun.*, 1983, **13**, 273 (*synth, ir, ms, pmr, cmr*)
Brown, R.F.C. *et al., Tetrahedron: Asymmetry*, 1993, **4**, 205 (*synth*)
Ross, S.A. *et al., J. Nat. Prod.*, 2005, **68**, 1297-1299 (*3-Methoxyaegeline, 7-Acetyl-3-methoxyaegeline*)
Narender, T. *et al., Bioorg. Med. Chem. Lett.*, 2007, **17**, 1808-1811 (*isol, activity*)
Faizi, S. *et al., Tetrahedron*, 2009, **65**, 998-1004 (*isol, pmr, cmr, ms*)

Aegicin A-232

*5,7-Dihydroxy-2-[4-[2-hydroxy-1-hydroxymethyl-2-(4-hydroxyphenyl)ethoxy]-3,5-dimethoxyphenyl]-4*H*-1-benzopyran-4-one, 9CI. Tricin 4′-*O*-(β-4-hydroxyphenylglyceryl) ether*



(7″R,8″R)-form

$C_{26}H_{24}O_{10}$ 496.47
Flavonolignan.

(7″R*,8″R*)-form [1217897-50-1]
threo-*form*. ***Calquiquelignan E***
Amorph. powder. Mp 247°. $[\alpha]_D^{25}$ +27 (c, 0.48 in MeOH). λ_{max} 201; 271; 329 (sh) (MeOH).

2S,3-Dihydro: [1217897-49-8] *Dihydrotricin 4′-O-(β-4-hydroxyphenylglyceryl) ether.* ***Calquiquelignan C***
$C_{26}H_{26}O_{10}$ 498.485
Pale yellow powder. Mp 146°. $[\alpha]_D^{25}$ -16 (c, 0.06 in MeOH). λ_{max} 202; 230; 286; 330 (sh) (MeOH).

3″-Methoxy: [369390-51-2] *Tricin 4′-O-(β-guaiacylglyceryl) ether.* ***Salcolin A***
$C_{27}H_{26}O_{11}$ 526.496
Isol. from oats (*Avena sativa*). Yellow solid. $[\alpha]_D^{24}$ -10 (c, 0.05 in MeOH). λ_{max} 272; 287 (sh); 303 (sh); 334 (MeOH).

*3″-Methoxy, 7-*O*-β-D-glucopyranoside:* [462100-43-2]
$C_{33}H_{36}O_{16}$ 688.638
Yellow solid. λ_{max} 270; 287 (sh); 340 (MeOH).

3″-Methoxy, 9″-Ac: [629646-28-2]
$C_{29}H_{28}O_{12}$ 568.533
Amorph. yellow solid. $[\alpha]_D^{20}$ -48.5 (c, 0.11 in MeOH). λ_{max} 310 (log ϵ 4.06) (MeOH).

*3″-Methoxy, 9″-*O*-(4-hydroxy-*E*-cinnamoyl):* [629646-41-9]
$C_{36}H_{32}O_{13}$ 672.641
Amorph. yellow solid. $[\alpha]_D^{20}$ +52.1 (c, 0.48 in MeOH). λ_{max} 312 (log ϵ 4.58) (MeOH).

3″-Methoxy, 7″-Me ether, 9″-Ac: [629646-35-1]
$C_{30}H_{30}O_{12}$ 582.56
Amorph. yellow solid. $[\alpha]_D^{20}$ +5.8 (c, 0.41 in MeOH). λ_{max} 272 (log ϵ 4.39); 322 (log ϵ 4.4) (MeOH).

*3″-Methoxy, 2*S*,3-dihydro:* [1217897-48-7] *Dihydrotricin 4′-*O*-(β-guaiacylglyceryl) ether.* ***Calquiquelignan B***
$C_{27}H_{28}O_{11}$ 528.512
Pale orange powder. Mp 118°. $[\alpha]_D^{25}$ +70 (c, 1.1 in MeOH). λ_{max} 203; 230; 288; 330 (sh) (MeOH).

(7″R*,8″S*)-form [65870-44-2]
erythro-*form.* ***Calquiquelignan D***
Cryst. ($CHCl_3$/MeOH). Mp 235-236° (218°). $[\alpha]_D^{25}$ -58 (c, 0.48 in MeOH) (Calquiquelignan D).

Penta-Ac: Mp 163-164°.

3″-Methoxy: [369390-52-3] ***Salcolin B***
Isol. from oats (*Avena sativa*). Yellow solid. $[\alpha]_D^{24}$ +15 (c, 0.05 in MeOH). λ_{max} 271; 288 (sh); 305 (sh); 335 (MeOH).

*3″-Methoxy, 7-*O*-β-D-glucopyranoside:* [462100-42-1]
Yellow solid. λ_{max} 270; 287 (sh); 340 (MeOH).

3″-Methoxy, 9″-Ac: [629646-32-8]
Amorph. yellow solid. $[\alpha]_D^{20}$ -70 (c, 0.15 in MeOH). λ_{max} 322 (log ϵ 3.94) (MeOH).

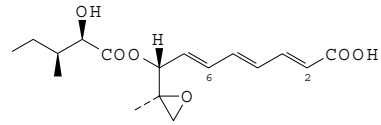
*3″-Methoxy, 9″-*O*-(4-hydroxy-*E*-cinnamoyl):* [629646-44-2]
Amorph. yellow solid. $[\alpha]_D^{20}$ -30.4 (c, 1.3 in dioxan). λ_{max} 310 (log ϵ 4.57) (MeOH).

3″-Methoxy, 7″-Me ether, 9″-Ac: [629646-37-3]
Amorph. yellow solid. $[\alpha]_D^{20}$ -13.8 (c, 0.25 in MeOH). λ_{max} 271 (log ϵ 4.21); 335 (log ϵ 4.2) (MeOH).

*3″-Methoxy, 2*S*,3-dihydro:* [1217897-47-6] ***Calquiquelignan A***
$C_{27}H_{28}O_{11}$ 528.512
Pale yellow powder. Mp 204°. $[\alpha]_D^{25}$ -33 (c, 0.21 in MeOH). λ_{max} 203; 230; 288; 330 (sh) (MeOH).

Cooper, R. *et al., Isr. J. Chem.*, 1977, **16**, 12-15 (*Aegicin*)
Syrchina, A.I. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1992, **28**, 155-158 (*Salcolins A,B*)
Bouaziz, M. *et al., Phytochemistry*, 2002, **60**, 515-520 (*Hyparrhenia hirta constits*)
Nakajima, Y. *et al., Tetrahedron*, 2003, **59**, 8011-8015 (*Sasa veitchii constits*)
Wenzig, E. *et al., J. Nat. Prod.*, 2005, **68**, 289-292 (*Salcolins A,B*)
Chang, C.-L. *et al., Phytochemistry*, 2010, **71**, 271-279 (*Calquiquelignans*)

AF Toxin II A-233



$C_{17}H_{24}O_6$ 324.373
Prod. by *Alternaria alternata* on strawberry. Phytotoxin specific to strawberry and pear.

(2E,4E,6E)-form [104420-17-9]
AF Toxin IIc
Oil (as Et ester). $[\alpha]_D^{23}$ -4.4 (c, 0.9 in EtOH) (Et ester). λ_{max} 289 (ϵ 27000) (MeOH) (Derep).

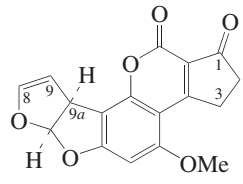
(2E,4E,6Z)-form [104363-99-7]
AF Toxin IIa
Oil (as Et ester). $[\alpha]_D^{23}$ +153 (c, 0.78 in EtOH) (Et ester). Major component of AF toxin complex. λ_{max} 289 (ϵ 27000) (MeOH) (Derep).

(2E,4Z,6E)-form
AF Toxin IIb λ_{max} 289 (ϵ 27000) (MeOH) (Derep).

Maekawa, N. *et al., Nippon Shokubutsu Byori Gakkaiho*, 1984, **50**, 610 (*props*)
Nakatsuka, S.-I. *et al., Tet. Lett.*, 1986, **27**, 2753 (*isol, struct*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2545 (*synth*)
Crombie, L. *et al., JCS Perkin 1*, 1991, 1511 (*synth*)

Aflatoxin B_1 A-234

*2,3,6*a*,9*a*-Tetrahydro-4-methoxycyclopenta[c]furo[3,2′:4,5]furo[2,3-*h*][1]benzopyran-1,11-dione, 9CI. Aflatoxin FB_1. Aflatoxin B* [1162-65-8]



Absolute Configuration

$C_{17}H_{12}O_6$ 312.278
CAS numbering shown. Other schemes have been used. Prod. by *Aspergillus flavus* and *Aspergillus parasiticus.* Toxin causing Turkey X disease. One of the most potent carcinogens known in animals. Potential food contaminant esp. in grains and nuts. Cryst. with blue fluor. Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 268-269° dec. $[\alpha]_D^{25}$ -562 (c, 0.115 in $CHCl_3$). Dimorphic. λ_{max} 220 (ϵ 25600); 265 (ϵ 13400); 362 (ϵ 21800) (MeOH) (Berdy). λ_{max} 223 (ϵ 25100); 265 (ϵ 13400); 362 (ϵ 21800) (EtOH) (Berdy).

▶ Human and exp. carcinogen; LD_{50} (rat, orl) 5 mg/kg. Exp. reprod. and teratogenic effects. Hepatotoxic. Crystalline material, e.g. from preparative tlc plates, presents an inhalation hazard because the crystals develop electrostatic charge and cling to dust particles. GY1925000

O-*De-Me:* [32215-02-4] ***Aflatoxin P_1***
$C_{16}H_{10}O_6$ 298.251
Metab. of Aflatoxin B_1. Pale yellow needles (MeOH/C_6H_6/hexane). Mp 320°. $[\alpha]_D^{20}$ -574 (c, 0.08 in MeOH).

▶ GY1775000

8α,9α-Epoxide: [67337-06-8]
$C_{17}H_{12}O_7$ 328.278
Prob. ultimate carcinogen of Aflatoxin B_1. Cryst. (Me_2CO/CH_2Cl_2). Mp 300° (phase transition at 230°). Stable at -10°, fairly stable at r.t.

▶ Presumed highly toxic and carcinogenic.

*1*R*-Alcohol:* [61740-00-9] *Aflatoxicol B. Aflatoxicol R_0*
Cryst. (C_6H_6/hexane). Dec. over broad range starting at 233°.

▶ GY1945000

*1*S*-Alcohol:* [29611-03-8] *Aflatoxicol A. Aflatoxin R_0*
Cryst. (C_6H_6/hexane). Mp 224-226°.

▶ Exp. carcinogen. GY1934000

8,9-Dihydro: [7220-81-7] ***Aflatoxin B_2***
$C_{17}H_{14}O_6$ 314.294
Metab. of *Aspergillus flavus.* Yellow cryst. with blue fluor. (MeOH). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 310° dec. $[\alpha]_D^{23}$ -492 (c, 0.1 in $CHCl_3$). λ_{max} 222 (ϵ 19600); 265 (ϵ 9200); 363 (ϵ 14700) (MeOH) (Berdy). λ_{max} 220 (ϵ 20800); 265 (ϵ 12700); 363 (ϵ 24000) (EtOH) (Berdy).

▶ Human and exp. carcinogen. LD_{50} (dck, orl) 1.7 mg/kg. Hepatotoxic. GY1722000

8,9-Dihydro, 8ξ-hydroxy: [17878-54-5] ***Aflatoxin B_{2a}.*** *Dihydrohydroxyaflatoxin B_1. Aflatoxin B_1-W*
$C_{17}H_{14}O_7$ 330.293
Metab. of *Aspergillus flavus.* Cryst. with blue fluor. ($CHCl_3$). Mp 217° (240° dec.).

▶ GY1718000

8,9-Dihydro, 8ξ-methoxy: [20421-12-9] ***Aflatoxin Ex_2B_1***
$C_{18}H_{16}O_7$ 344.32
Metab. of *Aspergillus flavus.* Cryst. ($CHCl_3$). Mp 240°. Doubtless and artifact of hemiacetal methylation.

8,9-Dihydro, 8ξ-ethoxy: [23402-20-2] ***Aflatoxin ExB_2***
$C_{19}H_{18}O_7$ 358.347
Isol. from *Aspergillus flavus.* Cryst. Mp 245°. Doubtless artifact.

2ξ-Hydroxy: [104700-21-2] ***Aflatoxin M_1***
$C_{17}H_{12}O_7$ 328.278
Isol. from cultures of *Aspergillus parasiticus.* Cryst.

3ξ-Hydroxy: [52819-96-2] ***Aflatoxin Q_1***
Mycotoxin. Metab. of Aflatoxin B. Cryst. ($CHCl_3$). Mp 265° dec., 280° dec.

▶ Carcinogen. GY1800000

9aα-Hydroxy: [6795-23-9] ***Aflatoxin M_1***
$C_{17}H_{12}O_7$ 328.278
Minor mycotoxin of *Aspergillus flavus*, also found in the milk of cows and sheep fed toxic meal. Metab. of Aflatoxin B_1, A-234. Cryst. (MeOH) exhibiting blue-violet fluor. Mp 299° dec. $[\alpha]_D^{20}$ -280 (c, 0.1 in DMF). λ_{max} 235 (ϵ 21200); 262 (ϵ 16300); 358 (ϵ 14000) (MeOH) (Berdy). λ_{max} 226; 265; 357 (EtOH) (Berdy).

▶ Exp. carcinogen. Hepatotoxic. Less potent carcinogen then Aflatoxin B_1. Possible human carcinogen (IARC 2B). GY1880000

9aα-Hydroxy, 8,9-dihydro: [6885-57-0] ***Aflatoxin M_2***
$C_{17}H_{14}O_7$ 330.293
Trace mycotoxin of *Aspergillus flavus*. Cryst. with violet fluor. (MeOH/$CHCl_3$). Mp 293° dec.

▶ GY1720000

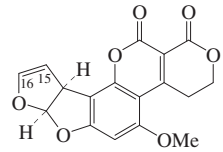
8,9-Dihydro. 8,9aα-dihydroxy: [36601-31-7] *Aflatoxin M_{2a}*
$C_{17}H_{14}O_8$ 346.293

[42583-46-0]

Asao, T. *et al., JACS*, 1965, **87**, 882-886 (*Aflatoxin B_1, struct, bibl*)
Dutton, M.F. *et al., Biochem. J.*, 1966, **101**, 21P-22P (*Aflatoxin B_{2a}*)
Holzapfel, C.W. *et al., Tet. Lett.*, 1966, **7**, 2799-2803 (*Aflatoxins M_1,M_2*)
Brechbühler-Bader, S. *et al., JOC*, 1967, **32**, 2641-2642 (*abs config*)
Roberts, J.C. *et al., JCS(C)*, 1968, 22-24 (*synth, uv, ir, ms*)
Lillehoj, E.B. *et al., Appl. Microbiol.*, 1969, **17**, 516-519 (*Aflatoxin B_{2a}*)
Dutton, M.F. *et al., Chem. Ind. (London)*, 1969, 983 (*Aflatoxin Ex_2B_1, Aflatoxin ExB_2*)
Büchi, G. *et al., JACS*, 1969, **91**, 5408-5409; 1971, **93**, 746-752; 1981, **103**, 3497-3501 (*Aflatoxin M_1, synth*)
Van Soest, T.C. *et al., Acta Cryst. B*, 1970, **26**, 1940-1947; 1947-1955 (*cryst struct, abs config*)
Cole, R.J. *et al., J. Agric. Food Chem.*, 1972, **20**, 1100-1102 (*Aflatoxicols*)
Stack, M.E. *et al., J. Assoc. Off. Anal. Chem.*, 1972, **55**, 313 (*Aflatoxin M_{2a}*)
Steyn, P.S. *et al., JCS Perkin 1*, 1974, 2551-2552 (*Aflatoxin Q_1*)
Büchi, G. *et al., JOC*, 1975, **40**, 3458-3460 (*Aflatoxin Q_1*)
IARC Monogr., 1976, **10**, 51; 1987, *Suppl. 6*, 40; *Suppl. 7*, 83 (*rev, tox*)
Pachler, K.G.R. *et al., JCS Perkin 1*, 1976, 1182-1189 (*cmr, biosynth*)
Pawlowski, N.E. *et al., J. Agric. Food Chem.*, 1977, **25**, 437-438 (*Aflatoxicols, synth*)
Cox, R.H. *et al., JOC*, 1977, **42**, 112-114 (*cmr*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*rev*)
Newton, M.G. *et al., J. Agric. Food Chem.*, 1979, **27**, 1339-1341 (*Aflatoxicols, stereochem, cryst struct*)
Brumley, W.C. *et al., Anal. Chem.*, 1981, **53**, 2003-2006 (*ms*)
Simpson, T.J. *et al., Chem. Comm.*, 1982, 631-632; 1983, 338-340 (*biosynth*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2220-2284 (*uv, ir, pmr, ms, cd*)
Moss, E.J. *et al., Biochem. Pharmacol.*, 1985, **34**, 3193-3197 (*metab*)
Castellino, A.J. *et al., JOC*, 1986, **51**, 1006-1011 (*Aflatoxin B_2, synth*)
Lafont, P. *et al., Microbiol., Aliments, Nutr.*, 1986, **4**, 65-74 (*Aflatoxin M_4*)
Weeratunga, G. *et al., Chem. Comm.*, 1988, 721-722 (*Aflatoxin B_2*)
Baertschi, S.W. *et al., JACS*, 1988, **110**, 7929-7931 (*epoxide*)
Townsend, C.A. *et al., JCS Perkin 1*, 1988, 839-861 (*biosynth*)
Sloan, C.P. *et al., Tet. Lett.*, 1988, **29**, 4685-4686 (*synth*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Horne, S. *et al., Chem. Comm.*, 1990, 39-41 (*Aflatoxin B_2, synth*)
Bhatnagar, D. *et al., Biochemistry*, 1991, **30**, 4343-4350 (*biosynth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1332
Koreeda, M. *et al., Synlett*, 1993, 555-556 (*Aflatoxin B_2, synth*)
Iyer, R.S. *et al., JACS*, 1994, **116**, 1603-1609 (*tox, activity*)
Chatterjee, M. *et al., JOC*, 1994, **59**, 4424-4429 (*biosynth*)
Toxicol. Aflatoxins, (eds. Eaton, D.L. *et al*), Academic Press, London, 1994, (*rev*)
Kraus, G.A. *et al., Tet. Lett.*, 1999, **40**, 8513-8514 (*Aflatoxin M_1, synth*)
Handbook of Secondary Fungal Metabolites, (ed. Cole, R.J. *et al*), Academic Press, 2003, **1**, 545-566
Henry, K.M. *et al., JACS*, 2005, **127**, 3300-3309 (*biosynth*)
Zhou, G. *et al., JACS*, 2005, **127**, 11958-11959 (*Aflatoxin B_2, synth*)
Eastham, S.A. *et al., Tetrahedron*, 2008, **64**, 936-948 (*Aflatoxin B_2, synth*)
IARC Monogr. (Web), http://monographs.iarc.fr
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEU250; AEW000; AEW500; AEU750

Aflatoxin G_1 A-235

Aflatoxin G [1165-39-5]



Absolute Configuration

$C_{17}H_{12}O_7$ 328.278
Mycotoxin prod. by *Aspergillus flavus* and *Aspergillus parasiticus*. Needles (MeOH) exhibiting green fluor. Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 257-259° (247-250°). $[\alpha]_D^{23}$ -556 (c, 0.1 in $CHCl_3$). λ_{max} 235 (ϵ 21200); 262 (ϵ 26300); 358 (ϵ 14000) (MeOH) (Berdy). λ_{max} 243 (ϵ 11500); 257 (ϵ 9900); 264 (ϵ 10000); 362 (ϵ 16100) (EtOH) (Berdy).

▶ Human and exp. carcinogen. LD_{50} (dck, orl) 0.79 mg/kg. LV1720000

15,16-Dihydro: [7241-98-7] ***Aflatoxin G_2***
$C_{17}H_{14}O_7$ 330.293
Minor mycotoxin prod. by *Aspergillus flavus*. Cryst. with green fluor. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. hexane. Mp 237-240°. $[\alpha]_D^{23}$ -473 (c, 0.084 in $CHCl_3$). λ_{max} 223; 265 (ϵ 11200); 363 (ϵ 19300) (EtOH) (Berdy).

▶ LD_{50} (dck, orl) 2.45 mg/kg. LV1700000

15,16-Dihydro, 16-hydroxy: [20421-10-7] ***Aflatoxin G_{2a}***
$C_{17}H_{14}O_8$ 346.293
Mycotoxin prod. by *Aspergillus flavus*. Cryst. with green fluor. Mp 190° dec.

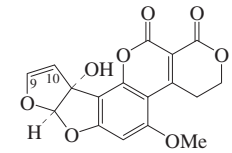
▶ LV1690000

15,16-Dihydro, 16-ethoxy: [23402-21-3] *Aflatoxin ExG*
$C_{19}H_{18}O_8$ 374.346
Mp 203°.

Nesbitt, B.E. *et al., Nature (London)*, 1962, **195**, 1062 (*isol*)
Asao, T. *et al., JACS*, 1963, **85**, 1706; 1965, **87**, 882 (*isol, uv, ir, ms, nmr, struct*)
Dutton, M.F. *et al., Biochem. J.*, 1966, **101**, 21P (*deriv*)
Brechbühler, S. *et al., JOC*, 1967, **32**, 2641 (*abs config*)
Dutton, M.F. *et al., Chem. Ind. (London)*, 1969, 983 (*Aflatoxin ExG*)
Büchi, G. *et al., JACS*, 1971, **93**, 746 (*uv, ms, synth*)
Heathcote, J.G. *et al., Chem. Ind. (London)*, 1976, 270 (*biosynth*)
IARC Monogr., 1976, **10**, 51; 1987, *Suppl. 6*, 49; *Suppl. 7*, 83; 1992, **56**, 245 (*rev, tox*)
Cox, R.H. *et al., JOC*, 1977, **42**, 112 (*cmr*)
Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*prop*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1332
Civitello, E.R. *et al., JOC*, 1994, **59**, 3775 (*synth, bibl*)
Toxicol. Aflatoxins, Eaton, D.L., *et al* Eds., Academic Press, London, 1994,
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 25; 45; 55
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEV000; AEV500

Aflatoxin GM_1 A-236

*3,4,7*a,*10*a-*Tetrahydro-10*a-*hydroxy-5-methoxy-1*H,*12*H-*furo[3′,2′:4,5]furo[2,3*-h*]pyrano[3,4-*c*][1]benzopyran-1,12-dione, 9CI* [23532-00-5]



Absolute Configuration

$C_{17}H_{12}O_8$ 344.277
Mycotoxin prod. by *Aspergillus flavus*. Cryst. ($CHCl_3$). Mp 276°.

Ac: Mp 280°.

9,10-Dihydro: ***Aflatoxin GM_2***
$C_{17}H_{14}O_8$ 346.293
Minor mycotoxin of *Aspergillus flavus*. Mp 270-272°.

Heathcote, J.G. *et al., Tetrahedron*, 1969, **25**, 1497 (*isol, uv, struct*)
IARC Monogr., 1972, **1**, 145; 1976, **10**, 51; 1987, *Suppl. 7*, 83 (*rev, tox*)
Heathcote, J.G. *et al., Biochem. Soc. Trans.*, 1974, **2**, 301 (*deriv*)
Heathcote, J.G. *et al., Chem. Ind. (London)*, 1976, 270 (*synth*)

Heathcote, J.G. *et al., Aflatoxins, Chemical and Biological Aspects*, Elsevier, 1978, (*rev*)
Betina, V. *et al., Mycotoxins: Chemical, Biological and Environmental Aspects*, Elsevier, 1989, 114 (*rev*)
Toxicol. Aflatoxins, (eds. Eaton, D.L. *et al*), Academic Press, London, 1994,

Agar A-237

Agar-agar. Gum agar. Gelose. Japan agar. Bengal isinglass. Ceylon isinglass. Chinese isinglass. Japan isinglass. FEMA 2012. E406 [9002-18-0]

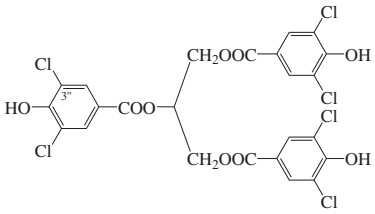
See also Agarose, A-242. Consists of a mixt. of 2 polysaccharides, Agarose, A-242 and Agaropectin, which has essentially the same struct. except that a variable proportion of the sugars in the polymer are replaced by 4,6-*O*-(1-carboxyethylidene)galactose or by sulfated or methylated sugar residues such as to retain the alternating sequence of 3-linked β-D- and 4-linked α-L- units. Distinguished from Carrageenan, C-179 by the presence of L-galacto residues and by the generally lower MW (mean ca. 120kDa but with a range of approx. 70-700). An important thickener, stabiliser and gelling agent in the food industry. Strips or fine powder. Sl. sol. in hot H_2O.

▶ AW7950000

Clark, R.E. *et al., Analyst (London)*, 1937, **62**, 661 (*detn, Sn*)
Bogan, E.J. *et al., Ind. Eng. Chem., Anal. Ed.*, 1942, **14**, 849 (*detn, $SO_4^{2\ominus}$*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, New York, 1948, **4**, (*use*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)
Duckworth, M. *et al., Carbohydr. Res.*, 1971, **18**, 1 (*struct, bibl*)
Davidson, R.L. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 7/1 (*rev*)
Glickmann, M. *et al., Food Hydrocolloids*, CRC Press, 1983, **2**, 73 (*rev*)
Rochas, C. *et al., Carbohydr. Res.*, 1994, **253**, 69 (*bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 53-56 (*use, props*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1470
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AEX250

Agaricoglyceride A A-238

Glycerol tris(3,5-dichloro-4-hydroxybenzoate)



$C_{24}H_{14}Cl_6O_9$ 659.085

Isol. from *Agaricus macrosporus* (horse mushroom).

3″-Dechloro: ***Agaricoglyceride B***
$C_{24}H_{15}Cl_5O_9$ 624.641
Isol. from *Agaricus macrosporus* (horse mushroom).

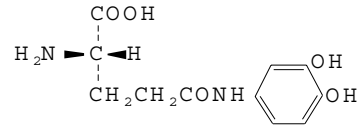
2-O-*Deacyl: Glycerol 1,3-bis(3,5-dichloro-4-hydroxybenzoate)*. ***Agaricoglyceride C***
$C_{17}H_{12}Cl_4O_7$ 470.088
Isol. from *Agaricus macrosporus* (horse mushroom).

2-O-*Deacyl, 2-Ac:* ***Agaricoglyceride D***
$C_{19}H_{14}Cl_4O_8$ 512.126
Isol. from *Agaricus macrosporus* (horse mushroom).

Stadler, M. *et al., J. Antibiot.*, 2005, **58**, 775-786 (*isol*)

Agaridoxin A-239

N-*(3,4-Dihydroxyphenyl)glutamine, 9CI. 3,4-Dihydroxy(γ-glutamyl)anilide* [58298-77-4]



$C_{11}H_{14}N_2O_5$ 254.242

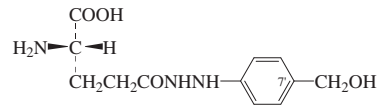
▶ MA2276100

(S)-form
L-form
Constit. of *Agaricus campestris* (field mushroom). Grey-white powder (MeOH aq.). Mp 220-221°.
Darkens in air.

Szent-Gyorgyi, A. *et al., JOC*, 1976, **41**, 1603 (*synth*)

Agaritine A-240

*β-N-(γ-Glutamyl)-4-hydroxymethylphenylhydrazine. Glutamic acid 5-2-(α-hydroxy-*p*-tolyl)hydrazide, 8CI* [2757-90-6]



$C_{12}H_{17}N_3O_4$ 267.284

▶ MA1284000

(S)-form
L-form
Constit. of some members of the family Agaricaceae, notably *Agaricus bisporus* (button mushroom). Cryst. (EtOH/butanol). Sol. MeOH, H_2O; poorly sol. EtOAc, hexane.
Mp 205-209° dec. $[\alpha]_D^{25}$ +7 (c, 0.8 in H_2O). pK_{a1} 3.4; pK_{a2} 8.86 (H_2O). λ_{max} 237 (ϵ 12000); 280 (ϵ 1400) (H_2O) (Berdy).

▶ A procarcinogen.

7′-Aldehyde: [114847-20-0] N^2-*(γ-Glutamyl)-4-formylphenylhydrazine.* ***Agaritinal***
$C_{12}H_{15}N_3O_4$ 265.268
Isol. from *Agaricus campestris* (field mushroom). Sol. H_2O, MeOH. λ_{max} 248 (ϵ 5750); 385 (ϵ 20000) (MeOH) (Berdy). λ_{max} 231 (ϵ 6200); 313 (ϵ 15500) (H_2O) (Berdy). λ_{max} 231 (ϵ 6200); 313 (ϵ 15500) (HCl) (Berdy).

7′-Carboxylic acid: [69644-85-5] N^2-*(γ-Glutamyl)-4-carboxyphenylhydrazine*
$C_{12}H_{15}N_3O_5$ 281.268
Isol. from *Agaricus bisporus* (button mushroom). Mp 175°.

▶ MA0955600

Daniels, E.G. *et al., JOC*, 1962, **27**, 3229 (*isol, synth*)
Levenberg, B. *et al., J. Biol. Chem.*, 1964, **239**, 2267 (*isol, struct*)
Chauhan, Y.S. *et al., J. Agric. Food Chem.*, 1984, **32**, 676; 1985, **33**, 817 (*deriv*)
Datta, S. *et al., Helv. Chim. Acta*, 1987, **70**, 1261 (*synth, ir, pmr, bibl*)
Chulia, A.J. *et al., Phytochemistry*, 1988, **27**, 929 (*Agaritinal*)
Baumgartner, D. *et al., Phytochemistry*, 1998, **49**, 465-474 (*biosynth*)
Espin, J.C. *et al., Phytochemistry*, 1999, **50**, 555-563 (*activity*)

Agaritine γ-glutamyltransferase A-241

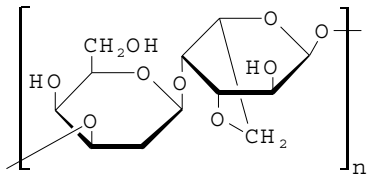
*E.C. 2.3.2.9. (γ-L-Glutamyl)-*N^1*-(4-hydroxymethylphenyl)hydrazine:(acceptor) γ-glutamyltransferase* [37257-25-3]

Aminoacyltransferase enzyme. Isol. from *Agaricus bisporus* (button mushroom).

Gigliotti, H.J. *et al., J. Biol. Chem.*, 1964, **239**, 2274-2284

Agarose A-242

Neutral agarose. Indubiose A4 [9012-36-6] [9036-61-7]



See also Agar, A-237. Composed of repeating units of β-D-Gal*p*-(1→4)-3,6-anhydro-α-L-Gal*p*-(1→3). Has a domain struct. of double helixes aggregating into a three-dimensional framework holding water molecules. There are two other polysaccharides in agar, one is similar to agarose but with 4,6-acetals of pyruvic acid at some of the D-galactose units. The other contains fewer 3,6-anhydro-L-galactose units and is sulfated.

Poly(6-aminohexyl) ether: [58856-73-8] *Agarose (6-aminohexyl)carbamimidate. Sepharose AH*
Non-stoichiometric.

Poly(5-carboxypentyl) ether: [55128-01-3] Non-stoichiometric.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 201C; 201D (*ir*)
Hegenauer, J.C. *et al., Biochim. Biophys. Acta*, 1965, **111**, 334 (*isol*)
BeMiller, J.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 65 (*purifn*)

Percival, E. *et al., The Carbohydrates*, 1970, **2B**, 553
Batey, J.F. *et al., Carbohydr. Res.*, 1975, **43**, 133
Turvey, J.R. *et al., Carbohydr. Res.*, 1976, **49**, 419
Rees, D. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214
Taylor, J.L. *et al., J. Chromatogr.*, 1983, **257**, 275-284 (*5-carboxypentyl ether*)
Szewezyk, A. *et al., Biochim. Biophys. Acta*, 1987, **89**, 252-260 (*6-aminohexyl ether*)
Kiwitt-Haschemie, K. *et al., Carbohydr. Res.*, 1993, **248**, 267
Arndt, E.R. *et al., Carbohydr. Res.*, 1997, **303**, 73-78 (*cd, struct*)
Gamini, A. *et al., Carbohydr. Res.*, 1997, **304**, 293-302 (*pmr, cmr, conformn*)

Agmatine N^4-coumaroyl-transferase A-243

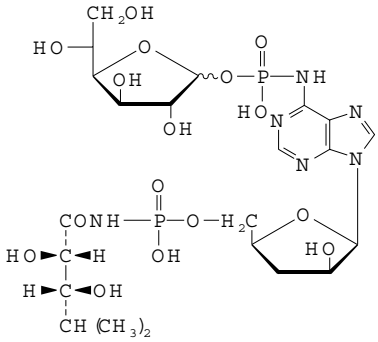
E.C. 2.3.1.64. 4-Coumaroyl-CoA:agmatine N^4-coumaroyl transferase [85030-72-4]

Enzyme. Isol. from barley seedlings (*Hordeum vulgare*).

Bird, C.R. *et al., Phytochemistry*, 1981, **20**, 2345-2346
Bird, C.R. *et al., Methods Enzymol.*, 1983, **94**, 344-347
Burhenne, K. *et al., J. Biol. Chem.*, 2003, **278**, 13919-13927

Agrocin 84, 9CI A-244

[59111-78-3]



$C_{22}H_{36}N_6O_{16}P_2$ 702.504

Nucleotide antibiotic. Bacteriocin active against *Agrobacterium tumefaciens*. λ_{max} 270 (ϵ 19000) (pH 1) (Derep). λ_{max} 264 (ϵ 19500); 270 (sh) (ϵ 15000) (pH 7 H_2O) (Derep). λ_{max} 270 (pH 1 buffer) (Berdy).

Heip, J. *et al., Arch. Int. Physiol. Biochim.*, 1975, **83**, 974 (*isol*)
Roberts, W.P. *et al., Nature (London)*, 1977, **265**, 379 (*struct*)
Das, P.K. *et al., J. Antibiot.*, 1978, **31**, 490 (*props*)
Thompson, R.J. *et al., Antimicrob. Agents Chemother.*, 1979, **16**, 293 (*isol, props*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711 (*rev*)
Filippov, D. *et al., Tet. Lett.*, 1998, **39**, 4891-4894 (*partial synth*)

Agrocin C58 A-245

[98667-77-7]

Struct. unknown. Bacteriocin prod. by *Agrobacterium tumefaciens*.

Necasek, J. *et al., Folia Microbiol. (Prague)*, 1985, **30**, 353-358

Agrocin D286 A-246

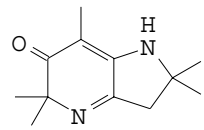
[86337-94-2]

Struct. unknown. Bacteriocin prod. by *Agrobacterium tumefaciens*. Sol. H_2O. λ_{max} 264 (H_2O).

Hendson, M. *et al., Appl. Environ. Microbiol.*, 1983, **45**, 1526-1532 (*isol, activity*)
Webster, J. *et al., Appl. Environ. Microbiol.*, 1986, **52**, 217-219 (*activity*)
Clere, B.G. *et al., Biotechnol. Ser.*, 1995, **28**, 619-632 (*rev*)

Agrocybenine A-247

1,2,3,5-Tetrahydro-2,2,5,5,7-pentamethyl-6H-pyrrolo[2,3-b]pyridin-6-one, 9CI [178764-92-6]



$C_{12}H_{18}N_2O$ 206.287

Alkaloid from the edible Korean mushroom yangimatusutake (*Agrocybe cylindracea*). Yellow powder. λ_{max} 223 (ϵ 16800); 333 (ϵ 9200) (MeOH).

3a,4-Dihydro: [1257392-35-0] ***Flavascensine***
$C_{12}H_{20}N_2O$ 208.303
Pale yellow powder. $[\alpha]_D^{20}$ -28 (c, 0.48 in MeOH). λ_{max} 295 (log ϵ 4.02) (MeOH).

Koshino, H. *et al., Tet. Lett.*, 1996, **37**, 4549-4550 (*Agrocybenine*)
Liu, X.-J. *et al., Fitoterapia*, 2010, **81**, 524-527 (*Flavascensine*)

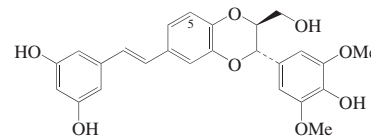
Agrocybin† A-248

Peptide. MW 9000. Isol. from fresh fruiting bodies of the edible mushroom *Agrocybe cylindracea*.

Ngai, P.H. *et al., Peptides (N.Y.)*, 2005, **26**, 191-196 (*Agrocybin*)

Aiphanol A-249

[353482-13-0]
[578020-29-8 ((±)-form)]



Absolute Configuration

$C_{25}H_{24}O_8$ 452.46

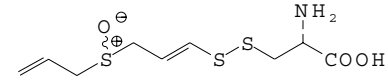
Stilbenolignan. Constit. of the seeds of *Aiphanes aculeata*. Brown powder. $[\alpha]_D^{20}$ -21.8 (c, 0.13 in MeOH). λ_{max} 233 (log ϵ 5.37); 322 (log ϵ 5.32) (MeOH).

5-Hydroxy: [1228276-51-4] ***5-Hydroxyaiphanol***
$C_{25}H_{24}O_9$ 468.459
Amorph. yellow powder. Optically inactive. λ_{max} 289 (log ϵ 3.97); 321 (log ϵ 4.07) (MeOH).

Lee, D. *et al., Org. Lett.*, 2001, **3**, 2169-2171 (*Aiphanol*)
Kuboki, A. *et al., Chem. Lett.*, 2003, **32**, 420-421 (*synth*)
Wang, X.L. *et al., Chin. Chem. Lett.*, 2004, **15**, 1036-1038 (*synth*)
Banwell, M.R. *et al., Tetrahedron: Asymmetry*, 2005, **16**, 1645-1654 (*synth, abs config*)
Lam, S.-H. *et al., Phytochemistry*, 2010, **71**, 792-797 (*5-Hydroxyaiphanol*)

Ajocysteine A-250

2-Amino-4,5,9-trithia-6,11-dodecadienoic acid 9-oxide



$C_9H_{15}NO_3S_3$ 281.42

Constit. of garlic (*Allium sativum*). No phys. props. reported.

Lawson, L.D. *et al., Planta Med. (Suppl.)*, 1993, **59**, A688 (*isol*)

Ajoene A-251

2-Propenyl 3-(2-propenylsulfinyl)-1-propenyl disulfide, 9CI. 4,5,9-Trithia-1,6,11-dodecatriene 9-oxide. Allyl 3-allylsulfinyl-1-propenyl disulfide [92285-01-3]

$H_2C{=}CHCH_2^9S(O)CH_2CH{=}CH\text{-}S\text{-}S\text{-}CH_2CH{=}CH_2$

$C_9H_{14}OS_3$ 234.407

Isol. from garlic (*Allium sativum*) extracts. Nutraceutical with anticancer props. λ_{max} 240 (MeOH) (Berdy).

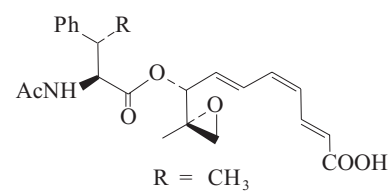
9-Oxide: [118590-71-9] *2-Propenyl 3-(2-propenylsulfonyl)-1-propenyl disulfide, 9CI. Allyl 3-(allylsulfonyl)-1-propenyl disulfide*
$C_9H_{14}O_2S_3$ 250.406
Isol. from garlic.

[92285-00-2, 72869-75-1, 92284-99-6]

Block, E. *et al., JACS*, 1984, **106**, 8295-8296; 1986, **108**, 7045-7055 (*synth, isol, E/Z-ajoene*)
Naganawa, R. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 4238-4242 (*activity*)
Yoshida, H. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 1014-1017; 1999, **63**, 588-590 (*activity*)
Gallwitz, H. *et al., J. Med. Chem.*, 1999, **42**, 364-372 (*props*)
Kyung, K.H. *et al., Curr. Opin. Biotechnol.*, 2012, (*rev, activity*)

AK toxin I A-252

N-*Acetyl-β-methyl-L-phenylalanine 7-carboxy-1-(2-methyloxiranyl)-2,4,6-heptatrienyl ester, 9CI* [85146-09-4]



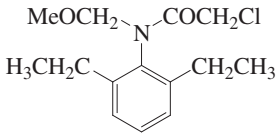
$C_{23}H_{27}NO_6$ 413.469

Prod. by *Alternaria alternata* Japanese pear pathotype. Cryst. (MeOH). Mp 168° dec. $[\alpha]_D^{25}$ +164 (c, 0.128 in MeOH). λ_{max} 285 (ε 27600) (MeOH) (Derep).

Nakashima, T. *et al., Agric. Biol. Chem.*, 1985, **49**, 807 (*isol, struct, props*)
Uemura, I. *et al., Tetrahedron*, 2002, **58**, 2351 (*synth*)

Alachlor, ANSI, BSI, ISO, JMAF, WSSA A-253

2-Chloro-N-*(2,6-diethylphenyl)*-N-*(methoxymethyl)acetamide, 9CI. 2-Chloro-2′,6′-diethyl*-N-*(methoxymethyl)acetanilide. Alagan. Alanex. Alatox. Bullet. Lasso. Pillarzo. Ralchlor. Satochlor. Alapaz. Nitala* [15972-60-8]



$C_{14}H_{20}ClNO_2$ 269.77
Selective preemergent herbicide used on food crops. Cryst. Spar. sol. H_2O; sol. Me_2CO, C_6H_6, EtOH, EtOAc. Mp 39.5-41.5°.

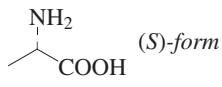
▶ LD_{50} (rat, orl) 1200 mg/kg. Possible skin allergen. AE1225000

[8070-94-8]

UK Pat., 1961, 1 008 851
Burow, M.D. *et al., Cryst. Struct. Commun.*, 1982, **11**, 747 (*cryst struct*)
Huppatz, J.L. *et al., Pestic. Sci.*, 1982, **13**, 78 (*synth, activity*)
Voyksner, R.D. *et al., J. Chromatogr.*, 1984, **312**, 221 (*hplc*)
Kimmel, E.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 157 (*metab*)
Supreck, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1987, **70**, 1014 (*gc*)
Chesters, G. *et al., Rev. Environ. Contam. Toxicol.*, 1989, **110**, 1 (*rev*)
Venkov, A.P. *et al., Synth. Commun.*, 1989, **19**, 2133 (*synth, pmr, ir*)
Dangerous Prop. Ind. Mater. Rep., 1990, **10**, 23 (*rev, tox*)
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A4
Warner, J.M. *et al., Compr. Anal. Profiles Important Pestic.*, 1993, 109 (*rev*)
Pesticide Manual, 11th edn., 1997, No. 14 (*props, use*)
Handbook of Pesticide Toxicology, (eds. Hayes, W.J. et al), Academic Press, 1991, 1341
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CFX000

Alanine, INN, USAN A-254

2-Aminopropanoic acid, 9CI. α-Alanine. Ala



(*S*)-*form*

$C_3H_7NO_2$ 89.094

(*S*)-*form* [56-41-7]
L-form
Dietary supplement, nutrient. Insol. EtOH; sol. H_2O (16.5g/100ml at 25°). Mp 297° dec. $[\alpha]_D$ +14.6 (c, 1 in 5*M* HCl). $[\alpha]_D$ +1.8 (c, 1 in H_2O). pK_{a1} 2.34; pK_{a2} 9.69 (NH_2). Isoelectric point 6.01. Sweet taste.

▶ AY2990000

N-*(5-Methyl-3-oxohexyl)*: N-*(5-Methyl-3-oxohexyl)alanine*
$C_{10}H_{19}NO_3$ 201.265
Constit. of *Cycas circinalis* (false sago) (Cycadaceae). Amorph. solid. $[\alpha]_D$ +100 (c, 1.1 in H_2O).

(±)-*form* [302-72-7]
Dietary supplement, nutrient, sweetening flavour enhancer in pickling spice mixts. Sweet tasting needles or prisms. Spar. sol. H_2O; insol. Et_2O. Mp 295° dec.

▶ AY2980000

[98204-12-7 (ξ-*N,N*-diethyl), 2134-48-7 (ξ-nitrile)]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 570D; 571A; 571B; 672A; 672B; 672C; **2**, 260D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 868C; 869B; 1069C; 1069B (*nmr*)
Org. Synth., Coll. Vol., 1, 1932, 20 (*synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1819 (*rev*)
Kost, A.N. *et al., Chem. Ind. (London)*, 1966, 1496-1497 (*Alanine, synth*)
Lehmann, M.S. *et al., JACS*, 1972, **94**, 2657-2660 (*L-Alanine, cryst struct*)
Okawara, T. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 1869-1872 (*L-Alanine, synth*)
Kopitsya, T.P. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1973, **9**, 916-620 (*Alanine, resoln*)
Kiyooka, S. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 1897-1900 (*Alanine, synth*)
Krapcho, A. *et al., Tet. Lett.*, 1976, **17**, 2205-2208 (*Alanine, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFH600; AFH625
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1035
Cong-Jun, L. *et al., Phytochemistry*, 1996, **42**, 443-445 (*N-5-methyl-3-oxohexyl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 57-59 (*use, props*)
Rosado, M.T.S. *et al., J. Mol. Struct.*, 1997, 343-348; 410-411 (*R-form, S-form, Raman, ir*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 11th edn., J. Wiley*, 2004, AFH600; AFM625

D-Alanine γ-glutamyltransferase A-255

E.C. 2.3.2.14. L-Glutamine:D-alanine γ-glutamyltransferase
Aminoacyltransferase enzyme. Isol. from pea seedlings (*Pisum sativum*).
Kawasaki, Y. *et al., Biochim. Biophys. Acta*, 1982, **716**, 194-200 (*Pisum sativum*)

Alanine transaminases A-256

Alanine aminotransferases
Aminotransferase enzymes.

Alanine transaminase [9000-86-6]
E.C. 2.6.1.2. L-Alanine:2-oxoglutarate aminotransferase. Alanine aminotransferase. Glutamic-pyruvic transaminase. Glutamic-alanine transaminase
Isol. from tomato and pig. Pyridoxal phosphate-dependent. Also acts on 2-aminobutanoate.

Alanine oxo-acid transaminase [9030-41-5]
E.C. 2.6.1.12. L-Alanine:2-oxo-acid aminotransferase. Alanine oxo-acid aminotransferase
Pyridoxal phosphate-dependent.

Alanine-glyoxylate transaminase [9015-67-2]
E.C. 2.6.1.44. L-Alanine:glyoxylate aminotransferase. Alanine-glyoxylic aminotransferase
Pyridoxal phosphate-dependent.

Alanine-oxomalonate transaminase [37277-96-6]
E.C. 2.6.1.47. L-Alanine:oxomalonate aminotransferase
Pyridoxal phosphate-dependent.

Green, D.E. *et al., J. Biol. Chem.*, 1945, **161**, 559-582 (*E.C. 2.6.1.2, pig heart*)
Rowsell, E.V. *et al., Biochem. J.*, 1956, **64**, 246-252 (*E.C. 2.6.1.12, rat liver*)
Sallach, H.J. *et al., J. Biol. Chem.*, 1956, **223**, 1101-1108 (*E.C. 2.6.1.12, dog liver*)
Nagayama, H. *et al., Nature (London)*, 1958, **181**, 417-418 (*E.C. 2.6.1.47, Bombyx mori*)
Saier, M.H. *et al., J. Biol. Chem.*, 1967, **242**, 91-100 (*E.C. 2.6.1.2, pig heart*)
Thompson, J.S. *et al., J. Biol. Chem.*, 1967, **242**, 3614-3619 (*E.C. 2.6.1.44, human liver*)
Segal, H.L. *et al., Methods Enzymol., Part A*, 1970, **17**, 153-159 (*E.C. 2.6.1.2, rat liver*)
Jenkins, W.T. *et al., Methods Enzymol., Part A*, 1970, **17**, 159-163 (*E.C. 2.6.1.2, pig heart*)
Richardson, K.E. *et al., Methods Enzymol., Part A*, 1970, **17**, 163-166 (*E.C. 2.6.1.44, human liver*)
Rech, J. *et al., Biochim. Biophys. Acta*, 1974, **350**, 392-399 (*E.C. 2.6.1.2, tomato*)
Noguchi, T. *et al., Biochem. J.*, 1978, **169**, 113-122 (*E.C. 2.6.1.44, mammalian liver*)
De Rosa, G. *et al., Biochim. Biophys. Acta*, 1979, **567**, 116-124 (*E.C. 2.6.1.2, pig liver, pig kidney*)
Okuno, E. *et al., Biochim. Biophys. Acta*, 1982, **715**, 97-104 (*E.C. 2.6.1.44, rat kidney*)

N-Alanylglutamine A-257

$H_3CCH(NH_2)CONHCH(COOH)–CH_2CH_2CONH_2$

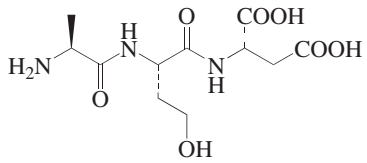
$C_8H_{15}N_3O_4$ 217.224

L-L-*form* [39537-23-0]
FEMA 4712
Dietary supplement. Metabolic source of glutamine esp. for parenteral use. Needles (EtOH aq.). Mp 215-216°. $[\alpha]_D^{20}$ +10.5 (c, 2.0 in H_2O). $[\alpha]_D^{20}$ -3.4 (c, 10 in 1*N* HCl).

Shimonishi, Y. *et al., Bull. Chem. Soc. Jpn.*, 1961, **34**, 739; 1962, **35**, 1966-1970; 1964, **37**, 200-203 (*synth*)
Eur. Pat., 1989, 311 057 (*synth, ir*)
Eur. Pat., 1994, 595 345 (*synth*)

Sano, T. *et al., Org. Process Res. Dev.*, 2000, **4**, 147-152 (*synth*)
Goeters, C. *et al., Crit. Care Med.*, 2002, **30**, 2032-2037 (*use, clin trials*)

Alanylhomoserinylaspartic acid A-258

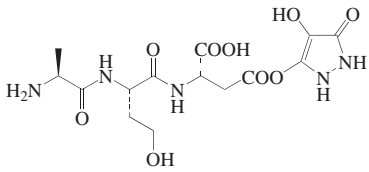


$C_{11}H_{19}N_3O_7$ 305.287

(*all-S*)-*form* [1094487-51-0]
Isol. from rice pathogen, *Burkholderia glumae*. Amorph. powder.
Mitchell, R.E. *et al., Phytochemistry*, 2008, **69**, 2704-2707 (*isol, pmr, cmr, ms*)

5-[(Alanylhomoserinyl-β-aspartyl)oxy]-1,2-dihydro-4-hydroxy-3*H*-pyrazol-3-one A-259

[1094487-53-2]



$C_{14}H_{21}N_5O_9$ 403.348
Isol. from rice pathogen *Burkholderia glumae*. Amorph. powder.
Mitchell, R.E. *et al., Phytochemistry*, 2008, **69**, 2704-2707 (*isol, pmr, cmr*)

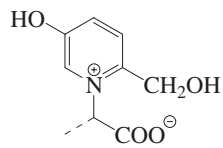
Alanylleucylglutamylprolyl A-260

[1175530-77-4]

Ala-Leu-Glu-Pro
$C_{19}H_{32}N_4O_7$ 428.484
Found in 11S-Globulin; a major constit. of the seeds of *Amaranthus hypochondriacus* (prince's feather).
Vecchi, B. *et al., Phytochemistry*, 2009, **70**, 864-870

Alapyridaine A-261

1-(1-Carboxyethyl)-5-hydroxy-2-(hydroxymethyl)pyridinium betaine [501421-91-6]
[566905-65-5]



(*S*)-*form*

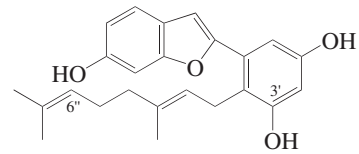
$C_9H_{11}NO_4$ 197.19

(*S*)-*form* [501007-16-5]
Taste enhancer. Present in beef broth. $[\alpha]_D^{20}$ +40.2 (c, 0.01 in NH_4 salt pH7).

(±)-*form*
Cryst. (EtOH). Mp 91°.
Ottinger, H. *et al., J. Agric. Food Chem.*, 2003, **51**, 1035-1041; 6791-6796 (*synth, pmr, cmr, occur*)
Villard, R. *et al., J. Agric. Food Chem.*, 2003, **51**, 4040-4045 (*synth, cryst struct*)

Albafuran A A-262

4-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI. 2-[3,5-Dihydroxy-2-(3,7-dimethyl-2,6-octadienyl)phenyl]-6-hydroxybenzofuran [84323-14-8]



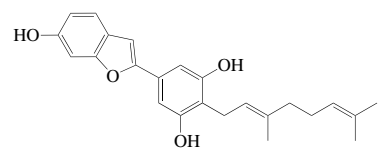
$C_{24}H_{26}O_4$ 378.467
Constit. of white mulberry (*Morus alba*). Cryst. Poorly sol. hexane. Mp 150-150.5°. λ_{max} 214 (ε 40300); 312 (ε 27300) (EtOH) (Berdy).

3′-Me ether: [68978-04-1] ***Mulberrofuran A***
$C_{25}H_{28}O_4$ 392.494
Constit. of white mulberry (*Morus alba*). Cryst. λ_{max} 216 (ε 32500); 311 (ε 23400) (EtOH). λ_{max} 328 (ε 23400) (EtOH/NaOH) (Berdy).

Δ7″-Isomer, 6″ξ-hydroxy: [1253190-72-5] ***Mornigrol D***
$C_{24}H_{26}O_5$ 394.466
Constit. of the bark of *Morus nigra* (black mulberry). Amorph. yellow powder. Mp 92-94°. λ_{max} 212 (log ε 4.59); 311 (log ε 4.39) (MeOH).
Nomura, T. *et al., Heterocycles*, 1978, **9**, 1593-1601 (*Mulberrofuran A*)
Takasugi, M. *et al., Chem. Lett.*, 1982, **11**, 1221-1222 (*Albafuran A*)
Jeong, S.H. *et al., J. Agric. Food Chem.*, 2009, **57**, 1195-1203 (*isol, pmr, cmr*)
Wang, L. *et al., J. Asian Nat. Prod. Res.*, 2010, **12**, 431-437 (*Mornigrol D*)

Albafuran B A-263

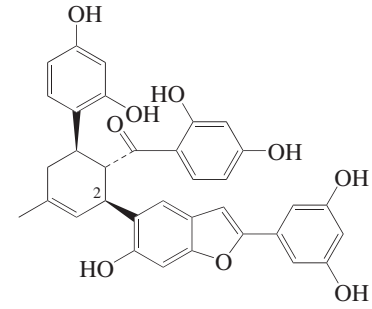
2-(3,7-Dimethyl-2,6-octadienyl)-5-(6-hydroxy-2-benzofuranyl)-1,3-benzenediol, 9CI. 2-[3,5-Dihydroxy-4-(3,7-dimethyl-2,6-octadienyl)phenyl]-6-hydroxybenzofuran [84323-15-9]



$C_{24}H_{26}O_4$ 378.467
Antifungal constit. of white mulberry (*Morus alba*). Cryst. Poorly sol. hexane. Mp 158-158.5°. λ_{max} 219 (ε 27000); 320 (ε 34000); 335 (ε 29000) (EtOH) (Berdy).
Takasugi, M. *et al., Chem. Lett.*, 1982, **11**, 1221-1222 (*Albafuran B*)

Albafuran C A-264

[84323-16-0]

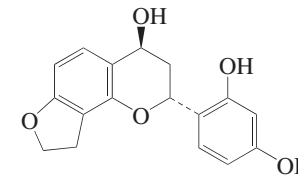


$C_{34}H_{28}O_9$ 580.59
Constit. of white mulberry bark *Morus alba*. Amorph. Sol. MeOH, Me_2CO, $CHCl_3$; poorly sol. hexane. $[\alpha]_D$ -302 (EtOH). λ_{max} 216 (ε 47000); 284 (ε 22300); 294 (ε 19600); 322 (ε 31700); 336 (ε 25700) (EtOH) (Berdy).

2-Epimer: [1001325-03-6] ***Australisin C***
$C_{34}H_{28}O_9$ 580.59
Yellow powder. $[\alpha]_D^{20}$ +340 (c, 0.27 in MeOH). Abs. config. known. λ_{max} 206 (log ε 4.87); 216 (sh) (log ε 4.83); 283 (log ε 4.46); 323 (log ε 4.67); 336 (sh) (log ε 4.62) (MeOH).
Takasugi, M. *et al., Chem. Lett.*, 1982, 1223-1224 (*Albafuran C*)
Zhang, Q.-J. *et al., Chem. Biodiversity*, 2007, **4**, 1533-1540 (*Australisin C*)

Albafuroflavan A A-265

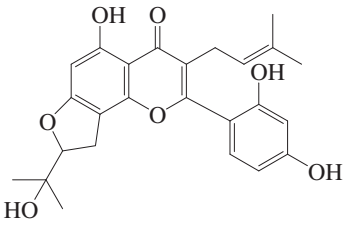
*2-(2,4-Dihydroxyphenyl)-3,4,8,9-tetrahydro-2*H*-furo[2,3-*h*]-1-benzopyran-4-ol* [1245744-43-7]



$C_{17}H_{16}O_5$ 300.31
Constit. of the leaves of *Morus alba* (white mulberry). Amorph. brown powder. Mp 106-108°. $[\alpha]_D^{20}$ -38 (c, 0.14 in MeOH). λ_{max} 210 (log ε 4.69); 235 (log ε 3.93); 277 (log ε 3.56); 286 (log ε 3.58) (MeOH).
Yang, Y. *et al., J. Asian Nat. Prod. Res.*, 2010, **12**, 194-198 (*Albafuroflavan A*)

Albanin C A-266

[73343-43-8]



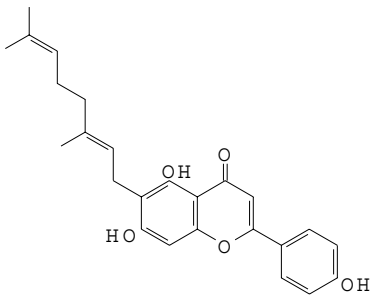
$C_{25}H_{26}O_7$ 438.476

Isol. from *Morus alba* (white mulberry) infected with *Fusarium solani*.

Takasugi, M. *et al., CA*, 1980, **92**, 160540d (*isol*)

Albanin D A-267

*6-(3,7-Dimethyl-2,6-octadienyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one, 9CI. 6-Geranyl-4′,5,7-trihydroxyflavone. 6-Geranylapigenin* [134955-26-3]



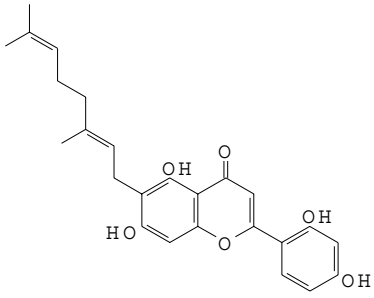
$C_{25}H_{26}O_5$ 406.477

Struct. revised in 1991. Isol. from *Morus alba* (white mulberry). Pale yellow prisms (Me_2CO). Mp 205-207°. λ_{max} 255; 288; 355 (EtOH) (Berdy).

Fukai, T. *et al., Heterocycles*, 1991, **32**, 499 (*synth, pmr, struct*)

Albanin E A-268

*2-(2,4-Dihydroxyphenyl)-6-(3,7-dimethyl-2,6-octadienyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one, 9CI. 6-Geranyl-2′,4′,5,7-tetrahydroxyflavone. 6-Geranylnorartocarpetin* [134955-27-4]



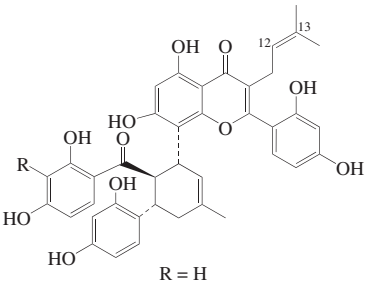
$C_{25}H_{26}O_6$ 422.477

Struct. revised in 1991. Isol. from *Morus alba* (white mulberry). Pale yellow prisms (C_6H_6/Me_2CO). Mp 174-177°. λ_{max} 269 (ϵ 13100); 348 (ϵ 11400) (MeOH) (Berdy). λ_{max} 213; 252; 271; 355 (EtOH) (Berdy).

Fukai, T. *et al., Heterocycles*, 1991, **32**, 499 (*synth, pmr, struct*)

Albanin F A-269

Kuwanon G. Moracenin B [75629-19-5]



R = H

$C_{40}H_{36}O_{11}$ 692.718

Abs. configs. do not appear certain. All isolates strongly laevorotatory. Authors' numbering shown. Constit. of white mulberry bark (*Morus alba*). Amorph. $[\alpha]_D$ -529 (MeOH). Log P 5.13 (calc).

12,13-Dihydro, 13-hydroxy: [78277-79-9] ***Moracenin D***

$C_{40}H_{38}O_{12}$ 710.733

Yellow amorph. powder. $[\alpha]_D^{18}$ -419 (c, 0.16 in MeOH). $[\alpha]_D$ -388 (c, 0.25 in MeOH). Log P 3.41 (calc).

Takasugi, M. *et al., Chem. Lett.*, 1980, 1577
Oshima, Y. *et al., Heterocycles*, 1981, **16**, 979 (*Moracenin D*)
Nomura, T. *et al., Heterocycles*, 1981, **16**, 983 (*Moracenin D*)
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90; 1984, **50**, 127 (*isol*)
Hano, Y. *et al., Heterocycles*, 1988, **27**, 2315 (*abs config*)
Mihara, S. *et al., Biochem. Biophys. Res. Commun.*, 1995, **213**, 594-599 (*Kuwanon G, pharmacol*)
Takayama, M. *et al., Rapid Commun. Mass Spectrom.*, 1995, **9**, 383 (*ms*)
Park, K.M. *et al., J. Ethnopharmacol.*, 2003, **84**, 181-185 (*Kuwanon G, pharmacol*)

Albanin G A-270

Kuwanon H. Moracenin A [76472-87-2]

As Albanin F, A-269 with R = $-CH_2CH{=}C(CH_3)_2$

$C_{45}H_{44}O_{11}$ 760.836

Constit. of white mulberry (*Morus alba*). $[\alpha]_D$ -455 (MeOH). Log P 7.13 (uncertain value) (calc).

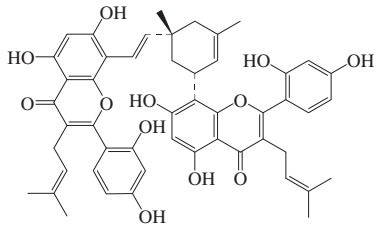
2‴-Deoxy: [886212-63-1] ***Mongolicin D***

$C_{45}H_{44}O_{10}$ 744.837

Amorph. yellow powder. $[\alpha]_D^{25}$ -227 (c, 0.11 in MeOH). λ_{max} 205; 264; 320 (MeOH).

Takasugi, M. *et al., Chem. Lett.*, 1980, 1577-1580 (*isol, struct*)
Nomura, T. *et al., Planta Med.*, 1983, **49**, 90-94; 1984, **50**, 127-130 (*isol*)
Mihara, S. *et al., Biochem. Biophys. Res. Commun.*, 1995, **213**, 594-599 (*pharmacol*)
Kang, J. *et al., Planta Med.*, 2006, **72**, 52-59 (*Mongolicin D*)

Albanin H A-271



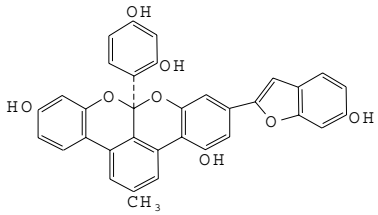
$C_{50}H_{48}O_{12}$ 840.922

Constit. of *Morus alba* (white mulberry). Yellow cryst. Mp 215° dec. Racemic.

Nomura, T. *et al., Prog. Chem. Org. Nat. Prod.*, 1988, **53**, 87-201 (*rev*)

Albanol B A-272

[87084-99-9]



$C_{34}H_{22}O_8$ 558.543

Artifact derived from Mulberrofuran I. Constit. of bark of white mulberry *Morus alba*. Yellow plates. Mp 248° dec.

Rao, A.V.R. *et al., Tet. Lett.*, 1983, **24**, 3013
Hano, Y. *et al., Heterocycles*, 1989, **28**, 745

Alcohol *O*-acetyltransferase A-273

E.C. 2.3.1.84. Acetyl-CoA:alcohol O-*acetyltransferase* [80237-89-4]

Enzyme. Isol. from *Saccharomyces cerevisiae*. Acts on short-chain aliphatic alcohols, incl. MeOH and EtOH.

Yoshioka, K. *et al., Agric. Biol. Chem.*, 1981, **45**, 483-490
Malcorps, P. *et al., Eur. J. Biochem.*, 1992, **210**, 1015-1022
Minetoki, T. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 2094-2098

Alcohol *O*-cinnamoyltransferase A-274

E.C. 2.3.1.152. 1-O-trans-*Cinnamoyl-β-D-glucopyranose:alcohol* O-*cinnamoyltransferase*

Enzyme. Isol. from seedlings of *Raphanus sativus* (radish). Alcohol substrates incl. MeOH, EtOH and 1-propanol. Also acts on 1-*O*-*trans*-cinnamoyl-β-D-gentiobiose.

Mock, H.P. *et al., Phytochemistry*, 1993, **32**, 575-579

Alcohol sulfotransferase A-275

E.C. 2.8.2.2. 3′-Phosphoadenylyl-sulfate:alcohol sulfotransferase. Hydroxysteroid sulfotransferase. Cholesterol sulfotransferase. HST [9032-76-2]

Sulfotransferase enzyme. Isol. from pig, rabbit. Primary and secondary

alcohols, incl. aliphatic alcohols and hydroxysteroids, can act as acceptors. Indistinguishable from Steroid sulfotransferase and Petromyzonol sulfotransferase, S-315 in CA.

Lyon, E.S. *et al., Methods Enzymol.*, 1981, **77**, 206-213 (*rat, rev*)
Yoshinari, K. *et al., J. Biochem. (Tokyo)*, 1998, **123**, 740-746 (*rabbit*)
Takehara, K. *et al., Arch. Biochem. Biophys.*, 2001, **394**, 201-208 (*mouse*)
Miki, Y. *et al., J. Clin. Endocrinol. Metab.*, 2002, **87**, 5760-5768 (*human*)
Lee, K.A. *et al., J. Biol. Chem.*, 2003, **278**, 44593-44599 (*human, cryst struct*)
Chen, W.T. *et al., Anal. Biochem.*, 2005, **339**, 54-60 (*pig, assay*)

Aldose 1-phosphate adenylyltransferase **A-276**

E.C. 2.7.7.36. ADP:α-D-aldose 1-phosphate adenylyltransferase. Sugar 1-phosphate adenylyltransferase. ADP aldose phosphorylase. Adenosine diphosphosugar phosphorylase [37278-27-6]

Nucleotidyltransferase enzyme. Isol. from wheat (*Triticum aestivum*). Enzyme activity range pH 7-10. At -15°, stable for several weeks.

Dankert, M. *et al., Biochim. Biophys. Acta*, 1964, **81**, 78-85 (*wheat*)

Aldose 1-phosphate nucleotidyltransferase **A-277**

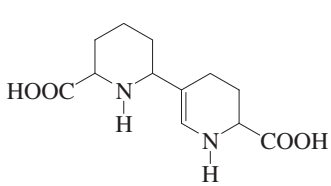
E.C. 2.7.7.37. NDP:α-D-aldose 1-phosphate nucleotidyltransferase. Sugar 1-phosphate nucleotidyltransferase. NDP aldose phosphorylase. Glucose 1-phosphate inosityltransferase. Nucleoside diphosphosugar phosphorylase [9033-61-8]

Nucleotidyltransferase enzyme. Isol. from baker's yeast (*Saccharomyces cerevisiae*). NDP sugar substrates incl. Uridine diphosphate mannose, Guanosine diphosphate mannose, ADP-D-mannose, dTDP-D-mannose and Uridine diphosphate glucose. Enzyme activity range pH 6.5-9.5. At -20°, the conc. enzyme fraction is stable for several months.

Cabib, E. *et al., J. Biol. Chem.*, 1965, **240**, 2114-2121 (*baker's yeast*)
Cabib, E. *et al., Methods Enzymol.*, 1966, **8**, 224-229 (*assay, props, purifn, rev*)

Aldosine **A-278**

5-(6-Carboxy-2-piperidinyl)-1,2,3,4-tetrahydro-2-pyridinecarboxylic acid, 9CI [142759-11-3]
[173653-73-1, 173449-61-1]

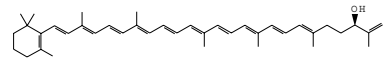


$C_{12}H_{18}N_2O_4$ 254.285
Hydrol. product from the aldol crosslinks of bovine elastin and collagen.

Suyama, K. *et al., Agric. Biol. Chem.*, 1991, **55**, 3147-3149
Nakamura, F. *et al., Arch. Biochem. Biophys.*, 1996, **325**, 167-173

Aleuriaxanthin **A-279**

1′,16′-Didehydro-1′,2′-dihydro-β,ψ-caroten-2′-ol [51599-07-6]



$C_{40}H_{56}O$ 552.882
Constit. of *Aleuria aurantia* (orange cup). Cryst. (Et_2O/petrol). Mp 122-122.5°.

Ac: [51276-30-3]
Purple prisms. Mp 134.5-135.5°.

Liaaen-Jensen, S. *et al., Phytochemistry*, 1965, **4**, 925 (*occur*)
Kjosen, H. *et al., Acta Chem. Scand.*, 1973, **27**, 2495 (*synth, uv, ir, pmr*)
Arpin, N. *et al., Phytochemistry*, 1973, **12**, 2751 (*struct, pmr, ir, uv*)
Buchecker, R. *et al., Phytochemistry*, 1976, **15**, 1013 (*struct*)
Eschenmoser, W. *et al., Helv. Chim. Acta*, 1983, **66**, 82 (*synth*)

Alexomycin, USAN **A-280**

U 82127. PNU 82127 [165101-50-8]

Mixt. composed mainly of isolate 10381b which contains several cyclic sulfur peptides prod. by *Streptomyces arginensis*. Major component is Sulfomycin I. Veterinary growth promoter used for poultry and swine.

Cromwell, G.L. *et al., J. Anim. Sci.*, 1996, **74**, 1284-1287 (*activity*)
Cho, B.-Y. *et al., J. Chromatogr., B*, 1997, **67**, 163-174 (*anal*)
Marshall, S.A. *et al., Diagn. Microbiol. Infect. Dis.*, 1999, **33**, 181-186 (*activity*)

Alfalfone **A-281**

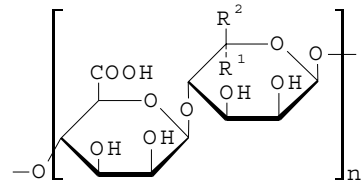
$C_{21}H_{42}O$ 310.562

Ketone of unknown struct. Constit. of the meal of *Medicago sativa* (alfalfa). Powder. Mp 88.5-88.8°.

Jacobson, C.A. *et al., JACS*, 1912, **34**, 300 (*isol*)

Alginic acid, BAN **A-282**

Gum levan. Levan gum. Kelacid. Norgine. Sazio. E400. Alginine† [9005-32-7]



R^1 = H , R^2 = COOH
or R^1 = COOH, R^2 = H

$[C_6H_8O_6]$
A polymer consisting of various proportions of β-D-Mannuronic acid and α-L-Guluronic acid linked 1 →4 and arranged in a block fashion. To a first approximation there are poly-M , poly-G and $(M\text{-}G)_n$ blocks of about 20 units with an overall degree of polymerisation of 1000-10,0000. Alginates are used to improve food texture, e.g. in ice cream, pie fillings. Emulsifier, stabiliser, thickener. $[\alpha]_D$ -120 (as Na salt in H_2O). Approx. 200 grades of the acid and its salts (ammonium, Ca, K, Na) commercially available. Alginates with the highest guluronic acid content display the strongest gel-forming activity.

▶ AZ5775000

Na salt: [9005-38-3] *Sodium alginate. Algin. E401*
Stabiliser, emulsifier, thickener, formulation aid. Pale yellow-brown powder. Sol. H_2O; poorly sol. EtOH, hexane. λ_{max} 260 (H_2O) (Berdy).

▶ AZ5820000

K salt: [9005-36-1] *Potassium alginate. E402*
Stabiliser, emulsifier, thickener, formulation aid. Insol. EtOH, Et_2O.

Ca salt: [9005-35-0] *Calcium alginate. E404*
Stabiliser, emulsifier, thickener, formulation aid. Sl. sol. EtOH; insol. H_2O, Et_2O.

NH_4 salt: [9005-34-9] *Ammonium alginate. E403*
Stabiliser, emulsifier, thickener, formulation aid. Insol. EtOH, Et_2O.

2-Hydroxypropyl ester. Propylene glycol alginate. Colloid 602™. Dricoid™. Kelcoloid™. FEMA 2941. E405. Many other trade names
[59125-52-9, 95328-14-6, 39306-87-1, 51374-11-9, 52441-26-6, 57762-73-9]
Stabiliser, emulsifier, thickener, formulation aid, surface active agent and flavouring adjunct or adjuvant for foodstuffs. White to yellowish fibrous or granular powder. Sol. H_2O. Composition varies acc. to the degree of esterification.

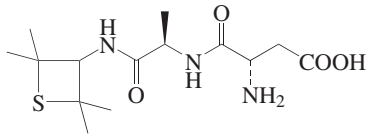
[9019-42-5, 9005-31-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1225B (*ir*)
Hirst, E. *et al., Chem. Ind. (London)*, 1963, 257
Haug, A. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 69 (*synth*)
Percival, E. *et al., The Carbohydrates*, (Pigman, W., Ed.), Academic Press, 1970, **2B**, 545
Ger. Pat., 1971, 2 046 966 (*2-hydroxypropyl ester, manuf*)
Rees, D.A. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 214 (*struct, rev*)
Grasdalen, H. *et al., Carbohydr. Res.*, 1977, **56**, C11; 1981, **89**, 179 (*nmr, cmr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 45 (*use*)
Cottrell, I.W. *et al., Handb. Water-Soluble Gums Resins*, McGraw-Hill, N.Y., 1980, 2/1-2/43 (*rev*)
Fed. Regist., 1982, **47**, 29946-29952 (*propylene glycol alginate*)
Martin, G. *et al., Sci. Aliments*, 1986, **6**, 473 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AFL000
Beale, J.M. *et al., Environ. Sci. Res.*, 1992, **44**, 209 (*rev, biosynth, struct*)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 10-11; 428-430
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1535
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 71-74; 2349-2352 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFL000; SEH000; CAM200; PKU700

Alitame, USAN A-283

L-α-Aspartyl-N-*(2,2,4,4-tetramethyl-3-thietanyl)-D-alaninamide, 9CI. CP 54802* [80863-62-3]



$C_{14}H_{25}N_3O_4S$ 331.435
Sweetening agent. Intensely sweet, approx. 2000 × sucrose. Use currently (1999) permitted in Australia, New Zealand, Indonesia and China. Solid + $2.5H_2O$. Log P -1.28 (calc). Use currently (1999) permitted in Australia, New Zealand, Indonesia and China.

[99016-42-9]

US Pat., 1983, (*(Pfizer)*)4 411 925 (*synth, use*)
Lawrence, J.F. *et al., J. Assoc. Off. Anal. Chem.*, 1988, **71**, 934-937 (*chromatog*)
Hendrick, M.E. *et al., Food Sci. Technol.*, 1991, **48**, 29-38 (*rev*)
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*rev*)
Auerbach, M.H *et al., Alternative Sweeteners*, 4th edn., (ed. O'Brien-Nabors, L.), CRC Press, 2011, 47-56 (*use, rev*)

Alkaline phosphatase A-284

E.C. 3.1.3.1. Phosphate-monoester phosphohydrolase (alkaline optimum). Alkaline phosphomonoesterase. Phosphomonoesterase†. *Glycerophosphatase*† [9001-78-9]

Phosphoric monoester hydrolase enzyme. Isol. from mammals, e.g. cow, pig, rabbit. Wide specificity. Zn- and Mg-dependent. Catalyses transphosphorylations. Human enzyme activity range pH 6.0-9.0. At -20°, 18% loss of activity after 2 years.

Stadtman, T.C. *et al., The Enzymes*, 2nd edn., (eds. Boyer, P.D. *et al*), Academic Press, 1961, **5**, 55-71 (*rev*)
Fernley, H.N. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1971, **4**, 417-447 (*rev*)
Goldstein, D.J. *et al., Nature (London)*, 1979, **280**, 602-605 (*mammals*)
Stinson, R.A. *et al., Adv. Protein Phosphatases*, 1987, **4**, 127-151 (*mammals, Escherichia coli*)
Fujimori-Arai, Y. *et al., Arch. Biochem. Biophys.*, 1991, **284**, 320-325 (*rabbit*)
Say, J.C. *et al., Biochim. Biophys. Acta*, 1991, **1074**, 256-262 (*rat*)
Savchenko, A. *et al., Methods Enzymol.*, 2001, **331**, 298-305 (*bacteria*)
Chen, Y.H. *et al., Protein Expr. Purif.*, 2004, **36**, 90-99 (*human*)

Gentiana Alkaloid V A-285

$C_{10}H_9NO_2$ 175.187
Struct. unknown. Monoterpene alkaloid. Alkaloid from *Gentiana lutea* (yellow gentian). Mp 240°.

Marekov, N. *et al., Dokl. Bulg. Akad. Nauk*, 1965, **18**, 999-1002 (*isol, ir*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)

Rosmarinus officinalis Alkaloid 2 A-286

$C_{20}H_{27}NO_4$ 345.438
Struct. unknown. Isol. from rosemary (*Rosmarinus officinalis*) using NH_3 during extraction. Cryst. (toluene). Mp 197-198° dec. $[\alpha]_D$ +36 (c, 1.48 in dioxan). Artifact.

Hydrochloride:
Cryst. (H_2O). Mp 214-216° dec.

N,O,O-*Tri-Ac:*
Cryst. (MeOH). Mp 291-292° dec.

Yakhontova, L.D. *et al., Khim. Prir. Soedin.*, 1967, **3**, 140; *Chem. Nat. Compd. (Engl. Transl.)*, 1967, **3**, 118

Alkane 1-monooxygenase A-287

E.C. 1.14.15.3. Alkane, reduced-rubredoxin:oxygen 1-oxidoreductase. Alkane 1-hydroxylase. Fatty acid ω-hydroxylase. ω-Hydroxylase. Laurate ω-hydroxylase [9059-16-9]

Oxidoreductase enzyme. Isol. from rabbit liver. Also hydroxylates fatty acids at the ω-position.

Cardini, G. *et al., J. Biol. Chem.*, 1970, **245**, 2789-2796 (*Corynebacterium*)
McKenna, E.J. *et al., J. Biol. Chem.*, 1970, **245**, 3882-3889 (*Pseudomonas oleovorans*)
Griffith, G.R. *et al., Methods Enzymol.*, 1978, **53**, 356-360 (*Pseudomonas oleovorans*)
Honeck, H. *et al., Biochem. Biophys. Res. Commun.*, 1982, **106**, 1318-1324 (*Lodderomyces elongisporus*)
Yoshimura, Y. *et al., J. Biochem. (Tokyo)*, 1990, **108**, 544-548 (*rabbit liver*)
May, S.W. *et al., Methods Enzymol.*, 1990, **188**, 3-10 (*Pseudomonas oleovorans*)
Okita, R.T. *et al., Curr. Drug Metab.*, 2001, **2**, 265-281 (*rev*)

1-Alkyl-2-acetylglycerophosphocholine esterase A-288

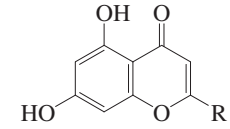
E.C. 3.1.1.47. 1-Alkyl-2-acetyl-sn-*glycero-3-phosphocholine acetohydrolase. 1-Alkyl-2-acetyllecithin deacetylase. Platelet-activating factor acetylhydrolase. LDL-associated phospholipase. PAF acetylhydrolase* [76901-00-3]

Carboxylic ester hydrolase enzyme. Isol. from mammals, e.g. cow, rabbit. Rat enzyme activity range pH 5.0-7.4.

Stafforini, D.M. *et al., J. Biol. Chem.*, 1987, **262**, 4223-4230; 1993, **268**, 3857-3865 (*human*)
Stafforini, D.M. *et al., Methods Enzymol.*, 1990, **187**, 344-357; 1991, **197**, 411-425 (*rev*)
Hattori, K. *et al., J. Biol. Chem.*, 1995, **270**, 22308-22313 (*ox*)
Tjoelker, L.W. *et al., Biochim. Biophys. Acta*, 2000, **1488**, 102-103 (*human, rat, rabbit*)
Chroni, A. *et al., Life Sci.*, 2000, **67**, 2807-2825 (*rat*)
Sheffield, P.J. *et al., Protein Eng.*, 2001, **14**, 513-519 (*cryst struct*)

2-Alkyl-5,7-dihydroxy-4*H*-1-benzopyran-4-ones A-289

2-Alkyl-5,7-dihydroxychromones



5,7-Dihydroxy-2-tritriacontyl-4*H*-1-benzopyran-4-one

5,7-Dihydroxy-2-tritriacontylchromone
$C_{42}H_{72}O_4$ 641.028

7-Me ether: [144049-68-3] *5-Hydroxy-7-methoxy-2-tritriacontyl-4*H*-1-benzopyran-4-one. 5-Hydroxy-7-methoxy-2-tritriacontylchromone*
$C_{43}H_{74}O_4$ 655.055
Constit. of *Agave americana*. Needles ($CHCl_3$/petrol). Mp 83°. λ_{max} 251 (MeOH) (Berdy).

Parmer, V.S. *et al., Tetrahedron*, 1992, **48**, 1281-1284 (*5-Hydroxy-7-methoxy-2-tritriacontylchromone*)

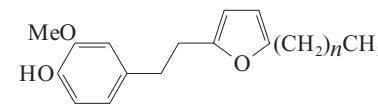
Alkylglycerophosphoethanolamine phosphodiesterase A-290

E.C. 3.1.4.39. 1-Alkyl-sn-*glycero-3-phosphoethanolamine ethanolaminehydrolase. Lysophospholipase D* [62213-15-4]

Phosphoric diester hydrolase enzyme. Isol. from rabbit, chicken. Also acts on acyl and choline analogues. Rat enzyme activity range pH 6.0-8.0.

Kawasaki, T. *et al., Biochim. Biophys. Acta*, 1987, **920**, 85-93 (*rabbit*)
Wykle, L. *et al., Methods Enzymol.*, 1991, **197**, 583-590 (*rat*)
Xie, Y. *et al., Cell. Signal.*, 2004, **16**, 975-981 (*human, rat, rabbit*)
Kehlen, A. *et al., Int. J. Cancer*, 2004, **109**, 833-838 (*human*)
Hama, K. *et al., J. Biol. Chem.*, 2004, **279**, 17634-17639 (*mouse*)
Morishige, J. *et al., Biochim. Biophys. Acta*, 2007, **1771**, 491-499 (*chicken*)

2-Alkyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furans A-291



n = 3, 5, 7

2-Butyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan [143114-90-3]

4-[2-(5-Butyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{17}H_{22}O_3$ 274.359

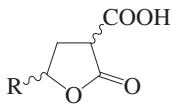
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 3.

2-Hexyl-5-[2-(4-hydroxy-3-methoxyphenyl)ethyl]furan [143114-91-4]
4-[2-(5-Hexyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{19}H_{26}O_3$ 302.413
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 5.

2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]-5-octylfuran [143114-92-5]
4-[2-(5-Octyl-2-furanyl)ethyl]-2-methoxyphenol, 9CI
$C_{21}H_{30}O_3$ 330.466
Isol. from dry rhizomes of ginger *Zingiber officinale*. *n* = 7.

Nakatani, N. *et al., Chem. Express*, 1992, **7**, 221 (*isol, pmr, cmr*)

5-Alkyltetrahydro-2-oxo-3-furancarboxylic acids A-292



5-Butyltetrahydro-2-oxo-3-furancarboxylic acid, 9CI
2-Carboxy-4-octanolide
$C_9H_{14}O_4$ 186.207
Possible latent butter aroma compd. Mp 48-50°.

5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-6-methyl-4-heptanolide
$C_9H_{14}O_4$ 186.207
Possible latent butter aroma compd. Mp 51-54°.

5-Pentyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-nonanolide
$C_{10}H_{16}O_4$ 200.234
Possible latent butter aroma compd. Mp 46-48°.

5-(3*E*-Pentenyl)tetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-7-nonen-4-olide
$C_{10}H_{14}O_4$ 198.218
Possible latent butter aroma compound. Mp 52.5-54°.

5-Hexyltetrahydro-2-oxo-3-furancarboxylic acid, 9CI
2-Carboxy-4-decanolide. α-Carboxy-γ-decalactone
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd. Mp 60.5-62.5°.

5-(1,3-Dimethylbutyl)tetrahydro-2-oxo-3-furancarboxylic acid
5-(4-Methyl-2-pentyl)tetrahydro-2-oxo-3-furancarboxylic acid. 2-Carboxy-5,7-dimethyl-4-octanolide
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd. Mp 100.5-105°.

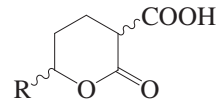
5-Heptyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-undecanolide
$C_{12}H_{20}O_4$ 228.288
Possible latent butter aroma compd. Mp 58-60°.

5-Octyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-dodecanolide. α-Carboxy-γ-dodecalactone
$C_{13}H_{22}O_4$ 242.314
Possible latent butter aroma compd. Mp 68.5-70.5°.

5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid
2-Carboxy-4-tridecanolide
$C_{14}H_{24}O_4$ 256.341
Possible latent butter aroma compd. Mp 68.5-69.5°.

Stoll, M. *et al., Nature (London)*, 1964, **202**, 350
Martin, J. *et al., Chem. Comm.*, 1970, 27 (*synth*)

6-Alkyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acids A-293



See also 5-Alkyltetrahydro-2-oxo-3-furancarboxylic acids, A-292.

6-Butyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acid
2-Carboxy-5-nonanolide. α-Carboxy-δ-nonalactone
$C_{10}H_{16}O_4$ 200.234
Possible latent butter aroma compd. Mp 79-80°.

6-Pentyltetrahydro-2-oxo-2*H*-pyran-3-carboxylic acid
2-Carboxy-5-decanolide. α-Carboxy-δ-decalactone
$C_{11}H_{18}O_4$ 214.261
Possible latent butter aroma compd. Mp 77-78°.

Stoll, M. *et al., Nature (London)*, 1964, **202**, 350 (*synth*)

Allantoic acid A-294

Bis[(aminocarbonyl)amino]acetic acid, 9CI. Diureidoacetic acid. Hidantoic acid (obsol.) [99-16-1]

$(H_2NCONH)_2CHCOOH$

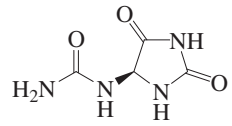
$C_4H_8N_4O_4$ 176.132
Isol. from coffee beans and leaves. Needles. Spar. sol. H_2O, org. solvs., dil. acids. Mp 173° dec. Sinters at 168°. Hot H_2O → Oxoacetic acid + Urea.

Et ester: [156217-60-6]
$C_6H_{12}N_4O_4$ 204.185
Needles. Sol. EtOH, hot H_2O. Dec. *ca.* 200°.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 675B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 805D (*ir*)
Behrend, R. *et al., Annalen*, 1909, **365**, 21-37 (*synth*)
Fosse, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1929, **189**, 716-717; 1933, **196**, 1264-1267 (*occur*)
Schlee, D. *et al., Phytochemistry*, 1963, **2**, 231-236 (*biosynth*)
Ringertz, H. *et al., Acta Cryst. B*, 1968, **24**, 1686-1692 (*cryst struct*)

Allantoin, BAN, USAN A-295

(2,5-Dioxo-4-imidazolidinyl)urea, 9CI. 5-Ureido-2,4-imidazolidinedione. Glyoxylic diureide. 5-Ureidohydantoin. Dermalex. Cordianin. Actinac. Alphosyl



(*R*)-*form*

$C_4H_6N_4O_3$ 158.116

(*R*)-*form* [7303-80-2]
Mod. sol. H_2O, more sol. org. solvs than (±)-form. Mp 226-229° dec. $[\alpha]_D^{30}$ -92 (c, 0.0075 in H_2O). pK_a 8.5 (25°).

(*S*)-*form* [3844-67-5]
Needles (H_2O). $[\alpha]_D^{29}$ +92 (H_2O).

(±)-*form* [5377-33-3]
Isol. from cows milk. Monoclinic prisms (H_2O). V. spar. sol. H_2O; spar. sol. org. solvs. Mp 238-240° dec. Log P -1.54 (calc). Component of numerous prepns. Actinac, Alphosyl, Dermalex.

▶ YT1600000

Dihydroxyaluminium compd.: [5579-81-7] ***Aldioxa, INN, USAN***. *Alanta-SF. Alarant. ALDA. Alkixa. Arlanto. Ascomp. Peptilate. RC-172. Many other names*
$C_4H_7AlN_4O_5$ 218.105
Greyish powder.

▶ BD0200000

Chlorotetrahydroxydialuminium compd.: [1317-25-5] ***Alcloxa, INN, USAN***. *Aluminium chlorhydroxy allantoinate. Isaropan. Ulfon. ALCA. RC-173*
Mp 240° dec.

▶ Eye irritant. BD0580000

1-Ac:
$C_6H_8N_4O_4$ 200.154
Leaflets (AcOH). Mp 236° dec.

1,3-Di-Ac:
$C_8H_{10}N_4O_5$ 242.191
Prisms (AcOH). Mp 247° dec.

1-Me: [22494-76-4] *α-Methylallantoin*
$C_5H_8N_4O_3$ 172.143
Cryst. Spar. sol. hot H_2O. Mp 255-259° dec.

3-Me: [22494-77-5] *β-Methylallantoin*
$C_5H_8N_4O_3$ 172.143
Prisms + H_2O (H_2O). Mp 226-227°.

1,3-Di-Me: [32282-45-4]
$C_6H_{10}N_4O_3$ 186.17
Prisms (EtOH). Mp 214°.

1,6-Di-Me:
$C_6H_{10}N_4O_3$ 186.17
Needles (AcOH). Mp 226-227° dec.

1,8-Di-Me:
$C_6H_{10}N_4O_3$ 186.17
Prisms (H_2O). Mp 220-223°.

3,8-Di-Me:
$C_6H_{10}N_4O_3$ 186.17
Prisms (H_2O). Mp 222-223°.

1,3,6-Tri-Me: Caffoline
$C_7H_{12}N_4O_3$ 200.197
Fine needles. Sol. H_2O. Mp 197°.

1,3,8-Tri-Me:
$C_7H_{12}N_4O_3$ 200.197
Prisms (EtOAc). Mp 152°.

[61504-48-1, 97-59-6 ((±)-*form*)]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 809A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1316C (*nmr*)
Biltz, H. *et al., Ber.*, 1911, **44**, 282-305 (*1,3,6-tri-Me*)
Fosse, R. *et al., C. R. Hebd. Seances Acad. Sci.*, 1934, **98**, 689; 1374-1376; 1953-1955 (*S-form, isol, resoln*)
Greenbaum, F.R. *et al., Am. J. Pharm.*, 1940, **112**, 205-216 (*rev*)
Org. Synth., Coll. Vol., 2, 1943, 21-23 (*synth, bibl*)
US Pat., 1956, 2 761 867 (*synth, Al compds*)
US Pat., 1967, 3 305 557 (*synth*)
Gravenmade, E.J. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1969, **88**, 929-939 (*R-form, synth*)
Abblard, J. *et al., Bull. Soc. Chim. Fr.*, 1971, 942-946 (*struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2569 (*occur*)
Mecca, S.B. *et al., Soap, Perfum. Cosmet.*, 1976, **49**, 434; 481; 483-485 (*rev*)
Coxon, B. *et al., JOC*, 1977, **42**, 3132-3140 (*cmr*)
Mecca, S.B. *et al., Cosmet. Toiletries*, 1978, **93**, 39-41 (*rev*)
Cook, A.F. *et al., JOC*, 1980, **45**, 4020-4025 (*isol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 184
Chen, K.J. *et al., Taiwan Kexue*, 1989, **42**, 21-24 ((±)-*form, isol*)
Modric, N. *et al., Tet. Lett.*, 1989, **30**, 5021-5024 (*cd*)
Hoffmann-Bohm, K. *et al., Planta Med.*, 1992, **58**, 544-548 ((±)-*form, isol*)
Mourabit, A.A. *et al., J. Nat. Prod.*, 1997, **60**, 290-291 ((±)-*form, isol*)
Shingfield, K.J. *et al., J. Chromatogr., B*, 1998, **706**, 342-346 (*hplc*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1078
Ferreira, D.T. *et al., Quim. Nova*, 2000, **23**, 42-46 (*isol*)

Allatostatin C A-296

Cb-AST-C1 [1189515-02-3]

5-Oxo-Pro-Ile-Arg-Tyr-His-Glu-Cys-Tyr-Phe-Asp-Pro-Ile-Ser-Cys-Phe-OH

$C_{88}H_{118}N_{22}O_{22}S_2$ 1900.166
Found in the nervous systems of crabs, lobsters and shrimp.

Stemmler, E.A. *et al., Gen. Comp. Endocrinol.*, 2010, **165**, 1-10 (*Allatostatin C*)

Allicepin A-297

Peptide. MW approx. 10 kDa. Isol. from onion (*Allium cepa*) bulbs.

Wang, H.X. *et al., J. Pept. Sci.*, 2004, **10**, 173-177 (*Allicepin*)

Allicin A-298

S-*2-Propenyl 2-propene-1-sulfinothioate, 9CI. Allitridi* [539-86-6]

$H_2C{=}CHCH_2\text{-}SO\text{-}S\text{-}CH_2CH{=}CH_2$
$C_6H_{10}OS_2$ 162.276
Isol. from garlic (*Allium sativum*). Nutraceutical. Yellow liq. Sol. H_2O, MeOH, Et_2O; fairly sol. hexane. d 1.11. λ_{max} 202; 240 (MeOH) (Berdy).

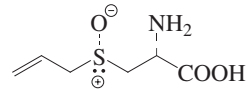
▶ LD_{50} (mus, scu) 120 mg/kg, LD_{50} (mus, ivn) 60 mg/kg. Can cause allergic contact dermatitis in sensitised individuals. UD1900000

[72869-75-1]

Cavallito, C.J. *et al., JACS*, 1944, **66**, 1950-1951 (*isol, struct, activity*)
Stoll, A. *et al., Helv. Chim. Acta*, 1948, **31**, 189; 1949, **32**, 197 (*synth*)
Virtanen, A.I. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 299 (*rev*)
Isenberg, N. *et al., Int. J. Sulfur Chem.*, 1973, **3**, 307 (*rev*)
Papageorgiou, C. *et al., Arch. Dermatol. Res.*, 1983, **275**, 229 (*tox*)
Block, E. *et al., JACS*, 1986, **108**, 7045-7055 (*synth, cmr, ir, pmr*)
Mayeux, P.R. *et al., Agents Actions*, 1988, **25**, 182 (*pharmacol*)
Makheja, A.N. *et al., Agents Actions*, 1990, **29**, 360 (*pharmacol*)
Gebhardt, R. *et al., Arzneim.-Forsch.*, 1991, **41**, 800 (*pharmacol*)
Gebhardt, R. *et al., Biochim. Biophys. Acta*, 1994, **1213**, 57 (*pharmacol*)
Calvey, E.M. *et al., J. Chromatogr. Sci.*, 1994, **32**, 93 (*chromatog*)
Block, E. *et al., Sulfur Compds. Foods, 1993*, (Eds. Mussinan, C.J. *et al*), American Chemical Society (*ACS Symp. Ser.* v564 1994), 1994, 63 (*rev*)
Nikolic, V. *et al., Pharmazie*, 2004, **59**, 10-14 (*synth, pmr, cmr*)
Kyung, K.H. *et al., Curr. Opin. Biotechnol.*, 2012, (*rev, activity*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AFS250

Alliin A-299

3-(2-Propenylsulfinyl)alanine, 9CI. β-Allysulfenylalanine. S-*Allylcysteine sulfoxide*



$C_6H_{11}NO_3S$ 177.224

(R)*$_C$*(S)*$_S$*-form [556-27-4]
Constit. of garlic oil (*Allium sativum*), also from ramsons (*Allium ursinum*). Needles (Me_2CO aq.). Mp 163° dec. $[\alpha]_D^{21}$ +67.7 (c, 2.0 in H_2O). Other stereoisomers have been prepared synthetically.

N-*(1-Deoxy-β-D-fructopyranosyl):*
[149340-22-7]
$C_{12}H_{21}NO_8S$ 339.366
Isol. from garlic (*Allium sativum*). Powder. $[\alpha]_D^{20}$ -25.4 (c, 0.41 in H_2O).

N-*Ac:* [38131-20-3]
Mp 188-198° dec. $[\alpha]_D^{21}$ -29 (c, 1.0 in MeOH).

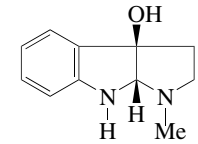
N-*Benzoyl:* Mp 152-153.5° dec. $[\alpha]_D^{20}$ -6 (c, 1.0 in MeOH).

N-*(4-Nitrobenzoyl):* Mp 180-182° dec. $[\alpha]_D^{20}$ -9 (c, 1.0 in 0.1*N* NaOH).

Stoll, A. *et al., Helv. Chim. Acta*, 1951, **34**, 481 (*synth*)
Virtanen, A.I. *et al., Angew. Chem., Int. Ed.*, 1962, **1**, 299 (*rev*)
Nishimura, H. *et al., Tetrahedron*, 1972, **28**, 4503 (*ms, ir*)
Freeman, G.G. *et al., Phytochemistry*, 1976, **15**, 521 (*synth*)
Muetsch-Eckner, M. *et al., J. Nat. Prod.*, 1993, **56**, 864 (*N-glycoside*)
Edwards, S.J. *et al., Phytochem. Anal.*, 1994, **5**, 4 (*anal*)
Keusgen, M. *et al., Planta Med.*, 1998, **64**, 736-740 (*anal*)
Kubec, R. *et al., J. Agric. Food Chem.*, 2000, **48**, 428-433 (*occur*)
Hughes, J. *et al., Phytochemistry*, 2005, **66**, 187-194 (*biosynth*)

Alline A-300

*2,3,8,8*a-*Tetrahydro-1-methylpyrrolo[2,3-*b*]indol-3*a*(1*H*)-ol, 9CI* [101053-34-3]



Relative Configuration

$C_{11}H_{14}N_2O$ 190.244
Alkaloid from Chinese chives (*Allium odorum*) and several other *Allium* spp. Mp 91-92°. $[\alpha]_D$ +136.3 (c, 1.218 in HCl). λ_{max} 245 (log ε 3.68); 303 (log ε 3.14) (no solvent reported).

Hydrochloride: Mp 196-197°.

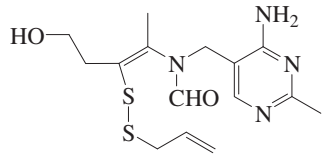
N-*De-Me,* O-*Ac:* [1147521-50-3] **O-*Acetyl*-N-*demethylalline***
$C_{12}H_{14}N_2O_2$ 218.255
Gum. $[\alpha]_D^{25}$ +84 (c, 0.24 in MeOH).

Me ether, N^8-*Me: 2,3,8,8*a-*Tetrahydro-3*a-*methoxy-1,8-dimethylpyrrolo[2,3-*b*]indole. **Alkaloid CPC 1**. CPC 1*
$C_{13}H_{18}N_2O$ 218.298
Amorph. solid. $[\alpha]_D^{26}$ -88 (c, 0.1 in MeOH). (3*aR*,8*aR*)-Config. determined. λ_{max} 205 (log ε 4.15); 251 (log ε 3.72); 301 (log ε 3.14) (MeOH).

Tashkhodzhaev, B. *et al., Khim. Prir. Soedin.*, 1985, **21**, 687-691; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 645-649 (*isol, cryst struct, uv*)
Samikov, K. *et al., Khim. Prir. Soedin.*, 1986, **22**, 383; *Chem. Nat. Compd. (Engl. Transl.)*, 1986, **22**, 362 (*occur*)
Antsupova, T.P. *et al., Rastit. Resur.*, 1987, **23**, 436 (*occur*)

Kitajima, M. *et al., Tet. Lett.*, 2006, **47**, 3199-3202 (*CPCI*)
Li, L.-Y. *et al., J. Asian Nat. Prod. Res.*, 2008, **10**, 765-770 (*N-de-Me O-Ac*)

Allithiamine **A-301**
N-*[(4-Amino-2-methyl-5-pyrimidinyl)-methyl]*-N-*[4-hydroxy-1-methyl-2-(2-propenyldithio)-1-butenyl]formamide, 9CI* [554-44-9]



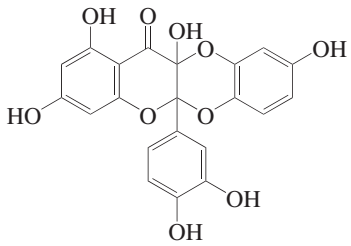
$C_{15}H_{22}N_4O_2S_2$ 354.496
Naturally-occurring open-chain thiamine analogue. Obt. from garlic (*Allium sativum*). Imparts meaty flavour to foods. Has vitamin B_1 activity. Investigated as a dietary supplement to enhance muscle performance in sports. Cryst. (C_6H_6). Mp 132-133° dec.

Matsukawa, T. *et al., Science (Washington, D.C.)*, 1953, **118**, 325 (*isol, struct*)
Matsukawa, T. *et al., CA*, 1955, **49**, 7572g (*synth*)
Baker, H. *et al., J. Nutr. Sci. Vitaminol.*, Suppl., 1976, **22**, 63-68 (*pharmacol*)
Doyle, M.R. *et al., Int. J. Sport Nutr.*, 1997, **7**, 39-47 (*use*)

Alliumin **A-302**
Protein. Isol. from multiple-cloved garlic bulbs (*Allium sativum*).

Xia, L. *et al., Peptides (N.Y.)*, 2002, **26**, 277-283 (*Alliumin*)

Alliuocide G **A-303**
[1058711-45-7]



$C_{21}H_{14}O_{10}$ 426.336
Constit. of the outer scales of onion bulbs (*Allium cepa*). Amorph. brown solid. Mp 292-293°. $[\alpha]_D$ +71.4 (c, 0.5 in MeOH). λ_{max} 290 (MeOH).

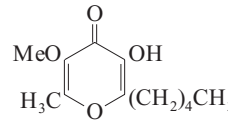
Mohamed, G.A. *et al., ARKIVOC*, 2008, **xi**, 202-209 (*isol, pmr, cmr*)

Allivin **A-304**
[459875-13-9]

Protein. Isol. from bulbs of the round-cloved garlic *Allium sativa* var. round clove.

Wang, H.X. *et al., Life Sci.*, 2001, **70**, 357-365 (*Allivin*)

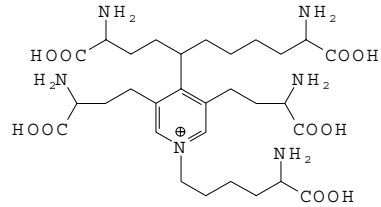
Allixin **A-305**
*3-Hydroxy-5-methoxy-6-methyl-2-pentyl-4*H-*pyran-4-one, 9CI* [125263-70-9]



$C_{12}H_{18}O_4$ 226.272
Constit. of garlic (*Allium sativum*). Potential nutraceutical. Needles (MeOH aq.). Mp 80-81°. λ_{max} 279 (no solvent reported).

Kodera, Y. *et al., Chem. Pharm. Bull.*, 1989, **37**, 1656 (*isol, struct*)
Arimoto, H. *et al., Tet. Lett.*, 1997, **38**, 7761-7762 (*synth*)
Matsumura, Y. *et al., Tet. Lett.*, 1998, **39**, 2339-2340 (*synth*)
Kodera, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 354-363; 405-407 (*pmr, cmr, ms, pharmacokinet*)

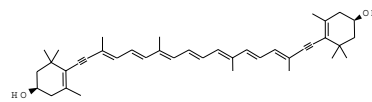
Allodesmosine **A-306**
[129717-82-4]



$C_{30}H_{51}N_6O_{10}^{\oplus}$ 655.767
Isol. from hydrolysate of bovine ligamentum nuchae elastin. Amorph. solid with faint yellow tinge. V. hygroscopic.

Suyuma, K. *et al., Biochem. Biophys. Res. Commun.*, 1990, **170**, 713 (*isol, uv, ms, pmr*)
Nakamura, F. *et al., Agric. Biol. Chem.*, 1991, **55**, 547 (*isol, pmr, ms*)

Alloxanthin **A-307**
7,7′,8,8′-Tetradehydro-β,β-carotene-3,3′-diol. Cynthiaxanthin. Cryptomonaxanthin. Manixanthin. Pectenoxanthin
[28380-31-6]



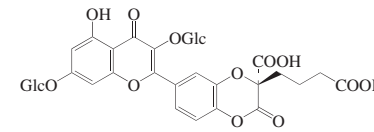
$C_{40}H_{52}O_2$ 564.85
Constit. of many shellfish including the giant scallop (*Pecten maximus*) and edible mussel (*Mytilus edulis*). Reddish needles (Me_2CO/petrol). Mp 188-190° (186-188°).

Enantiomer, di-Me ether: [166774-49-8]
7,7′,8,8′-Tetradehydro-3,3′-dimethoxy-β,β-carotene. ***Suberixanthin***
$C_{42}H_{56}O_2$ 592.903
λ_{max} 428 (sh); 452; 480 (Et_2O).

[26666-93-3 (Alloxanthin; unspecified form), 95343-66-1 (Alloxanthin; unspecified form)]

Chapman, D.J. *et al., Phytochemistry*, 1966, **5**, 1331-1333 (*Alloxanthin*)
Campbell, S.A. *et al., Chem. Comm.*, 1967, 941-942 (*Alloxanthin*)
De Ville, T.E. *et al., Chem. Comm.*, 1969, 1311-1312 (*Alloxanthin, struct*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*Alloxanthin, cmr*)
Liaaen-Jensen, S. *et al., Biochem. Syst. Ecol.*, 1982, **10**, 167-174 (*Alloxanthin, occur, sponges*)
Davies, A.J. *et al., JCS Perkin 1*, 1984, 2147-2157 (*(±)-Alloxanthin, synth*)
Pennington, F.C. *et al., Biochem. Syst. Ecol.*, 1985, **13**, 215-219 (*Alloxanthin, cd*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495-503 (*Alloxanthin, pmr, uv*)
Aiello, A. *et al., J. Prakt. Chem.*, 1995, **337**, 397-400 (*Suberixanthin, abs config*)
Chinese Pat., 2008, 101 293 863 (*Alloxanthin, synth*)

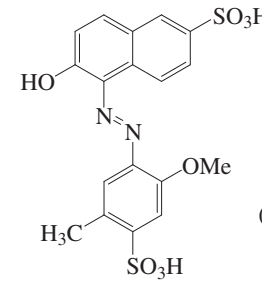
Alluceposide **A-308**
[1016883-43-4]



$C_{34}H_{36}O_{22}$ 796.645
Constit. of the bulbs of red onion (*Allium cepa*).

Zaghloul, M.G. *et al., Mansoura J. Pharm. Sci.*, 2007, **23**, 61-71 (*isol*)

Allura red AC **A-309**
6-Hydroxy-5-[(2-methoxy-5-methyl-4-sulfophenyl)azo]-2-naphthalenesulfonic acid, 9CI. FD and C Red No. 40. C.I. 16035. C.I. Food Red 17. Allura Red. E129 [25956-17-6]



(*E*)-*form*

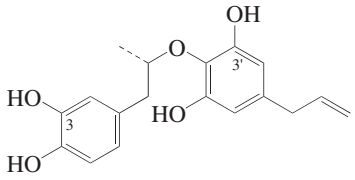
$C_{18}H_{16}N_2O_8S_2$ 452.465
Colour additive used in gelatins, puddings, custards, beverages, sauces, toppings, fruits, dairy products, bakery products, jams, jellies, condiments, meat and poultry. Dark red powder. Strictly the name Allura red AC applies to the disodium salt. Banned in EEC, Norway and Japan.

▶ QK2260000

UK Pat., 1970, 1 164 249 (*synth*)
Borzelleca, J.F. *et al., Food Chem. Toxicol.*, 1989, **27**, 701 (*tox*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1078-1080 (*use, props*)
Merck Index, 13th edn., 2001, No. 281 (*bibl*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG100

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4-dihydroxyphenyl)propane A-310



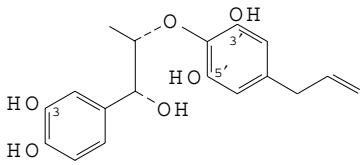
$C_8H_{20}O_5$ 196.243

(*S*)-*form*

Tetra-Me ether: [1246343-70-3] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)propane*
$C_{22}H_{28}O_5$ 372.46
Constit. of the seeds of *Myristica fragrans* (nutmeg).

Yang, X. *et al., Zhongguo Zhongyao Zazhi*, 2008, **33**, 397-402 (*tetra-Me ether*)

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4-dihydroxyphenyl)-1-propanol A-311



$C_{18}H_{20}O_6$ 332.352
Neolignan numbering shown.

(*R,*S**)-*form***

3,3′,5′-Tri-Me ether: [52190-21-3] *α-[1-[2,6-Dimethoxy-4-(2-propenyl)phenoxy]ethyl]-4-hydroxy-3-methoxybenzenemethanol, 9CI. 2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol*
$C_{21}H_{26}O_6$ 374.433
From seed kernels of *Myristica fragrans* (nutmeg). Mp 96.5-97.5°.

3,3′,5,5′-Tetra-Me ether: [41535-92-6] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_6$ 388.46
From *Myristica fragrans* (nutmeg). Cryst. Mp 65-66°.

3,4-Methylene, 3′,5′-di-Me ether: [50354-29-5] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4-methylenedioxyphenyl)-1-propanol*
$C_{21}H_{24}O_6$ 372.417
Constit. of *Myristica fragrans* (nutmeg). Oil.

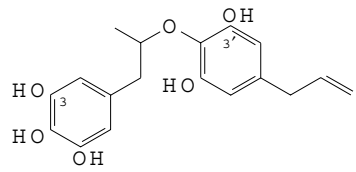
3,4-Methylene, 3′,5′-di-Me ether, Ac:
$C_{23}H_{26}O_7$ 414.454
Consit. of *Myristica fragrans* (nutmeg). Oil.

3,4-Methylene, 3′,5′-di-Me ether, benzoyl:
$C_{28}H_{28}O_7$ 476.525
Constit. of *Myristica fragrans* (nutmeg). Oil.

[52190-19-9, 41535-95-9]

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 1479 (*isol, ir, uv, pmr, ms*)
Forrest, J.E. *et al., JCS Perkin 1*, 1974, 205 (*isol, uv, pmr, ms*)
Kasahara, H. *et al., Phytochemistry*, 1995, **40**, 1515 (*abs config*)

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4,5-trihydroxyphenyl)propane A-312



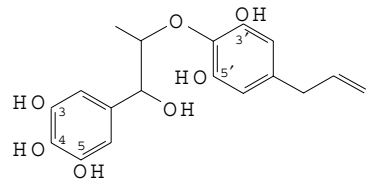
$C_{18}H_{20}O_6$ 332.352
Neolignan numbering shown.

Penta-Me ether: [124151-41-3] ***Virolongin B****. β-O-Dilignol*
$C_{23}H_{30}O_6$ 402.486
Constit. of *Myristica fragrans* (nutmeg). Oil. Identity of isolated samples not establ., may not be stereochemically identical.

3,4-Methylene, 3′,5,5′-tri-Me ether: [126223-32-3] ***Virolongin C***
$C_{22}H_{26}O_6$ 386.444
Oil.

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 193; 889; 1479 (*isol, struct*)
Forrest, J.E. *et al., JCS Perkin 1*, 1974, 205 (*isol, synth, struct*)
Calvacante, S.H. *et al., Phytochemistry*, 1985, **24**, 1051 (*isol*)
Muhammed, I. *et al., J. Nat. Prod.*, 1989, **52**, 1177 (*isol, pmr, cmr*)
Ren, X. *et al., J. Chin. Chem. Soc. (Taipei)*, 2004, **51**, 969-974 (*Virolongin B, synth*)

2-(4-Allyl-2,6-dihydroxyphenoxy)-1-(3,4,5-trihydroxyphenyl)-1-propanol A-313



$C_{18}H_{20}O_7$ 348.352
Neolignan numbering shown.

3,3′,4,5′-Tetra-Me ether: [108907-57-9] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3-hydroxy-4,5-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_7$ 404.459
Constit. of oil of *Myristica fragrans* (nutmeg). Oil.

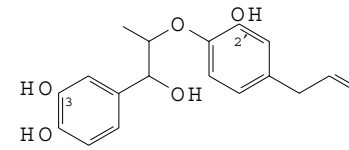
3,3′,5,5′-Tetra-Me ether: [108907-53-5] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(4-hydroxy-3,5-dimethoxyphenyl)-1-propanol*
$C_{22}H_{28}O_7$ 404.459
Constit. of oil of *Myristica fragrans* (nutmeg).

Penta-Me ether: [41551-58-0] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3,4,5-trimethoxyphenyl)-1-propanol*
$C_{23}H_{30}O_7$ 418.486
Constit. of *Myristica fragrans* (nutmeg). Mp 70-72° (66-66.5°).

4-Deoxy, 3,3′,5′-tri-Me ether: [1246343-73-6] *2-(4-Allyl-2,6-dimethoxyphenoxy)-1-(3-hydroxy-5-methoxyphenyl)-1-propanol*. ***Myrisisolignan***
$C_{21}H_{26}O_6$ 374.433
Constit. of the seeds of *Myristica fragrans* (nutmeg). Possesses (7*R**,8*R**)-config.

Isogai, A. *et al., Agric. Biol. Chem.*, 1973, **37**, 193-194; 889-895; 1479-1486 (*isol, struct, activity*)
Forrest, J.E. *et al., JCS Perkin 1*, 1974, 205-209 (*isol, struct*)
Hattori, H. *et al., Chem. Pharm. Bull.*, 1987, **35**, 668-674 (*tetra-Me ethers*)
Zacchino, S.A. *et al., J. Nat. Prod.*, 1988, **51**, 1261-1265 (*synth, ir, pmr, cmr, ms, abs config*)
Yang, X. *et al., Zhongguo Zhongyao Zazhi*, 2008, **33**, 397-402 (*Myrisisolignan*)

2-(4-Allyl-2-hydroxyphenoxy)-1-(3,4-dihydroxyphenyl)-1-propanol A-314



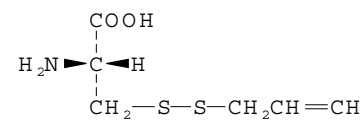
$C_{18}H_{20}O_5$ 316.353
Neolignan numbering shown.

2′,3-Di-Me ether: [108907-55-7] *2-(4-Allyl-2-methoxyphenoxy)-1-(4-hydroxy-3-methoxyphenyl)-1-propanol*
$C_{20}H_{24}O_5$ 344.407
Constit. of *Myristica fragrans* (nutmeg) oil. Oil.

Hattori, M. *et al., Chem. Pharm. Bull.*, 1987, **35**, 668

S-(Allylthio)cysteine A-315

3-(2-Propenyldithio)alanine, 9CI. 3-(Allyldithio)alanine, 8CI. 2-Amino-3-(2-propenyldithio)propanoic acid. S-*Allymercaptocysteine. 2-Amino-4,5-dithia-7-heptenoic acid. SAMC* [30910-60-2]



$C_6H_{11}NO_2S_2$ 193.29

(*R*)-*form* [2281-22-3]
L-form
Isol. from garlic (*Allium sativum*). Potential nutraceutical. Plates (Me_2CO aq.).

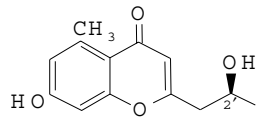
Mp 187-188° dec. $[\alpha]_D^{23.5}$ -107.9 (c, 0.4 in 6*M* HCl).

Cavallito, C.J. *et al., JACS*, 1944, **66**, 1952 (*synth*)

Sugii, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1114 (*isol, ir, struct*)

Aloesol A-316

*7-Hydroxy-2-(2-hydroxypropyl)-5-methyl-4*H*-1-benzopyran-4-one, 9CI. 7-Hydroxy-2-(2-hydroxypropyl)-5-methylchromone* [94356-35-1]



$C_{13}H_{14}O_4$ 234.251

Constit. of *Aloe* spp. and Chinese rhubarb. Cryst. (AcOH/MeOH). Mp 187.5-189°. $[\alpha]_D^{21}$ +38.4 (c, 0.89 in MeOH).

7-O-*β*-D-*Glucopyranoside:* [94356-36-2]
$C_{19}H_{24}O_9$ 396.393
Constit. of rhubarb *Rheum* sp. Needles + $1H_2O$ (MeOH/$CHCl_3$). Mp 191-193°. $[\alpha]_D^{24}$ -4.3 (c, 0.21 in MeOH).

2′-Ketone: [40738-40-7] ***Aloesone***
$C_{13}H_{12}O_4$ 232.235
Cryst. ($CHCl_3$). Mp 151-152°.

2′-Ketone, 7-O-*β*-D-*glucopyranoside:* [128701-04-2]
$C_{19}H_{22}O_9$ 394.377
Constit. of Chinese rhubarb (*Rheum* sp.). Needles (MeOH aq.). Mp 229-230°. $[\alpha]_D^{19}$ -50.6 (c, 0.37 in MeOH).

[104871-04-7, 135096-88-7]

Holdsworth, D.K. *et al., Planta Med.*, 1972, **22**, 54 (*isol*)

Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3493-3500 (*isol*)

Gramatica, P. *et al., Heterocycles*, 1986, **24**, 743 (*synth*)

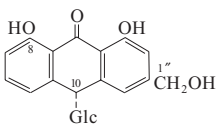
Kashiwada, Y. *et al., Phytochemistry*, 1990, **29**, 1007-1009 (*Aloesone 7-glucoside*)

Che, Q.M. *et al., Chem. Pharm. Bull.*, 1991, **39**, 704 (*occur*)

Xu, J. *et al., J. Nat. Prod.*, 2009, **72**, 662-665 (*isol, pmr*)

Aloin, BAN A-317

*10-β-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10*H*)-anthracenone, 9CI. Barbaloin. Socaloin. Ugandaloin. Jafaloin. Cafaloin* [8015-61-0]



(10*R*)–*form*

$C_{21}H_{22}O_9$ 418.399

Aloin as normally obt. is a mixt. of 10-epimers separable by hplc into Aloin A and the unstable Aloin B. Aloin A can also be obt. by cryst. from MeOH. Constit. of various *Aloe* spp. Sol. H_2O. Log P -1.88 (calc).

▶ LD_{50} (mus, ivn) 200 mg/kg.

(10*R*)-*form* [28371-16-6]
Aloin B*. Isobarbaloin. β-Barbaloin*Mp 138-140° (block). $[\alpha]_D^{30}$ -73 (c, 0.5 in MeOH). Negative CD at 295 nm. Pmr δ 5.27 (C-1′). Labile in soln. Isobarbaloin and β-Barbaloin were prob. not homogeneous.

1″-O-*α*-L-*Rhamnopyranoside:* [11006-91-0] ***Aloinoside B***
$C_{27}H_{32}O_{13}$ 564.542
Isol. from leaves of *Aloe* cf. *perryi*. Cryst. (Me_2CO aq.). Mp 233°. $[\alpha]_D^{20}$ -45.3 (c, 1.5 in 50% dioxan aq.).

8-O-*β*-D-*Glucopyranoside:* [53861-34-0] ***Cascaroside B***
$C_{27}H_{32}O_{14}$ 580.541
Isol. from *Rhamnus purshiana* (Cascara sagrada) bark. Cryst. + $2H_2O$. Mp 175-178°. $[\alpha]_D^{30}$ -104.4 (MeOH). Cascarosides A and B are a pair of 10-epimers corresponding to Aloins A and B but the configurational correspondence of Cascaroside B to Aloin B is not established, i.e. it could be (10*R*-).

1″-Carboxylic acid, 8-O-*β*-D-*glucopyranoside:* [111545-29-0] ***Rheinoside C***
$C_{27}H_{30}O_{15}$ 594.525
Isol. from rhubarb. Pale yellow powder + $2H_2O$. $[\alpha]_D^{25}$ -40 (c, 0.5 in MeOH).

7-Hydroxy: [82461-12-9] ***7-Hydroxyaloin B***
$C_{21}H_{22}O_{10}$ 434.399
Constit. of leaves of *Aloe vera*.

7-Hydroxy, 8-Me ether: ***7-Hydroxy-8-O-methylaloin B***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of leaves of *Aloe vera*. Amorph. yellowish solid. $[\alpha]_D^{25}$ -0.7 (c, 0.1 in MeOH). λ_{max} 204 (log ϵ 4.4); 221 (log ϵ 4.35); 294 (log ϵ 4.09); 345 (log ϵ 3.82) (MeOH).

1″-Deoxy, 8-O-*β*-D-*glucopyranoside:* [53861-35-1] ***Cascaroside D***
$C_{27}H_{32}O_{13}$ 564.542
From cascara sagrada (*Rhamnus purshiana*) bark.

1″-Deoxy, 6-hydroxy, 8-O-*β*-D-*glucopyranoside:* [164322-83-2] ***Cascaroside F***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of cascara sagrada (*Rhamnus purshiana*) bark. Mp 176-178°. $[\alpha]_D^{25}$ -69.5 (c, 0.1 in MeOH).

(10*S*)-*form* [1415-73-2]
Aloin A
Yellow needles (EtOH). Sol. H_2O. Mp 148° (block). $[\alpha]_D^{30}$ +10.2 (c, 0.5 in MeOH). Positive CD at 295 nm. Pmr δ 5.13 (C-1′).

▶ LD_{50} (mus, ivn) 200 mg/kg. LZ6520000

1″-O-*α*-L-*Rhamnopyranoside:* [56645-88-6] ***Aloinoside A***
$C_{27}H_{32}O_{13}$ 564.542
Constit. of *Aloe ferox* and other *Aloe* spp. λ_{max} 236 (ϵ 22400) (MeOH) (Derep).

8-O-*β*-D-*Glucopyranoside:* [53823-08-8] ***Cascaroside A***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of *Rhamnus purshiana* (Cascara sagrada) bark. Cryst. + $2H_2O$. Mp 184-187°. $[\alpha]_D^{30}$ +36.8 (MeOH).

1″-Carboxylic acid, 8-O-*β*-D-*glucopyranoside:* [111614-11-0] ***Rheinoside D***
$C_{27}H_{30}O_{15}$ 594.525
Constit. of rhubarb. Pale yellow powder + $2\frac{1}{2}H_2O$. $[\alpha]_D^{25}$ -56 (c, 0.5 in MeOH).

5-Hydroxy: [138373-23-6] ***5-Hydroxyaloin A***
$C_{21}H_{22}O_{10}$ 434.399
Constit. of *Aloe* spp. leaf. 10*R*-Config. (C-10 config. changes with addn. of C-5 hydroxy group).

7-Hydroxy, 8-Me ether: ***7-Hydroxy-8-O-methylaloin A***
$C_{22}H_{24}O_{10}$ 448.426
Constit. of *Aloe vera* leaf. Yellowish needles (Me_2CO/C_6H_6). Mp 218-224°. $[\alpha]_D^{30}$ +27.2 (c, 0.25 in MeOH). λ_{max} 206 (log ϵ 4.48); 221 (log ϵ 4.45); 294 (log ϵ 4.2); 345 (log ϵ 3.93) (MeOH).

1″-Deoxy, 8-O-*β*-D-*glucopyranoside:* [53823-09-9] ***Cascaroside C***
$C_{27}H_{32}O_{13}$ 564.542
From cascara sagrada *Rhamnus purshiana* bark. Cascarosides C and D are a pair of epimers resembling Cascarosides A and B.

1″-Deoxy, 6-hydroxy, 8-O-*β*-D-*glucopyranoside:* [164178-32-9] ***Cascaroside E***
$C_{27}H_{32}O_{14}$ 580.541
Constit. of cascara sagrada (*Rhamnus purshiana*) bark. Mp 197-199°. $[\alpha]_D^{25}$ -95.4 (c, 0.1 in MeOH).

(10ξ)-*form*

1″-Deoxy: [18262-45-8] ***Chrysaloin***. *11-Deoxyaloin*
$C_{21}H_{22}O_8$ 402.4
Isol. from *Rumex vesicarius* (bladder dock). Yellow powder (EtOAc). Mp 224-225° dec. $[\alpha]_D^{27}$ -9 (c, 1 in EtOH).

[5133-19-7, 73889-54-0, 138373-24-7]

Hay, J.E. *et al., JCS*, 1956, 3141-3147 (*struct, bibl*)

Hörhammer, L. *et al., Z. Naturforsch., B*, 1964, **19**, 222 (*Aloinoside B*)

Piox, A. *et al., Tetrahedron*, 1968, **24**, 3697 (*ms*)

Wagner, H. *et al., Z. Naturforsch., B*, 1976, **31**, 267 (*Cascarosides*)

Hata, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3792 (*Chrysaloin*)

Evans, F.J. *et al., Biomed. Mass Spectrom.*, 1979, **6**, 374 (*ms*)

Auterhoff, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1980, **313**, 113-120 (*Aloins A,B*)

Grün, M. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1982, **315**, 231-241 (*biosynth*)

Minocha, P.K. *et al., Proc. Natl. Acad. Sci., India, Sect. A*, 1982, **52**, 123 (*Deoxyaloin*)

Rauwald, H.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1984, **317**, 362 (*pmr*)

Rauwald, H.W. *et al., Angew. Chem., Int. Ed.*, 1989, **28**, 1528 (*cryst struct, bibl*)

Manitto, P. *et al., JCS Perkin 1*, 1990, 1297; 1993, 1577 (*abs config, pmr, cmr, conformn, Rheinosides, Cascarosides*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 869

Sigler, A. *et al., Z. Naturforsch., C*, 1994, **49**, 286 (*7-Hydroxyaloin*)

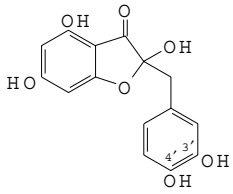
Manitto, P. *et al., J. Nat. Prod.*, 1995, **58**, 419-423 (*Cascarosides E,F*)

Dagne, E. *et al., Phytochemistry*, 1997, **44**, 1271-1274 (*Microstigmin A, 5-Hydroxyaloin A*)

Holzapfel, C.W. *et al., Phytochemistry*, 1997, **45**, 97-102 (*5-Hydroxyaloin A, 6′-Cinnamoyl-5-hydroxyaloin A*)
Okamura, N. *et al., Phytochemistry*, 1997, **45**, 1519-1522 (*7-Hydroxy-8-methylaloin, 10-Hydroxyaloin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAF825

Alphitonin A-318

2-[(3,4-Dihydroxyphenyl)methyl]-2,4,6-trihydroxy-3(2H)-benzofuranone, 9CI. 2,3′,4,4′,6-Pentahydroxybenzylcoumaranone [493-36-7]



$C_{15}H_{12}O_7$ 304.256
No data on abs. configs. in this series. Small opt rotns. reported for some compds., others appear to be racemic. Cryst. (H_2O). Mp 222-223°.

4-Deoxy, 4′-Me ether: 2,3′,6-Trihydroxy-4′-methoxybenzylcoumaran-3-one
$C_{16}H_{14}O_6$ 302.283
Isol. from quebracho. Cryst. (H_2O). Mp 196°. $[\alpha]_D^{23}$ -1.2 (50% Me_2CO aq.).

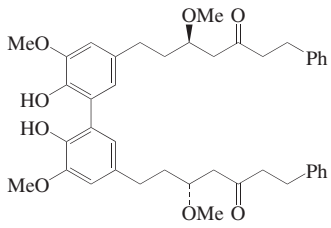
3′-Deoxy, 4-O-β-D-glucopyranoside: [210050-28-5] *Maesopsin 4-glucoside. **Hovetrichoside C***
$C_{21}H_{22}O_{11}$ 450.398
Constit. of *Ribes rubrum* (red currant) fruit. Amorph. powder. $[\alpha]_D^{25}$ -54.1 (c, 1.9 in MeOH). λ_{max} 210 (log ε 4.26); 228 (log ε 4.24); 280 (log ε 3.87) (MeOH).

3′-Deoxy, 6-O-β-D-glucopyranoside: [196102-61-1] ***Maesopsin 6-glucoside***
$C_{21}H_{22}O_{11}$ 450.398
Constit. of *Ceanothus americanus* (New Jersey tea). Powder (MeOH). $[\alpha]_D^{25}$ -43 (c, 0.9 in MeOH).

Roux, D.G. *et al., Biochem. J.*, 1961, **78**, 785-789 (*isol, 4-deoxy 4′-Me ether*)
King, H.G.C. *et al., JCS*, 1961, 3234-3239 (*4-deoxy 4′-Me ether*)
Li, X.-C. *et al., Phytochemistry*, 1997, **46**, 97-102 (*Maesopsin 6-glucoside*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 1998, **61**, 786-790 (*Hovetrichosides*)
Schwarz, B. *et al., J. Agric. Food Chem.*, 2007, **55**, 1394-1404 (*Hovetrichoside C*)

Alpinoid A A-319

[1005405-96-8]



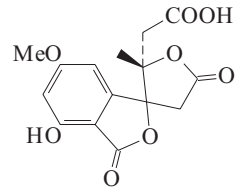
Absolute Configuration

$C_{42}H_{50}O_8$ 682.852
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal). Oil. $[\alpha]_D^{25}$ -6.1 (c, 0.01 in $CHCl_3$). λ_{max} 211 (log ε 3.6); 220 (log ε 3.5); 283 (log ε 0.9) (MeOH).

Sun, Y. *et al., Helv. Chim. Acta*, 2008, **91**, 118-123 (*isol, pmr, cmr*)

Altenuic acid II A-320

4,5-Dihydro-4′-hydroxy-6′-methoxy-2-methyl-3′,5-dioxospiro[furan-3(2H),1′(3′H)-isobenzofuran]-2-acetic acid, 9CI [1402-72-8]



$C_{15}H_{14}O_8$ 322.271
Plates (dioxan aq. or AcOH). Mp 245° dec. Racemic. Gives Altenuic acid III when treated with NaOH. λ_{max} 219 (log ε 4.62); 257 (log ε 4.21); 295 (log ε 4.62) (EtOH).

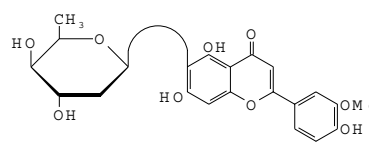
Stereoisomer (1): ***Altenuic acid I***
$C_{15}H_{14}O_8$ 322.271
Needles (H_2O or EtOH). Mp 183° Mp 224-230° dec. Gives Altenuic acid III on treatment with NaOH.

Stereoisomer (2): ***Altenuic acid III***
$C_{15}H_{14}O_8$ 322.271
Prisms (MeOH aq. or AcOH). Mp 198-202° Mp 225°.

Rosett, T. *et al., Biochem. J.*, 1957, **67**, 390-400 (*isol*)
Williams, D.J. *et al., Tet. Lett.*, 1973, **14**, 639-640 (*cryst struct*)
Handbook of Secondary Fungal Metabolites, (ed. Cole, R.J. *et al*), Academic Press, 2003, **1**, 712-714

Alternanthin A-321

6-(6-Deoxy-β-L-xylo-hexopyranosyl)-4′,5,7-trihydroxy-3′-methoxyflavone. 6-Boivinosylchrysoeriol [119269-48-6]



$C_{22}H_{22}O_9$ 430.41
The abs. config. is shown as β-D- in the struct. diagram but clearly stated to be β-L- in the text. Isol. from corn, *Zea mays*. Yellow needles (MeOH). Mp 225-227°. $[\alpha]_D$ +86.2 (c, 0.23 in MeOH). λ_{max} 271 (log ε 4.28); 346 (log ε 4.38) (MeOH).

7-O-β-D-Glucopyranoside:
$C_{28}H_{32}O_{14}$ 592.552
Isol. from the style of *Zea mays* (corn silk). Yellow amorph. solid. Mp 196-198°. $[\alpha]_D^{20}$ -24.9 (c, 0.61 in MeOH). λ_{max} 272 (log ε 4.23); 347 (log ε 4.55) (MeOH).

O-De-Me: [1015164-35-8] *6-Boivinosyl-luteolin*. ***Alternanthin B***
$C_{21}H_{20}O_9$ 416.384
Amorph. yellow solid. $[\alpha]_D^{25}$ +86.9 (c, 0.29 in MeOH). Config. of *Pogonatherum* isolate not confirmed. λ_{max} 271 (log ε 4.02); 335 (log ε 4.14) (MeOH).

O-De-Me, 4′-O-β-D-glucopyranoside: [1245447-09-9] ***Farobin B***
$C_{27}H_{30}O_{14}$ 578.526
Yellow powder. λ_{max} 272; 337 (MeOH aq.).

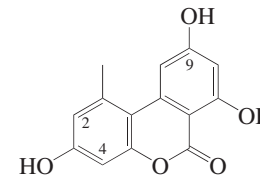
O-De-Me, 7-O-β-D-glucopyranoside: [1245447-08-8] ***Farobin A***
$C_{27}H_{30}O_{14}$ 578.526
Yellow powder. λ_{max} 257; 269 (sh); 347 (MeOH aq.).

Demethoxy, 7-O-β-D-glucopyranoside: [1207331-78-9] *6-Boivinosylapigenin 7-glucoside*
$C_{27}H_{30}O_{13}$ 562.526
Yellow powder. $[\alpha]_D^{24}$ -40 (c, 0.05 in MeOH). λ_{max} 285 (log ε 3.2); 333 (log ε 4.4) (MeOH).

Zhou, B.-N. *et al., Phytochemistry*, 1988, **27**, 3633-3636 (*Alternanthin*)
Suzuki, R. *et al., J. Nat. Prod.*, 2003, **66**, 564-565 (*Zea mays constits*)
Fang, J.-B. *et al., J. Asian Nat. Prod. Res.*, 2007, **9**, 511-515 (*Alternanthin B*)
Wang, G.-J. *et al., J. Ethnopharmacol.*, 2008, **118**, 71-78 (*Alternanthin B*)
Zhu, D. *et al., Chin. J. Nat. Med.*, 2009, **7**, 184-186 (*Boivinosylapigenin 7-glucoside*)
Van Hoyweghen, L. *et al., J. Nat. Prod.*, 2010, **73**, 1573-1577 (*Farobins A,B*)

Alternariol A-322

3,7,9-Trihydroxy-1-methyl-6H-dibenzo[b,d]pyran-6-one, 9CI. 3,4′,5-Trihydroxy-6′-methyldibenzo-α-pyrone [641-38-3]



$C_{14}H_{10}O_5$ 258.23
Occurs in mycelium of *Alternaria tenuis* responsible for alternaria cone disorder in hops and fruit spot on papaya (*Carica papaya*) and *Passiflora* spp. Needles (EtOH aq.). Sol. MeOH, bases, Et_2O; poorly sol. C_6H_6, hexane, H_2O. Mp 350° dec. Subl. 250 *in vacuo*. λ_{max} 213 (ε 21900); 258 (ε 41700); 290 (ε 10500); 303 (ε 11200); 336 (ε 11500) (MeOH).

▶ Exp. reprod. and teratogenic effects. HP8757000

9-O-Sulfate: [1030376-86-3] ***Alternariol 9-sulfate***
$C_{14}H_{10}O_8S$ 338.294
Reddish needles. λ_{max} 215; 250; 288; 345 (no solvent reported).

Tri-Ac:
Cryst. (EtOH). Mp 167-169°.

9-Me ether: [23452-05-3] *9*-O-*Methylalternariol*. ***Djalonensone***
$C_{15}H_{12}O_5$ 272.257
Needles (EtOH or dioxan). Mp 266-268° dec.
▶ Mutagen, teratogen.

9-Me ether, 3-O-*sulfate:* [1030376-87-4] ***9-O-Methylalternariol 3-sulfate***
$C_{15}H_{12}O_8S$ 352.321
Reddish needles. λ_{max} 203; 254; 285; 337 (no solvent reported).

9-Me ether, 3-Ac: [1093066-16-0] *3*-O-*Acetyl-9*-O-*methylalternariol*. ***Antibiotic 2240B***. *2240B*
$C_{17}H_{14}O_6$ 314.294
Amorph. powder. Mp 197-199°.

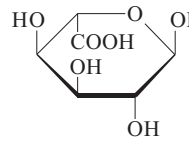
3,9-Di-Me ether: [13873-00-2] *3,9-Di*-O-*methylalternariol*
$C_{16}H_{14}O_5$ 286.284
Amorph. yellow powder. Mp 183-185°.

2-Chloro, 9-Me ether: ***Palmariol B***
$C_{15}H_{11}ClO_5$ 306.702
Powder. λ_{max} 208 (log ϵ 4.2); 218 (log ϵ 4.5); 257 (log ϵ 4.5); 282 (sh) (log ϵ 4.1); 302 (log ϵ 4); 344 (log ϵ 4) (MeOH).

4-Chloro, 9-Me ether: ***Palmariol A***
$C_{15}H_{11}ClO_5$ 306.702
Powder. λ_{max} 224 (log ϵ 4.6); 252 (log ϵ 4.6); 284 (sh) (log ϵ 4.3); 297 (log ϵ 4.2); 340 (log ϵ 4.2) (MeOH).

Raistrick, H. *et al., Biochem. J.*, 1953, **55**, 421-433 (*isol*)
Thomas, R. *et al., Proc. Chem. Soc., London*, 1959, 88 (*biosynth*)
Gatenbeck, S. *et al., Acta Chem. Scand.*, 1965, **19**, 65-71 (*synth*)
Sóti, F. *et al., Chem. Ber.*, 1977, **110**, 979-984 (*synth*)
Harris, T.M. *et al., JACS*, 1977, **99**, 1631-1637 (*synth*)
Abell, C. *et al., Chem. Comm.*, 1982, 1011-1013 (*biosynth*)
Leeper, F.J. *et al., JCS Perkin 1*, 1984, 1053-1059 (*synth*)
DiCosimo, F. *et al., Experientia*, 1985, **41**, 1188-1190 (*activity*)
Stinson, E.E. *et al., Can. J. Chem.*, 1986, **64**, 1590-1594 (*biosynth*)
Abell, C. *et al., Chem. Comm.*, 1986, 15-17 (*synth*)
Dasenbrock, J. *et al., Chem. Comm.*, 1987, 1235-1236 (*biosynth*)
An, Y.-H. *et al., J. Agric. Food Chem.*, 1989, **37**, 1341-1343 (*Djalonensone*)
Kanakam, C.C. *et al., JCS Perkin 1*, 1990, 2233-2237 (*synth*)
Onocha, P.A. *et al., Phytochemistry*, 1995, **40**, 1183-1189 (*Djalonensone*)
Handbook of Secondary Fungal Metabolites, (ed. Cole, R.J. *et al*), Academic Press, 2003, **1**, 703; 705
Schlörke, O. *et al., Dissertation*, Univ. of Göttingen, 2005, (*marine isol*)
Koch, K. *et al., JOC*, 2005, **70**, 3275-3276 (*synth*)
Tan, N. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2008, **44**, 296-300 (*2240B*)
Aly, A.H. *et al., J. Nat. Prod.*, 2008, **71**, 972-980 (*9-sulfates*)
Matumoto, T. *et al., Heterocycles*, 2010, **81**, 1231-1237 (*Palmariols A,B*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGW476

Altruronic acid, 9CI A-323



α–L–Pyranose–*form*

$C_6H_{10}O_7$ 194.141

L-*form* [39737-41-2]
Prod. during pectin saponification, by epimerisation of Galacturonic acid, G-63. Mp 124-127°. $[\alpha]_D^{18}$ +5.3 (c, 0.568 in H_2O).

[21675-51-4]

Fisher, F.G. *et al., Chem. Ber.*, 1959, **92**, 2184 (*synth*)
Carlsson, B. *et al., Acta Chem. Scand.*, 1969, **23**, 261 (*synth*)
Kjolberg, O. *et al., Acta Chem. Scand.*, 1972, **26**, 3245 (*synth*)
Bilik, V. *et al., Chem. Zvesti*, 1982, **36**, 831 (*synth*)
Zhan, D. *et al., Carbohydr. Res.*, 2001, **330**, 357-363 (*occur*)

Aluminium ammonium sulfate (1:1:2) A-324

Aluminium ammonium bis(sulfate). Burnt ammonium alum. Exsiccated ammonium alum. E523 [7784-25-0]

$NH_4Al(SO_4)_2$
$AlH_4NO_8S_2$ 237.147
Cryst. Dec. at 280°.

Dodecahydrate: [7784-26-1] *Ammonium alum*
[15614-99-0]
$AlH_{28}NO_{20}S_2$ 453.329
Used in foods as a buffer and neutralising agent. Cryst. (H_2O). Becomes anhyd. at *ca*. 250°.

[15710-63-1]

Franke, W. *et al., Acta Cryst.*, 1965, **19**, 870-871 (*synth, cryst struct*)
Larson, A.C. *et al., Acta Cryst.*, 1967, **22**, 793-800 (*dodecahydrate, cryst struct*)
Venkatesh, G.M. *et al., Indian J. Pure Appl. Phys.*, 1971, **9**, 39-43 (*dodecahydrate, ir*)
Bailey, W.C. *et al., J. Chem. Phys.*, 1974, **60**, 1952-1953 (*dodecahydrate, N-14 nmr*)
Abdeen, A.M. *et al., Z. Kristallogr.*, 1981, **157**, 147-166 (*dodecahydrate, cryst struct*)
Eckert, H. *et al., JACS*, 1986, **108**, 2140-2146 (*dodecahydrate, S-33 nmr*)
Bradley, S.M. *et al., Magn. Reson. Chem.*, 1993, **31**, 883-886 (*dodecahydrate, Al-27 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 108

Aluminium calcium silicate A-325

Calcium aluminosilicate. E554 [12251-31-9]

$CaAl_2(SiO_3)_4$
$Al_2CaO_{12}Si_4$ 398.376
Anticaking agent.

Mineral-*form* [1318-80-5]
Laumontite
[12251-34-2, 138329-32-5, 11126-82-2, 12330-25-5, 12026-15-2]
Zeolite-group mineral corresp. to $Al_2Ca(SiO_3)_4.4H_2O$ or $Al_2CaH_8(SiO_4)_4$. A partially dehydrated variety leonhardite also occurs naturally.

Mineral-*form* [12042-71-6]
Wairakite
[82828-52-2]
Zeolite-group mineral corresp. to $Al_2Ca(SiO_3)_4.2H_2O$; Ca analogue of Analcime.

Bartl, H. *et al., Neues Jahrb. Mineral., Monatsh.*, 1967, 33-42; 1970, 298-310 (*cryst struct, laumontite*)
Takeuchi, Y. *et al., Am. Mineral.*, 1979, **64**, 993-1001 (*cryst struct, wairakite*)
Armbruster, J. *et al., Neues Jahrb. Mineral., Monatsh.*, 1992, 385-397 (*cryst struct, leonhardite*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 108-109

Aluminium hydroxide, JAN, USAN A-326

[21645-51-2]
[12252-70-9]

$Al(OH)_3$
AlH_3O_3 78.003
Used in foods as a buffer, neutralising agent or firming agent. White solid (H_2O). Prac. insol. H_2O; sol. conc. aq. acids and alkalis. Forms gel on prolonged contact with H_2O.
▶ Gastrointestinal disturbances by ingestion. BD0940000

Gel-*form* [1330-44-5]
Algeldrate, INN, USAN. *Aluminium hydroxide hydrate. W 4600*

Mineral-*form* [14762-49-3]
Gibbsite. *Hydragillite*
Double layer of close packed OH of held by H bonds with Al in ⅔ octahedral holes. Colourless hexagonal platelets.

Mineral-*form* [20257-20-9]
Bayerite
Layer struct. with O approx. hcp and Al octahedrally coord. White powder, colourless monoclinic cryst.

Mineral-*form* [13840-05-6]
Nordstrandite
Double layers of AlO_6 octahedra with shared edges and corners linked by H bonds. Colourless, beige, pink and pale green cryst.

Mineral-*form*
Doyleite
Creamy or bluish white triclinic cryst.

[37317-08-1]

Thibon, H. *et al., Bull. Soc. Chim. Fr.*, 1951, 384 (*props*)
Calvet, E. *et al., Bull. Soc. Chim. Fr.*, 1953, 99 (*props*)
Brown, J.F. *et al., JCS*, 1953, 84 (*gibbsite, thermal dec*)
van Nordstrand, R.A. *et al., Nature (London)*, 1956, **177**, 713 (*nordstrandite*)
Papeé, D. *et al., Bull. Soc. Chim. Fr.*, 1958, 1301 (*props*)
Kroon, D.J. *et al., Nature (London)*, 1959, **183**, 944 (*gibbsite, bayerite, pmr*)
Wall, J.R.D. *et al., Nature (London)*, 1962, **196**, 264 (*nordstrandite*)

Hathaway, J.C. *et al., Nature (London)*, 1962, **196**, 265 (*nordstrandite*)
Hauschild, U. *et al., Z. Anorg. Allg. Chem.*, 1963, **324**, 15 (*synth, ir, powder struct, props*)
Lippens, C. *et al., Acta Cryst.*, 1964, **17**, 1312 (*phase trans*)
Beretka, J. *et al., JCS(A)*, 1967, 2106 (*bayerite, gibbsite, synth, props*)
Rothbauer, R. *et al., Z. Kristallogr.*, 1967, **125**, 317 (*bayerite, cryst struct, nd*)
Bosmans, H.J. *et al., Acta Cryst. B*, 1970, **26**, 649 (*nordstrandite, cryst struct*)
Sato, T. *et al., Z. Anorg. Allg. Chem.*, 1972, **391**, 69 (*synth*)
Singh, S.S. *et al., Soil Sci. Soc. Am. Proc.*, 1974, **38**, 415 (*soly, gibbsite*)
Saalfield, H.L. *et al., Z. Kristallogr.*, 1974, **139**, 129 (*gibbsite, cryst struct*)
Smyshiyaev, S.I. *et al., Russ. J. Phys. Chem. (Engl. Transl.)*, 1976, **50**, 528 (*thermodyn data*)
Chang, B.-T. *et al., Bull. Chem. Soc. Jpn.*, 1981, **54**, 1960 (*gibbsite, thermodyn data*)
Aluminium Chems. Sci. and Tech. Handbook, (Hart, D.Le.R., Ed.), Amer. Ceram. Soc., 1990,
Washington, N. *et al., Antacids and Anti-Reflux Agents*, CRC Press, 1991, 8 (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 869
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 110-111
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHC000

Aluminium potassium silicate A-327

Silicic acid (H_4SiO_4) aluminium potassium salt (1:1:1), 10CI. Potassium aluminosilicate ($KAlSiO_4$), 9CI. E555 [12003-49-5]

$AlK(SiO_4)$

$AlKO_4Si$ 158.163

Polymorphic; the 3 common polymorphs are kalsilite, metastable kaliophilite and a high-temp. rhombic phase. All are based on a tridymite framework. Anticaking agent; rarely used.

Schairer, J.F. *et al., Am. J. Sci.*, 1955, **253**, 681-746 (*synth*)
Deer, W.A. *et al., Rock Forming Minerals*, Longman, 1963, **4**, 231-270 (*mineral*)
Perotta, A.J. *et al., Mineral. Mag.*, 1965, **35**, 588-595 (*kalsilite, cryst struct*)
Abbott, R.N. *et al., Am. Mineral.*, 1984, **69**, 449-457 (*polymorphism*)
Food-Info, (*use*)

Aluminium potassium sulfate A-328 ($AlK(SO_4)_2$)

Sulfuric acid, aluminium potassium salt (2:1:1), 8CI. Aluminium potassium sulfate. Anhydrous alum. E522 [10043-67-1] [15007-61-1]

$KAl(SO_4)_2$

$AlKO_8S_2$ 258.207

Struct. comprises alternate layers of six coordinate $Al^{3\oplus}$ and $K^{\oplus}$ with $SO_4^{2\ominus}$ between. Colourless hexagonal plates (H_2SO_4). Sol. H_2O (7.74 g per 100 cm^3 at 30°); insol. EtOH. Corresp. $NH_4^{\oplus}$, $Rb^{\oplus}$, $Cs^{\oplus}$ salts also descr. ΔH_f° -2470 kJ mol^{-1}; ΔG_f° -2240 kJ mol^{-1}; S° 205 J K^{-1} mol^{-1}.

▶WS5650000

Dodecahydrate: [7784-24-9] *Potassium alum. **Kalinite**. Hexaaquaaluminium(3+) hexaaquapotassium(1+) bis(sulfate). α-Alum*

$AlH_{24}KO_{20}S_2$ 474.389

Used as an additive in the bleaching of milk and flour by benzoyl peroxide. Colourless cryst. (H_2O). Sol. H_2O (11 g per 100 cm^3 at 20°); insol. EtOH, Me_2CO. Mp 105°. Dec. on heating (-$9H_2O$ at 64.5°, -$12H_2O$ at 200°).

▶WS5690000

[14635-80-4]

Lipson, H. *et al., Proc. R. Soc. London, A*, 1935, **148**, 664; **151**, 347 (*cryst struct, dodecahydrate*)
Klug, H.P. *et al., JACS*, 1940, **62**, 1492 (*dodecahydrate, cryst struct*)
Young, F.E. *et al., JACS*, 1945, **67**, 257 (*synth, thermodyn props*)
Palmer, W.G. *et al., Experimental Inorganic Chemistry*, CUP, 1959, 216 (*synth, dodecahydrate*)
Burns, G. *et al., Phys. Rev.*, 1961, **123**, 64 (*dodecahydrate, pmr*)
Tret'yakov, Yu.D. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1961, 859 (*phase diagram*)
Haussühl, S. *et al., Z. Kristallogr.*, 1961, **116**, 371 (*props*)
Franke, W. *et al., Acta Cryst. B*, 1965, **19**, 870 (*anhydrous, cryst struct*)
Cromer, D.T. *et al., Acta Cryst.*, 1967, **22**, 800 (*nd, dodecahydrate*)
Vandorpe, B. *et al., C. R. Seances Acad. Sci., Ser. C*, 1968, **266**, 379 (*related compds*)
Manoli, J.-M. *et al., Bull. Soc. Chim. Fr.*, 1970, 98 (*synth, cryst struct*)
Rems, P. *et al., Inorg. Chim. Acta*, 1971, **5**, 33 (*ir*)
Gal, S. *et al., Therm. Anal., Proc. Int. Conf., 3rd, 1971 (1972)*, 1971, **2**, 559 (*dodecahydrate, thermal anal*)
Pannetier, G. *et al., Bull. Soc. Chim. Fr.*, 1972, 485 (*analogues*)
Strupler, N. *et al., Bull. Soc. Chim. Fr.*, 1974, 1830 (*dodecahydrate, ir*)
Eysel, H.H. *et al., Z. Anorg. Allg. Chem.*, 1976, **424**, 68 (*Raman*)
Hurlburt, H.Z. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 250
Couchot, P. *et al., Rev. Chim. Miner.*, 1978, **15**, 373 (*anhydrous, ir, Raman*)
Bhat, S.V. *et al., Curr. Sci.*, 1984, **53**, 27 (*Al-27 nmr, anhydrous*)
Eckert, H. *et al., JACS*, 1986, **108**, 2140 (*dodecahydrate, S-33 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 115-118
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHF100; AHF200

Aluminium sodium oxide A-329 ($AlNaO_2$)

Aluminium sodium oxide†. Sodium aluminate ($NaAlO_2$). Sodium aluminate† [1302-42-7]

$NaAlO_2$

$AlNaO_2$ 81.97

$NaFeO_2$ type struct. Food contaminant arising from its use as a boiler water additive in the prepn. of steam for food processing. White cryst. or powder. Mp 1700°. Various hydrated forms known. cf. also Aluminium sodium oxide (Al_5NaO_8). ΔH_{f298}° -1133.2 kJ mol^{-1}; S° 70.4 J K^{-1} mol^{-1}.

Théry, J. *et al., C. R. Hebd. Seances Acad. Sci.*, 1962, **254**, 2782 (*related compds*)
Reid, A.F. *et al., Inorg. Chem.*, 1968, **7**, 443 (*cryst struct*)
Peterson, G.E. *et al., J. Chem. Phys.*, 1969, **51**, 2610 (*Na-23 nqr*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 312
Müller, D. *et al., Chem. Phys. Lett.*, 1981, **79**, 59 (*Al-27 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2522

Aluminium sodium silicate A-330

Sodium aluminium silicate. Sodium aluminosilicate. Nepheline. E554 [1302-72-3] [1344-00-9, 12003-51-9, 12251-27-3]

$Na[AlSiO_4]$

$AlNaO_4Si$ 142.054

Stuffed tridymite struct. Anticaking agent. White cryst. (aq. melt). Hydrothermal synth. from Na_2O, Al_2O_3, SiO_2 gels.

Barrer, R.M. *et al., JCS*, 1952, 1561 (*synth*)
Hahn, T. *et al., Z. Kristallogr.*, 1955, **106**, 308 (*cryst struct*)
Brinkman, D. *et al., Z. Kristallogr.*, 1972, **135**, 208 (*Na-23, Al-27, Si-29 nmr*)
Klaska, R. *et al., Z. Kristallogr.*, 1975, **142**, 225 (*cryst struct*)
Lippmaa, E. *et al., JACS*, 1980, **102**, 4889; 1986, **108**, 1730 (*Si-29, Al-27 nmr*)
Wirsching, U. *et al., Clays Clay Miner.*, 1981, **29**, 171 (*synth, powder struct*)
Klinowski, J. *et al., J. Phys. Chem.*, 1981, **85**, 2590 (*Si-29 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2524-2525

Aluminium sodium sulfate A-331 ($AlNa(SO_4)_2$)

Sulfuric acid aluminium sodium salt (2:1:1), 8CI. Aluminium sodium sulfate. Sodium aluminium sulfate. E521 [10102-71-3]

$NaAl(SO_4)_2$

$AlNaO_8S_2$ 242.098

Orthorhombic cryst. V. sol. H_2O (40.9 g per 100 cm^3 at 20°).

Dodecahydrate: [7784-28-3] *Sodium alum. γ-Alum. Hexaaquaaluminium hexaaquasodium sulfate (1:1:2)*

$AlH_{24}NaO_{20}S_2$ 458.281

Food additive in baking powder, firming agent, buffer. May migrate to food from paper/board packaging. Cubic white cryst. Mp 61°. ΔH_f° -2353 kJ mol^{-1}. Formulated as $[Na(OH_2)_6][Al(OH_2)_6](SO_4)_2$.

Steele, F.A. *et al., Science (Washington, D.C.)*, 1928, **68**, 156 (*dodecahydrate, synth*)
Lipson, H. *et al., Proc. R. Soc. London, A*, 1935, **151**, 347 (*dodecahydrate, cryst struct*)
Cola, M. *et al., Gazz. Chim. Ital.*, 1960, **90**, 220 (*cryst struct, synth*)

Cromer, D.T. *et al., Acta Cryst.*, 1967, **22**, 182 (*dodecahydrate, cryst struct, nd*)
Petrov, K.I. *et al., Zh. Neorg. Khim.*, 1970, **15**, 2938 (*dodecahydrate, ir*)
Perret, R. *et al., C. R. Seances Acad. Sci., Ser. C*, 1972, **274**, 366 (*synth*)
Weiden, N. *et al., J. Magn. Reson.*, 1975, **20**, 279 (*dodecahydrate, Na-23, Al-27 nmr*)
Hurlburt, H.Z. *et al., Encycl. Chem. Process. Des.*, 1977, **3**, 120 (*rev, synth*)
W.H.O. Tech. Rep. Ser., 1978, **631**, 7 (*uses*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 244 (*dodecahydrate, rev*)

Aluminium sulfate, USAN A-332

Alunogenite. E520 [10043-01-3] [10199-21-0, 16828-11-8, 17927-65-0, 10124-29-5]

$Al_2(SO_4)_3$

$Al_2O_{12}S_3$ 342.154

Used in foods as a firming agent. White solid. Forms complex series of hydrates. Dec. at 450° to amorphous Al_2O_3 with high surface area. ΔH_{f298} -3435 kJ mol^{-1}. $Al(HSO_4)_3$ also known.

▶ BD1700000

Heptadecahydrate: ***Alunogen***
Colourless cryst.

Octadecahydrate: [7784-31-8]
Colourless hygroscopic cryst. (H_2O). Exact amount of H_2O uncertain. Gives anhyd. salt during 24h at 380°.

▶ WS5697000

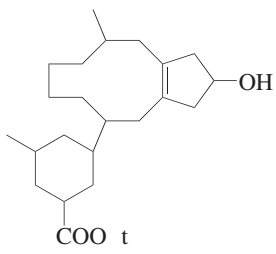
Sodium alum: see Aluminium sodium sulfate ($AlNa(SO_4)_2$), A-331

Potassium alum: see Aluminium potassium sulfate ($AlK(SO_4)_2$), A-328

Young, F.E. *et al., JACS*, 1945, **67**, 257 (*synth, thermodyn data*)
Bassett, H. *et al., JCS*, 1949, 2239 (*synth, phase diagram, powder struct, hydrates, props*)
Kellogg, H.H. *et al., Trans. Metall. Soc. AIME*, 1964, **230**, 1622 (*thermodyn data*)
Vandorpe, B. *et al., C. R. Seances Acad. Sci., Ser. C*, 1973, **277**, 1121 (*related compd*)
Akitt, J.W. *et al., JCS Dalton*, 1973, 1226 (*Al-27 nmr*)
Knutsen, G.F. *et al., J. Electrochem. Soc.*, 1978, **125**, 327 (*dec*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 120-122
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AHG750

Amadannulen A-333

[944707-16-8]



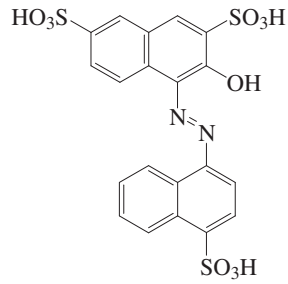
$C_{24}H_{40}O_3$ 376.578

Constit. of the rhizomes of *Curcuma amada* (mango-ginger). λ_{max} 242 ($CHCl_3$).

Policegoudra, R.S. *et al., J. Chromatogr., B*, 2007, **852**, 40-48 (*isol, uv, ir, pmr, cmr*)

Amaranth A-334

3-Hydroxy-4-[(4-sulfo-1-naphthalenyl)azo]-2,7-naphthalenedisulfonic acid, 9CI. C.I. Acid red 27, 8CI. Amaranth R. Amaranth S. Azorubine S. Bordeaux S. C.I. 16185. C.I. Food Red 9. FD and C Red No. 2. E123 [642-59-1] [915-67-3]



(*E*)-*form*

$C_{20}H_{14}N_2O_{10}S_3$ 538.536

Usually obt. as tri-Na salt, to which most synonyms refer. Used in food colouring. Dark red-brown powder (as tri-Na salt). Sol. H_2O, EtOH, 2-ethoxyethanol. Banned by FDA for use in food, drugs and cosmetics. Permitted in the UK and some other countries.

▶ Exp. weak reprod. and teratogenic effects (conflicting data).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 988B (*ir*)
Knecht, O. *et al., J. Soc. Dyers Colour.*, 1886, **2**, 24 (*synth*)
Lambert, J.L. *et al., Anal. Chem.*, 1954, **26**, 558-560; 1955, **27**, 800-801 (*detn, F,S*)
Nursten, H.E. *et al., J. Soc. Dyers Colour.*, 1973, **89**, 49-53 (*synth*)
Marmion, D.M. *et al., J. Assoc. Off. Anal. Chem.*, 1974, **57**, 495-507 (*synth*)
IARC Monogr., 1975, **8**, 41; 1987, *Suppl. 7*, 56 (*rev, tox*)
Fogg, A.G. *et al., Analyst (London)*, 1979, **104**, 723-729 (*anal*)
Clode, S.A. *et al., Food Chem. Toxicol.*, 1987, **25**, 937-946 (*tox*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 698
Yamada, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 494-499 (*hplc, pmr, cmr*)
Merck Index, 13th edn., 2001, No. 372 (*bibl, props*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 92
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, FAG020

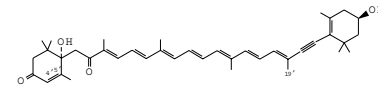
Amaranthin† A-335

Homodimeric protein. Isol. from seeds of *Amaranthus caudatus* (loves-lie-bleeding).

Rinderle, S.J. *et al., J. Biol. Chem.*, 1989, **264**, 16123-16131 (*isol*)

Amarouciaxanthin B A-336

7,8-Didehydro-7′,8′-dihydro-3,6′-dihydroxy-β,ε-carotene-3′,8′-dione. Sidnyaxanthin [92121-55-6]



$C_{40}H_{52}O_4$ 596.848

Dark reddish cryst. (Et_2O); reddish needles (petrol/Et_2O). Sol. MeOH, hexane; poorly sol. H_2O. Mp 88-89° Mp 154°. $[\alpha]_D$ +1.6 (c, 0.9 in $CHCl_3$). λ_{max} 230; 281; 463 (Et_2O).

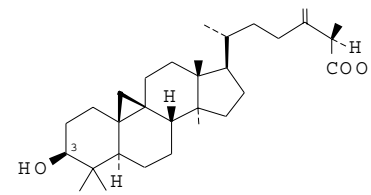
4,5β-Dihydro: [50906-60-0] *7,8-Didehydro-5′,6′,7′,8′-tetrahydro-3,6′-dihydroxy-β,β-carotene-3,8-dione.* ***Isomytiloxanthin***
$C_{40}H_{54}O_4$ 598.864
Isol. from the edible mussel (*Mytilus edulis*). Red gum. Tentative abs. config. λ_{max} 451 (no solvent reported).

19′-Hexanoyloxy, 4,5β-dihydro: ***19′-Hexanoyloxymytiloxanthin***
$C_{46}H_{64}O_6$ 713.008
Isol. from the edible mussel (*Mytilus edulis*).

Khare, A. *et al., Tet. Lett.*, 1973, **14**, 3921-3924 (*Isomytiloxanthin*)
Moss, G.P. *et al., Pure Appl. Chem.*, 1976, **47**, 97-102 (*Isomytiloxanthin, cmr*)
Belaud, C. *et al., Tet. Lett.*, 1984, **25**, 3087-3090 (*Sidnyaxanthin, struct*)
Matsuno, T. *et al., J. Nat. Prod.*, 1985, **48**, 606-613 (*Sidnyaxanthin, struct*)
Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495-503 (*19′-Hexanoyloxymytiloxanthin, struct*)
Khare, A. *et al., JCS Perkin 1*, 1988, 1389-1395 (*Isomytiloxanthin, struct*)
Partali, V. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1989, **92**, 239-246 (*Mytilus edulis constits, detn, metab*)

Ambolic acid A-337

*3β-Hydroxy-24-methylene-25*R*-cycloartan-26-oic acid* [13878-93-8]



$C_{31}H_{50}O_3$ 470.734

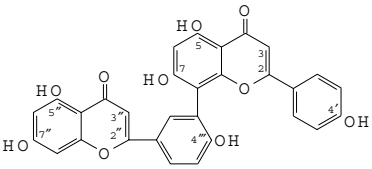
Constit. of *Mangifera indica* (mango). Cryst. ($CHCl_3$). Mp 168-170°. $[\alpha]_D$ +32.6 (c, 0.5 in $CHCl_3$).

3-Ketone: [17984-17-7] ***Ambonic acid***
$C_{31}H_{48}O_3$ 468.718
Constit. of *Mangifera indica* (mango). Cryst. (Et_2O/hexane). Mp 149-150°. $[\alpha]_D$ +9.4 (c, 0.7 in $CHCl_3$).

Corsano, S. *et al., Chem. Comm.*, 1968, 738 (*isol*)
Singh, C. *et al., Tetrahedron*, 1977, **33**, 817 (*synth*)

Amentoflavone A-338

4′,4‴,5,5″,7,7″-Hexahydroxy-3‴,8-biflavone, 8CI. 4′,5,7-Trihydroxyflavone(3′ → 8)-4′,5,7-trihydroxyflavone. 3′,8-Bi[4′,5,7-trihydroxyflavone] [1617-53-4]



$C_{30}H_{18}O_{10}$ 538.466

Numbering of the rings in the names of derivs. does not always follow the scheme shown here. Obt. from *Viburnum prunifolium* (black haw) and *Ginkgo biloba* (ginkgo). Yellow cryst. (EtOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 300°. $[\alpha]_D^{40}$ +9. Log P 1.7 (calc). Opt. rotn. of derivs. is variable owing to atropisomerism. λ_{max} 270 (ϵ 41600); 338 (ϵ 38900) (EtOH) (Berdy).

4‴-Me ether: [521-32-4] ***Bilobetin***
$C_{31}H_{20}O_{10}$ 552.493
From *Ginkgo biloba* (ginkgo). Cryst. Mp 320° dec. Softens at 245-53°, resolidifies at 278°.

4′,4‴-Di-Me ether: [548-19-6] ***Isoginkgetin***
$C_{32}H_{22}O_{10}$ 566.52
From leaves of *Ginkgo biloba* (ginkgo). Yellow cryst. (Me_2CO). Mp 210° (effervesces and resolidifies) Mp 245° (double Mp). λ_{max} 213 (ϵ 90000); 271 (ϵ 42000); 330 (ϵ 36500) (EtOH) (Berdy). λ_{max} 280 (ϵ 53000); 376 (ϵ 24300) (EtOH/NaOH) (Berdy).

4′,4‴-Di-Me ether, 7″-O-β-D-glucopyranoside: ***Isoginkgetin 7-glucoside***
$C_{38}H_{32}O_{15}$ 728.662
Constit. of the leaves of *Ginkgo biloba* (ginkgo). Amorph. yellow powder. $[\alpha]_D^{20}$ +0.8 (c, 0.003 in MeOH). λ_{max} 271 (log ϵ 4.68); 328 (log ϵ 4.58) (MeOH).

4‴,7″-Di-Me ether: [481-46-9] ***Ginkgetin***
$C_{32}H_{22}O_{10}$ 566.52
From *Ginkgo biloba* (ginkgo). Yellow plates (Me_2CO). Mp 336° Mp 350°.

4‴,7″-Di-Me ether, 7-O-β-D-glucopyranoside: ***Ginkgetin 7″-glucoside***
$C_{38}H_{32}O_{15}$ 728.662
Constit. of the leaves of *Ginkgo biloba* (ginkgo). Amorph. yellow powder. $[\alpha]_D^{20}$ +5.5 (c, 0.004 in MeOH). λ_{max} 270 (log ϵ 4.53); 330 (log ϵ 3.49) (MeOH).

5‴-Methoxy, 4‴-Me ether: [77053-35-1] ***5′-Methoxybilobetin***
$C_{32}H_{22}O_{11}$ 582.519
Isol. from *Ginkgo biloba* (ginkgo). Yellow cryst. (EtOH aq.). Mp 251°.

Nakazawa, K. *et al., Chem. Pharm. Bull.*, 1962, **10**, 1032 (*synth, derivs*)
Baker, W. *et al., JCS*, 1963, 1477 (*isol, struct, derivs*)
Batterham, R. *et al., Aust. J. Chem.*, 1964, **17**, 428-439 (*pmr, derivs*)
Beckmann, S. *et al., Phytochemistry*, 1971, **10**, 2465-2474 (*Metasequoia glypostroboides constits*)
Ilyas, N. *et al., Phytochemistry*, 1978, **17**, 987 (*derivs*)
Joly, M. *et al., Phytochemistry*, 1980, **19**, 1999 (*5′-Methoxybilobetin*)
Ahmad, I. *et al., Phytochemistry*, 1981, **20**, 1169 (*deriv*)
Ohmoto, T. *et al., Chem. Pharm. Bull.*, 1983, **31**, 919-924 (*Cryptomeria japonica constits*)
Kamil, M. *et al., Phytochemistry*, 1987, **26**, 1171 (*deriv*)
Konda, Y. *et al., J. Het. Chem.*, 1995, **32**, 1531 (*Ginkgetin, Sciadopitysin, cryst struct, pmr, cmr*)
Reddy, B.P. *et al., Indian J. Chem., Sect. B*, 1996, **35**, 283 (*Ginkgetin, Sciadopitysin*)
Muranaka, T. *et al., CA*, 1999, **130**, 322915n
Hyun, S.K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1200-1201 (*Ginkgetin 7″-glucoside, Isoginkgetin 7-glucoside*)

American oyster serine protease inhibitor A-339

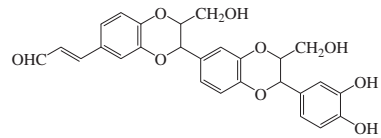
CVSI-1

Protein containing 71 amino acid residues incl. 12 cysteines. Isol. from the American oyster *Crassostrea virginica*.

Xue, Q.-G. *et al., Comp. Biochem. Physiol., B: Biochem. Mol. Biol.*, 2006, **145**, 16-26 (*isol, struct, activity*)

Americanin B A-340

[77053-44-2]



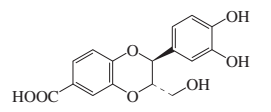
$C_{27}H_{24}O_9$ 492.481
Constit. of the seeds of *Phytolacca americana* (pokeberry). Mp 258-260°. $[\alpha]_D^{17}$ +1.7 (c, 0.3 in Py).

9-Alcohol: [362606-64-2] ***Artabotrycinol. Isoamericanol B***
$C_{27}H_{26}O_9$ 494.497
Cryst. (MeOH). Mp 194-196°. $[\alpha]_D^{20}$ -7 (c, 0.03 in MeOH). λ_{max} 236 (sh); 282 (MeOH).

Woo, W.S. *et al., Tet. Lett.*, 1980, **21**, 4255-4258
Yu, J.-G. *et al., Yaoxue Xuebao*, 2001, **36**, 281-286 (*isol, pmr, cmr, Artabotrycinol*)

Americanoic acid A† A-341

2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-hydroxymethyl-1,4-benzodioxin-6-carboxylic acid
[696603-06-2 (Me ester)]



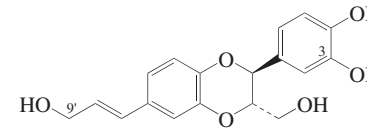
Relative Configuration

$C_{16}H_{14}O_7$ 318.282
Constit. of the seeds of *Phytolacca americana* (pokeberry). Amorph. (as Me ester). Racemic (Me ester). λ_{max} 206 (ϵ 30200); 261 (ϵ 4500); 290 (ϵ 3000) (EtOH) (Me ester).

Takahasi, H. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1377-1381 (*isol, pmr, cmr, ms*)

Americanol A A-342

3-[2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3-hydroxymethyl-1,4-benzodioxin-6-yl]-2-propen-1-ol [133838-65-0]



Absolute Configuration

$C_{18}H_{18}O_6$ 330.337
Isol. from seeds of *Phytolacca americana* (pokeberry) and *Morinda citrifolia* (noni). Prisms (Me_2CO/EtOAc). Mp 125-128°. Racemic.

9′-Me ether: ***9′-O-Methylamericanol A***
$C_{19}H_{20}O_6$ 344.363
Constit. of the seeds of *Phytolacca americana* (pokeberry). Powder. $[\alpha]_D^{23}$ -6.7. The *P. americana* isolate was racemic. λ_{max} 203 (ϵ 64300); 263 (ϵ 16700) (EtOH). λ_{max} 204 (log ϵ 4.7); 269 (log ϵ 3.32); 341 (log ϵ 2.73); 376 (log ϵ 2.48) (MeOH).

9′-Et ether: ***9′-O-Ethylamericanol A***
$C_{20}H_{22}O_6$ 358.39
Yellow powder. $[\alpha]_D^{23}$ -1.7 (c, 0.6 in MeOH). λ_{max} 206; 270; 380 (MeOH).

9′-Butyl ether: ***9′-O-Butylamericanol A***
$C_{22}H_{26}O_6$ 386.444
Yellow powder. $[\alpha]_D^{23}$ -7.9 (c, 1.4 in MeOH). λ_{max} 206; 270; 380 (MeOH).

9′-Aldehyde: [69506-79-2] ***Americanin A***
$C_{18}H_{16}O_6$ 328.321
Constit. of *Phytolacca americana* (pokeberry) and *Morinda citrifolia* (noni). Yellow plates (MeOH). Mp 246-247°. $[\alpha]_D^{17}$ +23.7.

9′-Carboxylic acid: [777061-45-7] ***Americanoic acid A***†
$C_{18}H_{16}O_7$ 344.32
Constit. of the fruit of *Morinda citrifolia* (noni). Pale yellow powder. $[\alpha]_D^{24}$ +26.2 (c, 0.7 in MeOH). λ_{max} 218 (log ϵ 4.33); 234 (log ϵ 4.24); 287 (log ϵ 4.18); 318 (log ϵ 4.1) (MeOH).

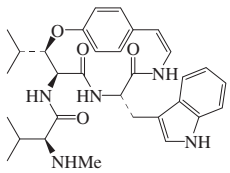
9′-Carboxylic acid, 3-Me ether: [1158294-48-4] *3-O-Methylamericanoic acid.* ***Arteminorin D***
$C_{19}H_{18}O_7$ 358.347
Amorph. powder. $[\alpha]_D^{25}$ -4.5 (c, 1.1 in MeOH). Only rel. config. determined.

Antus, S. *et al., Annalen*, 1986, 647-654 (*Americanin A*)
Fukuyama, Y. *et al., Chem. Pharm. Bull.*, 1992, **40**, 252-254 (*Americanol A*)
She, X.G. *et al., J. Chem. Res., Synop.*, 1998, 436-437 (*Americanin A, synth*)
Takahashi, H. *et al., Heterocycles*, 2002, **56**, 245-256 (*Americanol A, synth*)
Takahashi, H. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1377-1381 (*9′-O-Methylamericanol A*)

Waibel, R. *et al., Phytochemistry*, 2003, **62**, 805-811 (*Americanin A, isol, pmr, cmr, struct*)
Zhao, P.J. *et al., Chin. Chem. Lett.*, 2004, **15**, 921-924 (*Trewia nudiflora neolignans*)
Kamiya, K. *et al., J. Agric. Food Chem.*, 2004, **52**, 5843-5848 (*Americanoic acid A*)
He, Z.-Z. *et al., J. Nat. Prod.*, 2009, **72**, 1198-1201 (*Arteminorin D*)

Americine A-343

N-*[7-(1*H*-Indol-3-ylmethyl)-3-(1-methylethyl)-5,8-dioxo-2-oxa-6,9-diazabicyclo[10.2.2]hexadeca-10,12,14,15-tetraen-4-yl]-3-methyl-2-(methylamino)butanamide, 9CI* [18867-84-0]



Absolute Configuration

$C_{31}H_{39}N_5O_4$ 545.68
Alkaloid from the root bark of *Ceanothus americanus* (New Jersey tea). Mp 135.5-137°. $[\alpha]_D^{20}$ -198 (c, 0.51 in MeOH).

N-*Me:* [70403-89-3] **N-*Methylamericine***. *5-β-Indolylmethyl-8*N-(N,N-*dimethylvalyl)-9-isopropylphencyclopeptine*
$C_{32}H_{41}N_5O_4$ 559.707
Mp 233° (229°).

Klein, F.K. *et al., JACS*, 1968, **90**, 2398-2404 (*isol, uv, ir, pmr, ms, struct*)
Lagarias, J.C. *et al., J. Nat. Prod.*, 1979, **42**, 220-227; 663-668 (*N-Me*)

Amidicin A-344

[443769-50-4]

Val-His-Leu-Ser-Ala-Glu-Glu-Lys-Glu-Ala-Val-Leu-Gly-Leu-NH_2

$C_{66}H_{112}N_{18}O_{21}$ 1493.719
Widely distributed in porcine tissue; esp. abundant in pituitary gland, cardiac ventricle and spleen.

Ishiyama, Y. *et al., Biochem. Biophys. Res. Commun.*, 2002, **293**, 741-746 (*isol*)

Amidophosphoribosyltransferase A-345

*E.C. 2.4.2.14. 5-Phosphoribosylamine:diphosphate phospho-α-*D*-ribosyltransferase (glutamate-amidating). Glutamine phosphoribosyl-diphosphate amidotransferase. 5′-Phosphoribosyl-diphosphate amidotransferase. Glutamine PRPP amidotransferase* [9031-82-7]

Pentosyltransferase enzyme. Isol. from a variety of avian and mammalian sources, e.g. from chicken and pigeon livers. Involved in purine biosynth.

Hartman, S.C. *et al., J. Biol. Chem.*, 1958, **233**, 451-455 (*pigeon liver*)
Flaks, J.G. *et al., Methods Enzymol.*, 1963, **6**, 52-95 (*chicken liver*)
Lewis, J.M. *et al., Methods Enzymol.*, 1978, **51**, 171-178 (*chicken liver*)
Tsuda, M. *et al., J. Biochem. (Tokyo)*, 1979, **15**, 1347-1354 (*rat liver*)
Itakura, M. *et al., J. Biol. Chem.*, 1979, **254**, 333-338 (*human placenta*)
Messenger, L.J. *et al., J. Biol. Chem.*, 1979, **254**, 3382-3392 (*Escherichia coli*)
Wong, J.Y. *et al., Biochemistry*, 1981, **20**, 5669-5674 (*Bacillus subtilis*)
Zalkin, H. *et al., Methods Enzymol.*, 1985, **113**, 264-273 (*Escherichia coli*)
Yamaoka, T. *et al., Adv. Exp. Med. Biol., Sect. B*, 1989, **253**, 21-28 (*rat liver*)
Zalkin, H. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1993, **66**, 303-309 (*rev*)
Smith, J.L. *et al., Curr. Opin. Struct. Biol.*, 1998, **8**, 686-694 (*rev*)

Amine *N*-methyltransferase A-346

E.C. 2.1.1.49. S-*Adenosyl-*L*-methionine:amine* N-*methyltransferase. Nicotine* N-*methyltransferase. Tryptamine* N-*methyltransferase. Arylamine* N-*methyltransferase. Indolamine* N-*methyltransferase. Indoleethylamine* N-*methyltransferase. E.C. 2.1.1.81 (incorporated)* [51377-47-0]
[111694-10-1]

Methyltransferase enzyme. First isol. from rabbit lung; widely distributed in mammalian tissues, e.g. rabbit and bovine livers. Acts on a wide range of amines incl. Tryptamine, Aniline and (*S*)-nicotine.

Lyon, E.S. *et al., Methods Enzymol.*, 1981, **77**, 263-266 (*rabbit liver*)
Herman, K.S. *et al., J. Biol. Chem.*, 1985, **260**, 12336-12340 (*rabbit lung*)
Ansher, S.S. *et al., J. Biol. Chem.*, 1986, **261**, 3996-4001 (*rabbit liver*)
Ansher, S.S. *et al., Methods Enzymol.*, 1987, **142**, 660-667 (*rabbit liver*)
Bahnmaier, A.H. *et al., Chirality*, 1999, **11**, 160-165 (*bovine liver*)

Amine sulfotransferase A-347

E.C. 2.8.2.3. 3′-Phosphoadenylyl-sulfate:amine N-*sulfotransferase. Arylamine sulfotransferase* [9026-08-8]

Sulfotransferase enzyme. Isol. from rabbit. Many primary and secondary amines can act as acceptors, e.g. Aniline, 2-Naphthylamine, Cyclohexylamine, C-704 and 1-Octylamine.

Roy, A.B. *et al., Biochem. J.*, 1960, **74**, 49-56 (*mammals*)
Ramaswamy, S.G. *et al., J. Biol. Chem.*, 1987, **262**, 10039-10043 (*human, rat, rabbit, guinea pig*)
Ramaswamy, S.G. *et al., Methods Enzymol.*, 1987, **143**, 201-207 (*assay, rev*)
Maritomi, Y. *et al., Biol. Pharm. Bull.*, 1994, **17**, 1008-1011 (*rat*)
Yoshinari, K. *et al., J. Biochem. (Tokyo)*, 1998, **123**, 479-486 (*rabbit*)

D-Amino acid *N*-acetyltransferase A-348

*E.C. 2.3.1.36. Acetyl-CoA:*D*-amino acid* N-*acetyltransferase* [37257-15-1]

Enzyme. Isol. from *Saccharomyces cerevisiae.*

Zenk, M.H. *et al., Biochem. Z.*, 1965, **342**, 54-65

Amino acid *N*-acetyltransferase A-349

*E.C. 2.3.1.1. Acetyl-CoA:*L*-glutamate* N-*acetyltransferase.* N-*Acetylglutamate synthase* [9029-88-3]

Enzyme. Also acts on L-aspartate and more slowly on other amino acids.
▶ Isol. from mammalian liver.

Maas, W.K. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1953, **39**, 1004-1009 (*Escherichia coli*)
Lieberman, I. *et al., Methods Enzymol.*, 1955, **1**, 616-619 (*Clostridium kluyveri*)
Bachmann, C. *et al., Biochem. J.*, 1982, **205**, 123-127 (*human liver*)
Sonoda, T. *et al., J. Biol. Chem.*, 1983, **258**, 9839-9844 (*rat liver*)
Powers-Lee, S.G. *et al., Methods Enzymol.*, 1985, **113**, 27-35 (*rat liver*)

Amino acid dehydrogenases A-350

Oxidoreductase enzymes. Dehydrogenases specific for one amino acid have separate entries.

L-Amino-acid dehydrogenase [9029-13-4]
E.C. 1.4.1.5. L*-Amino-acid:NAD⊕ oxidoreductase (deaminating)*
Acts on aliphatic amino acids, such as L-valine and L-isoleucine.

D-Amino-acid dehydrogenase [37205-44-0]
E.C. 1.4.99.1. D*-Amino-acid:(acceptor) oxidoreductase (deaminating)*
FAD-dependent. Acts on all D-amino acids, except for D-aspartate and D-glutamate.

L-Amino-acid oxidase [9000-89-9]
E.C. 1.4.3.2. L*-Amino-acid:oxygen oxidoreductase (deaminating). Ophio-amino-acid oxidase. Escapin*
FAD-dependent.

D-Amino-acid oxidase [9000-88-8]
E.C. 1.4.3.3. D*-Amino-acid:oxygen oxidoreductase (deaminating)*
Isol. from sheep and pig kidney. FAD-dependent. Shows wide specificity; also acts on glycine.

Burton, K. *et al., Methods Enzymol.*, 1955, **2**, 199-204 (*E.C. 1.4.3.3, sheep kidney*)
Ratner, S. *et al., Methods Enzymol.*, 1955, **2**, 204-212 (*E.C. 1.4.3.2, Agkistrodon piscivorus, rat kidney*)
Wellner, D. *et al., J. Biol. Chem.*, 1960, **235**, 2013-2018 (*E.C. 1.4.3.2, Crotalus adamanteus*)
Tsukada, K. *et al., J. Biol. Chem.*, 1966, **241**, 4522-4528 (*E.C. 1.4.99.1, Pseudomonas fluorescens*)
Wellner, D. *et al., Methods Enzymol., Part B*, 1971, **17**, 597-600 (*E.C. 1.4.3.2, Crotalus adamanteus*)
Nakano, M. *et al., Methods Enzymol., Part B*, 1971, **17**, 601-605 (*E.C. 1.4.3.2, rat kidney*)
Yagi, K. *et al., Methods Enzymol., Part B*, 1971, **17**, 608-622 (*E.C. 1.4.3.3, hog kidney*)
Tsukada, K. *et al., Methods Enzymol., Part B*, 1971, **17**, 623-629 (*E.C. 1.4.99.1, Pseudomonas fluorescens*)
Nitta, Y. *et al., J. Bacteriol.*, 1974, **117**, 588-592 (*E.C. 1.4.1.5, Bacillus subtilis*)
Olsiewski, P.J. *et al., J. Biol. Chem.*, 1980, **255**, 4487-4494 (*E.C. 1.4.99.1, Escherichia coli*)
Konno, R. *et al., Int. J. Biochem.*, 1992, **24**, 519-524 (*E.C. 1.4.3.3, rev*)
Brunhuber, N.M.W. *et al., Crit. Rev. Biochem. Mol. Biol.*, 1994, **29**, 415-467 (*rev*)

Mattevi, A. *et al., Curr. Opin. Struct. Biol.*, 1997, **7**, 804-810 (*E.C. 1.4.3.3, rev*)
Pilone, M.S. *et al., Cell. Mol. Life Sci.*, 2000, **57**, 1732-1747 (*E.C. 1.4.3.3, rev*)
Du, X.Y. *et al., Toxicon*, 2002, **40**, 659-665 (*E.C. 1.4.3.2, rev*)
Yang, H. *et al., J. Exp. Biol.*, 2005, **208**, 3609-3622 (*E.C. 1.4.3.2, Aplysia californica constit*)
Kamio, M. *et al., Chem. Eur. J.*, 2009, **15**, 1597-1603 (*E.C. 1.4.3.2, Aplysia californica constit, props*)

Amino (methoxysulfinyl) pentasulfide, 9CI A-351

Methyl 5-aminopentasulfide 1-sulfinate [198898-37-2]

$H_2N–S–S–S–S–S(O)–OMe$

$CH_5NO_2S_6$ 255.452

Constit. of *Moringa oleifera* (horseradish tree).

Faizi, S. *et al., J. Nat. Prod.*, 1997, **60**, 1317-1321 (*isol, ms*)

2-Aminoacetophenone, 8CI A-352

2-Amino-1-phenylethanone, 9CI. Phenacylamine. Phenomydrol. Benzoylmethylamine. (Aminoacetyl)benzene [613-89-8]

$PhCOCH_2NH_2$

C_8H_9NO 135.165

Component of tortilla aroma and of other corn flour products. Cryst. (EtOH) (as picrate). Mp 174-176° dec. (picrate). Aroma threshold 0.2 ppb in H_2O.

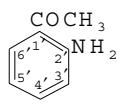
▶ Exp. reprod. effects. AM5775000

[25384-14-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 46D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 867A (*nmr*)
Tiffeneau, M. *et al., Bull. Soc. Chim. Fr.*, 1931, **49**, 1761 (*rev*)
Bellamy, L.J. *et al., Spectrochim. Acta A*, 1972, **28**, 1869 (*ir*)
Abdalla, G.M. *et al., J. Het. Chem.*, 1987, **24**, 297 (*synth, ir, pmr*)
Yamagama, C. *et al., Aust. J. Chem.*, 1989, **42**, 463 (*N-15 nmr*)
Baumstark, A.L. *et al., Chem. Comm.*, 1989, 767 (*O-17 nmr*)
Buttery, R.G. *et al., J. Agric. Food Chem.*, 1994, **42**, 1-2 (*occur, anal*)

2′-Aminoacetophenone, 8CI A-353

1-(2-Aminophenyl)ethanone, 9CI. FEMA 3906 [551-93-9]

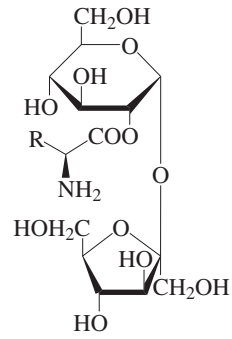


C_8H_9NO 135.165

Flavour compd. in stale dried milk. Responsible for the foxy odour of Concord grape (*Vitis lambrusca*). Flavour ingredient. Cryst. with grape-like odour. Mp 20°. Bp 250-252° slight dec. Bp_{13} 130° (lit quotes a pressure range). Steam-volatile.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 47C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 868C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1262D (*ir*)
Simpson, J.C.E. *et al., JCS*, 1945, 646 (*synth, bibl*)
Leonard, N.J. *et al., JOC*, 1946, **11**, 405 (*synth*)
Parks, O.W. *et al., Nature (London)*, 1964, **202**, 185 (*isol*)
Kozlov, N.S. *et al., CA*, 1969, **71**, 12833 (*synth*)
Arnold, R.G. *et al., J. Dairy Sci.*, 1969, **52**, 1097 (*occur*)
East Ger. Pat., 1971, 82 135 (*synth*)
Blum, M.S. *et al., Experientia*, 1981, **37**, 816 (*isol*)
Shure, K.B. *et al., J. Agric. Food Chem.*, 1994, **42**, 350-353 (*occur*)

2-*O*-(α-Aminoacyl)sucroses A-354



2-*O*-(2-Aminoacetyl)sucrose [908337-60-0]
2-O-*Glycylsucrose*

$C_{14}H_{25}NO_{12}$ 399.351

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ +0.07 (c, 0.003 in MeOH). R = H.

2-*O*-(2-Aminopropanoyl)sucrose [908337-58-6]
2-O-*Alanylsucrose*

$C_{15}H_{27}NO_{12}$ 413.378

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ +0.03 (c, 0.003 in MeOH). R = CH_3.

2-*O*-(2-Amino-3-methylbutanoyl)sucrose [908337-54-2]
2-O-*Valylsucrose*

$C_{17}H_{31}NO_{12}$ 441.431

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ +0.04 (c, 0.003 in MeOH). R = -$CH(CH_3)_2$.

2-*O*-(2*S*-Amino-3*R*-hydroxybutanoyl)sucrose [908337-56-4]
2-O-*Threonylsucrose*

$C_{16}H_{29}NO_{13}$ 443.404

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ -0.5 (c, 0.003 in MeOH). R = -$CH(OH)CH_3$.

2-*O*-Histidinylsucrose [908337-57-5]

$C_{18}H_{29}N_3O_{12}$ 479.44

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ +0.1 (c, 0.003 in MeOH). R = (3-imidazolyl)methyl.

2-*O*-L-Tyrosylsucrose [908337-55-3]

$C_{21}H_{31}NO_{13}$ 505.475

Constit. of *Ipomoea batatas* (sweet potato). $[\alpha]_D^{25}$ -0.8 (c, 0.003 in MeOH). R = 4-hydroxybenzyl.

2-*O*-L-Tryptophylsucrose [908337-59-7]

$C_{23}H_{32}N_2O_{12}$ 528.512

Constit. of *Ipomoea batatas* (sweet potato). R = (3-indolylmethyl).

Dini, I. *et al., J. Agric. Food Chem.*, 2006, **54**, 6089-6093

Aminoacyl-tRNA hydrolase A-355

E.C. 3.1.1.29. Aminoacyl-tRNA aminoacylhydrolase. Peptidyl-tRNA hydrolase [9054-98-2]

Carboxylic ester hydrolase enzyme. *Staphylococcus aureus* Enzyme activity range pH 6.0-8.5. *Artemia* Enzyme in 50% glycerol is stable for several months at -10°.

Neth, R. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1972, **353**, 117-121 (*human, rat*)
Morrisey, H. *et al., Methods Enzymol.*, 1974, **29**, 726-739 (*rev*)
Gallego, M.E. *et al., Biochim. Biophys. Acta*, 1982, **696**, 57-65 (*Artemia*)
Bonin, P.D. *et al., Protein Expr. Purif.*, 2002, **24**, 123-130 (*Staphylococcus aureus*)
Fromant, M. *et al., Biochemistry*, 2005, **44**, 4292-4301 (*cryst struct*)

2-Aminoadipate transaminase A-356

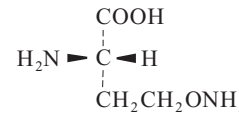
E.C. 2.6.1.39. L-2-Aminoadipate:2-oxoglutarate aminotransferase. 2-Aminoadipate aminotransferase [9033-00-5]

Aminotransferase enzyme. Isol. from baker's yeast and cow. Pyridoxal phosphate-dependent.

Matsuda, M. *et al., J. Biol. Chem.*, 1969, **244**, 3352-3358 (*Saccharomyces cerevisiae*)
Hartline, R.A. *et al., Methods Enzymol.*, 1985, **113**, 664-672 (*rat kidney*)
Deshmukh, D.R. *et al., Biochem. J.*, 1989, **261**, 761-768 (*bovine kidney*)
Mawal, M.R. *et al., Prep. Biochem.*, 1991, **21**, 63-73; 151-162 (*rat liver, rat kidney*)

2-Amino-4-(aminooxy)butanoic acid, 8CI A-357

O-*Aminohomoserine, 9CI. **Canaline***



(*S*)–*form*

$C_4H_{10}N_2O_3$ 134.135

(*S*)-*form* [496-93-5]
L-*form*
Present in *Canavalia ensiformis* (Jackbean). Needles (EtOH). Mp 214° dec. $[\alpha]_D^{21}$ -8.31.

Hydrochloride (1:2):
Cryst. (EtOH). Mp 166° dec.

Picrate: Mp 192-193° dec.

Dibenzoyl: Mp 99° dec.

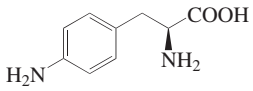
(±)-*form* [15985-61-2]
Cryst. (Me_2CO/EtOH/H_2O). Mp 195° dec. pK_{a1} 2.4; pK_{a2} 3.7; pK_{a3} 9.2 (25°).

Me ester:
$C_5H_{12}N_2O_3$ 148.161
Mp 165° dec. (as hydrochloride).

Gilon, C. *et al., Tetrahedron*, 1967, **23**, 4441 (*synth*)
Rahiala, E.-L. *et al., Acta Chem. Scand.*, 1973, **27**, 3861 (*synth*)
Williamson, J.D. *et al., Life Sci.*, 1974, **14**, 2481 (*isol*)
Rosenthal, G.A. *et al., Life Sci.*, 1978, **23**, 93 (*rev*)
Ozinskas, A.J. *et al., JOC*, 1986, **51**, 5047 (*synth*)
Barlos, K. *et al., Annalen*, 1986, 287

2-Amino-3-(4-aminophenyl)-propanoic acid A-358

α,4-Diaminobenzenepropanoic acid. 4-Aminophenylalanine, 9CI



(*S*)-*form*

$C_9H_{12}N_2O_2$ 180.206

(*R*)-*form* [102281-45-8]
D-form
Mp 245-248° Mp 268-270°. $[\alpha]_D^{20}$ +37 (c, 2 in H_2O).

Me ester:
$C_{10}H_{14}N_2O_2$ 194.233
$[\alpha]_D$ -5.9 (c, 2.02 in H_2O). Hygroscopic.

2-N,4′-N-Di-Ac, Me ester:
$C_{14}H_{18}N_2O_4$ 278.307
Yellow powder. $[\alpha]_D$ -40.1 (c, 0.85 in MeOH).

(*S*)-*form* [943-80-6]
L-form
Constit. of the famine food *Vigna vexillata*. Needles (H_2O). Mp 260-264° dec. $[\alpha]_D^{23}$ +1 (c, 0.3 in H_2O). $[\alpha]_{580}^{23}$ +28 (c, 0.3 in 1*N* HCl).

2-N,4′-N,4′-N-Tri-Me: 3-(4-Dimethylaminophenyl)-2-methylaminopropanoic acid. p-*Dimethylamino*-N-*methylphenylalanine*
$C_{12}H_{18}N_2O_2$ 222.286
Needles + ½H_2O (EtOH aq.). Mp 208°. $[\alpha]_D^{20}$ +22.6 (c, 0.5 in 1*M* HCl). $[\alpha]_D$ -3.2 (c, 1.076 in H_2O).

(±)-*form* [2922-41-0]
Cryst. (EtOH aq.). Mp 248°.

Et ester: [134733-85-0]
$C_{11}H_{16}N_2O_2$ 208.26
Pale yellow cryst. (EtOH/Et_2O) (as hydrochloride). Mp 232-233° (hydrochloride).

2-N,4′-N,4′-N-Tri-Me:
Needles. Mp 214°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 257D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1192A (*nmr*)
Pedrazzali, A. *et al., Helv. Chim. Acta*, 1957, **40**, 80 (*synth, resoln*)
Eastwood, F.W. *et al., JCS*, 1960, 2286-2292 (*2-N,4′-N,4′-N-tri-Me*)
Jollès, G. *et al., Bull. Soc. Chim. Fr.*, 1965, 2252-2259 (*2-N,4′-N,4′-N-tri-Me*)
Dardenne, G.A. *et al., Phytochemistry*, 1972, **11**, 2567-2570 (*S-form, isol, synth*)
Patel, V.F. *et al., J. Med. Chem.*, 1999, **42**, 2588-2603 (*R-form, Me ester, di-Ac, Me ester di-Ac, synth, pmr, ir, cmr*)
Ansari, A.M. *et al., Synth. Commun.*, 2008, **38**, 2330-2340 (*Et ester*)

4-Aminobenzoate 1-monooxygenase A-359

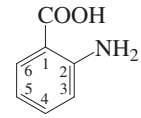
E.C. 1.14.13.27. 4-Aminobenzoate, NAD(P)H:oxygen oxidoreductase (1-hydroxylating, decarboxylating). 4-Aminobenzoate hydroxylase [98668-55-4]

FAD-dependent oxidoreductase enzyme. Isol. from *Agaricus bisporus* (button mushroom). Also acts on 2-Aminobenzoic acid and 4-aminosalicylate.

Tsuji, H. *et al., J. Biol. Chem.*, 1986, **261**, 13203-13209

2-Aminobenzoic acid, 9CI A-360

Anthranilic acid, 8CI. Vitamin L_1 [118-92-3]
[1321-11-5]



$C_7H_7NO_2$ 137.138
Leaflets. Sol. hot H_2O, EtOH, Et_2O. Mp 144-148°. pK_{a1} 1.97; pK_{a2} 4.79 (25°). pK_{a1} 2.17; pK_{a2} 4.85 (25°, 0.1*M* KCl). Sublimes, triboluminescent. λ_{max} 218 (ε 20200); 248 (ε 7000); 335 (ε 4700) (MeOH) (Berdy).

▶ LD_{50} (mus, orl) 1400 mg/kg. Exp. reprod. effects. CB2450000

β-D-Glucopyranosyl ester: [55798-72-6] *β-D-Glucopyranosyl anthranilate*
$C_{13}H_{17}NO_7$ 299.28
Constit. of the fruit of piñuela *Bromelia plumieri*.

Me ester: [134-20-3] *Methyl 2-aminobenzoate. FEMA 2682*
$C_8H_9NO_2$ 151.165
Found in essential oils, including bergamot, orange peel, lemon peel, jasmine, ylang-ylang and neroli. Also present in concord grape, strawberry, star fruit, wines, cocoa, black tea and rice bran. Flavouring agent. Cryst. Mp 24-25°. Bp_{15} 133.5°. pK_a 2.32 (25°, 1% EtOH aq.). Steam-volatile.

▶ Skin irritant. LD_{50} (rat, orl) 2910 mg/kg. Exp. reprod. effects. CB3325000

Et ester: [87-25-2] *Ethyl 2-aminobenzoate. FEMA 2421*
$C_9H_{11}NO_2$ 165.191
Flavouring ingredient. Present in orange juice, orange peel and concord grape. Liq. with faint orange-flower odour and flavour. d_4^{20} 1.12. Mp 13°. Bp 266-268° Bp_{15} 145-147°.

▶ DG2448000

2-Methylpropyl ester: [7779-77-3] *2-Methylpropyl 2-aminobenzoate. Isobutyl anthranilate. FEMA 2182*
$C_{11}H_{15}NO_2$ 193.245
Used in food flavouring. Liq. d 1.06. Bp 270° $Bp_{13.5}$ 169-170°.

2-Propenyl ester: [7493-63-2] *2-Propenyl 2-aminobenzoate. Allyl anthranilate. FEMA 2020*
$C_{10}H_{11}NO_2$ 177.202
Flavour ingredient. Bp_2 105°.

Butyl ester: [7756-96-9] *Butyl 2-aminobenzoate. FEMA 2181*
$C_{11}H_{15}NO_2$ 193.245
Used in fruit food flavouring. d 1.07. Bp 182°.

(Z)-3-Hexenyl ester: [65405-76-7] cis-*3-Hexenyl 2-aminobenzoate. FEMA 3925*
$C_{13}H_{17}NO_2$ 219.283
Flavouring ingredient for baked goods and candies. Bp_5 160°.

Cyclohexyl ester: [7779-16-0] *Cyclohexyl 2-aminobenzoate. Cyclohexyl anthranilate. FEMA 2350*
$C_{13}H_{17}NO_2$ 219.283
Flavouring ingredient. Liq. with a sweet, fruity taste. $d^{15.5}$ 1.02. Bp 318°.

2-Phenylethyl ester: [133-18-6] *2-Phenylethyl 2-aminobenzoate. Phenethyl anthranilate. FEMA 2859*
$C_{15}H_{15}NO_2$ 241.289
Flavouring ingredient. Cryst. Mp 42°. Bp 324°.

2-Naphthyl ester: [63449-68-3] *2-Naphthalenol 2-aminobenzoate. β-Naphthyl anthranilate. FEMA 2767*
$C_{17}H_{13}NO_2$ 263.295
Flavouring ingredient for beverages, baked goods and candies. Mp 118°. Bp 340°.

Amide: [88-68-6] *2-Aminobenzamide. Anthranilamide*
$C_7H_8N_2O$ 136.153
Acetaldehyde scavenger for polyethylene beverage bottles. Leaflets. Mp 109-111.5° dec.

▶ CU8993000

N-*Formyl, Me ester:* [41270-80-8] *Methyl 2-(formylamino)benzoate. FEMA 4171*
$C_9H_9NO_3$ 179.175
Aroma constit. of strawberry fruits. Flavour and fragrance agent. Mp 53°.

N-*Octadecanoyl:* [249620-87-9] N-*Octadecanoylanthranilic acid.* N-*Stearoylanthranilic acid.* ***Fistulosine***
$C_{25}H_{41}NO_3$ 403.604
Constit. of *Allium fistulosum* (Welsh onion) and *Allium porrum* (leek). Cryst. (hexane). Mp 81-82°. Struct. of Fistulosine revised in 2009.

N-*(Carboxyacetyl):* [53947-84-5] *2-[(Carboxyacetyl)amino]benzoic acid, 9CI.* ***2-(Malonylamino)benzoic acid***
$C_{10}H_9NO_5$ 223.185
Isol. from the leaves of the peanut (*Arachis hypogaea*). Cryst. (Me_2CO/hexane). Mp 190-192°.

N-*Me, 2-methylpropyl ester:* [65505-24-0] *Isobutyl* N-*methylanthranilate*
$C_{12}H_{17}NO_2$ 207.272
Possible flavour ingredient; reported in food additive surveys.

N-*Et, Et ester:* [38446-21-8] *Ethyl* N-*ethylanthranilate*
$C_{11}H_{15}NO_2$ 193.245

Possibly used as a flavouring agent; listed in the FDA inventory of substances added to food.

[117808-63-6, 99196-75-5, 99196-74-4, 552-37-4, 99197-00-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 189A; 301D; 302A; 368D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1066B; 1262B; 1262C; 1390C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1371A; 1371B (*ir*)
Bredt, J. *et al., Ber.*, 1900, **33**, 21-29 (*2-methylpropyl ester*)
Smith, P.A.S. *et al., JACS*, 1954, **76**, 431-436 (*synth*)
Adv. Chem. Ser., 1955, **15**, 513; 514 (*props, Me ester, Et ester*)
Forbes, W.F. *et al., Can. J. Chem.*, 1958, **36**, 1371-1380 (*uv*)
Staiger, R.P. *et al., JOC*, 1959, **24**, 1214-1219 (*2-naphthyl ester*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552-2556 (*pmr*)
Dhaneshwar, N.N. *et al., Acta Cryst. B*, 1972, **28**, 647-649 (*N-Me, cryst struct*)
Kimura, Y. *et al., Agric. Biol. Chem.*, 1974, **38**, 1507-1510 (*2-Malonylaminobenzoic acid*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 935-950 (*Me ester, rev, tox*)
Errede, L.A. *et al., JOC*, 1976, **41**, 1763-1765 (*synth*)
IARC Monogr., 1978, **16**, 265; 1987, *Suppl. 7*, 57 (*rev, tox*)
Pyysalo, T. *et al., J. Agric. Food Chem.*, 1979, **27**, 19-22 (*Me ester, N-formyl Me ester, occur*)
Parada, F. *et al., Phytochemistry*, 1996, **42**, 871-873 (*glucosyl ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 80; 751; 949; 981-982; 1445; 1456; 1717; 2156-2157 (*esters*)
Kobayashi, K. *et al., Chem. Lett.*, 2001, 602-603 (*N-formyl Me ester*)
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 38-39; 186-187; 365; 518-519; 760; 868-869; 1071-1072; 1278-1279; 1439 (*esters, use*)
Osvath, R. *et al., Food Chem. News*, 2001, **43(26)**, 30 (*amide, use*)
Clawson, R.W. *et al., Tetrahedron*, 2009, **65**, 8786-8793 (*Fistulosine*)

4-Aminobenzoic acid, 9CI A-361

Vitamin H'. Aminobenzoic acid, USAN. Amben. PABA [150-13-0]
[1321-11-5]

$C_7H_7NO_2$ 137.138
Listed in the EAFUS Food Additive Database (Jan. 2001) but with no reported use. Prisms. Sol. H_2O, alkalis, EtOH, Et_2O, C_6H_6. Mp 188-188.5°. pK_{a1} 2.5; pK_{a2} 4.87 (25°). Log P 0.98 (calc). Discolours to orange on exp. to air and light.

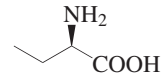
► Can cause contact and photocontact allergic dermatitis from topical use. LD_{50} (rbt, orl) 1830 mg/kg. Exp. reprod. effects. DG1400000

[577-48-0, 515-74-2, 138-84-1, 64059-66-1, 75106-10-4, 555-06-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 198C; 199A; 199C; 303A; 361B; 382D; 450D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1085B; 1086A; 1086C; 1264A; 1264B; 1371C; 1395C; 1413A; 1521B; 1524A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1372A; 1372B (*ir*)
Registry of Mass Spectral Data, Wiley-Interscience, 290 (*ms*)
Sadtler Standard C-13 NMR Spectra, 3466; 6429 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 15745; 16313 (*uv*)
Kremer, C.B. *et al., J. Chem. Educ.*, 1956, **33**, 71-72 (*synth*)
IARC Monogr., 1978, **16**, 249; 1987, *Suppl. 7*, 56 (*rev, tox*)
Dewick, P.M. *et al., Nat. Prod. Rep.*, 1993, **10**, 233-263 (*biosynth*)

2-Aminobutanoic acid, 9CI A-362

α-Aminobutyric acid. Butyrine. Quadrin [80-60-4]
[28805-76-7]



(*R*)-*form*

$C_4H_9NO_2$ 103.121

(*R*)-*form* [2623-91-8]
D-form
Constit. of seedlings of *Glycine max* (soybean), *Dolichos lablab* (hyacinth bean), *Canavalia gladiata* (swordbean), *Arachis hypogaea* (peanut), *Pisum sativum* (pea), *Phaseolus vulgaris* (kidney bean) and *Vigna sesquipedalis* (asparagus bean) after hydrol. Leaflets (EtOH aq.). Mp 292° dec. $[\alpha]_D^{20}$ -7.86 (H_2O) (5*M* HCl).

Hydrochloride: [67607-42-5]
$[\alpha]_D^{20}$ +14.1.

Me ester: [74645-03-7]
$C_5H_{11}NO_2$ 117.147
Bp_{15} 62°. $[\alpha]_D^{25}$ -19.44 (neat).

Me ester, hydrochoride: [85774-09-0]
Cryst. (MeOH/Et_2O). Mp 150°.

N-*Formyl:* [783357-29-9]
$C_5H_9NO_3$ 131.131
Cryst. (EtOH). Mp 126°. $[\alpha]_D^{20}$ +27.98 (H_2O).

N-*(2-Nitrobenzenesulfenyl), Me ester:* [151445-12-4]
$C_{11}H_{14}N_2O_4S$ 270.309
Yellow solid. Mp 99-100°.

N-*(2-Nitrobenzenesulfenyl), amide:* [151445-13-5] *2[[(2-Nitrophenyl)thio]amino]butanamide, 9CI*
$C_{10}H_{13}N_3O_3S$ 255.297
Yellow solid. Mp 150-152°.

(*S*)-*form* [1492-24-6]
L-form
Leaflets (EtOH aq.). Mp 292° dec. (303° in sealed tube). $[\alpha]_D^{20}$ +8 (H_2O) (5*M* HCl).

Hydrochloride: [5959-29-5]
Needles. $[\alpha]_D^{20}$ -14.

N-*Formyl:* [148261-29-4]
Cryst. (EtOH). Mp 126°. $[\alpha]_D^{20}$ -27.74 (H_2O).

(±)-*form* [2835-81-6]
Mp 304° (307° in sealed tube).

Hydrochloride: [40522-79-0]
Cryst.(EtOH aq.). Mp 179-180° (>230°).

Me ester: [2483-62-7]
Mp 139° (as hydrochloride).

Et ester: [5959-30-8]
$C_6H_{13}NO_2$ 131.174
Oil. Bp_{11} 61-62° ($Bp_{16\ 58°}$).

Et ester, hydrochloride: [55410-21-4]
Mp 148-150°.

Amide: [53726-14-0]
$C_4H_{10}N_2O$ 102.136
Prisms. Mp 74-75°.

Nitrile: [40651-89-6] *2-Aminobutanenitrile. 2-Cyanopropylamine*
$C_4H_8N_2$ 84.121
Mp 144-145° (as hydrochloride).

N-*Formyl:* [82413-57-8]
Needles (EtOH). Mp 153°.

N-*Benzoyl:* [5468-52-0]
$C_{11}H_{13}NO_3$ 207.229
Mp 145-146°.

N-*Me:* [70606-05-2] *2-(Methylamino)butanoic acid*
$C_5H_{11}NO_2$ 117.147
Prisms + $1H_2O$. V. sol. H_2O; insol. Et_2O. Mp 248° subl. Sweet taste.

N-*Me; hydrochloride:* Mp 150° dec.

N-*Me, Me ester:* [116496-48-1]
$C_6H_{13}NO_2$ 131.174
Bp_{30} 64.5°.

N,N-*Di-Me:* [10941-86-3] *2-(Dimethylamino)butanoic acid*
$C_6H_{13}NO_2$ 131.174
Hygroscopic needles. Sol. H_2O. Mp 179°.

N-*Ph:* [67832-70-6] *2-Anilinobutanoic acid*
$C_{10}H_{13}NO_2$ 179.218
Cryst. (MeOH/$CHCl_3$). Mp 141°.

N-*Ph, Et ester:* [73717-57-4]
$C_{12}H_{17}NO_2$ 207.272
Mp 26°. Bp 278°.

N-*Ph, amide:*
$C_{10}H_{14}N_2O$ 178.233
Mp 123°. No CAS no. found to 2008.

N-*Ph, nitrile:* [85599-84-4]
$C_{10}H_{12}N_2$ 160.218
Needles. Mp 39°.

N-*(2,4-Dinitrophenyl):* [31356-29-3]
Mp 143°.

[73689-74-4, 7682-20-4, 7682-18-0, 7324-11-0, 6367-34-6, 4470-69-3, 15399-22-1, 21685-47-2, 22621-37-0, 104652-77-9, 103765-03-3, 93554-80-4, 91462-82-7, 87068-75-5, 15399-11-8, 67942-91-0, 56545-22-3, 40916-98-1, 39540-29-9, 26815-92-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 572C; 572D; 573A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 871B; 871C; 872A (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2381-2406 (*synth, resoln*)
Junk, J.G. *et al., JACS*, 1963, **85**, 839-845 (*ms*)
Pachler, K.G.R. *et al., Spectrochim. Acta*, 1963, **19**, 2085-2092 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Ronwin, E. *et al., Can. J. Chem.*, 1968, **46**, 3013-3024 (*ir*)

Akimoto, T. *et al., Acta Cryst. B*, 1972, **28**, 3106-3107 (*cryst struct*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 191-193; 1865-1868 (*synth*)
Ogawa, T. *et al., Agric. Biol. Chem.*, 1976, **40**, 1661-1662 (*occur*)
Glowiak, T. *et al., Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1978, **26**, 43-51 (*cryst struct*)
Cooper, A.J.L. *et al., J. Biol. Chem.*, 1979, **254**, 2748-2753 (*synth*)
Compagnone, R.S. *et al., JOC*, 1986, **51**, 1713-1719 (*synth, pmr*)
Chenault, H.K. *et al., JOC*, 1987, **52**, 2608-2611 (*resoln, pmr*)
Bunse, M. *et al., Chem. Ber.*, 1993, **126**, 1499-1502 (*2-nitrobenzenesulfenyl derivs, synth, pmr*)
Stirling, I.R. *et al., JCS Perkin 1*, 1997, 677-680 (*synth*)
Cronin, J.R. *et al., Science (Washington, D.C.)*, 1997, **275**, 951-955 (*occur, meteorite*)
Pizzarello, S. *et al., Acc. Chem. Res.*, 2006, **39**, 231-237 (*occur, meteorites*)
Yajima, T. *et al., Biosci., Biotechnol., Biochem.*, 2007, **71**, 1338-1341 (*synth*)

3-Aminobutanoic acid, 9CI A-363

β-Homoalanine [541-48-0]
[28805-76-7]

(*R*)-*form*

$C_4H_9NO_2$ 103.121
Prod. by *Oryza sativa* (rice).

(*R*)-*form* [3775-73-3]
Prisms (MeOH). Mp 218-219°. $[\alpha]_D^{23}$ -39 (c, 0.4 in H_2O) (op).

(*S*)-*form* [3775-72-2]
Prisms (MeOH). Mp 215° (220° dec.). $[\alpha]_D^{19}$ +37 (c, 6.0 in H_2O).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 577B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 877B (*nmr*)
Aldrich Library of NMR Spectra, **3**, 4C (*pmr*)
Furukawa, M. *et al., Chem. Pharm. Bull.*, 1977, **25**, 1319-1325; 1978, **26**, 260-263 (*synth*)
Eur. Pat., 1985, 144 980 (*R-form, S-form, R-Me ester, S-Me ester, synth, resoln*)
Griesbeck, A. *et al., Helv. Chim. Acta*, 1987, **70**, 1326-1332 (*synth*)
Gmeiner, P. *et al., Annalen*, 1991, 501-502 (*R-form, synth, pmr*)
Bringmann, G. *et al., Synthesis*, 1991, 829-831 (*S-form, synth, pmr, ir, ms, S-Me ester*)
Amoroso, R. *et al., Heterocycles*, 1992, **34**, 349-355 (*R-form, S-form, synth, pmr, cmr*)
Juaristi, E. *et al., JOC*, 1992, **57**, 2396-2398 (*R-form, S-form, (±)-form, R-Me ester, S-Me ester, synth*)
Chu, K.S. *et al., Tetrahedron*, 1993, **49**, 9183-9190 (*S-form, synth, pmr, cmr, ir, ms*)
Davies, S.G. *et al., Chem. Comm.*, 1995, 1109-1110 (*S-form, synth*)
Cimarelli, C. *et al., Synth. Commun.*, 2001, **31**, 2943-2953 (*R-form, synth, ir, pmr, cmr*)
Agami, C. *et al., Tetrahedron*, 2001, **57**, 195-200 (*S-form, synth, pmr, cmr*)

4-Aminobutanoic acid, 9CI A-364

γ-Aminobutyric acid. Piperidinic acid. Piperidic acid. Aminalon. Gamalon. GABA. FEMA 4288 [56-12-2]
[28805-76-7]

$H_2NCH_2CH_2CH_2COOH$
$C_4H_9NO_2$ 103.121
Flavouring and cosmetic ingredient. Prisms (EtOH). V. sol. H_2O; sl. sol. EtOH, Me_2CO; insol. Et_2O. Mp 203° dec. Log P -3.33 (calc). Homopolymers (polyamides) are usually derived from the lactam 2-Pyrrolidinone.

▶ LD_{50} (mus, orl) 12680 mg/kg. ES6300000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 577C; 577D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 877C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 25 (*synth*)
Thompson, J.F. *et al., Arch. Biochem. Biophys.*, 1953, **46**, 248 (*synth*)
Taddei, F. *et al., JCS*, 1964, 1553 (*pmr*)
Voellmin, J. *et al., Microchem. J.*, 1966, **11**, 73 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2427 (*occur*)
Steward, E.G. *et al., Acta Cryst. B*, 1973, **29**, 2038; 2825 (*cryst struct*)
Tomita, K. *et al., Bull. Chem. Soc. Jpn.*, 1973, **46**, 2199 (*cryst struct*)
Weber, H.P. *et al., Acta Cryst. B*, 1983, **39**, 360 (*cryst struct*)
Erdoe, S.L. *et al., J. Neurochem.*, 1990, **54**, 363 (*rev*)
Bon, E. *et al., JOC*, 1994, **59**, 1904 (*synth, ir, pmr, cmr*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use*)

(4-Aminobutyl)guanidine, 9CI A-365

4-Guanidinobutylamine. 1-Amino-4-guanidinobutane. ***Agmatine*** [306-60-5]

$HN{=}^6C(NH_2)NH(CH_2)_3CH_2NH_2$
$C_5H_{14}N_4$ 130.192
Mp 101.5-103°.

Sulfate: [2482-00-0]
Cryst. Mp 229° (224-225°).

N^1-*Ac:* [3031-89-8] **N^1-*Acetylagmatine***
$C_7H_{16}N_4O$ 172.23

N^1-*(3S-Methyldecanoyl):* [164301-83-1] ***Aplysillamide B***
$C_{16}H_{34}N_4O$ 298.471
Oil. Sol. MeOH. $[\alpha]_D^{21}$ -2.4 (c, 0.1 in MeOH) (natural). $[\alpha]_D^{22}$ -5.1 (c, 1.6 in MeOH) (synthetic).

N^1-*(3-Methyl-2Z-decenoyl):* [164301-82-0] ***Aplysillamide A***
$C_{16}H_{32}N_4O$ 296.455
Oil. Sol. MeOH. λ_{max} 225 (ε 10000) (MeOH) (Berdy).

N^1-*(4-Hydroxy-*E*-cinnamoyl):* [47096-24-2] **N^1-trans-p-*Coumaroylagmatine***
[7295-86-5]
$C_{14}H_{20}N_4O_2$ 276.338
Isol. from barley seedlings. Sol. H_2O. Mp 215-217° (as picrate). λ_{max} 229 (ε 33100); 300 (ε 26300) (H_2O) (Berdy).

N^1-*(4-Hydroxy-Z-cinnamoyl):* [191330-81-1] **N^1-cis-p-*Coumaroylagmatine***
$C_{14}H_{20}N_4O_2$ 276.338
Syrup or powder. λ_{max} 278 (ε 2000) (H_2O).

N^1-*(4-Hydroxy-3-methoxy-*E*-cinnamoyl):* [188305-06-8] **N^1-trans-*Feruloylagmatine***
$C_{15}H_{22}N_4O_3$ 306.364
Isol. from *Triticum aestivum* (wheat) exposed to low temps.

N^1-*(3,4-Dimethoxycinnamoyl):* [128009-18-7] **N^1-*(3,4-Dimethoxycinnamoyl)agmatine***
[146072-40-4]
$C_{16}H_{24}N_4O_3$ 320.391

N^6-*Me:* [77414-15-4] N-*(4-Aminobutyl)*-N′-*methylguanidine.* **N^6-*Methylagmatine***
$C_6H_{16}N_4$ 144.219
Isol. from soybean and alfalfa.

N^6-*(3-Methyl-2-butenyl):* [128009-17-6] N-*(4-Aminobutyl)*-N′-*prenylguanidine.* **N^6-*(3-Methyl-2-butenyl)agmatine.*** N^6-*Prenylagmatine*
$C_{10}H_{22}N_4$ 198.311

N^4-*(3-Methyl-2-butenyl),* N^1-*(4-hydroxy-3-methoxy-*E*-cinnamoyl):* [1166170-66-6] N^1-trans-*Feruloyl*-N^4-*prenylagmatine.* ***Canarosine***
$C_{20}H_{30}N_4O_3$ 374.482
Pale yellow needles. Mp 235-237°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 821B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1330A (*nmr*)
Kossel, A. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1910, **66**, 257-261; **68**, 170-171 (*isol, struct, synth*)
Heyl, F.W. *et al., JACS*, 1919, **41**, 670-682 (*isol*)
Stoessl, A. *et al., Phytochemistry*, 1965, **4**, 973-976 (*isol, uv, struct, synth, N-coumaroyl*)
Boldt, A. *et al., Phytochemistry*, 1971, **10**, 731-738 (*biosynth*)
Smith, T.A. *et al., Phytochemistry*, 1978, **17**, 1093-1098 (*occur, N-coumaroyl*)
Kowabata, T. *et al., CA*, 1979, **89**, 178349 (*isol*)
Robin, Y. *et al., Oceanis*, 1980, **5**, 575-580 (N^1-*Acetylagmatine*)
Bird, C.R. *et al., Phytochemistry*, 1981, **20**, 2345-2346 (*biosynth, N-coumaroyl*)
Chandrasekhar, K. *et al., Acta Cryst. B*, 1982, **38**, 2538-2540 (*cryst struct*)
Cho, Y.B. *et al., Anal. Biochem.*, 1987, **160**, 429-433 (N^6-*Methylagmatine*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1313-1315 (N^6-*Methylagmatine*)
Hamana, K. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1991, **100**, 59-62 (*occur, hplc*)
Mitchinson, A. *et al., Chem. Comm.*, 1994, 2613-2614 (*synth*)
Honma, K. *et al., Tetrahedron*, 1995, **51**, 3745 (*Aplysillamides*)
Ueda, M. *et al., Biosci., Biotechnol., Biochem.*, 1998, **62**, 2133-2137 (*Z-coumaroyl*)
Reis, D.J. *et al., Ann. N.Y. Acad. Sci.*, 1999, **881**, 65-80 (*rev, activity*)
Monache, G.D. *et al., Bioorg. Med. Chem. Lett.*, 1999, **9**, 3249-3254 (*Prenylagmatine, Dimethoxycinnamoylagmatine*)
Jin, S. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1614-1617 (*Feruloylagmatine*)
Fairbanks, C.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 10584-10589 (*pharmacol*)
Reis, D.J. *et al., Trends Pharmacol. Sci.*, 2000, **21**, 187-193 (*pharmacol, rev*)
Demady, D.R. *et al., Mol. Pharmacol.*, 2001, **59**, 24-29 (*pharmacol*)
Cheng, X. *et al., Chem. Biodiversity*, 2008, **5**, 1335-1344 (*Feruloylagmatine*)
Pattamadilok, D. *et al., J. Asian Nat. Prod. Res.*, 2008, **10**, 915-918 (*Canarosine*)

(4-Aminobutyl)urea, 8CI A-366

N-*Carbamoylputrescine* [6851-51-0]

$H_2NCH_2(CH_2)_3NHCONH_2$

$C_5H_{13}N_3O$ 131.177

Alkaloid from *Hordeum vulgare* (barley) and *Sesamum indicum* (sesame).

Hydrochloride: Mp 185-186°.

Dipicrate: Mp 164-165°.

Linneweh, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1932, **205**, 126 (*synth*)
Smith, T.A. *et al., Phytochemistry*, 1964, **3**, 23 (*occur, synth*)
Crocomo, O.J. *et al., Phytochemistry*, 1970, **9**, 1487 (*occur*)

4-Aminobutyrate transaminase A-367

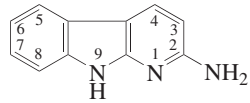
E.C. 2.6.1.19. 4-Aminobutanoate:2-oxoglutarate aminotransferase. β-Alanine oxoglutarate transaminase. β-Alanine aminotransferase. GABA aminotransferase. GABA transaminase. 4-Aminobutyrate aminotransferase [9037-67-6]

Aminotransferase enzyme. Isol. from pig and rabbit liver. Some preparations also act on β-alanine, 5-aminopentanoate and 3-amino-2-methylpropanoate.

Scott, E.M. *et al., J. Biol. Chem.*, 1959, **234**, 932-936 (*Pseudomonas fluorescens*)
Aurich, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1961, **326**, 25-33 (*Neurospora crassa*)
Jakoby, W.B. *et al., Methods Enzymol.*, 1962, **5**, 765-778 (*Pseudomonas fluorescens*)
Schousboe, A. *et al., Biochemistry*, 1973, **12**, 2868-2873 (*mouse brain*)
Maitre, M. *et al., Eur. J. Biochem.*, 1975, **52**, 157-169 (*rat brain*)
Buzenet, A.M. *et al., Biochim. Biophys. Acta*, 1978, **522**, 400-411 (*pig liver*)
Maitre, M. *et al., Adv. Exp. Med. Biol.*, 1979, **123**, 3-20 (*human brain*)
Yonaha, K. *et al., Arch. Biochem. Biophys.*, 1980, **200**, 159-164 (*Pseudomonas*)
Tamaki, N. *et al., J. Biochem. (Tokyo)*, 1982, **92**, 1009-1017 (*rabbit liver*)
Yonaha, K. *et al., Eur. J. Biochem.*, 1985, **146**, 101-106 (*Streptomyces griseus*)
Markovic-Housley, Z. *et al., J. Mol. Biol.*, 1990, **214**, 821-823 (*pig liver, cryst struct*)

2-Amino-α-carboline A-368

9H-Pyrido[2,3-b]indol-2-amine. 3-Amino-3-carboline (obsol.) [26148-68-5]



$C_{11}H_9N_3$ 183.212

Found in cooked foods as pyrol. prod. of tryptophan, esp. cooked meats. Cryst. ($CHCl_3$/hexane or EtOH). Mp 202-203°.

▶ Exp. carcinogen and mutagen. Possible human carcinogen (IARC 2B).

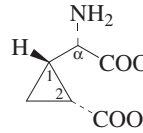
UU9351600

N^2-*Me:* [26148-70-9]
$C_{12}H_{11}N_3$ 197.239
Cryst. (C_6H_6/petrol). Mp 156-157°.

Stephenson, L. *et al., JCS(C)*, 1970, 1355 (*synth*)
Yoshida, D. *et al., Biochem. Biophys. Res. Commun.*, 1978, **83**, 915 (*cryst struct, tox*)
Matsumoto, T. *et al., Agric. Biol. Chem.*, 1979, **43**, 675 (*synth*)
Yoshida, D. *et al., Agric. Biol. Chem.*, 1979, **43**, 1769
Hibino, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 79 (*synth, pmr*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 68-78 (*detn, occur, ms, hplc*)
IARC Monogr. (Web), http://monographs.iarc.fr
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJD750

α-Amino-2-carboxycyclopropaneacetic acid, 8CI A-369

2-(Carboxycyclopropyl)glycine. 3,4-Methanoglutamic acid



(α*S*,1*S*,2*R*)-*form*

$C_6H_9NO_4$ 159.141

(α*S*,1*S*,2*R*)-*form* [117857-95-1]
L-cis-*form*
Cryst. (EtOH/Me_2CO/H_2O). $[\alpha]_D^{20}$ +25 (c, 1 in H_2O). $[\alpha]_D$ +58 (c, 0.5 in 5*M* HCl).

(α*S*,1*S*,2*S*)-*form* [117857-93-9]
L-trans-*form*. *L-CCG-I*
Isol. from seeds of *Blighia sapida* (akee apple). Cryst. $[\alpha]_D^{20}$ +107 (c, 2 in H_2O). $[\alpha]_D$ +146 (c, 1 in 5*M* HCl). Pharmacol. active isomer.

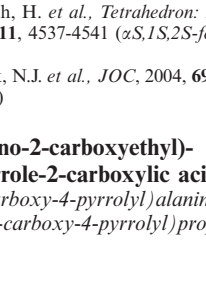
(α*S*,1*R*,2*S*)-*form* [117857-96-2]

[22255-17-0, 22255-18-1]

Fowden, L. *et al., Phytochemistry*, 1969, **8**, 437 (*isol, struct, pmr, ms, cryst struct*)
Fowden, L. *et al., JCS(C)*, 1971, 833 (*cd, ord*)
Kurokawa, N. *et al., Tet. Lett.*, 1985, **26**, 83 (*synth, pmr*)
Yamanoi, K. *et al., Tet. Lett.*, 1988, **29**, 1181 (*synth, biochem*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231 (*rev*)
Starratt, A.N. *et al., Phytochemistry*, 1995, **40**, 479 (*isol, bibl*)
Sagnard, I. *et al., Tet. Lett.*, 1995, **36**, 3149 (*synth*)
Pajouhesh, H. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 4537-4541 (*αS,1S,2S-form, synth, pmr*)
Wallcock, N.J. *et al., JOC*, 2004, **69**, 2997-3007 (*synth*)

4-(2-Amino-2-carboxyethyl)-1*H*-pyrrole-2-carboxylic acid A-370

3-(2-Carboxy-4-pyrrolyl)alanine. 2-Amino-3-(2-carboxy-4-pyrrolyl)propanoic acid



$C_8H_{10}N_2O_4$ 198.178

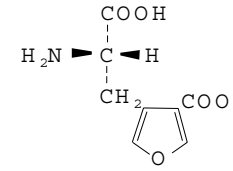
(*S*)-*form* [137309-97-8]
L-form
Mp 200-202° dec.

(±)-*form*
Mp 200-202° dec.

Yamano, K. *et al., Tetrahedron*, 1992, **48**, 1457 (*isol, synth, struct*)

α-Amino-4-carboxy-3-furanpropanoic acid, 9CI A-371

3-(3-Carboxy-4-furanyl)alanine



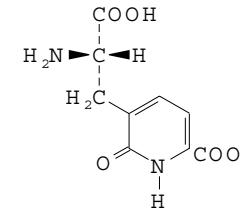
$C_8H_9NO_5$ 199.163

(*S*)-*form* [54836-90-7]
Isol. from the unpalatable mushrooms *Phyllotopsis nidulans* and *Tricholomopsis rutilans*. Cryst. (Me_2CO). Mp 227-228°.

Hatanaka, S. *et al., Mushroom Sci.*, (Publ. 1976), (Part 1), 1974, **9**, 809 (*isol*)
Doyle, R.R. *et al., Phytochemistry*, 1974, **13**, 2813 (*isol, struct*)

α-Amino-6-carboxy-2-oxo-3-pyridinepropanoic acid A-372

3-(6-Carboxy-2-oxo-3-pyridinyl)alanine



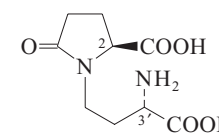
$C_9H_{10}N_2O_5$ 226.188
Sol. H_2O, MeOH; poorly sol. EtOAc, hexane. λ_{max} 241 (ε 12000); 315 (ε 13500) (H_2O).

(*S*)-*form* [148001-20-1]
$[\alpha]_D^{23}$ -5.8 (c, 0.13 in H_2O).

Yamano, K. *et al., Heterocycles*, 1992, **34**, 445-448; 1993, **35**, 125-128 (*isol, struct, activity*)
Yamano, K. *et al., Chem. Lett.*, 1993, 21 (*isol, biosynth*)
Yamano, K. *et al., Tetrahedron*, 1993, **49**, 2427-2436 (*isol*)
Adamczyk, M. *et al., Tetrahedron: Asymmetry*, 2001, **12**, 2385-2388 (*synth*)

α-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid, 9CI A-373

1-(3-Amino-3-carboxypropyl)-5-oxo-2-pyrrolidinecarboxyic acid. Lp-2 [115553-99-6]

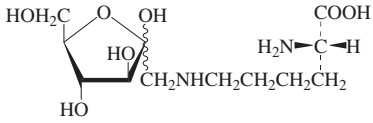


(2*S*,3′*S*)–*form*

$C_9H_{14}N_2O_5$ 230.22

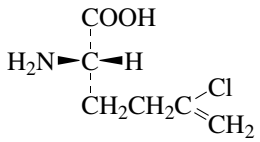
(2*S*,3′*S*)-*form*
Amino acid from the basidiomycete *Lactarius piperatus*. Amorph. solid. Sol. H_2O. $[\alpha]_D$ -17.5 (c, 0.939 in H_2O).
Fushiya, S. *et al., Chem. Pharm. Bull.*, 1988, **36**, 1366 (*isol, ir, pmr, cmr, synth*)

1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose, 9CI A-374
N^6-*(1-Deoxyfructos-1-yl)lysine. ϵ-Fructoselysine. ϵ-Deoxyfructosyllysine* [21291-40-7]



$C_{12}H_{24}N_2O_7$ 308.331
Amadori rearrangement prod. found in heated milk and other foodstuffs.
Acetate salt: [23931-62-6]
Mp 53-55°.
Finot, P.A. *et al., Helv. Chim. Acta*, 1969, **52**, 1488-1495 (*synth*)
Steinig, J. *et al., Z. Lebensm.-Unters. -Forsch.*, 1982, **174**, 453-457 (*synth, ms, detn*)
Dyer, D.G. *et al., J. Clin. Invest.*, 1993, **91**, 2463-2469; 2470-2478

2-Amino-5-chloro-5-hexenoic acid A-375
[66157-56-0]

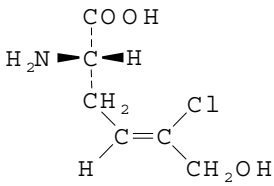


(*S*)-*form*

$C_6H_{10}ClNO_2$ 163.603

(*S*)-*form*
Isol. from the mushrooms *Amanita miculifera* and *Amanita onusta*.
Japan. Pat., 1977, 77 148 019 (*isol, ir*)
Hatanaka, S.-I. *et al., Phytochemistry*, 1998, **49**, 573-578 (*isol, synth, pmr, ms*)

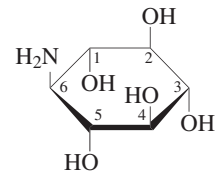
2-Amino-5-chloro-6-hydroxy-4-hexenoic acid A-376



$C_6H_{10}ClNO_3$ 179.603

(*S*,*Z*)-*form* [108101-63-9]
Isol. from toxic mushroom *Amanita abrupta*. Mp 200-212° dec. $[\alpha]_D^{20}$ -17.9 (c, 0.19 in H_2O).
Ohta, T. *et al., Phytochemistry*, 1987, **26**, 565-566 (*isol, pmr, struct*)

6-Amino-1,2,3,4,5-cyclohexanepentol A-377



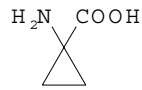
(1α,2β,3α,4β,5α,6β)-*form*

$C_6H_{13}NO_5$ 179.172
Numbering of inositols changes depending on stereochem. Numbering given below is based on the systemic numbering scheme shown.

(1α,2β,3α,4β,5α,6β)-*form* [16051-25-5]
1-Amino-1-deoxy-scyllo-*inositol, 9CI. Scylloinosamine. Inosamine SB. Bluensamine.* scyllo-*Inosamine.* s*Ia*
Present in alfalfa nodules (*Medicago sativa*). Cryst. Mp 300°. Opt. inactive (*meso*-).
2-Me: [151062-28-1] *1-Amino-1-deoxy-3-*O-*methyl-*L-scyllo-*inositol, 9CI. 3-*O-*Methyl-*L-scyllo-*inosamine.* ***Rhizopine***
$C_7H_{15}NO_5$ 193.199
Present in alfalfa nodules. Chiral compd.
Saint, C.P. *et al., J. Bacteriol.*, 1993, **175**, 5205-5215 (*Scylloinosamine, isol, genomics*)

Aminocyclopropanecarboxylate oxidase A-378
E.C. 1.14.17.4. 1-Aminocyclopropanecarboxylate, ascorbate:oxygen oxidoreductase (ethylene-forming). Ethylene-forming enzyme. ACC oxidase [98668-53-2]
Non-haem Fe-dependent oxidoreductase enzyme; requires CO_2 for activity. Present in higher plants, e.g. tomato (*Lycopersicon esculentum*) and apple (*Malus domestica*).
Dong, J.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1992, **89**, 9789-9793 (*apple*)
Zhang, Z.H. *et al., Biochem. J.*, 1995, **307**, 77-85 (*tomato*)
Pirrung, M.C. *et al., Acc. Chem. Res.*, 1999, **32**, 711-718 (*rev*)

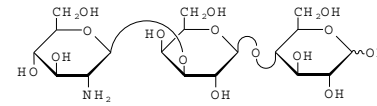
1-Aminocyclopropanecarboxylic acid, 9CI A-379
[22059-21-8]



$C_4H_7NO_2$ 101.105
Isol. from apple and pear juice and cranberries. Cryst. (EtOH aq.). Mp 229-231°.
▶ GZ1110000
N-*Malonyl:* [80550-27-2] *1-(Malonylamino)cyclopropanecarboxylic acid. MACC*
$C_7H_9NO_5$ 187.152
Constit. of numerous plant spp. including wheat, tomato and sweet corn. Mp 158-160°.
N-*(L-γ-Glutamyl):* [171437-78-8] *1-(γ-Glutamylamino)cyclopropanecarboxylic acid*
$C_9H_{14}N_2O_5$ 230.22
Isol. from tomato fruit (*Lycopersicon esculentum*).

[72784-48-6]
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 884A; 884B (*nmr*)
Vähätalo, M.L. *et al., Acta Chem. Scand.*, 1957, **11**, 741-743 (*isol*)
Berlinguet, L. *et al., Nature (London)*, 1962, **194**, 1082-1083 (*activity*)
Bregovec, I. *et al., Monatsh. Chem.*, 1972, **103**, 288-291 (*synth*)
Kollonitsch, J. *et al., JOC*, 1979, **44**, 771-777 (*synth*)
Ger. Pat., 1982, 3 122 240 (*synth*)
Baldwin, J.E. *et al., Chem. Comm.*, 1985, 206-207 (*props*)
Schöllkopf, U. *et al., Angew. Chem., Int. Ed.*, 1986, **25**, 754-755 (*synth*)
Isogai, K. *et al., Bull. Chem. Soc. Jpn.*, 1986, **59**, 2839-2842 (*synth, pmr, ir*)
Yang, S.F. *et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987)*, 1986, 92-101 (*rev*)
Amrhein, N. *et al., Conjugated Plant Horm.: Proc. Int. Symp., 1986 (1987)*, 1986, 102-110 (*rev*)
Wiesendanger, R. *et al., Experientia*, 1986, **42**, 207-209 (*biosynth*)
Strazewski, P. *et al., Synthesis*, 1987, 298-299 (*synth, pmr, cmr, ms*)
Wheeler, T.N. *et al., Synth. Commun.*, 1988, **18**, 141-149 (*synth, pmr, cmr*)
Vaidyanathan, G. *et al., JOC*, 1989, **54**, 1810-1815; 1815-1820 (*synth, Me ester, N,N-dibenzyl, N,N-di-Me, N-Me, N-benzyl, bibl*)
Salaün, J. *et al., JOC*, 1990, **55**, 4276-4281 (*synth, pmr*)
Stammer, H. *et al., Tetrahedron*, 1990, **46**, 2231-2254 (*rev*)
Cativiela, C. *et al., Synth. Commun.*, 1992, **22**, 2955-2963 (*synth*)
Alami, A. *et al., Bull. Soc. Chim. Fr.*, 1993, **130**, 5-24 (*rev*)
Angus, P.M. *et al., Chem. Comm.*, 1993, 979-980 (*synth*)
Zhu, X. *et al., Synth. Commun.*, 1998, **28**, 3159-3162 (*synth, ir, pmr, ms*)
Pirrung, M.C. *et al., Acc. Chem. Res.*, 1999, **32**, 711-718 (*rev*)
Fulop, F. *et al., Chem. Rev.*, 2001, **101**, 2181-2204 (*rev*)

2-Amino-2-deoxy-β-D-glucopyranosyl-(1 →3)-β-D-galactopyranosyl-(1 →4)-D-glucose A-380
3^2-Glucosaminyllactose



Pyranose-form

$C_{18}H_{33}NO_{15}$ 503.456
N-*Ac:* [75645-27-1] *2-Acetamido-2-deoxy-β-D-glucopyranosyl-(1 →3)-β-D-galactopyranosyl-(1 →4)-D-glucose. 3^2-β-N-Acetylglucosaminyllactose. Lacto-*N-*triose II*

$C_{20}H_{35}NO_{16}$ 545.494
Isol. from the partial acid hydrolysates of the tetra and higher saccharides obt. from human milk; does not occur free in milk. Mp 201-202°. $[\alpha]_D$ +40.7 (in H_2O).

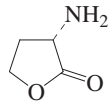
N-*Ac, phenylosazone:* Mp 230°.

[24741-60-4]

Kuhn, R. *et al., Chem. Ber.*, 1958, **91**, 364; 1960, **93**, 647; 1962, **95**, 513; 518 (*isol*)
Okuyama, T. *et al., CA*, 1961, **55**, 18817; 1962, **57**, 8880 (*isol*)
Acher, A.J. *et al., JOC*, 1970, **35**, 2436 (*synth*)
Koenderman, A.H.L. *et al., Biomed. Chromatogr.*, 1986, **1**, 104 (*synth*)

3-Aminodihydro-2(3*H*)-furanone, 9CI, 8CI A-381

2-Amino-4-butanolide. 2-Amino-4-hydroxybutanoic acid lactone. ***Homoserine lactone****. α-Amino-γ-butyrolactone* [1192-20-7]



(*S*)-*form*

$C_4H_7NO_2$ 101.105

(*S*)-*form* [2185-02-6]
L-form
Constit. of pea *Pisum sativum* seedlings. May be an artifact but most recent work indicates that it is prob. a genuine nat. prod.

N-*Butanoyl:* [67605-85-0] N-*(Tetrahydro-2-oxo-3-furanyl)butanamide, 9CI.* **N-*Butanoylhomoserine lactone****. PAI 2. C4-HSL*
$C_8H_{13}NO_3$ 171.196
Isol. from a *Pantoea* sp. found on maize leaves (*Zea mays*). Cryst. (CH_2Cl_2/hexane). Mp 120-121°. $[\alpha]_D^{25}$ +18.9 (c, 0.74 in $CHCl_3$).

N-*Hexanoyl:* [147852-83-3] N-*(Tetrahydro-2-oxo-3-furanyl)hexanamide, 9CI.* **N-*Hexanoylhomoserine lactone****. C6-HSL*
$C_{10}H_{17}NO_3$ 199.249
Prod. by an *Erwinia psidii* strain isol. on guava (*Psidium guajava*) and a *Pantoea* sp. on maize leaves (*Zea mays*). $[\alpha]_D^{20}$ -22.9 (c, 0.35 in MeOH).

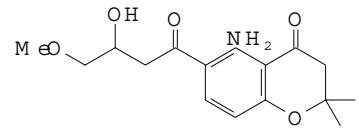
N-*Heptanoyl:* [177158-20-2] **N-*Heptanoylhomoserine lactone****. C7-HSL*
$C_{11}H_{19}NO_3$ 213.276
Prod. by an *Erwinia psidii* strain isol. on guava (*Psidium guajava*). $[\alpha]_D^{20}$ -18 (c, 0.42 in MeOH).

N-*(3*R*-Hydroxy-7Z-tetradecenoyl):* [172617-17-3] **N-*(3-Hydroxy-7-tetradecenoyl)homoserine lactone****. RLA1*
$C_{18}H_{31}NO_4$ 325.447
Bacteriocin. Prod. by *Rhizobium leguminosarum.*

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 700C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1139C (*nmr*)
Weiss, S. *et al., JACS*, 1951, **73**, 2497-2499 (*resoln*)
Saarivirta, M. *et al., Acta Chem. Scand.*, 1965, **19**, 1008-1009 (*isol*)
Jošt, K. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 2485-2490 (*synth*)
Natelson, S. *et al., Microchem. J.*, 1982, **27**, 466-483 (*occur*)
McGarvey, G.J. *et al., JACS*, 1986, **108**, 4943-4952 (*synth, pmr, ir*)
Buchardt, O. *et al., Synthesis*, 1993, 1065-1067 (*pmr*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2322-2325 (*resoln*)
Schripsema, J. *et al., J. Bacteriol.*, 1996, **178**, 366-371 (*3-hydroxytetradecenoyl*)
Pomini, A.M. *et al., J. Agric. Food Chem.*, 2005, **53**, 6262-6265; 2007, **55**, 1200-1204 (*N-butanoyl, N-hexanoyl, N-heptanoyl*)

5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxy-1-oxobutyl)-2,2-dimethyl-4*H*-1-benzopyran-4-one, 9CI A-382

*5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxybutanoyl)-2,2-dimethyl-4*H*-4-chromanone. TDP 6* [130767-47-4]

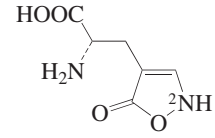


$C_{16}H_{21}NO_5$ 307.346
Isol. from rice cultures of *Fusarium equiseti.*

Xie, W. *et al., Appl. Environ. Microbiol.*, 1990, **56**, 2946-2948 (*isol, pmr, ms*)

α-Amino-2,5-dihydro-5-oxo-4-isoxazolepropanoic acid, 9CI A-383

α-Amino-5-oxo-3-isoxazoline-4-propionic acid, 8CI. 3-(Isoxazolin-5-on-4-yl)alanine. 4-Alanyl-3-isovalin-5-one. TAN 950A. Antibiotic TAN 950A



$C_6H_8N_2O_4$ 172.14
Exists in tautomeric equilibrium with Antibiotic TAN 950B.

(*S*)-*form* [127607-88-9]
L-form
Powder + $1H_2O$ (as Na salt). Sol. H_2O, DMSO, DMF; poorly sol. Me_2CO, $CHCl_3$, EtOAc. $[\alpha]_D^{23}$ -69.5 (c, 0.52 in H_2O) (as Na salt). λ_{max} 253 (ε 8060) (H_2O). λ_{max} 259 (E1%/1cm 421) (HCl) (Berdy).

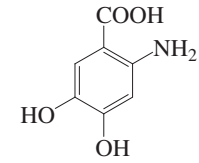
N^2-*β-D-Glucosyl:* [29790-46-3]
$C_{12}H_{18}N_2O_9$ 334.282
Isol. from *Pisum sativum* (peas). Cryst. (MeOH/propanol). Mp 182° dec.

[130621-61-3, 130620-29-0, 130621-42-0, 130621-41-9]

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1970, **40**, 557-564; 1974, **61**, 155-162 (*isol, struct, uv, pmr, ir*)
Murakoshi, I. *et al., Phytochemistry*, 1975, **14**, 1515-1517 (*biosynth*)
Eur. Pat., 1988, (*(Takeda)*)0 289 354 (*isol, activity*)
Eur. Pat., 1990, (*(Takeda)*)0 367 393 (*isol, activity*)
Tamura, N. *et al., Chem. Pharm. Bull.*, 1991, **39**, 1199-1212 (*synth, activity*)
Iwama, T. *et al., Eur. J. Pharmacol.*, 1991, **197**, 187-192 (*props*)
Tsubotani, S. *et al., Tetrahedron*, 1991, **47**, 8079-8090 (*synth, cryst struct*)
Hakoda, S. *et al., J. Antibiot.*, 1992, **45**, 854-860 (*isol*)

2-Amino-4,5-dihydroxybenzoic acid A-384

6-Aminoprotocatechuic acid. 4,5-Dihydroxyanthranilic acid [114874-99-6]



$C_7H_7NO_4$ 169.137

N-*Et, amide:* [127793-87-7] *2-(Ethylamino)-4,5-dihydroxybenzamide, 9CI*
$C_9H_{12}N_2O_3$ 196.205
Alkaloid from *Piper nigrum* (pepper).

4-Me ether: [31839-21-1] *2-Amino-5-hydroxy-4-methoxybenzoic acid. 2-Amino-5-hydroxy-*p*-anisic acid, 8CI*
$C_8H_9NO_4$ 183.163
Mp 214-215° (194-195°).

4-Me ether, N-*(4-hydroxy-3-methoxy-*E*-cinnamoyl):* [154992-25-3] ***Avenanthramide 2***
$C_{18}H_{17}NO_7$ 359.335
Constit. of *Avena sativa* (oat).

5-Me ether: [63407-32-9] *2-Amino-4-hydroxy-5-methoxybenzoic acid*
$C_8H_9NO_4$ 183.163
Mp 169-170°.

5-Me ether, Me ester: [848092-84-2]
$C_9H_{11}NO_4$ 197.19
Mp 148-149°.

Di-Me ether: [5653-40-7] *2-Amino-4,5-dimethoxybenzoic acid. 6-Aminoveratric acid*
$C_9H_{11}NO_4$ 197.19
Needles (EtOAc). Mp 186° (rapid heating).

Di-Me ether, Me ester: [26759-46-6] *Methyl 6-aminoveratrate*
$C_{10}H_{13}NO_4$ 211.217
Plates (C_6H_6) or cryst. (MeOH). Mp 133° (130°). Also named methyl 2-aminoveratrate in lit.

Di-Me ether, Et ester: [20323-74-4] *Ethyl 6-aminoveratrate*
$C_{11}H_{15}NO_4$ 225.244
Cryst. (petrol). Mp 88°.

Di-Me ether, amide: [5004-88-6] *2-Amino-4,5-dimethoxybenzamide*
$C_9H_{12}N_2O_3$ 196.205
Mp 127-128°.

Di-Me ether, anilide: [116241-64-6] *2-Amino-4,5-dimethoxy-*N*-phenylbenzamide*

$C_{15}H_{16}N_2O_3$ 272.303
Mp 158-160°.

Di-Me ether, nitrile: [26961-27-3] *2-Cyano-4,5-dimethoxyaniline. 6-Aminoveratronitrile*
$C_9H_{10}N_2O_2$ 178.19
Cryst. (MeOH). Mp 99-100°.

Di-Et ether: [20197-72-2]
$C_{11}H_{15}NO_4$ 225.244
Powder. Mp 120-126°.

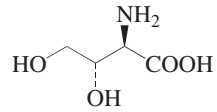
Di-Et ether, Et ester: [460750-27-0]
$C_{13}H_{19}NO_4$ 253.297
Solid. Mp 69-71°.

4-Benzyl ether, 5-Me ether:
$C_{15}H_{15}NO_4$ 273.288
Yellow solid. Mp 159-161°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 233A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1150B; 1541A (*nmr*)
Zincke, T. *et al., Annalen*, 1896, **293**, 175-193 (*di-Me ether Me ester, synth*)
Fetscher, C.A. *et al., JOC*, 1939, **4**, 71-87 (*di-Me ether, di-Me ether Et ester, synth*)
McKee, R.L. *et al., JACS*, 1946, **68**, 1902-1903 (*di-Me ether nitrile, synth*)
Wilson, C.V. *et al., JACS*, 1948, **70**, 1901-1903 (*di-Me ether nitrile, synth*)
Heacock, R.A. *et al., JCS*, 1963, 3574-3578 (*di-Me ether Et ester, synth*)
Carpenter, P.D. *et al., JCS Perkin 1*, 1979, 103 (*di-Me ether Me ester, synth, ir, pmr*)
Bandyopadhyay, C. *et al., J. Agric. Food Chem.*, 1990, **38**, 1696-1699 (*N-Et amide*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramide 2*)
Alvi, K.A. *et al., J. Antibiot.*, 1997, **50**, 264-266 (*isol*)
Hu, W.-P. *et al., JOC*, 2001, **66**, 2881-2883 (*4-benzyl-5-Me ether, pmr, cmr*)
Wright, S.W. *et al., J. Med. Chem.*, 2002, **45**, 3865-3877 (*di-Et ether Et ester, synth, pmr*)
Kumaraswamy, G. *et al., Org. Prep. Proced. Int.*, 2004, **36**, 341-345 (*di-Me ether Me ester, synth, pmr*)
VanBrocklin, H.F. *et al., J. Med. Chem.*, 2005, **48**, 7445-7456 (*di-Et ether*)
Wéber, C. *et al., Tetrahedron*, 2005, **61**, 9375-9380 (*4-Me ether*)
Sarojini, B.K. *et al., Acta Cryst. E*, 2007, **63**, o4553 (*di-Me ether nitrile, cryst struct*)
Stroganova, T.A. *et al., Synthesis*, 2008, 3088-3098 (*di-Me ether amide, di-Me ether anilide*)
Shankaraiah, N. *et al., Synthesis*, 2009, 2163-2170 (*5-Me ether, 5-Me ether Me ester*)

2-Amino-3,4-dihydroxybutanoic acid A-385

4-Hydroxythreonine [104111-37-7]



(2*R*,3*R*)-*form*

$C_4H_9NO_4$ 135.119

The stereoisomers can be named as 4-hydroxythreonines or 4-hydroxyallothreonines, but a change of Cahn-Ingold-Prelog priorities can lead to confusion.

(2*R*,3*R*)-*form* [21768-44-5]
(+)-threo-*form*
Isol. from the mushroom *Lyophyllum ulmarium*. Mp 214-215° (194°). $[\alpha]_D^{23}$ +13.6 (c, 4.8 in H_2O).

Lactone: [21768-48-9]
$C_4H_7NO_3$ 117.104
Cryst. (as hydrochloride). Mp 176.5° (hydrochloride). $[\alpha]_D^{23}$ -56.6 (c, 1.5 in H_2O).

4-Et ether: [98644-37-2] *2-Amino-4-ethoxy-3-hydroxybutanoic acid*
$C_6H_{13}NO_4$ 163.173
Isol. from the mushroom *Lyophyllum ulmarium*.

(2*R*,3*S*)-*form* [21768-46-7]
(-)-erythro-*form*
Mp 194-195° dec. $[\alpha]_D^{23}$ +11.3 (c, 1.5 in H_2O).

Lactone: Mp 176° dec. (as hydrochloride). $[\alpha]_D^{23}$ +55.6 (c, 1.5 in H_2O).

(2*S*,3*S*)-*form* [21768-43-4]
(-)-threo-*form*
Needles (EtOH aq.). Sol. EtOH; fairly sol. H_2O; poorly sol. butanol, hexane. Mp 210° dec. (194-195°). $[\alpha]_D^{25}$ -13.3 (c, 1 in H_2O).

Lactone: Mp 173-174° dec. (as hydrochloride). $[\alpha]_D^{23}$ -26.2 (c, 1 in H_2O).

Niemann, C. *et al., J. Biol. Chem.*, 1942, **143**, 191-202 (*synth*)
Hamel, E.E. *et al., JACS*, 1953, **75**, 1362-1368 (*config*)
Okawa, K. *et al., Bull. Chem. Soc. Jpn.*, 1969, **42**, 2720-2722 (*resoln*)
Westley, J.W. *et al., J. Antibiot.*, 1971, **24**, 330-331 (*isol*)
Katz, E. *et al., J. Antibiot.*, 1974, **27**, 952-955 (*isol*)
Ogawa, T. *et al., Phytochemistry*, 1984, **23**, 684-686; 1985, **24**, 1837-1838 (*isol*)
Pirrung, M.C. *et al., Bioorg. Med. Chem. Lett.*, 1993, **3**, 2095-2098 (*synth, abs config*)
Cativiela, C. *et al., Tetrahedron*, 1996, **52**, 9563-9574 (*synth*)
Fadnavis, N.W. *et al., Tetrahedron: Asymmetry*, 2001, **12**, 691-693 (*2S,3S-form, synth*)
Swift, M.D. *et al., Tet. Lett.*, 2007, **48**, 3771-3773 (*2R,3S-form, synth*)

2-Amino-3,4-dihydroxypentanedioic acid A-386

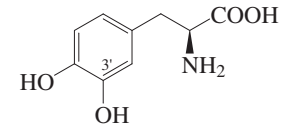
3,4-Dihydroxyglutamic acid
HOOCCH(OH)CH(OH)CH(NH_2)-COOH

$C_5H_9NO_6$ 179.129
Isol. from *Lepidium sativum* (garden cress) and *Rheum rhaponticum* (rhubarb). The (2*S*,3*S*,4*R*)- and (2*S*,3*S*,4*S*)-stereoisomers have been synthesised, but the abs. config. of the natural product is currently (2001) unknown.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1957, **11**, 182 (*isol*)
Mueller, A.L. *et al., Acta Chem. Scand.*, 1965, **19**, 1987 (*isol*)
Dauban, P. *et al., Tetrahedron*, 1999, **55**, 7589-7600 (*synth*)
Oba, M. *et al., Tet. Lett.*, 2001, **42**, 5901-5902 (*synth*)
Kim, H. *et al., Tetrahedron: Asymmetry*, 2008, **19**, 1965-1969 (*synth*)

2-Amino-3-(3,4-dihydroxyphenyl)propanoic acid A-387

3-Hydroxytyrosine, 9CI. 3,4-Dihydroxyphenylalanine. DOPA [587-45-1]



(*S*)-*form*

$C_9H_{11}NO_4$ 197.19
Log P -2.82 (uncertain value) (calc).

(*S*)-*form* [59-92-7]
L-form. ***Levodopa, BAN, INN, JAN, USAN***. *Bendopa. Brocadopa. Dopar. Larodopa. Levopa. Veldopa. Many other names*
Occurs in seedlings and pods of *Vicia faba*. Prisms, needles (H_2O + SO_2) or plates (EtOH aq.). Mp 285.5° dec. $[\alpha]_D^{20}$ -12.15 (c, 4 in 1*N* HCl). Pharmacol. active isomer. Rapidly turns green in air, aq. solns. darken in air. Green col. with $FeCl_3$. Reduces $AgNO_3$, NH_3 and acid $KMnO_4$. Component of Sinemet. High-mol.-wt. polymers have been synth.

▶ Systemic (e.g. CNS) and adverse effects when used therapeutically. LD_{50} (rat, orl) 1780 mg/kg. Exp. reprod. and teratogenic effects. AY5600000

3'-O-β-D-Glucopyranoside: [2275-95-8]
$C_{15}H_{21}NO_9$ 359.332
Isol. from *Pisum sativum* (peas) and *Vicia faba*. Resin or syrup.

N-*(4-Hydroxy-*E*-cinnamoyl):* [77201-64-0] **N-trans-p-*Coumaroyl-DOPA***
$C_{18}H_{17}NO_6$ 343.335
Constit. of roasted cocoa beans. $[\alpha]_D^{20}$ -24.2 (c, 1 in MeOH).

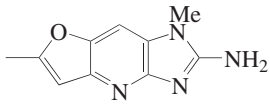
N-*Jasmonoyl:* [866421-54-7] **N-*Jasmonoyl DOPA***
$C_{21}H_{27}NO_6$ 389.447
Constit. of the flowers of *Vicia faba* (broad bean). For Jasmonoyl struct. see Jasmonic acid, J-9.

[127441-81-0 (*S*-form, potassium salt), 57308-51-7 (*S*-form, with (α,*S*)-α-hydrazinyl-3,4-dihydroxy-α-methylbenzenepropanoic acid)]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 257A; 257B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1190A; 1190B (*nmr*)
Andrews, R.S. *et al., Nature (London)*, 1965, **205**, 1213-1214 (*glucoside, struct*)
Vorbruggen, H. *et al., Chem. Ber.*, 1972, **105**, 1168-1173 (*L-DOPA, synth*)
Griffith, T. *et al., Phytochemistry*, 1973, **12**, 1651-1656 (*DOPA, biosynth*)
Mostad, A. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 1161-1168 (*L-DOPA hydrochloride, cryst struct*)
Renth, E.-O. *et al., Angew. Chem., Int. Ed.*, 1975, **14**, 361-363 (*L-DOPA, synth*)
Bartholini, G. *et al., Pharmacol. Ther., Part B*, 1975, **1**, 407-421 (*L-DOPA, rev, pharmacol*)
Gomez, R. *et al., Anal. Profiles Drug Subst.*, 1976, **5**, 189-223 (*L-DOPA, rev*)
Dardenne, G. *et al., Phytochemistry*, 1977, **16**, 1822-1824 (*Cortinarius brunneus constits*)
Danishevsky, S. *et al., Tetrahedron*, 1981, **37**, 4081-4086 (*L-DOPA, synth*)

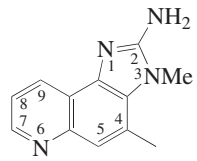
Nutt, J.G. *et al., Clin. Neuropharmacol.*, 1984, **7**, 35-49 (*L-DOPA, rev, metab*)
Kramell, R. *et al., J. Nat. Prod.*, 2005, **68**, 1345-1349 (*N-jasmonoyl, struct*)
Stark, T. *et al., J. Agric. Food Chem.*, 2006, **54**, 2859-2867 (*N-4-hydroxycinnamoyl, isol*)

2-Amino-1,6-dimethylfuro[3,2-*e*]imidazo[4,5-*b*]pyridine A-388
*1,6-Dimethyl-1*H-*furo[2,3-*b*]imidazo[4,5-*e*]pyridin-2-amine, 9CI. IFP* [132898-08-9]



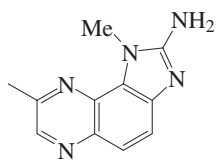
$C_{10}H_{10}N_4O$ 202.215
Isolated from cooked meats.
▶ Mutagenic.
Pais, P. *et al., J. Agric. Food Chem.*, 2000, **48**, 1721-1726 (*isol, struct*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*detn, occur*)

2-Amino-3,4-dimethylimidazo[4,5-*f*]quinoline A-389
Me-IQ [77094-11-2]



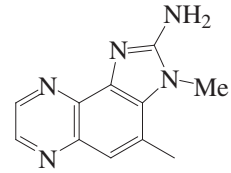
$C_{12}H_{12}N_4$ 212.254
Isol. from sardines and cooked meats. Mp 296-298° (sealed tube). λ_{max} 219; 265; 332 (no solvent reported).
▶ Highly mutagenic. Exp. carcinogenic data. Possible human carcinogen (IARC 2B). NJ5907000
Kasai, H. *et al., Chem. Lett.*, 1980, 1391 (*struct, bibl*)
Kasai, H. *et al., Bull. Chem. Soc. Jpn.*, 1982, **55**, 2233
Adolfsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 157 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*carcinogenicity*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*detn, occur*)
IARC Monogr. (Web), http://monographs.iarc.fr
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJQ600

2-Amino-1,8-dimethyl-1*H*-imidazo[4,5-*f*]quinoxaline A-390
*1,8-Dimethyl-1*H-*imidazo[4,5-*f*]quinoxalin-2-amine, 9CI. 1-Iso-8-MeIQx* [754203-16-2]



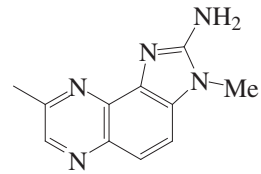
$C_{11}H_{11}N_5$ 213.241
Constit. of grilled/fried meats. No phys. props. reported.
Holland, R.D. *et al., Chem. Res. Toxicol.*, 2004, **17**, 1121-1136 (*synth, detn, pmr*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*occur*)

2-Amino-3,4-dimethyl-3*H*-imidazo[4,5-*f*]quinoxaline A-391
*3,4-Dimethyl-3*H-*imidazo[4,5-*f*]quinoxalin-2-amine. 4-MeIQx* [108354-48-9]



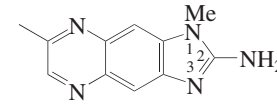
$C_{11}H_{11}N_5$ 213.241
Constit. of grilled/fried meats. Mp >300°.
▶ Weakly mutagenic.
Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521-528 (*synth, pmr, ms*)
Wyss, M. *et al., Physiol. Rev.*, 2000, **80**, 1107-1213 (*biol, rev*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*occur*)

2-Amino-3,8-dimethyl-3*H*-imidazo[4,5-*f*]quinoxaline A-392
*3,8-Dimethyl-3*H-*imidazo[4,5-*f*]quinoxalin-2-amine, 9CI. 8-MeIQx* [77500-04-0]



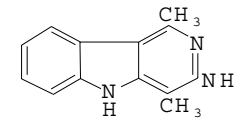
$C_{11}H_{11}N_5$ 213.241
Food-related mutagen isol. from cooked meats (esp. grilled/barbecued). Cryst. (Py). Mp 295-300° (sealed tube).
▶ Highly mutagenic. Exp. carcinogenic data. Possible human carcinogen (IARC 2B). NJ5925500
Kasai, H. *et al., Chem. Lett.*, 1981, 675 (*synth*)
Knapp, S. *et al., Tetrahedron*, 1989, **45**, 1293 (*synth*)
Grivas, S. *et al., Acta Chem. Scand.*, 1993, **43**, 521 (*synth, pmr, ms*)
Knize, M.G. *et al., J. Agric. Food Chem.*, 1998, **46**, 4648-4651 (*hplc*)
De Meester, C. *et al., Z. Lebensm.-Unters.-Forsch.*, 1998, **207**, 441-447 (*hplc*)
Fukushima, S. *et al., Cancer Lett.*, 1999, **143**, 157-159 (*tox*)
Schut, H.A. *et al., Carcinogenesis (London)*, 1999, **20**, 353-368 (*rev*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 68-78 (*occur, ms, hplc*)
IARC Monogr. (Web), http://monographs.iarc.fr
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJQ675

2-Amino-1,7-dimethyl-1*H*-imidazo[4,5-*g*]quinoxaline A-393
*1,7-Dimethyl-1*H-*imidazo[4,5-*g*]quinoxalin-2-amine, 9CI. 7-MeIgQx* [934333-16-1]



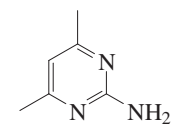
$C_{11}H_{11}N_5$ 213.241
One of the most abundant heterocyclic aromatic amines (HAAs) present in cooked meats esp. roasted/fried beef, pork and chicken.
Turesky, R.J. *et al., Chem. Res. Toxicol.*, 2007, **20**, 520-530 (*synth, detn, pmr, cmr, ms, biol*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*detn, ms*)

3-Amino-1,4-dimethyl-5*H*-pyrido[4,3-*b*]indole A-394
*1,4-Dimethyl-5*H-*pyrido[4,3-*b*]indol-3-amine, 9CI. 3-Amino-1,4-dimethyl-γ-carboline. Trp-P1* [62450-06-0]
[68808-54-8]



$C_{13}H_{13}N_3$ 211.266
Powerful mutacarcinogen found in cooked foods. Pale-brown needles or small prisms (EtOAc)(as acetate salt). Mp 252-262° (acetate salt).
▶ Highly mutagenic. Possible human carcinogen. LD_{50} (rat, orl) 100 mg/kg. Exp. carcinogen. UU9351900
Kosuge, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 611 (*isol, cryst struct, spectra*)
IARC Monogr., 1983, **31**, 247; 1987, *Suppl. 7*, 73 (*rev, tox*)
Akimoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 123 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 977 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AJR500; TNX275

2-Amino-4,6-dimethylpyrimidine A-395
4,6-Dimethyl-2-pyrimidinamine, 9CI [767-15-7]



$C_6H_9N_3$ 123.157
Cryst. (H_2O). Mod. sol. H_2O, EtOH; insol. Et_2O. Mp 153° (149-150°). Distils undec.
2-N-Ac: [15755-12-1]

$C_8H_{11}N_3O$ 165.194
Mp 124°.

2-N-*Me:* [15231-64-8]
$C_7H_{11}N_3$ 137.184
Cryst. (petrol). Mp 98°.

2-N-*Benzyl:* [106270-42-2]
$C_{13}H_{15}N_3$ 213.282
Cryst. Mp 110-112°.

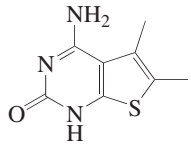
2-N-*Ph:* [53112-28-0] *2-Anilino-4,6-dimethylpyrimidine.* ***Pyrimethanil, BSI****. Mythos. Scala. SN 100309. ZK 100309*
$C_{12}H_{13}N_3$ 199.255
Fungicide used on grape vines. Cryst. (toluene). Mp 88-89°.

▶ LD_{50} (rat, orl) 4150-5971 mg/kg.

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 701D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 822D (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1555A (*ir*)
Hale, W.J. *et al., JACS*, 1918, **40**, 1046 (*synth*)
Short, L.N. *et al., JCS*, 1952, 168 (*ir*)
Alberola, A. *et al., Synth. Commun.*, 1987, **17**, 1309 (*synth*)
Neumann, G.L. *et al., Brighton Crop Prot. Conf. - Pests Dis.*, 1992, **1**, 395-402 (*pyrimethanil*)
Cobras, P. *et al., J. Agric. Food Chem.*, 1997, **45**, 2708-2710 (*pyrimethanil, detn*)
Pesticide Manual, 12th edn., 2000, No. 674 (*Pyrimethanil*)
Hemamalini, M. *et al., Acta Cryst. C*, 2005, **61**, o95-o97 (*cryst struct*)
Goswami, S. *et al., Bull. Chem. Soc. Jpn.*, 2009, **82**, 1175-1181 (*2-N-benzyl, 2-N-Ph*)

4-Amino-5,6-dimethylthieno[2,3-*d*]pyrimidin-2(1*H*)-one A-396

FEMA 4669 [121746-18-7]
[1033366-59-4 (hydrochloride)]

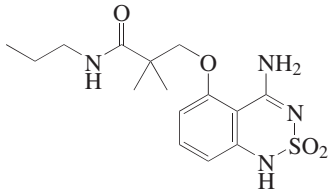


$C_8H_9N_3OS$ 195.245
Sweetness enhancer, esp. for foodstuffs contg. Sucralose, S-378. Solid.

Pat. Coop. Treaty (WIPO), 2009, 2009 100 333 (*FEMA 4669, synth, use*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4669, use*)

3-[(4-Amino-2,2-dioxido-1*H*-benzo[*c*][1,2,6]thiadiazin-5-yl)oxy]-2,2-dimethyl-*N*-propylpropanamide A-397

ADBT. FEMA 4701 [1093200-92-0]

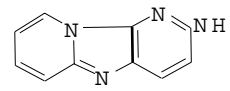


$C_{15}H_{22}N_4O_4S$ 354.429
Sweetness enhancer, esp. for Sucralose, S-378. Oil.

Pat. Coop. Treaty (WIPO), 2008, 2008 154 221 (*FEMA 4701, synth, props, use*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*FEMA 4701, use*)

2-Aminodipyrido[1,2-*a*:3′,2′-*d*]imidazole A-398

Dipyrido[1,2-a:3′,2′-d]imidazol-2-amine, 9CI. Glu-P-2 [67730-10-3]



$C_{10}H_8N_4$ 184.2
Parent compd. of a group of potent mutagens found in cooked foods.

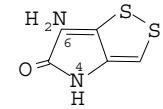
▶ Possible human carcinogen. Exp. carcinogen. Mutagen. JM5615000

Hydrobromide: Mp 286-287°.

Takeda, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2924 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
IARC Monogr., 1986, **40**, 235; 1987, *Suppl. 7*, 64 (*rev, tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 997 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DWW700

6-Amino-1,2-dithiolo[4,3-*b*]pyrrol-5(4*H*)-one, 9CI A-399

Holothin [488-03-9]



$C_5H_4N_2OS_2$ 172.231
Greenish-black cryst. (as hydrochloride). Mp 300° (hydrochloride).

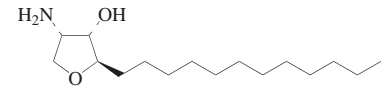
4-Me, N^6*-Ac:* [87-11-6] N-*Acetylpyrrothine.* ***Thiolutin****. Farcinicine*†*. Acetopyrrothine*
$C_8H_8N_2O_2S_2$ 228.295
Isol. from several strains of *Streptomyces albus* and *Streptomyces pimprina*. Antibiotic which inhibits microbiological growth in beer. Brilliant yellow needles (1-butanol). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, C_6H_6, Et_2O, hexane. Mp 273-276° dec. $Bp_{0.1}$ 200° subl. λ_{max} 248 (ε 6300); 311 (ε 5700); 388 (ε 10800) (MeOH) (Derep). λ_{max} 250 (ε 6030); 311 (ε 5600); 388 (ε 10960) (MeOH) (Berdy).

▶ LD_{50} (mus, scu) 25 mg/kg. JP1355000

Celmer, W.D. *et al., JACS*, 1952, **74**, 6304-6305; 1955, **77**, 2861-2865 (*Pyrrothine, Aureothricin, Thiolutin*)
Hagio, K. *et al., Bull. Chem. Soc. Jpn.*, 1974, **47**, 1484 (*Holothin, Thiolutin, Aureothricin, synth, ir, uv, pmr*)
Ninomiya, Y.T. *et al., Chem. Pharm. Bull.*, 1980, **28**, 3157-3162 (*Pyrrothine, Thiolutin, props, ms*)
Deb, P.R. *et al., Curr. Sci.*, 1984, **53**, 659 (*Thiolutin, props*)
Lamari, L. *et al., J. Antibiot.*, 2002, **55**, 696-701; 702-706 (*Saccharothrix SA 233 pyrrothines*)

4-Amino-2-dodecyltetrahydro-3-furanol A-400

4-Amino-2-dodecyl-3-hydroxytetrahydrofuran



$C_{16}H_{33}NO_2$ 271.442

(2R*,3S*,4S*)-form

N-*(2*R*-Hydroxyheptadecanoyl):*
[1067910-08-0] ***Suillumide***
$C_{33}H_{65}NO_4$ 539.881
Isol. from *Suillus luteus* (slippery jack). Amorph. solid. $[\alpha]_D^{25}$ +16.3 (c, 0.1 in $CHCl_3$).

León, F. *et al., Chem. Biodiversity*, 2008, **5**, 120-125 (*isol, pmr, cmr, ms*)

2-Aminoethanesulfonic acid, 9CI A-401

Taurine, 8CI, INN*. Aminoethylsulfonic acid. Ethylaminesulfonic acid. FEMA 3813* [107-35-7]

$H_2NCH_2CH_2SO_3H$
$C_2H_7NO_3S$ 125.148
Essential nutrient obt. from diet and by *in vivo* synth. from methionine and cysteine. Present in meats, fish, legumes, human milk, molluscs and other foodstuffs. Dietary supplement, e.g. in energy drinks. Monoclinic prismatic rods with sharp taste. Sol. H_2O; insol. EtOH. Mp 328° (320-325° dec.). pK_{a1} 1.5; pK_{a2} 8.74. Dec. at 300°.

▶ LD_{50} (mus, scu) 6000 mg/kg. WX0175000

Amide: [4378-70-5]
$C_2H_8N_2O_2S$ 124.163
Plates (EtOH) (as hydrochloride). Mp 133° (hydrochloride).

N-*Hexadecanoyl:* **N-*Hexadecanoyltaurine***
$C_{18}H_{37}NO_4S$ 363.561
Cryst. Mp 296.5-299°.

N-*(15-Methyl-9Z-hexadecenoyl):*
[679834-30-1] **N-*(15-Methyl-9-hexadecenoyl)taurine***
$C_{19}H_{37}NO_4S$ 375.572
Amorph. powder.

N-*(5Z,8Z,11Z,14Z-Eicosatetraenoyl):*
[679834-28-7] **N-*(5,8,11,14-Eicosatetraenoyl)taurine***
$C_{22}H_{37}NO_4S$ 411.605
Amorph. powder.

N-*(5*R*,15*S*-Dihydroxyeicosanoyl):*
[1290125-89-1] **N-*(5,15-Dihydroxyeicosanoyl)taurine***
$C_{22}H_{45}NO_6S$ 451.667
Powder.

N-*Phenylacetyl:* [33953-90-1] **N-*Phenylacetyltaurine***
$C_{10}H_{13}NO_4S$ 243.283
Oil.

N-*Me:* [107-68-6] **N-*Methyltaurine***
$C_3H_9NO_3S$ 139.175
Prisms. V. sol. H_2O; insol. EtOH, Et_2O. Mp 241-242°.

N,N-*Di-Me:* [637-95-6] **N-*Dimethyltaurine***
$C_4H_{11}NO_3S$ 153.202
Prisms (MeOH). V. sol. H_2O, AcOH; insol. EtOH, Et_2O. Mp 315-316° dec.

N,N-*Bis(2-chloroethyl):* [98277-87-3] *Taumustine*
$C_6H_{13}Cl_2NO_3S$ 250.145
Cryst. (H_2O). Mp 178-180°.

N-*(2,3-Dihydroxypropyl):* [65222-42-6] **N-*Glyceryltaurine***
$C_5H_{13}NO_5S$ 199.227
Cryst. (EtOH aq.). Mp 163-164°. $[\alpha]_D^{23}$ -21 (H_2O).

[4316-74-9, 7347-25-3]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 890A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1433C (*nmr*)
Org. Synth., Coll. Vol., 2, 1943, 563; 564 (*synth*)
Ishidate, M. *et al., Chem. Pharm. Bull.*, 1954, **2**, 275-279 (*synth*)
Lindberg, B. *et al., Acta Chem. Scand.*, 1955, **9**, 1093-1096; 1323-1326 (*isol, N-Me, N,N-di-Me*)
Wickberg, B. *et al., Acta Chem. Scand.*, 1956, **10**, 1097-1099 (*Glyceryltaurine*)
Sutherland, H.H. *et al., Acta Cryst.*, 1963, **16**, 897-901 (*cryst struct*)
Huxtable, R. *et al., Taurine, [Int. Symp.], 1st, 1975 (1976)*, (Eds.), Raven Press, New York, 1975, (*book*)
Utkina, N.K. *et al., Khim. Prir. Soedin.*, 1984, 124-125; *Chem. Nat. Compd. (Engl. Transl.)*, 1984, **20**, 126-127 (*N-Me, occur*)
Hashem, K.M.E. *et al., Bull. Soc. Chim. Belg.*, 1985, **94**, 735-754 (*cmr*)
Taurine: Nutritional Value and Mechanisms of Action, (eds. Lombardini, J.B. *et al*), Plenum Press, 1992, (*book*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1419
Fenaroli's Handbook of Flavor Ingredients, 4th edn., (ed. Burdock, G.A.), CRC Press, 2001, 1665-1666 (*use, occur*)
Merck Index, 13th edn., 2001, No. 9163 (*bibl*)
Hibbs, D.E. *et al., Chem. Eur. J.*, 2003, **9**, 1075-1084 (*cryst struct*)
Wang, W. *et al., Nat. Prod. Sci.*, 2003, **9**, 241-244 (*N-acyl marine constits*)
Wang, B. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2009, **45**, 137-138 (*N-Hexadecanoyltaurine*)
Wright, A.D. *et al., Mar. Drugs*, 2009, **7**, 565-575 (*N-Phenylacetyltaurine*)
Zhou, X. *et al., Biosci., Biotechnol., Biochem.*, 2010, **74**, 1089-1091 (*5,15-dihydroxyeicosanoyl*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TAG750

2-Aminoethanol, 9CI A-402

2-Hydroxyethylamine. Ethanolamine. Monoethanolamine. Colamine. Olamine [141-43-5]

$H_2NCH_2CH_2OH$
C_2H_7NO 61.083
Used in flume water for washing sugar beets prior to the slicing operation. Viscous, hygroscopic liq. Misc. H_2O, MeOH, Me_2CO; spar. sol. C_6H_6, Et_2O. d_4^{25} 1.01. Mp 10.5°. Bp 171°. n_D^{20} 1.4539. pK_a 9.47. Vp 0.48 mmHg (20°).

▶ Fl. p. 85°, autoignition temp. 410°. Corrosive and irritating to skin, eyes and mucous membranes. LD_{50} (rat, orl) 1720 mg/kg. Exp. teratogen. OES: long-term 3 ppm; short-term 6 ppm. KJ5775000

O-*Ac:* [1854-30-4] **O-*Acetylethanolamine***. *2-Acetoxyethylamine*
$C_4H_9NO_2$ 103.121
Isol. from seeds of *Lens culinaris* (lentil), also present in other Leguminosae. $Bp_{0.3}$ 134-135°.

N-*(9Z,12Z,15Z-Octadecatrienoyl):* [57086-93-8] N-*(2-Hydroxyethyl)-9,12,15-octadecatrienamide*. N-*(2-Hydroxyethyl)linolenamide*
$C_{20}H_{35}NO_2$ 321.502
Constit. of the pollen of *Brassica campestris* var. *oleracea* (oil-seed rape) and *Linum catharticum* (flax-seed oil). λ_{max} 208 (log ε 3.68) (MeOH).

N-*(5Z,8Z,11Z,14Z,17Z-Eicosapentaenoyl):* N-*(2-Hydroxyethyl)-5,8,11,14,17-eicosapentaenamide*
$C_{22}H_{35}NO_2$ 345.524
Constit. of *Linum catharticum* (flax-seed oil). λ_{max} 211 (log ε 3.87) (MeOH).

N-*(4Z,7Z,10Z,13Z,16Z,19Z-Docosahexaenoyl):* N-*(2-Hydroxyethyl)-4,7,10,13,16,19-docosahexaenamide*
$C_{24}H_{37}NO_2$ 371.562
Constit. of *Linum catharticum* (flax-seed oil). λ_{max} 215 (log ε 3.91) (MeOH).

N,N-*Di-Et:* [100-37-8] *2-Diethylaminoethanol, 9CI. 2-Hydroxytriethylamine. Pennad 150*
$C_6H_{15}NO$ 117.191
Boiler water additive. Sol. H_2O. Bp 163° Bp_{35} 75°.

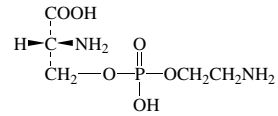
▶ Skin and severe eye irritant. Adverse gastrointestinal effects by inhalation. LD_{50} (rat, orl) 1300 mg/kg. LD_{50} (gpg, skn) 884 mg/kg. OES: long-term 10 ppm (Sk). KK5075000

[20739-39-3, 96-80-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 334A; 334B; 339D; 340A; 340C; 756B; 904B; 1280A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 535B; 543A; 543B; 544A; 545B; 545C; **2**, 457B; 591A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 423D; 430A; 430B; 430D; 432B; 1112C (*ir*)
Putokhin, N. *et al., CA*, 1929, **23**, 2938 (*synth*)
Sarneski, J.E. *et al., Anal. Chem.*, 1975, **47**, 2116-2124 (*cmr*)
Voronkov, M.G. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1978, **48**, 384-387 (*ms*)
Hayman, A.R. *et al., Phytochemistry*, 1987, **26**, 839-841 (*O-Acetylethanolamine*)
Van Oycke, S. *et al., Bull. Soc. Chim. Belg.*, 1988, **97**, 297-311 (*isol*)
Mootz, D. *et al., Acta Cryst. C*, 1989, **45**, 754-757 (*cryst struct*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1703
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 813; 1904-1905
Liu, J. *et al., JOC*, 2001, 5655-5663 (*OAc, synth, pmr*)
Karaulov, A.E. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2004, **40**, 222-226 (*Linum catharticum amides*)
Yang, N.-Y. *et al., J. Asian Nat. Prod. Res.*, 2009, **11**, 132-137 (*N-(2-Hydroxyethyl)linolenamide*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 0889
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 447; 578
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BQC000; DNP000; MGG000; HKM000; INN400; DHO500; EGA500; DDU600; EEC600

2-Aminoethyl seryl phosphate A-403

Serine ethanolamine phosphodiester. SEP [18635-48-8, 17871-37-3]



(*R*)-*form*

$C_5H_{13}N_2O_6P$ 228.141

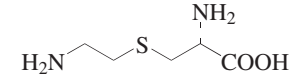
(*R*)-*form* [16106-04-0]
D-form
Cryst. (MeOH aq.). Mp 143-144° (dec.). $[\alpha]_D^{23}$ +18.2 (c, 0.7 in H_2O).

(*S*)-*form* [1186-34-1]
L-form
Isol. from numerous animals incl. chicken, fish and reptiles. Needles (MeOH aq.). Mp 142-143° (dec.). $[\alpha]_D^{23}$ -15 (c, 2 in H_2O).

(±)-*form* [114760-94-0]
Prisms (EtOH aq.). Mp 193-194° (dec.).
Ennor, A.H. *et al., J. Biochem. (Tokyo)*, 1960, **75**, 179-182
Beatty, I.M. *et al., JACS*, 1960, **82**, 4983-4989 (*synth*)
Rosenberg, H. *et al., J. Biochem. (Tokyo)*, 1961, **50**, 81-84 (*occur, biosynth*)
Allen, A.K. *et al., Biochim. Biophys. Acta*, 1968, **151**, 504-519; **152**, 208-210 (*biosynth*)
Euerby, M.R. *et al., J. Chem. Res., Synop.*, 1988, 394-395 (*synth, pmr, cmr, ms*)
Merchant, T.E. *et al., J. Lipid Res.*, 1990, **31**, 479-486 (*P-31 nmr*)

S-(2-Aminoethyl)cysteine, 9CI A-404

3-[(2-Aminoethyl)thio]alanine, 8CI. Thialysine. Thiosine [617-71-0]

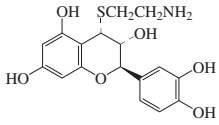


$C_5H_{12}N_2O_2S$ 164.228

(*R*)-*form* [2936-69-8]
L-form
Isol. from the edible mushroom *Rozites caperta*. Sol. H_2O; fairly sol. MeOH; poorly sol. Me_2CO, hexane.

► LD_{50} (mus, ipr) 300 mg/kg.
Matsumoto, N. *et al., CA*, 1985, **103**, 3724 (*isol*)

4-(2-Aminoethylthio)-3,3′,4′,5,7-pentahydroxyflavan A-405



(2*R*,3*R*,4*S*)-*form*

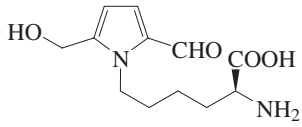
$C_{17}H_{19}NO_6S$ 365.406

(2*R*,3*R*,4*S*)-*form*
4β-(2-Aminoethylthio)catechin
Constit. of *Vitis vinifera* (wine grape).

(2*R*,3*S*,4*S*)-*form*
4β-(2-Aminoethylthio)epicatechin
Constit. of *Vitis vinifera* (wine grape).
3-O-*(3,4,5-Trihydroxybenzoyl):*
$C_{24}H_{23}NO_{10}S$ 517.512
Constit. of *Vitis vinifera* (wine grape).
Torres, J.L. *et al., J. Agric. Food Chem.*, 2001, **49**, 4627-4634

α-Amino-2-formyl-5-(hydroxymethyl)-1*H*-pyrrole-1-hexanoic acid, 9CI A-406

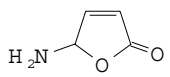
2-Formyl-5-(hydroxymethyl)pyrrole-1-norleucine. Lysylpyrroaldehyde. ϵ-Pyrrolelysine (incorr.) [126255-18-3]



$C_{12}H_{18}N_2O_4$ 254.285

(*S*)-*form* [74509-14-1]
Pyrraline
Maillard prod. Syrup.
► Mutagenic props.
Nakayama, T. *et al., Agric. Biol. Chem.*, 1980, **44**, 1201-1202 (*synth, uv, ms, pmr, cmr*)
Miller, R. *et al., Acta Chem. Scand., Ser. B*, 1984, **38**, 689-694; 1985, **39**, 717-723 (*synth, pmr, cmr*)
Schloesser, U. *et al., Z. Lebensm.-Unters. -Forsch.*, 1989, **189**, 138-140 (*synth*)
Henle, T. *et al., Z. Lebensm.-Unters. -Forsch.*, 1996, **202**, 72-74 (*synth, bibl*)

5-Amino-2(5*H*)-furanone A-407

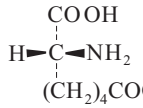


$C_4H_5NO_2$ 99.089
Parent compd. not known.

(±)-*form*
N-*Ac:* [16275-44-8] N-*(2,5-Dihydro-5-oxo-2-furanyl)acetamide, 9CI. 4-Acetamido-4-hydroxy-2-butenoic acid γ-lactone. 4-Acetamido-2-buten-4-olide*
$C_6H_7NO_3$ 141.126
Cryst. (EtOAc/cyclohexane).
Mp 116.5-118.5°.
► LU3455000
Yates, S.G. *et al., Tet. Lett.*, 1967, **8**, 621-625 (*N-Ac, isol, struct*)
Ružic-Toroš, Z. *et al., Acta Cryst. B*, 1982, **38**, 1664 (*cryst struct*)
Valla, A. *et al., Bull. Soc. Chim. Fr.*, 1997, **134**, 601-603 (*synth, pmr*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 898

2-Aminoheptanedioic acid, 8CI A-408

α-Aminopimelic acid [3721-85-5]



(*R*)–*form*

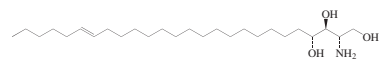
$C_7H_{13}NO_4$ 175.184
Isol. from *Ceratonia siliqua* (carob).

(*R*)-*form* [32224-57-0]
D-form
Cryst. (EtOH). Mp 219-220° dec. $[\alpha]_D^{25}$ -21 (c, 0.1 in 5*M* HCl). $[\alpha]_D^{26}$ -45.5 (c, 0.1 in 1*M* HCl). Rare occurrence of a D-aminoacid in higher plants. Forms a monohydrate.

(*S*)-*form* [26630-55-7]
L-form
Microcryst. Mp 204°. $[\alpha]_D^{25}$ +21.6 (c, 0.1 in 5*M* HCl). $[\alpha]_D^{26}$ +45 (c, 0.1 in 1*M* HCl). Forms a monohydrate.

(±)-*form* [627-76-9]
Mp 225°.
Virtanen, A.I. *et al., Acta Chem. Scand.*, 1954, **8**, 1085; 1725 (*isol*)
Wade, R. *et al., JACS*, 1957, **79**, 648 (*synth*)
Farkašová, H. *et al., Coll. Czech. Chem. Comm.*, 1965, **30**, 3117 (*synth*)
Jošt, K. *et al., Coll. Czech. Chem. Comm.*, 1971, **36**, 2795
Lerch, Ev. *et al., Helv. Chim. Acta*, 1974, **57**, 1584 (*ms, nmr*)
Rosowsky, A. *et al., J. Het. Chem.*, 1976, **13**, 729
Rabenstein, D.L. *et al., J. Magn. Reson.*, 1976, **24**, 27 (*nmr*)
Murakami, N. *et al., Phytochemistry*, 1983, **22**, 2735; 1985, **24**, 2291 (*isol, abs config*)
Phan, T. *et al., JOC*, 1994, **59**, 3676 (*synth, pmr, cmr*)

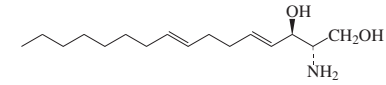
2-Amino-20-hexacosene-1,3,4-triol A-409



$C_{26}H_{53}NO_3$ 427.71

(2*S*,3*S*,4*R*,20*E*)-*form*
N-*(2R-Hydroxyhexadecanoyl):*
$C_{42}H_{83}NO_5$ 682.121
Isol. from the crown galls of *Panax quinquefolium* (American ginseng).
Cryst. powder. Mp 139-141°. $[\alpha]_D^{25}$ -1.3 (c, 0.0001 in $CHCl_3$).
Zhu, J.H. *et al., Fitoterapia*, 2010, **81**, 339-342 (*isol, pmr, cmr*)

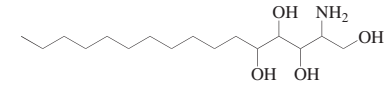
2-Amino-4,8-hexadecadiene-1,3-diol A-410



$C_{16}H_{31}NO_2$ 269.426

(2*S*,3*R*,4*E*,8*E*)-*form*
N-*(2R-Hydroxydocosanoyl), 1*-O-*β-D-glucopyranoside:* [946130-15-0] ***Ferocerebroside A***
$C_{44}H_{83}NO_9$ 770.141
Constit. of the seeds of *Euryale ferox* (foxnut). Amorph. powder. Mp 185-187°. $[\alpha]_D^{25}$ +11.2 (c, 0.08 in MeOH).
N-*(2R-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* [946130-16-1] ***Ferocerebroside B***
$C_{46}H_{87}NO_9$ 798.195
Constit. of the seeds of *Euryale ferox* (foxnut). Amorph. powder. Mp 187-189°. $[\alpha]_D^{25}$ +8.7 (c, 0.08 in MeOH).
Row, L.-C. *et al., J. Nat. Prod.*, 2007, **70**, 1214-1217 (*Ferocerebrosides A,B*)

2-Amino-1,3,4,5-hexadecanetetrol A-411

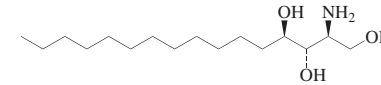


$C_{16}H_{35}NO_4$ 305.457

N-*(4E-Decenoyl):* [1292801-19-4]
$C_{26}H_{51}NO_5$ 457.693
Constit. of the leaves of *Citrus sinensis* 'Shukri' (orange). Amorph. powder. $[\alpha]_D$ +21.7 (c, 0.002 in MeOH).
Saleem, M. *et al., J. Asian Nat. Prod. Res.*, 2010, **12**, 702-706 (*Citrus sinensis constit*)

2-Amino-1,3,4-hexadecanetriol A-412

C_{16}-Phytosphingosine



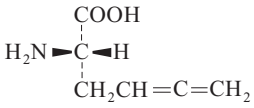
(2*S*, 3*S*, 4*R*)-*form*

$C_{16}H_{35}NO_3$ 289.457

(2*S*,3*S*,4*R*)-*form* [114379-45-2]
D-ribo-form
N-*(2R-Hydroxy-4E-hexacosenoyl), 1*-O-*β-D-glucopyranoside:* [1192057-20-7] ***Portulacerebroside A***
$C_{48}H_{93}NO_{10}$ 844.263
Constit. of *Portulaca oleracea* (purslane). Waxy solid. Mp 146-148°. $[\alpha]_D^{25}$ +20.5 (c, 0.1 in MeOH).
Xin, H.-L. *et al., Chin. J. Nat. Med.*, 2008, **6**, 401-403 (*Portulacerebroside A*)

2-Amino-4,5-hexadienoic acid, 9CI A-413

[18751-91-2]



(*S*)–*form*

$C_6H_9NO_2$ 127.143
Sol. H_2O; fairly sol. MeOH; poorly sol. MeOH, hexane.

(*S*)-*form* [22260-39-5]
Mp 174° dec. $[\alpha]_D^{22}$ -52.1 (c, 0.8 in H_2O).

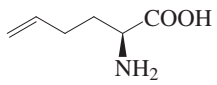
(±)-*form* [52521-29-6]
Powder.

3,5-Dinitrophenyl:
Yellow needles (EtOH aq.). Mp 177-180°.

Black, D.K. *et al., JCS(C)*, 1968, 283 (*synth*)
Chilton, W.S. *et al., Tet. Lett.*, 1968, 6283 (*isol, struct*)
Baldwin, J.E. *et al., Chem. Comm.*, 1984, 1284 (*synth*)
Hatanaka, S.-I. *et al., Phytochemistry*, 1998, **49**, 573-578 (*isol, bibl*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)

2-Amino-5-hexenoic acid, 9CI A-414

[16258-05-2]



(*S*)-*form*

$C_6H_{11}NO_2$ 129.158
Cryst. (H_2O). Mp 252-255°.

(*S*)-*form* [90989-12-1]
Powder. Mp 248° (dec.). $[\alpha]_D^{20}$ +13.6 (c, 0.9 in H_2O).

Hydrochloride:
Solid (MeOH/Et_2O). Mp 165-167°. $[\alpha]_D^{30}$ +30 (c, 0.97 in MeOH).

N-*Ac:*
$C_8H_{13}NO_3$ 171.196
Solid. Mp 114-116°. $[\alpha]_D^{20}$ -42.77 (c, 1.41 in $CHCl_3$) (78% ee).

N-tert-*Butyloxycarbonyl:* [208522-13-8]
$C_{11}H_{19}NO_4$ 229.275
Oil. $[\alpha]_D^{27}$ +37.24 (c, 0.5 in $CHCl_3$).

(±)-*form*
Cryst. (H_2O). Mp 275-276° (252-255°) dec.

Benzyl ester:
$C_{13}H_{17}NO_2$ 219.283
Oil.

Nitrile: [84673-59-6]
$C_6H_{10}N_2$ 110.158
No phys. props. reported.

N-*Ac:* [142034-37-5]
Solid. Mp 113.5-115°.

N-*Ac, Me ester:* [193223-81-3]
$C_9H_{15}NO_3$ 185.222
Fine needles (Et_2O/pentane). Mp 59.5-60.5°.

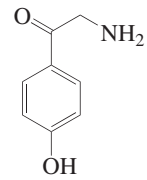
N-tert-*Butyloxycarbonyl:* [214206-61-8]
$C_{11}H_{19}NO_4$ 229.275
Solid (pentane). Mp 59-62°.

[141362-49-4, 103067-78-3]

Drinkwater, D.J. *et al., JCS(C)*, 1971, 1305-1307 (*synth*)
Kennewell, P.D. *et al., JCS Perkin 1*, 1982, 2553-2556 (*synth, ir, pmr*)
Bajgrowicz, J.A. *et al., Tetrahedron*, 1985, **41**, 1833-1843 (*nitrile*)
Baldwin, J.E. *et al., Chem. Comm.*, 1986, 273-275 (*synth*)
Baldwin, J.E. *et al., J. Chem. Res., Synop.*, 1992, 173; *J. Chem. Res., Miniprint*, 1992, 1517-1526 (*synth, S-form, pmr, cmr, ir, ms*)
Hatanaka, S.-I. *et al., Mycoscience*, 1994, **35**, 391 (*isol*)
Biagini, S.C.G. *et al., JCS Perkin 1*, 1998, 2485-2499 (*(±)-form, synth, (±)-N-Ac, (±)-N-BOC, ir, pmr, cmr, ms*)
Collet, S. *et al., JCS Perkin 1*, 2000, 177-182 (*S-form, synth, pmr, cmr*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)
Duggan, H.M.E. *et al., Org. Biomol. Chem.*, 2006, **3**, 2287-2295 (*S-form, synth, N-Boc*)

2-Amino-4′-hydroxyacetophenone A-415

2-Amino-1-(4-hydroxyphenyl)ethanone, 9CI. p-*Hydroxyphenacylamine* [77369-38-1]



$C_8H_9NO_2$ 151.165
Plates (EtOH). Mp 190-193° dec. A synthesis by Tutin *et al* (1910) could not be reproduced (Corrigan).

Hydrochloride: [19745-72-3]
Needles (HCl aq.), prisms (EtOH). Mp 241-245° Mp 249-251° dec.

N-*(9Z,12Z-Octadecadienoyl):* [1254277-87-6] ***Termitomycamide A***
$C_{26}H_{39}NO_3$ 413.599
Constit. of *Termitomyces titanicus.* Oil.

N-*(4-Hydroxy-3-methoxy*-E-*cinnamoyl):* [157536-49-7] ***Terrestriamide***
$C_{18}H_{17}NO_5$ 327.336
Light yellow cryst. Mp 218-220°.

N,N-*Di-Me:*
$C_{10}H_{13}NO_2$ 179.218
Prisms (Et_2O/petrol). Mp 142°.

Me ether: 2-Amino-4′-methoxyacetophenone
[3883-94-1 (hydrochloride)]
$C_9H_{11}NO_2$ 165.191
Cryst. (EtOH) (as hydrochloride). Mp 200-201° (hydrochloride).

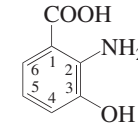
Me ether, N-*benzoyl:* [1823-86-5] *2-(Benzoylamino)-4′-methoxyacetophenone.* N-*(4-Methoxyphenacyl)benzamide.* ***Uguenenonamide***
$C_{16}H_{15}NO_3$ 269.299
Cryst. Mp 106-108°. λ_{max} 290 (log ε 4.53) ($CHCl_3$).

[40513-43-7]

Mannich, C. *et al., Ber.*, 1911, **44**, 1542-1552 (*synth*)
Voswinckel, H. *et al., Ber.*, 1912, **45**, 1004-1006 (*synth*)
Mannich, C. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1915, **253**, 181-195 (*synth*)
Corrigan, J.R. *et al., JACS*, 1945, **67**, 1894-1896 (*synth*)
Yinglin, H. *et al., Synthesis*, 1990, 615-618 (*Me ether*)
Ren, Y.J. *et al., Yaoxue Xuebao*, 1994, **29**, 204 (*Terrestriamide*)
Cheplogoi, P.K. *et al., Phytochemistry*, 2008, **69**, 1384-1388 (*Uguenenonamide*)
Choi, J.-H. *et al., Org. Lett.*, 2010, **12**, 5012-5015 (*Termitomycamide A*)

2-Amino-3-hydroxybenzoic acid A-416

3-Hydroxyanthranilic acid [548-93-6]



$C_7H_7NO_3$ 153.137
Isol. from *Brassica oleracea* (cauliflower). Leaflets (H_2O). Mp 164°. pK_{a2} 5.19; pK_{a3} 10.12 (20°).

▶ Exp. carcinogen. DG2625000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 206C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1098C; 1123C (*nmr*)
CRC Atlas of Spectral Data and Physical Constants, b842 (*uv, ir*)
Muelle, F. *et al., Planta*, 1961, **57**, 403-477 (*isol*)
Munsche, D. *et al., Phytochemistry*, 1965, **4**, 705-712 (*biosynth*)
Kuznezova, L.E. *et al., Nature (London)*, 1969, **222**, 484-485 (*props*)
Mohr, N. *et al., Annalen*, 1981, 1515-1518 (*isol*)
Okabe, N. *et al., Acta Cryst. C*, 1996, **52**, 2345-2347 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKE750

2-Amino-4-hydroxybenzoic acid A-417

4-Hydroxyanthranilic acid [38160-63-3]

$C_7H_7NO_3$ 153.137
Needles (H_2O). Mp 148° (dec.).

Hydrochloride:
Needles.

Me ester:
$C_8H_9NO_3$ 167.164
Needles. Mp 132-133°.

Me ether: [4294-95-5] *2-Amino-4-methoxybenzoic acid. 2-Aminoanisic acid. 4-Methoxyanthranilic acid*
$C_8H_9NO_3$ 167.164
Plates (EtOH). Mp 166° (dec.)
Mp 190°. pK_{a1} 2.06; pK_{a2} 4.88 (25°, 0.1*M* KCl).

N-*(4-Hydroxycinnamoyl)* (E-*): 4-Hydroxy*-N-*(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide G***
$C_{16}H_{13}NO_5$ 299.282

Stress metab. in oats (*Avena sativa*) induced by Victorin M. Cryst. + ¼ MeOH (MeOH/1% AcOH aq.). Mp 290-291°.

CRC Atlas of Spectral Data and Physical Constants, b843 (*uv*)
Drain, D.G. *et al., JCS*, 1949, 1489 (*synth*)
van der Stelt, C. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1953, **72**, 195 (*synth*)
Jilek, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 519 (*synth, uv, ir, pmr, deriv*)
Paulidis, V.H. *et al., Synth. Commun.*, 1994, **24**, 533 (*Me ether, synth, ir, pmr, cmr*)
Miyagawa, H. *et al., Phytochemistry*, 1996, **41**, 1473 (*Avenanthramide G*)
Boojamra, C.G. *et al., JOC*, 1997, **62**, 1240-1256 (*Me ether*)

2-Amino-5-hydroxybenzoic acid A-418

5-Hydroxyanthranilic acid [394-31-0]

$C_7H_7NO_3$ 153.137
Violet cryst. (H_2O). Mp 252° dec. pK_{a1} 2.72; pK_{a2} 5.37 (25°, 0.1*M* KCl). Log P 0.66 (calc).

N-*(4-Hydroxycinnamoyl)(*E-*):* [108605-70-5] *5-Hydroxy*-N-*(4-hydroxycinnamoyl)anthranilic acid.* ***Avenanthramide A****. Avenalumin I*
$C_{16}H_{13}NO_5$ 299.282
Isol. from the grains of oats (*Avena sativa*). Pale yellow needles (Me_2CO aq.). Mp 277°. Darkens at 235°. Originally descr. as Avenalumin I, given the wrong struct. λ_{max} 320 (ϵ 15400); 344 (ϵ 13400) (MeOH/HCl) (Derep). λ_{max} 366 (ϵ 16600) (MeOH/NaOH) (Derep). λ_{max} 317 (ϵ 15200); 336 (ϵ 15900) (MeOH) (Derep).

N-*(4-Hydroxycinnamoyl)(*Z-*):* [116764-20-6]
$C_{16}H_{13}NO_5$ 299.282
Isol. from oats (*Avena sativa*).

N-*(3,4-Dihydroxycinnamoyl)(*E-*):* [116764-15-9] N-*(3,4-Dihydroxycinnamoyl)-5-hydroxyanthranilic acid.* ***Avenanthramide C***
$C_{16}H_{13}NO_6$ 315.282
Isol. from oat grains.

N-*(3,4-Dihydroxycinnamoyl)(*Z-*):* [116764-22-8]
$C_{16}H_{13}NO_6$ 315.282
Isol. from oats (*Avena sativa*).

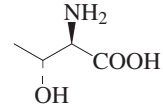
N-*(4-Hydroxy-3-methoxycinnamoyl)(*E-*):* [108605-69-2] N-*Feruloyl-5-hydroxyanthranilic acid.* ***Avenanthramide B****. Avenanthramide 1*
$C_{17}H_{15}NO_6$ 329.309
Isol. from oat grains. Long pale yellow needles (Me_2CO aq.). Mp 246°. λ_{max} 228; 315; 361; 392 (MeOH-NAOH) (Berdy).

N-*(4-Hydroxy-3-methoxycinnamoyl)(*Z-*):* [116764-21-7]
$C_{17}H_{15}NO_6$ 329.309
Isol. from oats (*Avena sativa*).

Collins, F.W. *et al., J. Agric. Food Chem.*, 1989, **37**, 60-66 (*Avenanthramides, isol, struct*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647-2648 (*Avenanthramides, synth*)
Dimberg, L.H. *et al., Cereal Chem.*, 1993, **70**, 637-641 (*Avenanthramides, rev, sar*)

2-Amino-3-hydroxybutanoic acid A-419

Threonine, 9CI. Thr [36676-50-3]



(2*R*,3*R*)-*form*

$C_4H_9NO_3$ 119.12

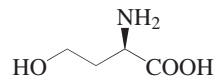
(2*S*,3*R*)-*form* [72-19-5]
L-Threonine*. FEMA 4710*
From wide variety of protein hydrolysates. Dietary supplement, nutrient. Cryst. (EtOH aq.). Sol. H_2O (20.5 g/100 ml at 25°). Mp 251-253° dec. $[\alpha]_D^{26}$ -33.9 (H_2O). pK_{a1} 2.71; pK_{a2} 9.62 (NH_2). Isoelectric point 6.16. Sweet taste.
▶ LD_{50} (rat, ipr) 3098 mg/kg. XO8590000

[2676-21-3, 4385-90-4, 71292-23-4, 62076-66-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 581A; 581B; 581C; 582A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 881C; 882B; 882A (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 2238-2258
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679-681 (*cd*)
Aruldhas, G. *et al., Spectrochim. Acta A*, 1967, **23**, 1345-1350 (*pmr*)
Pachler, K.G.R. *et al., Spectrochim. Acta A*, 1968, **24**, 1311-1316 (*pmr*)
Mallikarjunan, M. *et al., Acta Cryst. B*, 1969, **25**, 220-227 (*abs config*)
Maldonado, P. *et al., Bull. Soc. Chim. Fr.*, 1971, 2933-2938 (*synth*)
Soukup, M. *et al., Helv. Chim. Acta*, 1987, **70**, 232-236 (*2S,3R-form, synth*)
Seebach, D. *et al., Helv. Chim. Acta*, 1987, **70**, 237-261 (*2S,3R-form, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, TFU750
Jung, M.E. *et al., Tet. Lett.*, 1989, **30**, 6637-6640 (*synth*)
Shiraiwa, T. *et al., Bull. Chem. Soc. Jpn.*, 1990, **63**, 3296-3299; 1994, **67**, 1899-1903 (*resoln*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1050
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, TFU750

2-Amino-4-hydroxybutanoic acid A-420

Homoserine, 9CI [498-19-1]



(*R*)-*form*

$C_4H_9NO_3$ 119.12

(*S*)-*form* [672-15-1]
L-form
Present in germinating peas, Jack bean seeds (*Canavalia ensiformis*) and the seedlings of many leguminous plants. Mp 203° dec. $[\alpha]_D^{26}$ -8.8 (c, 5 in H_2O).

O-*Ac:* [7540-67-2] *4-Acetoxy-2-aminobutanoic acid.* **O-*Acetylhomoserine****. Homoserine acetate*
$C_6H_{11}NO_4$ 161.157
Found in green tissues of pea (*Pisum sativum*). Mp 200°. $[\alpha]_D^{20}$ +4.5 (c, 4 in H_2O).

O-*(3,4-Dihydroxy-*E*-cinnamoyl):* **O-*Caffeoylhomoserine***
$C_{13}H_{15}NO_6$ 281.265
Constit. of *Matteuccia struthiopteris* (ostrich fern). Prisms. Mp 224-225°. $[\alpha]_D^{20}$ -38.2 (c, 0.09 in MeOH aq.).

(±)-*form* [1927-25-9]
Needles (EtOH aq.). Mp 186-188° dec. Readily lactonises.

O-*Ac:* [6232-10-6]
Found in *Pisum sativum* (peas). Plates (EtOH). Mp 183-185°.

[55596-53-7, 53949-21-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 580C; 580D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 880B; 880C; 881A (*nmr*)
De Wald, H.A. *et al., JACS*, 1959, **81**, 4367-4370 (*(±)-O-Ac, synth*)
Drefahl, G. *et al., Chem. Ber.*, 1964, **97**, 159-164 (*(±)-form, synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1965, **3**, 2612 (*synth*)
Grobbelaar, N. *et al., Phytochemistry*, 1969, **8**, 553-559 (*S-form, S-form O-Ac, isol*)
Lawrence, J.M. *et al., Phytochemistry*, 1973, **12**, 2207-2209 (*S-form, isol*)
Curran, W.V. *et al., Prep. Biochem.*, 1981, **11**, 269-271 (*R-form, R-N-benzyloxycarbonyl, (±)-N-benzyloxycarbonyl, resoln*)
Baldwin, J.E. *et al., Tetrahedron*, 1988, **44**, 637-642 (*S-form, synth*)
Seebach, D. *et al., Annalen*, 1989, 1215-1232 (*S-form, synth, pmr, ir, ms*)
Shiraiwa, T. *et al., Chem. Pharm. Bull.*, 1996, **44**, 2322-2325 (*R-form, S-form, synth*)
Kimura, T. *et al., Phytochemistry*, 2004, **65**, 423-426 (*O-Caffeoylhomoserine*)

2-Amino-4-hydroxy-6-heptynoic acid A-421

[23840-14-4]

$HC{\equiv}CCH_2CH(OH)CH_2CH(NH_2)$-COOH
$C_7H_{11}NO_3$ 157.169
Found in *Euphoria longan* (Longan fruit). Cryst. (EtOH aq.). $[\alpha]_D^{20}$ -27 (c, 2 in H_2O).

Sung, M.L. *et al., Phytochemistry*, 1969, **8**, 1227
Scopes, P.M. *et al., JCS(C)*, 1971, 833 (*uv*)
Fowden, L. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1979, **50**, 117 (*rev*)

2-Amino-4-hydroxy-6-hydroxymethyldihydropteridine diphosphokinase A-422

E.C. 2.7.6.3. ATP:2-amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine 6′-diphosphotransferase. H_2-pteridine-CH_2OH pyrophosphokinase. 6-Hydroxymethyl-7,8-dihydropterin pyrophosphokinase. 7,8-Dihydro-6-hydroxymethylpterin diphosphokinase [37278-23-2]

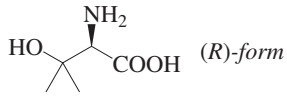
Diphosphotransferase enzyme. Isol. from baker's yeast. *Plasmodium falciparum* Enzyme activity range pH 8.5-10.5; *Escherichia coli* enzyme range pH 7.5-10.8. *Escherichia coli* Enzyme loses activity over a period of months

at -20°. *Plasmodium falciparum* Enzyme at -20° or -80°, in 20*mM* Tris-HCl, pH 8.0 buffer containing 10% or 20% glycerol, shows no loss of activity over 3 months; without glycerol, 30% or 50% of activity is lost when stored for 6 months at -80° or -20° respectively.

Richey, D.P. *et al., J. Biol. Chem.*, 1969, **244**, 1582-1592 (*Escherichia coli*)
Richey, D.P. *et al., Methods Enzymol., Part B*, 1971, **18**, 765-771 (*rev, assay, Escherichia coli*)
Walter, R.D. *et al., Methods Enzymol.*, 1980, **66**, 564-570 (*Plasmodium chabaudi*)
Talarico, T.L. *et al., J. Bacteriol.*, 1991, **173**, 7029-7031 (*Escherichia coli*)
Kasekarn, W. *et al., Mol. Biochem. Parasitol.*, 2004, **137**, 43-53 (*Plasmodium falciparum*)
Lawrence, M.C. *et al., J. Mol. Biol.*, 2005, **348**, 655-670 (*struct, baker's yeast*)

2-Amino-3-hydroxy-3-methylbutanoic acid A-423

3-Hydroxyvaline, 9CI. 2-Amino-3-hydroxyisovaleric acid [5174-30-1]



(*R*)-*form*

$C_5H_{11}NO_3$ 133.147

(*R*)-*form* [2280-48-0]
D-*form*
Mp 205°. $[\alpha]_D^{25}$ -13.5 (c, 4.82 in 5*M* HCl).
N-*Benzoyl:*
$C_{12}H_{15}NO_4$ 237.255
Mp 112°. $[\alpha]_D^{25}$ -30.5 (c, 2.01 in EtOH).

(*S*)-*form* [2280-27-5]
L-*form*
Isol. from *Pleurocybella porrigens* (angels wings). Mp 205°. $[\alpha]_D^{25}$ +13.5 (c, 0.64 in 6*M* HCl) (99.9% ee).
O-*[α-D-Glucopyranosyl-(1→1)-α-D-glucopyranos-6-yl]:*
$C_{17}H_{31}NO_{13}$ 457.431
Isol. from *Pleurocybella porrigens* (angels wings). $[\alpha]_D^{30}$ +130 (c, 0.1 in H_2O).
N-tert-*Butyloxycarbonyl:* [102507-13-1]
$C_{10}H_{19}NO_5$ 233.264
Cryst. Mp 125-126°. $[\alpha]_D^{20}$ -2.5 (c, 1.0 in MeOH) (≥99% ee).
Me ether: [2280-29-7] *2-Amino-3-methoxy-3-methylbutanoic acid*
$C_6H_{13}NO_3$ 147.174
Isol. from *Pleurocybella porrigens* (angels wings). $[\alpha]_D^{30}$ +4 (c, 0.2 in H_2O).
Et ether: [1207383-84-3] *2-Amino-3-ethoxy-3-methylbutanoic acid*
$C_7H_{15}NO_3$ 161.2
Isol. from *Pleurocybella porrigens* (angels wings). Mp 180-182°. $[\alpha]_D^{30}$ +9.4 (c, 0.2 in H_2O).
O-*(2ξ,3-Dihydroxypropyl) ether:* [1207613-15-7] *2-Amino-3-(2,3-dihydroxypropoxy)-3-methylbutanoic acid*
$C_8H_{17}NO_5$ 207.226
Isol. from *Pleurocybella porrigens* (angels wings). Mp 175-177°. $[\alpha]_D^{30}$ +12 (c, 0.08 in H_2O).

(±)-*form* [2280-28-6]
Plates (EtOH aq. or MeOH). Mp 221-223°.
N-*Benzoyl:* Mp 156° dec.
N-*Benzoyl, Me ester:*
$C_{13}H_{17}NO_4$ 251.282
Mp 105°. $Bp_{3.5}$ 185-190° (lit. gives a pressure range).
Me ether:
$C_6H_{13}NO_3$ 147.174
Plates. Mp 258-260° dec.
Me ether, Me ester:
$C_7H_{15}NO_3$ 161.2
Bp 94-95°.

Ohhashi, J. *et al., Bull. Chem. Soc. Jpn.*, 1966, **39**, 2287-2289 (*synth, resoln, abs config*)
Berse, C. *et al., Can. J. Chem.*, 1971, **49**, 2610-2611 (*synth*)
Ito, S. *et al., J. Antibiot.*, 1972, **25**, 360-361 (*isol*)
Aoyagi, Y. *et al., Phytochemistry*, 1988, **27**, 3306-3307 (*isol*)
Belokon, Y.N. *et al., Tetrahedron: Asymmetry*, 2001, **12**, 481-485 (*S-form, synth*)
Dettwiler, J.E. *et al., JOC*, 2003, **68**, 177-179 (*S-form, N-butyloxycarbonyl, synth*)
Kawaguchi, T. *et al., Tetrahedron*, 2010, **66**, 504-507 (*Pleurocybella porrigens constits*)

3-Amino-2-hydroxy-3-methylbutanoic acid A-424

β-Amino-α-hydroxyisovaleric acid
$(H_3C)_2C(NH_2)CH(OH)COOH$
$C_5H_{11}NO_3$ 133.147

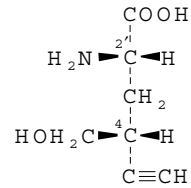
(+)-*form* [62000-66-2]
Isol. from the edible mushroom *Pleurocybella porrigens* (angels wings). $[\alpha]_D^{30}$ +12 (c, 0.07 in H_2O).

(±)-*form* [114043-75-3]
Mp 279-280° dec.

Danilov, S.N. *et al., Zh. Obshch. Khim.*, 1952, **22**, 1572-1576; *J. Gen. Chem. USSR (Engl. Transl.)*, 1952, **22**, 1615-1618 (*synth*)
Kaneko, T. *et al., Nippon Kagaku Zasshi*, 1961, **82**, 743-747 (*synth*)
Kaji, E. *et al., Bull. Chem. Soc. Jpn.*, 1976, **49**, 3181-3184 (*synth*)
Fringuelli, F. *et al., JOC*, 2003, **68**, 7041-7045 (*synth*)
Kawaguchi, T. *et al., Tetrahedron*, 2010, **66**, 504-507 (*Pleurocybella porrigens constit*)

2-Amino-4-hydroxymethyl-5-hexynoic acid, 8CI A-425

[23840-13-3]



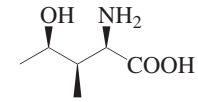
$C_7H_{11}NO_3$ 157.169

(2*S*,4*R*)-*form*
Isol. from *Euphoria longan* (Longan fruit). $[\alpha]_D^{20}$ -27 (c, 2 in H_2O). $[\alpha]_D$ -13 (c, 1 in 5*M* HCl). Tentative abs. config.

Sung, M.L. *et al., Phytochemistry*, 1969, **8**, 1227 (*isol, struct*)
Scopes, P.M. *et al., JCS(C)*, 1971, 833 (*uv*)

2-Amino-4-hydroxy-3-methylpentanoic acid A-426

2-Amino-2,3,5-trideoxy-3-methylpentonic acid. 4-Hydroxyisoleucine [50764-07-3]



(2*R*,3*R*,4*R*)-*form*

$C_6H_{13}NO_3$ 147.174

(2*R*,3*R*,4*R*)-*form* [60010-78-8]
D-xylo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-D-xylonic acid*
Cryst. (EtOH aq.). Mp *ca.*230°. $[\alpha]_D^{20}$ -35.6 (c, 1.12 in D_2O).
1,4-Lactone: 3-Aminodihydro-4,5-dimethyl-2(3H)-furanone
$C_6H_{11}NO_2$ 129.158
Cryst. (EtOH/petrol) (as hydrochloride). Mp 222° (hydrochloride). $[\alpha]_D^{25}$ +88.7 (c, 1 in MeOH).
1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 140°. $[\alpha]_D^{25}$ +88 (c, 1 in DMSO).

(2*R*,3*R*,4*S*)-*form* [60010-73-3]
L-arabino-*form. 2-Amino-2,3,5-trideoxy-3-methyl-L-arabinonic acid*
Minor amino acid constit. of *Trigonella foenum-graecum* (fenugreek) seeds. $[\alpha]_D^{20}$ +1 (c, 1 in H_2O).
Orginally thought to be the 2*R*,3*R*,4*R*-form.
1,4-Lactone:
Cryst. (as hydrochloride). Mp 170-175° (hydrochloride).
1,4-Lactone, N-*Ac:* [60010-74-4] *3-Acetamidodihydro-4,5-dimethyl-2(3H)-furanone.* ***Desmodilactone***
$C_8H_{13}NO_3$ 171.196
Cryst. Mp 84-85°. $[\alpha]_D^{18}$ -16.4 (c, 0.11 in MeOH).

(2*S*,3*R*,4*R*)-*form* [55399-92-3]
D-lyxo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-D-lyxonic acid*
Cryst. (EtOH aq.). Mp *ca.*220°. $[\alpha]_D^{20}$ -24.9 (c, 1.17 in D_2O).
1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 255° (hydrochloride). $[\alpha]_D^{25}$ +24.3 (c, 1 in MeOH).
1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 141°.

(2*S*,3*R*,4*S*)-*form* [55399-93-4]
L-ribo-*form. 2-Amino-2,3,5-trideoxy-3-methyl-L-ribonic acid*
Major constit. of *Trigonella foenum-graecum* (fenugreek). Cryst. (EtOH aq.). Mp 224-225°. $[\alpha]_D^{20}$ +31 (c, 1 in H_2O). Stereochem. revised in 1989.
1,4-Lactone:
Needles (EtOH/petrol) (as hydrochloride). Mp 230° (hydrochloride). $[\alpha]_D^{25}$ -15.5 (c, 1 in MeOH).

1,4-Lactone, N-*Ac:*
Needles (EtOH). Mp 94°.

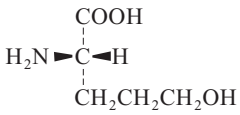
(2*S*,3*S*,4*R*)-*form* [21704-86-9]
D-arabino-*form. 2-Amino-2,3,5-trideoxy-3-methyl-*D*-arabinonic acid*Mp 205-207°. $[\alpha]_D^{27}$ +2.9 (c, 0.1 in H_2O). λ_{max} 197 (ϵ 250) (H_2O).

1,4-Lactone: [71392-28-4]
[90693-46-2]
Powder (as hydrochloride). Mp 212-215° (hydrochloride). $[\alpha]_D^{25}$ -14.8 (c, 0.7 in MeOH).

Fowden, L. *et al., Phytochemistry*, 1973, **12**, 1707-1711 (*Trigonella foenum-graecum constits*)
Gieren, A. *et al., Annalen*, 1974, 1561-1569 (*synth*)
Hasan, M. *et al., Annalen*, 1976, 781-787 (*lactone, synth, pmr*)
Raffauf, R.F. *et al., JOC*, 1984, **49**, 2714-2718 (*Quararbea funebris constit*)
Alcock, N.W. *et al., Phytochemistry*, 1989, **28**, 1835-1841 (*struct*)
Inghardt, T. *et al., Tetrahedron*, 1991, **47**, 6469-6482 (*2R,3R,4R-form, 2R,3R,4R-1,4-lactone, 2S,3R,4R-form, 2S,3R,4R-1,4-lactone, synth, cryst struct, pmr, cmr*)
Yang, J. *et al., Yaoxue Xuebao*, 1993, **28**, 197-201 (*Desmodilactone*)
Sauvaire, Y. *et al., Diabetes*, 1998, **47**, 206-210 (*pharmacol*)
Wang, Q. *et al., Eur. J. Org. Chem.*, 2002, 834-839 (*synth, pmr, cmr*)
Rolland-Fulcrand, V. *et al., Eur. J. Org. Chem.*, 2004, 873-877 (*synth, pmr, cmr*)
Aouadi, K. *et al., Synthesis*, 2007, 3399-3405 (*2S,3R,4R-form, synth, pmr, cmr, ms*)
Jette, L. *et al., Curr. Opin. Invest. Drugs*, 2009, **10**, 353-358 (*pharmacol*)

2-Amino-5-hydroxypentanoic acid, 9CI A-427

2-Amino-5-hydroxyvaleric acid. Pentahomoserine. 5-Hydroxynorvaline



(*S*)–*form*

$C_5H_{11}NO_3$ 133.147

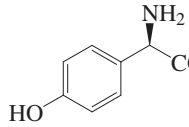
(*S*)-*form*
L-*form*
Present in jack bean seeds (*Canavalia ensiformis*). Mp 231.5°. $[\alpha]_D^{25}$ +22.6 (c, 2 in 0.5*M* HCl).

(±)-*form*
Needles (MeOH aq.). Sol. H_2O; spar. sol. EtOH, Me_2CO. Mp 223-224°.

Sörensen, S.P.L. *et al., Chem. Zentralbl.*, 1905, **2**, 398
Thompson, J.F. *et al., J. Biol. Chem.*, 1964, **239**, 1122 (*isol, synth*)
Barlos, K. *et al., Chem. Comm.*, 1987, 1583 (*synth, bibl*)
Hill, R.E. *et al., J. Nat. Prod.*, 1993, **56**, 1246 (*isol, ms, synth*)
Garcia, M. *et al., Tetrahedron: Asymmetry*, 2000, **11**, 991-994 (*S-form, synth, pmr, cmr, ms*)
Carmo-Silva, A.E. *et al., Phytochemistry*, 2009, **70**, 664-671 (*isol, synth, pmr, ms*)

2-Amino-2-(4-hydroxyphenyl)acetic acid A-428

*α-Amino-4-hydroxybenzeneacetic acid, 9CI. 2-(*p*-Hydroxyphenyl)glycine, 8CI.* ***Oxfenicine, BAN, INN, USAN*** [938-97-6]



(*R*)-*form*

$C_8H_9NO_3$ 167.164

(*R*)-*form* [22818-40-2]
D-*form*
Cryst. Mp 240° dec. $[\alpha]_D^{25}$ -158.4 (c, 1 in 1M HCl).

N-tert-*Butyloxycarbonyl:* [27460-85-1]
$C_{13}H_{17}NO_5$ 267.281
Cryst. (EtOAc). Mp 199° (dec. from 160°). $[\alpha]_D^{24}$ -130 (c, 1.08 in EtOH).

N-*Benzoyl:* [37784-33-1]
$C_{15}H_{13}NO_4$ 271.272
Cryst. (H_2O). Mp 223°. $[\alpha]_D^{18}$ -137.9 (c, 1.0 in THF).

(*S*)-*form* [32462-30-9]
UK 25842

Me ether: [24593-48-4] *2-Amino-2-(4-methoxyphenyl)acetic acid*
$C_9H_{11}NO_3$ 181.191
Mp 260° dec. $[\alpha]_D^{20}$ +139.1 (c, 1 in 1*M* HCl) (96.5% ee).

Me ether, N-*Me:* [865244-82-2] *2-(4-Methoxyphenyl)-2-(methylamino)acetic acid*
$C_{10}H_{13}NO_3$ 195.218
Mp 177° dec. $[\alpha]_D^{25}$ +131.8 (c, 0.5 in 1*M* HCl) (76% ee).

(±)-*form* [6324-01-2]
Plates (H_2O). Spar. sol. H_2O, insol. Et_2O. Dec. at 200° without melting.

Amide:
[73226-87-6 (non-stereospecific), 53958-19-3 (*S*-form), 72151-95-2 ((±)-form), 54397-23-8 (*R*-form)]
$C_8H_{10}N_2O_2$ 166.179

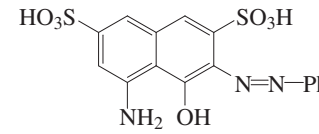
N-*Carbamoyl:* [32507-69-0]
[72500-37-9]
$C_9H_{10}N_2O_4$ 210.189
Isol. from leaves of *Vicia faba.*

Me ether: [19789-59-4]
[2540-53-6]
Mp 200° dec.

Lomakina, N.N. *et al., Khim. Prir. Soedin.*, 1969, **5**, 43-46; *Chem. Nat. Compd. (Engl. Transl.)*, 1969, **5**, 36 (*occur, abs config*)
Larsen, P.O. *et al., Biochim. Biophys. Acta*, 1975, **381**, 397-408 (*isol*)
Smith, G.A. *et al., JCS Perkin 1*, 1975, 2108-2115 (*isol*)
Clark, J.C. *et al., JCS Perkin 1*, 1976, 475-481 (*resoln*)
US Pat., 1977, (*(Nippon Kayaku)*)4 002 666 (*resoln*)
Yamada, S. *et al., Agric. Biol. Chem.*, 1979, **43**, 395-396 (*synth*)
Blackburn, K.J. *et al., Br. J. Pharmacol.*, 1979, **66**, 443P-444P (*S-form, pharmacol*)
Eur. Pat., 1979, (*(Beecham)*)1 319 (*(±)-form, synth*)
McGahren, W.J. *et al., JACS*, 1980, **102**, 1671-1684 (*isol*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 13061
US Pat., 1982, (*(ICI)*)4 350 826 (*(±)-form, synth*)
Yoshioka, R. *et al., Bull. Chem. Soc. Jpn.*, 1987, **60**, 649-652; 4321-4323 (*resoln, bibl*)
US Pat., 1987, (*(Beecham)*)4 647 692 (*resoln*)
Salituro, G.M. *et al., JACS*, 1990, **112**, 760-770 (*N-tert-butyloxycarbonyl*)
Eur. Pat., 1991, (*(Stamicarbon)*)442 584 (*(±)-amide, resoln*)
Bhattacharya, A. *et al., Synth. Commun.*, 1994, **24**, 2449-2459 (*resoln, pmr, cmr*)
Beller, M. *et al., Chem. Eur. J.*, 1998, **4**, 935-941 (*Me ether, synth, ir, pmr*)
Tokic-Vujosevic, Z. *et al., Synth. Commun.*, 2005, **35**, 435-447 (*R-form, N-benzoyl*)
Wang, M.-X. *et al., Tetrahedron: Asymmetry*, 2005, **16**, 2409-2416 (*S-form, N-Me Me ether*)

5-Amino-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic acid, 9CI A-429

Acid Fuchsin Fast B. Acid Fuchsine D. Azofuchsin. Fast Acid Magenta. C.I. Acid Red 33. C.I. Food Red 12. C.I. 17200. D and C Red No. 33 [2203-16-9]
[3567-66-6, 112524-65-9, 126212-64-4]

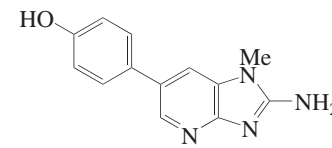


$C_{16}H_{13}N_3O_7S_2$ 423.427
Normally encountered as Na salt, to which the trade names refer. Food dye. Na salt sol. H_2O. Exists in soln. as an equilib. mixt. of azo and hydrazone tautomers with the naphthoquinone hydrazone predominating.

Krasovitskii, B.M. *et al., Ukr. Khim. Zh. (Russ. edn.)*, 1961, **27**, 94-97 (*synth, uv*)
Colour Index, 3rd edn., 1971, **4**, 4105 (*synth*)
Lycka, A. *et al., Dyes Pigm.*, 1987, **8**, 315-325 (*pmr, cmr, N-15 nmr, tautom*)

2-Amino-6-(4-hydroxyphenyl)-1-methyl-1*H*-imidazo[4,5-*b*]pyridine A-430

*4-(2-Amino-1-methyl-1*H*-imidazo[4,5-b]pyridin-6-yl)phenol, 9CI. 4′-OH-PhIP*
[126861-72-1]



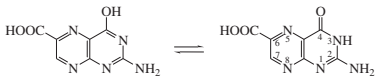
$C_{13}H_{12}N_4O$ 240.264
Present in fried chicken and broiled beef. Cryst. (DMF). Shows low level mutagenicity in *Salmonella* assays. λ_{max} 239; 275; 321 (MeOH).

Kurusaka, R. *et al., Jpn. J. Cancer Res.*, 1992, **83**, 919-922 (*detn, synth, pmr, uv*)
Frandsen, H. *et al., Food Chem. Toxicol.*, 2007, **45**, 863-870 (*metab*)

Busquets, R. *et al., J. Agric. Food Chem.*, 2007, **55**, 9318-9324 (*detn, occur, bibl*)

2-Amino-4-hydroxy-6-pteridinecarboxylic acid A-431

*2-Amino-1,4-dihydro-4-oxo-6-pteridinecarboxylic acid. 2-Amino-4(3*H*)-pteridinone-6-carboxylic acid. Pterin-6-carboxylic acid. Ranachrome 5* [948-60-7]



$C_7H_5N_5O_3$ 207.148
Isol. from various biol. sources incl. fish and soybeans. Cream cryst. Mp 360°.

Me ester: [31010-61-4]
$C_8H_7N_5O_3$ 221.175
Cryst. (DMF). Mp 285° dec.

2-N-*Ac:* [31010-65-8]
$C_9H_7N_5O_4$ 249.185
Cryst. (MeOH). Mp 210°.

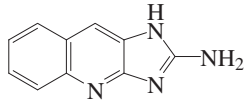
2-N-*Ac, Me ester:* [31010-67-0]
$C_{10}H_9N_5O_4$ 263.212
Mp 283°.

7,8-Dihydro: ***7,8-Dihydropterin-6-carboxylic acid***
$C_7H_8N_5O_3$ 210.172

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 896C (*ir*)
Baugh, C.M. *et al., JOC*, 1964, **29**, 3610 (*synth*)
Pfleiderer, W. *et al., Annalen*, 1970, **741**, 64 (*synth, derivs*)
Iwanami, Y. *et al., Tet. Lett.*, 1972, 3219 (*ms*)
Nair, M.G. *et al., JOC*, 1973, **38**, 2185 (*synth*)
Mengel, R. *et al., Chem. Ber.*, 1978, **111**, 3790 (*synth*)
Kohashi, M. *et al., J. Biochem. (Tokyo)*, 1980, **87**, 1581 (*isol*)
Zeitler, M. *et al., Methods Enzymol.*, 1986, **122**, 273 (*isol*)
Sato, N. *et al., J. Het. Chem.*, 1988, **25**, 1737 (*synth, derivs*)
Suga, T. *et al., J. Nat. Prod.*, 1988, **51**, 713 (*isol*)
Kuse, M. *et al., Bioorg. Med. Chem. Lett.*, 2001, **11**, 1037-1040 (*7,8-dihydro*)

2-Aminoimidazo[4,5-*b*]quinoline A-432

*Imidazo[4,5-*b*]quinolin-2-amine, 9CI*



$C_{10}H_8N_4$ 184.2

1*H-form* [156215-58-6]
Isol. from grilled meats. Pale yellow needles (EtOH aq.). Mp >300°.

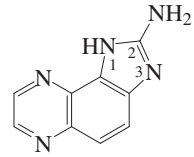
*1-Me: 1-Methyl-1*H*-imidazo[4,5-*b*]quinolin-2-amine, 9CI. 2-Amino-1-methylimidazo[4,5-*b*]quinoline. IQ[4,5-*b*]*
$C_{11}H_{10}N_4$ 198.227
Constit. of cooked meats.

1-Me, 2-N-*Ac:*
$C_{13}H_{12}N_4O$ 240.264
Mp 210-212°.

Ronne, E. *et al., Commun.*, 1994, **24**, 1363-1366 (*synth, pmr, ms, N-Ac*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 68-78 (*isol, ms, 1-Me, detn, occur*)

2-Amino-3*H*-imidazo[4,5-*f*]quinoxaline A-433

*3*H*-Imidazo[4,5-*f*]quinoxalin-2-amine, 9CI*



1*H-form*

$C_9H_7N_5$ 185.188

1*H-form*

1-Me: [851759-16-5] *1-Methyl-1*H*-imidazo[4,5-*f*]quinoxalin-2-amine. 2-Amino-1-methyl-1*H*-imidazo[4,5-*f*]quinoxaline. 1-Iso-IQx*
$C_{10}H_9N_5$ 199.215
Isol. from cooked meats. No phys. props. reported.

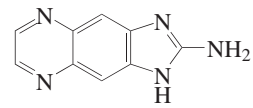
3*H-form*

3-Me: [108354-47-8] *3-Methyl-3*H*-imidazo[4,5-*f*]quinoxalin-2-amine. 2-Amino-3-methyl-3*H*-imidazo[4,5-*f*]quinoxaline. Iqx*
$C_{10}H_9N_5$ 199.215
Mutagen found in cooked beef and pork.
▶ Mutagenic.

Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521-528 (*synth*)
Solyakov, A. *et al., Food Chem. Toxicol.*, 1999, **32**, 1-11 (*occur*)
Guy, P.A. *et al., J. Chromatogr.*, 2000, **883**, 89-102 (*occur*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 67-78 (*1-Me, 3-Me, occur, synth, ms, pmr*)

2-Amino-1*H*-imidazo[4,5-*g*]quinoxaline A-434

*1*H*-Imidazo[4,5-*g*]quinoxalin-2-amine, 9CI*



$C_9H_7N_5$ 185.188

1-Me: [1004510-30-8] *IgQx*
$C_{10}H_9N_5$ 199.215
Constit. of roast/fried meats. No phys. props. reported.

Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*1-Me, synth, occur, pmr, ms*)

5-Aminolevulinate transaminase A-435

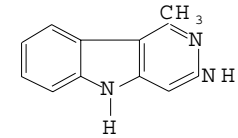
E.C. 2.6.1.43. 5-Aminolevulinate:pyruvate aminotransferase. 5-Aminolevulinate aminotransferase. 4,5-Dioxovalerate transaminase. 4,5-Dioxovalerate aminotransferase [9012-46-8]

Aminotransferase enzyme. Isol. from chicken and cow. Pyridoxal phosphate-dependent.

Neuberger, A. *et al., Biochim. Biophys. Acta*, 1963, **67**, 342-345 (*Rhodopseudomonas sphaeroides*)
Varticovski, L. *et al., J. Biol. Chem.*, 1980, **255**, 3742-3747 (*bovine liver*)
Bajkowski, A.S. *et al., J. Biol. Chem.*, 1982, **257**, 2207-2211 (*Clostridium tetanomorphum*)
Shanker, J. *et al., Biochem. Int.*, 1983, **7**, 23-31 (*rat liver*)
Shioi, Y. *et al., Arch. Biochem. Biophys.*, 1984, **234**, 117-124 (*Chlorella regularis*)
Singh, N.K. *et al., Biochim. Biophys. Acta*, 1985, **827**, 305-309 (*rat kidney*)
Rhee, H. *et al., J. Biochem. (Tokyo)*, 1988, **103**, 1045-1049 (*Pseudomonas riboflavina*)
Ades, I.Z. *et al., Int. J. Biochem.*, 1989, **21**, 679-687 (*chicken liver*)
Tyagi, R.K. *et al., Protein Expr. Purif.*, 1994, **5**, 527-533 (*rat kidney*)

3-Amino-1-methyl-γ-carbazole A-436

*1-Methyl-5*H*-pyrido[3,4-*b*]indol-1-amine, 9CI. Trp-P2* [62450-07-1]
[72254-58-1]



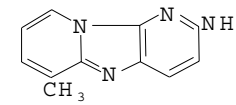
$C_{12}H_{11}N_3$ 197.239
Isol. from protein pyrolysates contg. tryptophan. Mutagenic potential food contaminant. Prisms (as acetate salt). Mp 242-247° (acetate salt).
▶ Possible human carcinogen. Exp. carcinogen and mutagen. UU9354000

[75074-77-0]

IARC Monogr., 1983, **31**, 255; 1987, *Suppl. 7*, 73 (*rev, tox*)
Akimoto, H. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 123 (*synth, bibl, ir, uv*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALD500; ALE750

2-Amino-6-methyldipyrido[1,2-*a*:3′,2′-*d*]imidazole A-437

*6-Methyldipyrido[1,2-*a*:3′,2′-*d*]imidazol-2-amine, 9CI. Glu-P-1* [67730-11-4]



$C_{11}H_{10}N_4$ 198.227

Powerful mutagen presumed present in cooked foods. Yellow prisms (MeOH/EtOAc).

▶ Highly mutagenic. Possible human carcinogen. Exp. carcinogen. JM5620000

Hydrobromide: [68739-12-8]
Cryst. + $1H_2O$. Mp 290-292°.

Takeda, K. *et al., Chem. Pharm. Bull.*, 1978, **26**, 2924
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*tox*)
IARC Monogr., 1986, **40**, 223; 1987, *Suppl. 7*, 64 (*rev, tox*)
Stavric, B. *et al., Food Chem. Toxicol.*, 1994, **32**, 997 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKS250

4-Amino-2-methylenebutanoic acid, 9CI A-438

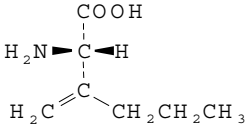
γ-Amino-α-methylenebutyric acid [65370-67-4]

$H_2C{=}C(COOH)CH_2CH_2NH_2$
$C_5H_9NO_2$ 115.132
Found in *Arachis hypogaea* (peanut). Cryst. (EtOH aq. or EtOH/Me_2CO). Mp 152° dec Mp 170-179° dec.

Fowden, L. *et al., Biochem. J.*, 1953, **55**, 548
Marcus, A. *et al., Arch. Biochem. Biophys.*, 1963, **100**, 80
Hatanaka, S. *et al., Phytochemistry*, 1977, **16**, 1820 (*synth, nmr*)

2-Amino-3-methylenehexanoic acid A-439

3-Methylenenorleucine, 8CI. 2-Amino-3-propyl-3-butenoic acid



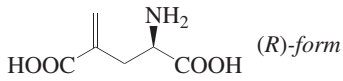
$C_7H_{13}NO_2$ 143.185

(*S*)-*form* [29784-96-1]
L-form
Found in carpophores of *Amanita vaginata* (grisette). Cryst. (EtOH aq.). Mp 171°. $[\alpha]_D^{20}$ +158 (c, 0.51 in 1*M* HCl). $[\alpha]_D^{20}$ +148 (c, 0.56 in H_2O).

Vervier, R. *et al., Phytochemistry*, 1970, **9**, 2059

2-Amino-4-methylenepentanedioic acid A-440

4-Methyleneglutamic acid. 4-Amino-1-butene-2,4-dicarboxylic acid. 2-Amino-4-methyleneglutaric acid



(*R*)-*form*

$C_6H_9NO_4$ 159.141

(*R*)-*form* [2517-06-8]
D-form
$[\alpha]_D$ -13.7 (5*M* HCl).

(*S*)-*form* [16804-57-2]
L-form
Constit. of peanuts (*Arachis hypogaea*) and other plants, notably tulips and hops. $[\alpha]_D$ +13.7 (5*M* HCl).

Hydrobromide: [888324-05-8]
Cryst. Mp *ca.*200° dec. $[\alpha]_D^{17}$ +12 (c, 1.0 in 3*M* HCl).

γ-Amide: γ-Methyleneglutamine
$C_6H_{10}N_2O_3$ 158.157
Isol. from peanuts and other plant sources. Amorph. $[\alpha]_D^{18}$ 0 (H_2O). $[\alpha]_D$ +21 (6*M* HCl).

N-tert-*Butyloxycarbonyl, di-Me ester:* [95049-80-2]
$C_{13}H_{21}NO_6$ 287.312
Oil. $[\alpha]_D^{20}$ +15.2 (c, 1.2 in $CHCl_3$).

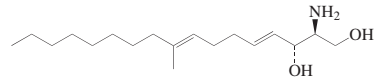
(±)-*form* [7150-74-5]
Mp 203-210° dec.

Hydrochloride: Mp 179-180° dec.

N-*Ac:*
$C_8H_{11}NO_5$ 201.179
Mp 88.5°.

Virtanen, A.I. *et al., Acta Chem. Scand.*, 1955, **9**, 553-554 (*isol*)
Wailes, P.C. *et al., JCS*, 1955, 3636 (*struct, synth*)
Marcus, A. *et al., Arch. Biochem. Biophys.*, 1963, **100**, 80-85 (*isol, S-form, R-form, (±)-form, synth*)
Blake, J. *et al., Biochem. J.*, 1964, **92**, 136-142 (*isol, S-form, abs config, amide*)
Meier, L.K. *et al., Phytochemistry*, 1979, **18**, 1173-1175 (*isol, S-form*)
Moody, C.M. *et al., JCS Perkin 1*, 1997, 3519-3530 (*synth, ir, pmr, cmr*)
Dieterich, P. *et al., Org. Biomol. Chem.*, 2006, **4**, 1492-1496 (*S-form, synth, N-BOC di-Me ester*)
Kang, S. *et al., Tetrahedron*, 2010, **66**, 4326-4329 (*S-form, synth*)

2-Amino-9-methyl-4,8-heptadecadiene-1,3-diol A-441



$C_{18}H_{35}NO_2$ 297.48

(2*S*,3*R*,4*E*,8*E*)-*form*
N-*Hexadecanoyl, 1*-O-α-D-*glucopyranoside:* [251565-82-9] ***Thraustochytroside C***
$C_{40}H_{75}NO_8$ 698.034

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{38}H_{71}NO_9$ 685.98
Amorph. powder (MeOH). $[\alpha]_D^{20}$ +3.5 (c, 0.15 in $CHCl_3$).

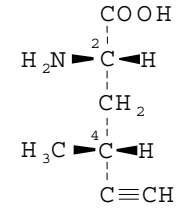
N-*(2*R*-Hydroxyoctadecanoyl):* [959929-63-6] ***Ramariaceramide A***
$C_{36}H_{69}NO_4$ 579.945
Constit. of the fruiting bodies of *Ramaria botrytis* (pink-tipped coral). Amorph. powder. $[\alpha]_D^{21}$ +7.4 (c, 0.41 in $CHCl_3$).

N-*(2*R*-Hydroxy-3-octadecenoyl), 1*-O-β-D-*glucopyranoside:* [1184182-48-6] ***Alternaroside B***
$C_{42}H_{77}NO_9$ 740.072
Amorph. powder. $[\alpha]_D^{20}$ -9 (c, 0.1 in MeOH). λ_{max} 202 (log ε 3.2) (MeOH).

Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside C*)
Liu, J.-K. *et al., Lipids*, 2003, **38**, 669-675 (*Cortinarius glycolipid*)
Yaoita, Y. *et al., J. Nat. Med. (Tokyo)*, 2007, **61**, 205-207 (*Ramariaceramide A*)
Wang, W. *et al., J. Nat. Prod.*, 2009, **72**, 1695-1698 (*Alternaroside B*)

2-Amino-4-methyl-5-hexynoic acid, 9CI A-442

[23840-12-2]



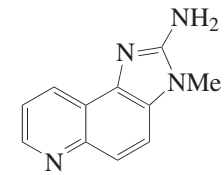
$C_7H_{11}NO_2$ 141.169

(2*S*,4*R*)-*form*
Obt. from *Euphoria longan* (longan fruit). Cryst. (EtOH aq.). $[\alpha]_D^{20}$ -33 (c, 2 in H_2O). $[\alpha]_D$ -27 (c, 1 in 5*M* HCl). Tentative config.

Sung, M.L. *et al., Phytochemistry*, 1969, **8**, 1227 (*isol, struct*)
Scopes, P.M. *et al., JCS(C)*, 1971, 833 (*uv*)
Coulter, A.W. *et al., Mol. Pharmacol.*, 1974, **10**, 293

2-Amino-3-methylimidazo[4,5-*f*]quinoline A-443

IQ [76180-96-6]



$C_{11}H_{10}N_4$ 198.227
Isol. from cooked foods, e.g. sardines, beef extract, var. cooked meats. Cryst. (MeOH aq.). Mp 300°.

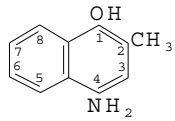
▶ Highly mutagenic. Probable human carcinogen (IARC 2A). Exp. carcinogen. NJ5910000

Kasai, H. *et al., JCS Perkin 1*, 1981, 2290
Adolfsson, L. *et al., Acta Chem. Scand., Ser. B*, 1983, **37**, 157 (*synth*)
Ohgaki, H. *et al., Environ. Health Perspect.*, 1986, **67**, 129 (*carcinogenicity*)
Ronne, E. *et al., Acta Chem. Scand.*, 1994, **48**, 823 (*synth, bibl, ms, hplc*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 68-78 (*detn, occur, ms, hplc*)
Wang, F. *et al., JACS*, 2006, **128**, 10085-10095 (*props, bibl*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*chromatog, detn*)
IARC Monogr. (Web), http://monographs.iarc.fr, (*tox*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKT600

4-Amino-2-methyl-1-naphthol, 8CI A-444

4-Amino-2-methyl-1-naphthalenol, 9CI. Vitamin K_5 [83-70-5]

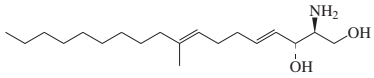


$C_{11}H_{11}NO$ 173.214
Vitamin. Used as a food preservative. Log P 1.92 (calc).
▶ LD_{50} (mus, ipr) 250 mg/kg. QL3350000
Hydrochloride: [130-24-5] *Synkamine. Kayvisyn*
Needles (HCl aq.). Mp 280-282° dec. (darkens at 260°).
N-*Ac:* [523-68-2] *4-Acetamido-2-methyl-1-naphthol*. ***Acetyl-Vitamin K_5***. *Kavitrat*. *K-Vitrat*
$C_{13}H_{13}NO_2$ 215.251
Prothrombogenic vitamin. Needles. Mp 208-210°. Log P 2.17 (calc).

Sah, P.P.T. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1941, **60**, 373 (*synth*)
Veldstra, H. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1943, **62**, 75 (*synth*)
Gaultier, J. *et al., C. R. Seances Acad. Sci., Ser. C*, 1967, **264**, 766 (*cryst struct*)
Madelmont, J.C. *et al., J. Labelled Compd. Radiopharm.*, 1978, **14**, 281 (*synth*)
Prenzel, U. *et al., J. Chromatogr.*, 1982, **242**, 9 (*hplc*)
Martindale, The Extra Pharmacopoeia, 28th/29th edn., Pharmaceutical Press, 1982, 7909
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AKX500

2-Amino-9-methyl-4,8-octadecadiene-1,3-diol A-445

9-Methyl-4,8-sphingadienine



$C_{19}H_{37}NO_2$ 311.507

(2S,3R,4E,8E)-form

N-*Hexadecanoyl:* [105243-35-4]
$C_{35}H_{67}NO_3$ 549.919
Amorph. powder. $[\alpha]_D^{21}$ -11.6 (c, 0.09 in $CHCl_3$).

N-*Hexadecanoyl, 1*-O-α-D-*glucopyranoside:* [251565-81-8] ***Thraustochytroside B***
$C_{41}H_{77}NO_8$ 712.061
Amorph. solid.

N-*(2*E*-Octadecenoyl), 1*-O-β-D-*glucopyranoside:* [849544-01-0]
$C_{43}H_{79}NO_8$ 738.099

N-*(9Z,12Z-Octadecadienoyl):* [448933-55-9]
$C_{37}H_{67}NO_3$ 573.941
Amorph. powder. $[\alpha]_D^{30}$ -13.3 (c, 0.08 in $CHCl_3$).

N-*(2*R*-Hydroxytridecanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{38}H_{71}NO_9$ 685.98

N-*(2*R*-Hydroxytetradecanoyl):* [448933-57-1]
$C_{33}H_{63}NO_4$ 537.865
Amorph. powder. $[\alpha]_D^{20}$ +6.3 (c, 0.2 in $CHCl_3$).

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{39}H_{73}NO_9$ 700.007

N-*(2*R*-Hydroxypentadecanoyl):* [448933-56-0]
$C_{34}H_{65}NO_4$ 551.892
Amorph. powder. $[\alpha]_D^{21}$ +7 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxypentadecanoyl), 1*-O-β-D-*glucopyranoside:*
$C_{40}H_{75}NO_9$ 714.034

N-*(2*R*-Hydroxyhexadecanoyl):* [95673-08-8]
$C_{35}H_{67}NO_4$ 565.919
Isol. from the mushroom *Lepista nuda* (wood blewit). Amorph. powder. $[\alpha]_D^{19}$ +7.5 (c, 0.1 in $CHCl_3$).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-β-D-*glucopyranoside:* [88642-46-0] ***Cerebroside B***
$C_{41}H_{77}NO_9$ 728.061
From *Clitocybe* spp. Mp 180-190°. $[\alpha]_D^{20}$ +5.2 (c, 1 in MeOH). $[\alpha]_D^{19}$ -7.4 (c, 0.3 in $CHCl_3$).

N-*(2*R*-Hydroxy-3-hexadecenoyl), 1*-O-β-D-*glucopyranoside:* [115681-40-8] ***Cerebroside A***
$C_{41}H_{75}NO_9$ 726.045
Cryst. Sol. MeOH. Mp 170-178°. $[\alpha]_D^{20}$ -6.7 (c, 1 in MeOH).

N-*(2*R*-Hydroxyheptadecanoyl), 1*-O-β-D-*glucopyranoside:* [120029-71-2]
$C_{42}H_{79}NO_9$ 742.087
Amorph. powder. Mp 154-156°. $[\alpha]_D^{26}$ +4.9 (c, 0.4 in MeOH).

N-*(2*R*-Hydroxyoctadecanoyl):* [372178-04-6] ***Lactariamide B***
$C_{37}H_{71}NO_4$ 593.972
Isol. from the fungus *Lactarius volemus* (tawny milkcap mushroom). Amorph. powder. $[\alpha]_D^{20}$ +8.4 (c, 0.39 in MeOH). Stereochem. not confirmed.

N-*(2*R*-Hydroxyoctadecanoyl), 1*-O-β-D-*glucopyranoside:* [113773-89-0] ***Cerebroside D***
$C_{43}H_{81}NO_9$ 756.114
Cryst. Sol. MeOH. Mp 178-189°. $[\alpha]_D^{20}$ +4.9 (c, 1 in MeOH).

N-*(2*R*-Hydroxy-3*E*-octadecenoyl), 1*-O-β-D-*glucopyranoside:* [98677-33-9] ***Cerebroside C***
$C_{43}H_{79}NO_9$ 754.098
Cryst. Mp 159-169°. $[\alpha]_D^{20}$ -6.2 (c, 1 in MeOH).

N-*(2*R*-Hydroxynonadecanoyl), 1*-O-β-D-*glucopyranoside:* [852627-54-4]
$C_{44}H_{83}NO_9$ 770.141
Solid. Mp 218-220°. $[\alpha]_D^{28}$ -13.2 (c, 0.05 in MeOH).

N-*(2*R*-Hydroxyeicosanoyl), 1*-O-β-D-*glucopyranoside:* [854008-50-7] ***Ircicerebroside***
$C_{45}H_{85}NO_9$ 784.168
Amorph. powder. $[\alpha]_D^{20}$ +9.1 (c, 0.02 in MeOH).

N-*(2*R*-Hydroxyheneicosanoyl), 1*-O-β-D-*glucopyranoside:* ***Sarcoehrenoside B***
$C_{46}H_{87}NO_9$ 798.195
Amorph. powder. $[\alpha]_D^{23}$ +51.3 (c, 0.3 in MeOH).

N-*(2*R*-Hydroxydocosanoyl), 1*-O-β-D-*glucopyranoside:* [120040-25-7] ***Cortenuamide C***
$C_{47}H_{89}NO_9$ 812.221
Powder.

N-*(2*R*-Hydroxytricosanoyl), 1*-O-β-D-*glucopyranoside:* [120029-72-3] ***Cortenuamide B***
$C_{48}H_{91}NO_9$ 826.248
Powder.

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-β-D-*glucopyranoside:* [96848-45-2] ***Cortenuamide A***
$C_{49}H_{93}NO_9$ 840.275
Powder.

N-*(2*R*-Hydroxy-17Z-tetracosenoyl), 1*-O-β-D-*glucopyranoside:* ***Catacerebroside A***
$C_{49}H_{91}NO_9$ 838.259
Amorph. solid. $[\alpha]_D^{20}$ -5 (c, 1.1 in MeOH).

Kawai, G. *et al., Biochim. Biophys. Acta*, 1982, **719**, 612; 1983, **754**, 243 (*isol*)
Kawai, G. *et al., Agric. Biol. Chem.*, 1985, **49**, 2137 (*isol, pmr*)
Kawai, G. *et al., J. Lipid Res.*, 1985, **26**, 338 (*struct*)
Mori, K. *et al., Tetrahedron*, 1985, **41**, 2369; 2379 (*synth*)
Kawai, G. *et al., J. Biol. Chem.*, 1986, **261**, 779-784 (*isol*)
Fogeldal, M. *et al., CA*, 1987, **160**, 29746 (*isol*)
Sitrin, R.D. *et al., J. Antibiot.*, 1988, **41**, 469 (*isol, pmr, cmr, ms, struct*)
Keusgen, M. *et al., Biochem. Syst. Ecol.*, 1996, **24**, 465-468 (*Cerebroside C, isol, marine fungus*)
Striegler, S. *et al., Monatsh. Chem.*, 1996, **127**, 755-761 (*activity*)
Koga, Y. *et al., J. Biol. Chem.*, 1998, **273**, 31985-31991 (*activity, pmr, cmr*)
Jenkins, K.M. *et al., Tet. Lett.*, 1999, **40**, 7637-7640 (*Thraustochytroside B*)
Wang, X.-Z. *et al., JOC*, 2000, **65**, 8146-8151 (*synth*)
Yue, J.-M. *et al., J. Nat. Prod.*, 2001, **64**, 1246-1248 (*Lactariamide B*)
Gao, J.M. *et al., Lipids*, 2001, **36**, 521-527 (*Polyporus ceramide*)
Dmitrenok, A.S. *et al., Russ. Chem. Bull. (Engl. Transl.)*, 2001, **50**, 1474-1477 (*Cladiella/Sinularia cerebrosides*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2002, **50**, 681-684 (*hexadecanoyl, 2-hydroxyacyl, octadecadienoyl*)
Batrakov, S.G. *et al., Chem. Phys. Lipids*, 2002, **117**, 45-51 (*Mortierella alpina cerebrosides*)
Zhan, Z.-J. *et al., J. Nat. Prod.*, 2003, **66**, 1013-1016 (*Catacerebroside A*)
Tan, J.W. *et al., Lipids*, 2003, **38**, 81-84 (*Cortenuamides A-C*)
Zhu, F. *et al., CA*, 2005, **142**, 370451c (*N-2-octadecenoyl glucoside*)
Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2005, **53**, 168-171 (*N-2-hydroxynonadecanoyl 1-glucoside*)
Zhang, G.-W. *et al., Helv. Chim. Acta*, 2005, **88**, 885-890 (*Ircicerebroside*)
Dong, J.-Y. *et al., Chem. Biodiversity*, 2009, **6**, 569-577 (*Cerebroside C*)

Cheng, S.-Y. *et al., J. Nat. Prod.*, 2009, **72**, 465-468 (*Sarcoehrenoside B*)

(Aminomethyl)phosphonic acid, 9CI A-446

[1066-51-9]

$H_2NCH_2P(O)(OH)_2$

CH_6NO_3P 111.037

Free acid exists in dipolar form. Metab. of Glyphosine and Glyphosate in plants. Cryst. Mp 308-310°. pK_{a1} 0.44; pK_{a2} 5.39; pK_{a3} 10.05 (25°,H_2O). pK_{a1} 1.85; pK_{a2} 5.35; pK_{a3} 10.

Di-Et ester: [50917-72-1] *Diethyl (aminomethyl)phosphonate*
$C_5H_{14}NO_3P$ 167.144
Yellowish liq. Dec. on attempted distn.

N-*Ac, di-Me ester: Dimethyl [(*N-*acetylamino)methyl]phosphonate*
$C_5H_{12}NO_4P$ 181.128
Solid. Mp 46-47°. $Bp_{0.008}$ 117-120°.

N-*Ac, di-Et ester: Diethyl [(*N-*acetylamino)methyl]phosphonate*
$C_7H_{16}NO_4P$ 209.181
Solid. Mp 38-39°. $Bp_{0.006}$ 122-123°.

N-*Benzoyl: (*N-*Benzoylaminomethyl)-phosphonic acid*
$C_8H_{10}NO_4P$ 215.145
Solid. Mp 182°.

N-*Benzoyl, di-Et ester: Diethyl [(*N-*benzoylamino)methyl]phosphonate*
$C_{12}H_{18}NO_4P$ 271.252
Solid. Mp 40-41°. $Bp_{0.006}$ 170-172°.

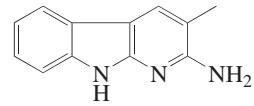
N-*Benzyl:* [49622-09-5] N-*(Benzylaminomethyl)phosphonic acid*
$C_8H_{12}NO_3P$ 201.161
Cryst. (H_2O). Mp 270-272°.

N-*Benzyl, di-Et ester:* [50917-70-9] *Diethyl [(benzylamino)methyl]phosphonate*
$C_{12}H_{20}NO_3P$ 257.269
Liq. $Bp_{0.02}$ 124-125°. n_D^{20} 1.5010.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1475C (*nmr*)
Chambers, J.R. *et al., JOC*, 1964, **29**, 832 (*synth*)
Ivanov, B.E. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1970, 2627; 1971, 2493, 2773; 1972, 2768; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1970, 2475; 1971, 2364, 2629; 1972, 2698 (*amides, synth*)
Garrigan-Lagrange, C. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1970, **67**, 1646 (*ir*)
Destrade, C. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1970, **67**, 2013 (*ir*)
Harvey, D.J. *et al., J. Chromatogr.*, 1973, **79**, 65 (*silyl derivs, ms*)
Darriet, M. *et al., Acta Cryst. B*, 1975, **31**, 469 (*cryst struct*)
Yamauchi, K. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 3285 (*di-Et ester, ir, pmr*)
Bel'skii, V.E. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1975, 1047; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1975, 958 (*derivs, synth, pmr, nmr*)
Rueppel, M.L. *et al., Org. Magn. Reson.*, 1976, **8**, 19 (*pmr, P-31 nmr*)
Kahovec, J. *et al., Org. Prep. Proced. Int.*, 1978, **10**, 285 (*synth*)
Wozniak, W. *et al., Talanta*, 1979, **26**, 1135 (*complexes*)
Oleksyszyn, J. *et al., Synthesis*, 1980, 906 (*synth*)
Latajka, Z. *et al., J. Mol. Struct.*, 1981, **70**, 49 (*struct*)
Kurguzova, A.M. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1982, 1265; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1982, 1126 (*derivs, props*)
Appleton, T.G. *et al., Aust. J. Chem.*, 1984, **37**, 1833 (*pmr, cmr, P-31 nmr*)
Tyka, R. *et al., Synthesis*, 1984, 218 (*synth*)
Constantin, E. *et al., Org. Mass Spectrom.*, 1986, **21**, 431 (*ms*)
Org. Synth., 1987, **65**, 119 (*synth, pmr*)
Soroka, M. *et al., Synthesis*, 1988, 370 (*di-Me ester*)
Harris, R.K. *et al., Magn. Reson. Chem.*, 1989, **27**, 470 (*cmr, P-31 nmr, cryst struct*)
Glowacki, Z. *et al., Magn. Reson. Chem.*, 1989, **27**, 897 (*cmr, P-31 nmr*)
Matczak-Jon, E. *et al., Inorg. Chim. Acta*, 1990, **173**, 85 (*complexes, cmr, P-31 nmr*)
Gajda, T. *et al., Synth. Commun.*, 1992, **22**, 2193-2203 (*di-Et ester*)
Ali, M.M. *et al., Chem. Eur. J.*, 2008, **14**, 7250-7248 (*di-Et ester*)
Reddy, K.N. *et al., J. Agric. Food Chem.*, 2008, **56**, 2125-2130 (*detn, glc*)
Goldeman, W. *et al., ARKIVOC*, 2010, **xi**, 360-369 (*synth*)

2-Amino-3-methyl-9*H*-pyrido[2,3-*b*]indole A-447

*3-Methyl-1*H*-pyrido[2,3-*b*]indol-2-amine, 9CI. 2-Amino-3-methyl-α-carboline. Glob-P-1. MeA-α-C* [68006-83-7]



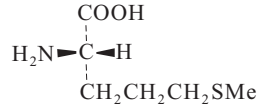
$C_{12}H_{11}N_3$ 197.239
Constit. of cooked beef and chicken. Cryst. ($CHCl_3$/hexane). Sol. MeOH, DMSO. Mp 215-218°.

▶ Mutagen. Possible human carcinogen. Exp. carcinogen. UU9354380

Yoshida, D. *et al., Biochem. Biophys. Res. Commun.*, 1978, **83**, 915 (*cryst struct, tox*)
Yoshida, D. *et al., Agric. Biol. Chem.*, 1979, **43**, 1769
Matsumoto, T. *et al., Agric. Biol. Chem.*, 1981, **45**, 2031 (*synth, ms*)
IARC Monogr., 1986, **40**, 253; 1987, *Suppl. 7*, 65 (*rev, tox*)
Hibino, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 79 (*synth, pmr*)
Venishi, J. *et al., JOC*, 1993, **58**, 4382 (*synth, pmr*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*occur, hplc, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALD750

2-Amino-5-(methylthio)pentanoic acid A-448

5-(Methylthio)norvaline, 9CI, 8CI. Homomethionine [5632-95-1]



(*S*)–*form*

$C_6H_{13}NO_2S$ 163.24

(S)-form [25148-30-5]
L-form
Isol. from cabbage and horseradish. Plates (EtOH aq.). Mp 235° Mp 247-248° dec. $[\alpha]_D^{25.5}$ +21 (c, 0.3 in 6*M* HCl).

(±)-form [6094-76-4]
Hexagonal plates (EtOH). Mp 247-248°.

Kjaer, A. *et al., Acta Chem. Scand.*, 1955, **9**, 721 (*synth*)
Sugii, M. *et al., Chem. Pharm. Bull.*, 1964, **12**, 1115 (*isol*)
Suketa, Y. *et al., Chem. Pharm. Bull.*, 1970, **18**, 249 (*isol, ord, biosynth*)
Vriesema, B.K. *et al., Tet. Lett.*, 1986, **27**, 2045 (*resoln, cd, abs config*)

Aminomethyltransferase A-449

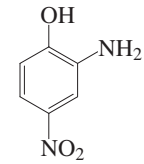
E.C. 2.1.2.10. Protein-S*-aminomethyldihydrolipoyllysine:tetrahydrofolate aminomethyltransferase (ammonia-forming)* [37257-08-2]

Enzyme. Isol. from chicken liver. Forms the T-protein component of the glycine cleavage system (glycine synthase).

Okamura-Ikeda, K. *et al., J. Biol. Chem.*, 1982, **257**, 137-139 (*chicken liver*)
Lokanath, N.K. *et al., Acta Cryst. D*, 2004, **60**, 1450-1452 (*Pyrococcus horikoshii, cryst struct*)

2-Amino-4-nitrophenol, 9CI A-450

[99-57-0]



$C_6H_6N_2O_3$ 154.125
Orange prisms. Mp 142-143° Mp 176-177° Mp 195-198°.

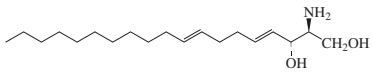
▶ Eye irritant. LD_{50} (mus, orl) 850 mg/kg. Exp. neoplastic agent. SJ6300000

Propyl ether: [553-79-7] *5-Nitro-2-propoxyaniline. P 4000*
$C_9H_{12}N_2O_3$ 196.205
Once proposed for use as an artificial sweetener but now prohibited from use in food.

Propyl ether, N-*Ac:* [553-20-8] N-*(5-Nitro-2-propoxyphenyl)acetamide, 9CI. 5′-Nitro-2′-propoxyacetanilide, 8CI. Acetylaminonitropropoxybenzene.* ***Falimint***
$C_{11}H_{14}N_2O_4$ 238.243
Sweetening agent. Cryst. Mp 102-103° Mp 202-203°.

UK Pat., 1948, 597 835 (*synth, Falimint*)
Hannig, E. *et al., Arzneim.-Forsch.*, 1953, **3**, 310 (*pharmacol, Falimint*)
Becher, M. *et al., Pharmazie*, 1989, **44**, 56; 1990, **45**, 440; 534 (*metab, Falimint*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2079 (*propyl ether*)

2-Amino-4,8-nonadecadiene-1,3-diol A-451

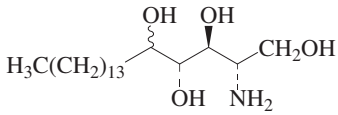


$C_{19}H_{37}NO_2$ 311.507

(2S,3R,4E,8E)-form

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-*β-D-glucopyranoside:* [189272-90-0] ***Lucyobroside***
$C_{39}H_{73}NO_9$ 700.007
Constit. of *Luffa cylindrica* (smooth luffa). Mp 140-142°.
Fang, Z. *et al., CA*, 1997, **126**, 303677n (*isol, struct, Lucyobroside*)

2-Amino-1,3,4,5-nonadecanetetrol A-452

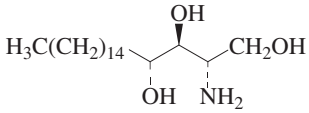


$C_{19}H_{41}NO_4$ 347.537

(2S,3S,4R,5ξ)-form

N-*(6Z-Tetracosenoyl):* [921604-68-4] ***Longifoamide B***
$C_{43}H_{85}NO_5$ 696.148
Constit. of *Mentha longifolia* (wild mint). Powder. Mp 90°. $[\alpha]_D^{28}$ +17.3 (c, 0.33 in Py).
Ali, M.S. *et al., Nat. Prod. Res.*, 2006, **20**, 953-960 (*isol, pmr, cmr, ms*)

2-Amino-1,3,4-nonadecanetriol A-453



$C_{19}H_{41}NO_3$ 331.538

(2S,3S,4R)-form

N-*Hexadecanoyl:* [906478-03-3]
$C_{35}H_{71}NO_4$ 569.95

N-*Heptadecanoyl:* [906478-06-6]
$C_{36}H_{73}NO_4$ 583.977

N-*Docosanoyl:* [636589-64-5]
$C_{41}H_{83}NO_4$ 654.111

N-*(6Z-Tetracosenoyl):* ***Longifoamide A***
$C_{43}H_{85}NO_4$ 680.149
Constit. of *Mentha longifolia* (wild mint). Powder. Mp 98-100°. $[\alpha]_D^{28}$ +16.1 (c, 0.61 in Py).

N-*(2*R*-Hydroxynonadecanoyl):*
$C_{38}H_{77}NO_5$ 628.03
Cryst. (MeOH). Mp 101-103°. $[\alpha]_D^{25}$ +8.5 (c, 0.1 in Py).

N-*(2*R**,3*S**-Dihydroxyoctacosanoyl), 1*-O-*β-D-glucopyranoside:*
$C_{53}H_{105}NO_{11}$ 932.413

N-*(2*R**,3*S**-Dihydroxyoctacosanoyl), 1*-O-*[β-D-galactopyranosyl-(1→4)-β-D-glucopyranoside]:*
$C_{59}H_{115}NO_{16}$ 1094.555

N-*(2*R**,3*S**-Dihydroxyoctacosanoyl), 1*-O-*[α-D-fucopyranosyl-(1→3)-[α-D-galactopyranosyl-(1→4)]-β-D-glucopyranoside]:*
$C_{65}H_{125}NO_{20}$ 1240.697

Muralidhar, P. *et al., Chem. Pharm. Bull.*, 2003, **51**, 1193-1195 (*N-docosanoyl*)
Aiello, A. *et al., Eur. J. Org. Chem.*, 2003, 734-739 (*Microcosmus sulcatus constits*)
Krishna, N. *et al., J. Nat. Prod.*, 2004, **67**, 1423-1425 (*N-2-hydroxynonadecanoyl*)
Ali, M.S. *et al., Nat. Prod. Res.*, 2006, **20**, 953-960 (*Longifoamide A*)
Guzii, A.G. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2006, **32**, 288-294 (*Oceanapia constits*)

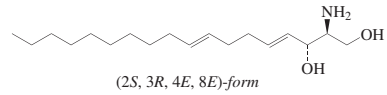
2-Amino-11-nonadecene-1,3,4-triol A-454

$H_3C(CH_2)_6CH{=}CH(CH_2)_6CH(OH)$-$CH(OH)CH(NH_2)CH_2OH$
$C_{19}H_{39}NO_3$ 329.522

N-*(2-Hydroxyeicosanoyl), 1*-O-*β-D-glucopyranoside:* [230295-19-9] ***Culinariside***
$C_{45}H_{87}NO_{10}$ 802.183
Constit. of the seeds of *Lens culinaris* (lentil). Stereochem. not determined.
Hong, Y. *et al., J. Chin. Pharm. Sci.*, 1999, **8**, 8-10

2-Amino-4,8-octadecadiene-1,3-diol A-455

4,8-Sphingadiene. 4,8-Octadecasphingadiene. 4,8-Sphingadienine



(2S, 3R, 4E, 8E)-form

$C_{18}H_{35}NO_2$ 297.48

(2S,3R,4E,8E)-form

N-*Hexadecanoyl:* [141980-53-2]
$C_{34}H_{65}NO_3$ 535.892
Isol. from *Vigna angularis* (azuki bean). Solid. Mp 82-83°. $[\alpha]_D^{25}$ -8 (c, 0.5 in $CHCl_3$).

N-*(2*R*-Hydroxytetradecanoyl), 1*-O-*β-D-glucopyranoside:* [212777-97-4] *AS 1-1*
$C_{38}H_{71}NO_9$ 685.98
Isol. from garlic bulbs. Amorph. powder. Mp 197-200°. $[\alpha]_D^{28}$ +5.2 (c, 0.25 in propanol).

N-*(2*R*-Hydroxypentadecanoyl), 1*-O-*β-D-glucopyranoside:* [212777-98-5] *AS 1-2*
$C_{39}H_{73}NO_9$ 700.007
Isol. from garlic bulbs. Amorph. powder. Mp 195-200°. $[\alpha]_D^{28}$ +8.8 (c, 0.13 in 1-propanol).

N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* [114297-20-0] ***Soyacerebroside I***. *AS 1-4*
$C_{40}H_{75}NO_9$ 714.034
Isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and bulbs of *Allium sativum* var. *sativum* (garlic). Hygroscopic granules or amorph. solid. Mp 184-186° Mp 193-197°. $[\alpha]_D^{24}$ +10.5 (c, 0.30 in MeOH/$CHCl_3$, 3:2).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* [606125-06-8] ***Longancerebroside I***
$C_{48}H_{91}NO_9$ 826.248
Constit. of *Euphoria longana* (longan). Cryst. (MeOH). Mp 184-186°. $[\alpha]_D^{25}$ +17.2 (c, 1.1 in MeOH).

(2S,3R,4E,8Z)-form

N-*Hexadecanoyl, 1*-O-*β-D-glucopyranoside:* [127842-89-1]
$C_{40}H_{75}NO_8$ 698.034
Constit. of *Lycium chinense* (Chinese boxthorn). Amorph. powder. $[\alpha]_D^{25}$ +1.2 (c, 0.1 in MeOH).

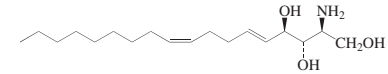
N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β-D-glucopyranoside:* [115074-93-6] ***Soyacerebroside II***. *AS 1-3*
$C_{40}H_{75}NO_9$ 714.034
Isol. from *Tetragonia tetragonoides* (New Zealand spinach), *Glycine max* (soybean) and bulbs of *Allium sativum* var. *sativum* (garlic). Hygroscopic granules or amorph. solid. Mp 192-194° (183°). $[\alpha]_D^{24}$ +13.4 (c, 0.43 in MeOH/$CHCl_3$ 3:2) (+4.6).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:* [220873-86-9] ***Stenochlaena cerebroside***. *Longancerebroside II*
$C_{48}H_{91}NO_9$ 826.248
Constit. of *Euphoria longana* (longan). $[\alpha]_D^{25}$ +7.9 (c, 0.09 in MeOH).

[127912-01-0]

Mori, K. *et al., Annalen*, 1988, 807-814 (*abs config, ir, pmr, cmr, synth, bibl, Soyacerebroside*)
Shibuya, H. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2933-2938 (*Soyacerebrosides*)
Shin, J. *et al., J. Nat. Prod.*, 1995, **58**, 948-953 (*N-hexadecanoyl*)
Kim, S.Y. *et al., J. Nat. Prod.*, 1997, **60**, 274-276 (*Lycium chinense constit*)
Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS compounds*)
Liu, H. *et al., Phytochemistry*, 1998, **49**, 2403-2408 (*Stenochlaena cerebroside*)
Anjaneyulu, V. *et al., Indian J. Chem., Sect. B*, 1999, **38**, 457-460 (*N-hexadecanoyl*)
Ryu, J. *et al., Arch. Pharmacal Res.*, 2003, **26**, 138-142 (*Longancerebrosides I,II*)

2-Amino-5,9-octadecadiene-1,3,4-triol A-456



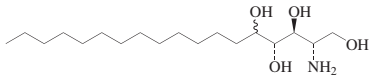
$C_{18}H_{35}NO_3$ 313.479

(2S,3S,4R,5E,9Z)-form

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β-D-glucopyranoside:*
$C_{48}H_{91}NO_{10}$ 842.248
Constit. of the flowers of *Sesamum indicum* (sesame).
Hu, Y.-M. *et al., Yaoxue Xuebao*, 2007, **42**, 286-291 (*isol, pmr, cmr*)

2-Amino-1,3,4,5-octadecanetetrol A-457

4,5-Dihydro-4,5-dihydroxysphingosine



(2*S*,3*S*,4*R*,5ξ)-*form*

$C_{18}H_{39}NO_4$ 333.51

(2*S*,3*S*,4*R*,5ξ)-*form*

N-*(6*E-*Tetracosenoyl), 3*-O-*β*-D-*glucopyranoside:* ***Longifoside A***
$C_{48}H_{93}NO_{10}$ 844.263
Constit. of *Mentha longifolia* (horsemint). $[\alpha]_D^{28}$ +111.8 (c, 0.76 in $CHCl_3$) (as per-Ac).

(*all*-ξ)-*form*

N-*Hexadecanoyl:* [141364-80-9] *UF 131*
$C_{34}H_{69}NO_5$ 571.923
Mp 143-144°. $[\alpha]_D$ +8.2 (c, 0.5 in MeOH).

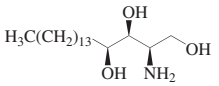
N-*Tetracosanoyl:* [302953-31-7] ***Coelarthenol***
$C_{42}H_{85}NO_5$ 684.137
Powder. Mp 133.5-135°. $[\alpha]_D$ +11.4 (c, 0.18 in Py).

N-*Pentacosanoyl:* [155230-16-3]
$C_{43}H_{87}NO_5$ 698.164
Mp 148-149°.

Garg, H.S. *et al., Tet. Lett.*, 1992, **33**, 1641-1644 (*N-hexadecanoyl*)
Rao, C.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 97-98 (*N-pentacosanoyl*)
Ali, M. *et al., Nat. Prod. Sci.*, 2000, **6**, 61-65 (*Coelarthenol*)
Ali, M.S. *et al., Nat. Prod. Res.*, 2006, **20**, 715-723 (*Longifoside A*)

2-Amino-1,3,4-octadecanetriol, 8CI A-458

C_{18}-Phytosphingosine. 4-Hydroxysphinganine



(2*R*,3*S*,4*S*)-*form*

$C_{18}H_{39}NO_3$ 317.511

(2*S*,3*S*,4*R*)-*form* [554-62-1]
D-ribo-*form*
Amorph. powder. Mp 103° (95-97°). $[\alpha]_D^{20}$ +10.3 (Py) (+9.4).

N-*Hexadecanoyl:* [111149-09-8] ***Armillaramide***
$C_{34}H_{69}NO_4$ 555.923
Isol. from *Armillaria mellea* (honey mushroom). Amorph. powder. Mp 113-117°. $[\alpha]_D^{26}$ +14.3 (c, 0.21 in Py).

N-*(9*Z,*12*Z-*Octadecadienoyl):* [173059-97-7]
$C_{36}H_{69}NO_4$ 579.945
Isol. from the mushroom *Grifola frondosa* (maitake). $[\alpha]_D^{24}$ +20 (c, 0.05 in Py).

N-*Nonadecanoyl:* [844866-88-2]
$C_{37}H_{75}NO_4$ 598.004
Isol. from *Tuber indicum* (Chinese truffle). Solid. Mp 122-124°. $[\alpha]_D^{28}$ +19.2 (c, 0.5 in $CHCl_3$).

N-*(2*R-*Hydroxydocosanoyl):* [305363-08-0]
$C_{40}H_{81}NO_5$ 656.084
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{22}$ +12.9 (c, 0.1 in Py).

N-*Tricosanoyl:* [844866-89-3]
$C_{41}H_{83}NO_4$ 654.111
Isol. from *Tuber indicum* (Chinese truffle).

N-*(2*R-*Hydroxytricosanoyl):* [305363-09-1]
$C_{41}H_{83}NO_5$ 670.11
Isol. from the mushroom *Grifola frondosa* (maitake) and the truffle *Tuber indicum*. Amorph. powder. $[\alpha]_D^{20}$ +14.9 (c, 0.07 in Py).

N-*(2*R-*Hydroxypentacosanoyl):* [305363-10-4]
$C_{43}H_{87}NO_5$ 698.164
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. Mp 145°. $[\alpha]_D^{21}$ +13.8 (c, 0.1 in Py).

N-*(2*R-*Hydroxyhexacosanoyl):* [164988-96-9]
$C_{44}H_{89}NO_5$ 712.191
Isol. from the mushroom *Grifola frondosa* (maitake). Amorph. powder. $[\alpha]_D^{22}$ +11.1 (c, 0.1 in Py).

(2ξ,3ξ,4ξ)-*form*

N-*(2ξ-Hydroxytetracosanoyl):* [859513-39-6] ***Soyasphingosine B***
$C_{42}H_{85}NO_5$ 684.137
Constit. of the stems of *Glycine max* (soya). Cryst. ($CHCl_3$). Mp 150-151°.

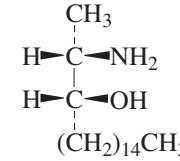
N-*(2ξ-Hydroxypentacosanoyl):* [859513-38-5] ***Soyasphingosine A***
$C_{43}H_{87}NO_5$ 698.164
Constit. of the stems of *Glycine max* (soya). Cryst. ($CHCl_3$). Mp 150-151°.

N-*(2ξ,3ξ-Dihydroxy-?-tetracosenoyl):* [260545-65-1] ***Tuberceramide***
$C_{42}H_{83}NO_6$ 698.121
Constit. of the seeds of *Allium tuberosum* (Chinese chives). Amorph. powder. Mp 148-149°. $[\alpha]_D^{21}$ +28 (c, 0.02 in MeOH). Posn. of double bond not determined.

Prostenik, M. *et al., Tetrahedron*, 1965, **21**, 651-655 (*synth*)
Gigg, J. *et al., JCS(C)*, 1966, 1872-1876; 1876-1879 (*2S,3S,4R-form, synth*)
Schmidt, R.R. *et al., Carbohydr. Res.*, 1988, **174**, 169-179 (*stereoisomers, synth*)
Lin, G. *et al., Tetrahedron*, 1996, **52**, 2187-2192 (*synth*)
Zou, Z.-M. *et al., J. Asian Nat. Prod. Res.*, 1999, **2**, 55-61 (*Tuberceramide*)
Yaoita, Y. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1356-1358 (*Grifola frondosa ceramides*)
Gao, J.M. *et al., Chin. Chem. Lett.*, 2001, **12**, 139-140; 2002, **13**, 325-326 (*Armillaramide, Tuber indicum ceramide*)
Yaoita, Y. *et al., Nat. Med. (Tokyo)*, 2003, **57**, 189-191 (*N-9,12-octadecadienoyl*)
Du, C. *et al., Zhongguo Yaoke Daxue Xuebao*, 2003, **34**, 506-508 (*Soyasphingosines A,B*)
Gao, J.-M. *et al., Chem. Phys. Lipids*, 2004, **131**, 205-213 (*N-nonadecanoyl, N-tricosanoyl*)

2-Amino-3-octadecanol A-459

Spisulosine*. ES 285*
[247067-50-1 2S,3S, 378754-86-0 2R,3S]



$C_{18}H_{39}NO$ 285.512

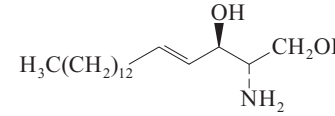
(2*S*,3*R*)-*form* [196497-48-0]
Isol. from the clam *Spisula polynyma*. Solid (as hydrochloride). Mp 66-67°. $[\alpha]_D^{26}$ +24.9 (c, 1 in $CHCl_3$).

[378753-73-2 (hydrochloride)]

Pat. Coop. Treaty (WIPO), 1999, 99 52 521 (*isol, synth*)
Cuadros, R. *et al., Cancer Lett.*, 2000, **152**, 23-29 (*isol, activity*)
Jimeno, J.M. *et al., Anti-Cancer Drugs*, Suppl. 1, 2002, **13**, S15-S19 (*rev*)
Den Brok, M.W. *et al., J. Chromatogr., A*, 2003, **1020**, 251-258 (*anal*)
Stokvis, E. *et al., J. Mass Spectrom.*, 2003, **38**, 548-554 (*anal*)
Yun, J.M. *et al., JOC*, 2003, **68**, 7675-7680 (*synth*)
Allepuz, A.C. *et al., Eur. J. Org. Chem.*, 2009, 6172-6178 (*synth*)
Amarante, G.W. *et al., Tet. Lett.*, 2010, **51**, 2597-2599 (*synth*)
Ghosal, P. *et al., Tet. Lett.*, 2010, **51**, 4140-4142 (*synth*)
Dinda, S.K. *et al., Tetrahedron*, 2010, **66**, 9304-9309 (*synth*)
Malik, G. *et al., JOC*, 2011, **76**, 7438-7448 (*synth*)

2-Amino-4-octadecene-1,3-diol, 9CI A-460

4-Sphingenine. C_{18}*-Sphingosine*



(2*S*,3*R*,4*E*)−*form*

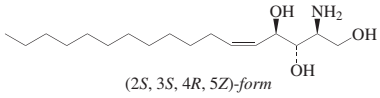
$C_{18}H_{37}NO_2$ 299.496
Many syntheses reported of various stereoisomers.

(2*S*,3*R*,4*E*)-*form* [123-78-4]
D-erythro-trans-*form*
Cryst. (Et_2O). Mp 80-84° (79-81°).

N-*(2*R-*Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:* [154967-87-0] *AS 1-5*
$C_{40}H_{77}NO_9$ 716.05
Constit. of *Allium sativum* (garlic) bulbs. Amorph. powder. Mp 205-210°. $[\alpha]_D^{28}$ +8.3 (c, 0.15 in propanol).

Inagaki, M. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1153-1156 (*AS 1-5*)

2-Amino-5-octadecene-1,3,4-triol A-461



(2*S*, 3*S*, 4*R*, 5*Z*)-*form*

$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,5*Z*)-*form*

N-*(6*E*-Tetracosenoyl), 3*-O-*β*-D-*glucopyranoside:* ***Longifoside B***
$C_{48}H_{91}NO_9$ 826.248
Constit. of *Mentha longifolia* (horsemint). $[\alpha]_D^{28}$ +109 (c, 0.3 in $CHCl_3$) (as per-Ac).

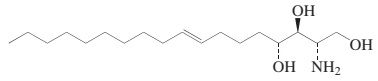
(2ξ,3ξ,4ξ,5*E*)-*form*

N-*(2-Hydroxyhexadecanoyl):* [479411-46-6]
$C_{34}H_{67}NO_5$ 569.907
Cryst. ($CHCl_3$/MeOH). Mp 144-145°. $[\alpha]_D^{25}$ +7.2 (c, 0.1 in MeOH).

Parvataneni, R. *et al., J. Indian Chem. Soc.*, 2002, **79**, 732-738 (*N-2-hydroxyhexadecanoyl*)
Ali, M.S. *et al., Nat. Prod. Res.*, 2006, **20**, 715-723 (*Longifoside B*)

2-Amino-8-octadecene-1,3,4-triol, 9CI A-462

[81520-97-0]



(2*S*,3*S*,4*R*, *E*)-*form*

$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,8*E*)-*form* [3687-54-5]
D-ribo-trans-*form*. *Dehydrophytosphingosine*
Present in soybean phospholipids. Cryst. (Et_2O). Mp 92-94°. $[\alpha]_D^{25}$ +8.5 (c, 1.2 in EtOH).

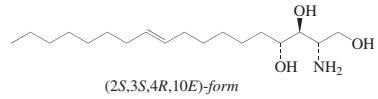
N-*(2*R*-Hydroxyhexadecanoyl), 1*-O-*β*-D-*glucopyranoside:* [239449-41-3] ***Araliacerebroside***
$C_{40}H_{77}NO_{10}$ 732.049
Constit. of the root bark of *Aralia elata* (Japanese angelica tree). Amorph. powder. Mp 215-216°. $[\alpha]_D^{20}$ +14.6 (c, 0.53 in MeOH).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* [606125-07-9] ***Momorcerebroside I***
$C_{48}H_{93}NO_{10}$ 844.263
Constit. of *Momordica charantia* (bitter melon). Powder. Mp 203-205°. $[\alpha]_D^{20}$ +12.7 (c, 0.1 in $CHCl_3$/MeOH).

[25277-37-6, 51153-53-8]

Carter, H.E. *et al., Biochemistry*, 1963, **2**, 389-393 (*Dehydrophytosphingosine, isol, struct*)
Kang, S.S. *et al., J. Nat. Prod.*, 1999, **62**, 1059-1060 (*Araliacerebroside*)
Yinggang, Y. *et al., Lipids*, 2004, **39**, 907-913 (*Momorcerebroside I*)

2-Amino-10-octadecene-1,3,4-triol A-463



(2*S*,3*S*,4*R*,10*E*)-*form*

$C_{18}H_{37}NO_3$ 315.495

(2*S*,3*S*,4*R*,10*E*)-*form*

N-*(2*R*-Hydroxydocosanoyl), 1*-O-*β*-D-*glucopyranoside:* [1206850-06-7] ***Gynuraoside***
$C_{46}H_{89}NO_{10}$ 816.21
Amorph. powder. Mp 123-125°. $[\alpha]_D^{20}$ +35.8 (c, 0.75 in Py).

N-*(2*R*-Hydroxytricosanoyl), 1*-O-*β*-D-*glucopyranoside:* [1214258-36-2]
$C_{47}H_{91}NO_{10}$ 830.237
Amorph. powder. Mp 123-125°.

N-*(2*R*-Hydroxytetracosanoyl):*
$C_{42}H_{83}NO_5$ 682.121
Amorph. powder. $[\alpha]_D^{20}$ +11.1 (c, 1 in Py).

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* [1198320-81-8]
$C_{48}H_{93}NO_{10}$ 844.263
Constit. of the stems of *Cucumis sativus* (cucumber).

N-*(2ξ,3ξ-Dihydroxytetracosanoyl):* [1198320-80-7]
$C_{42}H_{83}NO_6$ 698.121
Constit. of the stems of *Cucumis sativus* (cucumber).

(2*S*,3*S*,4*R*,10*Z*)-*form*

N-*(2*R*-Hydroxytetracosanoyl), 1*-O-*β*-D-*glucopyranoside:* [1244547-34-9]
$C_{48}H_{93}NO_{10}$ 844.263
Amorph. powder. Mp 123-125°. $[\alpha]_D^{20}$ +35.8 (c, 0.75 in Py). There is a large degree of coincidence in the data between this compd. and Gynuraoside which has 2 less CH_2 groups in its struct.

Zhan, Z.-J. *et al., Zhiwu Xuebao (Acta Bot. Sin.)*, 2003, **45**, 248-252 (*Engleromyces constit*)
Chen, L. *et al., Chin. Chem. Lett.*, 2009, **20**, 1091-1093 (*Gynuraoside*)
Chen, L. *et al., Fitoterapia*, 2009, **80**, 517-520 (*N-hydroxytricosanoyl 1-glucoside*)
Chen, L. *et al., Nat. Prod. Res.*, 2009, **23**, 1330-1336 (*N-hydroxytetracosanoyl 1-glucoside*)
Tang, J. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2009, **21**, 66-69 (*Cucumis sativus constits*)

4-Aminooctanoic acid A-464

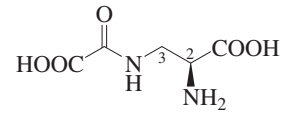
4-Aminocaprylic acid
$H_3C(CH_2)_3CH(NH_2)CH_2CH_2COOH$
$C_8H_{17}NO_2$ 159.228
Isol. is tentative.

(±)-*form*
Mp 147-149°.
Hydrochloride: Mp 136-137°.
N-*4-Methylbenzenesulfonyl:* Mp 100-101°.

Gol'dfarb, Y.L. *et al., CA*, 1957, **51**, 1839g (*synth*)
Jadhav, K.A. *et al., J. Univ. Bombay, Sci.*, 1960, **29**, 11 (*isol*)
Fabrichnyi, B.P. *et al., Zh. Obshch. Khim.*, 1964, **34**, 3878 (*synth*)

2-Amino-3-(oxalylamino)propanoic acid A-465

3-[(Carboxycarbonyl)amino]alanine, 9CI. (2-Amino-2-carboxyethyl)oxamic acid, 8CI. 2,3-Diamino-3-N-*oxalylpropanoic acid*. ***Dencichin***. *β-ODAP* [7554-90-7]



$C_5H_8N_2O_5$ 176.129

(*S*)-*form* [5302-45-4]
L-*form*
Isol. from *Lathyrus sativus* (chickling pea) and *Panax notoginseng* (sanchi). Cryst. (H_2O) (dimorph.). Mp 206° dec. $[\alpha]_D^{27}$ -36.9 (c, 0.66 in 4*N* HCl).
▶ Neurotoxin. RO4555000

[58086-31-0, 120963-05-5, 61238-52-6]

Rao, S.L.R. *et al., Biochemistry*, 1964, **3**, 432 (*isol, synth*)
Murti, V.V.S. *et al., Phytochemistry*, 1964, **3**, 73 (*ir*)
Bell, E.A. *et al., Phytochemistry*, 1966, **5**, 1211 (*occur*)
Rao, S.L.N. *et al., Biochemistry*, 1975, **14**, 5218 (*synth*)
O'Brien, P. *et al., Phytochemistry*, 1982, **21**, 2001 (*dimorphism, ir, bibl*)
Euerby, M.R. *et al., J. Chromatogr.*, 1989, **466**, 407 (*hplc, resoln*)
Davis, A.J. *et al., J. Inorg. Biochem.*, 1990, **39**, 209 (*isol*)
Davis, A.J. *et al., Phytochemistry*, 1991, **30**, 3635 (*cryst struct*)
Yan, Z.-Y. *et al., Phytochemistry*, 2006, **67**, 107-121 (*rev, chem, biosynth, activity*)

3-Amino-2-(oxalylamino)propanoic acid A-466

3-Amino-N-*(carboxycarbonyl)alanine, 9CI. (2-Amino-1-carboxyethyl)oxamic acid, 8CI. 2,3-Diamino-2*-N-*oxalylpropanoic acid* [7554-89-4]

$C_5H_8N_2O_5$ 176.129

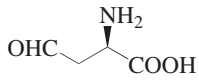
(*S*)-*form* [61277-72-3]
L-*form*
Present in seeds of *Lathyrus sativus* (chickling pea). Cryst. + ½H_2O. Mp 170-172°. $[\alpha]_D^{21}$ +14.7 (c, 2 in 1*M* KOH).

[61238-53-7]

Bell, E.A. *et al., Phytochemistry*, 1966, **5**, 1211 (*isol*)
Roy, D.N. *et al., Curr. Sci.*, 1968, **37**, 395 (*isol*)
Wu, G. *et al., Phytochemistry*, 1976, **15**, 1257 (*synth*)

2-Amino-4-oxobutanoic acid, 9CI A-467

2-Aminosuccinaldehydic acid. 2-Amino-4,4-dihydroxybutanoic acid. β-Aspartaldehydic acid. Aspartic semialdehyde. Aspartyl semialdehyde. β-Formylalanine. Aspartal. ASA† [498-20-4]



(*R*)-*form*

$C_4H_7NO_3$ 117.104

Exists predominantly as the covalent hydrate in aq. soln. Fails to undergo normal aldehyde condensation reactions.

(*R*)-*form*

N-*Benzyloxycarbonyl, Me ester:* [112229-40-0]
Mp 161-163°. $[\alpha]_D$ -21 (in $CHCl_3$).

(*S*)-*form* [2338-03-6]
L-form
Isol. from pea *Pisum sativum*. $[\alpha]_D^{20}$ +3.2 (H_2O). Reasonably stable in acid soln., dec. in neutral soln. or on drying.

N-tert-*Butyloxycarbonyl, Me ester:* [87884-14-8]
$C_{10}H_{17}NO_5$ 231.248
Oil. $[\alpha]_D$ +34 (c, 2.1 in $CHCl_3$).

N-*Benzyloxycarbonyl, Me ester:* [60684-59-5]
Mp 161-163°. $[\alpha]_D$ +21 (in $CHCl_3$).

N-*Phthaloyl, Me ester:* [137278-36-5]
$C_{13}H_{11}NO_5$ 261.234
Solid. Mp 64-68°. $[\alpha]_D^{20}$ -50.5 (c, 1.7 in $CHCl_3$).

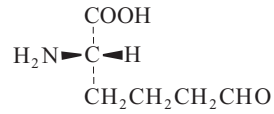
N-*Phthaloyl, Et ester:* [155095-04-8]
$C_{14}H_{13}NO_5$ 275.26
Oil. $[\alpha]_D^{20}$ -26.2 (c, 1.07 in $CHCl_3$).

(±)-*form* [15106-57-7]
Reasonably stable in acid soln. In neutral soln. or in dry state dec. in a few hours. Usual aldehyde derivs. are not readily formed.

Black, S. *et al., J. Biol. Chem.*, 1955, **213**, 39-50 (*synth*)
Gilvarg, C. *et al., J. Biol. Chem.*, 1962, **237**, 482-484 (*biochem*)
Neuberger, A. *et al., JCS*, 1962, 3963-3968 (*synth*)
Shames, S.L. *et al., Arch. Biochem. Biophys.*, 1984, **235**, 359-370 (*biochem*)
Eur. Pat., 1987, 230 037 (*synth, esters*)
Baldwin, J.E. *et al., Tet. Lett.*, 1987, **28**, 3605-3608 (*synth*)
Dehmlow, E.V. *et al., Synthesis*, 1993, 1225-1226 (*phthalimides*)
Meffre, P. *et al., Synthesis*, 1995, 1111-1114 (*phthalimides*)
Coulter, C.V. *et al., Tetrahedron*, 1996, **52**, 7127-7136 (*S-form, synth, nmr, props*)
Org. Synth., 1999, **76**, 123-132 (*N-phthalimide Me ester*)
Roberts, S.J. *et al., ARKIVOC*, 2004, **x**, 166-177 (*S-form, synth*)
Dondoni, A. *et al., JOC*, 2007, **72**, 7677-7687 (*S-form, N-Boc Me ester*)

2-Amino-6-oxohexanoic acid A-468

6-Oxonorleucine, 9CI. 5-Formylnorvaline, 8CI. α-Aminoadipic semialdehyde. 2-Aminoadipaldehydic acid. Allysine [1962-83-0]



(*S*)–*form*

$C_6H_{11}NO_3$ 145.158

In equil. with the anhydro-form 2,3,4,5-Tetrahydro-2-pyridinecarboxylic acid. Does not show typical aldehyde reactions.

(*S*)-*form*
L-form
Found in collagen, elastin and heart muscle. $[\alpha]_D^{25}$ -5.1 (c, 3 in H_2O) (ca. 90% pure).

(±)-*form*
Obt. only in soln.

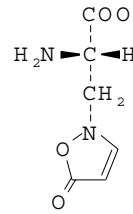
2,4-Dinitrophenylhydrazone:
Cryst. (EtOH). Mp 116-117°. Formed only slowly (5 days at 5°).

N-*Ac:*
$C_8H_{13}NO_4$ 187.195
Mp 95-96°.

Aspen, A.J. *et al., Biochemistry*, 1962, **1**, 600
Basso, L.V. *et al., J. Biol. Chem.*, 1962, **237**, 2239
Rodwell, V.W. *et al., Methods Enzymol., Part B*, 1971, **17**, 188 (*synth, bibl*)

α-Amino-5-oxo-2(5*H*)-isoxazolepropanoic acid, 9CI A-469

α-Amino-5-oxo-3-oxazoline-2-propionic acid, 8CI. β-(Isoxazolin-5-on-2-yl)alanine. 2-Alanyl-3-isoxazolin-5-one



$C_6H_8N_2O_4$ 172.14

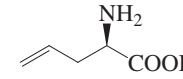
(*S*)-*form* [59476-61-8]
L-form
Amino acid from the roots of pea seedlings (*Pisum* spp.). Fairly sol. H_2O. Mp 203-205° dec. $[\alpha]_D^{20}$ -62 (c, 1.4 in H_2O). Base-labile. λ_{max} 265 (ϵ 12300) (pH 2 buffer) (Berdy). λ_{max} 267 (ϵ 13190) (pH 10 buffer) (Berdy).

N-*(4-Amino-4-carboxybutanoyl):* [142115-24-0] *γ-Glutamyl-β-(isoxazolin-5-on-2-yl)alanine*
$C_{11}H_{15}N_3O_7$ 301.255
Constit. of *Lens culinaris* (lentil).
Cryst. (Me_2CO aq.).

Lambein, F. *et al., Biochem. Biophys. Res. Commun.*, 1969, **37**, 375 (*isol*)
Lambein, F. *et al., Heterocycles*, 1976, **4**, 567 (*isol*)
Baldwin, J.E. *et al., Tet. Lett.*, 1985, **26**, 5931 (*synth, pmr, ir*)
Lambein, F. *et al., Phytochemistry*, 1992, **31**, 887 (*glutamyl deriv*)
Kuo, Y.-H *et al., Phytochemistry*, 1998, **49**, 43-48 (*occur, metab, biosynth*)

2-Amino-4-pentenoic acid, 9CI A-470

Allylglycine. 2-(2-Propenyl)glycine [1069-48-3]



(*R*)-*form*

$C_5H_9NO_2$ 115.132

(*R*)-*form* [54594-06-8]
D-form
Cryst. (EtOH aq.).
Mp 240-241° dec. $[\alpha]_D^{24}$ +37.8 (c, 4 in H_2O). $[\alpha]_D^{24}$ +5.7 (c, 2 in 6*M* HCl).

N-*Ac:* [121786-40-1]
$C_7H_{11}NO_3$ 157.169
Cryst. (Me_2CO/petrol). $[\alpha]_D^{22}$ -42 (c, 4 in H_2O).

(*S*)-*form* [16338-48-0]
L-form
Isol. from *Amanita pseudoporphyria* and *Amanita abrupta*. Cryst. (EtOH aq.).
Mp 275-280° (241-243°) dec. $[\alpha]_D^{24}$ -37.1 (c, 4 in H_2O). $[\alpha]_D^{24}$ -5.7 (c, 2 in 6*M* HCl).

Hydrochloride: [195316-72-4]
Solid (MeOH/Et_2O). Mp 154-156° dec. $[\alpha]_D^{23}$ +196.6 (c, 0.5 in MeOH).

Me ester: [50299-15-5]
[173723-62-1 (hydrochloride)]
$C_6H_{11}NO_2$ 129.158
Solid (hydrochloride). Mp 91-92° (hydrochloride). $[\alpha]_D^{20}$ +8.3 (c, 1.07 in MeOH) (hydrochloride).

N-tert-*Butyloxycarbonyl:* [90600-20-7]
$C_{10}H_{17}NO_4$ 215.249
Viscous oil. $[\alpha]_D^{23}$ +11.9 (c, 1.4 in MeOH). $[\alpha]_D^{23}$ -3.9 (c, 1 in CH_2Cl_2). $[\alpha]_D^{20}$ +14.5 (c, 1.28 in $CHCl_3$).

N-*Benzyl, Et ester:* [635300-09-3]
$C_{14}H_{19}NO_2$ 233.31
Oil. $[\alpha]_D^{20}$ -18 (c, 0.28 in $CHCl_3$).

(±)-*form* [7685-44-1]
Cryst. (MeOH). Mp 243-245° dec.

Me ester: [70837-19-3]
Liq. $Bp_{1.1}$ 69-70°.

Et ester: [68843-72-1]
[89077-49-6 (deleted)]
$C_7H_{13}NO_2$ 143.185
Liq. Bp_{15} 75-78°.

Et ester, oxalate:
Cryst. (EtOH aq.). Mp 111-112°.

N-*Ac:* [50299-14-4]
Mp 114°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 574D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 874C; 875A (*nmr*)
Black, S. *et al., J. Biol. Chem.*, 1955, **213**, 39-50 (*synth, resoln*)

Japan. Pat., 1977, 77 54 085 (*isol*)
Sasaki, N.A. *et al., Tet. Lett.*, 1989, **30**, 1943-1946 (*synth*)
Mooiweer, H.H. *et al., Tetrahedron*, 1989, **45**, 4627-4636 (*synth, ir, pmr, Me ester*)
Broxterman, Q.B. *et al., JOC*, 1992, **57**, 6286-6294 (*resoln, pmr, cmr*)
Dragovich, P.S. *et al., J. Med. Chem.*, 1996, **39**, 1872-1884 (*Me ester, synth, ir, pmr*)
Org. Synth., 1999, **76**, 57-76 (*S-form, synth, ir, pmr, cmr*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)
Koch, C.-J. *et al., Eur. J. Org. Chem.*, 2003, 1244-1263 (*R-form, synth*)
Org. Synth., 2003, **80**, 31-37 (*N-butyloxycarbonyl, synth, ir, pmr*)
Saniére, L. *et al., Tetrahedron*, 2004, **60**, 5889-5897 (*S-form, synth*)
Kaul, R. *et al., JOC*, 2005, **70**, 3838-3844 (*S-form, N-Boc, Me ester*)
Duggan, H.M.E. *et al., Org. Biomol. Chem.*, 2005, **3**, 2287-2295 (*S-form, synth, pmr, cmr*)
Sugiura, M. *et al., JACS*, 2006, **128**, 11038-11039; s1-s47 (*S-form, synth*)
Ansari, A.M. *et al., Synth. Commun.*, 2008, **38**, 2330-2340 (*Et ester, pmr, ir*)

(5-Aminopentyl)guanidine, 9CI A-471

1-Amino-5-guanidinopentane. ***Homoagmatine*** [18431-52-2]

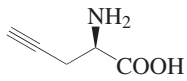
$HN{=}C(NH_2)NH(CH_2)_4CH_2NH_2$
$C_6H_{16}N_4$ 144.219
Constit. of *Lathyrus sativus* (chickling pea). Mp 135-137° (as hydrochloride).

N^5-*Ac:* [180251-16-5] ***Acetylhomoagmatine***
$C_8H_{18}N_4O$ 186.256
Yellow amorph. solid. λ_{max} 206 (log ϵ 3.23) (MeOH).

Ramakrishna, S. *et al., Phytochemistry*, 1973, **12**, 2691-2695 (*isol, synth, ir*)
Lenis, L.A. *et al., Nat. Prod. Lett.*, 1996, **8**, 15-23 (*Acetylhomoagmatine*)
Castellanos, L. *et al., Mar. Drugs*, 2006, **4**, 286-289 (*Acetylhomoagmatine, synth*)

2-Amino-4-pentynoic acid, 9CI A-472

Propargylglycine



(*R*)-*form*

$C_5H_7NO_2$ 113.116
Sol. H_2O; poorly sol. butanol, hexane.

(*R*)-*form* [23235-03-2]
Mp 221° dec.
$[\alpha]_D^{25}$ +25.7 (c, 0.8 in H_2O).
Me ester: [78342-50-4]
$C_6H_9NO_2$ 127.143
Bp_{10} 80-85°. $[\alpha]_D^{20}$ +1.7 (c, 1.0 in EtOH).

(*S*)-*form* [23235-01-0]
L-form
Isol. from *Amanita pseudoporphyria*.
Mp 230° (dec. from 210°)
(248-249° dec.). $[\alpha]_D^{20}$ -35 (c, 1 in H_2O).
N-*Phthaloyl, dicyclohexylamine salt:*
Mp 205°. $[\alpha]_D^{20}$ -29.4 (c, 1 in EtOH).
N-*Phthaloyl, Me ester:*
Cryst. (petrol). Mp 112°. $[\alpha]_D^{20}$ -63.2 (c, 1 in EtOH).

(±)-*form* [50428-03-0]
Mp 235-237° dec.
Hydrochloride: [61172-65-4]
Cryst. (2-propanol/diisopropyl ether). Mp 195°.
Me ester: [166734-65-2]
[70837-20-6]
Characterised by ir, pmr and cmr only.
N-*Phthaloyl,* tert-*butyl ester:* Mp 97°.
[198774-27-5]

Scannell, J.P. *et al., J. Antibiot.*, 1971, **24**, 239-244 (*isol, synth*)
Tun-kyi, A. *et al., Helv. Chim. Acta*, 1976, **59**, 2181-2183 (*synth*)
Fauchére, J.-L. *et al., Helv. Chim. Acta*, 1979, **62**, 1385-1395 (*synth, resoln*)
Diuric, S. *et al., Tet. Lett.*, 1981, **22**, 1787-1790 (*synth*)
Church, N.J. *et al., JCS Perkin 1*, 1998, 1475-1482 (*R-form, S-form, synth, pmr, ir*)
Wolf, L.B. *et al., Adv. Synth. Catal.*, 2001, **343**, 662-674 (*S-form, synth, ir, pmr, cmr*)
Knight, D.W. *et al., JCS Perkin 1*, 2002, 622-628 (*Me ester, synth, ir, pmr, cmr*)
Struthers, H. *et al., Chem. Eur. J.*, 2008, **14**, 6173-6183 (*synth, ir, pmr, cmr*)
Bucuroaia, C. *et al., Eur. J. Org. Chem.*, 2009, 3605-3612 (*R-form, Me ester*)

Aminopeptidase I A-473

E.C. 3.4.11.22. Aminopeptidase III. Leucine aminopeptidase IV. Vacuolar aminopeptidase I. Aminopeptidase yscI. Yeast aminopeptidase I
[9031-94-1]

Aminopeptidase enzyme. Isol. from baker's yeast, barley, pig. Aminoacyl-arylamides are poor substrates. Activity is stimulated by $Zn^{2\oplus}$ and $Cl^{\ominus}$ ions. Yeast enzyme activity range pH 4.0-9.0. At 4°, in 50*mM* Tris-HCl buffer, pH 7.2, 38% and 81% loss of activity after 4 and 11 days respectively.

Tisljar, U. *et al., FEBS Lett.*, 1993, **322**, 191-196 (*yeast, activity, stability*)
Cristofoletti, P.T. *et al., Biochim. Biophys. Acta*, 2000, **1479**, 185-190 (*Tenebrio molitor*)
Desimone, M. *et al., J. Chromatogr., B*, 2000, **737**, 285-293 (*barley*)
Handb. Proteolytic Enzymes, 2nd edn., (eds. Barrett, A.J. *et al*), Elsevier Academic Press, 2004, **1**, 316-318; 940-941; 968-970 (*yeast, Bacillus stearothermophilus*)
Russo, S. *et al., J. Biol. Chem.*, 2004, **279**, 51275-51281 (*cryst struct, Pyrococcus*)
Chang, S.C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2005, **102**, 17107-17112 (*pig*)
York, I.A. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2006, **103**, 9202-9207 (*mouse*)

Aminopeptidase B A-474

E.C. 3.4.11.6. Arginine aminopeptidase. Arginyl aminopeptidase. Arylamidase II. Cytosol aminopeptidase IV [9073-92-1]

Aminopeptidase enzyme. Isol. from cow, pig. Also acts on arylamides of Arg and Lys. Cow enzyme activity range pH 5.0-7.0. At -20°, stable for 10 days; after 30 days, exhibits 25% activity.

Kawata, S. *et al., J. Biochem. (Tokyo)*, 1980, **88**, 1025-1032; 1601-1605 (*pig*)
Blahovec, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 1249-1257 (*cow, stability*)
Lauffart, B. *et al., Biochem. Soc. Trans.*, 1988, **16**, 849-850 (*human*)
Foulon, T. *et al., Handb. Proteolytic Enzymes*, 2nd edn., (eds. Barrett, J. *et al*), Elsevier Academic Press, 2004, **1**, 328-332 (*rat, human*)
Hwang, S.R. *et al., J. Neurochem.*, 2007, **100**, 1340-1350 (*cow, rat, activity*)

Aminopeptidase Ey A-475

E.C. 3.4.11.20
[9031-94-1]

Aminopeptidase enzyme. Isol. from chicken egg yolk. A Zn glycoprotein.

Ichishima, E. *et al., Agric. Biol. Chem.*, 1989, **53**, 1867-1872 (*chicken*)
Tanaka, T. *et al., Int. J. Biochem.*, 1993, **25**, 1681-1688 (*chicken*)
Midorikawa, T. *et al., Comp. Biochem. Physiol., B: Biochem. Mol. Biol.*, 1998, **119**, 513-520 (*chicken*)

Aminopeptidase Y A-476

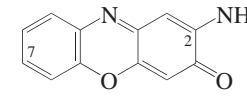
E.C. 3.4.11.15. Lysyl aminopeptidase. Aminopeptidase (cobalt-activated). Aminopeptidase Co [114796-97-3]

Aminopeptidase enzyme. Isol. from baker's yeast. Requires $Co^{2\oplus}$. Inhibited by $Zn^{2\oplus}$ and $Mn^{2\oplus}$. *Yarrowia lipolytica* Yeast enzyme activity range pH 7.0-8.0.

Yasuhara, T. *et al., J. Biol. Chem.*, 1994, **269**, 13644-13650 (*Saccharomyces cerevisiae*)
Pan, D. *et al., Food Chem.*, 2004, **88**, 511-516 (*Lactobacillus helveticus*)
Nakai, T. *et al., Handb. Proteolytic Enzymes*, 2nd edn., (eds. Barrett, A.J. *et al*), Elsevier Academic Press, 2004, **1**, 956-957 (*Saccharomyces cerevisiae*)
Hernandez-Montanez, Z. *et al., FEMS Microbiol. Lett.*, 2007, **268**, 178-186 (*Yarrowia lipolytica, activity*)
Munih, P. *et al., J. Inorg. Biochem.*, 2007, **101**, 1099-1107 (*cryst struct, Vibrio proteolyticus*)

2-Amino-3*H*-phenoxazin-3-one, 9CI, 8CI A-477

Questiomycin A. *AV toxin C* [1916-59-2]



$C_{12}H_8N_2O_2$ 212.207
Isol. from *Calocybe gambosa* (St George's mushroom). Dark brown or red cryst. (EtOH). Sol. EtOH. Mp 250-251°. Subl. 255-257. Sometimes occurs in amorph. form with Mp 296-297°. E° + 0.372V (pH 0.92, 23°). λ_{max} 235 (ϵ 28400); 467 (ϵ 1700) (0.25*N* HCl) (Derep). λ_{max} 335 (ϵ 1230) (0.1*N* KOH) (Derep). λ_{max} 240 (ϵ 26300); 435 (ϵ 2330) (pH 7.4) (Derep).
▶ LD_{50} (mus, ipr) 200 mg/kg. SP7695000
N-*β-D-Glucopyranosyl:* [218150-62-0] **N-*β-D-Glucopyranosylquestiomycin A***
$C_{18}H_{18}N_2O_7$ 374.349

Red powder. Sol. DMSO, Py; fairly sol. MeOH; poorly sol. $CHCl_3$, EtOAc. Mp >195° dec. $[\alpha]_D^{28}$ +16.5 (c, 0.1 in Py). λ_{max} 240 (log ϵ 4.33); 423 (log ϵ 4.23) (MeOH).

N-*Ac:* [1916-55-8] N-*(3-Oxo-3*H*-phenoxazin-2-yl)acetamide, 9CI. 2-Acetamido-3*H*-phenoxazin-3-one.* **N-*Acetylquestiomycin A***
$C_{14}H_{10}N_2O_3$ 254.245
Orange cryst. Sol. EtOH, Et_2O, C_6H_6, MeOH; poorly sol. H_2O. Mp 295-297°. Subl. 165. E° + 0.375V (pH 0.84, 23°). λ_{max} 240 (E1%/1cm 1400); 405 (E1%/1cm 1100) (EtOH) (Berdy).

N-*(2-Hydroxyethyl):* [16061-92-0]
$C_{14}H_{12}N_2O_3$ 256.26
Mp 203-205° (204-207°). λ_{max} 238; 422; 438 (EtOH).

N-*Hydroxyacetyl:* [664355-13-9] N-*(Hydroxyacetyl)questiomycin A.* ***Chandrananimycin B***
$C_{14}H_{10}N_2O_4$ 270.244
Orange solid. λ_{max} 238 (log ϵ 3.85); 399 (log ϵ 3.66) (MeOH).

N-*Me:* [41688-04-4] **N-*Methylquestiomycin A***
$C_{13}H_{10}N_2O_2$ 226.234
Red-brown needles.

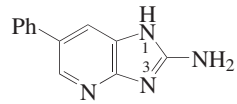
6-Hydroxy: [900531-66-0] *2-Amino-6-hydroxy-3*H*-phenoxazin-3-one.* ***6-Hydroxyquestiomycin A***
$C_{12}H_8N_2O_3$ 228.207
Red solid. λ_{max} 236 (log ϵ 3.93); 277 (log ϵ 3.75); 430 (log ϵ 3.72) (MeOH). λ_{max} 230 (log ϵ 3.91); 284 (log ϵ 3.61); 464 (log ϵ 3.5) (MeOH/HCl).

9-Hydroxy, N-*Ac:* [664355-12-8] N-*Acetyl-9-hydroxyquestiomycin A.* ***Chandrananimycin A***
$C_{14}H_{10}N_2O_4$ 270.244
Orange solid. λ_{max} 226 (log ϵ 4.52); 270 (log ϵ 4.38); 423 (log ϵ 4.45) (MeOH).

7,8-Dimethoxy: [261162-39-4] *2-Amino-7,8-dimethoxy-3*H*-phenoxazin-3-one. 7,8-Dimethoxyquestiomycin A.* ***Peristrophine***
$C_{14}H_{12}N_2O_4$ 272.26
Mp 250° dec. λ_{max} 235; 280 (sh); 484 (MeOH). λ_{max} 239; 273 (sh); 320 (sh); 544 (sh); 583 (MeOH/HCl).

Fischer, O. *et al., Ber.*, 1894, **27**, 2782-2785 (*synth*)
Gerber, N.N. *et al., Biochemistry*, 1964, **3**, 598-602 (*isol, N-Ac, synth, uv*)
Gerber, N.N. *et al., JOC*, 1967, **32**, 4055-4057 (*isol, N-(2-hydroxyethyl), uv, synth*)
Ruzička, E. *et al., Mikrochim. Acta*, 1967, **55**, 277-286 (*use*)
Ruzička, E. *et al., CA*, 1968, **69**, 40930j (*stannometry*)
Ikekawa, T. *et al., Chem. Pharm. Bull.*, 1968, **16**, 1705-1708 (*synth, ir*)
Hishida, T. *et al., Chem. Lett.*, 1974, 293-296 (*synth, uv*)
Schlunegger, U.P. *et al., Helv. Chim. Acta*, 1976, **59**, 1383-1388 (*synth, pmr, ir, ms, Calocybe gambosa constit*)
Motohashi, N. *et al., Yakugaku Zasshi*, 1983, **103**, 364-371 (*pharmacol*)
Bolognese, A. *et al., J. Het. Chem.*, 1986, **23**, 1003-1006 (*synth, N-Ac, pmr, cmr, uv ir, ms*)
Kinjo, J. *et al., Tet. Lett.*, 1987, **28**, 3697-3698 (*isol, pmr, cmr, ir, ms*)
Simandi, L.I. *et al., Tet. Lett.*, 1993, **34**, 717-720 (*synth*)
Igarashi, Y. *et al., J. Antibiot.*, 1998, **51**, 915-920 (*Glucosylquestiomycin A*)
Qin, J.P. *et al., Yaoxue Xuebao*, 1999, **34**, 599-603 (*Peristrophine*)
Kim, D.S. *et al., Planta Med.*, 2000, **66**, 78-79 (*Questiomycin A, isol, activity*)
Bolognese, A. *et al., J. Med. Chem.*, 2002, **45**, 5205-5216 (*synth, N-Ac, uv, pmr*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 622-629 (*Chandrananimycins A,B*)
Bitzer, J. *et al., J. Antibiot.*, 2006, **59**, 86-92 (*6-Hydroxyquestiomycin A*)
Giurg, M. *et al., Pol. J. Chem. (Rocz. Chem.)*, 2006, **80**, 297-306 (*synth*)
Giurg, M. *et al., Synth. Commun.*, 2007, **37**, 1779-1789 (*synth, ir, uv, pmr*)
Liu, W.-H. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2008, **44**, 503-505 (*N-Methylquestiomycin A*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, QCJ275

2-Amino-6-phenylimidazo[4,5-*b*]pyridine A-478



1*H-form*

$C_{12}H_{10}N_4$ 210.238

1*H-form*

1-Me: [105650-23-5] *1-Methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridin-2-amine, 9CI. 2-Amino-1-methyl-6-phenyl-1*H*-imidazo[4,5-*b*]pyridine. PhIP*
$C_{13}H_{12}N_4$ 224.265
Food-related mutagen, reported to be the most abundant heterocyclic amine found in cooked meat and fish. Solid. Mp 327-328°.

▶ Mutagen. Exp. carcinogen. Possible human carcinogen (IARC 2B).

3*H-form*

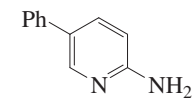
3-Me: [107351-87-1] *2-Amino-3-methyl-6-phenyl-3*H*-imidazo[4,5-*b*]pyridine*
$C_{13}H_{12}N_4$ 224.265
Cryst. (2-propanol). Mp 217°.

▶ Mutagen.

Knize, M.G. *et al., Heterocycles*, 1986, **24**, 1815-1819 (*1-Me, 3-Me, synth, pmr, cmr, ir, uv, ms, activity*)
Lindström, S. *et al., Acta Chem. Scand.*, 1993, **47**, 805-812 (*1-Me, 3-Me, synth*)
Lindström, S. *et al., Acta Chem. Scand.*, 1995, **49**, 361-363 (*1-Me, synth*)
Lang, N.P. *et al., Cancer Lett.*, 1999, **143**, 135-138 (*metab*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*1-Me, detn, occur*)
Vanhaecke, L. *et al., J. Agric. Food Chem.*, 2006, **54**, 3454-3461 (*1-Me, metab*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*1-Me, detn, occur*)
Chrisman, W. *et al., J. Het. Chem.*, 2008, **45**, 1641-1649 (*1-Me, 3-Me, synth, pmr, cmr, ir, ms*)
IARC Monogr. (Web), http://monographs.iarc.fr

2-Amino-5-phenylpyridine, 8CI A-479

5-Phenyl-2-pyridinamine, 9CI. Phe-P-1
[33421-40-8]



$C_{11}H_{10}N_2$ 170.213
Mutagen found in cooked food. Cryst. (H_2O). Mp 136-137° (134-135°).

▶ Mutagen. US2145000

N-*Acetoxy:* [124392-12-7] *2-Acetoxyamino-5-phenylpyridine. 5-Phenyl-2(1*H*)-pyridinone,* O-*acetyloxime, 9CI*
[189894-03-9]
$C_{13}H_{12}N_2O_2$ 228.25
Cryst. Mp 124-126°.

▶ Proximate carcinogen of the parent compd.

Beyer, H. *et al., Chem. Ber.*, 1958, **91**, 247-256 (*synth, ir*)
Butler, D.E. *et al., J. Med. Chem.*, 1971, **14**, 575 (*synth*)
Kosuge, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 611 (*tox*)
US Pat., 1983, 4 386 209 (*synth*)
Stavenuiter, J.F.C. *et al., Carcinogenesis (London)*, 1985, **6**, 13-19 (*synth, pmr, ms*)
Lutgerink, J.T. *et al., Carcinogenesis (London)*, 1989, **10**, 1957-1960 (*N-acetyloxy, synth, pmr, ms*)
Ojala, W.H. *et al., Acta Cryst. C*, 1997, **53**, 634-637 (*N-acetyloxy, cryst struct*)
Stoll, I. *et al., Tetrahedron*, 2008, **64**, 3813-3825 (*synth, pmr*)
Darweesh, A.F. *et al., Synthesis*, 2010, 3163-3173 (*synth, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ALY000

2-Amino-1,3-propanediol, 9CI, 8CI A-480

Serinol [534-03-2]

$(HOCH_2)_2CHNH_2$
$C_3H_9NO_2$ 91.11
Present in sugarcane *Saccharum officinarum* clone 51NG97. Mp 128°. Bp 264-265° $Bp_{0.06}$ 115-120°.

Hydrochloride: [73708-65-3]
Mp 104°.

Oxalate: [24070-20-0]
Hygroscopic cryst. Mp 202-203°.

O-*Phosphate:*
$C_3H_{10}NO_5P$ 171.09
Present in sugarcane *Saccharum officinarum* clone 51NG97.

N-*Ac:* [2655-79-0]
$C_5H_{11}NO_3$ 133.147
Mp 89-90°.

N-*(11ξ-Methyloctadecanoyl):* [1131838-96-4] N-*(11-Methyloctadecanoyl)serinol.* ***Inconspicamide***
$C_{22}H_{45}NO_3$ 371.602
Powder. $[\alpha]_D^{23}$ -6.3 (c, 0.17 in MeOH).

N-*(*tert*-Butyloxycarbonyl):* [125414-41-7]
$C_8H_{17}NO_4$ 191.227
Needles (hexane/EtOAc). Mp 84-85°.

N-*(2-Hydroxybenzoyl):* [758724-18-4] N-*(2-Hydroxybenzoyl)serinol*. **N-*Salicyloylserinol***
$C_{10}H_{13}NO_4$ 211.217
Amorph. solid. λ_{max} 225 (log ϵ 4.32); 283 (sh) (log ϵ 3.54); 302 (sh) (log ϵ 3.5) (MeOH).

N-*(2-Hydroxybenzoyl), 1-Ac:*
$C_{12}H_{15}NO_5$ 253.254
Yellow amorph. solid. $[\alpha]_D^{25}$ -29 (c, 0.14 in MeOH). λ_{max} 228 (log ϵ 4.56); 282 (sh) (log ϵ 4.17); 301 (sh) (log ϵ 4.13) (MeOH).

N-*Benzyl:* [124613-28-1]
$C_{10}H_{15}NO_2$ 181.234
Solid (Et_2O). Mp 72-73°.

Dibenzyl ether:
$C_{17}H_{21}NO_2$ 271.358
Oil.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 551B (*nmr*)
Den Otter, H.P. *et al., Recl. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1938, **57**, 13 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1948, **31**, 1617-1623 (*synth*)
Langenbeck, W. *et al., Naturwissenschaften*, 1955, **42**, 389 (*synth*)
Szammer, J. *et al., Acta Chim. Acad. Sci. Hung.*, 1969, **61**, 417 (*synth*)
Japan. Pat., 1976, 76 67 788 (*biosynth*)
Pinkerton, F. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 1976, **73**, 4007-4011 (*isol*)
Babczinski, P. *et al., Plant Physiol.*, 1978, **61**, 46-49 (*phosphate*)
US Pat., 1985, (*(Eprova AG)*)4 503 252 (*synth*)
Rai, B.L. *et al., J. Med. Chem.*, 1998, **41**, 3347-3359 (*dibenzyl ether*)
Neri, C. *et al., Adv. Synth. Catal.*, 2003, **345**, 835-848 (*tert-butyloxycarbonyl*)
US Pat., 2003, (*(SK Corp., Seoul)*)6 509 504 (*synth*)
Hossain, M.S. *et al., Phytochemistry*, 2004, **65**, 2147-2151 (*N-salicyloyl amides*)
Gu, K. *et al., Bioorg. Med. Chem.*, 2006, **14**, 1339-1347 (*synth, pmr, cmr*)
Ueoka, R. *et al., Biosci., Biotechnol., Biochem.*, 2008, **72**, 3055-3058; 2009, **73**, E2 (*Inconspicamide*)
Fujisaki, F. *et al., Heterocycles*, 2008, **75**, 1681-1694 (*N-benzyl*)

3-Aminopropanoic acid A-481

β-Alanine, 9CI. FEMA 3252 [107-95-9]

$H_2NCH_2CH_2COOH$

$C_3H_7NO_2$ 89.094
Widely distributed in plants including algae, fungi and many higher plants. Flavouring ingredient. Cryst. (H_2O). Sol. H_2O; almost insol. Et_2O, Me_2CO. Mp 200° (197-198°). pK_{a1} 3.7; pK_{a2} 10.1 (30°).

Amide: [4726-85-6] *3-Aminopropanamide, 9CI*
$C_3H_8N_2O$ 88.109
Present in raw potato. Precursor of formation of Acrylamide in P-685 cooked potato. Needles or oil. Mp 41°.

Nitrile: [151-18-8] *3-Aminopropanenitrile, 9CI. 3-Cyanopropylamine. β-Aminopropionitrile*
$C_3H_6N_2$ 70.094
Constit. of chickling pea (*Lathyrus sativus*). Bp_{23} 89° $Bp_{0.1}$ 50-55°.

▶ LD_{50} (mus, ipr) 1152 mg/kg. Exp. reprod. and teratogenic effects. Polymerises to an explosive yellow solid. Storage hazard. UG0350000

N-*Benzoyl:* [3440-28-6] N-*Benzoyl-β-alanine, 9CI*. ***Betamipron, INN***. *3-Benzamidopropanoic acid*
$C_{10}H_{11}NO_3$ 193.202
Artificial sweetener. Leaflets or prisms (H_2O). Mp 120°. Log P 0.69 (calc).

▶ AY3272500

Org. Synth., Coll. Vol. 3, 1955, 93 (*3-Aminopropanenitrile*)
Kircz, M. *et al., Rev. Chim. (Bucharest)*, 1959, **10**, 78 (*rev*)
Jose, P. *et al., Acta Cryst. C*, 1965, **18**, 806 (*cryst struct*)
Voellmin, J. *et al., Microchem. J.*, 1966, **11**, 73 (*ms*)
Zilkha, A. *et al., JOC*, 1968, **33**, 1686 (*synth*)
Becke, F. *et al., Annalen*, 1970, **735**, 27 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2425 (*occur*)
Shirai, T. *et al., Synth. Prod. Util. Amino Acids*, (Kaneko, T. *et al*, Ed.), Kodansha, Ltd., Tokyo, 1974, 67 (*rev*)
Garrigou-Lagrange, C. *et al., Can. J. Chem.*, 1978, **56**, 663 (*ir, Raman*)
Blagoeva, I. *et al., Synthesis*, 1982, 967 (*synth*)
Ishibashi, N. *et al., Agric. Biol. Chem.*, 1988, **52**, 819 (*synth, use, Betamipron*)
Tamura, M. *et al., J. Agric. Food Chem.*, 1989, **37**, 737; 1990, **38**, 1368 (*synth, activity, Betamipron*)
Barluenga, J. *et al., Tetrahedron*, 1989, **45**, 2183 (*synth, Betamipron*)
Rosado, M.T.S. *et al., J. Mol. Struct.*, 1997, 343-348; 410-411 (*Raman, ir*)
Granvogl, M. *et al., J. Agric. Food Chem.*, 2004, **52**, 4751-4757 (*amide, occur, hplc*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 1139
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 212
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AMB500; DPU000; AMB750

(3-Aminopropoxy)guanidine, 9CI A-482

γ-Guanidinooxypropylamine [97091-01-5]

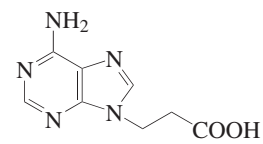
$HN{=}C(NH_2)NHOCH_2CH_2CH_2NH_2$

$C_4H_{12}N_4O$ 132.165
Constit. of *Canavalia gladiata* (sword-bean).

Hamana, K. *et al., Biochem. Biophys. Res. Commun.*, 1985, **129**, 46 (*isol*)
Matsuzaki, S. *et al., Phytochemistry*, 1990, **29**, 1311 (*isol*)

6-Amino-9*H*-purine-9-propanoic acid, 9CI A-483

3-(9-Adeninyl)propionic acid [4244-47-7]



$C_8H_9N_5O_2$ 207.191
Isol. from *Lentinus edodes* (shiitake). Mp 277-278° dec. λ_{max} 262 (ϵ 14400) (0.1*N* NaOH). λ_{max} 259 (ϵ 13800) (0.1*N* HCl).

Me ester: [70259-15-3]
$C_9H_{11}N_5O_2$ 221.218
Cryst. (Et_2O/MeOH). Mp 182-183°.

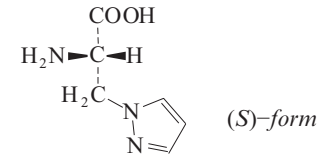
Et ester: [7083-40-1]
$C_{10}H_{13}N_5O_2$ 235.245
Solid. Mp 167-168°.

Nitrile: [4244-45-5] *6-Amino-9-(2-cyanoethyl)purine*
$C_8H_8N_6$ 188.191
Solid (H_2O). Mp 258-261° (245-247°).

Lira, E.P. *et al., JOC*, 1966, **31**, 2188-2191 (*synth, Et ester, nitrile*)
Chakraborti, S.K. *et al., Indian J. Chem.*, 1969, **7**, 426 (*synth*)
Saito, Y. *et al., Tet. Lett.*, 1970, 4863-4866 (*isol, struct, synth*)
Holy, A. *et al., Coll. Czech. Chem. Comm.*, 1978, **43**, 3444-3465 (*synth, Me ester*)
Poritere, S.E. *et al., Khim. Geterotsikl. Soedin.*, 1982, 539-541; *Chem. Heterocycl. Compd. (Engl. Transl.)*, 1982, 415-417 (*nitrile*)
Zaré, A. *et al., Synth. Commun.*, 2009, **39**, 139-157 (*Et ester*)

2-Amino-3-(1-pyrazolyl)propanoic acid A-484

*α-Amino-1*H*-pyrazole-1-propanoic acid, 9CI. β-Pyrazol-1-ylalanine* [10162-27-3] [28024-60-4]



(*S*)–*form*

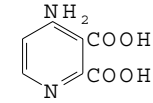
$C_6H_9N_3O_2$ 155.156

(*S*)-*form* [2734-48-7]
L-form
Amino acid present in seeds of *Citrullus vulgaris* (watermelon). Cryst. (EtOH aq.). Mp 243° dec. $[\alpha]_D^{20}$ -73 (c, 3.4 in H_2O).

Noe, F.F. *et al., Biochem. J.*, 1960, **77**, 543 (*isol, synth*)
Sugimoto, N. *et al., Tetrahedron*, 1960, **11**, 231 (*synth*)
Dunnill, P.M. *et al., Biochem. J.*, 1963, **86**, 388 (*isol*)
Takeshita, M. *et al., J. Biol. Chem.*, 1963, **238**, 660 (*isol, synth*)
Dunnill, P.M. *et al., Phytochemistry*, 1965, **4**, 933 (*occur*)
Frisch, D.M. *et al., Phytochemistry*, 1967, **6**, 921 (*biosynth*)
Murakoshi, I. *et al., Chem. Pharm. Bull.*, 1972, **20**, 609; 1980, **34**, 1473 (*synth*)
Brown, E.G. *et al., Phytochemistry*, 1982, **21**, 863 (*biosynth*)
Arnold, L.D. *et al., JACS*, 1988, **110**, 2237-2241 (*synth, pmr*)

4-Amino-2,3-pyridinedicarboxylic acid, 9CI A-485

[122475-55-2]



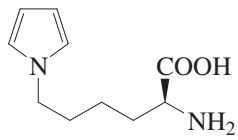
$C_7H_6N_2O_4$ 182.135
Cryst. (H_2O). Sol. H_2O, MeOH; poorly sol. Me_2CO, hexane. λ_{max} 262 (ϵ 9550)

(0.1*N* HCl). λ_{max} 245 (sh) (ε 8710); 290 (ε 2090) (H_2O at pH 11). λ_{max} 252 (ε 10000) (MeOH). λ_{max} 265 (ε 9800); 290 (ε 2080) (H_2O).

Hirayama, F. *et al., Phytochemistry*, 1989, **28**, 1133-1135 (*isol, struct, synth*)
US Pat., 2002, 6 395 903 (*prodn*)

α-Amino-1*H*-pyrrole-1-hexanoic acid, 9CI A-486

N$^{\epsilon}$-*Pyrrolylnorleucine. Pyrrole-1-norleucine. 1-(5′-Amino-5′-carboxypentyl)pyrrole*



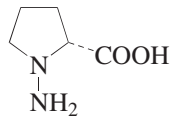
$C_{10}H_{16}N_2O_2$ 196.249

(*S*)-*form* [156539-32-1]
L-form
Widely distributed in fresh foodstuffs, e.g. meats, fish, vegetables, nuts, and processed foods. Component of nonenzymic browning reaction models. Characterised spectroscopically.

Chiang, G.H. *et al., J. Agric. Food Chem.*, 1988, **36**, 506-509 (*hplc, occur*)
Zamora, R. *et al., Lipids*, 1994, **29**, 243-249; 1995, **30**, 477-483 (*synth, detn, pmr, cmr*)
Zamora, R. *et al., Biochim. Biophys. Acta*, 1995, **1258**, 319-327 (*formn*)
Hidalgo, F.J. *et al., J. Agric. Food Chem.*, 1995, **43**, 1023-1028 (*occur, formn*)
Zamora, R. *et al., J. Agric. Food Chem.*, 1999, **47**, 1942-1947 (*occur*)

1-Amino-2-pyrrolidinecarboxylic acid A-487

1-Aminoproline, 9CI



(*R*)-*form*

$C_5H_{10}N_2O_2$ 130.146
Log P -0.97 (calc).

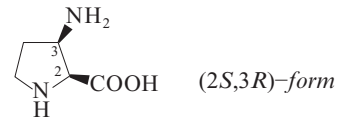
(*R*)-*form* [10139-05-6]
D-*form*
Obt. from linseed meal. Pale yellow cryst. (EtOH). Mp 155° dec. $[\alpha]_D^{25}$ +113 (c, 2 in 0.5M HCl).
► TW3588500

N-γ-L-*Glutamyl:* [10139-06-7] *1-[*N-*(*γ-L-*Glutamyl)amino]-*D-*proline.* ***Linatine***
$C_{10}H_{17}N_3O_5$ 259.261
Isol. from *Linum usitatissimum* (flax). Amorph. solid. Sol. H_2O; poorly sol. butanol, hexane. $[\alpha]_D^{24}$ +46.4 (c, 2.75 in H_2O).
► MA2275500

(*S*)-*form* [15265-22-2]
L-*form*
Mp 155-156°. $[\alpha]_D^{24}$ -111 (c, 1.6 in 0.5*M* HCl).
Parsons, J.L. *et al., Antimicrob. Agents Chemother. (1961-70)*, 1967, 415-421
Klosterman, H.J. *et al., Biochemistry*, 1967, **6**, 170-177 (*synth, Linatine*)
Achiwa, K. *et al., Tet. Lett.*, 1974, 1799-1802 (*synth*)
Klosterman, H.J. *et al., Methods Enzymol.*, 1979, **62**, 483-495 (*props*)

3-Amino-2-pyrrolidinecarboxylic acid A-488

3-Aminoproline, 9CI [24279-08-1]



(2*S*,3*R*)–*form*

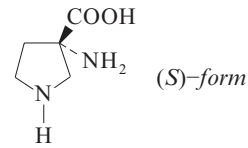
$C_5H_{10}N_2O_2$ 130.146

(2*S*,3*R*)-*form* [25876-88-4]
L-cis-*form*
Isol. from *Morchella esculenta* (common morel). Pale yellow powder (H_2O). Mp 215° (190°). $[\alpha]_D^{20}$ +22.5 (c, 0.9 in 6*M* HCl).

Baldwin, J.E. *et al., Tetrahedron*, 1995, **51**, 5169 (*synth, pmr, 2S,3R-form*)

3-Amino-3-pyrrolidinecarboxylic acid, 9CI A-489

Cucurbitine



(*S*)–*form*

$C_5H_{10}N_2O_2$ 130.146
Log P -2.15 (calc).

(*S*)-*form* [6807-92-7]
Isol. from pumpkin seeds. Cryst. (EtOH aq.). Mp 239-241° dec. $[\alpha]_D^{25}$ -19.96 (c,1 in H_2O). Pharmacol. active isomer.

Hydrochloride:
Cryst. (EtOH aq.). $[\alpha]_D^{19.5}$ -15 (c, 1 in H_2O). Dec. at 275°.

Perchlorate:
Cryst. $[\alpha]_D^{20.5}$ -13.08 (c, 10.4 in H_2O). Dec. above 275°.

N,N′-*Dibenzoyl:*
$C_{19}H_{18}N_2O_4$ 338.362
Cryst. (MeOH aq.). Mp 207-208°. $[\alpha]_D^{24.5}$ -1.63 (c, 4.83 in MeOH).

(±)-*form*

Hydrochloride:
Cryst. Dec. *ca.* 280°.

Hydrobromide:
Cryst. Dec. at 286°.

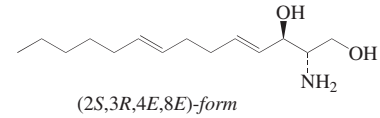
Perchlorate:
Cryst. Dec. above 280°.

N,N′-*Di-Ac:*
$C_9H_{14}N_2O_4$ 214.221
Cryst. (EtOH aq.). Mp 243-244°.

N,N′-*Dibenzoyl:*
Cryst. (MeOH aq.). Mp 226-227°.

Bis-4-nitrobenzoyl:
Cryst. (MeOH aq.). Mp 255-256°.
Fan, H.-F. *et al., CA*, 1965, **63**, 109 (*cryst struct, abs config*)
Dunnill, P.M. *et al., Phytochemistry*, 1965, **4**, 933 (*occur*)
Morimoto, Y. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3845 (*synth*)
Williams, R.M. *et al., Tet. Lett.*, 1992, **33**, 6755-6758 (*synth, pmr*)
Paik, S. *et al., Bull. Korean Chem. Soc.*, 2000, **21**, 131-132 (*synth*)

2-Amino-4,8-tetradecadiene-1,3-diol A-490



(2*S*,3*R*,4*E*,8*E*)-*form*

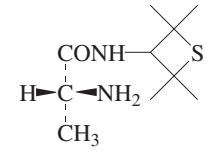
$C_{14}H_{27}NO_2$ 241.373

(2*S*,3*R*,4*E*,8*E*)-*form*
N-*Eicosanoyl:* [910546-29-1] ***Corticeramide***
$C_{34}H_{65}NO_3$ 535.892

(2*S*,3*R*,4*E*,8*Z*)-*form*
N-*(2*R-*Hydroxytetracosanoyl), 1*-O-β-D-*glucopyranoside:* [1253258-42-2]
$C_{44}H_{83}NO_9$ 770.141
Constit. of the radix of *Cyperus rotundus* (nutgrass). Amorph. powder. Mp 190-191°. $[\alpha]_D^{26}$ +10.4 (c, 0.1 in MeOH).

Ahmed, S. *et al., Bull. Pharm. Sci., Assiut Univ.*, 2006, **29**, 151-165 (*Corticeramide*)
Liu, P. *et al., Chin. Chem. Lett.*, 2010, **21**, 606-609 (*Cyperus rotundus cerebroside*)

2-Amino-*N*-(2,2,4,4-tetramethyl-3-thietanyl)propanamide, 9CI A-491



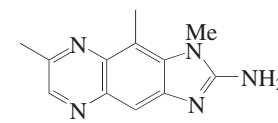
$C_{10}H_{20}N_2OS$ 216.347

(*R*)-*form* [80875-07-6]
Aqueous degradn. prod. of Alitame, A-283. Oil.

Eur. Pat., 1989, 325 485 (*synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*occur*)

2-Amino-1,7,9-trimethylimidazo[4,5-*g*]quinoxaline A-492

7,9-DiMeIgQx



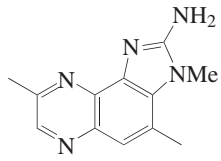
$C_{12}H_{13}N_5$ 227.268
Isol. from beef extract and various cooked meats. Mp 250°.

▶ Mutagenic.

Achiwa, I. *et al., Chem. Pharm. Bull.*, 1994, **42**, 408 (*synth, pmr, uv*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258; 2008, **56**, 68-78 (*occur, ms, hplc*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*detn, occur*)

2-Amino-3,4,8-trimethyl-3*H*-imidazo[4,5-*f*]quinoxaline A-493

*3,4,8-Trimethyl-3*H-*imidazo[4,5-*f*]quinoxalin-2-amine, 9CI. 4,8-Di-MeIQx*
[95896-78-9]



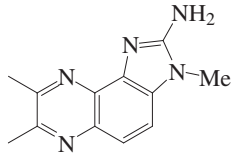
$C_{12}H_{13}N_5$ 227.268
Pyrolysis prod. from creatine, threonine and glucose in cooked food, esp. cooked meats. Mp 300°.

▶ Mutagen. NJ5920400

Knapp, S. *et al., Tetrahedron*, 1989, **45**, 1293 (*synth*)
Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521 (*synth, pmr, ms*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*occur, ms, hplc*)
Ni, W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*detn, occur*)

2-Amino-3,7,8-trimethyl-3*H*-imidazo[4,5-*f*]quinoxaline, 9CI A-494

7,8-DiMeIQx



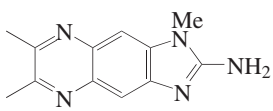
$C_{12}H_{13}N_5$ 227.268
Constit. of fried meats. No phys. props. reported.

▶ Mutagenic.

Grivas, S. *et al., Acta Chem. Scand.*, 1993, **47**, 521-528 (*synth*)
Wyss, M. *et al., Physiol. Rev.*, 2000, **80**, 1107-1213 (*biol, rev*)
Turesky, R.J. *et al., J. Agric. Food Chem.*, 2005, **53**, 3248-3258 (*occur*)

2-Amino-1,6,7-trimethyl-1*H*-imidazo[4,5-*g*]quinoxaline A-495

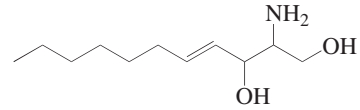
*1,6,7-Trimethyl-1*H-*imidazo[4,5-*g*]quinoxalin-2-amine, 9CI. 6,7-DiMeIgQx*
[1004510-31-9]



$C_{12}H_{13}N_5$ 227.268
Present in roasted/fried meats esp. beef, pork and chicken. No phys. props. reported.

Ni, N.W. *et al., J. Agric. Food Chem.*, 2008, **56**, 68-78 (*synth, pmr, ms, detn*)

2-Amino-4-undecene-1,3-diol A-496



$C_{11}H_{23}NO_2$ 201.308

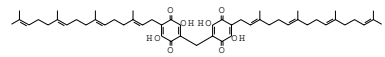
(2ξ,3ξ,4E)-form

N-*(2ξ-Hydroxy-4*E*-decenoyl), 1-*O*-β-D-glucopyranoside:* [1240641-07-9] ***Panajaponin***
$C_{27}H_{49}NO_9$ 531.685
Struct. incorrectly drawn in ref. Constit. of the roots of *Panax japonicus* (Japanese ginseng). Needles. Mp 116-118°. $[\alpha]_D^{20}$ +29.5 (c, 0.2 in $CHCl_3$).

Guo, Z. *et al., Nat. Prod. Res.*, 2010, **24**, 86-91 (*Panajaponin*)

Amitenone A-497

2,2′-Methylenebis[3,6-dihydroxy-5-(3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraenyl)]-2,5-cyclohexadiene-1,4-dione, 9CI. Methylenebis[2,5-dihydroxy-4-geranylgeranyl-3,6-benzoquinone]
[21682-47-3]



$C_{53}H_{72}O_8$ 837.147
Pigment from the edible mushroom Amitake (*Suillus bovinus*). Yellow-orange cryst. Mp 187-188°.

Minami, K. *et al., Tet. Lett.*, 1968, 5067 (*isol, struct*)
Azawa, K. *et al., Mokuzai Gakkaishi*, 1971, **17**, 384 (*struct, synth*)

AML 1 A-498

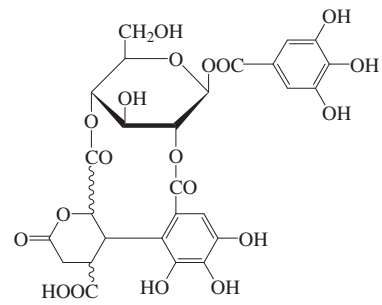
[125147-23-1]

$C_{35}H_{62}O_4$ 546.872
Acetogenin. Struct. unknown. Constit. of *Annona muricata* (soursop). Powder. Sol. MeOH, hexane; poorly sol. H_2O. No further reports to 2009.

Japan. Pat., 1989, 1 050 892 (*isol*)

Amlaic acid A-499

[17278-02-3]



$C_{27}H_{24}O_{19}$ 652.475
Constit. of the leaves of *Phyllanthus emblica* (emblic). Cryst. (butanol/Et_2O). Mp 206°. $[\alpha]_D$ -289.

Theresa, Y.M. *et al., Leather Sci. (Madras)*, 1967, **14**, 16-17

Ammonia, 11CI A-500

Azane. Ammine. Amine. FEMA 4494
[7664-41-7]

NH_3 (C_{3v})
H_3N 17.03
Pyramidal. Interatomic distance: H–N 101.2 pm; angle: HNH 106.7°. Acidity regulator for foodstuffs. Colourless alkaline nonflammable gas with v. pungent odour. V. sol. H_2O, $CHCl_3$, Et_2O. Mp -77.8°. Bp -33.5°. pK_a 9.25 (25°). T_{crit} 133.0; P_{crit} 111.5 atm. FEMA no. also includes Ammonium chloride ($(NH_4)Cl$), A-504.

▶ Corrosive, toxic, irritant. BO0875000

Trideutero compd.: [13550-49-7] *Ammonia-*d_3. *Perdeuteroammonia*
D_3N 20.049
Colourless gas, similar to NH_3. Mp -73.6°. Bp -31.1°. pK_a 9.76 (20°). T_{crit} 132.3°.

Hydrate: see Ammonium hydroxide ($(NH_4)(OH)$), A-505

[13767-16-3, 13587-49-0, 19496-55-0, 34819-78-8]

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 363A (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1928, **8**, 144; 1964, **8/II/1**, 240 (*rev*)
Helminger, P. *et al., J. Mol. Spectrosc.*, 1971, **39**, 94 (*struct*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 15 (*use*)
Brauer, G. *et al., Handbuch Prp. Anorg. Chem.*, 3rd edn., Ferdinand Enke Verlag, 1975, **1**, 152; 445 (*synth ND_3, NH_3*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 470 (*rev*)
Urban, S. *et al., J. Mol. Spectrosc.*, 1984, **106**, 29 (*ND_3, ir, microwave*)
Encyclopedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 185-192 (*use*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AMY500

Ammonia kinase A-501

E.C. 2.7.3.8. ATP:ammonia phosphotransferase. Phosphoramidate adenosine diphosphate phosphotransferase. Phosphoramidate ADP phosphotransferase
[37278-16-3]

Phosphotransferase enzyme with nitrogen acceptor. Isol. from baker's yeast. Has wide specificity. In the reverse direction, *N*-phosphoglycine and *N*-phosphohistidine can also act as phosphate donors; Adenosine diphosphate, dADP, Guanosine 5′-diphosphate, Cytidine 5′-diphosphate, dCDP, IDP and UDP can act as phosphate acceptors (in decreasing order of activity). Baker's yeast enzyme exhibits 50% maximal activity at pH 6.5 and 40% at pH 8.5.

Dowler, M.J. *et al., J. Biol. Chem.*, 1968, **243**, 1434-1440 (*baker's yeast*)

Ammonium acetate A-502

[631-61-8]

NH_4OAc

$C_2H_7NO_2$ 77.083

Struct. is a 3-D H-bonded network with each O atom accepting 2 H bonds. Listed in the EAFUS Food Additive Database (Jan 2001) but with no reported use. Hygroscopic cryst. Mp 114°.

Zuffanti, S. *et al., JACS*, 1941, **63**, 3123-3124 (*synth*)
Gutowsky, H.S. *et al., J. Chem. Phys.*, 1954, **22**, 1782-1783 (*pmr*)
Schmidt, B.M. *et al., J. Mol. Spectrosc.*, 1958, **2**, 539-550 (*N-14 nmr*)
Vratny, F. *et al., Anal. Chem.*, 1961, **33**, 1455 (*ir*)
Nahringbauer, I. *et al., Acta Cryst.*, 1967, **23**, 956-965 (*cryst struct*)

Ammonium carbonate, USAN A-503

Carbonic acid ammonium salt. Diammonium carbonate. Hartshorn. Sal volatile. E503(i) [10361-29-2]
[8000-73-5]

$(NH_4)_2CO_3$

$CH_8N_2O_3$ 96.086

As normally obt., contains large amounts of Carbamic acid, from which it is formed on hydration. Used in baking powder; acidity regulator, raising agent. Colourless cryst. Strong odour of NH_3. Sharp taste. V. sol. H_2O. Mp 58° dec. Dec. in air → $NH_3 + CO_2 + H_2O$. Converts to Ammonium bicarbonate, in C-121. The name E503 is also used for Ammonium bicarbonate.

▶ LD_{50} (mus, ivn) 96 mg/kg. BP1925000

Monohydrate: [16799-91-0]
$CH_{10}N_2O_4$ 114.101
Colourless cubes. V. sol. cold H_2O; dec. hot H_2O.

Compd. with H_2O_2: [76261-70-6] *Ammonium carbonate peroxohydrate*
$CH_{10}N_2O_5$ 130.1
Colourless cryst.

[506-87-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1272B (*ir*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1964, **8/IA**, 459 (*rev*)
Jones, D.P. *et al., JCS Dalton*, 1980, 2526 (*synth, ir, Raman*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 743
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 131-132 (*props, use*)
Merck Index, 13th edn., 2001, No. 508 (*props, use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANE000

Ammonium chloride A-504

($(NH_4)Cl$), 11CI, JAN, USAN

Sal ammoniac. Amchlor. Darammon. Ammonium muriate. Salmiac. FEMA 4494 [12125-02-9]

$[NH_4]Cl$

ClH_4N 53.491

Has CsCl struct. below 184.3° and NaCl above this temp. Dough conditioner and strengthener, flavour enhancer, leavening agent, processing aid and yeast food. Used in sanitising solns. Hygroscopic white solid. V. sol. H_2O. V.p. 758 mm at 338°. Subl. when heated. FEMA no. also includes Ammonia, A-500.

▶ Irritant. BP4550000

[12015-14-4]

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1521D (*ir*)
*Gmelin Handbook Inorg. Chem., Syst. No.*23, 1936, 150 (*bibl*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1964, **8/I**, *Part* 1; 378 (*rev*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **2**, 520 (*rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 135-136
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANE500

Ammonium hydroxide A-505

($(NH_4)(OH)$), 11CI, 10CI, 9CI

Ammonium hydroxide. Ammonia aqueous. Aqua ammonia. E527 [1336-21-6]

$NH_3.H_2O$ rather than NH_4OH

H_5NO 35.046

Name given to aq. soln. of Ammonia, A-500. Used in food processing as a leavening agent, pH control agent, surface-finishing agent, and boiler water additive. Colourless liq. Sol. H_2O. d^{20} 0.89. Mp -77°.

▶ Corrosive. V. pungent odour, poison by ingestion. Severe eye irritant. Can inflict burns. BQ9625000

Penta-deutero compd.: [12168-30-8]
D_5NO 40.077

Mellor Compr. Treat. Inorg. Theor. Chem., 1928, 194; 1964, **8/I**, 311 (*rev*)
Gmelin Handbook Inorg. Chem., Syst. No. 23, 1936, 42 (*bibl*)
Herber, R.H. *et al., Inorg. Isot. Synth.*, Benjamin, 1962, 47 (*deutero deriv*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **2**, 224 (*struct, rev*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 137-138
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANK250

Ammonium phosphate A-506

($(NH_4)(H_2PO_4)$)

Monoammonium phosphate, 9CI, 8CI. Ammonium phosphate†. Ammonium dihydrogen phosphate [7722-76-1]
[10124-31-9]

$(NH_4)(H_2PO_4)$

H_6NO_4P 115.025

Thermally the most stable of the ammonium orthophosphates. Each $NH_4^{\oplus}$ cation is coord. by 8 oxygens forming two interpenetrating tetragonal disphenoids. Mean P–O 153.7 pm. Used in food as a source of acidity, pH control agent, buffering agent, leavening agent, dough strengthener and nutrient source; also used as a yeast nutrient in wine production and to start secondary fermentations in the production of sparkling wines. Colourless, transparent tetragonal prisms (H_2O). Mp 190°. Low temp. orthorhombic, antiferroelectric phase transforms at -125° (rising temp.) into tetragonal, paraelectric phase.

[93454-16-1, 93454-15-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266C (*ir*)
Miller, F.A. *et al., Spectrochim. Acta A*, 1960, **16**, 135 (*ir*)
Kolomiichuk, V.N. *et al., Kristallografiya*, 1968, **13**, 519; *Sov. Phys. Crystallogr. (Engl. Transl.)*, 1968, **13**, 4221 (*ed*)
Mullin, J.W. *et al., J. Appl. Chem.*, 1970, **20**, 153 (*synth*)
Khan, A.A. *et al., Acta Cryst. B*, 1973, **29**, 2721 (*cryst struct*)
Nicholson, J.Y. *et al., J. Chem. Phys.*, 1974, **60**, 715 (*pmr*)
Ratcliffe, C.I. *et al., Chem. Phys. Lett.*, 1985, **120**, 427 (*N-15 nmr*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **70**, 408 (*P-31 nmr*)
Bréhat, F. *et al., J. Phys. C: Solid State Phys.*, 1986, **19**, 6893 (*ir*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 335 (*P-31 nmr*)
Mohanial, S.K. *et al., Cryst. Res. Technol.*, 1987, **22**, 21 (*synth*)
Pastor, A.C. *et al., Ferroelectrics*, 1987, **71**, 61 (*rev*)
Cerreta, M.K. *et al., J. Cryst. Growth*, 1987, **84**, 577 (*Raman*)
Hattori, T. *et al., J. Phys. Soc. Jpn.*, 1987, **56**, 781 (*Raman*)
Fukami, T. *et al., J. Phys. Soc. Jpn.*, 1987, **56**, 2223; 4388 (*cryst struct*)
Kim, J.J. *et al., Phys. Rev. B*, 1987, **36**, 5651 (*Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 142-143

Ammonium phosphate A-507

($(NH_4)_2(HPO_4)$)

Diammonium phosphate, 9CI, 8CI. Ammonium phosphate, USAN†. Diammonium hydrogen phosphate [7783-28-0]
[10124-31-9]

$(NH_4)_2(HPO_4)$

$H_9N_2O_4P$ 132.056

Struct. has discrete $PO_4H^{2\ominus}$ and $NH_4^{\oplus}$ tetrahedra with P–O 151.9-158.7 pm, angle: OPO 103.6-113.2°. Dough strengthener, firming agent, leavening agent, pH control agent, processing aid, nutrient source, yeast nutrient and a starter for secondary fermentation in the production of sparkling wines. Mp 185° dec.

▶ TB9375000

α-form

High temp.-form
Orthorhombic cell at 120°. Reverts to β-form at *ca.* 100°.

β-form

Low temp.-form
Monoclinic cell. Colourless cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1266D (*ir*)
Thompson, H.L. *et al., Ind. Eng. Chem.*, 1950, **42**, 2176 (*props, manuf*)

Smith, P. *et al., Acta Cryst.*, 1957, **10**, 709 (*cryst struct*)
Coates, R.V. *et al., Acta Cryst.*, 1967, **23**, 504 (*synth, cryst struct*)
Nabiev, M.N. *et al., Zh. Neorg. Khim.*, 1969, **14**, 2950; *Russ. J. Inorg. Chem. (Engl. Transl.)*, 1969, **14**, 1556 (*synth, props*)
Khan, A.A. *et al., Acta Cryst. B*, 1972, **28**, 2065 (*cryst struct*)
Hamann, S.D. *et al., Aust. J. Chem.*, 1978, **31**, 11 (*ir*)
Neels, J. *et al., Z. Anorg. Allg. Chem.*, 1982, **495**, 65 (*P-31 nmr*)
Ratcliffe, C.I. *et al., Chem. Phys. Lett.*, 1983, **99**, 177 (*N-15 nmr*)
Mudrakovskii, I.L. *et al., J. Phys. Chem. Solids*, 1986, **47**, 338 (*P-31 nmr*)
Videnova-Adrabinska, V. *et al., J. Mol. Struct.*, 1988, **175**, 295 (*ir, Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 140-145
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ANR500

Ammonium sulfide $((NH_4)_2S)$, 10CI, 9CI A-508

Ammonium sulfide. Diammonium sulfide. FEMA 2053 [12135-76-1]

$[NH_4]_2S$

H_8N_2S 68.143

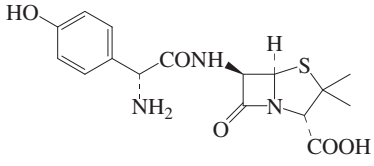
Flavouring ingredient. Used in baked goods, meat products, condiments and gravies. Yellow hygroscopic cryst.; stable below -18°. Sol. H_2O. Dec. to NH_3 + NH_4SH, polysulfides.

▶ Toxic. Pyrophoric in air. BS4920000

Mellor Compr. Treat. Inorg. Theor. Chem., 1928, **2**, 645; *Part 1*, 1964, **8/1**, 469 (*rev*)
Encyclopedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 197-199 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 146-147
Merck Index, 13th edn., 2001, No. 560
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 82 (*use*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 7th edn., Van Nostrand Reinhold*, 1989, 243; 244 (*haz*)

Amoxicillin, INN, JAN, USAN A-509

6-[[2-Amino(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 9CI. 6-(α-Amino-4-hydroxyphenylacetamido)penicillanic acid. ρ-Hydroxyampicillin. ***Amoxycillin, BAN****. Almodan. Amix. Amopen. Amoram. Amoxid. Amoxil. Amoxymed. Amrit. Biomox. Cemoxin. Clamoxyl (SKB). Flemoxin. Galenamox. Imacillin. Moxatag. Polymox. Rimoxallin. Sauracillin. Trimox. Wymox. BRL 2333. Many other names* [26787-78-0]
[61336-70-7]



$C_{16}H_{19}N_3O_5S$ 365.409

Potential contaminant in cow's milk arising from its veterinary use. Cryst. + $3H_2O$. Sol. H_2O. $[\alpha]_D^{20}$ +246 (c, 0.1 in H_2O). Log P -1.94 (uncertain value) (calc).

▶ Hypersensitivity reactions and gastrointestinal effects reported when used therapeutically. LD_{50} (rat, ipr) 2870 mg/kg (trihydrate). XH8300000

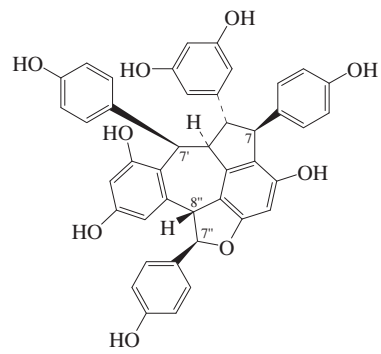
Na salt: [34642-77-8] ***Amoxicillin sodium, USAN****. Amoxycillin sodium, BAN*Used in combination with clavulanate potassium #BDT59-S and marketed as Augmentin.

[79198-29-1]

Neu, H. *et al., Antimicrob. Agents Chemother. (1961-70)*, 1970, 407; *Antimicrob. Agents Chemother.*, 1970, 411; 416; 423, (*props*)
UK Pat., 1970, 1 241 844 (*synth*)
Long, A. *et al., JCS(C)*, 1971, 1920 (*synth*)
Boles, M.O. *et al., Acta Cryst. B*, 1978, **34**, 461 (*cryst struct*)
Bhattacharyya, P.K. *et al., Anal. Profiles Drug Subst.*, 1978, **7**, 19 (*rev*)
Owen, R.T. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 163 (*rev, pharmacol*)
Bird, A.E. *et al., JCS Perkin 1*, 1982, 563 (*pmr, cd*)
Kawamori, M. *et al., Agric. Biol. Chem.*, 1983, **47**, 2503 (*biosynth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4027 (*synonyms*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, A0A100
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 129 (*rev*)
Vega, J.M. *et al., Allergy*, 1994, **49**, 317 (*tox*)
Bird, A.E. *et al., Anal. Profiles Drug Subst.*, 1994, **23**, 1 (*rev*)
Aguilar, L. *et al., Antimicrob. Agents Chemother.*, 1997, **41**, 1403-1405 (*amoxicillin sodium-clavulanic acid*)
Ang, C.Y.W. *et al., J. Agric. Food Chem.*, 1997, **45**, 4351-4356 (*occur, anal*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 151
Easton, J. *et al., Drugs*, 2003, **63**, 311-340 (*rev*)
McCormack, P.L. *et al., Drugs*, 2005, **65**, 121-136 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, A0A100

Ampelopsin C A-510

[130518-20-6]



$C_{42}H_{32}O_9$ 680.709

Oligostilbene. Mp 268-269°. $[\alpha]_D$ +24 (c, 1.04 in MeOH). λ_{max} 282 (ε 10700) (MeOH) (Derep).

▶ Hepatotoxin.

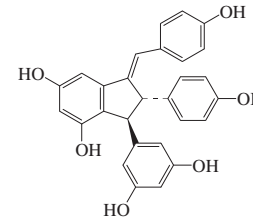
7-Epimer: [625096-18-6] ***Viniferol D***
$C_{42}H_{32}O_9$ 680.709
Constit. of the stems of *Vitis vinifera* 'Kyohou'. Amorph. solid. $[\alpha]_D$ +101.4 (c, 0.27 in MeOH). λ_{max} 201 (log ε 5.02); 227 (sh) (log ε 4.73); 284 (log ε 4.04) (MeOH).

7′,7″,8″-Triepimer: [174291-95-3] ***Davidiol A***
$C_{42}H_{32}O_9$ 680.709
Powder. $[\alpha]_D^{29}$ -272 (c, 0.18 in MeOH). λ_{max} 219 (log ε 4.83); 285 (log ε 4.08) (MeOH).

Oshima, Y. *et al., Tetrahedron*, 1990, **46**, 5121-5126 (*isol, pmr, cmr, struct*)
Tanaka, T. *et al., Phytochemistry*, 2000, **53**, 1009-1014 (*Davidiol A*)
Takaya, Y. *et al., Heterocycles*, 2003, **60**, 1433-1439 (*Viniferol D*)
He, Y.-H. *et al., Heterocycles*, 2006, **68**, 93-100 (*Davidiol A, abs config*)

Ampelopsin D A-511

[149418-37-1]



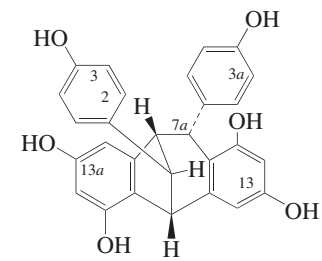
Absolute Configuration

$C_{28}H_{22}O_6$ 454.478

Constit. of *Vitis vinifera* (wine grape). Amorph. powder. $[\alpha]_D^{22}$ -5 (c, 0.27 in MeOH).

Oshima, Y. *et al., Phytochemistry*, 1993, **33**, 179-182 (*isol, pmr, cmr*)
Adesanya, S.A. *et al., J. Nat. Prod.*, 1999, **62**, 1694-1695 (*struct*)
Niwa, M. *et al., Heterocycles*, 2000, **53**, 1475-1478 (*pmr, cmr, abs config*)
Takaya, Y. *et al., Tetrahedron*, 2002, **58**, 7259-7265 (*abs config*)

Ampelopsin F A-512



( )-*form*

$C_{28}H_{22}O_6$ 454.478

(+)-*form* [151487-08-0]
Pale brown powder. Mp 223°. $[\alpha]_D$ +14 (c, 1.98 in MeOH).

*13*a-O-*β-D-Glucopyranoside:* [849699-44-1] ***Upunoside C***
$C_{34}H_{32}O_{11}$ 616.62
Yellow powder. $[\alpha]_D$ -68 (c, 0.18 in MeOH). λ_{max} 225 (log ε 4.7); 281 (log ε 4.1) (MeOH).

*2*b-*Hydroxy:* [361444-42-0] ***2b-Hydroxyampelopsin F***
$C_{28}H_{22}O_7$ 470.478
Pale brown powder. $[\alpha]_D$ +12 (c, 0.1 in MeOH). λ_{max} 215 (log ε 4.1); 283 (log ε 3.5); 325 (sh) (MeOH).

*7*a-*Epimer:* [212967-52-7] ***Isoampelopsin F***
$C_{28}H_{22}O_6$ 454.478
Pale brown solid. $[\alpha]_D$ -56.7 (c, 0.2 in MeOH). λ_{max} 232; 279 (MeOH).

*7*a-*Epimer, 2*b-*hydroxy:* [256415-40-4] ***Gnetuhainin C***
$C_{28}H_{22}O_7$ 470.478
Amorph. powder. $[\alpha]_D^{25}$ +16.7 (c, 0.03 in MeOH). λ_{max} 280 (log ε 4.3) (MeOH).

(-)-*form* [354528-90-8]
Amorph. yellow powder. Mp 164-166°. $[\alpha]_D^{20}$ -4.6 (c, 0.14 in MeOH). λ_{max} 282 (log ε 4.03) (MeOH).

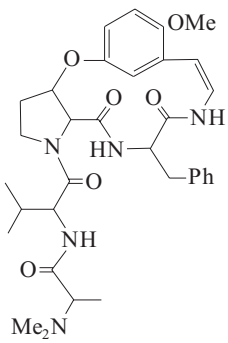
*3*a,*3*b-*Dimethoxy:* [560085-55-4] ***Gnemonol M***
$C_{30}H_{26}O_8$ 514.531
Constit. of the roots of *Gnetum gnemon* (bago). Amorph. powder. $[\alpha]_D$ -28 (c, 0.12 in MeOH). λ_{max} 207 (log ε 4.9); 230 (sh); 282 (log ε 4.4) (MeOH).

*7*a-*Epimer:* [354553-38-1]
Amorph. yellow powder. Mp 185-187°. $[\alpha]_D^{20}$ +30.6 (c, 0.77 in MeOH). λ_{max} 281 (log ε 4.11) (MeOH).

Oshima, Y. *et al., Tetrahedron*, 1993, **49**, 5801-5804 (*isol, pmr, cmr*)
Tanaka, T. *et al., Phytochemistry*, 1998, **48**, 1241-1243 (*Isoampelopsin F*)
Huang, K.-S. *et al., J. Nat. Prod.*, 2000, **63**, 86-89 (*Gnetuhainin C*)
Tanaka, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 858-862 (*2b-Hydroxyampelopsin F*)
Luo, H.F. *et al., Tetrahedron*, 2001, **57**, 4849-4854 (*(+)-Ampelopsin F, (+)-Isoampelopsin F*)
Takaya, Y. *et al., Tetrahedron*, 2002, **58**, 7259-7265 (*abs config*)
Iliya, I. *et al., Phytochemistry*, 2003, **62**, 601-606 (*Gnemonol M*)
Ito, C. *et al., Helv. Chim. Acta*, 2005, **88**, 23-34 (*Upunoside C*)
Li, W. *et al., Synthesis*, 2010, 3822-3826 (*Gnemonol M, synth*)

Amphibine H A-513

[52659-55-9]



$C_{33}H_{43}N_5O_6$ 605.733

Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Cryst. ($CHCl_3$/petrol). Mp 205°. $[\alpha]_D^{20}$ -570 (c, 0.12 in MeOH).

N-*De-Me:* [53947-96-9] ***Nummularine B.*** N-*Demethylamphibine H. Daechuine S27*
$C_{32}H_{41}N_5O_6$ 591.706
Alkaloid from the stem bark of *Zizyphus jujuba* (Chinese date). Needles (MeOH). Mp 230-231°. $[\alpha]_D^{20}$ -390 (c, 0.2 in $CHCl_3$).

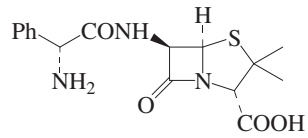
N-*De-Me,* N-*formyl:* [99694-95-8] ***Nummularine T***
$C_{33}H_{41}N_5O_7$ 619.716
Granules (MeOH). Mp 188-190°.

Dihydro:
Needles (CH_2Cl_2/Me_2CO). Mp 281°. $[\alpha]_D^{20}$ -381 (c, 0.15 in MeOH).

Tschesche, R. *et al., Chem. Ber.*, 1974, **107**, 686; 3180 (*isol, uv, ir, pmr, ms, struct*)
Tschesche, R. *et al., Phytochemistry*, 1976, **15**, 541; 1979, **18**, 702 (*isol*)
Pandey, V.B. *et al., Phytochemistry*, 1984, **23**, 2118 (*isol*)
Han, B.H. *et al., Pure Appl. Chem.*, 1989, **61**, 443 (*isol, Nummularine B*)
Pandey, V.B. *et al., Planta Med.*, 1990, **56**, 649 (*activity*)
Singh, B. *et al., Phytochemistry*, 1995, **38**, 271 (*Nummularine T*)
Panseeta, P. *et al., Phytochemistry*, 2011, **72**, 909-915 (*Nummularine B*)

Ampicillin, BAN, INN, JAN, USAN A-514

6-[(Aminophenylacetyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]-heptane-2-carboxylic acid, 9CI. D-α-Aminobenzylpenicillin. 6-(α-Aminophenylacetamido)penicillanic acid. Ampicillin anhydrous, JAN. Amblosin. Amfipen. Binotal. Magnapen. Marcillin. Omnipen. Penbristol. Pentritin. Penicline. Tolomol. Viccillin. Vidocillin. Vidopen. AY 6108. BRL 1341. NSC 528986 [69-53-4]
[7177-48-2]



$C_{16}H_{19}N_3O_4S$ 349.41
Semisynthetic penicillin. Potential contaminant of cow's milk arising from its veterinary use. Mp 199-202° dec. $[\alpha]_D^{23}$ +287.9 (H_2O). pK_{a1} 2.52; pK_{a2} 7.24 (25°). Log P -1.27 (uncertain value) (calc). Constit. of Unasyn.
▶ Hypersensitivity reactions reported when used therapeutically. LD_{50} (rat, ipr) 4500 mg/kg. Exp. teratogen. XH8350000

Na salt: [69-52-3] *Ampicillin sodium, JAN, USAN. Omnipen. Embacillin C*
▶ LD_{50} (mus, ipr) 3480 mg/kg. XH8400000

[94935-63-4]

Doyle, F. *et al., JCS*, 1962, 1440 (*synth*)
Austin, K. *et al., Nature (London)*, 1965, **208**, 99
Ivashkiv, E. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 1 (*rev*)
Boles, M. *et al., Acta Cryst. B*, 1976, **32**, 2279; 1978, **34**, 461 (*cryst struct*)
Kaifež, F. *et al., J. Het. Chem.*, 1976, **13**, 561 (*synth*)
Bird, A.E. *et al., JCS Perkin 1*, 1982, 563 (*pmr, cd*)
Akita, H. *et al., Chem. Pharm. Bull.*, 1984, **32**, 4317 (*synth*)
Humber, D.C. *et al., Tetrahedron*, 1984, **40**, 4153 (*synth*)
Cooper, J. *et al., Tetrahedron*, 1984, **40**, 4153 (*synth*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 4026 (*synonyms*)
IARC Monogr., 1990, **50**, 153 (*rev, tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **3**, 129 (*rev*)
Ang, C.Y.W. *et al., J. Agric. Food Chem.*, 1997, **45**, 4351-4356 (*occur, anal*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 153; 154
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AIV500; SEQ000; AOD125

Amygdalin β-glucosidase A-515

E.C. 3.2.1.117. Amygdalin β-D-glucohydrolase. Amygdalase. Amygdalinase. Amygdalin hydrolase [51683-43-3]

Glycosidase enzyme. Isol. from black cherry and plum. Highly specific. Stored at 4°, 10*mM* histidine-HCl buffer at pH 6.0.

Li, C.P. *et al., Plant Physiol.*, 1992, **100**, 282-290 (*Prunus serotina, stability*)
Swain, E. *et al., Plant Physiol.*, 1992, **100**, 291-300; 1994, **106**, 437-445 (*Prunus serotina*)
Poulton, J.E. *et al., Plant Physiol.*, 1994, **104**, 29-35 (*Prunus domestica*)
Brimer, L. *et al., World J. Microbiol. Biotechnol.*, 1994, **10**, 203-206 (*Penicillium*)
Brimer, L. *et al., Appl. Microbiol. Biotechnol.*, 1998, **49**, 182-188 (*Endomyces fibuliger*)

α-Amylase A-516

Alpha Amylase, USAN. Fortizyme. Amylopsin. Buclamase. Maxilase. Amylase THC250. Glycogenase†. E.C. 3.2.1.1. 4-α-D-Glucan glucanohydrolase. 1,4-α-D-Glucan glucanohydrolase [9000-90-2]

Glycosidase enzyme. Isol. from mammals, e.g. pig, and from plants, e.g. pea. Used for the hydrol. of starch in the sugar, brewing and distilling industries. Improves baking quality and fermentation. Acts on starch, glycogen and related oligo- and polysaccharides in a random manner. The term α- refers to the initial anomeric config. of the free sugar released and not to the config. of the link hydrolysed. *Vibrio* Enzyme activity range pH 4.5-8.5. Purified enzyme at -20°, in 20*mM* MES, pH 6.5, is stable for at least 4 months.

Manners, D.J. *et al., Adv. Carbohydr. Chem.*, 1962, **17**, 371-430 (*rev*)
Thoma, J.A. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1971, **5**, 115 (*rev*)
Methods Enzym. Anal., 2nd edn., (ed. Bergmeyer, H.U.), Verlag Chemie, 1974, **1**, 923-927; 927-931; 931-936; 936-943 (*human, mouse, rat*)

Pierrot, M. *et al., FEBS Lett.*, 1977, **79**, 105 (*cryst struct*)
Ingle, M.B. *et al., Adv. Appl. Microbiol.*, 1978, **24**, 257 (*rev, bacterial amylase*)
Karn, R.C. *et al., Adv. Comp. Physiol. Biochem.*, 1978, **7**, 1 (*rev, animal amylase*)
Beers, E.P. *et al., Plant Physiol.*, 1990, **92**, 1154-1163 (*pea*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1337
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 149-153
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1549
Aguilar, G. *et al., Enzyme Microb. Technol.*, 2000, **27**, 406-413 (*Lactobacillus constit*)
Ranawala, A.P. *et al., Physiol. Plant.*, 2000, **109**, 388-395 (*tulip*)
Zhuo, H. *et al., Protein J.*, 2004, **23**, 379-387 (*cryst struct, pig*)
Najafi, M.F. *et al., Enzyme Microb. Technol.*, 2005, **36**, 535-539 (*Vibrio constit, activity, stability*)

β-Amylase, 9CI A-517

E.C. 3.2.1.2. 4-α-D-Glucan maltohydrolase. Glycogenase†. *1,4-α-D-Glucan maltohydrolase. Saccharogen amylase* [9000-91-3]

Glycosidase enzyme, MW 206 000 ± 1000; tryptophan residues are involved at the active site. Used in the prodn. of alcoholic beverages and sugar syrups. Isol. from various plants, e.g. pea, broad bean, sweet potato, wheat, barley, soybean. Acts on starch, glycogen and related oligo- and polysaccharides to prod. β-maltose. Term β refers to the initial anomeric config. of the free sugar group released and not to config. of link hydrolysed. *Vicia faba* Enzyme activity range pH 3.0-9.0. At 3°, with 0.05*M* β-mercaptoethanol, 50% loss of activity in 1 week.

French, D. *et al., The Enzymes*, 2nd edn., (eds. Boyer, P.D. *et al.*), Academic Press, 1960, **4**, 345-368 (*rev, wheat, barley, Ipomoea constit, soybean*)
Manners, D.J. *et al., Adv. Carbohydr. Chem.*, 1962, **17**, 371-430 (*rev*)
Thoma, J. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.), Academic Press, 1971, **5**, 115-189 (*rev*)
Chapman, G.W. *et al., Biochim. Biophys. Acta*, 1972, **276**, 491-507 (*Vicia faba constit, activity, stability*)
Vihinen, M. *et al., Crit. Rev. Biochem. Mol. Biol.*, 1989, **24**, 329-418 (*rev*)
Lizotte, P.A. *et al., Plant Physiol.*, 1990, **92**, 615-621 (*pea*)
Ray, R.R. *et al., Crit. Rev. Microbiol.*, 1996, **22**, 181-199 (*rev*)
Sohn, C.B. *et al., J. Food Sci.*, 1996, **61**, 230-234 (*Bacillus polymyxa constit*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 151-152 (*use*)
Oyama, T. *et al., J. Biochem. (Tokyo)*, 2003, **133**, 467-474 (*Bacillus cereus constit, cryst struct*)

Amylo-α-1,6-glucosidase A-518

E.C. 3.2.1.33. Glycogen phosphorylase-limit dextrin 6-α-glucohydrolase. Amylo-1,6-glucosidase. Dextrin 6-α-D-glucosidase [9012-47-9]

Glycosidase enzyme. Isol. from cow, pig, rabbit and baker's yeast. Acts on branch points of amylopectin and glycogen. Rabbit enzyme activity range pH 5.0-8.0. Stable for 2 months at 0°, 50*mM* glycerophosphate, 2*mM* EDTA, 1*mM* dithiothreitol, pH 7.0.

Gordon, R.B. *et al., Biochim. Biophys. Acta*, 1972, **289**, 97-107 (*rabbit, activity*)
Lee, E.Y.C. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1972, **5**, 191-234 (*rev, mammals, yeast*)
Bates, E.J. *et al., FEBS Lett.*, 1975, **58**, 181-185 (*rabbit, stability*)
Narahara, E. *et al., J. Biochem. (Tokyo)*, 2001, **130**, 465-470 (*ox*)
Makino, Y. *et al., Biosci., Biotechnol., Biochem.*, 2006, **70**, 907-915 (*pig*)

Amylovorin L A-519

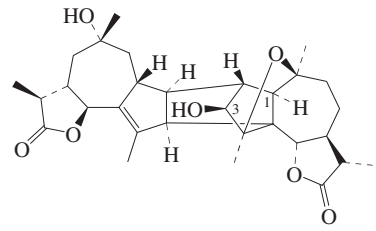
Amylovorin L471. Lactobin A [176634-12-1]
[185568-35-8 (Lactobin A)]

Peptide containing 50 unmodified amino acid residues. Prod. by *Lactobacillus amylovorus* isol. from corn steep liquor. Bacteriocin.

Contreras, B.G.L. *et al., Appl. Environ. Microbiol.*, 1997, **63**, 13-20 (*Lactobin A*)
Callewaert, R. *et al., Microbiology (Reading, U.K.)*, 1999, **145**, 2559-2568 (*Amylovorin L471*)
De Vuyst, L. *et al., Int. J. Food Microbiol.*, 2004, **90**, 93-106 (*Amylovorin L*)
Moreno, M.R. *et al., FEMS Microbiol. Lett.*, 2008, **286**, 199-206 (*activity*)

Anabsin A-520

[72542-39-3]



$C_{30}H_{40}O_7$ 512.642
Constit. of *Artemisia absinthium* (wormwood). Cryst. Mp 276° dec. $[\alpha]_D^{25}$ +110 (c, 1.7 in Me_2CO).

3-Deoxy: [6903-12-4] ***Anabsinthin***
$C_{30}H_{40}O_6$ 496.642
Isol. from *Artemisia absinthium* (wormwood). Cryst. (C_6H_6). Mp 267° (260°). $[\alpha]_D^{20}$ +113 ($CHCl_3$).

3-Deoxy, 1α-hydroxy: [244179-05-3] ***Seemarin***
$C_{30}H_{40}O_7$ 512.642
Cryst. Mp 256-257°. $[\alpha]_D$ +114.5 (c, 0.1 in MeOH/$CHCl_3$).

10′,11′-Diepimer, 3-deoxy: [314763-54-7] ***Caruifolin D***
$C_{30}H_{40}O_6$ 496.642
Amorph. powder. $[\alpha]_D^{24}$ +108 (c, 0.29 in $CHCl_3$).

Kasyrov, Sh.Z. *et al., Khim. Prir. Soedin.*, 1979, **15**, 495; *Chem. Nat. Compd. (Engl. Transl.)*, 1979, **15**, 430 (*struct, bibl*)
Ullah, N. *et al., Phytochemistry*, 1999, **51**, 559-562 (*Seemarin, Anabsinthin*)
Ma, C.-M. *et al., J. Nat. Prod.*, 2000, **63**, 1626-1629 (*Caruifolin D*)
Ali, M.S. *et al., Nat. Prod. Lett.*, 2002, **16**, 179-186 (*Anabsinthin, pmr, cmr*)

Ananain A-521

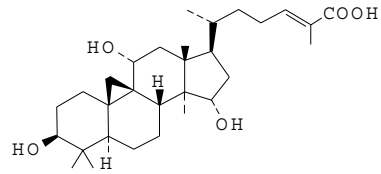
E.C. 3.4.22.31 [119129-70-3]

Cysteine endopeptidase enzyme. Isol. from *Ananas comosus* (pineapple). Activity range pH 3.0-9.5. At -20°, stable when stored dry. Inhibited by chicken cystatin, thus differing from E.C. 3.4.22.32 and E.C. 3.4.22.33 (see Bromelains, B-281).

Napper, A.D. *et al., Biochem. J.*, 1994, **301**, 727-735 (*Ananas comosus, purifn*)
Rowan, A.D. *et al., Methods Enzymol.*, 1994, **244**, 555-568 (*Ananas comosus, stability*)
Lee, K.L. *et al., Biochem. J.*, 1997, **327**, 199-202 (*Ananas comosus*)
Carter, C.E. *et al., Biochemistry*, 2000, **39**, 11005-11013 (*Ananas comosus, activity*)

Ananasic acid A-522

*3β,11α,15α-Trihydroxycycloart-24*E*-en-26-oic acid* [60877-02-3]

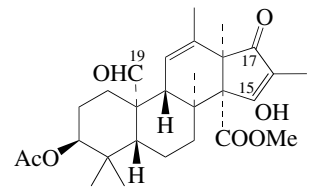


$C_{30}H_{48}O_5$ 488.706
Constit. of pineapple stems. Cryst. (MeOH). Mp 194-197.5°. $[\alpha]_D^{25}$ +4.23.

Takata, R.H. *et al., Tetrahedron*, 1976, **32**, 1077

Andrastin A A-523

[174232-42-9]



$C_{28}H_{38}O_7$ 486.604
Tautomeric with 15-oxo-17*OH* form. Isol. from *Penicillium roqueforti* in blue cheese. Powder. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. Mp 131-135°. $[\alpha]_D^{26}$ -46.4 (c, 0.6 in MeOH). λ_{max} 211 (ε 10580); 286 (ε 10580) (MeOH). λ_{max} 209 (ε 9370); 258 (ε 10558) (MeOH/HCl). λ_{max} 286 (ε 14330) (MeOH/NaOH).

19-Alcohol: [174232-43-0] ***Andrastin B***
$C_{28}H_{40}O_7$ 488.62
Isol. from *Penicillium roqueforti* in blue cheese. Powder. Sol. MeOH, $CHCl_3$, EtOAc; poorly sol. H_2O. Mp 136-139°. $[\alpha]_D^{26}$ -27.9 (c, 1 in MeOH). λ_{max} 211 (ε 12200); 286 (ε 11310) (MeOH). λ_{max} 207 (ε 10260); 235 (ε 8430); 258 (ε 7740) (MeOH/HCl). λ_{max} 286 (ε 11970) (MeOH/NaOH).

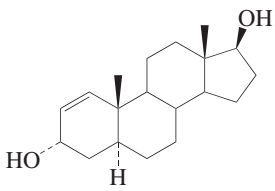
19-Deoxo: [174232-44-1] ***Andrastin C***
$C_{28}H_{40}O_6$ 472.62
Isol. from *Penicillium roqueforti* in blue cheese. Powder. Sol. MeOH, $CHCl_3$,

EtOAc; poorly sol. H_2O. Mp 115-120°. $[\alpha]_D^{26}$ -30.3 (c, 1 in MeOH). λ_{max} 211 (ϵ 11820); 286 (ϵ 11440) (MeOH). λ_{max} 207 (ϵ 10630); 235 (ϵ 7878); 258 (ϵ 7970) (MeOH/HCl). λ_{max} 286 (ϵ 13100) (MeOH/NaOH).

3-O-*De-Ac, 3-ketone, 19-deoxo:* [184432-08-4] ***Andrastin D***
$C_{26}H_{36}O_5$ 428.567
Isol. from *Penicillium roqueforti* in blue cheese. Mp 114-120°. $[\alpha]_D$ -69.6 (c, 1 in MeOH). λ_{max} 211 (ϵ 11130); 235 (sh) (ϵ 3600); 255 (ϵ 2960); 290 (sh) (ϵ 2440) (MeOH).

Omura, S. *et al., J. Antibiot.*, 1996, **49**, 414-417; 418-424 (*isol, uv, ir, pmr, cmr, ms, cryst struct*)
Uchida, R. *et al., J. Antibiot.*, 1996, **49**, 1278-1280 (*Andrastin D*)
Shiomi, K. *et al., Tet. Lett.*, 1996, **37**, 1265-1268 (*isol, pmr, cmr, cryst struct*)
Nielsen, K.F. *et al., J. Agric. Food Chem.*, 2005, **53**, 2908-2911 (*isol*)
Overy, D.P. *et al., Mycol. Res.*, 2005, **109**, 1243-1249 (*isol, props*)

Androst-1-ene-3,17-diol, 9CI A-524



(3α, 5α)-*form*

$C_{19}H_{30}O_2$ 290.445

(3α,5α,17β)-*form* [38859-38-0]
Cryst. (Me_2CO). Mp 217-219°. $[\alpha]_D^{23}$ -86 (c, 1.00 in $CHCl_3$).

17-Ac: [14291-94-2]
$C_{21}H_{32}O_3$ 332.482
Cryst. (EtOAc). Mp 187-190°. $[\alpha]_D$ -64.9 (c, 1.00 in $CHCl_3$).

Di-Ac: [63109-27-3]
$C_{23}H_{34}O_4$ 374.519
Cryst. (2-propanol). Mp 131-132°. $[\alpha]_D^{23}$ -74.4 (c, 1.00 in $CHCl_3$).

(3β,5α,17β)-*form* [5323-27-3]
Constit. of pig fat. Cryst. (MeOH aq.). Mp 161-163°. $[\alpha]_D^{26}$ +38 ($CHCl_3$).

17-Ac: [51505-46-5]
Cryst. (petrol). Mp 111-112° and 139-141° (double Mp). $[\alpha]_D^{25}$ +33.4 ($CHCl_3$).

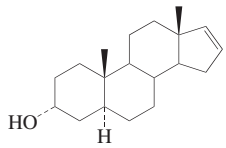
Di-Ac: [55206-08-1]
Cryst. (MeOH aq.). Mp 92-93°. $[\alpha]_D^{26}$ +41 ($CHCl_3$).

17-Me ether: [17925-67-6] *17-Methoxyandrost-1-en-3-ol*
$C_{20}H_{32}O_2$ 304.472
Mp 164.5-166°. $[\alpha]_D^{20}$ +9 (c, 0.16 in $CHCl_3$).

[34220-64-9, 23633-67-2]

Counsell, E. *et al., JOC*, 1962, **27**, 248 (*synth, 3β,5α,17β-form*)
Klein, U. *et al., Chem. Ber.*, 1977, **110**, 994 (*synth, ir, pmr, 3α,5α,17β-form*)
McGregor, S.J. *et al., J. Nat. Prod.*, 2003, **66**, 1147-1148 (*isol*)
Parr, M.K. *et al., Steroids*, 2007, **72**, 545-551 (*synth*)

Androst-16-en-3-ol, 9CI A-525



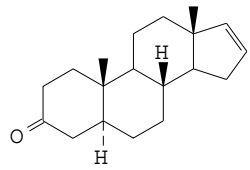
(3α,5α)-*form*

$C_{19}H_{30}O$ 274.445

(3α,5α)-*form* [1153-51-1]
Aroma substance from the Perigord truffle tuber. Cryst. (petrol). Mp 143.5-144°. $[\alpha]_D^{20}$ +15 (c, 1.33 in $CHCl_3$).

Ruzicka, L. *et al., Helv. Chim. Acta*, 1943, **26**, 975; 1947, **30**, 3080
Prelog, V. *et al., Helv. Chim. Acta*, 1945, **28**, 618
Fishman, J. *et al., JOC*, 1963, **28**, 1443 (*synth, 3α,5α-form*)
Hudec, J. *et al., Tetrahedron*, 1976, **32**, 2475 (*ord, cd*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1983, **66**, 192 (*synth, ir, pmr*)

Androst-16-en-3-one A-526



$C_{19}H_{28}O$ 272.43

5α-*form* [18339-16-7]
Androgen metabolite which causes "boar taint" in pigmeat products. Cryst. (pentane). Mp 140-141°. $[\alpha]_D^{17}$ +38 (c, 2.08 in $CHCl_3$).

(5α,13α)-*form* [86335-08-2]
Cryst. (petrol). Mp 120-122°. $[\alpha]_D$ -86.8 (c, 8.5 in $CHCl_3$).

(5α,14β)-*form* [88930-98-7]
Mp 101.5-103°.

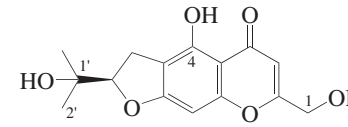
(5β,8α,9β,10α,13α,14β)-*form* [86362-77-8]
Cryst. (pentane). Mp 140-141°. $[\alpha]_D$ -38.5 (c, 1 in $CHCl_3$).

[82209-82-3, 66263-13-6, 82209-84-5, 82209-77-6]

Prelog, V. *et al., Helv. Chim. Acta*, 1944, **27**, 66 (*synth*)
Zalkow, L.H. *et al., Tet. Lett.*, 1964, 217 (*synth*)
Patterson, R.L.S. *et al., J. Sci. Food Agric.*, 1968, **19**, 31 (*occur*)
Kingsbury, A.E. *et al., Horm. Res.*, 1978, **9**, 254 (*metab*)
Kagan, M.Z. *et al., Bioorg. Khim.*, 1979, **5**, 1158 (*synth*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1983, **66**, 192 (*synth, epimers, isomers*)
Turner, A.B. *et al., Tet. Lett.*, 1983, **24**, 4589 (*14β-form*)
Cox, P.J. *et al., Tetrahedron*, 1984, **40**, 3153 (*synth, cryst struct, bibl*)

Angelicain A-527

2,3-Dihydro-4-hydroxy-7-(hydroxymethyl)-2-(1-hydroxy-1-methylethyl)-5H-furo[3,2-g][1]benzopyran-5-one, 9CI. Norcimifugin [64519-22-8]



(*R*)-*form*

$C_{15}H_{16}O_6$ 292.288
Numbering systems vary.

(R)-form

1′-Deoxy, 1′,2′-didehydro: [17398-06-0] ***Umtatin***
$C_{15}H_{14}O_5$ 274.273
Cryst. (MeOH). Mp 178-180°. $[\alpha]_D^{21}$ -56.3 (c, 0.13 in $CHCl_3$).

(S)-form [49624-66-0]
Constit. of *Angelica archangelica* (angelica). Cryst. Mp 208-209°. $[\alpha]_D$ +49.

1″-O-β-D-Glucopyranoside: [85889-15-2] **prim-O-*Glucosylangelicain***
$C_{21}H_{26}O_{11}$ 454.43
Needles (EtOH). Mp 130-132°. $[\alpha]_D^{22}$ +13.7 (c, 0.580 in EtOH).

1″-Angeloyl: [173994-06-4] ***Angeliticin A***
$C_{20}H_{22}O_7$ 374.39
Cryst. Mp 177-178°.

4-Me ether: [37921-38-3] ***Cimifugin***. *Cimitin*
$C_{16}H_{18}O_6$ 306.315
Needles (MeOH). Mp 107-109°. $[\alpha]_D$ +79.2 (c, 0.8 in $CHCl_3$).

4-Me ether, 1″-O-β-D-glucopyranoside: [80681-45-4] **prim-O-*Glucosylcimifugin***
$C_{22}H_{28}O_{11}$ 468.457
Cryst. ($CHCl_3$). Mp 118-120° (113°-115°). $[\alpha]_D^{24}$ +33.3 (c, 0.6 in $CHCl_3$).

1″-Carboxylic acid: 2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-oxo-5H-furo[3,2-g][1]benzopyran-7-carboxylic acid. Norcimifugin acid

1″-Carboxylic acid, 4-Me ether: Cimifugin acid. ***Divaricatacid***
$C_{16}H_{16}O_7$ 320.298
λ_{max} 243; 306 (EtOAc).

1″-Carboxylic acid, 4-Me ether, Et ester: [1049708-13-5] ***Divaricataester B***
$C_{18}H_{20}O_7$ 348.352
Brown powder. $[\alpha]_D^{25}$ +32.2 (c, 0.09 in MeOH). λ_{max} 243; 314 (EtOH). λ_{max} 218 (log ϵ 4.19); 243 (sh) (log ϵ 3.83); 314 (log ϵ 3.61) (MeOH).

2′-Hydroxy: [864814-09-5] ***2′-Hydroxyangelicain***
$C_{15}H_{16}O_7$ 308.287
Needles (MeOH). Mp 196-198°. $[\alpha]_D^{25}$ +83 (c, 0.04 in MeOH). C-1′ config. not determined. Called 6′-hydroxy in the lit. λ_{max} 215 (log ϵ 3.76); 233 (log ϵ 2.67); 251 (log ϵ 2.36); 300 (log ϵ 1.78) (MeOH).

1″-Deoxy: ***Visamminol***
$C_{15}H_{16}O_5$ 276.288
Needles (hexane/EtOAc). Mp 160-

160.5°. $Bp_{0.002}$ 140°. $[\alpha]_D^{17}$ +133.3 (c, 0.08 in EtOH). λ_{max} 233 (log ϵ 4.33); 250 (log ϵ 4.27); 257 (log ϵ 4.26); 296 (log ϵ 4.15) (EtOH).

1″-Deoxy, 4-Me ether: [80681-42-1] ***5-O-Methylvisamminol***
$C_{16}H_{18}O_5$ 290.315
Needles (EtOAc/hexane). Mp 141-142°. $[\alpha]_D^{25}$ +91.8 (c, 0.90 in $CHCl_3$). λ_{max} 224 (log ϵ 4.39); 238 (log ϵ 4.35); 241 (log ϵ 4.29); 387 (log ϵ 4.2) (EtOH).

*1″-Deoxy, 4-Me ether, 1′-*O*-β-D-gluco-pyranoside:* [84272-85-5] *5-*O*-Methyl-visamminol glucoside*
$C_{22}H_{28}O_{10}$ 452.457
Needles (H_2O). Mp 151-156°. $[\alpha]_D^{25}$ +104 (c, 0.05 in MeOH).

1″-Deoxy, 4-Me ether, 1′-angeloyl: [1082971-50-3] ***4′-O-Angeloyl-5-O-methylvisamminol***
$C_{21}H_{24}O_6$ 372.417
Oil. $[\alpha]_D$ +59 (c, 0.1 in $CHCl_3$). λ_{max} 214 (log ϵ 4.33); 286 (log ϵ 3.93) (EtOH).

*1″-Deoxy, 4-Me ether, 1′-*O*-(3-methyl-2-butenoyl):* [1082971-52-5] ***5-O-Methyl-4′-O-senecioylvisamminol***
$C_{21}H_{24}O_6$ 372.417
Oil. $[\alpha]_D$ +42 (c, 0.4 in $CHCl_3$). λ_{max} 212 (log ϵ 4.49); 284 (log ϵ 3.92) (EtOH).

(±)-*form*
Mp 197-198°.

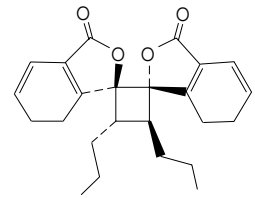
(ξ)-*form*

1″-Deoxy, 2′-hydroxy (1′ξ): [103629-81-8] ***Cnidimol B***
$C_{15}H_{16}O_6$ 292.288
Needles. Mp 214-215°. $[\alpha]_D$ -112.8 (c, 0.24 in MeOH).

Bencze, W. *et al., Helv. Chim. Acta*, 1956, **39**, 923-944 (*Visamminol*)
Neilsen, B.E. *et al., Acta Chem. Scand.*, 1964, **18**, 2111-2114 (*Visamminol, abs config*)
Dean, F.M. *et al., Tet. Lett.*, 1967, **8**, 2737-2740 (*Umtatin*)
Kondo, Y. *et al., Chem. Pharm. Bull.*, 1972, **20**, 1940-1944 (*Cimicifugin*)
Kirtany, J.K. *et al., Indian J. Chem.*, 1973, **11**, 505 (*struct*)
Grundon, M.F. *et al., JCS Perkin 1*, 1975, 150 (*Visamminol, synth*)
Chatterjee, A. *et al., Indian J. Chem., Sect. B*, 1977, **15**, 212 (*isol*)
Baba, K. *et al., Chem. Pharm. Bull.*, 1981, **29**, 2565-2570 (*Angelica japonica constits*)
Sasaki, H. *et al., Chem. Pharm. Bull.*, 1982, **30**, 3555-3562 (*Ledebouriella constits*)
Kozawa, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 64-69 (*Angelicain glucoside*)
Kopp, B. *et al., Helv. Chim. Acta*, 1991, **74**, 611 (*Cimifugin glucoside*)
Baba, K. *et al., Phytochemistry*, 1992, **31**, 1367-1370 (*Cnidimol B, isol*)
Lemmich, J. *et al., Phytochemistry*, 1995, **38**, 427-432 (*Diplolophium constits*)
Mi, C.F. *et al., Yaoxue Xuebao*, 1995, **30**, 910 (*Angelicitin A*)
Lal, B. *et al., Indian J. Chem., Sect. B*, 1998, **37**, 881-893 (*isol, synth, pmr, activity*)
Cai, J.-N. *et al., J. Nat. Prod.*, 2000, **63**, 485-488 (*Cnidimol B*)
Cao, P. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 145-149 (*6′-Hydroxyangelicain*)
Yamaguchi, S. *et al., Bull. Chem. Soc. Jpn.*, 2008, **81**, 863-868 (*Umtatin, synth, abs config*)
Kang, J. *et al., J. Asian Nat. Prod. Res.*, 2008, **10**, 971-976 (*Divaricataester B*)
Torres-Valencia, J.M. *et al., J. Nat. Prod.*, 2008, **71**, 1956-1960 (*Prionosciadium thapsoides constits, abs config*)
Kang, J. *et al., Rapid Commun. Mass Spectrom.*, 2008, **22**, 1899-1911 (*Norcimifugin acid derivs*)

Angelicolide A-528

3,3′,8,8′-Diligustilide [90826-58-7]

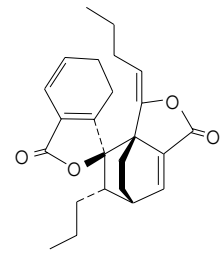


$C_{24}H_{28}O_4$ 380.483
Constit. of roots of *Angelica glauca*. Prisms (Me_2CO/petrol). Mp 157°.

Banerjee, S.K. *et al., Annalen*, 1984, 888 (*cryst struct*)

Angeolide A-529

[81957-73-5]



$C_{24}H_{28}O_4$ 380.483
Constit. of *Angelica glauca*. Cryst. (C_6H_6/hexane). Mp 130°. $[\alpha]_D^{25}$ 0 ($CHCl_3$).

Banerjee, S.K. *et al., Annalen*, 1982, 699-707 (*cryst struct*)

Triakis scyllia Angiotensin I A-530

Dogfish angiotensin I [152839-32-2]

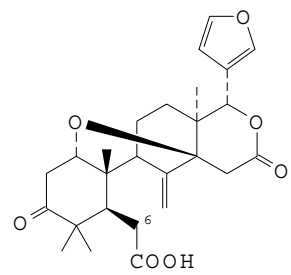
Asn-Arg-Pro-Tyr-Ile-His-Pro-Phe-Gln-Leu

$C_{61}H_{89}N_{17}O_{14}$ 1284.48
Isol. from plasma and kidney extracts of the dogfish *Triakis scyllia*.

Takei, Y. *et al., J. Endocrinol.*, 1993, **139**, 281-285 (*isol*)

Angolensic acid A-531

[3242-10-2]



$C_{26}H_{32}O_7$ 456.535
Cryst. (MeOH). Mp 272°. $[\alpha]_D$ -46 (c, 1 in $CHCl_3$).

Me ester: [2629-14-3] ***Methyl angolensate***
$C_{27}H_{34}O_7$ 470.561
Cryst. (MeOH). Mp 212-214°. $[\alpha]_D^{30}$ -43 (c, 2 in $CHCl_3$).

8,30-Dihydro, 8α-hydroxy, Me ester: [1019983-91-5]
$C_{27}H_{36}O_8$ 488.577
Amorph. powder. $[\alpha]_D^{20}$ +50 (c, 0.105 in MeOH). λ_{max} 210 (sh) (log ϵ 3.74) (MeOH).

6-Hydroxy: 6-Hydroxyangolensic acid
Cryst. Mp 275°.

6ξ-Hydroxy, Me ester: [23984-30-7]
$C_{27}H_{34}O_8$ 486.561
Cryst. (MeOH aq.). Mp 235-238°. $[\alpha]_D$ -85 (c, 0.95 in $CHCl_3$).

6ξ-Acetoxy, Me ester: [16566-88-4]
$C_{29}H_{36}O_9$ 528.598
Cryst. (MeOH aq.).
Mp 172-174°. $[\alpha]_D$ -82 (c, 1.6 in $CHCl_3$).

6ξ,12α-Diacetoxy, Me ester: [37144-86-8] ***Methyl 6,12-diacetoxyangolensate***
$C_{31}H_{38}O_{11}$ 586.635
Cryst. (MeOH). Mp 249-251°. $[\alpha]_D^{26}$ -59.6.

*17-Epimer, 6*S*-hydroxy, Me ester:* [1011244-46-4] ***Intybusoloid***
$C_{27}H_{34}O_8$ 486.561
Constit. of *Cichorium intybus* (chicory). Amorph. powder. $[\alpha]_D^{25}$ -88 (c, 0.21 in MeOH). λ_{max} 206 (log ϵ 4.1) (MeOH).

Chan, W.R. *et al., JCS(C)*, 1967, 171-177 (*Methyl angolensate*)
Connolly, J.D. *et al., Tetrahedron*, 1967, **23**, 4035-4039 (*6-hydroxy derivs*)
Adesogan, E.K. *et al., JCS(C)*, 1968, 1974-1981 (*Khaya senegalensis constits*)
Connolly, J.D. *et al., JCS Perkin 1*, 1972, 1145 (*Methyl diacetoxyangolensate*)
Connolly, J.D. *et al., JCS Perkin 1*, 1973, 2407-2413 (*synth*)
Taylor, D.A.H. *et al., JCS Perkin 1*, 1974, 437-441 (*cmr*)
Kadota, S. *et al., Chem. Pharm. Bull.*, 1990, **38**, 639-651 (*pmr, cmr*)
Njar, V.C.O. *et al., Planta Med.*, 1995, **61**, 91-92 (*Methyl angolensate, activity*)
Mootoo, B.S. *et al., J. Nat. Prod.*, 1996, **49**, 544 (*Methyl angolensate, activity*)
Bickii, J. *et al., J. Ethnopharmacol.*, 2000, **69**, 27-33 (*Methyl angolensate, activity*)
Abdelgaleil, S.A.M. *et al., Tetrahedron*, 2001, **57**, 119-126 (*pmr, cmr*)
Atta-ur-Rahman, *et al., J. Nat. Prod.*, 2008, **71**, 910-913 (*Intybusoloid*)
Wang, X.-N. *et al., Phytochemistry*, 2008, **69**, 1319-1327 (*Trichilia connaroides constit*)

Angularin† A-532

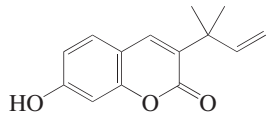
[436084-54-7]

Peptide. Struct. not reported. Isol. from adzuki beans.

Ye, X.Y. *et al., J. Pept. Sci.*, 2002, **8**, 101-106

Angustifolin† A-533

*3-(1,1-Dimethyl-2-propenyl)-7-hydroxy-2*H*-1-benzopyran-2-one, 9CI. 3-(1,1-Dimethylallyl)-7-hydroxycoumarin* [56881-08-4]



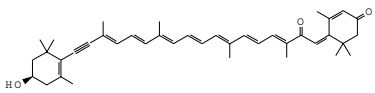
$C_{14}H_{14}O_3$ 230.263
Gum.

Me ether: [20958-63-8] *3-(1,1-Dimethyl-2-propenyl)-7-methoxy-2*H*-1-benzopyran-2-one. 3-(1,1-Dimethylallyl)-7-methoxycoumarin.* ***3-(1,1-Dimethylallyl)herniarin***
$C_{15}H_{16}O_3$ 244.29
Isol. from roots of *Ruta graveolens* (rue). Cryst. (MeOH or hexane). Mp 126-128°. λ_{max} 216 (log ϵ 4.11); 251 (sh) (log ϵ 3.36); 295 (sh) (log ϵ 3.96); 321 (log ϵ 4.25) (MeOH).

Reisch, J. *et al., Tet. Lett.*, 1968, **9**, 4395-4398 (*Me ether, isol*)
Raj, K. *et al., Indian J. Chem.*, 1975, **13**, 404 (*synth*)
Del Castillo, J.B. *et al., Phytochemistry*, 1984, **23**, 2095-2096 (*Angustifolin, isol*)
Galán, R.H. *et al., Heterocycles*, 1989, **29**, 297-300 (*synth*)
Macias, F.A. *et al., Acta Cryst. C*, 1990, **46**, 2482-2484 (*cryst struct*)

Anhydroamarouciaxanthin B A-534

6′,7,7′,8-Tetrahydro-6′,8′-dihydro-3-hydroxy-β,ϵ-carotene-3′,8′-dione [119286-10-1]

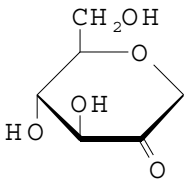


$C_{40}H_{50}O_3$ 578.833
Constit. of *Mytilus edulis* (blue mussel). λ_{max} 458; 485 (hexane).

Hertzberg, S. *et al., Acta Chem. Scand., Ser. B*, 1988, **42**, 495 (*occur, uv, ms, pmr*)

1,5-Anhydrofructose, 9CI A-535

1,5-Anhydro-arabino-*hex-2-ulose*



$C_6H_{10}O_5$ 162.142
In aq. soln. the oxo form illus. is in equilib. with the 2-enol form, the 2,3-enediol form and the 3,3-diol covalent hydrate, which is the predominating species. In nonaqueous solvs. exists as a mixt. of two dimers. Acetylation gives spiro-dimers.

D-*form* [75414-43-6]
Isol. from *Morchella vulgaris* (morel). Amorph. solid. Mp 107-112°. $[\alpha]_D^{20}$ -32.9 (c, 0.86 in H_2O).

Oxime: [75414-31-2]
$C_6H_{11}NO_5$ 177.157
Mp 178-180°. $[\alpha]_D^{21}$ -43 (c, 0.3 in H_2O).

*Tri-Ac: 3,4,6-Tri-*O*-acetyl-1,5-anhydro-*D*-*arabino*-hex-2-ulose*
$C_{12}H_{16}O_8$ 288.254
Mp 93-94° (86-88°). $[\alpha]_D$ -7.2 (c, 1.5 in $CHCl_3$).

Tribenzoyl: [75414-32-3] *1,5-Anhydro-3,4,6-tri-*O*-benzoyl-*D*-fructose*
$C_{27}H_{22}O_8$ 474.466
Mp 126-127°. $[\alpha]_D^{20}$ -24 (c, 0.8 in $CHCl_3$).

Tri-Ac, oxime: [88851-59-6] [75414-20-9]
$C_{12}H_{17}NO_8$ 303.268
Mp 89-90°. $[\alpha]_D^{21}$ -52.9 (c, 0.3 in $CHCl_3$).

Tribenzoyl, oxime: [82569-81-1] [75414-21-0]
$C_{27}H_{23}NO_8$ 489.481
Mp 176-177°. $[\alpha]_D^{21}$ -39 (c, 0.4 in $CHCl_3$).

*4,6-Benzylidene, 3-(*tert*-butyldimethylsilyl):* [89872-98-0] *1,5-Anhydro-4,6-*O*-benzylidene-3-*O*-(*tert*-butyldimethylsilyl)-*D*-fructose*
$C_{19}H_{28}O_5Si$ 364.513
Syrup + $1H_2O$. $[\alpha]_D^{20}$ -49.9 (c, 2.7 in $CHCl_3$).

Di-Et dithioacetal: [75414-37-8]
$C_{10}H_{20}O_4S_2$ 268.398
Needles (Et_2O). Mp 93-94°. $[\alpha]_D^{24}$ -49.8 (c, 1 in $CHCl_3$).

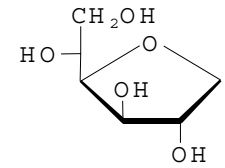
Tribenzyl: [1017968-98-7] *1,5-Anhydro-3,4,6-tri-*O*-benzyl-*D*-fructose*
$C_{27}H_{28}O_5$ 432.515
Cryst. (diisopropyl ether). Mp 85°. $[\alpha]_D^{20}$ -16.1 (c, 1.1 in $CHCl_3$).

*Tribenzyl, oxime (*E*-):* [1017968-93-2]
$C_{27}H_{29}NO_5$ 447.53
Mp 64-65°. $[\alpha]_D^{20}$ -29 (c, 1.1 in $CHCl_3$).

Lichtenthaler, F.W. *et al., Tet. Lett.*, 1980, **21**, 1429-1432 (*synth, tri-Ac, tribenzoyl*)
Tulshian, D.B. *et al., JOC*, 1984, **49**, 2347-2355 (*benzylidene butyldimethylsilyl*)
Deffieux, G. *et al., Phytochemistry*, 1987, **26**, 1391-1393 (*biosynth, isol, oxime, cryst struct*)
Baute, M.A. *et al., Phytochemistry*, 1991, **30**, 1419-1423 (*biosynth*)
Yu, S. *et al., Carbohydr. Res.*, 1998, **305**, 73-82 (*anal, bibl*)
Kopper, S. *et al., Chem. Eur. J.*, 1998, **4**, 2442-2455 (*synth*)
Andersen, S.M. *et al., J. Carbohydr. Chem.*, 1998, **17**, 1027-1035 (*acetyl dimers, cryst struct*)
Andersen, S.M. *et al., J. Carbohydr. Chem.*, 2000, **19**, 717-723; 2002, **21**, 569-578 (*synth, struct, tri-Ac, props*)
Andersen, S.M. *et al., Carbohydr. Res.*, 2002, **337**, 873-890 (***rev***)
Yamaji, K. *et al., Planta Med.*, 2002, **68**, 16-19 (*activity*)
Lichtenthaler, F.W. *et al., Eur. J. Org. Chem.*, 2003, 3094-3104 (*tribenzoyl*)
Yu, S. *et al., Food Chem. Toxicol.*, 2004, **42**, 1677-1686 (*anal, metab, toxicol*)
Brehm, M. *et al., Tetrahedron: Asymmetry*, 2008, **19**, 358-373 (*oxime derivs, di-Et dithioacetal, tri-Ac, tribenzoyl, tribenzyl*)

1,4-Anhydroglucitol, 9CI, 8CI A-536

1,4-Anhydrosorbitol. Arlitan. Sorbitan [27299-12-3]
[12441-09-7]



$C_6H_{12}O_5$ 164.158

D-*form*
Cryst. (2-propanol). Mp 115-116°. $[\alpha]_D^{27}$ -21.9 (c, 2.5 in H_2O).

*6-*O*-Dodecanoyl:* [1338-39-2] *Sorbitan monolaurate, BAN, USAN.* ***Sorbitan laurate, INN****. Sorbester P12. Span 20. E493*
$C_{18}H_{34}O_6$ 346.463
Food emulsifier, solubiliser, crystallisation retarder, dough improver, antifoam agent, stabiliser.
▶ Eye irritant. LD_{50} (rat, orl) 33600 mg/kg. WG2920000

*6-*O*-Hexadecanoyl:* [26266-57-9] *Sorbitan monopalmitate, BAN, USAN.* ***Sorbitan palmitate, INN****. Sorbester P16. Span 40. E495*
$C_{22}H_{42}O_6$ 402.57
Food emulsifier, stabiliser.
▶ WG2932900

*6-*O*-Octadecanoyl:* [1338-41-6] *Sorbitan monostearate, BAN, USAN.* ***Sorbitan stearate, INN****. Sorbester P18. Span 60. FEMA 3028. E491*
$C_{24}H_{46}O_6$ 430.624
Food emulsifier, stabiliser, defoaming agent, flavouring and flavour modifier, rehydration agent for active dried yeast, coating for fruit and vegetables and other food uses.
▶ Skin irritant. LD_{50} (rat, orl) 31000 mg/kg. WG2933500

*6-*O*-(9-Octadecenoyl):* [1338-43-8] *Sorbitan monooleate, BAN, USAN.* ***Sorbitan oleate, INN****. Sorbester P17. Span 80. NSC 406239. E494*
$C_{24}H_{44}O_6$ 428.608
Emulsifier and clarification agent in food preparations (sugar liquor or juice).
▶ Skin irritant. WG2932400

3,5,6-Trioctadecanoyl: [26658-19-5] ***Sorbitan tristearate, BAN, USAN****. Sorbester P38. Span 65. E492*
$C_{60}H_{114}O_8$ 963.556
Food emulsifier, stabiliser.

3,5,6-Tris(9-octadecenoyl): [5960-06-5] ***Sorbitan trioleate, BAN, USAN****. Sorbester P37. Span 85*
[26266-58-0]
$C_{60}H_{108}O_8$ 957.508
Food emulsifier.

*5,6-*O*-Isopropylidene:* [55730-73-9] *1,4-Anhydro-5,6-*O*-isopropylidene-*D*-glucitol*
$C_9H_{16}O_5$ 204.222
Mp 68-70°. $[\alpha]_D^{20}$ -6 (c, 1 in $CHCl_3$).

*5,6-*O*-Isopropylidene, 2-mesyl:* [55730-74-0] *1,4-Anhydro-5,6-*O*-isopropylidene-2-*O*-mesyl-*D*-glucitol*
$C_{10}H_{18}O_7S$ 282.314
Mp 112°.

*5,6-*O*-Isopropylidene, 2,3-dimesyl:* [55730-75-1] *1,4-Anhydro-5,6-*O*-isopropylidene-2,3-di-*O*-mesyl-*D*-glucitol*
$C_{11}H_{20}O_9S_2$ 360.406
Mp 163-163.5°.

*Tetra-Me: 1,4-Anhydro-2,3,5,6-tetra-*O*-methyl-*D*-glucitol*
$C_{10}H_{20}O_5$ 220.265
Bp_{14} 170-174°. $[\alpha]_D^{22}$ -43 (c, 4.84 in EtOH).

Mixt. of partial esters, mono- and dianhydrides with oleic acid: [8007-43-0] ***Sorbitan sesquioleate, BAN, USAN.*** *Arlacel C*
[37318-79-9]
Oily viscous liq.

▶ Potent allergen.

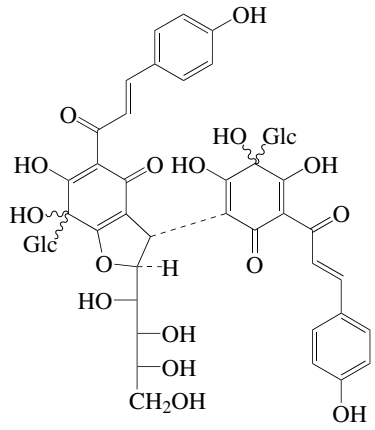
9-Octadecenoyl (2:3): Crill 43™. Sorgen 30™. Nikkol SO-15™
Water in oil emulsifier, wetting agent, pigment dispersant. Mixt. of mono- and diesters of oleic acid.

[54392-26-6, 51938-44-4, 36521-89-8]

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1055A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 727B (*ir*)
Goldsmith, H.A. *et al., Chem. Ind. (London)*, 1943, **52**, 326-328 (*sorbitan sesquioleate*)
Soltzberg, S. *et al., JACS*, 1946, **68**, 919 (*D-form, synth, D-tetra-Me*)
Sherman, P. *et al., J. Colloid Sci.*, 1953, **8**, 35-37 (*sorbitan sesquioleate*)
Que, L. *et al., Biochemistry*, 1974, **13**, 146 (*cmr*)
Hanessian, S. *et al., Tet. Lett.*, 1974, 3983 (*D-isopropylidene mesyl, D-isopropylidene dimesyl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **22**, 332 (*esters, use*)
Sato, S. *et al., Anal. Lett.*, 1981, **14**, 531 (*use*)
Sato, S. *et al., Anal. Chim. Acta*, 1982, **142**, 319 (*use*)
Larni, E. *et al., Contact Dermatitis*, 1988, **19**, 368-371 (*sorbitan sesquioleate*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, SKV100; SKU700
Duclos, A. *et al., Synthesis*, 1994, 1087 (*D-isopropylidene*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2620; 2621-2624 (*monooleate, monostearate, use, props*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1328
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1847 (*monooctadecanoate*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SKV000; SKV100; SKV150

Anhydrosafflor Yellow B A-537

[184840-84-4]

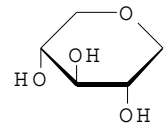


$C_{48}H_{52}O_{26}$ 1044.923
Isol. from fresh florets of safflower (*Carthamus tinctorius*). Amorph. yellow powder. λ_{max} 230 (log ϵ 4.33); 410 (log ϵ 4.62) (MeOH).

Kazuma, K. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 1588-1599

1,5-Anhydroxylitol A-538

[39102-78-8]



$C_5H_{10}O_4$ 134.132
A *meso* compd. Isol. from leaves of *Olea europaea* (common olive). Prisms (EtOH). Sol. H_2O; insol. EtOAc, petrol. Mp 90-91° Mp 116-117°.

2,3,4-Triphosphate:
$C_5H_{13}O_{13}P_3$ 374.071
Cryst. + $1H_2O$ (MeOH/2-propanol) (as pentakis(cyclohexylammonium) salt). Mp 187.5-190° (pentakis(cyclohexylammonium) salt).

Tri-Ac: [19200-32-9] *2,3,4-Tri-*O*-acetyl-1,5-anhydroxylitol*
$C_{11}H_{16}O_7$ 260.243
Mp 122-123°.

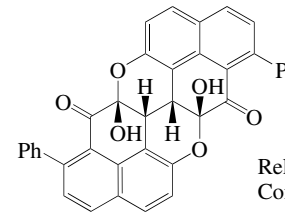
Tribenzoyl: [15023-21-9] *1,5-Anhydro-2,3,4-tri-*O*-benzoylxylitol*
$C_{26}H_{22}O_7$ 446.456
Cryst. (EtOH). Mp 146-147°.

3,4-Dibenzyl: [174226-13-2] *1,5-Anhydro-3,4-di-*O*-benzyl-*D*-xylitol*
$C_{19}H_{22}O_4$ 314.38
Cryst. (hexane/EtOAc). Mp 50-52°. $[\alpha]_D$ -9.2 (c, 1.3 in $CHCl_3$).

Fletcher, H.G. *et al., JACS*, 1947, **69**, 921 (*synth*)
Soman, E. *et al., Carbohydr. Res.*, 1972, **24**, 173 (*synth*)
Kondo, Y. *et al., Carbohydr. Res.*, 1982, **103**, 154; 1983, **111**, 325 (*derivs*)
Regeling, H. *et al., Carbohydr. Res.*, 1993, **244**, 187 (*triphosphate*)
Murali, R. *et al., Carbohydr. Res.*, 1996, **280**, 351-355 (*synth, 3,4-dibenzyl*)
Elvebak, L.E. *et al., Carbohydr. Res.*, 1997, **299**, 143-149 (*derivs*)
Campeol, E. *et al., Carbohydr. Res.*, 2004, **339**, 2731-2732 (*isol*)

Anigorootin A-539

[221287-38-3]
[193892-60-3, 193892-39-6]



Relative Configuration

$C_{38}H_{22}O_6$ 574.588
Phenalene dimer showing 2-fold rotational symmetry. Compd. 2 of Luis *et al*, 1997, has been reassigned this struct. (2002). Constit. of *Musa acuminata* (dwarf banana). Yellow solid. λ_{max} 249 (log ϵ 3.9); 284 (log ϵ 3.4); 358 (log ϵ 1.5); 448 (log ϵ 1.5) (MeOH).

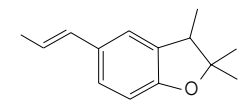
4′-Hydroxy: ***4′-Hydroxyanigorootin***
$C_{38}H_{22}O_7$ 590.588
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Pale yellow solid. Contains a *p*-hydroxyphenyl residue. Formerly assigned an isomeric struct.

4′,4″-Dihydroxy: ***4′,4″-Dihydroxyanigorootin***
$C_{38}H_{22}O_8$ 606.587
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Pale yellow solid. Compd. 3 of Luis *et al*, 1997, was reassigned this struct. (2002).

Luis, J.G. *et al., Tetrahedron*, 1997, **53**, 8249-8256 (*isol*)
Hoelscher, D. *et al., Phytochemistry*, 1999, **50**, 155-161 (*isol, uv, ir, pmr, cmr*)
Otalvaro, F. *et al., Phytochemistry*, 2002, **60**, 61-66 (*isol, pmr, cmr, cryst struct*)

Anisoxide A-540

2,3-Dihydro-2,2,3-trimethyl-5-(1-propenyl)benzofuran, 9CI [643-49-2]



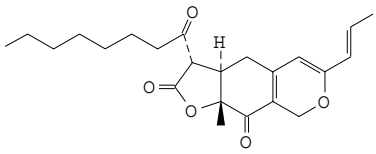
$C_{14}H_{18}O$ 202.296

(±)-*form*
Isol. from oil of star anise (*Illicium verum*) after thermal fractionation. Mp 34-37°. Bp_{14} 142-143°. An artifact resulting from rearr. of Foeniculin (see 4-(1-Propenyl)phenol, P-715).

Jackson, R.W. *et al., JCS*, 1937, 513 (*isol*)
Barton, D.H.R. *et al., JCS*, 1958, 4393 (*synth*)
Okely, H.M. *et al., JCS Perkin 1*, 1981, 897

Ankaflavin A-541

3a,4,8,9a-Tetrahydro-9a-methyl-3-(1-oxooctyl)-6-(1-propenyl)-2H-furo[3,2-g][2]benzopyran-2,9(3H)-dione, 9CI
[50980-32-0]

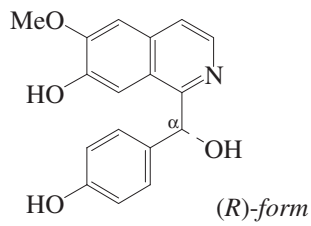


$C_{23}H_{30}O_5$ 386.487
Constit. of red-mold rice. Mp 120-121°. $[\alpha]_D^{25}$ +454 (c, 1.01 in $CHCl_3$). λ_{max} 212 (ϵ 14300); 228 (ϵ 16400); 382 (ϵ 13200) (dioxan).

Manchand, P.S. *et al., Phytochemistry*, 1973, **12**, 2531-2532 (*isol, struct*)
Whalley, W.B. *et al., JCS Perkin 1*, 1976, 1366 (*abs config*)
Martinkova, L. *et al., Food Addit. Contam.*, 1999, **16**, 15-24 (*activity*)
Akihisa, T. *et al., J. Agric. Food Chem.*, 2005, **53**, 562-565 (*isol, activity*)
Hsu, Y.-W. *et al., J. Agric. Food Chem.*, 2010, **58**, 8211-8216 (*isol, pmr, cmr*)

Annocherine A A-542

Annocherine C



$C_{17}H_{15}NO_4$ 297.31
Annocherine A was the *S*-enantiomer and Annocherine C the *R*-form.

(*R*)-*form* [431982-10-4]
Alkaloid from the leaves of *Annona cherimola* (cherimoya). Yellow amorph. powder. Mp 123-125°. $[\alpha]_D^{25}$ -125 (c, 0.3 in $CHCl_3$). λ_{max} 260; 300; 331 (MeOH).

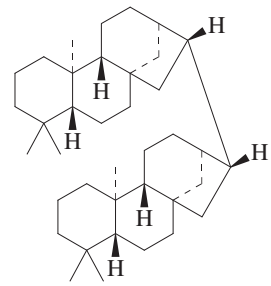
(*S*)-*form*
Alkaloid from *Annona cherimola* (cherimoya). Yellow needles. Mp 156-158°. $[\alpha]_D^{24}$ +135 (c, 0.1 in $CHCl_3$). λ_{max} 260 (log ϵ 3.41); 300 (log ϵ 3.1); 330 (log ϵ 3.52) (MeOH).

α-Me ether: ***Annocherine B***
$C_{18}H_{17}NO_4$ 311.337
Alkaloid from *Annona cherimola* (cherimoya). Amorph. yellow powder. Mp 196-198°. $[\alpha]_D^{24}$ +115 (c, 0.1 in $CHCl_3$). λ_{max} 260 (log ϵ 3.32); 300 (log ϵ 3.11); 331 (log ϵ 3.6) (MeOH).

Chen, C.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 2001, **48**, 1203-1206 (*Annocherine C*)
Chen, C.-Y. *et al., Phytochemistry*, 2001, **56**, 753-757 (*Annocherine A,B*)

Annoglabayin A-543

[819050-87-8]

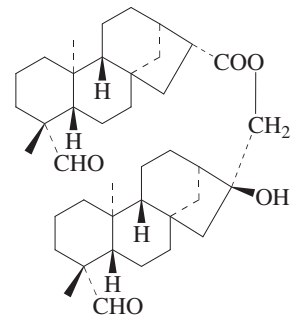


$C_{38}H_{62}$ 518.908
Constit. of fruits of *Annona glabra* (pond apple). Powder. Mp 125-127°. $[\alpha]_D^{25}$ -5.2 (c, 0.75 in $CHCl_3$).

Chen, C.-H. *et al., J. Nat. Prod.*, 2004, **67**, 1942-1946 (*isol, pmr, cmr*)

Annomosin A A-544

[474250-95-8]

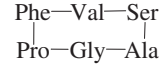


$C_{40}H_{60}O_5$ 620.911
Constit. of *Annona squamosa* (sugar apple). Cryst. Mp 170-171°. $[\alpha]_D^{25}$ -49.3 (c, 0.12 in $CHCl_3$).

Yang, Y.-L. *et al., J. Nat. Prod.*, 2002, **65**, 1462-1467 (*isol, pmr, cmr*)

Annomuricatin A A-545

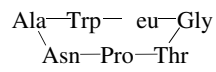
[173994-05-3]



$C_{27}H_{38}N_6O_7$ 558.633
Cyclic peptide. Constit. of the seeds of *Annona muricata* (soursop). Needles (MeOH). Mp 285-287°. $[\alpha]_D^{23}$ +11.28 (c, 0.4 in Py). λ_{max} 202 (ϵ 2800) (EtOH).

Li, C.-M. *et al., Yunnan Zhiwu Yanjiu*, 1995, **17**, 459-462 (*isol, pmr, ms*)

Annomuricatin B A-546

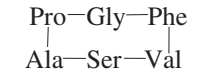


$C_{35}H_{49}N_9O_9$ 739.827
Cyclic peptide. Constit. of the seeds of *Annona muricata* (soursop). Needles ($CHCl_3$/MeOH). Mp 213°. $[\alpha]_D^{19}$ -37.2 (c, 0.5 in MeOH). λ_{max} 204 (log ϵ 3.49); 221 (log ϵ 3.53); 282 (log ϵ 2.65); 290 (log ϵ 2.61) (MeOH).

Li, C.-M. *et al., Phytochemistry*, 1998, **48**, 555-556 (*isol, uv, ir, pmr, cmr, ms*)

Annomuricatin C A-547

[828283-33-6]

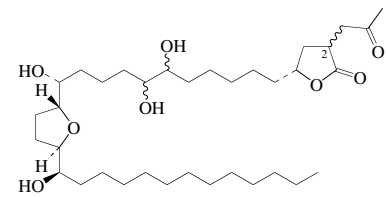


$C_{27}H_{38}N_6O_7$ 558.633
Isol. from seeds of *Annona muricata* (soursop). Mp 284-285°. $[\alpha]_D^{22}$ -2.7 (0.1 in MeOH).

Wélé, A. *et al., C. R. Chim.*, 2004, **7**, 981-988 (*isol*)
Chuang, P.-H. *et al., J. Nat. Prod.*, 2008, **71**, 1365-1370 (*isol, activity*)

Annomuricin-D-one A-548

[184093-47-8, 184093-48-9]

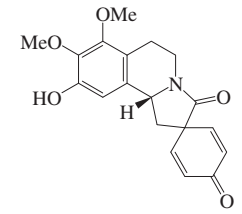


$C_{35}H_{64}O_8$ 612.886
Constit. of *Annona muricata* (soursop). Powder. $[\alpha]_D^{25}$ +15 (c, 10 in $CHCl_3$). Obt. as a 1:1 mixture of C-2 epimers. λ_{max} 205 (ϵ 7750) (MeOH).

Zeng, L. *et al., J. Nat. Prod.*, 1996, **59**, 1035-1042 (*isol, uv, ir, pmr, cmr, ms*)

Annosqualine A-549

[770737-96-7]



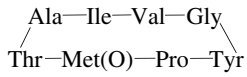
Absolute Configuration

$C_{19}H_{19}NO_5$ 341.363
Alkaloid from the stems of *Annona squamosa* (sugar apple). Syrup. $[\alpha]_D^{27}$ +56 (c 0.19 in MeOH).

Yang, Y.-L. *et al., Helv. Chim. Acta*, 2004, **87**, 1392-1399 (*isol, pmr, cmr, ms*)
Shigehisa, H. *et al., Tet. Lett.*, 2006, **47**, 7301-7306 (*synth*)

Annosquamosin A† **A-550**

[192584-48-8]



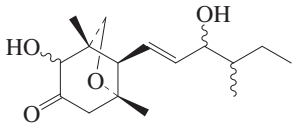
$C_{39}H_{60}N_8O_{11}S$ 849.016

Cyclic peptide. Constit. of the seeds of *Annona squamosa* (sugar apple). Needles (MeOH). Mp 215-216°. $[\alpha]_D^{24}$ -65.3 (c, 0.4 in MeOH).

Chao-Ming, L. *et al., Phytochemistry*, 1997, **45**, 521-523 (*isol, ir, pmr, cmr, ms*)

Annuionone H **A-551**

[866925-33-9]



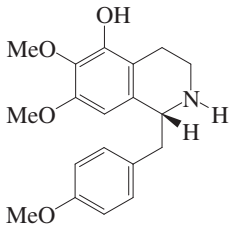
$C_{16}H_{26}O_4$ 282.379

Constit. of *Helianthus annuus* (sunflower). Oil.

Anjum, T. *et al., Phytochemistry*, 2005, **66**, 1919-1921

Anomuricine **A-552**

1,2,3,4-Tetrahydro-6,7-dimethoxy-1-[(4-methoxyphenyl)methyl]-5-isoquinolinol, 9CI. 1,2,3,4-Tetrahydro-5-hydroxy-6,7-dimethoxy-1-(4-methoxybenzyl)isoquinoline [78416-89-4]



$C_{19}H_{23}NO_4$ 329.395

(*R*)-*form*

Me ether, N,N-*di-Me:* **N,N-*Dimethylanomurine***
Amorph. powder (as perchlorate). $[\alpha]_D^{22}$ -26.3 (c, 0.32 in MeOH) (perchlorate). λ_{max} 277 (log ϵ 3.49); 283 (log ϵ 3.47) (MeOH) (perchlorate).

(ξ)-*form*

Minor alkaloid from the root and stem barks of *Annona muricata* (soursop). Noncryst.

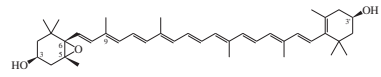
Me ether: [78478-27-0] *1,2,3,4-Tetrahydro-5,6,7-trimethoxy-1-[(4-methoxyphenyl)methyl]isoquinoline, 9CI.* ***Anomurine***
$C_{20}H_{25}NO_4$ 343.422
Minor alkaloid from the root and stem bark of *Annona muricata* (soursop). Noncryst.

Leboeuf, M. *et al., Planta Med.*, 1981, **42**, 37 (*Anomurine, Anomuricine*)

Nishiyama, Y. *et al., Phytochemistry*, 2004, **65**, 939-944 (*N,N-Dimethylanomurine*)

Antheraxanthin **A-553**

5,6-Epoxy-5,6-dihydro-β,β-carotene-3,3′-diol, 9CI. Zeaxanthin epoxide. 5,6-Epoxyzeaxanthin



(3S,3′R,5S,6R,9E)-form

$C_{40}H_{56}O_3$ 584.881

(3*S*,3′*R*,5*S*,6*R*,9*E*)-*form* [25494-44-4]
Antheraxanthin A
Constit. of *Capsicum* fruit; potential nutraceutical. Cryst. (MeOH). Mp 197°.

(3*S*,3′*R*,5*S*,6*R*,9*Z*)-*form* [68831-78-7]
cis-*Antheraxanthin*
Cryst. (MeOH). Mp 108°.

(3*S*,3′*R*,5*R*,6*S*)-*form* [640-03-9]
Antheraxanthin B λ_{max} 420; 445; 475 (Et_2O).

Tappi, G. *et al., Helv. Chim. Acta*, 1949, **32**, 50 (*isol*)
Bartlett, L. *et al., JCS(C)*, 1969, 2527 (*synth, pmr, ms, uv, ord*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 1841 (*occur*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1982, **65**, 2198 (*abs config*)
Molnar, P. *et al., Acta Chim. Hung.*, 1983, **112**, 477 (*cmr*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 231 (*bibl*)
Tsushima, M. *et al., J. Nat. Prod.*, 2000, **63**, 960-964 (*Antheraxanthin B*)

Anthocyanidin 3-*O*-glucosyltransferase **A-554**

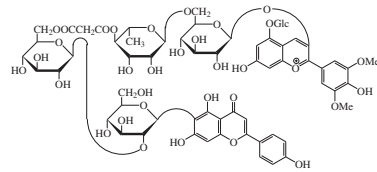
E.C. 2.4.1.115. UDP-D-glucose:anthocyanidin 3-O-*β-D-glucosyltransferase* [65607-32-1]

Hexosyltransferase enzyme. Isol. from wine grape. Acts on a variety of anthocyanidins, incl. delphinidin and pelargonidin.

Kamsteeg, J. *et al., Biochem. Genet.*, 1978, **16**, 1045-1058 (*Silene dioica*)
Ford, C.M. *et al., J. Biol. Chem.*, 1998, **273**, 9224-9233 (*Vitis vinifera*)

***Oxalis* Anthocyanin-flavone dimer** **A-555**

[934754-96-8]

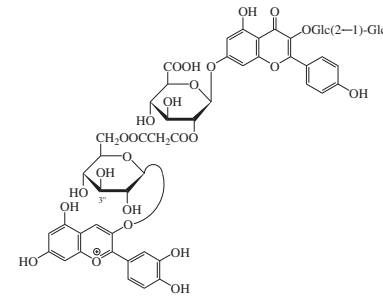


$C_{65}H_{75}O_{38}^{\oplus}$ 1464.285

Constit. of the leaves of *Oxalis triangularis.* λ_{max} 276; 310; 346 (MeOH/0.1% HCl).

Fossen, T. *et al., Phytochemistry*, 2007, **68**, 652-662 (*isol, uv, pmr, cmr, ms*)

***Allium schoenoprasum* Anthocyanin-flavonol** **A-556**



$C_{57}H_{59}O_{35}^{\oplus}$ 1304.072

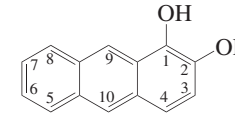
Constit. of the flowers of *Allium schoenoprasum* (chives).

3″-Ac:
$C_{59}H_{61}O_{36}^{\oplus}$ 1346.109
Constit. of the flowers of *Allium schoenoprasum* (chives).

Fossen, T. *et al., Phytochemistry*, 2000, **54**, 317-323

1,2-Anthracenediol, 9CI **A-557**

1,2-Dihydroxyanthracene. 1,2-Anthradiol [577-95-7]



$C_{14}H_{10}O_2$ 210.232

Leaflets (MeOH). Mp 160-162°.

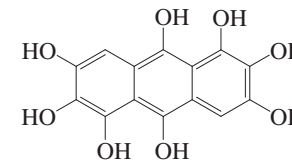
Di-Ac: [74877-26-2]
$C_{18}H_{14}O_4$ 294.306
Cryst. (EtOAc/petrol). Mp 157-157.5°.

1-Me ether: [344452-71-7] *1-Methoxy-2-anthracenol. 2-Hydroxy-1-methoxyanthracene.* ***Orizaanthracenol***
$C_{15}H_{12}O_2$ 224.259
Isol. from rice hulls (*Oryza sativa*). Yellow semi-solid. $[\alpha]_D^{25}$ +8.9. Opt. rotation unaccounted for.

Hall, J. *et al., JCS*, 1923, **123**, 2029 (*synth*)
Jain, A.C. *et al., J. Sci. Ind. Res., Sect. B*, 1956, **15**, 61 (*synth*)
Boldt, P. *et al., JCS Perkin 1*, 1996, 2615 (*pmr, cmr*)
Chung, I.-M. *et al., Bull. Korean Chem. Soc.*, 2006, **27**, 995-1000 (*Orizaanthracenol*)

1,2,3,5,6,7,9,10-Anthraceneoctol **A-558**

1,2,3,5,6,7,9,10-Octahydroxyanthracene



$C_{14}H_{10}O_8$ 306.228

Likely to show tautomerism with 9-oxo form.

*2-Me ether, 7-*O*-α-L-rhamnopyranoside:* [1152440-40-8]
$C_{21}H_{22}O_{12}$ 466.398
Constit. of the aerial parts of *Rhodomyrtus tomentosa* (hill gooseberry). Amorph. yellow powder. $[\alpha]_D^{20}$ +17 (c, 0.5 in MeOH). λ_{max} 223 (log ε 2.24); 235 (log ε 2.54) (MeOH).

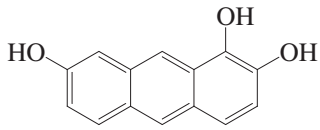
*2,6-Di-Me ether, 3-*O*-α-L-rhamnopyranoside:* [870486-73-0]
$C_{22}H_{24}O_{12}$ 480.424
Cryst. (MeOH). Mp 296-298°. $[\alpha]_D^{22}$ -36 (c, 0.02 in MeOH). λ_{max} 227; 238 (MeOH).

*2,3,6-Tri-Me ether, 7-*O*-β-D-glucopyranoside:* [1152440-38-4]
$C_{23}H_{26}O_{13}$ 510.451
Constit. of the aerial parts of *Rhodomyrtus tomentosa* (hill gooseberry). Amorph. yellow powder. $[\alpha]_D^{20}$ +27.9 (c, 0.5 in MeOH). λ_{max} 226 (log ε 2.13); 238 (log ε 2.41) (MeOH).

Rana, V.S. *et al., Chem. Biodiversity*, 2005, **2**, 792-798 (*Mallotus roxburghianus constit*)
Tung, N.H. *et al., Arch. Pharmacal Res.*, 2009, **32**, 515-520 (*Rhodomyrtus tomentosa glycosides*)

1,2,7-Anthracenetriol A-559

1,2,7-Trihydroxyanthracene



$C_{14}H_{10}O_3$ 226.231

*7-*O*-(3,7-Dimethyloctanoyl), 2-*O*-β-D-glucopyranoside:* [916588-96-0]
$C_{30}H_{38}O_9$ 542.625
Isol. from rice hulls (*Oryza sativa*). Yellow semi-solid. $[\alpha]_D^{25}$ +18.9.

*7-*O*-(3,7,11,15,19-Pentamethyltricosanoyl), 2-*O*-β-D-glucopyranoside:*
$C_{48}H_{74}O_9$ 795.107
Isol. from rice hulls (*Oryza sativa*). Dark yellow semi-solid. $[\alpha]_D^{25}$ +28.1.

Chung, I.-M. *et al., Bull. Korean Chem. Soc.*, 2006, **27**, 995-1000 (*isol, pmr, cmr, ms*)

1,3,10-Anthracenetriol A-560

*1,3,10-Trihydroxyanthracene. 2,4-Dihydroxyanthrone. 2,4-Dihydroxy-9(10*H*)-anthracenone, 9CI*

$C_{14}H_{10}O_3$ 226.231

Tautomeric, anthrone form predominates.

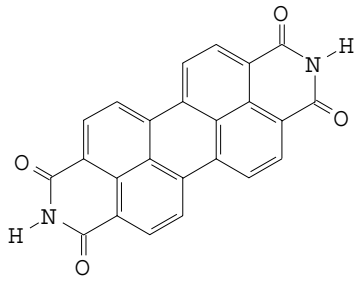
Oxo-*form*

Di-Me ether: 2,4-Dimethoxyanthrone
$C_{16}H_{14}O_3$ 254.285
Constit of the fruit of *Morinda citrifolia* (noni). Mp 209-212°. λ_{max} 255 (log ε 4.16); 275 (sh) (log ε 4.08); 343 (log ε 3.42) (MeOH).

Horii, Z. *et al., Chem. Pharm. Bull.*, 1962, **10**, 1013
Inoue, K. *et al., Phytochemistry*, 1984, **23**, 307-311 (*di-Me ether*)
Siddiqui, B.S. *et al., Nat. Prod. Res.*, 2008, **22**, 1128-1136 (*di-Me ether, isol*)

Anthra[2,1,9-*def*:6,5,10-*d′e′f′*]diisoquinoline-1,3,8,10(2*H*,9*H*)-tetrone, 9CI A-561

Perylene-3,4:9,10-tetracarboxdiimide. C.I. Pigment Violet 29 [81-33-4]



$C_{24}H_{10}N_2O_4$ 390.354

N,N′-*Di-Me:* [5521-31-3] *Indanthrene Red GG. Perylene maroon. C.I. Pigment Red 179. C.I. Vat Red 23*
$C_{26}H_{14}N_2O_4$ 418.408
Red-violet needles.

N,N′-*Bis(tridecyl):* [95689-92-2]
$C_{50}H_{62}N_2O_4$ 755.051
Mp 300°.

N,N′-*Bis(3,5-dimethylphenyl):* [4948-15-6] *C.I. Pigment Red 149*
$C_{40}H_{26}N_2O_4$ 598.656
FDA approved colourant for food contact polymers. Red prisms (quinoline). Mp >300°.

N,N′-*Bis(4-methoxyphenyl):* [6424-77-7] *Indanthrene Scarlet R. Perylene red. Perylene scarlet. C.I. Pigment Red 190. C.I. Vat Red 29*
$C_{38}H_{22}N_2O_6$ 602.602

N,N′-*Bis(2-phenylethenyl):* [97540-34-6] *Perylene green*
$C_{40}H_{22}N_2O_4$ 594.625

N-*Amino,* N′-*(1-butylpentyl):*
$C_{33}H_{29}N_3O_4$ 531.61
Mp >350°.

Ger. Pat., 1959, 1 115 386 (*synth*)
Manukian, B.K. *et al., Helv. Chim. Acta*, 1971, **54**, 2924-2929 (*struct, ir, ms, pmr*)
Rademacher, A. *et al., Chem. Ber.*, 1982, **115**, 2927-2934 (*synth, ms*)
Langhals, H. *et al., Chem. Ber.*, 1985, **118**, 4641-4645; 1991, **124**, 529-535 (*synth, ir, uv, pmr*)
Haedicke, E. *et al., Acta Cryst. C*, 1986, **42**, 189-195; 195-198 (*cryst struct*)
Akers, K. *et al., Spectrochim. Acta A*, 1988, **44**, 1129-1135 (*ir, uv, Raman*)
Quante, H. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 1323-1325 (*bibl*)
Langhals, H. *et al., Chem. Eur. J.*, 1998, **4**, 2110-2116 (*N-amino derivs, synth, ir, pmr, cmr, ms, use*)
Osvath, R. *et al., Food Chem. News*, 2001, **43(19)**, 6 (*C.I. Pigment Red 149, use*)

Anthranilate *N*-malonyltransferase A-562

E.C. 2.3.1.113. Malonyl-CoA:anthranilate N*-malonyltransferase* [94489-98-2]

Enzyme. Isol. from peanut seedlings (*Arachis hypogaea*).

Matern, U. *et al., Arch. Biochem. Biophys.*, 1984, **235**, 218-227

Anthranilate *N*-methyltransferase A-563

E.C. 2.1.1.111. S-*Adenosyl-L-methionine:anthranilate* N*-methyltransferase. Anthranilic acid* N*-methyltransferase* [123779-15-7]

Methyltransferase enzyme. Isol. from *Ruta graveolens* (rue) and other plants. Involved in biosynth. of acridine alkaloids.

Eilert, U. *et al., Plant Cell, Tissue Organ Cult.*, 1989, **18**, 1-18 (*Ruta graveolens*)
Baumert, A. *et al., J. Plant Physiol.*, 1991, **139**, 224-228 (*Ruta graveolens*)

Anthranilate phosphoribosyltransferase A-564

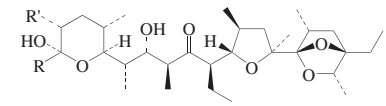
E.C. 2.4.2.18. N-*(5-Phospho-D-ribosyl)anthranilate:diphosphate phospho-α-D-ribosyltransferase. Phosphoribosyl-anthranilate pyrophosphorylase* [9059-35-2]

Pentosyltransferase enzyme. Isol. from yeast, e.g. *Saccharomyces cerevisiae.*

Ito, J. *et al., J. Bacteriol.*, 1969, **97**, 734-742 (*Escherichia coli*)
Creighton, T.E. *et al., Methods Enzymol., Part A*, 1970, **17**, 365-380 (*Escherichia coli*)
Marcus, S.L. *et al., Methods Enzymol.*, 1974, **34**, 377-385 (*Salmonella typhimurium*)
Largen, M. *et al., Eur. J. Biochem.*, 1976, **67**, 31-36 (*Serratia marcescens*)
Edwards, S.L. *et al., J. Mol. Biol.*, 1988, **203**, 523-524 (*Hafnia alvei*)
Hummel, U. *et al., Eur. J. Biochem.*, 1989, **180**, 33-40 (*Saccharomyces cerevisiae*)
Ivens, A. *et al., Eur. J. Biochem.*, 2001, **268**, 2246-2252 (*Sulfolobus sulfataricus*)

Antibiotic X 14889D A-565

X 14889D [97671-94-8]



R = CH_2CH_3, R' = CH_3

$C_{33}H_{58}O_7$ 566.817
Ruminant antibiotic feed additive. Sol. MeOH, C_6H_6; fairly sol. hexane; poorly sol. H_2O. Mp 117°.

Eur. Pat., 1985, 143 438 (*isol*)
Westley, J.W. *et al., J. Antibiot.*, 1986, **39**, 1704-1711 (*struct*)
Liu, C.-M. *et al., J. Antibiot.*, 1993, **46**, 275-279; 280-286 (*isol, cryst struct*)

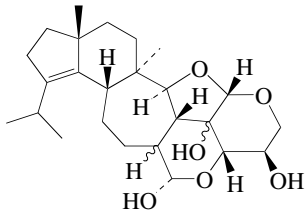
Antibiotic AC1 A-566

Protein, MW 5.4 kDa, comprising a single polypeptide chain. Isol. from *Lactobacillus acidophilus* AC 1. Shows antimicrobial activity.

Mehta, A.M. *et al., Microbios*, 1983, **38**, 73-81

Antibiotic CJ 14258 A-567

CJ 14258



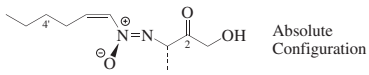
$C_{25}H_{38}O_6$ 434.572

Related to *O*-Demethylstriatin C, D-111. Prod. by *Hericium ramosum*. Powder. $[\alpha]_D^{25}$ -73.4 (c, 0.74 in MeOH).

Saito, T. *et al., J. Antibiot.*, 1998, **51**, 983-990 (*isol, ir, pmr, cmr*)

Antibiotic LL-BH872α A-568

[3-(1-Hexenyl)-ONN-*azoxy]-1-hydroxy-2-butanone, 9CI. LL-BH872α* [24397-77-1]



$C_{10}H_{18}N_2O_3$ 214.264

Light yellow oil. $[\alpha]_D^{25}$ +157 (c, 1.7 in MeOH). Dec. v. readily. λ_{max} 238 (ϵ 9000) (MeOH) (Berdy).

Ac: [36846-66-9] More stable than parent compd.

2ξ-Alcohol: [131205-70-4] ***[3-(1-Hexenyl)*-ONN-*azoxy]-1,2-butanediol*** [637035-36-0]
$C_{10}H_{20}N_2O_3$ 216.28
Prod. by an *Actinomadura* sp. isol. from the roots of *Prunus armeniaca* (apricot). Yellow oil. $[\alpha]_D^{25}$ -30 (c, 0.2 in MeOH). Stereochemical information incomplete. The two isolates may be stereoisomeric. λ_{max} 228 (ϵ 9900) (EtOH).

4′ξ-Hydroxy, 2ξ-alcohol: [131205-71-5] *3-[(4-Hydroxy-1-hexenyl)*-ONN-*azoxy]-1,2-butanediol*. ***Antibiotic MH 072***. *MH 072*
$C_{10}H_{20}N_2O_4$ 232.279

McGahren, W.J. *et al., JACS*, 1969, **91**, 2808-2810; 1970, **92**, 1587-1590 (*isol, cd*)
McGahren, W.J. *et al., JOC*, 1972, **37**, 902-906 (*cd, struct*)
US Pat., 1972, 3 647 776 (*isol, synth*)
Japan. Pat., 1990, 90 202 867 (*Streptomyces misonensis isolates*)
Bianchi, G. *et al., Planta Med.*, 2003, **69**, 574-576 (*2-alcohol, isol, pmr, cmr*)

Phytolacca americana Antifungal peptide A-569

PAFP-S [227622-06-2]

$C_{163}H_{253}N_{51}O_{51}S_6$ 3935.499

Contains 38 amino acids and 3 disulfide bonds. Isol. from the seeds of *Phytolacca americana* (pokeberry).

Shao, F. *et al., Biochim. Biophys. Acta*, 1999, **1430**, 262-268 (*isol, struct*)

Raphanus sativus Antifungal peptides A-570

RS-AFP

Highly-basic polypeptides; rich in cysteine. Four components characterised.

RS-AFP 1

Isol. from radish seeds (*Raphanus sativus*). Contains 51 amino acids. Reduced form shown.

RS-AFP 2

Isol. from radish seeds (*Raphanus sativus*). Contains 51 amino acids. Reduced form shown.

RS-AFP 3

Isol. from radish seeds (*Raphanus sativus*) infected with *Alternaria brassicola*. Terras *et al* indicate struct. contains 51 amino acids, but only provide a 50 one letter code struct.

RS-AFP 4

Isol. from radish seeds (*Raphanus sativus*) infected with *Alternaria brassicola*. Contains 48 amino acids. Reduced form shown.

Terras, F.R. *et al., J. Biol. Chem.*, 1992, **267**, 15301-15309 (*AFP 1, AFP 2, isol, struct*)
Terras, F.R. *et al., Plant Cell*, 1995, **7**, 573-588 (*AFP 3, AFP 4, isol, struct*)
Fant, F. *et al., J. Mol. Biol.*, 1998, **279**, 257-270 (*AFP 1, struct, pmr, cmr*)

Amaranthus caudatus Antimicrobial peptides A-571

Ac-AMP

Peptides; sequences highly homologous to the cysteine/glycine-rich domain occurring in many chitin-binding proteins. Reduced forms shown. Isol. from seeds of *Amaranthus caudatus* (loves-lie-bleeding).

Ac-AMP-1 [139632-17-0]

Contains 29 amino acid residues including 6 cysteines.

Ac-AMP-2 [139632-18-1]

Broekaert, W.F. *et al., Biochemistry*, 1992, **31**, 4308-4314 (*isol, struct*)
Martins, J.C. *et al., J. Mol. Biol.*, 1996, **258**, 322-323 (*pmr, struct*)
El Bouyoussef, M. *et al., J. Pept. Res.*, 1997, **49**, 336-340 (*disulfide bonds*)

Pharbitis nil Antimicrobial peptides A-572

Pn-AMP

Two peptides, Pn-AMP-1 (41 residues) and Pn-AMP-2 (40 residues) with 4 disulfide bonds. Isol. from seeds of *Pharbitis nil*. Analogues of Hevein.

[205394-99-6, 205394-98-5]

Koo, J.C. *et al., Biochim. Biophys. Acta*, 1998, **1382**, 80-90 (*Pn-AMP*)

Misgurnus anguillicaudatus Antimicrobial polypeptide A-573

MAPP

Single-chain polypeptide antibiotic.

Dong, X.Z. *et al., Chin. Chem. Lett.*, 2003, **14**, 54-57 (*isol*)

Allium cepa Antimicrobial protein 1 A-574

Ace-AMP 1 [450374-32-0]

Cationic protein containing 93 amino acid residues and 4 disulfide bonds. Isol. from onion seeds.

Cammue, B.P. *et al., Plant Physiol.*, 1995, **109**, 445-455 (*isol, struct*)
Tassin, S. *et al., Biochemistry*, 1998, **37**, 3623-3637 (*pmr, soln struct*)
Wu, Y. *et al., Appl. Microbiol. Biotechnol.*, 2011, **90**, 1303-1310 (*activity*)

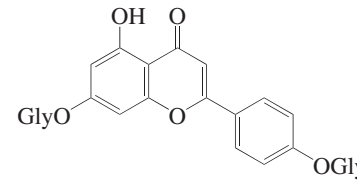
Capsicum annuum Antimicrobial protein 1 A-575

Ca AMP 1

Protein. Shows antifungal activity. Isol. from *Capsicum annuum*.

Pat. Coop. Treaty (WIPO), 1994, 94 11 511 (*isol*)

Apigenin 4′,7-diglycosides A-576



Glycosides of 4′,5,7-Trihydroxyflavone, T-763 with sugar residues at both C-4′ and C-7.

4′-O-β-D-Glucopyranoside, 7-O-[β-D-galacturonopyranosyl-(1→?)-β-D-galacturonopyranoside]: [126207-51-0] *Apigenin 7-digalacturonoside 4′-glucoside*
$C_{33}H_{36}O_{22}$ 784.634
Isol. from *Cuminum cyminum* (cumin).

4′-O-β-D-Glucuronopyranoside, 7-O-[β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:
$C_{33}H_{34}O_{23}$ 798.618
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 182-183° dec. $[\alpha]_D^{20}$ -50.8 (c, 0.05 in MeOH aq.).

*4′-O-β-D-Glucuronopyranoside, 7-O-[4-hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 205-206°. $[\alpha]_D^{20}$ -13.8 (c, 0.1 in MeOH). λ_{max} 271; 323 (MeOH).

*4′-O-[4-Hydroxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 7-O-β-D-glucuronopyranoside:*
$C_{42}H_{40}O_{25}$ 944.763
Constit. of alfalfa (*Medicago sativa*). Amorph. powder. Mp 197-198°. $[\alpha]_D^{20}$ -52.4 (c, 0.1 in MeOH). λ_{max} 272 (sh); 314 (MeOH).

*4′-O-[4-Hydroxy-3-methoxy-*E*-cinnamoyl-(→2)-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside], 7-O-β-D-glucuronopyranoside:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 197-198°.

$[\alpha]_D^{20}$ -10.2 (c, 0.1 in MeOH). λ_{max} 270 (sh); 319 (MeOH).

The Flavonoids: Advances in Research Since 1980, (ed. Harborne, J.B.), Chapman and Hall, 1988,
El-Negoumy, S.I. *et al., CA*, 1990, **112**, 175645x (*cumin glycoside*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 753-758 (*alfalfa glucuronides*)
Stochmal, A. *et al., Phytochemistry*, 2001, **57**, 1223-1226 (*alfalfa glucuronides*)
Flavonoids: Chemistry and Biochemistry, (ed. Andersen, O.M. *et al*), CRC Press, 2005,

Apigenin 7-glycosides A-577

Glycosides of 4′,5,7-Trihydroxyflavone, T-763 with sugar residues at *O*-7 only. See also Cosmosiin, C-546.

7-O-*(6*-O-*Ethyl-β-D-glucuronopyranoside):* [62268-42-2] *Apigenin 7*-O-*ethylglucuronide*
$C_{23}H_{22}O_{11}$ 474.42
Isol. from *Silybum marianum* (milk thistle). Cryst. ($CHCl_3$/EtOH). Mp 220-223°.

7-O-*[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [26544-34-3] ***Apiin***. *7-(2-Apiosylglucosyl)apigenin*
$C_{26}H_{28}O_{14}$ 564.499
Constit. of parsley (*Petroselinum crispum*) and of the flowers of *Anthemis nobilis* (Roman chamomile). First isol. in 1843. Cryst. (EtOH). Mp 236-237°. $[\alpha]_D$ -130 (c, 0.12 in MeOH). λ_{max} 267 (ϵ 15136); 342 (ϵ 19950) (MeOH) (Berdy).

7-O-*[β-D-Apiofuranosyl-(1→2)-6*-O-*acetyl-β-D-glucopyranoside]:* ***6″-Acetylapiin***
$C_{28}H_{30}O_{15}$ 606.536
Constit. of parsley. Powder. $[\alpha]_D^{25}$ -151.6 (c, 0.4 in MeOH). λ_{max} 269 (log ϵ 4); 334 (log ϵ 4.1) (MeOH).

7-O-*[β-D-Apiofuranosyl-(1→2)-6*-O-*malonyl-β-D-glucopyranoside]:* [60478-75-3] ***6″-Malonylapiin***
$C_{29}H_{30}O_{17}$ 650.546
Isol. from parsley.

7-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-glucopyranoside]:* [17306-46-6] *Apigenin 7-neohesperidoside.* ***Rhoifolin***. *Rhoifoloside*
$C_{27}H_{30}O_{14}$ 578.526
Isol. from *Citrus aurantium* (Seville orange). Cryst. + $6H_2O$ (H_2O). Mp 245° (anhyd. 205-208°) Mp 251-253°. $[\alpha]_D^{29}$ -110 (c, 0.21 in MeOH).

7-O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [552-57-8] *Apigenin 7*-O-*rutinoside.* ***Isorhoifolin***
$C_{27}H_{30}O_{14}$ 578.526
Isol. from leaves of *Citrus paradisi* (grapefruit) and other plant spp.; constit. of artichoke heads. Small needles (MeOH). Mp 269-270°. $[\alpha]_D^{23}$ -98.2 (c, 1.19 in Py).

7-O-*[α-L-Rhamnopyranosyl-(1→2)-β-D-galacturonopyranoside]:* [124167-97-1]
$C_{27}H_{28}O_{15}$ 592.509
Isol. from flowers of *Silybum marianum* (milk thistle).

7-O-*[β-D-Galactopyranosyl-(1→4)-β-D-mannopyranoside]:* [84638-36-8]
$C_{27}H_{30}O_{15}$ 594.525
Isol. from seeds of carrot (*Daucus carota*). Cryst. (MeOH). Mp 268-270°.

7-O-*[β-D-Mannopyranosyl-(1→2)-β-D-allopyranoside]:* [956586-41-7]
$C_{27}H_{30}O_{15}$ 594.525
Constit. of the fruit of *Prunus armeniaca* (apricot). Yellow powder. Mp 162°. λ_{max} 272; 333 (MeOH).

7-O-*[β-D-Galacturonopyranosyl-(1→?)-β-D-glucopyranoside]:* [126254-76-0]
$C_{27}H_{28}O_{16}$ 608.509
Isol. from *Cuminum cyminum* (cumin).

7-O-*[β-D-Galacturonopyranosyl-(1→?)-β-D-galacturonopyranoside]:* [126254-75-9] *Apigenin 7-digalacturonoside*
$C_{27}H_{26}O_{17}$ 622.492
Isol. from seeds of *Cuminum cyminum* (cumin).

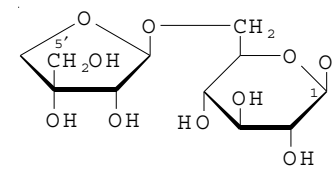
7-O-*[4-Hydroxy*-E-*cinnamoyl-(→2)-[β-D-glucuronopyranosyl-(1→3)]-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{42}H_{40}O_{25}$ 944.763
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 203-204°. $[\alpha]_D^{20}$ -61 (c, 0.1 in MeOH). λ_{max} 271; 323 (MeOH).

7-O-*[4-Hydroxy-3-methoxy*-E-*cinnamoyl-(→2)-[β-D-glucuronopyranosyl-(1→3)]-β-D-glucuronopyranosyl-(1→2)-β-D-glucuronopyranoside]:*
$C_{43}H_{42}O_{26}$ 974.789
Constit. of alfalfa, *Medicago sativa*. Amorph. yellow powder. Mp 210-211°. $[\alpha]_D^{20}$ -50.8 (c, 0.1 in MeOH). λ_{max} 271; 323 (MeOH).

4′-O-*(3,4-Dihydroxy*-E-*cinnamoyl), 7*-O-*[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranoside]:* [14637-28-6] ***Menthoside***
$C_{36}H_{36}O_{17}$ 740.67
Isol. from *Mentha piperita* (peppermint) leaves. Cryst. (EtOH). Mp 271-273°. $[\alpha]_D^{18}$ -89 (c, 0.1 in DMF).

Coussio, J.D. *et al., Experientia*, 1964, **20**, 562 (*Rhoifolin*)
Coussio, J.D. *et al., An. Asoc. Quim. Argent. (1921-2001)*, 1965, **53**, 257-259 (*Rhoifolin*)
Hulyalkar, R.H. *et al., Can. J. Chem.*, 1965, **43**, 2085 (*Apiin*)
Gella, E.V. *et al., Farm. Zh. (Kiev)*, 1967, **22**, 80-85 (*Menthoside*)
Nordby, H.E. *et al., Phytochemistry*, 1968, **7**, 1653-1657 (*Isorhoifolin*)
Wagner, H. *et al., Chem. Ber.*, 1969, **102**, 2083-2088; 1971, **104**, 2681-2687 (*Isorhoifolin, 7-glucuronoside*)
Ezekiel, A.D. *et al., JCS(C)*, 1971, 2907 (*Apiin, synth*)
Schmid, R.D. *et al., Tetrahedron*, 1972, **28**, 3259-3269 (*Apiin, ms*)
Kanao, M. *et al., Yakugaku Zasshi*, 1978, **98**, 366 (*Rhoifolin*)
Gupta, K.R. *et al., Planta Med.*, 1982, **46**, 240 (*4-galactosylmannoside*)
Voigtländer, H.W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1983, **316**, 219 (*Rhoifolin, synth*)
Picher, M.T. *et al., Phytochemistry*, 1984, **23**, 1995-1998 (*ethylglucuronoside*)
El-Negoumy, S.I. *et al., Grasas y Aceites (Sevilla)*, 1989, **40**, 87-89 (*Cuminum cyminum constits*)
Ahmed, A.A. *et al., Phytochemistry*, 1989, **28**, 1751-1753 (*2-rhamnosylgalacturonide, ethylglucuronide, glucuronide*)
Eckey-Kaltenbach, H. *et al., Phytochemistry*, 1993, **34**, 687-691 (*Apiin, 6″-Malonylapiin*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 2000, **48**, 1039-1044 (*6″-Acetylapiin*)
Stochmal, A. *et al., J. Agric. Food Chem.*, 2001, **49**, 753-758 (*alfalfa glucuronides*)
Rashid, F. *et al., Arch. Pharmacal Res.*, 2007, **30**, 932-937 (*7-mannosylalloside*)

6-*O*-β-D-Apiofuranosyl-D-glucose A-578



$C_{11}H_{20}O_{10}$ 312.273

β-D-Pyranose-*form*

1-O-*(3-Methylbutanoyl):* [467242-31-5]
$C_{16}H_{28}O_{11}$ 396.391
Constit. of green coffee beans (*Coffea arabica*).

1-O-*(3-Methyl-2-butenoyl):* [467242-32-6]
$C_{16}H_{26}O_{11}$ 394.375
Constit. of green coffee beans (*Coffea arabica*).

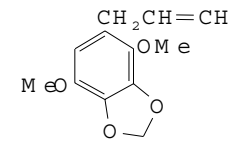
1-O-*Benzoyl, 5′*-O-*(3,4-dihydroxycinnamoyl)(*E-*):* [166990-09-6] ***Psydroside***
$C_{27}H_{30}O_{14}$ 578.526
$[\alpha]_D^{25}$ -45 (c, 0.5 in MeOH).

Me glycoside: Methyl β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside
$C_{12}H_{22}O_{10}$ 326.3
Constit. of cumin (*Cuminum cyminum*). Syrup. $[\alpha]_D^{21}$ -81 (c, 0.4 in MeOH).

Nahrstedt, A. *et al., Phytochemistry*, 1995, **39**, 375 (*Psydroside*)
Weckerle, B. *et al., Phytochemistry*, 2002, **60**, 409-414 (*coffee constits*)
Takayanagi, T. *et al., Phytochemistry*, 2003, **63**, 479-484 (*Me glycoside, isol*)

Apiole A-579

4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole, 9CI. 1-Allyl-2,5-dimethoxy-3,4-methylenedioxybenzene. Parsley apiole. Parsley camphor [523-80-8]



$C_{12}H_{14}O_4$ 222.24
Occurs in *Sassafras albidum* (sassafras), *Anethum graveolens* (dill), *Petroselinum crispum* (parsley) and many other plants. Needles. d_4^{20} 1.02. Mp 30°. Bp 294° Bp_{33} 179°. Log P 2.5 (calc). 2 unstable modifications Mps. 18° and 27.5°. λ_{max} 280 (no solvent reported).

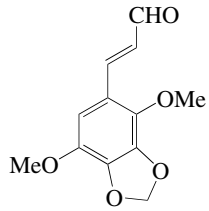
▶ CY2500000

Baker, W. *et al., JCS*, 1938, 1602-1608 (*synth*)

Kasting, R. *et al., Phytochemistry*, 1972, **11**, 2277-2282 (*isol*)
Sethi, M.L. *et al., Phytochemistry*, 1976, **15**, 1773-1775 (*isol*)
Goeckeritz, D. *et al., Pharmazie*, 1979, **34**, 426-429 (*isol*)
MacLeod, A.J. *et al., Phytochemistry*, 1985, **24**, 2623-2627 (*occur*)
Santos, B.V. de O. *et al., Phytochemistry*, 1998, **49**, 1381-1384 (*isol, uv, pmr, cmr*)
Benevides, P.J.C. *et al., Phytochemistry*, 1999, **52**, 339-343 (*isol, pmr*)
Atta-ur-Rahman, *et al., Phytochemistry*, 1999, **52**, 495-499 (*isol, pmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AGE500

Apional A-580

3-(2,5-Dimethoxy-3,4-methylenedioxyphenyl)-2-propenal. 2,5-Dimethoxy-3,4-methylenedioxycinnamaldehyde

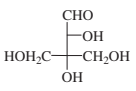


$C_{12}H_{12}O_5$ 236.224
Constit. of parsley (*Petroselinum hortense*). Yellow needles (Et_2O). Mp 99°.

Appendino, G. *et al., Phytochemistry*, 1998, **49**, 1719-1722 (*isol, ir, pmr, cmr, ms*)

Apiose, 9CI, 8CI A-581

*2,3,4-Trihydroxy-3-(hydroxymethyl)butanal. 3-*C*-(Hydroxymethyl)-*glycero*-tetrose. Tetrahydroxyisovaleraldehyde*



D-*form*

β-D-erythro-Tetrofuranose-*form*

$C_5H_{10}O_5$ 150.131
Care needed with naming and numbering of derivs. C-3 is not a chiral centre in the acyclic sugar. In L-Apio-α-D-furanose for example, L- defines the config. at C-2 (L-apiose), while D-defines the config. at C-3 (D-furanosyl stereoisomeric form of L-apiose).

D-*form* [639-97-4]
*(*R*)-form*
First found in parsley as the glycoside Apiin, also present in celery. Syrup. $[\alpha]_D$ +7.6 (c, 0.7 in H_2O).

Benzylphenylhydrazone:
Cryst. ($CHCl_3$). Mp 138-139°. $[\alpha]_D^{20}$ -94 (c, 4.6 in Py). $[\alpha]_D$ -29 (c, 1.1 in MeOH).

*2,3-*O*-Isopropylidene:* [94943-41-6] *2,3-*O*-Isopropylidene-D-apiose*
$C_8H_{14}O_5$ 190.196
Syrup. $[\alpha]_D$ -35 (c, 0.87 in MeOH).

α-D-*erythro*-Tetrofuranose-*form* [30738-01-3]
*D-Apio-α-D-furanose, 9CI. 3-*C*-Hydroxymethyl-α-D-*erythro*-tetrofuranose*

*1,2-*O*-Isopropylidene:* [25018-74-0] *1,2-*O*-Isopropylidene-D-apio-α-D-furanose. 1,2-*O*-Isopropylidene-α-D-*erythro*-tetrofuranose*
$C_8H_{14}O_5$ 190.196
Needles (Et_2O/hexane). Mp 118-120°. $[\alpha]_D^{29}$ +54.5 (c, 0.8 in EtOH).

*1,2-*O*-Isopropylidene, di-Ac:* [33962-41-3] *1′,3-Di-*O*-acetyl-1,2-*O*-isopropylidene-D-apio-α-D-furanoside. 1′,3-Di-*O*-acetyl-1,2-*O*-isopropylidene-α-D-*erythro*-tetrofuranose*
$C_{12}H_{18}O_7$ 274.27
Needles (hexane). Mp 110-111°. $[\alpha]_D$ +64 (c, 1.4 in $CHCl_3$).

*1,2:1′,3-Di-*O*-isopropylidene:* [25904-06-7] *1,2:1′,3-Di-*O*-isopropylidene-D-apio-α-D-furanoside. 1,2:1′,3-Di-*O*-isopropylidene-α-D-*erythro*-tetrofuranose*
$C_{11}H_{18}O_5$ 230.26
Cryst. (Et_2O/hexane). Mp 46-49° Mp 52-54°. $[\alpha]_D$ +62.4 (c, 1.0 in $CHCl_3$). $[\alpha]_D^{28}$ +76.5 (c, 3.0 in EtOH).

*Me glycoside, 1′,2,3-tri-Me: Methyl 1′,2,3-tri-*O*-methyl-D-apio-α-D-furanoside. Methyl 3-*C*-(methoxymethyl)-2,3-di-*O*-methyl-α-D-*erythro*-tetrofuranoside*
$C_9H_{18}O_5$ 206.238
$[\alpha]_D^{26}$ +116 ($CHCl_3$).

β-D-*erythro*-Tetrofuranose-*form* [36465-64-2]
*D-Apio-β-D-furanose, 9CI. 3-*C*-Hydroxymethyl-β-D-*erythro*-tetrofuranose*
Syrup.

*2,3-*O*-Isopropylidene:* [70147-50-1] *2,3-*O*-Isopropylidene-D-apio-β-D-furanose. 3-*C*-Hydroxymethyl-2,3-*O*-isopropylidene-β-D-*erythro*-tetrofuranose*
$C_8H_{14}O_5$ 190.196
Cryst. (Et_2O/hexane). Mp 72°. $[\alpha]_D$ -40 (c, 1.5 in $CHCl_3$).

*Me glycoside, 2,3-*O*-isopropylidene, 1′-tosyl:* [32445-78-6] *Methyl 2,3-*O*-isopropylidene-1′-tosyl-D-apio-β-D-furanoside*
$C_{16}H_{22}O_7S$ 358.412
Cryst. (Et_2O/hexane). Mp 90-91°. $[\alpha]_D^{28}$ -82.1 (c, 4.0 in $CHCl_3$).

*Me glycoside, 1′-Me, 2,3-*O*-isopropylidene:* [4098-02-6] *Methyl 2,3-*O*-isopropylidene-1′-methyl-D-apio-β-D-furanoside. 2,3-*O*-Isopropylidene-3-*C*-(methoxymethyl)-3-*O*-methyl-β-D-*erythro*-tetrofuranose*
$C_{10}H_{18}O_5$ 218.249
Bp_2 70°. $[\alpha]_D^{25}$ -106 (c, 2.4 in $CHCl_3$).

*Me glycoside, 1′,2,3-tri-Me: Methyl 1′,2,3-tri-*O*-methyl-D-apio-β-D-furanoside. Methyl 3-*C*-(methoxymethyl)-2,3-di-*O*-methyl-β-D-*erythro*-tetrofuranoside*
$C_9H_{18}O_5$ 206.238
Syrup. $[\alpha]_D$ -79 ($CHCl_3$). CAS no. not found to 2010.

β-L-*threo*-Tetrofuranose-*form*

*1,2-*O*-Isopropylidene:* [14048-35-2] *1,2-*O*-Isopropylidene-L-apio-β-L-furanose. 1,2-*O*-Isopropylidene-3-*C*-hydroxymethyl-β-L-*threo*-tetrofuranose*
$C_8H_{14}O_5$ 190.196
Needles (CH_2Cl_2/hexane). Mp 124-125°. $[\alpha]_D^{29}$ +46 (c, 1.0 in EtOH).

*1,2-*O*-Isopropylidene, di-Ac:* [14048-36-3] *1′,3-Di-*O*-acetyl-1,2-*O*-isopropylidene-D-apio-β-L-furanose. 1′,3-Di-*O*-acetyl-1,2-*O*-isopropylidene-β-L-*threo*-tetrofuranose*
$C_{12}H_{18}O_7$ 274.27
Cubes (cyclohexane). Mp 88-89.5°. $[\alpha]_D^{29}$ +75 (c, 1.4 in $CHCl_3$).

*1,2-*O*-Isopropylidene, 1′-tosyl: 1,2-*O*-Isopropylidene-1′-*O*-tosyl-β-D-apio-β-L-furanose. 1,2-*O*-Isopropylidene-1′-*O*-tosyl-β-L-*threo*-tetrofuranose*
$C_{15}H_{20}O_7S$ 344.385
Cryst. (Et_2O). Mp 137-138°. $[\alpha]_D$ +43.2 (c, 4.4 in $CHCl_3$).

*1,2:1′,3-Di-*O*-isopropylidene:* [14854-36-5] *1,2:1′,3-Di-*O*-isopropylidene-D-apio-β-L-furanose. 1,2:1′,3-Di-*O*-isopropylidene-3-*C*-(hydroxymethyl)-β-L-*threo*-tetrofuranose*
[34724-16-8]
$C_{11}H_{18}O_5$ 230.26
Needles (H_2O/NH_3). Mp 80-82°. $[\alpha]_D^{29}$ +59 (c, 1.0 in EtOH).

*1′,3-Di-Me, 1,2-*O*-isopropylidene:* [32445-76-4] *1,2-*O*-Isopropylidene-1′,3′-di-*O*-methyl-D-apio-β-L-furanose. 1,2-*O*-Isopropylidene-1′,3′-di-*O*-methyl-β-L-*threo*-tetrofuranose*
$C_{10}H_{18}O_5$ 218.249
Oil. $Bp_{0.1}$ 60°.

*1′,3-Dibenzyl, 1,2-*O*-isopropylidene:* [34339-65-6] *1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-L-apio-β-L-furanose. 1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-β-L-*threo*-tetrofuranose*
$C_{22}H_{26}O_5$ 370.444
Mp 38-39°. $[\alpha]_D^{22}$ +54.5 (c, 1.2 in $CHCl_3$).

L-*form* [6477-44-7]
Syrup. $[\alpha]_D^{20}$ -5 (c, 8.0 in H_2O).

Benzylphenylhydrazone:
Cryst. Mp 136-137°. $[\alpha]_D^{20}$ +94 (c, 1.0 in Py).

α-L-*erythro*-Tetrofuranose-*form*
*L-Apio-α-L-furanose, 9CI. 3-*C*-Hydroxymethyl-α-L-*erythro*-tetrofuranose*

*1,2-*O*-Isopropylidene:* [22403-90-3] *1,2-*O*-Isopropylidene-L-apio-α-L-furanose*
$C_8H_{14}O_5$ 190.196
Cryst. (EtOAc/hexane). Mp 116-118°. $[\alpha]_D^{20}$ -43.8 (c, 1.5 in EtOH).

*1′,3-Dibenzyl, 1,2-*O*-isopropylidene: 1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-L-apio-α-L-furanose. 1′,3-Di-*O*-benzyl-1,2-*O*-isopropylidene-α-L-*erythro*-tetrofuranose*
$C_{22}H_{26}O_5$ 370.444
Cryst. (Et_2O/petrol). Mp 60-61°. $[\alpha]_D^{19}$ -58 (c, 1.5 in $CHCl_3$).

DL-*form* [42927-70-8]
Syrup.

[41546-47-8, 41546-49-0, 41546-43-4, 41546-44-5, 30912-14-2, 41546-46-7]

Bell, D.J. *et al., JCS*, 1954, 3702-3706 (*Posidonia australis constit*)
Weygand, F. *et al., Chem. Ber.*, 1959, **92**, 535-540 (*L-form, synth*)

Schaffer, R. *et al., JACS*, 1959, **81**, 5452-5454 (*L-form*)
Bell, D.J. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 260-263 (*Posidonia australis constit*)
Williams, D.T. *et al., Can. J. Chem.*, 1964, **42**, 69-72 (*D-form, isol, synth, D-isopropylidene*)
Carey, F.A. *et al., Carbohydr. Res.*, 1966, **3**, 205-213 (*α-L-fur derivs*)
Ball, D.H. *et al., Carbohydr. Res.*, 1969, **10**, 121-128; 1971, **17**, 165-174; 1975, **45**, 91-103 (*α-D-Me gly tri-Me, β-D-Me gly tri-Me, β-D-Me gly derivs, 1,2, 3,3′-diisopropylidene*)
Ezekiel, A.D. *et al., Tet. Lett.*, 1969, 1635-1638 (*α-D-isopropylidene, α-D-isopropylidene di-Ac*)
Overend, W.G. *et al., Carbohydr. Res.*, 1970, **15**, 185-195 (*L-form, synth*)
Medicino, J. *et al., J. Biol. Chem.*, 1970, **245**, 6113-6124 (*D-Apio-β-L-furanose*)
Tronchet, J.M.J. *et al., Helv. Chim. Acta*, 1971, **54**, 1466-1479 (*1,2-O-isopropylidene*)
Ezekiel, A.D. *et al., JCS(C)*, 1971, 2907-2911 (*β-L-dibenzyl isopropylidene*)
Kinoshita, T. *et al., Carbohydr. Res.*, 1973, **28**, 175-179 (*β-L-threo-isopropylidene, β-L-threo diisopropylidene*)
Tronchet, J.M.T. *et al., Carbohydr. Res.*, 1974, **33**, 237-248 (*β-L-threo isopropylidene*)
Watson, R.R. *et al., Adv. Carbohydr. Chem. Biochem.*, 1975, **31**, 135-184 (***rev***)
Vyas, D.M. *et al., Can. J. Chem.*, 1975, **53**, 2748-2754 (*apiose derivs, cmr*)
Ho, P.-T. *et al., Can. J. Chem.*, 1979, **57**, 381-383 (*D-form, L-form, synth, β-D-isopropylidene*)
Koos, M. *et al., Carbohydr. Res.*, 1986, **146**, 335-341 (*Apiose, !synth*)
Snyder, J.R. *et al., Carbohydr. Res.*, 1987, **166**, 85-99 (*DL-form, spectral anal*)
Polsterer, J.P. *et al., Nucleosides Nucleotides*, 1991, **10**, 621-622 (*apiofuranoses*)
Polle, A. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2001, **27**, 45-49 (*Tanacetum vulgare constit*)
Koos, M. *et al., Tet. Lett.*, 2002, **43**, 5405-5406 (*D-Apio-D-furanose, synth*)
Yun, M. *et al., Tet. Lett.*, 2005, **46**, 5903-5905 (*L-apiose, synth*)
Su, Y. *et al., Tianran Chanwu Yanjiu Yu Kaifa*, 2006, **18**, 878-882 (*Conyza constit*)

β-Apiosyl-β-glucosidase A-582

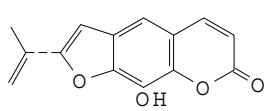
E.C. 3.2.1.161. 7-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranosyloxy]isoflavonoid β-D-apiofuranosyl-(1→6)-D-glucohydrolase. Isoflavonoid 7-O-β-apiosyl-glucoside β-glucosidase. Isoflavonoid-7-O-β-[D-apiosyl-(1→6)-β-D-glucoside] disaccharidase. Furcatin hydrolase [1000598-83-3]
[39346-29-7]

Glycosidase enzyme. Isol. from chickpea. *Dalbergia nigrescens* Enzyme activity range pH 3.5-6.5.

Hosel, W. *et al., Eur. J. Biochem.*, 1975, **57**, 607-616 (*Cicer arietinum*)
Ahn, Y.O. *et al., J. Biol. Chem.*, 2004, **279**, 23405-23414 (*Viburnum furcatum*)
Chuankhayan, P. *et al., Phytochemistry*, 2005, **66**, 1880-1889 (*Dalbergia nigrescens, activity*)

Apiumetin A-583

2,3-Dihydro-9-hydroxy-2-(1-methylethenyl)-7H-furo[3,2-g][1]benzopyran-7-one, 9CI. Leptophyllidin [70610-24-1]



$C_{14}H_{12}O_4$ 244.246

(R)-form

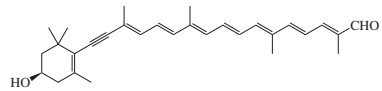
Constit. of the seeds of *Apium graveolens*. Needles. Mp 198°. $[\alpha]_D^{19}$ -68.29 (c, 0.41 in $CHCl_3$).

O-β-D-Glucopyranoside: [115356-05-3]
$C_{20}H_{22}O_9$ 406.388
Constit. of *Apium graveolens*. Needles (EtOH). Mp 165°. $[\alpha]_D^{20}$ -60 (c, 0.16 in $CHCl_3$).

Garg, S.K. *et al., Phytochemistry*, 1978, **17**, 2135 (*isol, struct*)
Sharma, B.R. *et al., Indian J. Chem., Sect. B*, 1979, **17**, 647 (*Leptophyllidin*)
Ahluwalia, V.K. *et al., Phytochemistry*, 1988, **27**, 1181 (*deriv*)
Elgamal, M.H.A. *et al., Phytochemistry*, 1993, **34**, 819 (*isol, pmr*)

Apoalloxanthinal A-584

7,8-Didehydro-3-hydroxy-8′-apo-β-caroten-8′-al [190849-79-7]

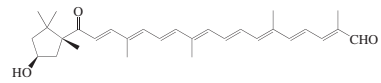


$C_{30}H_{38}O_2$ 430.629
Isol. from the mussel *Mytilus coruscus* and the oyster *Crassostrea gigas*.

Maoka, T. *et al., J. Nat. Prod.*, 1997, **60**, 616-617 (*isol, cd, pmr, ms*)

8′-Apocapsorubinal A-585

[336105-83-0]

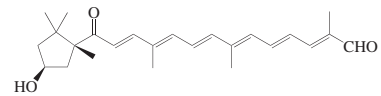


$C_{30}H_{40}O_3$ 448.644
Constit. of fruits of red paprika (*Capsicum annuum*). λ_{max} 428; 458; 485 (Et_2O).

Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*8′-Apocapsorubinal*)

12′-Apocapsorubinal A-586

[336105-82-9]

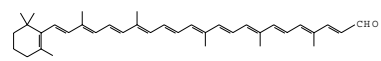


$C_{25}H_{34}O_3$ 382.542
Constit. of fruits of red paprika (*Capsicum annuum*). λ_{max} 313; 413; 437 (Et_2O).

Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*12′-Apocapsorubinal*)

2′-Apo-β-carotenal, 8CI A-587

β-Apo-2′-carotinal [5525-46-2]

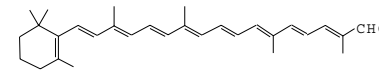


$C_{37}H_{48}O$ 508.786
Trace constit. of *Citrus* spp. Violet cryst. (petrol). Mp 160-161°. λ_{max} 498 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1949, **42**, 854 (*synth*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951 (*isol*)
Enzell, C.R. *et al., Acta Chem. Scand.*, 1969, **23**, 727 (*ms*)

8′-Apo-β-caroten-8′-al A-588

β-Carotinal. *β-Apo-2-carotinal. C.I. Food Orange 6* [1107-26-2]



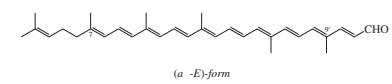
$C_{30}H_{40}O$ 416.645
Constit. of orange peel, spinach, marigolds and egg yolks. Colour additive. Violet cryst. (MeOH). Mp 139°.

8′-Carboxylic acid, Et ester: [1109-11-1]
all-trans *Carophyll yellow. C.I. Food Orange 7*
$C_{32}H_{44}O_2$ 460.698
Colour additive for foods, e.g. egg yolks. Dark red cryst. (CH_2Cl_2/EtOH). Mp 137-138°. λ_{max} 445; 470 (petrol).

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854-864 (*synth*)
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951-2965 (*isol*)
Isler, O. *et al., Chimia*, 1961, **15**, 208-226 (*synth*)
Schwieter, H. *et al., Helv. Chim. Acta*, 1966, **49**, 369-390 (*carboxylic acid, Et ester, uv*)
Englert, G. *et al., Helv. Chim. Acta*, 1975, **58**, 2367-2390 (*cmr*)
Sharma, R.V. *et al., Biochim. Biophys. Acta*, 1977, **486**, 183-194 (*biochem*)
Straub, O. *et al., Key to Carotenoids*, 2nd edn., Birkhauser Verlag, Basel and Boston, 1987, 482 (*bibl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AQO300
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 192-193 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQO300

6′-Apo-ψ-caroten-6′-al A-589

Apo-6′-lycopenal. Lycopenal. Apo-2-lycopenal



(a -E)-form

$C_{32}H_{42}O$ 442.683

(all-E)-form [22255-36-3]
Isol. from *Lycopersicon esculentum* (tomato). Dark red plates (EtOH). Mp 147°. λ_{max} 475 (EtOH). λ_{max} 569 (CS_2). λ_{max} 455; 486; 519 (petrol).

6′-Carboxylic acid, Me ester: [22255-21-6]
Methyl apo-6′-lycopenate. *Methyl 6′-apo-γ-carotenoate, 8CI*
$C_{33}H_{44}O_2$ 472.709
Constit. of the seeds of *Bixa orellana* (annatto). Cryst. (C_6H_6/MeOH). Mp 141-144° (137-145°). λ_{max} 471; 503 (petrol). λ_{max} 445; 469 (Me_2CO).

(9′Z)-form

6′-Carboxylic acid: ***6′-Apo-ψ-caroten-6′-oic acid***

$C_{32}H_{42}O_2$ 458.683

6′-Carboxylic acid, Me ester: [174206-07-6] ***Methyl 6′-apo-9′Z-lycopen-6′-oate***
$C_{33}H_{44}O_2$ 472.709
Constit. of the seeds of *Bixa orellana* (annatto). λ_{max} 342; 360; 439 (sh); 460; 493 (sh) (no solvent reported).

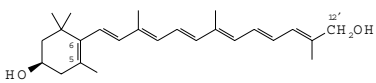
(7Z,9Z,9′Z)-form

6′-Carboxylic acid, Me ester: [188738-88-7]
Isol. from the seeds of *Bixa orellana* (annatto).

Kuhn, R. *et al., Ber.*, 1932, **65**, 898 (*synth*)
Karrer, P. *et al., Helv. Chim. Acta*, 1939, **22**, 69
Winterstein, A. *et al., Chem. Ber.*, 1960, **93**, 2951 (*isol*)
Kjosen, H. *et al., Phytochemistry*, 1969, **8**, 483-491 (*Methyl apo-6′-lycopenate*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759-2764 (*isol*)
Mercadante, A.Z. *et al., Phytochemistry*, 1996, **41**, 1201-1203 (*9Z-carboxylic acid Me ester*)
Mercadante, A.Z. *et al., J. Agric. Food Chem.*, 1997, **45**, 1050-1054 (*7Z,9Z,9′Z-carboxylic acid Me ester*)

12′-Apo-β-carotene-3,12′-diol A-590

[120021-87-6]



$C_{25}H_{36}O_2$ 368.558
Constit. of peaches (*Prunus persica*).

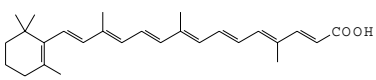
5α,6α-Epoxide: [80952-82-5] *5,6-Epoxy-5,6-dihydro-12′-apo-β-carotene-3,12′-diol*. ***Persicaxanthin***
$C_{25}H_{36}O_3$ 384.558
Isol. from plums *Prunus domestica*. Yellow plates (C_6H_6/petrol). Mp 92°.

12′-Aldehyde, 5α,6α-epoxide: 5,6-Epoxy-5,6-dihydro-3β-hydroxy-12′-apo-β-caroten-12′-al. ***Apo-12′-violaxanthal***
$C_{25}H_{34}O_3$ 382.542
Isol. from plums *Prunus domestica*. Yellow pigment.

Gross, J. *et al., Phytochemistry*, 1981, **20**, 2267 (*Persicaxanthin*)
Molnár, P. *et al., Phytochemistry*, 1987, **26**, 1493 (*abs config*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1988, **71**, 1689 (*isol, pmr, uv*)

10′-Apo-β-caroten-10′-oic acid A-591

10′-Apo-β,ψ-carotenoic acid, 9CI. β-Apo-10′-carotenic acid [6880-01-9]



$C_{27}H_{36}O_2$ 392.58
Constit. of flowers of *Boronia megastigma* (brown boronia). Cryst. (C_6H_6). Mp 186-187°. λ_{max} 430 (petrol).

Me ester: [69774-12-5]
$C_{28}H_{38}O_2$ 406.607
Constit. of flowers of *Boronia megastigma* (brown boronia).

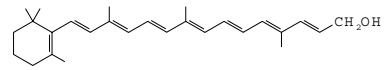
Isler, O. *et al., Helv. Chim. Acta*, 1959, **42**, 864 (*synth*)
Sharma, R.V. *et al., Biochim. Biophys. Acta*, 1977, **486**, 183 (*biochem*)
Cooper, C.M. *et al., J. Agric. Food Chem.*, 2003, **51**, 2384-2389 (*isol*)

Apo-β-carotenoid-14′,13′-dioxygenase A-592

E.C. 1.13.12.12. 8′-Apo-β-carotenol:oxygen oxidoreductase
Thiol-dependent oxidoreductase enzyme. Isol. from rabbit intestine.

Dmitrovskii, A.A. *et al., Biochemistry (Moscow) (Engl. Transl.)*, 1997, **62**, 787-792

10′-Apo-β-caroten-10′-ol A-593



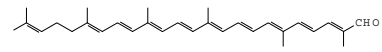
$C_{27}H_{38}O$ 378.597

10′-Aldehyde: [640-49-3] ***10′-Apo-β-caroten-10′-al***. *β-Apo-3-carotenal*
$C_{27}H_{36}O$ 376.581
Constit. of oranges and other citrus fruits. Red cryst. (petrol). Mp 97-98°.

Rüegg, R. *et al., Helv. Chim. Acta*, 1959, **42**, 854 (*synth*)
Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*isol*)
Singh, H. *et al., Biochem. J.*, 1972, **128**, 11P (*synth*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1987, **70**, 1988 (*isol*)

Apo-8′-lycopenal A-594

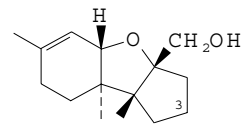
2,6,11,15,19,23-Hexamethyl-2,4,6,8,10,12,14,16,18,22-tetracosadecaenal. 8′-Apo-ψ-caroten-8′-al. Apo-3-lycopenal [2213-22-1]



$C_{30}H_{40}O$ 416.645
Isol. from *Lycopersicon esculentum* (tomato). Purple plates (C_6H_6/MeOH). Mp 141°. λ_{max} 280; 475; 505 (cyclohexane).

Karrer, P. *et al., Helv. Chim. Acta*, 1939, **22**, 69 (*synth*)
Surmatis, J.D. *et al., JOC*, 1966, **31**, 186 (*synth*)
Ben-Aziz, A. *et al., Phytochemistry*, 1973, **12**, 2759 (*isol*)
Johansen, J.E. *et al., Acta Chem. Scand., Ser. B*, 1974, **28**, 301 (*synth*)

Apotrichothecene A-595



$C_{15}H_{24}O_2$ 236.353
Mycotoxin of *Fusarium culmorum*.

3α-Hydroxy: [104148-45-0] ***Apotrichodiol***. *3-Hydroxyapotrichothecene. Secodeoxysambucinol*
$C_{15}H_{24}O_3$ 252.353
Mycotoxin of *Fusarium culmorum*, *Fusarium sambucinum* and *Fusarium crookwellense*. Glass.

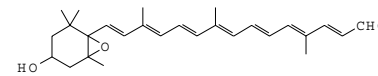
3β-Hydroxy:
$C_{15}H_{24}O_3$ 252.353
Mycotoxin prod. by *Fusarium sambucinum*. Glass. λ_{max} 197 (ϵ 7800) (MeCN).

3-Oxo: ***3-Ketoapotrichothecene***
$C_{15}H_{22}O_3$ 250.337
Mycotoxin from *Fusarium sambucinum*. Glass. λ_{max} 197 (ϵ 3600) (MeCN) (Berdy).

Lauren, D.R. *et al., J. Agric. Food Chem.*, 1987, **35**, 884 (*isol*)
Zamir, L.O. *et al., J. Biol. Chem.*, 1987, **262**, 15348; 15354 (*isol, pmr*)
Greenhalgh, R. *et al., J. Agric. Food Chem.*, 1989, **37**, 699 (*cryst struct*)
Sanson, D.R. *et al., JOC*, 1989, **54**, 4313 (*isol, deriv*)
Zamir, L.O. *et al., Tet. Lett.*, 1992, **33**, 5181 (*isol, pmr, cmr*)

Apo-10′-violaxanthal A-596

5,6-Epoxy-5,6-dihydro-3-hydroxy-10′-apo-β,ψ-carotenal, 9CI. 5,6-Epoxy-3-hydroxy-5,6-dihydro-10′-apo-β-caroten-10′-al. Apoviolaxanthinal [17237-68-2]

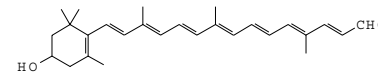


$C_{27}H_{36}O_3$ 408.58
Isol. from Valencia orange peels. λ_{max} 403; 424; 448 (hexane). λ_{max} 440 (EtOH).

Curl, A.L. *et al., J. Food Sci.*, 1967, **32**, 141 (*isol*)
Gross, J. *et al., Phytochemistry*, 1974, **13**, 1917

10′-Apozeaxanthal A-597

3-Hydroxy-10′-apo-β,ψ-carotenal, 9CI. 3-Hydroxy-β-apo-10′-carotenal. Apo-3-zeaxanthinal [79709-31-2]



$C_{27}H_{36}O_2$ 392.58
Isol. from Sinton citrangequat and the fruits of red paprika (*Capsicum annuum*). λ_{max} 444 (EtOH).

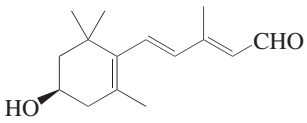
10′-Carboxylic acid: [521303-91-3] *3-Hydroxy-10′-apo-β-carotenoic acid*
$C_{27}H_{36}O_3$ 408.58
Constit. of flowers of *Boronia megastigma* (brown boronia).

10′-Carboxylic acid, Me ester: [521303-92-4]
$C_{28}H_{38}O_3$ 422.606
Constit. of flowers of *Boronia megastigma* (brown boronia).

Yokoyama, H. *et al., Phytochemistry*, 1966, **5**, 1159 (*isol*)
Ellis, P.R. *et al., Helv. Chim. Acta*, 1981, **64**, 1092 (*synth*)
Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*paprika constit*)
Cooper, C.M. *et al., J. Agric. Food Chem.*, 2003, **51**, 2384-2389 (*Boronia megastigma constits*)

11-Apozeaxanthinal A-598

[260244-86-8]



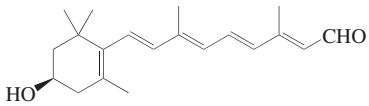
$C_{15}H_{22}O_2$ 234.338

Constit. of fruits of red paprika (*Capsicum annuum*). λ_{max} 300 (Et_2O).

Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*11-Apozeaxanthinal*)

15-Apozeaxanthinal A-599

3-Hydroxyretinal [60046-53-9]



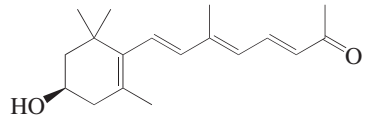
$C_{20}H_{28}O_2$ 300.44

Constit. of fruits of red paprika (*Capsicum annuum*). Oil. λ_{max} 378 (Et_2O).

Barua, R.K. *et al., Biochem. J.*, 1966, **101**, 250
Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*15-Apozeaxanthinal*)
van Wijk, A.A.C. *et al., Eur. J. Org. Chem.*, 2003, 863-868 (*synth*)
Dominguez, M. *et al., Org. Biomol. Chem.*, 2006, **4**, 155-164 (*synth*)

13-Apozeaxanthinone A-600

[336105-81-8]



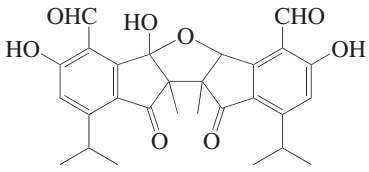
$C_{18}H_{26}O_2$ 274.402

Constit. of fruits of red paprika (*Capsicum annuum*). λ_{max} 338 (Et_2O).

Maoka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 1601-1606 (*13-Apozeaxanthinone*)

Aquatidial A-601

[929258-34-4]



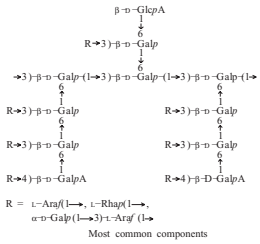
$C_{28}H_{28}O_8$ 492.524

Constit. of *Pachira aquatica* (Malabar chestnut). Cryst. ($CHCl_3$). Mp 230-231°.

Paula, V.F. *et al., J. Braz. Chem. Soc.*, 2007, **17**, 1443-1446 (*Aquatidial*)

Arabic acid, 9CI, 8CI A-602

[32609-14-6]



Most common components

A highly branched polysaccharide composed of L-arabinose, D-galactose, L-rhamnose and D-gluconic acid in an approx. 3:3:1:1 ratio. Main chain consists of (1 →3)- and (1 →6)-linked β-D-Galp units with (1 →6)-linked β-D-GlcpA units. Side branches may contain α-L-Rhap, β-D-GlcpA, β-D-Galp and α-L-Araf with (1 →3)-, (1 →4)- and (1 →6)-glycosidic linkages. High water soly. and low viscosity w.r.t. other gums. Protein moiety of gum arabic is responsible for surface activity, foaming and emulsifying props.

Mixed salts: [9000-01-5] *Gum arabic. Australian gum. Acacia gum. Wattle gum. E 414. FEMA 2001*
Stabiliser for soft drink and flavour emulsions; encapsulating agent to protect lipid or liposoluble materials that are sensitive to decomposition; texturising or filming agent in confectionary; gelling agent or carrier in reduced calorie applications; clarification and stabilising aid in wines. Yellowish-amber lumps. Dissolves slowly in H_2O.

▶ CE5945000

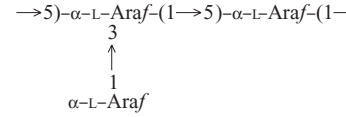
Me ester: $[\alpha]_D^{19}$ -47 (c, 1.0 in $CHCl_3$).

Per-Ac: $[\alpha]_D$ -21 (c, 0.94 in $CHCl_3$).

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 202A (*ir*)
Smith, F. *et al., JCS*, 1939, 1724-1738; 1940, 1035-1051 (*composition, Me ester, per-Ac*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, NY, 1948, **4**, 303 (*use*)
Aspinall, G.O. *et al., JCS*, 1963, 1696-1702 (*struct*)
Aspinall, G.O. *et al., The Carbohydrates*, 2nd edn., (eds. Pigman, W. *et al*), Academic Press, 1970, **2B**, 515-536 (*rev*)
Churms, S.C. *et al., Carbohydr. Res.*, 1983, **123**, 267-269 (*struct*)
Defaye, J. *et al., Carbohydr. Res.*, 1986, **150**, 221-231 (*cmr, struct, bibl*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1-5 (*Gum arabic*)
Draget, K. *et al., Handbook of Hydrocolloids*, (eds. Phillips, G.O. *et al*), CRC Press, 2000, 379-395 (*rev*)
Izydorczyk, M. *et al., Food Carbohydrates*, (ed. Cui, S.W.), CRC Press, 2005, (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQQ500

Arabinan, 9CI, 8CI A-603

Araban [11078-27-6]



Portion of idealised structure

$C_5H_8O_4$ 132.116

A polymer of linearly α-(1 →5)-linked L-arabinofuranose units with single L-arabinofuranose α-(1 →3)-linked to the main chain at intervals. Polymeric. Minimum formula given. Arabinans devoid of other sugars have been isol. from mustard seeds. Heteroarabinans have been found in sugar beet and apples. $[\alpha]_D$ -157. $[\alpha]_D$ -114. $[\alpha]_D$ -129 (H_2O).

Ac: $[\alpha]_D^{20}$ -90 (Me_2CO).

[9060-75-7]

Hirst, E.L. *et al., JCS*, 1939, 452; 454; 1865
Hirst, E.L. *et al., Adv. Carbohydr. Chem.*, 1947, **2**, 235 (*rev*)
Hirst, E.L. *et al., Biochem. J.*, 1965, **95**, 453 (*isol*)
Roudier, A.J. *et al., Bull. Soc. Chim. Fr.*, 1965, 460
Jones, J.K.N. *et al., Methods Carbohydr. Chem.*, 1965, **5**, 74 (*synth*)
Aspinal, G.O. *et al., The Carbohydrates*, (Pigman W. etal, Ed.), Academic Press, 1970, **2B**, 517
Radha, A. *et al., Carbohydr. Res.*, 1997, **298**, 105-115 (*cryst struct, conformn*)

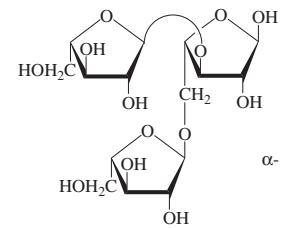
α-*N*-Arabinofuranosidase A-604

E.C. 3.2.1.55. α-L-Arabinofuranoside arabinofuranohydrolase. α-L-Arabinofuranosidase hydrolase. Arabinosidase. E.C. 3.2.1.79 (incorporated) [9067-74-7]

Glycosidase enzyme. Isol. from plants, e.g. carrot, soybean. *Scopolia japonica* Enzyme activity range pH 3.5-6.3. Shows 5% loss of activity after 1 month at 4°, pH 5.5.

Tagawa, K. *et al., Methods Enzymol.*, 1988, **160**, 707-712 (*Aspergillus niger*)
Uchida, T. *et al., Methods Enzymol.*, 1988, **160**, 712-719 (*Scopolia japonica*)
Hatanaka, H. *et al., Agric. Biol. Chem.*, 1991, **55**, 2599-2605 (*carrot, Japanese belladonna, soybean*)
Matsuo, N. *et al., Biochem. J.*, 2000, **346**, 9-15 (*bacteria*)
Miyanaga, A. *et al., J. Biol. Chem.*, 2004, **279**, 44907-44914 (*cryst struct*)

α-L-Arabinofuranosyl-(1 → 3)-[α-L-arabinofuranosyl-(1 →5)]-L-arabinose A-605



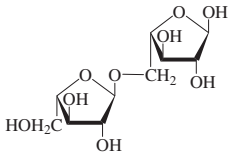
α- uranose-*form*

$C_{15}H_{26}O_{13}$ 414.363

Constit. of the anti-complementary arabinogalactan (AG IIb-1), isol. from the roots of *Angelica acutiloba* (Dong Dang Gui).

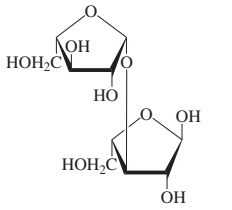
α-Furanose-*form* [114226-47-0]
Syrup.
Kiyohara, H. *et al., Carbohydr. Res.*, 1987, **167**, 221 (*isol, glc, ms, chromatog*)

5-*O*-α-L-Arabinofuranosyl-L-arabinose A-606


α- uranose-*form*

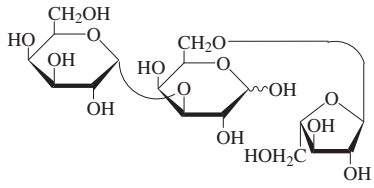
$C_{10}H_{18}O_9$ 282.247
From stem mucilage of *Opuntia ficus-indica* (Indian fig). Isol. from partial acid hydrolysates of sugar beet araban. $[\alpha]_D^{18}$ -87 (c, 0.5 in H_2O). $[\alpha]_D$ -98.4 (H_2O).
Andrews, P. *et al., Chem. Ind. (London)*, 1956, 658 (*isol, sugarbeet*)
Smith, F. *et al., JCS*, 1961, 4892 (*isol*)
Tanaka, M. *et al., Biochim. Biophys. Acta*, 1981, **658**, 377
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, synth*)

3-*O*-β-L-Arabinofuranosyl-L-arabinose, 9CI A-607
Arabinofuranobiose [52287-00-0]


β- uranose-*form*

$C_{10}H_{18}O_9$ 282.247
Formed on partial acid hydrolysis of sugar beet araban and certain plant gums. $[\alpha]_D$ +94 (H_2O).
Phenylosazone: Mp 200°.
Andrews, P. *et al., Chem. Ind. (London)*, 1956, 658 (*isol*)
Aspinall, G.O. *et al., JCS*, 1959, 1697 (*isol*)
Sarkar, M. *et al., Indian J. Chem.*, 1974, **11**, 1129
Sarkar, M. *et al., Indian J. Chem., Sect. B*, 1978, **16**, 369 (*isol, pmr*)

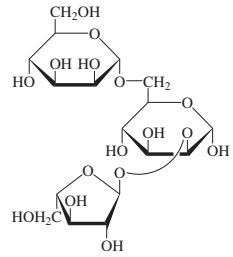
α-L-Arabinofuranosyl-(1 → 6)-[β-D-galactopyranosyl-(1 →3)]-D-galactose A-608



$C_{17}H_{30}O_{15}$ 474.415
Principal oligosaccharide of sanqi (*Panax notoginseng*).

Me α-glycoside:
Solid. $[\alpha]_D$ +23 (c, 1 in MeOH).
Yang, F. *et al., Carbohydr. Res.*, 2002, **337**, 485-491 (*synth, pmr, cmr, ms*)

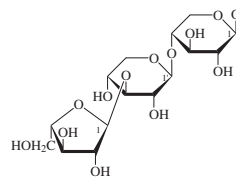
α-L-Arabinofuranosyl-(1 → 2)-[α-D-mannopyranosyl-(1 →6)]-D-mannose A-609


α-Pyranose-*form*

$C_{17}H_{30}O_{15}$ 474.415
Residue present in tomato oligosaccharides.

α-form
Allyl glycoside:
Amorph. solid. $[\alpha]_D$ +8 (c, 1 in H_2O).
Utille, J.P. *et al., Carbohydr. Res.*, 2000, **329**, 431-439 (*occur, synth*)

α-L-Arabinofuranosyl-(1 → 3)-β-D-xylopyranosyl-(1 →4)-D-xylose A-610
[66186-04-7]


β-Pyranose-*form*

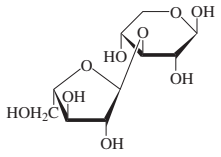
$C_{15}H_{26}O_{13}$ 414.363
Prod. of partial enzymic hydrol. of xylans found in foods, e.g. rye flour. Pentahydrate. $[\alpha]_D^{20}$ -72 (c, 0.5 in H_2O). $[\alpha]_D$ -15 (H_2O).

Pyranose-*form*
5′′-(4-Hydroxy-E-*cinnamoyl):* [102254-69-3]
$C_{24}H_{32}O_{15}$ 560.508
Enzym. hydrol. product of bamboo shoot (*Phyllostachys edulis*) cell wall and of barley straw cell walls. Syrup.

α-Pyranose-*form*
Benzyl glycoside, heptabenzyl: [99388-77-9]
$C_{71}H_{74}O_{13}$ 1135.358
$[\alpha]_D^{20}$ +14 (c, 1.5 in $CHCl_3$).

β-Pyranose-*form*
Me glycoside: [93130-20-2] *Methyl α-L-arabinofuranosyl-(1→3)-β-D-xylopyranosyl-(1→4)-β-D-xylopyranoside*
$C_{16}H_{28}O_{13}$ 428.389
Cryst. (MeOH/Me_2CO). Mp 146-147°. $[\alpha]_D^{22}$ -121 (c, 1.0 in H_2O).
Me glycoside, 2′′,3′′,4′′-tribenzoyl, 2,2′,3,4′-tetra-Ac:
$C_{45}H_{48}O_{20}$ 908.862
Amorph. $[\alpha]_D^{22}$ -48 (c, 1.0 in $CHCl_3$).
Bishop, C.T. *et al., JACS*, 1956, **78**, 2840 (*isol*)
Aspinall, G.O. *et al., JCS*, 1960, 3881 (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 2713
Shambe, T. *et al., Carbohydr. Res.*, 1983, **113**, 125
Hirsch, J. *et al., Carbohydr. Res.*, 1984, **131**, 219 (*β-Me gly synth, cmr*)
Schraml, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1605 (*pmr, cmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1464 (*enzymic synth, α-deriv synth*)
Mueller-Harvey, I. *et al., Carbohydr. Res.*, 1986, **148**, 71 (*coumaroyl, isol, pmr, cmr, ms*)
Ishii, T. *et al., Carbohydr. Res.*, 1990, **206**, 297 (*coumaroyl, isol, cmr, pmr*)

3-*O*-α-L-Arabinofuranosyl-D-xylose, 9CI A-611
[66186-03-6]


β-Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247

β-Pyranose-*form*
Me glycoside: [93130-21-3] *Methyl 3*-O-*α-L-arabinofuranosyl-β-D-xylopyranoside*
$C_{11}H_{20}O_9$ 296.274
Sesquihydrate. $[\alpha]_D^{20}$ -113 (c, 1.2 in H_2O).
Me glycoside, pentabenzyl: [99388-70-2] *Methyl 2,4-di*-O-*benzyl-3*-O-*(2,3,5-tri*-O-*benzyl-α-L-arabinofuranosyl)-β-D-xylopyranoside*
$C_{46}H_{50}O_9$ 746.896
$[\alpha]_D^{20}$ -7 (c, 1.1 in $CHCl_3$).
2′-O-*(4-Hydroxy-3-methoxycinnamoyl)*(E-):
$C_{20}H_{26}O_{12}$ 458.418
Isol. from corn hulls. Powder. λ_{max} 230; 279 (MeOH).
2′-Me ether, 5′-O-*(4-hydroxy-3-methoxycinnamoyl)*(E):
$C_{21}H_{28}O_{12}$ 472.445
Isol. from corn hulls. Powder. λ_{max} 228; 284 (MeOH).
2′-Me ether, 5′-O-*(4-hydroxy-3-methoxycinnamoyl)*(Z-):
$C_{21}H_{28}O_{12}$ 472.445
Isol. from corn hulls. Powder. λ_{max} 215; 272 (MeOH).
Kusakabe, I. *et al., Nippon Nogei Kagaku Kaishi*, 1977, **51**, 669 (*isol*)
Kusakabe, I. *et al., Agric. Biol. Chem.*, 1983, **47**, 2713
Sahrami, J. *et al., Coll. Czech. Chem. Comm.*, 1984, **49**, 1605 (*nmr*)
Koto, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 1464 (*Me gly*)
Hosny, M. *et al., J. Nat. Prod.*, 1997, **60**, 219 (*feruloyl derivs*)

Arabinogalactan A-612

D-Galacto-L-arabinan. Larch gum. FEMA 3254 [9036-66-2]

A complex polymer of arabinose and galactose in a 1:6 ratio. Also contains a small proportion of uronic acid units. Emulsifier, stabiliser.

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 194-195

Ponder, G.R. *et al., J. Carbohydr. Chem.*, 1997, **16**, 181-193; 195-211 (*struct, bibl*)

Arabinokinase A-613

Phosphotransferase enzymes with alcohol acceptor.

D-*form* [37278-02-7]

*D-Arabinokinase. E.C. 2.7.1.54. ATP:D-arabinose 5-phosphotransferase*Shows 40% maximum activity at pH 5.5, 60% at pH 10.5. During purifn., 0.1*M* ammonium sulfate used for stabilisation. At 0°, crude extract stable for several weeks, but partially purified enzyme loses 46% activity after 1 week and is completely inactive after 2 weeks.

L-*form* [37277-99-9]

L-Arabinokinase. E.C. 2.7.1.46. ATP:L-arabinose 1-phosphotransferase

Isol. from mung bean (*Phaseolus aureus*). V. unstable; complete loss of activity in 24h at 4°.

Neufeld, E.F. *et al., J. Biol. Chem.*, 1960, **235**, 906-909 (*L-form, Phaseolus aureus*)

Volk, W.A. *et al., J. Biol. Chem.*, 1962, **237**, 19-23 (*D-form, Propionibacterium pentosaceum*)

Volk, W.A. *et al., Methods Enzymol.*, 1966, **9**, 442-445 (*D-form, assay, props*)

Chan, H.P. *et al., Anal. Biochem.*, 1975, **64**, 372-379 (*L-form, Phaseolus aureus*)

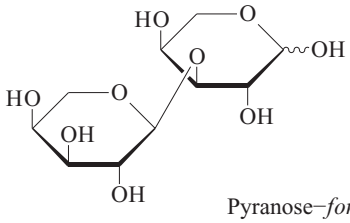
Dolezal, O. *et al., Plant Physiol.*, 1991, **96**, 1255-1260 (*L-form, Arabidopsis thaliana*)

Gy, I. *et al., Gene*, 1998, **209**, 201-210 (*L-form, Arabidopsis thaliana*)

Sherson, S. *et al., Plant Mol. Biol.*, 1999, **39**, 1003-1012 (*L-form, Arabidopsis thaliana*)

3-*O*-α-L-Arabinopyranosyl-L-arabinose, 9CI A-614

[79435-28-2]



Pyranose–*form*

$C_{10}H_{18}O_9$ 282.247

Hydrolytic product of the mucilage from the stems of *Opuntia ficus-indica* (Indian fig). Syrup. $[\alpha]_D$ +76 (c, 0.63 in H_2O).

α-Pyranose-*form*

Me glycoside: [105261-00-5] *Methyl 3-O-α-L-arabinopyranosyl-α-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Mp 211°. $[\alpha]_D$ +34.4 (c, 3.9 in H_2O).

Me glycoside, penta-Ac: [105453-49-4] *Methyl 2,4-di-O-acetyl-3-O-(2,3,4-tri-O-acetyl-α-L-arabinopyranosyl)-α-L-arabinopyranoside, 9CI*
$C_{21}H_{30}O_{14}$ 506.46
Mp 70°. $[\alpha]_D$ +1.78 (c, 4.8 in $CHCl_3$).

β-Pyranose-*form*

Me glycoside: [105260-96-6] *Methyl 3-O-α-L-arabinopyranosyl-β-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
Mp 194°. $[\alpha]_D$ +156 (c, 0.8 in H_2O).

Me glycoside, penta-Ac: [105260-90-0]
$C_{21}H_{30}O_{14}$ 506.46
Mp 154°. $[\alpha]_D$ +89.3 (c, 2.0 in $CHCl_3$).

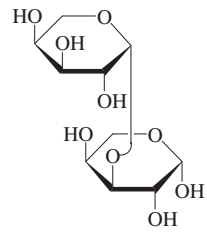
McGarvie, D. *et al., Carbohydr. Res.*, 1981, **94**, 57 (*isol, pmr*)

Kochetkov, N.K. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 200 (*Me gly, pmr, cmr*)

Shashkov, A.S. *et al., Magn. Reson. Chem.*, 1988, **26**, 735 (*cmr*)

3-*O*-β-L-Arabinopyranosyl-L-arabinose, 9CI, 8CI A-615

Arabinopyranobiose [20546-04-7]



β-Pyranose-*form*

$C_{10}H_{18}O_9$ 282.247

Isol. from partial acid hydrolysates of golden apple (*Spondias cytherea*), lemon, peach, cherry. Also major disaccharide product from the acid reversion of L-arabinose. $[\alpha]_D$ +210 (c, 1.0 in H_2O). $[\alpha]_D$ +164 (c, 1.0 in H_2O). $[\alpha]_D$ +193 (c, 3.8 in H_2O).

Phenylosazone: Mp 235° (221°).

α-Pyranose-*form*

Me glycoside: [105260-99-9] *Methyl 3-O-β-L-arabinopyranosyl-α-L-arabinopyranoside, 9CI*
$C_{11}H_{20}O_9$ 296.274
$[\alpha]_D$ +140 (c, 2.6 in MeOH).

Me glycoside, penta-Ac: [105260-92-2]
$C_{21}H_{30}O_{14}$ 506.46
$[\alpha]_D$ +115 (c, 2.3 in $CHCl_3$).

β-Pyranose-*form*

Me glycoside, penta-Ac: [105260-89-7]
Mp 211°. $[\alpha]_D$ +148 (c, 0.3 in $CHCl_3$).

Jones, J.K.N. *et al., JCS*, 1953, 1672; 1958, 27 (*isol, synth*)

Andrews, P.A. *et al., JCS*, 1953, 4090

Aspinall, G.O. *et al., JCS*, 1955, 1106; 1965, 2685 (*isol*)

Smith, F. *et al., Chemistry of Plant Gums and Mucilages*, Reinhold, New York, 1959,

Haq, S. *et al., Can. J. Chem.*, 1961, **39**, 1563 (*isol*)

Chalk, R.C. *et al., Can. J. Chem.*, 1968, **46**, 2311 (*isol*)

Aspinall, G.O. *et al., Carbohydr. Res.*, 1968, **7**, 421 (*isol*)

Kubala, J. *et al., Coll. Czech. Chem. Comm.*, 1977, **42**, 2809 (*isol*)

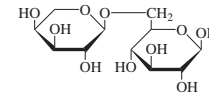
Kochetkov, N.K. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, 200 (*deriv, synth, pmr, cmr*)

Shashkov, A.S. *et al., Magn. Reson. Chem.*, 1988, **26**, 735 (*cmr*)

Verkerk, R. *et al., Natural Toxicants in Food*, (ed. Watson, R.), Sheffield Academic Press, 1998, 29-53 (*rev*)

6-*O*-α-L-Arabinopyranosyl-D-glucose, 9CI, 8CI A-616

Vicianose [14116-69-9]



α-D-Pyranose-*form*

$C_{11}H_{20}O_{10}$ 312.273

Mp 210° dec. $[\alpha]_D^{20}$ +56.5 → +39.7 (H_2O).

Occurs in Geoside, M-373.

β-Pyranose-*form*

Hepta-Ac: [14260-08-3]
$C_{25}H_{34}O_{17}$ 606.533
Mp 158.5-160.5°. $[\alpha]_D$ +15 ($CHCl_3$).

Benzyl glycoside: [148031-67-8] ***Benzyl β-vicianoside***
$C_{18}H_{26}O_{10}$ 402.397
Constit. of the fruit of *Passiflora edulis* (passion fruit).

Helferich, B. *et al., Annalen*, 1928, **465**, 166-184 (*synth*)

Kochetkov, N.K. *et al., J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 315-319 (*synth*)

Psenak, M. *et al., Planta Med.*, 1972, **22**, 93-96 (*Geum urbanum constit*)

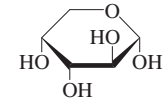
Balan, N.F. *et al., Bioorg. Khim.*, 1980, **5**, 1657-1666 (*hepta-Ac*)

Bartlett, P.A. *et al., JACS*, 1980, **102**, 337-342 (*synth*)

Chassagne, D. *et al., Phytochemistry*, 1996, **41**, 1497-1500 (*benzyl glycoside*)

Arabinose A-617

Aloinose. Aloe sugar. Pectinose [147-81-9]



α-D-Pyranose-*form*

$C_5H_{10}O_5$ 150.131

L-*form* [5328-37-0]

FEMA 3255

[87-72-9]

Flavouring agent. Mp 160°. $[\alpha]_D^{20}$ +190.6 → +104.5 (c, 4 in H_2O). Sweetness = 0.37 × sucrose.

[28697-53-2, 1768-95-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 188D (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 293B (*nmr*)

Tollens, B. *et al., Kurzes Handbuch der Kohlenhydrate, 4th edn., J.A. Barth*, 1935, 120 (*rev*)

White, E.V. *et al., Methods Carbohydr. Chem.*, 1962, **1**, 76 (*synth, L-form*)

Staněk, J. *et al., The Monosaccharides*, Academic Press, 1963, (*rev*)

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn.,*

Birkhuser Verlag, 1972, nos. 583; 584 (*occur*)
Schaffer, R. *et al., The Carbohydrates*, 1972, **1A**, 69 (*occur*)
Benesi, A.J. *et al., Carbohydr. Res.*, 1994, **258**, 27 (*pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 196
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 113 (*use*)

β-L-Arabinosidase A-618

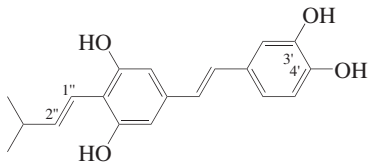
E.C. 3.2.1.88. β-L-Arabinoside arabinohydrolase. Vicianosidase [39361-63-2]

Glycosidase enzyme. Isol. from seeds of *Cajanus indicus* (pigeon pea). Activity range pH 2.0-6.5. Enzyme assayed with the chromogenic substrate *p*-nitrophenyl β-L-arabinoside.

Dey, P.M. *et al., Biochim. Biophys. Acta*, 1973, **302**, 393-398; 1983, **746**, 8-13 (*Cajanus indicus, activity*)

Arachidin 1 A-619

4-[2-[3,5-Dihydroxy-4-(3-methyl-1-butenyl)phenyl]ethenyl]-1,2-benzenediol, 9CI. 3,3′,4′,5-Tetrahydroxy-4-(3-methyl-1-butenyl)stilbene [79147-73-2]



$C_{19}H_{20}O_4$ 312.365
Stilbene numbering shown.

(E,E)-form [98391-38-9]
Constit. of peanuts (*Arachis hypogaea*).

3′-Deoxy: [87320-15-8] *5-[2-(4-Hydroxyphenyl)ethenyl]-2-(3-methyl-1-butenyl)-1,3-benzenediol, 9CI. 3,4′,5-Trihydroxy-4-(3-methyl-1-butenyl)stilbene.* ***Arachidin 3***
$C_{19}H_{20}O_3$ 296.365
Isol. from peanuts (*Arachis hypogaea*).

*3′-Deoxy, 1′′,2′′-dihydro, 2′′*R*,3′′-dihydroxy:* [1114548-06-9] *2-(2,3-Dihydroxy-3-methylbutyl)-5-[2-(4-hydroxyphenyl)ethenyl]-1,3-benzenediol.* ***Arahypin 3***
$C_{19}H_{22}O_5$ 330.38
Constit. of peanuts (*Arachis hypogaea*) infected with *Aspergillus caelatus*. Yellowish cryst. (EtOAc). Mp 213-216°. $[\alpha]_D$ +20 (c, 0.5 in MeOH).

3′,4′-Dideoxy: [1114548-05-8] *2-(3-Methyl-1-butenyl)-5-(2-phenylethenyl)-1,3-benzenediol.* ***Arahypin 1***
$C_{19}H_{20}O_2$ 280.366
Constit. of peanuts (*Arachis hypogaea*) infected with *Aspergillus caelatus*. Yellowish oil.

*3′,4′-Dideoxy, 1′′,2′′-dihydro, 2′′*R*,3′′-dihydroxy:* [1114548-07-0] *2-(2,3-Dihydroxy-3-methylbutyl)-5-(2-phenylethenyl)-1,3-benzenediol.* ***Arahypin 4***
$C_{19}H_{22}O_4$ 314.38
Constit. of peanuts (*Arachis hypogaea*) infected with *Aspergillus caelatus*. Yellowish oil. $[\alpha]_D$ +9.5 (c, 0.25 in MeOH).

[79147-71-0]

Aguamah, G.E. *et al., Phytochemistry*, 1981, **20**, 1381-1383 (*isol, pmr*)
Wotton, H.R. *et al., J. Gen. Microbiol.*, 1985, **131**, 487 (*isol*)
Sobolev, V.S. *et al., Phytochem. Anal.*, 2006, **17**, 312-322 (*isol, ms*)
Sobolev, V.S. *et al., J. Agric. Food Chem.*, 2009, **57**, 62-68 (*Arahypins 1,3,4*)
Park, B.H. *et al., J. Nat. Prod.*, 2011, **74**, 644-649 (*synth*)

Arachidonate lipoxygenases A-620

Fe-dependent oxidoreductase enzymes.

Arachidonate 5-lipoxygenase [80619-02-9]
E.C. 1.13.11.34. Arachidonate:oxygen 5-oxidoreductase. 5-Lipoxygenase. Leukotriene A_4 synthase
Isol. from potato tubers.

Arachidonate 8-lipoxygenase [100900-72-9]
E.C. 1.13.11.40. Arachidonate:oxygen 8-oxidoreductase. 8-Lipoxygenase

Arachidonate 12-lipoxygenase [82391-43-3]
E.C. 1.13.11.31. Arachidonate:oxygen 12-oxidoreductase. 12-Lipoxygenase
Isol. from bovine platelets.

Arachidonate 15-lipoxygenase [82249-77-2]
E.C. 1.13.11.33. Arachidonate:oxygen 15-oxidoreductase. 15-Lipoxygenase. ω-6 Lipoxygenase
Isol. from soybean and from rabbit reticulocytes.

Nugteren, D.H. *et al., Biochim. Biophys. Acta*, 1975, **380**, 299-307 (*E.C. 1.13.11.31, blood platelets*)
Wallach, D.P. *et al., Biochim. Biophys. Acta*, 1981, **663**, 361-372 (*E.C. 1.13.11.31, human blood platelets*)
Nugteren, D.H. *et al., Methods Enzymol.*, 1982, **86**, 49-54 (*E.C. 1.13.11.31, bovine platelets*)
Bundy, G.L. *et al., J. Biol. Chem.*, 1986, **261**, 747-751 (*E.C. 1.13.11.40, Pseudoplexaura porosa*)
Shibata, D. *et al., J. Biol. Chem.*, 1987, **262**, 10080-10085 (*E.C. 1.13.11.33, soybean*)
Ohishi, N. *et al., J. Biol. Chem.*, 1987, **262**, 10200-10205 (*E.C. 1.13.11.34, human lung*)
Sigal, E. *et al., J. Biol. Chem.*, 1988, **263**, 5328-5332 (*E.C. 1.13.11.33, human leucocytes*)
Soberman, R.J. *et al., Methods Enzymol.*, 1988, **163**, 344-349 (*E.C. 1.13.11.33, E.C. 1.13.11.34, human leukocytes*)
Sloane, D.L. *et al., Biochem. Biophys. Res. Commun.*, 1990, **173**, 507-513 (*E.C. 1.13.11.33, rabbit reticulocytes*)
Reddanna, P. *et al., Methods Enzymol.*, 1990, **187**, 268-277 (*E.C. 1.13.11.34, potato tubers*)
Rouzer, C.A. *et al., Methods Enzymol.*, 1990, **187**, 312-319 (*E.C. 1.13.11.34, human leukocytes*)
Ford-Hutchinson, A.W. *et al., Eicosanoids*, 1991, **4**, 59-74 (*E.C. 1.13.11.33, rev*)
Ford-Hutchinson, A.W. *et al., Annu. Rev. Biochem.*, 1994, **63**, 383-417 (*E.C. 1.13.11.34, rev*)
Kuhn, H. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 157-170 (*E.C. 1.13.11.33, rev*)
Radmark, O. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 171-184 (*E.C. 1.13.11.34, rev*)
Yoshimoto, T. *et al., J. Lipid Mediators Cell Signalling*, 1995, **12**, 195-212 (*E.C. 1.13.11.31, rev*)
Yamamoto, S. *et al., Prog. Lipid Res.*, 1997, **36**, 23-41 (*E.C. 1.13.11.31, rev*)
Dailey, L.A. *et al., Curr. Med. Chem.*, 1999, **6**, 389-398 (*E.C. 1.13.11.31, rev*)
Radmark, O. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 211-234 (*E.C. 1.13.11.34, rev*)
Furstenburger, C. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 235-243 (*E.C. 1.13.11.40, rev*)
Yoshimoto, H. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 245-262 (*E.C. 1.13.11.31, rev*)
Kuhn, H. *et al., Prostaglandins Other Lipid Mediat.*, 2002, **68-69**, 263-290 (*E.C. 1.13.11.33, rev*)
Peters-Golden, M. *et al., Prostaglandins, Leukotrienes, Essent. Fatty Acids*, 2003, **69**, 89-97 (*E.C. 1.13.11.34, rev*)

Arachidoside A-621

Struct. unknown. Flavonoid glucoside. Poss. a glycoside of Dihydroisorhamnetin. Isol. from shells of peanuts (*Arachis hypogaea*). Brown-red powder.

Tuyeau, F. *et al., C. R. Hebd. Seances Acad. Sci.*, 1947, **224**, 290

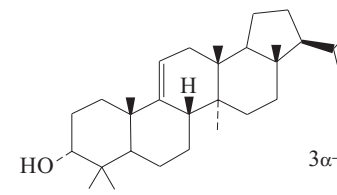
Aralkylamine *N*-acetyltransferase A-622

E.C. 2.3.1.87. Acetyl-CoA:2-arylethylamine N*-acetyltransferase. Serotonin acetyltransferase. Serotonin acetylase. AANAT* [92941-56-5]

Enzyme. Isol. from sheep pineal gland. Substrates incl. 5-Hydroxytryptamine, H-1075, Tryptamine, T-1134 and 2-Phenylethylamine, P-371. Participates in melatonin biosynth. and plays a major role in the regulation of melatonin circadian rhythm.

Voisin, P. *et al., J. Biol. Chem.*, 1984, **259**, 10913-10918 (*isol*)

9(11)-Arborinen-3-ol A-623



3α–*form*

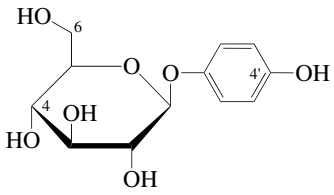
$C_{30}H_{50}O$ 426.724

(3β,21βH)-form [90582-44-8]
Sorghumol
Constit. of *Sorghum bicolor* (sorghum). Cryst. Mp 277-282°.

Nes, W.D. *et al., Chem. Comm.*, 1984, 223 (*Sorghumol*)

Arbutin A-624

4-Hydroxyphenyl β-D-glucopyranoside, 9CI, 8CI. Hydroquinone-glucose. Arbutoside. Ericolin [497-76-7]



$C_{12}H_{16}O_7$ 272.254
Constit. of pear leaves (*Pyrus communis*). Mp 199-200° (163-165°). $[\alpha]_D^{22}$ -55.8 (c, 0.56 in MeOH). Log P -1.83 (calc). λ_{max} 291 (MeOH) (Berdy). λ_{max} 294 (EtOH) (Berdy).

▶ Exp. reprod. and teratogenic effects (v. large doses). CE8863000

2-O-β-D-Glucopyranosyl: [1085850-98-1] *4-Hydroxyphenyl β-sophoroside*
$C_{18}H_{26}O_{12}$ 434.396
Constit. of ripe cherry tomato (*Lycopersicon esculentum* var. *cerasiforme*). Amorph. powder. $[\alpha]_D^{28}$ -7.9 (c, 0.4 in Py). Misnamed in ref.

6-O-β-D-Glucopyranosyl: [7013-25-4] *4-Hydroxyphenyl β-gentiobioside*
$C_{18}H_{26}O_{12}$ 434.396
Constit. of the leaves of *Vaccinium vitis-idaea* (cowberry). Cryst. Mp 265.5-267.5°. $[\alpha]_D^{22}$ -58.3 (c, 0.75 in H_2O). λ_{max} 283 (ϵ 2000) (H_2O).

6-O-[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranosyl]: [54522-15-5]
$C_{24}H_{36}O_{17}$ 596.538
Constit. of wheat germ (*Triticum aestivum*). Powder. λ_{max} 192 (log ϵ 4.68); 222 (log ϵ 3.97); 284 (log ϵ 3.46) (MeOH/AcOH aq.).

2-Ac: [15794-91-9] ***2-O-Acetylarbutin***. *Isopyroside*
$C_{14}H_{18}O_8$ 314.291
Constit. of *Vaccinium vacillans* (blueberry). Cryst. Mp 172-174°. $[\alpha]_D^{22}$ -22. $[\alpha]_D$ -21.2 (c, 0.9 in MeOH).

6-Ac: [10338-88-2] ***6-O-Acetylarbutin***. *Pyroside*
$C_{14}H_{18}O_8$ 314.291
Constit. of the leaves of immature pear (*Pyrus communis*) and mountain cranberry (*Vaccinium vitis-idaea*). Mp 214-216°. $[\alpha]_D^{23}$ -58.8 (c, 2.0 in H_2O).

*2-O-(3,4-Dihydroxy-*E*-cinnamoyl):* [230955-36-9] ***2-O-trans-Caffeoylarbutin***
[14477-53-3]
$C_{21}H_{22}O_{10}$ 434.399
Isol. from leaves of *Vaccinium vitis-idaea* (mountain cranberry). Prisms. Mp 165°.

Haslam, E. *et al., JCS*, Suppl. I, 1964, 5649-5654 (*2-O-Caffeoylarbutin*)

Durkee, A.B. *et al., J. Food Sci.*, 1968, **33**, 461-463 (*Arbutin, 6-Acetylarbutin, isol, pear*)

Haslam, E. *et al., Tetrahedron*, 1968, **24**, 4015-4020 (*synth*)

Frenzel, H. *et al., Pharmazie*, 1969, **24**, 235-236; 236-237 (*4-Hydroxyphenyl gentiobioside*)

Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, nos. 204; 205; 2610 (*occur*)

Perol, G.W. *et al., JCS Perkin 1*, 1979, 239-243 (*Eximin*)

Lutterbach, R. *et al., Helv. Chim. Acta*, 1992, **75**, 2009-2011 (*enzymic synth*)

Ek, S. *et al., J. Agric. Food Chem.*, 2006, **54**, 9834-9842 (*2-O-Caffeoylarbutin*)

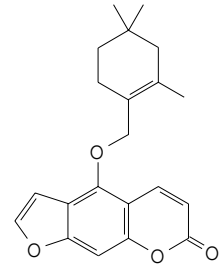
Ono, M. *et al., Chem. Pharm. Bull.*, 2008, **56**, 1499-1501 (*4-Hydroxyphenyl sophoroside*)

Zhokhov, S.S. *et al., J. Nat. Prod.*, 2009, **72**, 656-661 (*wheat germ triglucoside*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HIH100

Archangelin A-625

*4-[(2,4,4-Trimethyl-1-cyclohexen-1-yl)-methoxy]-7*H*-furo[3,2-g][1]benzopyran-7-one, 9CI. Iselin* [21174-75-4]



$C_{21}H_{22}O_4$ 338.402
Constit. of the root of *Angelica archangelica* (angelica). Thick rods (MeOH). Mp 132°. $[\alpha]_D^{30}$ +14 ($CHCl_3$).

Chatterjee, A. *et al., Tet. Lett.*, 1964, 1961 (*isol, struct*)

Chatterjee, A. *et al., Indian J. Chem.*, 1968, **6**, 415 (*isol, struct*)

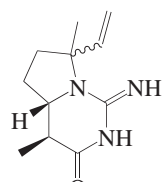
Bates, R.B. *et al., Tet. Lett.*, 1972, 3811 (*rev*)

Dukhovlinova, L.I. *et al., Khim. Prir. Soedin.*, 1974, **10**, 308; *Chem. Nat. Compd. (Engl. Transl.)*, 1974, **10**, 316 (*isol*)

Magotra, D. *et al., Acta Cryst. C*, 1995, **51**, 2196 (*cryst struct*)

Arenaine A-626

[35471-10-4]

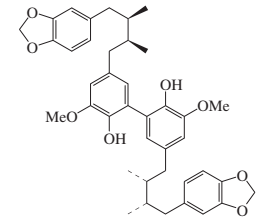


Relative Configuration

$C_{11}H_{17}N_3O$ 207.275
Alkaloid from seeds of *Plantago arenaria* (sand plantain). Mp 208-210°. $[\alpha]_D^{22}$ +305 (c, 1.7 in $CHCl_3$).

Rabaron, A. *et al., JACS*, 1971, **93**, 6270-6271 (*uv, ir, pmr, cmr, struct*)

Argenteane A-627



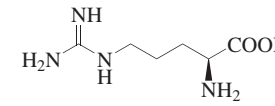
Relative Configuration

$C_{40}H_{46}O_8$ 654.799
Constit. of mace, *Myristica argentea*. Oil. λ_{max} 220 (log ϵ 1.53); 250 (sh); 289 (log ϵ 1.04) (MeOH).

Filleur, F. *et al., Nat. Prod. Lett.*, 2002, **16**, 1-7 (*isol, pmr, cmr*)

Arginine, INN, USAN A-628

2-Amino-5-[(aminoiminomethyl)amino]-pentanoic acid. 2-Amino-5-guanidinovaleric acid. Arg [7004-12-8]



(*S*)-*form*

$C_6H_{14}N_4O_2$ 174.202
Dietary supplement. Log P -4.79 (calc).

(S)-form [74-79-3]
L-form. L-Arginine. FEMA 3819
Dietary supplement, nutrient. Plates or prisms + $2H_2O$ (H_2O), plates (EtOH). Sol. H_2O (15.0g/100g at 21°). Mp 207° Mp 244° dec. (anhyd. 105°). $[\alpha]_D$ +21.8 (H_2O). $[\alpha]_D^{25}$ +48.1 (c, 1 in 5*M* HCl). pK_{a1} 2.17; pK_{a2} 9.04; pK_{a3} 12.48 (guanido). Isoelectric point 10.76. Bitter taste. *N*-Protected derivs. useful in peptide synth. have been listed alphabetically elsewhere.

▶ CF1934200

Hydrochloride: [1119-34-2] ***Arginine hydrochloride, USAN***
[15595-35-4]
Dietary supplement, nutrient.
Mp 222° dec. (235°). $[\alpha]_D^{20}$ +12.1 (H_2O).

▶ LD_{50} (rat, orl) 12000 mg/kg. Exp. teratogen. CF1995500

N^2-*β-D-Fructopyranos-1-yl:* [162966-07-6] N^2-*Fructopyranosylarginine. UK III*
$C_{12}H_{24}N_4O_7$ 336.344
Constit. of Korean red ginseng.

N^2-*[α-D-Glucopyranosyl-(1→4)-β-D-fructopyranos-1-yl]:* [162966-06-5] N^2-*Maltulosylarginine. UK II*
[185351-34-2]
$C_{18}H_{34}N_4O_{12}$ 498.486
Constit. of Korean red ginseng.
Powder. Mp 158-160°.

N^2-*(3-Carboxypropanoyl):* [2478-02-6] ***N^2-Succinoylarginine***
$C_{10}H_{18}N_4O_5$ 274.276

Constit. of the shoots of pear trees.

N^2-*Oxalyl:* [90250-86-5] **N^2-*Oxalylarginine***
$C_8H_{14}N_4O_5$ 246.222
Constit. of the shoots of apple and pear trees (*Malus* spp.).

N^2-*(3-Carboxy-2-hydroxypropanoyl):* [87605-92-3] **N^2-*(2-Hydroxysuccinoyl)arginine***. N^2-*(3-Carboxy-2-hydroxy-1-oxopropyl)arginine*
$C_{10}H_{18}N_4O_6$ 290.275
Constit. of the seeds of *Vicia faba* and the shoots of apple and pear trees.

N^2-*(3-Carboxy-3-hydroxypropanoyl):* [90250-85-4] **N^2-*(3-Hydroxysuccinoyl)arginine***
$C_{10}H_{18}N_4O_6$ 290.275
Constit. of the shoots of apple and pear trees.

N^2-*[3-Carboxy-2-(carboxymethyl)-2-hydroxypropanoyl]:* [87605-91-2] **N^2-*(2-Carboxymethyl-2-hydroxysuccinoyl)arginine***
$C_{12}H_{20}N_4O_8$ 348.312
Constit. of the shoots of apple and pear trees.

[14975-30-5, 32042-43-6, 78851-84-0, 63238-98-2, 50912-92-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 785A; 785D; 786A; 786B; **2**, 259C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1281A (*nmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1841 (*rev*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Bak, B. *et al., J. Mol. Spectrosc.*, 1968, **26**, 78 (*pmr*)
Voelter, W. *et al., Z. Naturforsch., B*, 1971, **26**, 213 (*cmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2392 (*occur*)
Lehmann, M.S. *et al., JCS Perkin 2*, 1973, 133 (*cryst struct*)
Torgerson, D.F. *et al., Biochem. Biophys. Res. Commun.*, 1974, **60**, 616 (*ms*)
Kasai, T. *et al., Phytochemistry*, 1983, **22**, 147-149; 1984, **23**, 19-22 (*N-succinoyl derivs*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, AQV 980; AQW 000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 197-198
Zheng, Y.-N. *et al., J. Chin. Pharm. Sci.*, 1998, **7**, 7-10 (*Maltulosylarginine*)

Arginyltransferase A-629

E.C. 2.3.2.8. *L-Arginyl-tRNA:protein arginyltransferase* [37257-24-2]

Aminoacyltransferase enzyme. Isol. from mammalian tissues, e.g. from rabbit reticulocytes and liver and hog kidney.

Soffer, R.L. *et al., J. Mol. Biol.*, 1969, **43**, 163-175 (*rabbit liver*)
Soffer, R.L. *et al., J. Biol. Chem.*, 1970, **245**, 731-737 (*rabbit liver*)
Kato, M. *et al., Anal. Biochem.*, 1984, **143**, 361-367 (*hog kidney*)
Ciechanover, A. *et al., J. Biol. Chem.*, 1988, **263**, 11155-11167 (*rabbit reticulocytes*)

Argon A-630

E938 [7440-37-1]

Ar
Ar 39.948

Atomic No. 18. Ground state electron config. [Ne]$3s^2 3p^6$. Discovered in air in 1894 by Sir W. Ramsey and M.W. Travers. There are 8 isotopes of which 3 are natural. Abundance: 9300 ppm in air (by vol.). Solid state struct. is ccp or hcp (metastable). Inert atmosphere for wine and fruit or vegetable juice containers. Generally recognised as safe (GRAS) in the USA. Colourless, odourless, tasteless, monatomic gas. Forms no true chemical compds. Forms clathrates with H_2O and hydroquinone. Forms complex with HBr. Sol. H_2O (33.6 cm^3 kg^{-1} at 20°). Mp -189.4°. Bp -185.9°. Forms clathrate compds. with phenols.

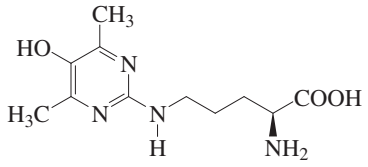
▶ CF2300000

[16740-17-3, 16249-22-2, 15099-26-0, 14864-12-1, 14791-69-6, 16904-17-9, 12595-59-4, 37352-46-8, 34247-59-1, 16941-40-5, 17428-37-4, 16941-44-9, 61762-54-7, 26603-53-2, 15801-88-4, 17596-58-6, 20499-74-5, 12650-44-1, 11130-84-0, 14343-01-2, 18973-74-5, 15056-24-3]

Mellor Compr. Treat. Inorg. Theor. Chem., 1927, **7**, 889 (*rev, bibl*)
Gmelin Handbook Inorg. Chem., Syst. No. 1, *Suppl. Vol.*, 1970, 16; 133 (*rev, bibl*)
Compr. Inorg. Chem., Pergamon, Oxford, 1973, **1**, 139 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **12**, 249 (*rev, bibl*)
Greenwood, N.N. *et al., Chemistry of the Elements*, Pergamon, Oxford, 1986, 1042 (*rev*)
Emsley, J. *et al., The Elements*, 3rd edn., Clarendon Press, 1998, 24; 235
Osvath, R. *et al., Food Chem. News*, 2000, **42**, 3-5 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, AQW250

Argpyrimidine A-631

N^5-*(5-Hydroxy-4,6-dimethyl-2-pyrimidinyl)ornithine*



$C_{11}H_{18}N_4O_3$ 254.288

(*S*)-*form*
Found in beer.

Glomb, M.A. *et al., J. Agric. Food Chem.*, 2001, **49**, 366-372 (*isol, synth, ms*)

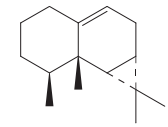
Arietin A-632

[470688-19-8]

Peptide. Struct. not reported. Isol. from seeds of the chickpea *Cicer arietinum*.

Ye, X.Y. *et al., Peptides (N.Y.)*, 2002, **23**, 817-822 (*isol*)

9-Aristolene A-633



( )-*form*

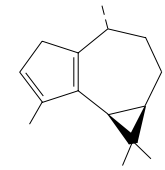
$C_{15}H_{24}$ 204.355

(+)-*form* [27862-07-3]
ent-*9-Aristolene*. **α-*Ferulene***
Oil. Bp_8 110°. $[\alpha]_D$ +68 (neat). $[\alpha]_D$ +40 (c, 0.1 in $CHCl_3$).

(-)-*form* [6831-16-9]
Aristolene
Constit. of calarene from sweet flag oil. Oil. $[\alpha]_D$ -98.7 (neat).

Pesnelle, P. *et al., Bull. Soc. Chim. Fr.*, 1963, 912 (*isol*)
Carboni, S. *et al., Tet. Lett.*, 1965, 3017 (*isol*)
Weinheimer, A.J. *et al., Chem. Comm.*, 1968, 1070 (*isol*)
Hirota, H. *et al., Tetrahedron*, 1996, **52**, 2359 (*isol, pmr, cmr*)

1(5),3-Aromadendradiene A-634

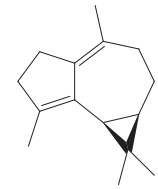


$C_{15}H_{22}$ 202.339

(6α,7α,10α)-*form* [111778-06-4]
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Flavouring agent. Oil.

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753

1(10),4-Aromadendradiene A-635



(6α,7α)-*form*

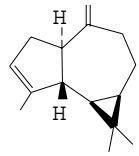
$C_{15}H_{22}$ 202.339

(6α,7α)-*form* [112362-74-0]
Constit. of Tolu balsam (from *Balsamum tolutanum*). Oil.

(6β,7β)-*form* [783350-51-6]
Constit. of *Myroxylon balsamum* (Tolu balsam). Oil.

Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753
Von Reuss, S.H. *et al., Phytochemistry*, 2004, **65**, 2277-2291 (*isol, pmr, cmr*)

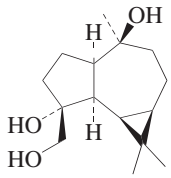
3,10(14)-Aromadendradiene A-636



$C_{15}H_{22}$ 202.339

(1α,5β,6α,7α)-*form* [53526-64-0]
β-Spathulene
Constit. of the the oil of *Schinus molle* (California peppertree).
Terhune, S.J. *et al., Phytochemistry*, 1974, **13**, 865
Büchi, G. *et al., JACS*, 1969, **91**, 6473-6478 (*Globulol, Ledol, Viridiflorol, synth, abs config*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 1908 (*occur*)
Marshall, J.A. *et al., JOC*, 1974, **39**, 1971-1973 (*Globulol, synth*)
Pakrashi, S.C. *et al., JOC*, 1980, **45**, 4765-4767 (*(+)-Ledol, isol*)
El-Seedi, H. *et al., Phytochemistry*, 1994, **35**, 1495-1497 (*Ledol, cmr*)
Gwaltney, S.L. *et al., JOC*, 1996, **61**, 7438-7451 (*Ledol, synth*)
Topçu, G. *et al., Phytochemistry*, 1997, **44**, 1393 (*Ledol, pmr, cmr*)
Cao, S.-G. *et al., Nat. Prod. Lett.*, 2000, **14**, 447-452 (*Ledol, synth*)
Kaplan, M.A.C. *et al., Phytochemistry*, 2000, **55**, 749-753 (*Ledol, struct, bibl*)

4,10,15-Aromadendranetriol A-637

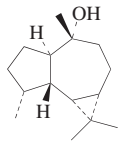


$C_{15}H_{26}O_3$ 254.369

(1α,4α*OH*,5α,6α,7α,10β*OH*)-*form*
[1224881-32-6]
Constit. of *Valeriana officinalis* (valerian). Amorph. powder.
Zhou, Y. *et al., Chin. J. Nat. Med.*, 2009, **7**, 270-273 (*Valeriana officinalis constit*)

10-Aromadendranol A-638

*Decahydro-1,1,4,7-tetramethyl-1*H*-cyclo-prop[e]azulen-4-ol, 9CI* [19078-39-8]



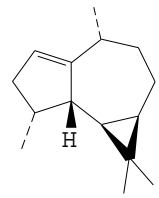
(1α,4α,5β,6β,7β,10α)-*form*

$C_{15}H_{26}O$ 222.37

(1α,4α,5β,6β,7β,10α)-*form* [489-41-8]
Globulol
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Needles (EtOH aq.). Mp 88.5°. Bp 283°. $[\alpha]_D^{20}$ -35.3 ($CHCl_3$).

(1β,4α,5β,6α,7α,10α)-*form* [577-27-5]
Ledol. *Ledum camphor. Porschcamphor*
Constit. of *Valeriana officinalis* (valerian), *Piper* spp. and others. Cryst. (petrol). Mp 105°. Bp 282-283°. $[\alpha]_D$ +8 (EtOH). Stereochem. revised in 2000.
Birch, A.J. *et al., Aust. J. Chem.*, 1955, **8**, 550-551 (*Viridiflorol, isol*)
Büchi, G. *et al., Tet. Lett.*, 1959, **No. 6**, 14-19 (*Globulol, Ledol, Viridiflorol, struct, synth*)
Graham, B.A. *et al., Aust. J. Chem.*, 1960, **13**, 372-379 (*Globulol, Ledol, struct*)

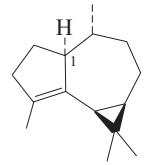
1-Aromadendrene A-639



$C_{15}H_{24}$ 204.355

(4α,5β,6α,7α,10α)-*form* [111821-79-5]
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ +42 (c, 0.2 in pentane).
Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753
Tanaka, T. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1243 (*synth*)

4-Aromadendrene A-640



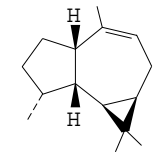
(1α,6α,7α,10α)–*form*

$C_{15}H_{24}$ 204.355

(1α,6α,7α,10α)-*form* [112421-19-9]
1-Epi-α-gurjunene
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ -68 (c, 0.2 in pentane).

(1β,6α,7α,10α)-*form* [489-40-7]
α-Gurjunene. *Gurjunene*
Oil. Bp_{10} 114-116° Bp_3 75-77°. $[\alpha]_D$ -179.5.
Streith, J. *et al., Bull. Soc. Chim. Fr.*, 1963, 1950-1956 (*α-Gurjunene*)
Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753-1759 (*1-Epi-α-gurjunene*)
Calancea, M. *et al., Eur. J. Org. Chem.*, 2009, 3134-3137 (*synth*)

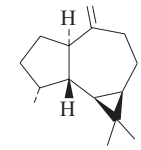
9-Aromadendrene A-641



$C_{15}H_{24}$ 204.355

(1β,4α,5β,6α,7α)-*form* [112421-20-2]
Constit. of Tolu balsam (*Myroxylon balsamum* var. *balsamum*). Food flavouring. Oil. $[\alpha]_D^{25}$ -78 (c, 0.6 in pentane).
Friedel, H.D. *et al., Helv. Chim. Acta*, 1987, **70**, 1753

10(14)-Aromadendrene A-642



(1α,4α,5β,6α,7α)–*form*

$C_{15}H_{24}$ 204.355

(1α,4α,5β,6α,7α)-*form* [14682-34-9]
(-)-Aromadendrene. *β-Diploalbicene* [72747-25-2]
Constit. of *Bixa orellana* (annatto). Oil. $[\alpha]_D$ -11 (EtOH).

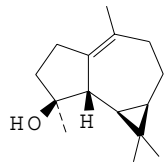
10β,14-Epoxide: [85710-39-0] *10,14-Epoxyaromadendrane.* ***Aromadendrene epoxide***
$C_{15}H_{24}O$ 220.354
Constit. of hops.

(1β,4α,5β,6β,7β)-*form* [25246-27-9]
Alloaromadendrene. *α-Aromadendrene* [72747-25-2]
Constit. of essential oils of *Eucalyptus globulus* (Tasmanian blue gum). Oil. Bp_2 96°. $[\alpha]_D^{20}$ -21.6. n_D^{18} 1.5010.

10β,14-Epoxide: [85760-81-2] ***Alloaromadendrene epoxide***
$C_{15}H_{24}O$ 220.354

(1β,4β,5α,6β,7β)-*form* [489-39-4]
(+)-Aromadendrene
[72747-25-2]
Oil. Bp 260-265°. $[\alpha]_D$ +24.5.
Dolejš, L. *et al., Coll. Czech. Chem. Comm.*, 1960, **25**, 1483 (*isol*)
Büchi, G. *et al., JACS*, 1969, **91**, 6473 (*synth, abs config, bibl*)
Braeckman, J.C. *et al., Experientia*, 1977, **33**, 993 (*Alloaromadendrene, isol, coral*)
Tressl, R. *et al., J. Agric. Food Chem.*, 1983, **31**, 892 (*Aromadendrene epoxide*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 1950 (*Alloaromadendrene epoxide*)
Zafra-Polo, M.C. *et al., J. Chromatogr.*, 1990, **518**, 230 (*Aromadendrene epoxide*)
Williams, H.J. *et al., Phytochemistry*, 1995, **40**, 1633 (*pmr, cmr, ms*)
Tanaka, T. *et al., Tetrahedron*, 1996, **52**, 4257 (*synth*)

1(10)-Aromadendren-4-ol A-643



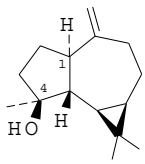
$C_{15}H_{24}O$ 220.354

(4β,5β,6α,7α)-*form* [88395-46-4]
Isospathulenol
Constit. of Clary sage oil (*Salvia sclarea*). Cryst. Mp 69-70.5°. $[\alpha]_D$ +99 (c, 0.6 in $CHCl_3$).

Maurer, B. *et al., Helv. Chim. Acta*, 1983, **66**, 2223-2235 (*Isospathulenol*)

10(14)-Aromadendren-4-ol A-644

[72203-24-8]



(1α,4β,5β,6α,7α)

$C_{15}H_{24}O$ 220.354

(1α,4β,5β,6α,7α)-*form* [6750-60-3]
Spathulenol†
Constit. of *Salvia sclarea* (clary sage). Oil. Sol. MeOH, C_6H_6; poorly sol. H_2O, hexane. $[\alpha]_D$ +56.

Ac: [1170109-32-6] ***Acetylspathulenol***
$C_{17}H_{26}O_2$ 262.391
$[\alpha]_D$ +23 (c, 1 in MeOH).

2-Methyl-2-butenoyl: [1170109-34-8]
$C_{20}H_{30}O_2$ 302.456
$[\alpha]_D$ +27 (c, 1 in MeOH). Geom. of double bond unknown.

3,5-Dinitrobenzoyl:
Cryst. Mp 148°.

(1β,4α,5β,6β,7β)-*form*
Epispathulenol
Cryst. Mp 102-103°. $[\alpha]_D$ +2 (c, 0.7 in Me_2CO).

(1β,4α,5α,6β,7β)-*form* [77171-55-2]
ent-*Spathulenol*
$[\alpha]_D$ -20 (c, 1 in $CHCl_3$). Prob. an artifact as it is readily prod. by autoxidation of bicyclogermacrene (see Bicyclogermacrene, B-108).

Bowyer, R.C. *et al., Chem. Ind. (London)*, 1963, 1245-1246 (*Eucalyptus spathulata constit, struct*)
Asakawa, Y. *et al., Phytochemistry*, 1980, **19**, 2141-2145 (*Plagiochila yokogurensis constit, struct*)
Surburg, H. *et al., Chem. Ber.*, 1981, **114**, 118-131 (*ent-Spathulenol, synth*)
Hubert, T.D. *et al., Phytochemistry*, 1985, **24**, 1197-1198 (*insect repellant activity*)
Van Lier, F.P. *et al., Tet. Lett.*, 1985, **26**, 2109-2110 (*synth*)
Richardson, D.P. *et al., J. Chem. Ecol.*, 1989, **15**, 731-747 (*Dipterocarpus kerri constit*)
Ulubelen, A. *et al., Phytochemistry*, 1994, **36**, 971-974 (*Salvia sclarea consitit*)
Tringali, C. *et al., Phytochemistry*, 1995, **40**, 827-831 (*Epispathulenol*)
Toyota, M. *et al., Phytochemistry*, 1996, **41**, 1347-1350 (*Dicranolejeunea yoshingana constit*)
Goud, V.T. *et al., Biochem. Syst. Ecol.*, 2002, **30**, 493-495 (*Sinularia kavarattiensis constit*)
Vassallo, A. *et al., Nat. Prod. Commun.*, 2008, **3**, 1967-1970 (*Salvia palaestina constits*)

Arsenite methyltransferase A-645

E.C. 2.1.1.137. S-*Adenosyl-L-methionine:arsenite* As-*methyltransferase. E.C. 2.1.1.138 (deleted)* [167140-41-2]

Methyltransferase enzyme. Isol. from rabbit liver.

Zakharyan, R.A. *et al., Chem. Res. Toxicol.*, 1995, **8**, 1029-1038; 1999, **121**, 1278-1283 (*isol*)

Arsenobetaine A-646

(Carboxymethyl)trimethylarsonium hydroxide inner salt, 9CI [64436-13-1]

$Me_3As^{\oplus}CH_2COO^{\ominus}$
$C_5H_{11}AsO_2$ 178.062
Found in algae, lobsters, sharks, etc. Deliquescent cryst. (Me_2CO/MeOH). Mp 204-210° dec. Low mammalian toxicity, excreted unchanged e.g. from seafood sources.

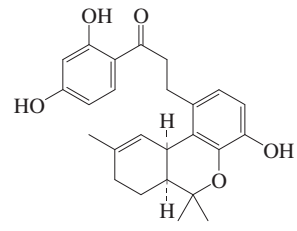
▶ LD_{50} (mus, orl) 10000 mg/kg.
CH9750000

Hydrobromide: [71642-15-4]
$C_5H_{12}AsBrO_2$ 258.974
Non-hygroscopic white shiny cryst. (EtOH at 5°).

Edmonds, J.S. *et al., Tet. Lett.*, 1977, 1543-1546 (*synth, pmr, cryst struct*)
Cannon, J.R. *et al., Aust. J. Chem.*, 1981, **34**, 787-798 (*isol, synth*)
Edmonds, J.S. *et al., Chemosphere*, 1981, **10**, 1041-1044 (*isol, ir, pmr*)
Norin, H. *et al., Chemosphere*, 1982, **11**, 287-298 (*isol, ms, pmr, reaction*)
Luten, J.B. *et al., Chemosphere*, 1983, **12**, 131-141 (*isol, ms, reaction*)
Edmonds, J.S. *et al., JCS Perkin 1*, 1983, 2375-2382 (*pmr, cmr*)
Edmonds, J.S. *et al., Appl. Organomet. Chem.*, 1988, **2**, 297-302 (*biosynth, occur, uv*)
Hanaoka, K. *et al., Appl. Organomet. Chem.*, 1988, **2**, 371-376 (*occur, metab*)
Ismail, H. *et al., Pertanika J. Trop. Agric. Sci.*, 1988, **11**, 437-439 (*synth, cmr*)
Siu, K.W.M. *et al., Rapid Commun. Mass Spectrom.*, 1988, **2**, 69-71 (*ms*)
Beauchemin, D. *et al., J. Anal. At. Spectrom.*, 1989, **4**, 285-289 (*hplc, ms*)
Arsenic Environ., Part II:, (ed. Nriagu, J.O.), J. Wiley, 1994, (*rev, props*)
Minhas, R. *et al., Appl. Organomet. Chem.*, 1998, **12**, 635-641 (*synth, pmr, cmr, ms*)

Artaltilin A A-647

[943029-47-8]

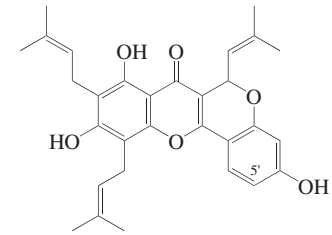


$C_{25}H_{28}O_5$ 408.493
Constit. of the leaves of *Artocarpus altilis* (breadfruit). Yellowish oil. $[\alpha]_D^{20}$ +11.3 (c, 0.4 in MeOH). λ_{max} 279 (log ϵ 4.16); 316 (log ϵ 3.83); 341 (log ϵ 3.62) (MeOH).

Wang, Y. *et al., Phytochemistry*, 2007, **68**, 1300-1306 (*isol, pmr, cmr*)

Artelastin A-648

[182052-05-7]



$C_{30}H_{32}O_6$ 488.579

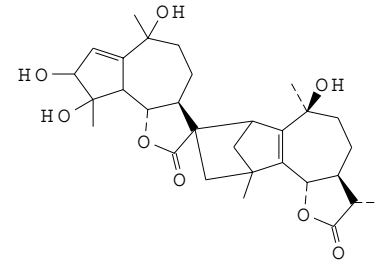
(ξ)-*form*
Orange-red gum. λ_{max} 207 (log ϵ 4.8); 260 (log ϵ 4.2); 276 (log ϵ 4.2); 369 (log ϵ 4.1) (MeOH).

5′-Hydroxy: [1174017-37-8] ***Artoheterophyllin B***. *Cyclorigidol*
[1225288-93-6]
$C_{30}H_{32}O_7$ 504.579
Constit. of *Artocarpus heterophyllus* (jackfruit). Amorph. yellow powder (hexane). $[\alpha]_D^{20}$ +20 (c, 0.2 in CH_2Cl_2). λ_{max} 228 (log ϵ 4.28); 282 (log ϵ 4.35); 386 (log ϵ 4.21) (CH_2Cl_2).

Kijjoa, A. *et al., Phytochemistry*, 1996, **43**, 691-694 (*Artelastin*)
Cidade, H.M. *et al., Planta Med.*, 2001, **67**, 867-870 (*activity*)
Pedro, M. *et al., Life Sci.*, 2005, **77**, 293-311 (*activity*)
Zheng, Z.-P. *et al., J. Agric. Food Chem.*, 2009, **57**, 6649-6655 (*Artoheterophyllin B*)
Ren, Y. *et al., J. Nat. Prod.*, 2010, **73**, 949-955 (*Cyclorigidol*)

Artenolide A-649

[113807-34-4]

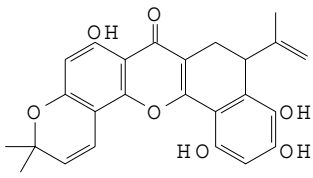


$C_{30}H_{40}O_8$ 528.641
Constit. of *Artemisia absinthium* (wormwood). Cryst. (EtOH). Mp 163-174°.

Ovezdurdyev, A. *et al., Khim. Prir. Soedin.*, 1987, **23**, 667; *Chem. Nat. Compd. (Engl. Transl.)*, 553 (*isol, pmr, cmr*)

Artobiloxanthone A-650

*8,9-Dihydro-6,10,11,13-tetrahydroxy-3,3-dimethyl-9-(1-methylethenyl)-3*H,*7*H-*benzo[c]pyrano[3,2-*h*]xanthen-7-one, 9CI. KB 1* [121748-25-2]
[133813-53-3]

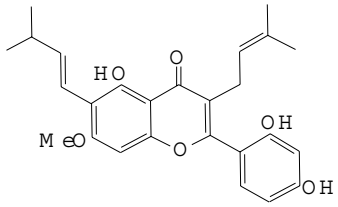


$C_{25}H_{22}O_7$ 434.445
Constit. of *Artocarpus communis* (breadfruit). Yellow solid. Mp 162-164°. λ_{max} 265 (log ϵ 4.34); 285 (log ϵ 4.35); 315 (sh) (log ϵ 4.07); 394 (log ϵ 4.02) ($CHCl_3$/MeOH).

Sultanbawa, M.U.S. *et al., Phytochemistry*, 1989, **28**, 599-605 (*isol, uv, pmr, cmr*)
Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1787-1789 (*isol*)
Jayasinghe, U.L.B. *et al., Fitoterapia*, 2008, **79**, 37-41 (*isol, pmr, cmr*)

Artocarpin A-651

*2-(2,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-6-(3-methyl-1-butenyl)-3-(3-methyl-2-butenyl)-4*H*-1-benzopyran-4-one, 9CI* [7608-44-8]



$C_{26}H_{28}O_6$ 436.504
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow needles (Me_2CO, C_6H_6 or MeOH). Mp 174-175° Mp 250°.

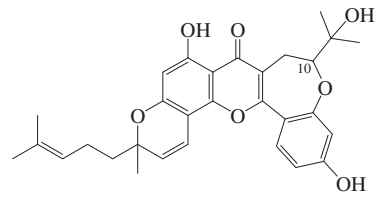
O-*De-Me:* ***Norartocarpin***
$C_{25}H_{26}O_6$ 422.477
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder. Mp 158-159°. λ_{max} 278 (log ϵ 4.74); 321 (log ϵ 4.33); 395 (log ϵ 3.47) (MeOH).

$\Delta^{3''}$-Isomer, 2''ξ-hydroxy: ***Artogomezianone***
$C_{26}H_{28}O_7$ 452.503
Yellow powder. $[\alpha]_D^{20}$ +28.4 (c, 0.1 in MeOH). λ_{max} 278 (log ϵ 4.57); 324 (log ϵ 3.1) (MeOH).

Lin, C.-N. *et al., Phytochemistry*, 1995, **39**, 1447-1451 (*Artocarpin*)
Wang, Y.-H. *et al., J. Nat. Prod.*, 2004, **67**, 757-761 (*Artocarpin*)
Likhitwitayawuid, K. *et al., Chem. Biodiversity*, 2006, **3**, 1138-1143 (*Artogomezianone*)
Arung, E.T. *et al., Planta Med.*, 2006, **72**, 847-850 (*Norartocarpin*)
Chantrapromma, S. *et al., Acta Cryst. E*, 2007, **63**, o1864-o1866 (*Artocarpin, cryst struct*)

Artocarpol B A-652

[317821-24-2]



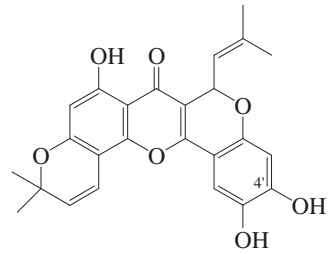
$C_{30}H_{32}O_7$ 504.579
Amorph. yellow powder (cyclohexane/Me_2CO). $[\alpha]_D^{25}$ -2.4 (c, 0.1 in Me_2CO). λ_{max} 210 (log ϵ 4.6); 231 (log ϵ 4.51); 289 (log ϵ 4.56); 307 (sh) (log ϵ 4.42); 348 (log ϵ 4.44) (MeOH).

10-Epimer: ***Artocommunol CC***
$C_{30}H_{32}O_7$ 504.579
Constit. of the roots of *Artocarpus communis* (breadfruit). Amorph. yellow powder. $[\alpha]_D^{25}$ +43.1 (c, 0.1 in MeOH). λ_{max} 240 (log ϵ 4.58); 275 (log ϵ 4.61); 340 (log ϵ 4.34) (MeOH).

Ko, H.-H. *et al., Helv. Chim. Acta*, 2000, **83**, 3000-3005 (*isol, pmr, cmr*)
Chan, S.-C. *et al., J. Nat. Prod.*, 2003, **66**, 427-430 (*Artocommunol CC*)

Artochamin A A-653

*6,11,12-Trihydroxy-3,3-dimethyl-8-(2-methyl-1-propenyl)-3*H,*7*H,*8*H*-bis[1]-benzopyrano[4,3-b:6′,5′-*e*]pyran-7-one, 9CI. Artoindonesianin D* [656832-73-4]



$C_{25}H_{22}O_7$ 434.445
Flavonoid numbering shown. Orange prisms (Me_2CO/petrol). Mp 238-240°. Racemic. λ_{max} 227 (log ϵ 4.41); 270 (log ϵ 4.39); 282 (sh) (log ϵ 4.34); 407 (log ϵ 4.17) (MeOH).

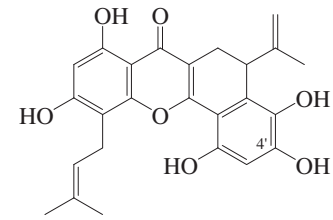
4′-Me ether: [135023-19-7] ***Cycloartomunin***
$C_{26}H_{24}O_7$ 448.471
Isol. from the root bark of *Artocarpus communis* (breadfruit). Yellow needles (MeOH). Mp 278-280°. Racemic. λ_{max} 211 (log ϵ 4.75); 260 (log ϵ 4.3); 400 (log ϵ 3.67) (MeOH).

4′-Me ether, di-Ac:
Needles ($CHCl_3$). Mp 274-276°.

Lin, C.-N. *et al., Phytochemistry*, 1991, **30**, 1669-1671; 1996, **41**, 1215-1217 (*Cycloartomunin*)
Achmad, S.A. *et al., CA*, 2003, **140**, 160452 (*Artoindonesianin D*)
Wang, Y.-H. *et al., J. Nat. Prod.*, 2004, **67**, 757-761 (*Artochamin A*)

Artochamin E A-654

*5,6-Dihydro-1,3,4,8,10-pentahydroxy-11-(3-methyl-2-butenyl)-5-(1-methylethenyl)-7*H*-benzo[c]xanthen-7-one, 9CI. 5,6-Dihydro-1,3,4,8,10-pentahydroxy-5-isopropenyl-11-prenyl-7*H*-benzo[c]-xanthen-7-one* [697234-29-0]



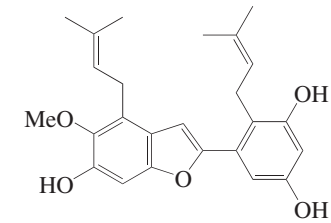
$C_{25}H_{24}O_7$ 436.46
Amorph. yellow powder. Racemic. λ_{max} 196 (log ϵ 4.02); 220 (log ϵ 4.3); 255 (log ϵ 4.32); 280 (sh) (log ϵ 4.06); 315 (log ϵ 4.23) (MeOH).

4′-Me ether: [886757-32-0] ***Dihydroartomunoxanthone***
$C_{26}H_{26}O_7$ 450.487
Constit. of the roots of *Artocarpus communis* (breadfruit). Orange powder. $[\alpha]_D^{25}$ +33 (c, 1 in Me_2CO). λ_{max} 220 (log ϵ 4.9); 260 (log ϵ 4.84); 375 (log ϵ 4.68) (MeOH). λ_{max} 250 (log ϵ 5.08); 330 (log ϵ 4.47); 420 (log ϵ 4.69) (MeOH/$AlCl_3$).

Wang, Y.-H. *et al., J. Nat. Prod.*, 2004, **67**, 757-761 (*Artochamin E*)
Weng, J.-R. *et al., Phytochemistry*, 2006, **67**, 824-829 (*Dihydroartomunoxanthone*)

Artoheterophyllin A A-655

2-[3,5-Dihydroxy-2-(3-methyl-2-butenyl)phenyl]-5-methoxy-4-(3-methyl-2-butenyl)-6-benzofuranol. 2-(3,5-Dihydroxy-2-prenylphenyl)-6-hydroxy-5-methoxy-4-prenylbenzofuran [1174017-36-7]

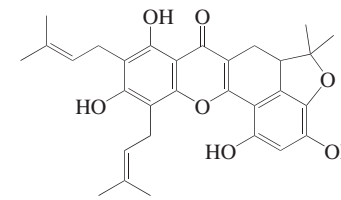


$C_{25}H_{28}O_5$ 408.493
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder.

Zheng, Z.-P. *et al., J. Agric. Food Chem.*, 2009, **57**, 6649-6655 (*isol, pmr, cmr*)

Artoheterophyllin C A-656

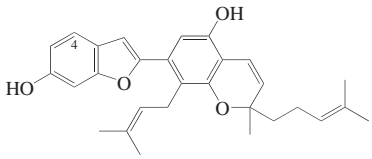
[1174017-38-9]



$C_{30}H_{32}O_7$ 504.579
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder.

Zheng, Z.-P. *et al., J. Agric. Food Chem.*, 2009, **57**, 6649-6655 (*isol, pmr, cmr*)

Artolakoochol A-657



$C_{29}H_{32}O_4$ 444.569

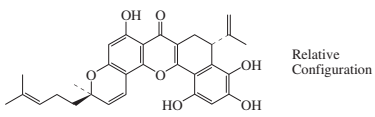
(-)-*form* [1245824-04-7]
Constit. of the root bark of *Artocarpus lakoocha* (lakoocha). Amorph. yellow solid. $[\alpha]_D^{20}$ -86.1 (c, 0.03 in MeOH). λ_{max} 234 (log ϵ 3.16); 339 (log ϵ 3.23) (MeOH).

4-Hydroxy: [1245824-06-9] ***4-Hydroxyartolakoochol***
$C_{29}H_{32}O_5$ 460.569
Constit. of the root bark of *Artocarpus lakoocha* (lakoocha). Powder. $[\alpha]_D^{20}$ -117.6 (c, 0.03 in MeOH). λ_{max} 240 (log ϵ 3.04); 341 (log ϵ 3.02) (MeOH).

Sritularak, B. *et al., Molecules*, 2010, **15**, 6548-6558 (*Artolakoochol, 4-Hydroxyartolakoochol*)

Artomunoisoxanthone A-658

[886757-34-2]

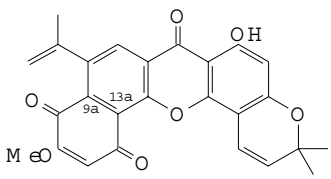


$C_{30}H_{30}O_7$ 502.563
Constit. of the roots of *Artocarpus communis* (breadfruit). Yellow powder. $[\alpha]_D^{25}$ +58 (c, 1 in Me_2CO). λ_{max} 213 (log ϵ 4.63); 270 (log ϵ 4.61); 380 (log ϵ 0.28) (MeOH). λ_{max} 250 (log ϵ 5.16); 450 (log ϵ 4.06) (MeOH/$AlCl_3$).

Weng, J.-R. *et al., Phytochemistry*, 2006, **67**, 824-827 (*isol, uv, pmr, cmr*)

Artomunoxanthentrione A-659

[139921-73-6]



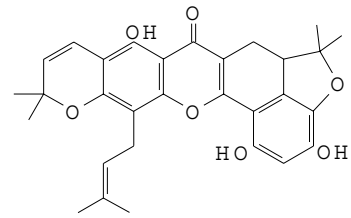
$C_{26}H_{20}O_7$ 444.44
Constit. of *Artocarpus communis* (breadfruit). Red cryst. (EtOAc). Mp 230-232°.

9a,13a-Epoxide: [143522-33-2] *Artomunoxanthentrione epoxide*
$C_{26}H_{22}O_8$ 462.455
Isol. from the root bark of *Artocarpus communis* (breadfruit). Orange needles (EtOAc). Mp 248-251°. CA numbering.

Shieh, W.-L. *et al., Phytochemistry*, 1992, **31**, 364 (*isol, pmr, cmr*)
Lin, C.-N. *et al., Phytochemistry*, 1992, **31**, 2563 (*epoxide*)

Artonin A A-660

[124721-15-9]

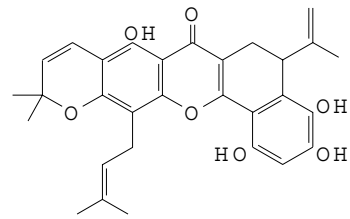


$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 239-240°. $[\alpha]_D^{23}$ -6 (c, 0.1 in Me_2CO).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 1447 (*isol, pmr, cmr, ms, cryst struct*)
Wei, B.-L. *et al., J. Agric. Food Chem.*, 2005, **53**, 3867-3871 (*isol, pmr, cmr*)

Artonin B A-661

[124693-70-5]

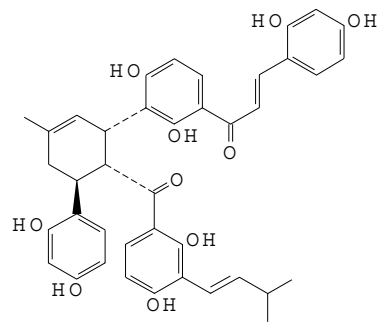


$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow needles (C_6H_6). Mp 219-222° (202-204°). $[\alpha]_D^{22}$ -4 (c, 0.1 in Me_2CO).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 1447 (*isol, pmr, cmr, ms*)
Wei, B.-L. *et al., J. Agric. Food Chem.*, 2005, **53**, 3867-3871 (*isol, pmr, cmr*)

Artonin C A-662

[128553-97-9]

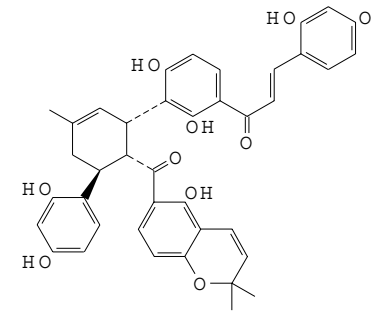


$C_{40}H_{38}O_{10}$ 678.734
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder. Mp 169-171°. $[\alpha]_D^{22}$ +20 (c, 0.09 in MeOH).

Hano, Y. *et al., J. Nat. Prod.*, 1990, **53**, 391 (*isol, pmr, cmr, ir, uv, ms*)

Artonin D A-663

[128532-95-6]

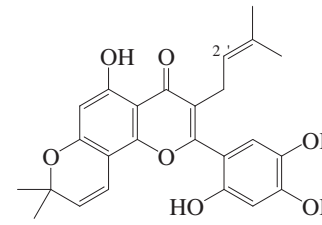


$C_{40}H_{36}O_{10}$ 676.718
Constit. of *Artocarpus heterophyllus* (jackfruit). Yellow powder. Mp 140-143°. $[\alpha]_D$ +77 (c, 0.172 in MeOH).

Hano, Y. *et al., J. Nat. Prod.*, 1990, **53**, 391 (*isol, pmr, cmr, ir, uv, ms*)

Artonin E A-664

KB 3 [129683-93-8]



$C_{25}H_{24}O_7$ 436.46
Numbering systems vary. Constit. of *Artocarpus communis* (breadfruit). Yellow needles (C_6H_6/Me_2CO). Mp 244-248°. λ_{max} 233; 274 (EtOH).

2′-Me ether: [1058721-47-3] ***2′-O-Methylartonin E***
$C_{26}H_{26}O_7$ 450.487
Mp 97°. λ_{max} 252; 290; 349 (EtOH).

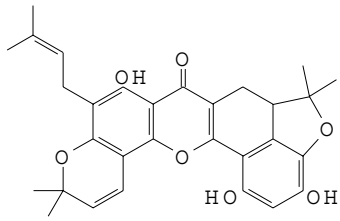
3‴-Hydroxy, 2‴,3‴-dihydro: [133740-64-4] ***KB 2***
$C_{25}H_{26}O_8$ 454.476
Constit. of *Artocarpus communis* (breadfruit). Mp 166-168°.

4‴-Hydroxy: ***14-Hydroxyartonin E***
$C_{25}H_{24}O_8$ 452.46
Yellow powder. λ_{max} 211 (log ϵ 4.45); 270 (log ϵ 4.35); 314 (sh) (log ϵ 3.6); 387 (log ϵ 3.55) (MeOH).

Fujimoto, Y. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1787-1789 (*isol, deriv*)
Hano, Y. *et al., Heterocycles*, 1990, **31**, 877 (*isol, pmr, cmr*)
Cao, S. *et al., Nat. Prod. Res.*, 2003, **17**, 79-81 (*14-Hydroxyartonin E*)
Jayasinghe, U.L.B. *et al., Fitoterapia*, 2008, **79**, 37-41 (*2′-O-Methylartonin E*)

Artonin F A-665

[129683-94-9]

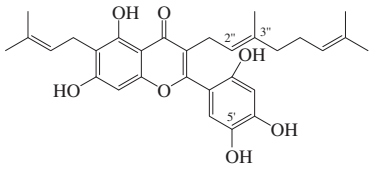


$C_{30}H_{30}O_7$ 502.563
Constit. of *Artocarpus communis* (breadfruit). Yellow needles (C_6H_6/Me_2CO). Mp 248°.

Hano, Y. *et al., Heterocycles*, 1990, **31**, 877 (*isol, pmr, cmr*)

Artonin H A-666

3-Geranyl-2′,4′,5,5′,7-pentahydroxy-6-prenylflavone [133866-94-1]



$C_{30}H_{34}O_7$ 506.594
Amorph powder. λ_{max} 206 (ϵ 48980); 258 (ϵ 27540); 302 (ϵ 11220) (MeOH) (Berdy).

5′-Deoxy: [54835-67-5] ***Rubraflavone C***
$C_{30}H_{34}O_6$ 490.595
Constit. of *Morus rubra* (red mulberry). Yellow solid.

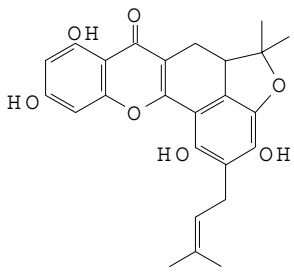
5′-Deoxy, 2″,3″-dihydroxy, 2″,3″-dihydro: [459155-95-4] ***Artocarpol H***
$C_{30}H_{36}O_8$ 524.61
Yellow needles (Me_2CO). Mp 199-200°. $[\alpha]_D^{27}$ -13.5 (c, 0.1 in Me_2CO). λ_{max} 215 (log ϵ 3.53); 291 (log ϵ 3.16) (MeOH).

Hano, Y. *et al., Heterocycles*, 1990, **31**, 2173 (*isol, struct*)

Lu, Y.-H. *et al., Helv. Chim. Acta*, 2002, **85**, 1626-1632 (*Artocarpol H, Rubraflavone C*)

Artonin J A-667

[148719-51-1]



$C_{25}H_{24}O_7$ 436.46
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 281-282°. Racemic.

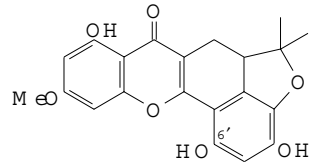
7-Me ether: [161017-03-4] ***Artonin T***
$C_{26}H_{26}O_7$ 450.487
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow needles (Me_2CO). Mp 252°. Racemic.

Aida, M. *et al., Heterocycles*, 1993, **36**, 575 (*isol, pmr, cmr*)

Aida, M. *et al., Heterocycles*, 1994, **39**, 847 (*Artonin T*)

Artonin K A-668

[148719-61-3]



$C_{21}H_{18}O_7$ 382.369
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (Me_2CO). Mp 312-314°. Racemic.

6′-Me ether: [148719-52-2] ***Artonin L***
$C_{22}H_{20}O_7$ 396.396
Constit. of the root bark of *Artocarpus heterophyllus* (jackfruit). Yellow prisms (MeOH). Mp 249-250°. Racemic.

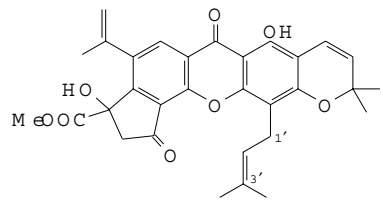
O-*De-Me:* [148719-53-3] ***Artoindonesianin P***
$C_{20}H_{16}O_7$ 368.342
Yellow cryst. (EtOAc). $[\alpha]_D^{25}$ +1.5 (c, 0.1 in MeOH). Mp >300°. λ_{max} 210 (log ϵ 5.03); 228 (log ϵ 4.81); 264 (log ϵ 4.79); 324 (log ϵ 4.33); 380 (log ϵ 4.62); 388 (log ϵ 3.62) (MeOH).

Aida, M. *et al., Heterocycles*, 1993, **36**, 575 (*isol, pmr, cmr*)

Hakim, E.H. *et al., Fitoterapia*, 2002, **73**, 668-673 (*Artoindonesianin P*)

Artonin Q A-669

[161017-00-1]



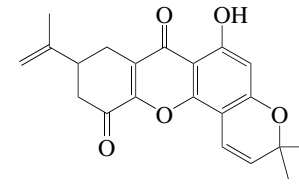
$C_{31}H_{30}O_8$ 530.573
Constit. of the bark of *Artocarpus heterophyllus* (jackfruit). Yellow cryst. (hexane/Et_2O). Mp 57-59°. Racemic. λ_{max} 205 (ϵ 30900); 225 (ϵ 25120); 250 (sh) (ϵ 26300); 302 (ϵ 27540); 350 (ϵ 8910); 390 (ϵ 4070) (MeOH).

Δ$^{1'}$-Isomer, 3′-hydroperoxy: [161017-01-2] ***Artonin R***
$C_{31}H_{30}O_{10}$ 562.572
Isol. from *Artocarpus heterophyllus* (jackfruit). Yellow cryst. (hexane/Et_2O). Mp 173°. λ_{max} 202 (ϵ 7940); 226 (ϵ 7410); 298 (ϵ 6310); 350 (ϵ 2090); 400 (ϵ 830) (MeOH).

Aida, M. *et al., Heterocycles*, 1994, **39**, 847 (*isol, uv, ir, ms, pmr, cmr*)

Artonol A A-670

[186824-57-7]

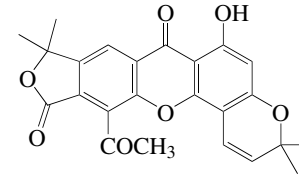


$C_{21}H_{20}O_5$ 352.386
Constit. of the bark of *Artocarpus communis* (breadfruit). Orange prisms (Me_2CO). Mp 189-196°. Racemic. λ_{max} 236 (log ϵ 4.45); 279 (log ϵ 4.31); 337 (log ϵ 3.57) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol B A-671

[186824-58-8]

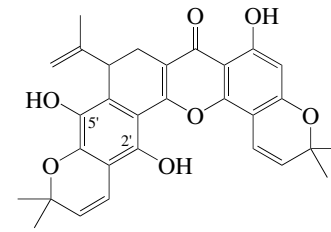


$C_{24}H_{20}O_7$ 420.418
Constit. of the bark of *Artocarpus communis* (breadfruit). Orange needles (C_6H_6). Mp 267-273°. λ_{max} 246 (log ϵ 4.1); 284 (log ϵ 3.99); 338 (log ϵ 3.5); 405 (log ϵ 3.1) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol C A-672

[186824-59-9]



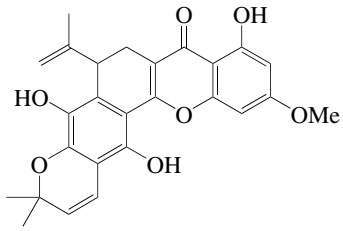
$C_{30}H_{28}O_7$ 500.547
Constit. of the bark of *Artocarpus communis* (breadfruit). Yellow needles (MeOH/C_6H_6). Mp 182-184°. Racemic. λ_{max} 237 (log ϵ 4.36); 281 (log ϵ 4.44); 345 (log ϵ 3.9); 386 (log ϵ 4.11) (MeOH).

2′,5′-Quinone: [186824-60-2] ***Artonol D***
$C_{30}H_{26}O_7$ 498.531
Constit. of the bark of *Artocarpus communis* (breadfruit). Reddish needles (Me_2CO). Mp 130°. λ_{max} 235 (log ϵ 4.33); 265 (log ϵ 4.43); 337 (log ϵ 3.84) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*isol, uv, ir, pmr, cmr*)

Artonol E A-673

[186824-61-3]



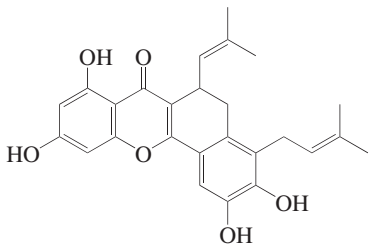
$C_{26}H_{24}O_7$ 448.471
Constit. of the bark of *Artocarpus communis* (breadfruit). Yellow needles (EtOAc). Mp 224-227°. λ_{max} 211 (log ϵ 4.31); 271 (log ϵ 4.26); 377 (log ϵ 4.09) (MeOH).

O-*De-Me:* ***De*-O-*methylartonol E***. *Artelastoxanthone*
$C_{25}H_{22}O_7$ 434.445
Constit. of the root bark of *Artocarpus rigidus* ssp. *rigidus* (monkey-jackfruit). Pale yellow-brown powder or orange gum. Mp 224-226°. $[\alpha]_D^{26}$ -7.6 (c, 0.29 in MeOH). $[\alpha]_D^{28}$ -67 (c, 0.2 in Me_2CO). λ_{max} 210 (log ϵ 4.54); 265 (sh) (log ϵ 4.45); 275 (log ϵ 4.5); 390 (log ϵ 4.08) (MeOH).

Aida, M. *et al., Heterocycles*, 1997, **45**, 163-175 (*Artonol E*)
Ko, H.-H. *et al., J. Nat. Prod.*, 2005, **68**, 1692-1695 (*Artelastoxanthone*)
Namdaung, U. *et al., Chem. Pharm. Bull.*, 2006, **54**, 1433-1436 (*De-O-methylartonol E*)

Artosimmin A-674

[1253589-99-9]



$C_{26}H_{26}O_6$ 434.488
Constit. of *Artocarpus odoratissimus* (marang). Mp 213-215°.

Ee, G.C.L. *et al., Lett. Org. Chem.*, 2010, **7**, 240-244 (*Artosimmin*)

Aryl sulfotransferase A-675

E.C. 2.8.2.1. 3′-Phosphoadenylyl-sulfate:-phenol sulfotransferase. Phenol sulfotransferase. Sulfokinase. PST [9026-09-9]

Sulfotransferase enzyme. Isol. from cow, pig. A number of aromatic compds. can act as acceptors. Partially purified rat enzyme undergoes 20% loss of activity in 7 days at -20°.

Foldes, A. *et al., Biochim. Biophys. Acta*, 1973, **327**, 365-374 (*rat*)
Sekura, R.D. *et al., Methods Enzymol.*, 1981, **77**, 197-206 (*rat*)
Fernando, P.H.P. *et al., Biochem. Mol. Biol. Int.*, 1993, **30**, 433-441 (*ox*)
Tsoi, C. *et al., Arch. Biochem. Biophys.*, 2002, **401**, 125-133 (*dog*)
Lin, Z. *et al., Mamm. Genome*, 2004, **15**, 218-226 (*pig*)
Liu, M.Y. *et al., Arch. Biochem. Biophys.*, 2005, **437**, 10-19 (*zebrafish*)
Lu, J.H. *et al., Biochem. Biophys. Res. Commun.*, 2005, **335**, 417-423 (*human, cryst struct*)

Arylamine *N*-acetyltransferase† A-676

E.C. 2.3.1.5. Acetyl-CoA:arylamine N-*acetyltransferase. Arylamine acetylase* [9027-33-2]

Enzyme. Isol. from rabbit liver. Shows wide specificity. Plays an important role in the detoxification and activation of many therapeutic drugs and carcinogens.

Weber, W.W. *et al., Methods Enzymol., Part B*, 1971, **17**, 805-811 (*rabbit liver*)
Barenholz, Y. *et al., Methods Enzymol.*, 1975, **35**, 247-253 (*Hansenula ciferri*)
Sim, E. *et al., Biochem. Soc. Trans.*, 1992, **20**, 304-309 (*rev*)
Upton, A. *et al., Trends Pharmacol. Sci.*, 2001, **22**, 140-146 (*rev*)
Dupret, J.M. *et al., Curr. Med. Chem.*, 2005, **12**, 311-318 (*rev*)

Arylamine glucosyltransferase A-677

E.C. 2.4.1.71. UDP-glucose:arylamine N-*D-glucosyltransferase* [37277-72-8]

Hexosyltransferase enzyme. Isol. from soybean. Involved in the metab. of herbicides.

Frear, D.S. *et al., Phytochemistry*, 1968, **7**, 381-390

Aryldialkylphosphatase A-678

E.C. 3.1.8.1. Aryltriphosphate dialkylphosphohydrolase. A-esterase†. Aryltriphosphatase. Paraoxon hydrolase. Paraoxonase†. Phosphotriesterase [117698-12-1]

Phosphoric triester hydrolase enzyme. Isol. from cow, pig, rabbit. Substrates incl. organophosphorus compds. Requires divalent cations for activity. Inhibited by chelating agents. Previously regarded as identical with Arylesterase, A-679. Rat enzyme activity range pH 7.0-9.0. At 4° or -20°, rat plasma enzyme is more stable than rat liver enzyme.

Mackness, M.I. *et al., Biochem. J.*, 1987, **245**, 293-296 (*rev*)
Furlong, C.E. *et al., Biochemistry*, 1991, **30**, 10133-10140 (*rabbit, human*)
Gil, F. *et al., Chem. Biol. Interact.*, 1993, **87**, 149-154 (*rat, stability*)
Rodrigo, L. *et al., Biochem. J.*, 1997, **321**, 595-601 (*rat, activity*)
Yeung, D.T. *et al., Biochim. Biophys. Acta*, 2004, **1702**, 67-77 (*human*)

Arylesterase A-679

E.C. 3.1.1.2. Aryl ester hydrolase. A-esterase†. Paraoxonase†. Aromatic esterase [9032-73-9]

Carboxylic ester hydrolase enzyme. Isol. from ox, sheep. Acts on many phenolic esters. Guinea pig enzyme activity range pH 7.0-9.0; rat enzyme at -20° to -70°, stable for several months.

Bosmann, H.B. *et al., Biochim. Biophys. Acta*, 1972, **276**, 180-191 (*guinea pig*)
Don, M.M. *et al., Biochem. J.*, 1975, **151**, 625-630 (*ox*)
Mackness, M.I. *et al., Biochem. Soc. Trans.*, 1985, **13**, 135-136 (*human, sheep*)
Johnson, K.G. *et al., Methods Enzymol.*, 1988, **160**, 551-560 (*rev*)
Kim, K.K. *et al., Proteins*, 1993, **15**, 213-215 (*cryst struct*)
Rodrigo, L. *et al., Biochem. J.*, 2003, **376**, 261-268 (*rat*)

Arylsulfatase A-680

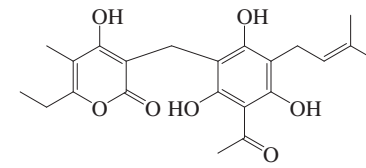
E.C. 3.1.6.1. Aryl sulfate sulfohydrolase. Sulfatase [9016-17-5]

Sulfuric ester hydrolase enzyme. Arylsulfatase is the general enzyme in a category and also represents a group of enzyme with similar specificities. Isol. from cow, pig, sheep, chicken. Rat enzyme activity range pH 5.0-7.0. Chicken enzyme stable for 2 months at -20°.

Shapira, E. *et al., Arch. Biochem. Biophys.*, 1975, **170**, 179-187 (*human*)
Sakurai, Y. *et al., Agric. Biol. Chem.*, 1980, **44**, 1-7 (*Aspergillus*)
Farooqui, A.A. *et al., Biochem. J.*, 1987, **242**, 97-102 (*chicken, stability*)
Toennes, S.W. *et al., Clin. Chem. (Winston-Salem, N.C.)*, 1999, **45**, 2173-2182 (*clin use*)
Chen, W.T. *et al., Anal. Biochem.*, 2005, **339**, 54-60 (*assay, rat, pig, Escherichia coli*)
Kilic, M. *et al., Int. Dairy J.*, 2006, **16**, 88-91 (*ox, sheep, goat*)

Arzanol A-681

Homoarenol [32274-52-5]



$C_{22}H_{26}O_7$ 402.443
The struct. of Homoarenol was revised in 2007 and shown to be identical to Arzanol. Constit. of *Helichrysum italicum* var. *microphyllum* (curry plant). Pale yellow powder ($CHCl_3$/petrol). Mp 146°.

Appendino, G. *et al., J. Nat. Prod.*, 2007, **70**, 608-612 (*isol, pmr, cmr*)

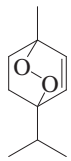
Ascalin A-682

Peptide. Struct. not reported. Isol. from shallot bulbs (*Allium ascalonicum*).

Wang, H.X. *et al., Peptides (N.Y.)*, 2002, **23**, 1025-1029 (*isol*)

Ascaridole A-683

*1-Methyl-4-(1-methylethyl)-2,3-dioxabicyclo[2.2.2]oct-5-ene, 9CI. 1-Isopropyl-4-methyl-7-oxabicyclo[2.2.1]hept-2-ene. 1,4-Epidioxy-*p*-menth-2-ene. Kebal II. Uncinacina. Ascapurin. Ascarisin* [512-85-6]



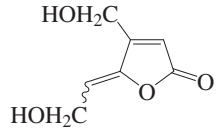
$C_{10}H_{16}O_2$ 168.235
Said to be the major constit. of oil of *Peumus boldus* (boldo). Oil. d_4^{20} 1.01. Mp 3.3°. Bp_{15} 115° $Bp_{0.2}$ 39-40°. Log P 1.34 (uncertain value) (calc). Unstable.

▶ Explodes on heating or on treatment with acids. LD_{50} (rat, orl) 200 mg/kg. Shows neoplastic activity.
OT0175000

Schenk, G.O. *et al., Angew. Chem.*, 1952, **64**, 12 (*synth*)
Beckett, A.H. *et al., J. Pharm. Pharmacol.*, 1955, **7**, 55 (*purifn*)
Swern, D. *et al., Anal. Chem.*, 1969, **41**, 412 (*pmr*)
Bernhard, R.A. *et al., Phytochemistry*, 1971, **10**, 177 (*isol*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426 (*cmr*)
Haynes, R.K. *et al., Aust. J. Chem.*, 1978, **31**, 131 (*synth*)
Masilamani, D. *et al., JOC*, 1983, **48**, 4918 (*synth*)
Zagorski, M.G. *et al., JOC*, 1985, **50**, 4484 (*cmr, O-17 nmr*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 40
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARM500

Ascladiol A-684

*5-(2-Hydroxyethylidene)-4-(hydroxymethyl)-2(5*H*)-furanone, 9CI* [32013-85-7]



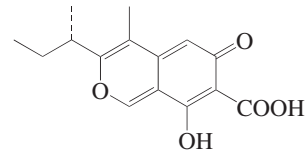
$C_7H_8O_4$ 156.138
Toxin from *Aspergillus clavatus* in wheat flour. Cryst. ($Me_2CO/CHCl_3$). Mp 65-66°. V. hygroscopic. λ_{max} 271 (MeOH) (Berdy).

▶ Toxic.

Suzuki, T. *et al., Chem. Pharm. Bull.*, 1971, **19**, 1786-1788 (*isol, struct*)
Handbook of Secondary Fungal Metabolites, (ed. Cole, R.J. *et al*), Academic Press, 2003, 744
Lykakis, I.N. *et al., JOC*, 2009, **74**, 6339-6342 (*synth*)

Ascochitin A-685

Ascochytin



$C_{15}H_{16}O_5$ 276.288
Polyketide.

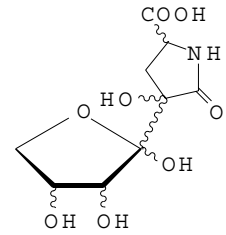
(*S*)-*form* [3615-05-2]
Causes brown rot in broad beans. Yellow cryst. Mp 196-198°. $[\alpha]_D^{25}$ -86 ($CHCl_3$). λ_{max} 220 (ϵ 20617); 286 (ϵ 17550); 415 (ϵ 5700) (EtOH).

(±)-*form*
Yellow prisms (CCl_4/CH_2Cl_2). Mp 203°.

Iwai, I. *et al., Chem. Ind. (London)*, 1965, 186-187 (*struct*)
Galbraith, M.N. *et al., JCS(C)*, 1971, 3557-3559 (*struct, synth, bibl*)
Colombo, L. *et al., JCS Perkin 1*, 1980, 675-676; 2549-2553 (*cmr, struct, biosynth*)
Marcinowska, J. *et al., J. Phytopathol.*, 1991, **131**, 253-258 (*occur*)
Foremska, E. *et al., Acta Biotechnol.*, 1992, **12**, 461-465 (*manuf, purifn, activity*)
Beed, F.D. *et al., Mycol. Res.*, 1994, **98**, 1069-1076 (*manuf*)
Seibert, S.F. *et al., Org. Biomol. Chem.*, 2006, **4**, 2233-2240 (*isol*)

Ascorbalamic acid, 9CI A-686

[41679-87-2]

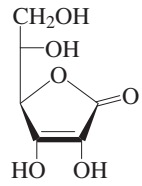


$C_9H_{13}NO_8$ 263.204
Constit. of cabbage (*Brassica oleracea*). $[\alpha]_D^{26}$ +24 (c, 1.25 in H_2O). pK_a 1.

Couchman, R. *et al., Phytochemistry*, 1973, **12**, 707 (*isol*)

Ascorbic acid, BAN, INN, USAN A-687

threo-*Hex-2-enonic acid γ-lactone, 9CI, 8CI.* threo-*Hexulosono-1,4-lactone-2,3-enediol. Hexuronic acid. Lyxoascorbic acid. Xyloascorbic acid*



-form

$C_6H_8O_6$ 176.126
Log P -2.21 (calc).

L-*form* [50-81-7]
***Vitamin C**. Vitamin C*[3]*. Ascorbicap. Cebione. Celaskon. Cenolate. Cevalin. Cevital. Citrovit. Roscorbic. Vitacimin. Vitascorbol. E300*
Occurs widely in animals and plants. Good sources are citrus fruits and hip berries. Isol. from ox adrenal cortex, lemons and paprika. Prod. industrially on a large scale from glucose. Vitamin (antiscorbutic), antioxidant, nutrient, preservative consistency enhancer. Used to reduce discoloration, mainly browning caused by polyphenol oxidase, in fruit and vegetable products. Used to enhance colour formn. and to reduced the formn. of nitrosamines in meat products. Used synergistically with Sulfur dioxide, S-404 in wine and beer as a preservative. Assists formn. of the gluten network in bread making, thus enhancing bread volume. Mp 190-192°. $[\alpha]_D^{25}$ +24 (c, 1 in H_2O). $[\alpha]_D^{18}$ +49 (MeOH). pK_{a1} 4.04; pK_{a2} 11.34 (25°, 0.1*M* KNO_3). Component of numerous preparations.

▶ Human systemic effects when administered intravenously. Exp. reprod. and teratogenic effects (v. large doses). LD_{50} (rat, orl) 11900 mg/kg. CI7650000

Na salt: [134-03-2] ***Sodium ascorbate, INN**. E301*
Antioxidant. $[\alpha]_D$ +24 (c, 3 in H_2O).

▶ CI7671000

Ca salt (2:1): [5743-27-1] *Calcium ascorbate. E302*
Antioxidant. $[\alpha]_D^{10}$ +91 (c, 0.3 in H_2O).

*Fe(*II*) salt:* [24808-52-4] *Ferrous ascorbate*
Dietary supplement.

*2-*O*-α-D-Glucopyranoside:* [129499-78-1] *Ascorbic acid 2-α-D-glucoside. AA-2G*
Isol. from kimchi. $[\alpha]_D^{20}$ +189.6 (c, 5.0 in H_2O).

*2-*O*-β-D-Glucopyranoside:* [562043-82-7] *Ascorbic acid 2-β-D-glucoside*
$C_{12}H_{18}O_{11}$ 338.268
Constit. of the fruit of *Lycium barbarum* (box thorn). Amorph. cryst. λ_{max} 259 (H_2O).

*6-*O*-β-D-Glucopyranoside:* [1043475-91-7] *Ascorbic acid 6-β-D-glucoside*
$C_{12}H_{18}O_{11}$ 338.268
Constit. of the fruit of *Cucurbita pepo* (zucchini). λ_{max} 265 (H_2O).

6-Hexadecanoyl: [137-66-6] ***Ascorbyl palmitate, USAN**. E304*
$C_{22}H_{38}O_7$ 414.538
Antioxidant. Mp 107-117°. $[\alpha]_D^{20}$ +22.9 (c, 2 in MeOH).

▶ CI7671040

6-Octadecanoyl: [10605-09-1] ***Ascorbyl stearate***
[25395-66-8]
$C_{24}H_{42}O_7$ 442.592
Preservative for margarine.

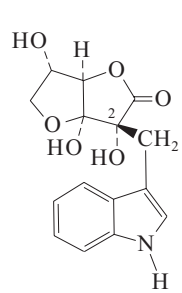
3-Et: [86404-04-8] *Ethylascorbic acid*
$C_8H_{12}O_6$ 204.179
Antioxidant. Mp 111-115°.

[25395-66-8, 6730-29-6, 5743-28-2, 124928-57-0, 6485-44-5, 299-36-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 702B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1149C; 1150C; 1151B; 1151A (*nmr*)
Herbert, R.W. *et al., JCS*, 1933, 1270-1290 (*struct*)
Reichstein, T. *et al., Helv. Chim. Acta*, 1934, **17**, 311-328 (*synth*)
Hirst, E.L. *et al., Fortschr. Chem. Org. Naturst.*, 1939, **2**, 132-159
Sawyer, D.T. *et al., Anal. Chem.*, 1966, **38**, 192-199 (*pmr*)
Pilipenko, A.T. *et al., Zavod. Lab.*, 1966, **32**, 3 (*rev, use*)
Hvoslef, J. *et al., Acta Cryst. B*, 1969, **25**, 2214-2223 (*cryst struct*)
Berger, S. *et al., Tetrahedron*, 1977, **33**, 1587-1589 (*cmr*)
Crawford, T.C. *et al., Adv. Carbohydr. Chem.*, 1980, **37**, 79-155 (*rev*)
Sieb, P.A. *et al., Adv. Chem. Ser.*, 1982, **200**, 1-585 (*rev*)
Ascorbic acid: Chemistry, Metabolism and Uses (Adv. Chem. Ser. no. 200), ACS, 1982, (*book*)
Eur. Pat., 1985, (*(Takeda)*)146 121 (*CV 3611, synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN000
Davies, M.B. *et al., Vitamin C: its Chemistry and Biochemistry*, RSC, 1991,
Parviainen, M.T. *et al., Chromatogr. Sci.*, 1992, **60**, 235-260 (*rev, chromatog*)
Barili, P.L. *et al., Tetrahedron*, 1992, **48**, 6273-6284 (*synth*)
Csiba, M. *et al., JOC*, 1993, **58**, 7281-7282 (*synth*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 15-18; 19-20; 431-432
Ruchmann, A. *et al., Magn. Reson. Chem.*, 1996, **34**, 116-122 (*O-17 nmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 205; 212; 213; 369-370; 1106-1107; 2526-2527 (*salts, rev*)
Jun, H.-K. *et al., J. Microbiol. Biotechnol.*, 1998, **8**, 710-713 (*2-glucoside, isol*)
Loewus, F.A. *et al., Phytochemistry*, 1999, **52**, 193-210 (*rev, biosynth, metab*)
Yamamoto, I. *et al., J. Med. Chem.*, 2002, **45**, 462-468 (*2-α-D-glucoside, bibl*)
Toyoda-Ono, Y. *et al., J. Agric. Food Chem.*, 2004, **52**, 2092-2096 (*2-β-D-glucoside*)
Jin, S. *et al., Acta Cryst. E*, 2008, **64**, o860 (*3-Et ether, synth, cryst struct*)
Hancock, R.D. *et al., Phytochemistry*, 2008, **69**, 1850-1858 (*6-glucoside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN000; ARN125; CAM600

Ascorbigen A-688

2-C-(1H-Indol-3-ylmethyl)-3-hexulofuranosonic acid γ-lactone, 9CI [8075-98-7]



(2*R*)–*form*

$C_{15}H_{15}NO_6$ 305.287
Present in plants, esp. cabbage and other crucifers.

(2*R*)-*form* [26548-49-2]
β-L-lyxo-*form*. ***Ascorbigen B***
Light yellow amorph. powder.
Mp 70° (sinters). $[\alpha]_D^{25}$ +12.5 (c, 1.0 in MeOH).

(2*S*)-*form* [26676-89-1]
β-L-xylo-*form*. ***Ascorbigen A***
Amorph. powder. Mp *ca.*65° (sinters).
$[\alpha]_D^{25}$ +11 (c, 2.0 in EtOH).

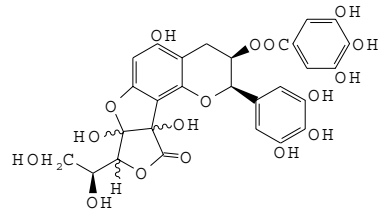
N-*Methoxy:* [331754-99-5] ***Neoascorbigen***
$C_{16}H_{17}NO_7$ 335.313
Isol. from *Brassica* spp. Powder. $[\alpha]_D^{20}$ +8 (c, 0.05 in EtOH).

[29400-26-8]

Piironen, E. *et al., Acta Chem. Scand.*, 1962, **16**, 1286-1287 (*synth, bibl*)
Kiss, G. *et al., Helv. Chim. Acta*, 1966, **49**, 989-992 (*synth, ir, uv, pmr, struct*)
Preobrazhenskaya, M.N. *et al., Pharmacol. Ther.*, 1993, **60**, 303-313 (*activity*)
Musk, S.R.R. *et al., Mutat. Res. Lett.*, 1994, **323**, 69-74 (*tox*)
Agerbirk, N. *et al., J. Agric. Food Chem.*, 1998, **46**, 1563-1571 (*Neoascorbigen*)
Yudina, L.N. *et al., Chem. Heterocycl. Compd. (Engl. Transl.)*, 2000, **36**, 144-151 (*Neoascorbigen*)

8-*C*-Ascorbylepigallocatechin 3-*O*-gallate A-689

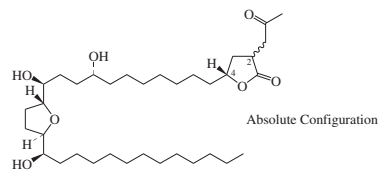
[126715-87-5]



$C_{28}H_{24}O_{17}$ 632.487
Constit. of commercial oolong tea (*Camellia sinensis* var. *viridis*). Off-white amorph. powder + ½H_2O. $[\alpha]_D^{21}$ -215.1 (c, 1.0 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 3255 (*struct, ir, pmr, cmr*)

Asitrocinone A-690

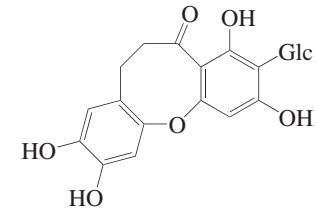


$C_{35}H_{64}O_7$ 596.886
Constit. of the seeds of *Asimina triloba* (pawpaw). Powder. $[\alpha]_D^{23}$ +13.2 (c, 0.005 in CH_2Cl_2). Mixt. of 2,4-*cis*-and *trans*-isomers. λ_{max} 205 (log ϵ 3.6) (MeOH).

Kim, E.-J. *et al., J. Nat. Prod.*, 2000, **63**, 1503-1506

Aspalalinin A-691

[910252-00-5]

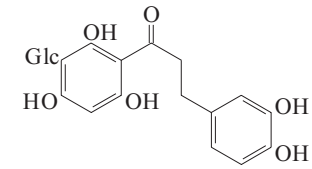


$C_{21}H_{22}O_{11}$ 450.398
Cyclised dihydrochalcone. Constit. of the leaves of *Aspalathus linearis* (rooibos). Plates + ½H_2O (MeOH aq.). Mp 219-221°. $[\alpha]_D^{23}$ +26.2 (c, 1 in MeOH).

Shimamura, N. *et al., Biol. Pharm. Bull.*, 2006, **29**, 1271-1274 (*isol, cd, pmr, cmr, cryst struct*)

Aspalathin A-692

1-(3-C-β-D-Glucopyranosyl-2,4,6-trihydroxyphenyl)-3-(3,4-dihydroxyphenyl)-1-propanone. 3′-Glucosyl-2′,3,4,4′,6′-pentahydroxydihydrochalcone



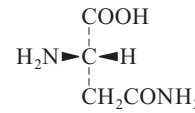
$C_{21}H_{24}O_{11}$ 452.414
Constit. of *Aspalathus linearis* (rooibos). Amorph. Sol. H_2O. $[\alpha]_D^{20}$ +34.7 (c, 2.14 in EtOH). $[\alpha]_D$ +58.4 (c, 2.21 in Me_2CO).

Nona-Ac:
Fine needles (EtOH). Mp 153-154°.
$[\alpha]_D^{25}$ -35.8 (c, 2.16 in Me_2CO).

Koeppen, B.H. *et al., Tet. Lett.*, 1965, 3497; *Biochem. J.*, 1966, **99**, 604 (*isol, struct*)
Yepremyan, A. *et al., Org. Lett.*, 2010, **12**, 1580-1583 (*synth*)

Asparagine, 9CI A-693

2,4-Diamino-4-oxobutanoic acid. Aspartic acid β-monoamide. β-Asparagine. Asparamide. Altheine. Asn [7006-34-0]



(*S*)–*form*

$C_4H_8N_2O_3$ 132.119
Derivs. labelled *N* (here and in 9CI) refer to those subst. on the amide (or N^4) nitrogen; N^2 refers to subst. on amino group.

(*R*)-*form* [2058-58-4]
D-form
[5794-24-1]
Cryst. + 1H_2O. Mp 234-235°. $[\alpha]_D^{15}$ +5.4 (H_2O).

(*S*)-*form* [70-47-3]
L-form
One of the nonessential amino acids.

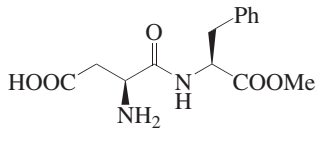
Dietary supplement, nutrient. Widely distributed in the plant kingdom. Isol. from asparagus, beetroot, peas, beans, etc. Rhombic hemihedral cryst. + $1H_2O$ (H_2O). Mod. sol. H_2O (3.1g/100g at 25°). Mp 226-227° dec. (slow heat) Mp 234-235° (rapid heat). $[\alpha]_D^{25}$ -7.4 (c, 2 in H_2O). $[\alpha]_D$ +33.2 (3*M* HCl). pK_{a1} 2.02; pK_{a2} 8.6 (NH_2). Isoelectric point 5.41. Bitter taste.

(±)-*form* [3130-87-8]
Cryst. + $1H_2O$ (EtOH/HCl aq.). Loses H_2O at 210°; dec. at 280-5°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 782A; 782B; 782C; **2**, 263A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1277C; 1278A (*nmr*)
Aldrich Library of NMR Spectra, **3**, 10A; 121C (*pmr*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **2**, 1257; **3**, 1856 (*occur, isol, synth*)
Gray, D.O. *et al., Nature (London)*, 1961, **189**, 401-402 (*N-Et, isol*)
Biochem. Prep., 1963, **10**, 10
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679 (*cd*)
Ramanadham, M. *et al., Acta Cryst. B*, 1972, **28**, 3000-3005 (*cryst struct*)
Verbis, J.J. *et al., Acta Cryst. B*, 1972, **28**, 3006-3013 (*cryst struct*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2370 (*occur*)
Toi, K. *et al., Synth. Prod. Util. Amino Acids*, 1974, 75 (*rev*)
Tome, D. *et al., Int. J. Pept. Protein Res.*, 1981, **17**, 501 (*cmr*)
Yoshifuji, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 2994-3001 (*synth*)
Sieciechowicz, K.A. *et al., Phytochemistry*, 1988, **27**, 663-671 (*rev, metab*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN810
Casado, J. *et al., J. Mol. Struct.*, 1995, **349**, 57 (*ir, Raman*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 213-214
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN810

Aspartame, BAN, INN, USAN A-694

N-α-*Aspartyl-L-phenylalanine 1-methyl ester, 9CI. Methyl aspartylphenylalanine. Nutrasweet. Canderel. α-APM. SC-18862. E951* [22839-47-0]



$C_{14}H_{18}N_2O_5$ 294.307
Compd. with 100 times the sweetness of sucrose. Artificial sweetener permitted in foods in EU at 300-5500 ppm. Also permitted in USA. Widely used in foods, beverages and pharmaceutical formulations. ADI 50 mg/kg (1984). Cryst. (EtOH aq. or H_2O). Sl. sol H_2O; insol. fats, oils. Mp 190° Mp 245-247° (double Mp) (235-236° dec.). $[\alpha]_D$ 0 (H_2O). $[\alpha]_D^{22}$ +32 (c, 1 in AcOH). Log P -2.16 (calc).

▶ WM3407000

Hydrochloride: [5910-52-1]
Mp 127-128° dec. (partly melts at 103°). $[\alpha]_D^{25}$ +1.3 (c, 2 in H_2O).

Hydrobromide: [36771-92-3]
Mp 155° dec. $[\alpha]_D^{25}$ +1 (c, 2 in H_2O).

3-N-tert-*Butyloxycarbonyl:* [40944-73-8]
$C_{19}H_{26}N_2O_7$ 394.424
Cryst. (EtOAc/Et_2O). Mp 164-166° (149-151°). $[\alpha]_D^{18}$ -34.5 (c, 0.5 in DMF).

3-N-*Benzyloxycarbonyl:* [33605-72-0]
$C_{22}H_{24}N_2O_7$ 428.441
Cryst. Mp 120-124°. $[\alpha]_D^{25}$ -14.4 (c, 1 in MeOH).

[53906-69-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 267D (*ir*)
Neuman, M. *et al., Drugs of Today (Barcelona)*, 1980, **16**, 63-67 (*rev*)
Shvachkin, Y.P. *et al., Zh. Obshch. Khim.*, 1982, **52**, 2791-2792 (*synth*)
Fujii, N. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3503-3514 (*tert-butyloxycarbonyl*)
Stegink, L.D. *et al., Food Sci. Technol.*, Aspartame: Physiol. Biochem., Dekker, N.Y., 1984, **12**, (*book*)
Renwick, A.G. *et al., Food Chem.*, 1985, **16**, 281-301 (*metab*)
Hatada, M. *et al., JACS*, 1985, **107**, 4279-4282 (*cryst struct*)
Tou, J.S. *et al., JOC*, 1985, **50**, 4982-4984 (*synth*)
Fuganti, C. *et al., JOC*, 1986, **51**, 1126-1128 (*synth*)
Görbitz, C.H. *et al., Acta Chem. Scand., Ser. B*, 1987, **41**, 87-92 (*hydrochloride, cryst struct*)
Nakanishi, K. *et al., Food Biotechnol.*, 1988, **2**, 219-249 (*rev, synth*)
Chen, S.T. *et al., JOC*, 1988, **53**, 4589-4590 (*tert-butyloxycarbonyl*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN825
Keirs, D. *et al., Heterocycles*, 1989, **28**, 841-848 (*synth*)
Kuhl, P. *et al., Pharmazie*, 1990, **45**, 881-887 (*rev, synth*)
Homler, B.E. *et al., Food Sci. Technol.*, 1991, **48**, 39-69 (*rev*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 21-23
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1354
Ager, D.J. *et al., Angew. Chem., Int. Ed.*, 1998, **37**, 1803-1817 (*rev, synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*degradn, rev*)
Prankerd, R.J. *et al., Anal. Profiles Drug Subst.*, 2002, **29**, 7-55 (*rev*)
Abegaz, E.G. *et al., Alternative Sweeteners*, 4th edn., (ed. O'Brien-Nabors, L.), CRC Press, 2011, 57-76 (*use, rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, ARN825

Aspartate kinase A-695

E.C. 2.7.2.4. ATP:L-aspartate 4-phosphotransferase. Aspartokinase. Aspartic kinase [9012-50-4]

Phosphotransferase enzyme with carboxy acceptor. Isol. from maize, rice, spinach, baker's yeast. *Streptococcus mutans* Enzyme optimum activity range pH 6.0-9.0. At -20°, can be stored for several months; at 4°, over 24 hours, shows substantial loss of activity. *Escherichia coli* Enzyme is a multifunctional protein.

Black, S. *et al., Methods Enzymol.*, 1962, **5**, 820-827 (*baker's yeast*)
Paulus, H. *et al., J. Biol. Chem.*, 1967, **242**, 4980-4986 (*Bacillus polymyxa*)
Véron, M. *et al., Eur. J. Biochem.*, 1972, **28**, 520-527 (*Escherichia coli*)
Truffa-Bachi, P. *et al., The Enzymes*, 3rd edn., (ed. Boyer, P.D.), Academic Press, 1973, **8**, 509-553 (*rev, microbial*)
Moir, D. *et al., J. Biol. Chem.*, 1977, **252**, 4648-4654 (*Bacillus subtilis*)
McCarron, R.M. *et al., J. Bacteriol.*, 1978, **134**, 483-491 (*Streptococcus mutans, purifn, props, regulation*)
Kochhar, S. *et al., Biochim. Biophys. Acta*, 1986, **880**, 220-225 (*spinach*)
Dotson, S.B. *et al., Plant Physiol.*, 1990, **93**, 98-104 (*maize, purifn*)
Lugli, J. *et al., Plant Sci. (Shannon, Irel.)*, 2000, **150**, 51-58 (*rice*)
Marina, P. *et al., Biochem. Biophys. Res. Commun.*, 2004, **321**, 584-591 (*baker's yeast*)
Curien, G. *et al., FEBS J.*, 2007, **274**, 164-176 (*thale cress*)

Aspartate oxidases A-696

FAD-dependent oxidoreductase enzymes.

D-Aspartate oxidase [9029-20-3]
E.C. 1.4.3.1. D-Aspartate:oxygen oxidoreductase (deaminating)
Isol. from beef and rabbit kidney.

L-Aspartate oxidase [69106-47-4]
*E.C. 1.4.3.16. L-Aspartate:oxygen oxidoreductase (deaminating)*A component of the bacterial quinolinate synthase system.

Still, J.L. *et al., J. Biol. Chem.*, 1949, **179**, 831-837 (*E.C. 1.4.3.1, rabbit kidney*)
Dixon, M. *et al., Biochim. Biophys. Acta*, 1967, **146**, 54-76 (*E.C. 1.4.3.1, rabbit kidney*)
Dixon, M. *et al., Methods Enzymol., Part A*, 1970, **17**, 713-718 (*E.C. 1.4.3.1, rabbit kidney*)
Nasu, S. *et al., J. Biol. Chem.*, 1982, **257**, 626-632 (*E.C. 1.4.3.16, Escherichia coli*)
Negri, A. *et al., J. Biol. Chem.*, 1987, **262**, 10026-10034 (*E.C. 1.4.3.1, beef kidney*)
Yamada, R. *et al., Biochim. Biophys. Acta*, 1996, **1294**, 153-158 (*E.C. 1.4.3.1, Cryptococcus humicolus*)
Bacchella, L. *et al., Acta Cryst. D*, 1999, **55**, 549-551 (*E.C. 1.4.3.16, Escherichia coli*)

Aspartate transaminase A-697

E.C. 2.6.1.1. L-Aspartate:2-oxoglutarate aminotransferase. Aspartate aminotransferase. Glutamic-aspartic transaminase. Transaminase A. Glutamate-oxalacetate aminotransferase. AAT [9000-97-9]

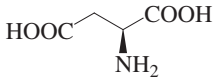
Aminotransferase enzyme. Isol. from chicken and pig, and from kidney bean. Pyridoxal phosphate-dependent. Also acts on L-tyrosine, L-phenylalanine and L-tryptophan. Exists in 2 isozyme forms: m (mitochondrial) and c (cytosolic).

Sizer, I.W. *et al., Methods Enzymol.*, 1962, **5**, 677-684 (*pig heart*)
Bertland, L.H. *et al., Biochemistry*, 1968, **7**, 134-142 (*chicken heart*)

Forest, J.C. *et al., Can. J. Biochem.*, 1973, **50**, 813-829 (*Phaseolus vulgaris*)
Mavrides, C. *et al., J. Biol. Chem.*, 1975, **250**, 4128-4133 (*Escherichia coli*)
Lowe, P.N. *et al., Biochem. J.*, 1985, **232**, 689-695 (*Trichomonas vaginalis*)

Aspartic acid, INN, USAN A-698

Aminobutanedioic acid, 9CI. Aminosuccinic acid. Asparagic acid. Asparaginic acid. Asp [6899-03-2]



(*S*)-*form*

$C_4H_7NO_4$ 133.104

(*S*)-*form* [56-84-8]
L-*form. FEMA 3656*
Found in sugar cane and sugar beet molasses and proteins/peptides. Dietary supplement, nutrient. Leaflets (H_2O). Spar. sol. H_2O (0.5g/100g at 25°). Mp 269-271° dec. $[\alpha]_D^{25}$ +5.05 (c, 1 in H_2O). $[\alpha]_D$ +25.4 (c, 1 in 5*M* HCl). pK_{a1} 2.09 (COOH); pK_{a2} 3.86 (4-COOH); pK_{a3} 9.82 (1-COOH) (25°). Isoelectric point 2.77. Bitter taste.
▶ LD_{50} (mus, ipr) 6000 mg/kg. CI9098500

N-*Benzoyl:* [4631-12-3]
Constit. of pea (*Pisum sativum*). Mp 171-173°. $[\alpha]_D^{20}$ +37 (c, 10 in 1*M* NaOH).

N-*(2-Hydroxybenzoyl):* [56145-94-9] **N-*Salicyloylaspartic acid***
$C_{11}H_{11}NO_6$ 253.211
Constit. of kidney beans (*Phaseolus vulgaris*) and grape (*Vitis* spp.). λ_{max} 238; 305 (MeOH) (Berdy).
▶ CI9455500

N-*(*E*-Cinnamoyl):* [860295-30-3]
$C_{13}H_{13}NO_5$ 263.249
Constit. of roasted cocoa beans. Powder. $[\alpha]_D^{20}$ +1.7 (c, 1 in MeOH).

N-*(4-Hydroxycinnamoyl):* [151435-24-4] **N-p-*Coumaroylaspartic acid***
$C_{13}H_{13}NO_6$ 279.249
Constit. of roasted cocoa beans and coffee powder. $[\alpha]_D^{20}$ +1.2 (c, 1 in MeOH).

N-*(3,4-Dihydroxy*-E-*cinnamoyl):* [860295-20-1] N-*Caffeoylaspartic acid*
$C_{13}H_{13}NO_7$ 295.248
Constit. of roasted cocoa beans. Powder. $[\alpha]_D^{20}$ +9.3 (c, 1 in H_2O).

N-*(4-Hydroxy-3-methoxycinnamoyl):* [135068-96-1] **N-*Feruloylaspartic acid***
$C_{14}H_{15}NO_7$ 309.275
Constit. of beet (*Beta vulgaris*) and roasted cocoa beans. $[\alpha]_D^{20}$ +10.9 (c, 1 in H_2O).

N-*Phenylacetyl:* [2752-32-1] N-*Phenylacetylaspartic acid*
$C_{12}H_{13}NO_5$ 251.238
Constit. of pea (*Pisum sativum*). Mp 136°.

[17090-93-6, 14007-45-5, 3792-50-5, 1115-63-5]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 496C; 496D; 497A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 588D; 589B; 589A (*ir*)
Vickery, H.B. *et al., Biochem. Prep.*, 1952, **2**, 71-73 (L-*form, synth*)
Greenstein, J.P. *et al., Chemistry of the Amino Acids*, Wiley, N.Y., 1961, **3**, 1856-1878; 2759 (*synth, resoln, rev*)
Org. Synth., Coll. Vol., 4, 1963, 55-58 (*synth*)
Fujiwara, S. *et al., Bull. Chem. Soc. Jpn.*, 1964, **37**, 344-349 (*pmr*)
Legrand, M. *et al., Bull. Soc. Chim. Fr.*, 1965, 679-681 (*cd*)
Young, D.P. *et al., Chem. Ind. (London)*, 1967, 1251 (*synth*)
Zintel, J.A. *et al., Can. J. Chem.*, 1969, **47**, 411-415 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 2369 (*occur*)
Rao, S.T. *et al., Acta Cryst. B*, 1973, **29**, 1718-1720 (*cryst struct*)
Sergeev, G.M. *et al., CA*, 1977, **89**, 208521r (*use*)
Gianfagna, T.J. *et al., Phytochemistry*, 1980, **19**, 959-961 (*isol, N-benzoyl, N-phenylacetyl*)
Hardin, E.D. *et al., Anal. Chem.*, 1981, **53**, 1492-1497 (*ms*)
Harada, K. *et al., Bull. Chem. Soc. Jpn.*, 1983, **56**, 653-654 (*resoln*)
Zahradnik, J. *et al., Coll. Czech. Chem. Comm.*, 1985, **50**, 2122-2133 (*manuf*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, ARN830; ARN850
Bokern, M. *et al., Phytochemistry*, 1991, **30**, 3261-3265 (*N-Feruloylaspartic acid*)
Bourne, D.J. *et al., Phytochemistry*, 1991, **30**, 4041-4044 (*N-Salicyloylaspartic acid*)
Mock, H.-P. *et al., Phytochemistry*, 1993, **34**, 157-159 (*N-Coumaroylaspartic acid*)
Castro, J.L. *et al., J. Mol. Struct.*, 1995, **349**, 113-116 (*ir, Raman*)
Stark, T. *et al., J. Agric. Food Chem.*, 2005, **53**, 5407-5418; 5419-5428; 2006, **54**, 2859-2867 (*cocoa cinnamamides, isol, synth*)
Bendeif, E.-E. *et al., Acta Cryst. C*, 2007, **63**, o361-o364 (*cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, ARN830; 1992, ARN850

Aspartyl aminopeptidase A-699

E.C. 3.4.11.21
[9074-83-3]

Aminopeptidase enzyme. Isol. from pig, rabbit. Pig enzyme activity range pH 4.5-8.5.

Danielsen, E.M. *et al., Biochem. J.*, 1980, **189**, 591-603 (*pig, activity*)
Nathan, P.B. *et al., Biochem. Soc. Trans.*, 1989, **17**, 354 (*Escherichia coli*)
Wilk, S. *et al., J. Biol. Chem.*, 1998, **273**, 15961-15970 (*human, rabbit, rat*)
Simmons, W.H. *et al., Handb. Proteolytic Enzymes*, 2nd edn., (eds. Barrett, A.J. *et al*), Elsevier Academic Press, 2004, **1**, 937-939 (*rabbit, human*)

N^{β}-Aspartylglycine, 9CI A-700

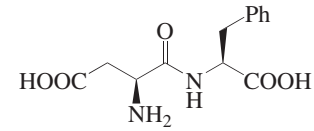
$HOOCCH(NH_2)CH_2CONHCH_2COOH$
$C_6H_{10}N_2O_5$ 190.155

D-*form* [67176-36-7]
Mp 210-228°. $[\alpha]_D^{28}$ -8.9 (c, 1 in 50% AcOH).

L-*form* [3790-52-1]
Cryst. (H_2O). Mp 160-168°. $[\alpha]_D^{28}$ +18.1 (c, 1 in 1*M* HCl).

Takashi, A. *et al., Biochem. Biophys. Res. Commun.*, 1978, **82**, 707
Welling, G.W. *et al., Biochem. J.*, 1978, **175**, 807
Welling, G.W. *et al., J. Chromatogr.*, 1982, **232**, 55 (*anal*)

N^{α}-Aspartylphenylalanine A-701



$C_{13}H_{16}N_2O_5$ 280.28

L-L-*form* [13433-09-5]
Degradn. product of Aspartame, A-694. Mp 232-235°. $[\alpha]_D$ +16 (c, 1 in DMF).

Me ester: see Aspartame, A-694

N-*(3,3-Dimethylbutyl), Me ester:* [165450-17-9] *Neotame*
$C_{20}H_{30}N_2O_5$ 378.467
Potential high-intensity sweetener, sweetness variously stated to be 40 x sucrose and 7000-13000 x sucrose. ADI 2mg/kg. Widely used in foods and beverages. Cryst. + $1H_2O$ (EtOAc/hexane). V. sol EtOH. Mp 80-83° (monohydrate). $[\alpha]_D$ -54.84 (c, 1 in MeOH). Other diastereomers do not exhibit sweetening power.

Davey, J.M. *et al., JCS(C)*, 1966, 555 (*deriv*)
Mazur, R.H. *et al., JACS*, 1969, **91**, 2684 (*synth*)
Roberts, G.C.K. *et al., Biochem. J.*, 1971, **125**, 88P (*pmr*)
Yasutake, A. *et al., Bull. Chem. Soc. Jpn.*, 1977, **50**, 2413 (*deriv*)
US Pat., 1996, 5 510 508 (*Neotame*)
Wink, D.J. *et al., Acta Cryst. C*, 1999, **55**, 1365-1368 (*Neotame, synth, pmr, cryst struct*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261
Mayhew, D.A. *et al., Alternative Sweeteners*, 4th edn., (ed. O'Brien-Nabors, L.), CRC Press, 2011, 133-150 (*Neotame, use, rev*)

Aspartylserylglyclisoleucyl-serylprolylarginine A-702

[81317-15-9]

H-Asp-Ser-Gly-Ile-Ser-Pro-Arg-OH
$C_{29}H_{50}N_{10}O_{12}$ 730.774

Grataroli, R. *et al., Eur. J. Biochem.*, 1982, **122**, 111-117 (*struct*)

Aspergillomarasmine A A-703

N-*[2-(2-Amino-2-carboxyethyl)amino]-2-carboxyaspartic acid, 9CI. Toxin C* [3484-65-9]

$HOOCCH_2CH(COOH)NHCH_2CH(COOH)NHCH_2CH(NH_2)COOH$
$C_{10}H_{17}N_3O_8$ 307.26
Metab. of the cereal fungus (*Aspergillus flavus*), found only in young cultures. Sol. acids, bases; poorly sol. H_2O, butanol, hexane. Mp 230-236° dec. $[\alpha]_D^{20}$ -48 (phosphate buffer, pH 7).

► LD_{50} (mus, ivn) 250 mg/kg. CI9098825

Barter, M. *et al., Bull. Soc. Chim. Fr.*, 1962, 187

Bogdanovsky, O. *et al., Bull. Soc. Chim. Fr.*, 1965, 832 (*synth*)

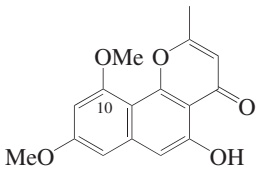
Haenni, A.L. *et al., Helv. Chim. Acta*, 1965, **48**, 729 (*struct*)

Mikami, Y. *et al., Agric. Biol. Chem.*, 1983, **47**, 2693 (*activity*)

Matsuura, A. *et al., Jpn. J. Pharmacol.*, 1993, **63**, 187-193 (*activity*)

Asperxanthone† A-704

*5-Hydroxy-8,10-dimethoxy-2-methyl-4*H*-naphtho[1,2-*b*]pyran-4-one, 9CI.* ***Flavasperone****. Antibiotic TMC 256C$_2$. TMC 256C$_2$* [3566-99-2]



$C_{16}H_{14}O_5$ 286.284

Isol. from *Aspergillus niger* infected mango fruits and peanuts. Yellow needles ($CHCl_3$/EtOH). Mp 204° (203-204°) . λ_{max} 241 (ϵ 44670); 282 (ϵ 25700); 370 (ϵ 4570) (MeOH).

*10-*O*-De-Me, 10-*O*-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [200127-93-1] *10-*O*-Demethylflavasperone 10-gentiobioside. Isorubrofusarin 10-gentiobioside*

$C_{27}H_{32}O_{15}$ 596.541

Constit. of the seeds of *Cassia tora* (charota). Yellow powder. $[\alpha]_D$ -14 (c, 0.1 in Py). λ_{max} 240 (log ϵ 4.49); 248 (sh) (log ϵ 4.39); 279 (log ϵ 4.35); 313 (sh) (log ϵ 3.84); 367 (log ϵ 3.5) (MeOH).

Lund, N.A. *et al., JCS*, 1953, 2434-2439 (*isol*)

Bycroft, B.W. *et al., JCS*, 1962, 40-44; 1963, 4868-4872 (*struct, synth*)

Tanaka, H. *et al., Agric. Biol. Chem.*, 1966, **30**, 107-113 (*isol*)

Ghosal, S. *et al., J. Agric. Food Chem.*, 1979, **27**, 1347-1351 (*isol, props*)

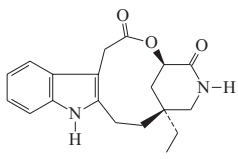
Gorst-Allman, C.P. *et al., JCS Perkin 1*, 1980, 2474-2479 (*isol, uv, ir, pmr, cmr*)

Lee, H.J. *et al., Arch. Pharmacal Res.*, 1997, **20**, 513-515 (*Isorubrofusarin gentiobioside*)

Hatano, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1121-1127 (*Isorubrofusarin 10-gentiobioside*)

Aspidochibine A-705

Alkaloid AQC2 [139955-86-5]



Relative configuration

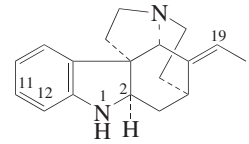
$C_{19}H_{22}N_2O_3$ 326.394

New structural class of the quebrachamine series. Alkaloid from cell cultures of *Aspidosperma quebracho-blanco* (quebracho). Amorph.

Aimi, N. *et al., Tet. Lett.*, 1991, **32**, 4949 (*isol, pmr, cmr, struct*)

Aspidospermatidine A-706

14,19-Didehydrocondyfolan, 9CI [3890-05-9]



Absolute Configuration

$C_{18}H_{22}N_2$ 266.385

Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Cryst. (Et_2O/hexane). Mp 168-170° Mp 184-186°. λ_{max} 242 (log ϵ 3.83); 296 (log ϵ 3.48) (EtOH).

N-*Ac:* **N-*Acetylaspidospermatidine***

$C_{20}H_{24}N_2O$ 308.422

Noncryst. $[\alpha]_D$ -28 (EtOH). λ_{max} 210; 253; 289 ($CHCl_3$).

N-*Me:* **N-*Methylaspidospermatidine***

$C_{19}H_{24}N_2$ 280.412

Alkaloid in *Aspidosperma quebracho-blanco* (quebracho). Amorph.

1,2-Didehydro, 19,20β-dihydro: [3408-40-0] *Condyfoline*

$C_{18}H_{22}N_2$ 266.385

Cryst. (Et_2O). Mp 76-80°. $[\alpha]_D^{21}$ +348 (c, 0.67 in EtOAc). Semisynthetic. λ_{max} 250 (Et_2O).

11-Hydroxy, N-*Ac:* **N-*Acetyl-11-hydroxyaspidospermatidine***

$C_{20}H_{24}N_2O_2$ 324.422

Noncryst. λ_{max} 218 (log ϵ 4.23); 252 (log ϵ 3.89); 294 (log ϵ 3.65); 300 (log ϵ 3.65) (EtOH).

12-Hydroxy, N-*Ac:* [11035-45-3] ***Limatinine***

[19046-21-0]

$C_{20}H_{24}N_2O_2$ 324.422

Prisms (Et_2O/pentane). Mp 162-163° (158-160°). $[\alpha]_D^{22}$ +170 (c, 0.24 in EtOH). $[\alpha]_D^{25}$ +162 (c, 0.83 in $CHCl_3$). 19-Config. uncertain. λ_{max} 220 (log ϵ 4.36); 259 (log ϵ 3.85); 290 (log ϵ 3.49) (EtOH).

12-Hydroxy, N-*Ac, picrate:*

Cryst. (Me_2CO/MeOH or Me_2CO aq.). Mp 250° dec.

12-Hydroxy, N-*propanoyl:* ***Limatine***

$C_{21}H_{26}N_2O_2$ 338.449

Cryst. (Me_2CO/hexane). Mp 175-176°. $[\alpha]_D^{20}$ +166 (c, 0.85 in $CHCl_3$). 19-Config. uncertain. λ_{max} 220 (log ϵ 4.66); 259 (log ϵ 4.51); 290 (log ϵ 3.83) (EtOH).

12-Hydroxy, N-*propanoyl, picrate:*

Cryst. (Me_2CO/EtOAc or Me_2CO aq.). Mp 265° dec.

11-Methoxy, 12-hydroxy: [11044-89-6] ***11-Methoxylimatine***

$C_{22}H_{28}N_2O_3$ 368.475

Prisms (MeOH/Et_2O/pentane). Mp 75-78°. $[\alpha]_D^{23}$ +168 (c, 0.21 in $CHCl_3$). 19-Config. uncertain. λ_{max} 227 (log ϵ 4.39); 262 (log ϵ 3.91) (EtOH).

11-Methoxy, 12-hydroxy, N-*Ac:* [11035-48-6] ***11-Methoxylimatinine***

$C_{21}H_{26}N_2O_3$ 354.448

Prisms (Et_2O/pentane or Me_2CO/hexane). Mp 139-140°. $[\alpha]_D^{23}$ +181 (c, 0.17 in $CHCl_3$). 19-Config. uncertain. λ_{max} 229 (log ϵ 4.38); 261 (log ϵ 3.77) (EtOH).

11-Methoxy, 12-hydroxy, N-*Ac, picrate:*

Cryst. (Me_2CO/EtOH). Mp 238-244° dec.

11-Methoxy, 12-hydroxy, N-*propanoyl, picrate:*

Cryst. (Me_2CO/EtOH). Dec. >250° without melting.

12-Methoxy, N-*Ac:* [5794-14-9] ***Aspidospermatine***

$C_{21}H_{26}N_2O_2$ 338.449

Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 162° (157-159°). $[\alpha]_D$ -73 (EtOH). 19-Config. uncertain. λ_{max} 219 (log ϵ 4.54); 255 (log ϵ 4.1); 290 (log ϵ 3.62) (EtOH).

12-Methoxy, 19,20-dihydro, N-*Ac:* ***Dihydroaspidospermatine***

$C_{21}H_{28}N_2O_2$ 340.464

Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Noncryst.

Schumann, D. *et al., Helv. Chim. Acta*, 1963, **46**, 1996-2003 (*Condyfoline*)

Biemann, K. *et al., JACS*, 1963, **85**, 631-638 (*Aspidospermatidine, N-Methylaspidospermatidine, Aspidospermatine, Dihydroaspidospermatine*)

Walser, A. *et al., Helv. Chim. Acta*, 1965, **48**, 391-404 (N-*Acetylaspidospermatidine*)

Pinar, M. *et al., Helv. Chim. Acta*, 1965, **48**, 822-825; 1967, **50**, 89-93 (*Aspidosperma limae alkaloids*)

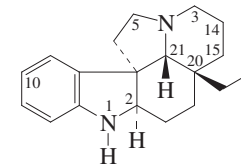
Gilbert, B. *et al., Tetrahedron*, 1965, **21**, 1141-1166 (N-*Acetyl-11-hydroxyaspidospermatidine*)

Klyne, W. *et al., Helv. Chim. Acta*, 1966, **49**, 833-841 (*Limatine, abs config*)

Arndt, R.R. *et al., Phytochemistry*, 1967, **6**, 1653-1658 (*Limatinine, abs config*)

Zeches, M. *et al., Planta Med.*, 1995, **61**, 89-91 (*Aspidospermatine*)

Aspidospermidine A-707



( )-*form*

$C_{19}H_{26}N_2$ 282.428

(+)-*form* [2912-09-6]

Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). Mp 119.5-121°. $[\alpha]_D^{23}$ +21 (EtOH).

Biemann, K. *et al., JACS*, 1963, **85**, 631-638 (*ms*)

Smith, G.F. *et al., JCS*, 1963, 4002-4004 (*Rhazya stricta constits, uv*)

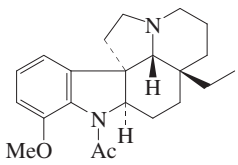
Klyne, W. *et al., Helv. Chim. Acta*, 1968, **51**, 1169-1184 (*ord*)

Laronze, J.-Y. *et al., Tet. Lett.*, 1974, **15**, 491-494 (*(±)-form, synth*)

Seki, K. *et al., Tet. Lett.*, 1975, **16**, 723-726 (*1-Acetylaspidospermidine, synth*)
Paccioni, J.P. *et al., Phytochemistry*, 1978, **17**, 2146-2147 (*Geissospermum argenteum constit*)
Gallagher, T. *et al., JACS*, 1983, **105**, 4750-4757 (*(±)-form, synth*)
Mandal, S.B. *et al., JOC*, 1988, **53**, 4236-4241 (*(±)-form, synth*)
Node, M. *et al., JOC*, 1990, **55**, 517-521 (*(-)-form, synth*)
Le Ménez, P. *et al., JOC*, 1991, **56**, 2915-2918 (*(±)-form, synth*)
Desmaële, D. *et al., JOC*, 1994, **59**, 2292-2303 (*(+)-form, synth*)
Wenkert, E. *et al., JOC*, 1994, **59**, 7677-7682 (*(±)-form, synth*)
Forns, P. *et al., JOC*, 1996, **61**, 7882-7888 (*(-)-form, synth*)
Schultz, A.G. *et al., JOC*, 1997, **62**, 6855-6861 (*(-)-form, synth*)
Callaghan, O. *et al., JCS Perkin 1*, 1999, 995-1001 (*(±)-form, synth*)
Callaghan, O. *et al., Tet. Lett.*, 1999, **40**, 161-164; 2225 (*synth, bibl*)
Toczko, M.A. *et al., JOC*, 2000, **65**, 2642-2645 (*(±)-form, synth*)
Kozmin, S.A. *et al., JACS*, 2002, **124**, 4628-4641 (*(+)-form, synth*)

Aspidospermine A-708

1-Acetyl-17-methoxyaspidospermidine, 9CI [466-49-9]



(-)-*form*

$C_{22}H_{30}N_2O_2$ 354.491
Alkaloid from *Aspidosperma quebracho-blanco* (quebracho). λ_{max} 218 (ϵ 37500); 255 (ϵ 11000); 285 (ϵ 3400) (MeOH) (Berdy).

▶ LD_{50} (mus, ipr) 40 mg/kg.

N-*De-Ac:* [2447-50-9] ***Deacetylaspidospermine***. *Deformylvallesine. 17-Methoxyaspidospermidine*
$C_{20}H_{28}N_2O$ 312.454
Cryst. (pentane). Mp 107-109°. $[\alpha]_D^{20}$ +8 (MeOH).

N-*De-Ac, hydroiodide (1:2):*
Prisms. Mp 243° (after sintering from 235°).

N-*De-Ac,* N-*formyl:* [466-46-6] ***Vallesine***
$C_{21}H_{28}N_2O_2$ 340.464
Needles (Me_2CO/Et_2O). Mp 154-155°. $[\alpha]_D$ -92 (c, 0.12 in $CHCl_3$).

N-*De-Ac,* N-*propanoyl:* [466-48-8] ***Palosine***
$C_{23}H_{32}N_2O_2$ 368.518
Needles (Et_2O/petrol). Mp 149-152°. $[\alpha]_D^{24}$ -85.9 (c, 0.734 in $CHCl_3$).

O-*De-Me:* [2122-21-6] ***Demethylaspidospermine***
$C_{21}H_{28}N_2O_2$ 340.464
Needles. Mp 112-114°. $[\alpha]_D^{20}$ +114 ($CHCl_3$).

O-*De-Me, perchlorate:*
Cryst. + 1 MeOH (MeOH). Mp 170° dec. $[\alpha]_D^{25}$ +94 (c, 0.98 in MeOH).

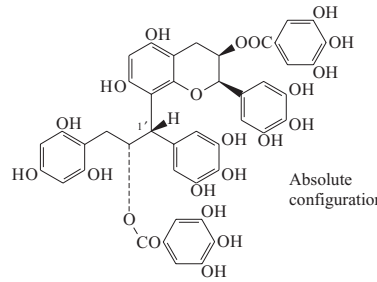
O-*De-Me,* N-*de-Ac:* [466-47-7] ***Aspidosine***
$C_{19}H_{26}N_2O$ 298.427
Mp 255.5-257.5° (250-253°). $[\alpha]_D^{20}$ -12 (EtOH). λ_{max} 246 (log ϵ 3.91); 289 (log ϵ 3.42) (MeOH).

O-*De-Me,* N-*de-Ac,* N-*propanoyl:* [16049-40-4] **O-*Demethylpalosine***
$C_{22}H_{30}N_2O_2$ 354.491
Mp 169°. $[\alpha]_D^{20}$ +118 (c, 0.36 in $CHCl_3$).

Ewins, A.J. *et al., JCS*, 1914, **105**, 2738 (*synth*)
Schlittler, E. *et al., Helv. Chim. Acta*, 1948, **31**, 446 (*synth, uv*)
Witkop, B. *et al., JACS*, 1954, **76**, 5603 (*synth, uv*)
Chalmers, J.R. *et al., JCS*, 1957, 1115 (*uv*)
Conroy, H. *et al., JACS*, 1958, **80**, 5178 (*ir, pmr*)
Schmutz, J. *et al., Helv. Chim. Acta*, 1959, **42**, 874 (*Palosine*)
Taylor, W.I. *et al., Helv. Chim. Acta*, 1959, **42**, 2750 (*Palosine*)
Holker, J.S.E. *et al., JOC*, 1959, **24**, 314 (*Vallesine*)
Gilbert, B. *et al., Chem. Ind. (London)*, 1962, 1949 (*Demethoxypalosine*)
Ferreira, J.M. *et al., Experientia*, 1963, **19**, 585 (*uv, ir, pmr, ms, struct, deriv*)
Biemann, K. *et al., JACS*, 1963, **85**, 631 (*ms*)
Walser, A. *et al., Helv. Chim. Acta*, 1965, **48**, 391 (*deriv*)
Klyne, W. *et al., Helv. Chim. Acta*, 1965, **48**, 443; 1966, **49**, 833 (*ord, uv, abs config*)
Ban, Y. *et al., Tet. Lett.*, 1965, 2261 (*synth*)
Gilbert, B. *et al., Tetrahedron*, 1965, **21**, 1141 (*isol*)
Achenbach, H. *et al., Tet. Lett.*, 1966, 5027 (*Demethylpalosine*)
Craven, B.M. *et al., Experientia*, 1968, **24**, 770 (*cryst struct, abs config*)
Sakabe, N. *et al., Tet. Lett.*, 1969, 2527 (*cryst struct*)
Stevens, R.V. *et al., Chem. Comm.*, 1971, 857 (*synth*)
Paccioni, J.P. *et al., Phytochemistry*, 1978, **17**, 2146 (*isol*)
Laguna, A. *et al., Coll. Czech. Chem. Comm.*, 1980, **45**, 1419-1423 (*Vallesine, Aspidosine, Demethylaspidospermine*)
Meyers, A.I. *et al., JOC*, 1989, **54**, 4673 (*synth*)
Campbell, W.E. *et al., Spectrosc. Lett.*, 1993, **26**, 707 (*pmr, cmr*)
Mitaine, A.C. *et al., Planta Med.*, 1996, **62**, 458 (*Palosine, isol, pmr, cmr*)
Fukuda, Y.-I. *et al., Org. Lett.*, 2003, **5**, 749-751 (*synth*)

Assamicain A A-709

[121795-66-2]



Absolute configuration

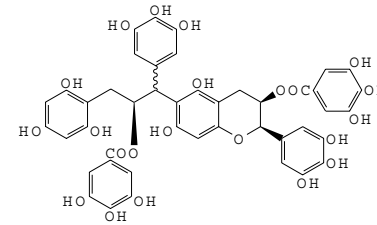
$C_{44}H_{36}O_{22}$ 916.755
Isol. from the leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $3H_2O$. $[\alpha]_D^{17}$ -120 (c, 1.0 in Me_2CO).

1′-Epimer: [121844-27-7] ***Assamicain B***
$C_{44}H_{36}O_{22}$ 916.755
Isol. from leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{17}$ -54.3 (c, 1.0 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 77 (*isol, pmr, cmr*)

Assamicain C A-710

[121795-67-3]



$C_{44}H_{36}O_{22}$ 916.755
Derived from the leaves of *Camellia sinensis* var. *assamica* (Assam tea). Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{17}$ +60.5 (c, 1.3 in Me_2CO).

Hashimoto, F. *et al., Chem. Pharm. Bull.*, 1989, **37**, 77 (*isol, pmr, cmr, synth*)

Astacidin 1 A-711

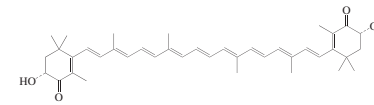
[511511-06-1]

$C_{90}H_{136}N_{28}O_{21}$ 1946.239
Isol. from freshwater crayfish *Pacifastacus leniusculus*.

Lee, S.Y. *et al., J. Biol. Chem.*, 2003, **278**, 7927-7933 (*isol*)

Astaxanthin A-712

3,3′-Dihydroxy-β,β-carotene-4,4′-dione. 3,3′-Dihydroxycanthaxanthin. 3,3′-Dihydroxy-4,4′-diketo-β-carotene. Ovoester [7542-45-2]



(3*R*,3*R*′)-*form*

$C_{40}H_{52}O_4$ 596.848
Present as mono- and diesters of fatty acids in the shrimp (*Pandalus borealis*).

(3*R*,3′*R*)-*form* [60760-95-4]
Mp 222-223°. CD:$\Delta\epsilon_{385}$ -6.2, $\Delta\epsilon_{324}$ +24.0. λ_{max} 492 ($CHCl_3$).

(3*S*,3′*S*)-*form* [472-61-7]
Food colourant. Mp 223-225°. λ_{max} 472 (MeOH) (Berdy). λ_{max} 466 (hexane) (Berdy). λ_{max} 485 ($CHCl_3$) (Berdy). λ_{max} 492 ($CHCl_3$).

Disodium disuccinate salt: [605666-03-3] ***Cardax***
[605666-04-4 (3*R*,3′*S*-form), 605666-02-2 (3*R*,3′*R*-form)]
Solid; characterised by pmr and cmr. Cardax synth. as a mixt. of stereoisomers. CAS indexes cardax under the (3*S*,3*S*′)-form.

3-O-*β*-D-*Glucopyranoside:*
$C_{46}H_{62}O_9$ 758.99
λ_{max} 487 (C_6H_6).

Di-O-*α*-L-*rhamnopyranoside:* [1184301-65-2]
$C_{52}H_{72}O_{12}$ 889.134
λ_{max} 471 (ϵ 130000) (Et_2O/2-methylbutane/EtOH).

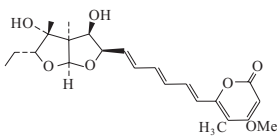
(*3′RS,3′SR*)-*form* [71772-51-5]
Used in fish farming to induce trout flesh colouring. Red food dye. Mp 216-219°. *meso*-Isomer.

[74601-68-6]

Andrewes, A.G. *et al., Phytochemistry*, 1976, **15**, 1009-1011 (*R,R-form, isol*)
Müller, R.K. *et al., Helv. Chim. Acta*, 1980, **63**, 1654-1664 (*isol, synth, hplc*)
Zell, R. *et al., Helv. Chim. Acta*, 1981, **64**, 2447-2462 (*synth*)
Renstrom, B. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 249 (*isol, isomers*)
Berger, H. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1982, **71**, 253 (*isol*)
Yokoyama, A. *et al., J. Nat. Prod.*, 1995, **58**, 1929-1933 (*glucoside*)
Breithaupt, D.E. *et al., J. Agric. Food Chem.*, 2004, **52**, 3870-3875 (*isol, shrimp*)
Gross, G.J. *et al., Life Sci.*, 2004, **75**, 215-224; 2006, **79**, 162-174 (*cardax, pharmacol*)
Frey, D.A. *et al., Org. Process Res. Dev.*, 2004, **8**, 796-801 (*cardax, synth*)
Pat. Coop. Treaty (WIPO), 2004, (*(Hawaii Biotech)*)04 011 423 (*cardax, synth, pharmacol*)
Lauver, D.A. *et al., J. Pharmacol. Exp. Ther.*, 2005, **314**, 686-692 (*cardax, pharmacol*)
Choi, S. *et al., JOC*, 2005, **70**, 3328-3331 (*synth*)
Hussein, G. *et al., J. Nat. Prod.*, 2006, **69**, 443-449 (*rev*)
Asker, D. *et al., J. Antibiot.*, 2009, **62**, 397-399 (*dirhamnoside*)

Asteltoxin A-713

[79663-49-3]



Absolute configuration

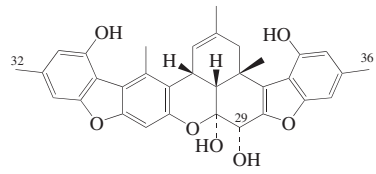
$C_{23}H_{30}O_7$ 418.486
Mycotoxin of *Aspergillus stellatus* and *Emericella varicolor*. Small pale-yellow needles. Mp 130-132°. $[\alpha]_D^{23}$ +20 (c, 1.15 in MeOH). λ_{max} 267 (ϵ 29300); 273 (ϵ 29400); 367 (ϵ 32800) (MeOH) (Derep).

▶ Hepatotoxin, neurotoxin. UQ0860000

Kruger, G.J. *et al., Chem. Comm.*, 1979, 441-442 (*isol, spectra, cryst struct*)
Schreiber, S.L. *et al., JACS*, 1983, **105**, 6723-6724; 1984, **106**, 4186-4188 (*synth*)
Steyn, P.S. *et al., Chem. Comm.*, 1984, 977-979 (*biosynth*)
De Jesus, A.E. *et al., Chem. Comm.*, 1985, 1633-1635 (*biosynth, cmr*)
Schreiber, S.L. *et al., Tet. Lett.*, 1986, **27**, 2575-2578 (*abs config*)
Tadano, K. *et al., Tetrahedron*, 1990, **46**, 2353-2366 (*synth*)
Raman, J.V. *et al., Tet. Lett.*, 1995, **36**, 3095-3098 (*synth*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 317-332 (*bibl, synth*)
Eom, K.D. *et al., JACS*, 2003, **125**, 5415-5421 (*synth*)

Asticolorin A A-714

[93376-70-6]



Absolute Configuration

$C_{33}H_{30}O_7$ 538.596
Mycotoxin prod. by *Aspergillus multicolor*. Cryst. (Me_2CO). Sol. MeOH, EtOAc. Mp 320°. $[\alpha]_D^{20}$ -120.5 (c, 0.2 in Me_2CO). λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 13300); 304 (ϵ 12700); 316 (ϵ 20500) (MeOH) (Derep).

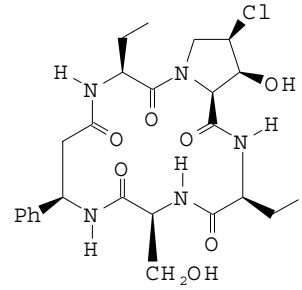
29-Ketone: [93376-71-7] ***Asticolorin B***
$C_{33}H_{28}O_7$ 536.58
Mycotoxin from *Aspergillus multicolor*. Cryst. Sol. MeOH, EtOAc. Mp 320°. λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 13300); 304 (ϵ 12700); 316 (ϵ 20500) (MeOH) (Derep).

32,36-Dihydroxy, 29-ketone: [93395-44-9] ***Asticolorin C***
$C_{33}H_{28}O_9$ 568.579
Mycotoxin of *Aspergillus multicolor*. Cryst. Sol. MeOH, EtOAc. Mp 320°. λ_{max} 225 (ϵ 81400); 263 (ϵ 28100); 290 (ϵ 23300); 304 (ϵ 12700); 316 (ϵ 20500) (EtOH) (Derep).

Rabie, C.J. *et al., Chem. Comm.*, 1984, 764-765 (*isol, struct*)
Steyn, P.S. *et al., Chem. Comm.*, 1984, 765-767 (*nmr, biosynth*)

Astin I A-715

[161162-22-7]

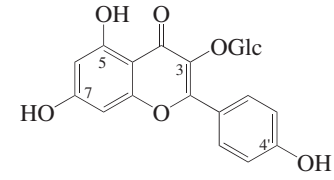


$C_{25}H_{34}ClN_5O_7$ 552.026
Cyclic peptide antibiotic. Constit. of *Actinidia kolomikta* (kiwi fruit). Mp 174.1-176.5°. $[\alpha]_D$ -78.8 (c, 0.1 in MeOH).

Morita, H. *et al., Chem. Lett.*, 1994, **23**, 2009-2010 (*isol, pmr, cmr*)
Wang, Y. *et al., CA*, 1995, **122**, 156308e (*isol*)

Astragalin A-716

3-O-*β*-D-*Glucopyranosyloxy-4′,5,7-trihydroxyflavone. Kaempferol 3-glucoside* [480-10-4]



$C_{21}H_{20}O_{11}$ 448.382
Present in red wine and tea. Isol. from many plant spp. Yellow needles. Mp 178°. $[\alpha]_D^{18}$ +16.9 (c, 0.62 in MeOH).
Log P -2.32 (calc).

▶ DJ3080000

Mono-Ac: [36310-43-7] ***Acetylastragalin***
$C_{23}H_{22}O_{12}$ 490.42
Isol. from liquorice (*Glycyrrhiza glabra*). Full struct. not determined. May be identical with the 6″-Ac above.

6″-O-*Malonoyl:* [81149-02-2] ***6″-Malonylastragalin***
$C_{24}H_{22}O_{14}$ 534.429
Constit. of *Cicer* sp. and pears.

6″-O-*(4-Carboxy-3-hydroxy-3-methylbutanoyl):* [157407-84-6] *Kaempferol 3-[6-O-(3-hydroxy-3-methylglutaroyl)-glucoside]*. ***6″-O-(3-Hydroxy-3-methylglutaroyl)astragalin***
$C_{27}H_{28}O_{15}$ 592.509
Constit. of aged callus cultures of lime (*Citrus aurantifolia*). Yellow powder (MeOH). Mp 210-213°. λ_{max} 305 (log ϵ 4.2); 350 (log ϵ 4.3) (MeOH).

2″-O-*(4-Hydroxy*-E-*cinnamoyl):* [137018-32-7] *Kaempferol 3-(2*-E-p-*coumaroylglucoside)*. ***2″-O-trans-p-Coumaroylastragalin***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from *Lithocarpus polystachya* tea.

6″-O-*(4-Hydroxy*-E-*cinnamoyl):* [20316-62-5] ***Tiliroside***. *6″*-O-trans-*p-Coumaroylastragalin*
$C_{30}H_{26}O_{13}$ 594.528
Isol. from strawberries (*Fragaria ananassa*). Pale yellow needles (MeOH aq.). Mp 269-271°. $[\alpha]_D^{26}$ -62 (c, 0.28 in MeOH). This struct. was formerly assigned to Tribuloside isol. from *Tribularia* spp.

▶ UD3375250

6″-O-*(4-Hydroxy*-Z-*cinnamoyl): 6″*-O-cis-p-*Coumaroylastragalin*. **cis-*Tiliroside***
$C_{30}H_{26}O_{13}$ 594.528
Isol. from strawberries (*Fragaria ananassa*). $[\alpha]_D^{26}$ -57 (c, 0.04 in MeOH). λ_{max} 208 (sh) (log ϵ 4.4); 227 (log ϵ 4.3); 267 (log ϵ 4.4); 315 (log ϵ 4.5) (MeOH).

7-O-*(4-Hydroxycinnamoyl):* [51795-36-9]
$C_{30}H_{26}O_{13}$ 594.528
Constit. of *Elaeagnus angustifolia* (Russian olive).

2″,4″-Bis-O-*(4-hydroxycinnamoyl):* [85122-24-3]
$C_{39}H_{32}O_{15}$ 740.673

Isol. from *Quercus ilex* (holly oak). Needles (MeOH aq.). Dec. above 280°.

2″,4″-Bis-O-*(4-Hydroxycinnamoyl), 3″,6″-di*-O-*Ac:* [94474-72-3]
$C_{43}H_{36}O_{17}$ 824.747
Constit. of leaves of *Quercus ilex* (holly oak). Needles (MeOH aq.). Mp 280° dec.

2″,6″-Bis-O-*(4-hydroxy*-E-*cinnamoyl):*
[121651-61-4]
[94474-74-5]
$C_{39}H_{32}O_{15}$ 740.673
Isol. from *Quercus ilex* (holly oak). Mp 180-182°. $[\alpha]_D^{25}$ -162 (c, 0.39 in MeOH). λ_{max} 268; 315; 355 (sh) (MeOH).

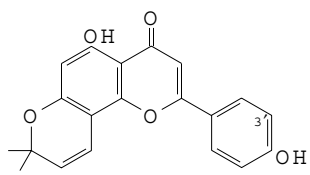
6″-O-*(3,4-Dihydroxy*-E-*cinnamoyl):*
[190328-43-9] *6″*-O-*Caffeoylastragalin*
$C_{30}H_{26}O_{14}$ 610.527
Constit. of young bracken fronds (*Pteridium aquilinium*).

[94535-60-1]

Markham, K.R. *et al., Tetrahedron*, 1978, **34**, 1389-1397 (*cmr*)
Imperato, F. *et al., Chem. Ind. (London)*, 1981, 695-696; 1983, 204-205 (*6″-Malonylastragalin, 3″-sulfate, 6″-sulfate*)
Vermes, B. *et al., Helv. Chim. Acta*, 1981, **64**, 1964-1967 (*Tiliroside*)
Piegay, I. *et al., Pharmazie*, 1986, **41**, 524-525 (*Acetylastragalin*)
Merfort, I. *et al., Phytochemistry*, 1988, **27**, 3281-3284 (*6″-O-Acetylastragalin*)
Romussi, G. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1991, **324**, 519-524 (*Quercus dicoumarates*)
Yang, D. *et al., CA*, 1991, **115**, 228326q (*4-hydroxycinnamoyl esters*)
The Flavonoids: Advances in Research Since 1986, (ed. Harborne, J.B.), Chapman & Hall, 1993,
Berhow, M.A. *et al., Phytochemistry*, 1994, **36**, 1225-1227 (*Citrus hydroxymethylglutarate*)
Imperato, F. *et al., Phytochemistry*, 1997, **45**, 199-200 (*6″-Caffeoylastragalin*)
Afifi, M.S. *et al., Bull. Fac. Pharm. (Cairo Univ.)*, 1999, **37**, 119-124 (*isol, activity*)
Liu, H. *et al., J. Nat. Prod.*, 1999, **62**, 70-75 (*Stenopalustrosides*)
Tsukamoto, S. *et al., J. Nat. Prod.*, 2004, **67**, 1839-1841 (*Tiliroside,* cis-*Tiliroside*)
Wu, H. *et al., Food Chem.*, 2009, **115**, 592-595 (*isol, pmr, cmr*)

Atalantoflavone A-717

*5-Hydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-4*H,*8*H-*benzo[1,2*-b:*3,4*-b′*]dipyran-4-one, 9CI. Limonianin*
[119309-02-3]



$C_{20}H_{16}O_5$ 336.343
Isol. from rootbark of lemon trees. Yellow needles (Me_2CO/hexane). Mp 289-290° (275-277°). Physical data varies between Atalantoflavone and Limonianin. λ_{max} 233 (log ϵ 4.51); 277 (log ϵ 4.45); 312 (log ϵ 4.42); 328 (sh) (log ϵ 4.27) (MeOH).

Di-Ac:
Needles (Me_2CO/petrol). Mp 230-232° (221-223°).

4′-Me ether: [1205687-49-5] ***4′-O-Methylatalantoflavone***
$C_{21}H_{18}O_5$ 350.37
Yellow oil. λ_{max} 231; 276; 312; 326 (sh); 360 (sh) (MeOH aq.).

Di-Me ether:
Pale yellow cryst. (Me_2CO/hexane). Mp 207-209° (185-188°).

3′-Hydroxy: [697234-27-8] ***Artochamin C***
$C_{20}H_{16}O_6$ 352.343
Amorph. yellow powder. λ_{max} 236 (log ϵ 4.42); 272 (log ϵ 4.37); 344 (log ϵ 4.17) (MeOH).

1″,2″-Dihydro, 1″ξ,2″ξ-dihydroxy:
$C_{20}H_{18}O_7$ 370.358
λ_{max} 270; 317 (sh); 339 (MeOH).

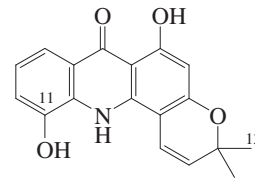
5-Deoxy, 4′-Me ether: [1020409-03-3] *2-(4-Methoxyphenyl)-8,8-dimethyl-4*H,*8*H-*benzo[1,2*-b:*3,4*-b′*]dipyran-4-one*
$C_{21}H_{18}O_4$ 334.371
Amorph. solid.

3′-Methoxy: [106055-12-3] ***Racemoflavone***
$C_{21}H_{18}O_6$ 366.37
Yellow cryst. (Me_2CO/hexane). Mp 236-237°. λ_{max} 236 (log ϵ 4.13); 274 (log ϵ 4.07); 338 (log ϵ 3.9) (MeOH).

Banerji, A. *et al., Phytochemistry*, 1988, **27**, 3637-3640 (*Atalantoflavone, Racemoflavone, isol, synth, uv, pmr, ms*)
Chang, S.-H. *et al., Phytochemistry*, 1990, **29**, 351-353 (*Limonianin*)
Banerji, A. *et al., Spectrosc. Lett.*, 1990, **23**, 555-565 (*pmr, struct*)
Subramanian, M. *et al., J. Nat. Prod.*, 1992, **55**, 1213-1229 (*Atalantoflavone, synth*)
Vijayalakshmi, C.S. *et al., Z. Naturforsch., B*, 1992, **47**, 1021 (*synth*)
Prasad, K.J.R. *et al., J. Nat. Prod.*, 1993, **56**, 208-214 (*synth*)
Kassem, M. *et al., Fitoterapia*, 2000, **71**, 649-654 (*1″,2″-dihydrodihydroxy*)
Wang, Y.-H. *et al., J. Nat. Prod.*, 2004, **67**, 757-761 (*Artochamin C*)
Magalhaes, A.F. *et al., An. Acad. Bras. Cienc.*, 2007, **79**, 351-367 (*5-deoxy 4′-Me ether*)
Bacher, M. *et al., Magn. Reson. Chem.*, 2010, **48**, 83-88 (*4′-Me ether*)

Atalaphyllidine† A-718

*3,12-Dihydro-6,11-dihydroxy-3,3-dimethyl-7*H-*pyrano[2,3*-c*]acridin-7-one, 9CI* [57959-88-3]



$C_{18}H_{15}NO_4$ 309.321
Mp 275° dec.

N-*Me:* [27067-70-5] **N-*Methylatalaphyllidine*.** *5-Hydroxynoracronycine*
$C_{19}H_{17}NO_4$ 323.348
Red needles (Et_2O/petrol). Mp 252-254°.

N-*Me, di-Ac:*
Prisms (Et_2O/petrol). Mp 178-181°.

11-Me ether: Mp 200°.

11-Me ether, N-*Me:* see 11-Methoxy, *O*-de-Me, in Acronycine, A-188

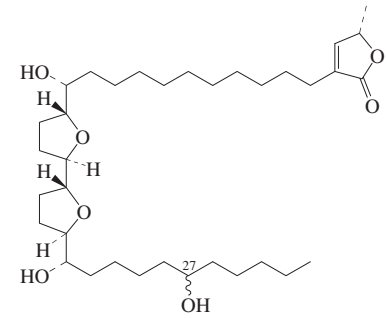
Di-Me ether, N-*Me: 5-Methoxyacronycine*
Yellow needles (Et_2O/petrol). Mp 97-98°.

13-Hydroxy, N-*Me:* [904327-13-5] ***5,13-Dihydroxynoracronycine***
$C_{19}H_{17}NO_5$ 339.347
Alkaloid from the stem bark of *Citrus maxima* (pummelo). Yellow. Mp 162-163°. λ_{max} 266 (log ϵ 4.34); 283 (log ϵ 4.21) (MeOH).

Sullivan, H.R. *et al., J. Med. Chem.*, 1970, **13**, 904 (*isol, deriv*)
Fraser, A.W. *et al., JCS Perkin 1*, 1973, 1173 (*isol, uv, ir, nmr, ms, struct, deriv*)
Basa, S.C. *et al., Experientia*, 1975, **31**, 1387 (*isol, uv, ir, pmr, ms, struct*)
Adams, J.H. *et al., J. Nat. Prod.*, 1976, **39**, 399 (*synth, deriv*)
Wu, T.-S. *et al., Heterocycles*, 1982, **19**, 273 (*isol, deriv*)
Teng, W.-Y. *et al., J. Chin. Chem. Soc. (Taipei)*, 2005, **52**, 1253-1255 (*5,13-Dihydroxynoracronycine*)

Atemoyacin B A-719

[164991-85-9]

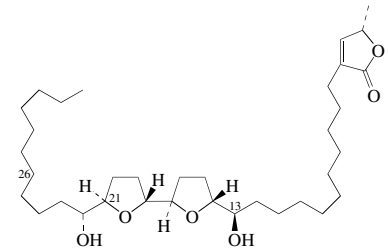


$C_{35}H_{62}O_7$ 594.871
Constit. of the seeds of *Annona atemoya* (custard apple). Cytotoxic. Wax. $[\alpha]_D$ +12.9 (c, 0.02 in MeOH). λ_{max} 210 (ϵ 7150) (MeOH).

Chen, W.-S. *et al., Huaxue Xuebao*, 1995, **53**, 516

Atemoyin A-720

Squamocin K [161169-70-6]
[159993-38-1]



$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona squamosa* (sugar apple) and the seeds of *Annona atemoya*

(custard apple). Wax. $[\alpha]_D^{25}$ +20.5 (c, 0.5 in MeOH).

13-Epimer: [159993-37-0] ***Squamocin I***
$C_{35}H_{62}O_6$ 578.871
Constit. of *Annona squamosa* (sugar apple). Needles (MeOH aq.). Mp 68.5-71°. $[\alpha]_D^{24}$ +22.2 (c, 0.5 in MeOH).

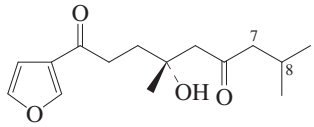
21-Epimer, 26ξ-hydroxy: ***Carolin C***
$C_{35}H_{62}O_7$ 594.871
Oil. $[\alpha]_D^{20}$ +8 (c, 0.5 in $CHCl_3$). λ_{max} 205 (log ϵ 4) (EtOH). λ_{max} 208 (ϵ 10000) (MeOH) (Berdy).

[161025-06-5]

Sahai, M. *et al., Chem. Pharm. Bull.*, 1994, **42**, 1163-1174 (*Squamocins*)
Duret, P. *et al., Nat. Prod. Lett.*, 1995, **5**, 295-302 (*isol, uv, pmr, cmr, ms*)
Queiroz, E.F. *et al., J. Nat. Prod.*, 1998, **61**, 34-39 (*Carolin C*)

Athanagrandione A-722

1-(3-Furanyl)-4-hydroxy-4,8-dimethyl-1,6-nonanedione, 9CI. 4-Hydroxymyoporone



$C_{15}H_{22}O_4$ 266.336

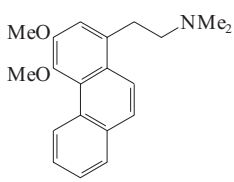
(*R*)-*form* [69926-93-8]
Prod.by sweet potato tubers (*Ipomoea batatas*) infected by *Fusarium solani*. Oil.

7,8-Didehydro: [72896-64-1] *4-Hydroxydehydromyoporone, 9CI. Furopinnatin* [135029-99-1, 63955-86-2]
Prod.by sweet potatoes infected by *Fusarium solani*. Oil. The abs. config. of Furopinnatin was not determined, and no opt. rotn. was reported for it.

Burka, L.T. *et al., Tet. Lett.*, 1974, 4017 (*struct*)
Inoue, H. *et al., Phytochemistry*, 1977, **16**, 1063-1065 (*4-Hydroxydihydromyoporone*)
Burka, L.T. *et al., Phytochemistry*, 1977, **16**, 2022 (*biosynth*)
Bohlmann, F. *et al., Phytochemistry*, 1978, **17**, 1595 (*isol, struct*)
Oba, K. *et al., Plant Cell Physiol.*, 1979, **20**, 819 (*biosynth*)
Dimitriadis, E. *et al., Phytochemistry*, 1984, **23**, 1325 (*abs config*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 1161 (*Furopinnatin*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 736

Atherosperminine A-723

*3,4-Dimethoxy-*N,N*-dimethyl-1-phenanthreneethanamine, 9CI. 1-Dimethylaminoethyl-3,4-dimethoxyphenanthrene*
[5531-98-6]
[98900-05-1]



$C_{20}H_{23}NO_2$ 309.407
Alkaloid from the stem bark of *Annona muricata* (soursop). Needles (Me_2CO/petrol). Mp 199-200°.

Hydrochloride: [54749-97-2]
Mp 234-235° dec.

Picrate: [5531-99-7]
Yellow needles (Me_2CO/MeOH). Mp 189-190°.

N-*Oxide:* [91174-15-1] ***Atherosperminine* N-*oxide***
$C_{20}H_{23}NO_3$ 325.407
Noncryst.

N-*Me:* [98900-03-9] **N-*Methylatherosperminium***
[98900-04-0, 5532-00-3]
$C_{21}H_{26}NO_2^{\oplus}$ 324.442
Needles (EtOH)(as iodide). Mp 282-284° (iodide).

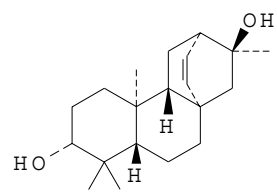
N-*De-Me:* [74606-53-4] ***Noratherosperminine***
$C_{19}H_{21}NO_2$ 295.38
Mp 180°.

2-O-*De-Me:* [16625-57-3] *1-[2-(Dimethylamino)ethyl]-4-methoxy-3-phenanthrenol. 1-(2-Dimethylaminoethyl)-3-hydroxy-4-methoxyphenanthrene.* ***Argentinine***
$C_{19}H_{21}NO_2$ 295.38
Oil.

2-O-*De-Me,* N-*oxide:* [138690-45-6] ***Argentinine* N-*oxide***
$C_{19}H_{21}NO_3$ 311.38
Oil. Possible artifact.

Cooke, R.G. *et al., Aust. J. Chem.*, 1954, **7**, 99 (*isol, uv*)
Bick, I.R.C. *et al., Aust. J. Chem.*, 1956, **9**, 111; 1965, **18**, 1997 (*isol, pmr, uv*)
Priestap, H.A. *et al., Chem. Comm.*, 1967, 754 (*Argentinine, Atherosperminine*)
Aguilar-Santos, G. *et al., Philipp. J. Sci.*, 1967, **96**, 399 (*isol*)
Priestap, H.A. *et al., An. Asoc. Quim. Argent. (1921-2001)*, 1972, **60**, 309 (*Argentinine, Atherosperminine*)
Roblot, F. *et al., Plant. Med. Phytother.*, 1978, **12**, 259
Guinaudeau, H. *et al., J. Nat. Prod.*, 1979, **42**, 325 (*Noratherosperminine*)
Leboeuf, M. *et al., Planta Med.*, 1980, **38**, 33; 1981, **42**, 37
Castedo, L. *et al., Heterocycles*, 1982, **19**, 209 (*Noratherosperminine, synth*)
Hocquemiller, R. *et al., J. Nat. Prod.*, 1984, **47**, 353 (*Atherosperminine N-oxide*)
Lu, S.T. *et al., Phytochemistry*, 1985, **24**, 1829 (*N-Methylatherosperminium*)
Achenbach, H. *et al., J. Nat. Prod.*, 1991, **54**, 1331 (*Argentinine N-oxide*)
Chen, K.-S. *et al., J. Nat. Prod.*, 1996, **59**, 531-534 (*activity*)
Lopez-Martin, J. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1613-1615 (*Argentinine, isol, pmr, cmr*)

13-Atisene-3,16-diol A-724



$C_{20}H_{32}O_2$ 304.472

(*ent*-3β,16α)-*form*
Cryst. (diisopropyl ether/EtOAc). Mp 192-193°.

3-Ketone: [119642-81-8] *16-Hydroxy-13-atisen-3-one.* ***Yucalexin A16***
$C_{20}H_{30}O_2$ 302.456
Gum. Stress metab. of cassava root (*Manihot esculenta*).

13,14-Dihydro: [87013-77-2] ***13,16-Atisanediol***
$C_{20}H_{34}O_2$ 306.487
Cryst. (C_6H_6). Mp 205-206°. $[\alpha]_D$ -28 (c, 0.22 in $CHCl_3$).

13,14-Dihydro, 3-ketone: [87039-25-6] ***16-Hydroxy-3-atisanone***
$C_{20}H_{32}O_2$ 304.472
Cryst. Mp 157-158°. $[\alpha]_D^{25}$ -33 (c, 0.1 in $CHCl_3$).

Schmitz, F.J. *et al., JOC*, 1983, **48**, 3941
Delgado, G. *et al., Phytochemistry*, 1984, **23**, 2285
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexin A16*)
De Heluani, C.S. *et al., Magn. Reson. Chem.*, 1998, **36**, 947-950 (*Yucalexin A16, pmr, cmr*)
Kang, J. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 729-734 (*Excoecaria agallocha constit*)

ATP adenylyltransferase A-725

E.C. 2.7.7.53. ADP:ATP adenylyltransferase. Bis(5′-nucleosyl) tetraphosphate phosphorylase (NDP-forming). Diadenosine tetraphosphate α,β-phosphorylase. AP-4-A phosphorylase. Adenine triphosphate adenylyltransferase [96697-71-1]

Nucleotidyltransferase enzyme. Isol. from baker's yeast. Guanosine 5′-triphosphate and Adenosine 5′-tetraphosphate can also act as adenylyl acceptors. Baker's yeast enzyme activity range pH 6.5-9.0.

Guranowski, A. *et al., J. Biol. Chem.*, 1985, **260**, 3542-3547; 1986, **261**, 5943-5946 (*baker's yeast*)
Brevet, A. *et al., Biochemistry*, 1987, **26**, 4763-4768 (*baker's yeast*)
Guranowski, A. *et al., Int. J. Biochem.*, 1988, **20**, 449-455 (*Euglena gracilis*)
McLennan, A.G. *et al., Biochem. J.*, 1994, **300**, 183-189 (*Scenedesmus, Chlorella vulgaris*)

ATP citrate synthase A-726

E.C. 2.3.3.8. Acetyl-CoA:oxaloacetate C-*acetyltransferase [(*pro-S*)-carboxymethyl-forming, ADP-phosphorylating]. ATP citrate lyase. Citrate cleaving enzyme. E.C. 4.1.3.8 (transferred)* [9027-95-6]

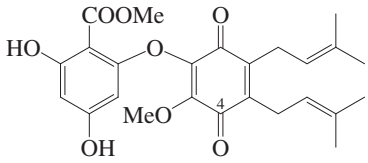
Acyltransferase enzyme. Isol. from mammalian tissues, e.g. chicken liver. An important enzyme in lipid biosynth. Can be dissociated into several components, two of which are identical with E.C. 4.1.3.14 (citryl-CoA lyase) and E.C. 6.2.1.18 (citrate-CoA ligase).

Srere, P.A. *et al., Methods Enzymol.*, 1962, **5**, 641-644 (*chicken liver*)

Plowman, K.A. *et al., J. Biol. Chem.*, 1967, **242**, 4239-4247 (*rat liver*)
Takeda, Y. *et al., Methods Enzymol.*, 1969, **13**, 153-160 (*rat liver*)
Srere, P.A. *et al., Curr. Top. Cell. Regul.*, 1972, **5**, 229-283 (*rev*)
Mahlen, A. *et al., Eur. J. Biochem.*, 1973, **36**, 342-346 (*Penicillium spiculisporum*)
Srere, P.A. *et al., Adv. Enzymol. Relat. Areas Mol. Biol.*, 1975, **43**, 57-101 (*rev*)
Linn, T.C. *et al., J. Biol. Chem.*, 1979, **254**, 1691-1698 (*rat liver*)
Szutowicz, A. *et al., Arch. Biochem. Biophys.*, 1983, **221**, 168-174 (*rat brain*)
Houston, B. *et al., Biochem. J.*, 1984, **224**, 437-443 (*rat liver*)
Shashi, K. *et al., Biochim. Biophys. Acta*, 1990, **1033**, 23-30 (*Rhodotorula gracilis*)
Adams, I.P. *et al., Biochim. Biophys. Acta*, 2002, **1597**, 36-41 (*Aspergillus nidulans*)

Atrovirinone A-727

[356053-82-2]

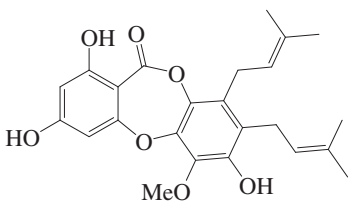


$C_{25}H_{28}O_8$ 456.491
Constit. of the roots of *Garcinia atroviridis* (gelugor). Red needles ($CHCl_3$/hexane). Mp 124-125°. λ_{max} 204 (log ϵ 5.14); 221 (log ϵ 5.1); 273 (log ϵ 5.04) (EtOH).

Hydroquinone, 4-Me ether: ***4-O-Methylhydroatrovirinone***
$C_{26}H_{32}O_8$ 472.534
Constit. of the roots of *Garcinia atroviridis* (gelugor). Amorph. yellow solid ($CHCl_3$/hexane). Mp 120-121°. λ_{max} 205 (log ϵ 3.59); 270 (log ϵ 3.13) (MeOH).

Permana, D. *et al., J. Nat. Prod.*, 2001, **64**, 976-979 (*isol, pmr, cmr*)
Permana, D. *et al., Z. Naturforsch., B*, 2003, **58**, 322-335 (*4-Methylhydroatrovirinone*)

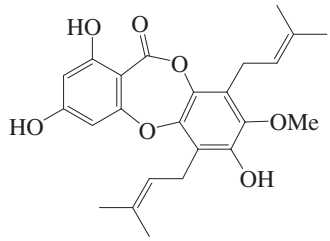
Atrovirisidone A-728



$C_{24}H_{26}O_7$ 426.465
Constit. of the roots of *Garcinia atroviridis* (gelugor). Cryst. ($CHCl_3$/hexane). Mp 75-76°. λ_{max} 207 (log ϵ 4.93); 269 (log ϵ 4.36) (EtOH).

Permana, D. *et al., J. Nat. Prod.*, 2001, **64**, 976-979

Atrovirisidone B A-729

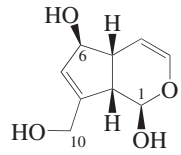


$C_{24}H_{26}O_7$ 426.465
Constit. of the roots of *Garcinia atroviridis* (gelugor). Cryst. (CH_2Cl_2/hexane). Mp 156-158°. λ_{max} 210 (log ϵ 4.87); 311 (log ϵ 4.49) (MeOH).

Permana, D. *et al., Z. Naturforsch., C*, 2005, **60**, 523-526 (*isol, pmr, cmr, ms*)

Aucubigenin A-730

Rhinanthogenin [64274-28-8]



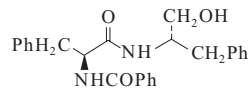
$C_9H_{12}O_4$ 184.191
Oil. Unstable. λ_{max} 204 (ϵ 1300) (MeOH) (Berdy).

10-O-(4-Hydroxybenzoyl), 1-O-β-D-glucopyranoside: [11027-63-7] ***Agnuside.*** *Agnoside. Buddlejoside A*
$C_{22}H_{26}O_{11}$ 466.441
Isol. from *Vitex agnus-castus* (agnus castus). Cryst. (H_2O). Mp 146°. $[\alpha]_D^{20}$ -91.5 (EtOH).

Hänsel, R. *et al., Phytochemistry*, 1965, **4**, 19-27 (*Agnuside*)

Aurantiamide A-731

N-*Benzoylphenylalanylphenylalaninol. Antibiotic TMC 58B. TMC 58B* [58115-31-4]



Absolute configuration

$C_{25}H_{26}N_2O_3$ 402.492
Cryst. (C_6H_6). Mp 194° (184°). $[\alpha]_D^{30}$ -51 ($CHCl_3$).

O-*Ac:* [56121-42-7] ***Asperglaucide.*** *Anomalamide. Lyciumamide. Aurantiamide acetate. Antibiotic TMC 58A. TMC 58A. Saropeptate*
$C_{27}H_{28}N_2O_4$ 444.529
Alkaloid from *Acanthophora spicifera* (lumikaro). Mp 185-186°. $[\alpha]_D^{30}$ -45 ($CHCl_3$).

O-*Benzoyl:* [150881-02-0] ***Aurantiamide benzoate.*** O-*Benzoylaurantiamide* [150881-03-1]
$C_{32}H_{30}N_2O_4$ 506.6
Needles (C_6H_6/cyclohexane). Mp 211°. $[\alpha]_D^{30}$ -26.3 ($CHCl_3$).

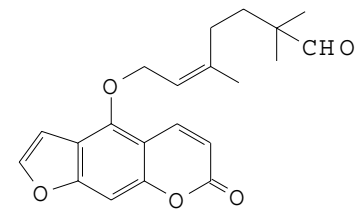
L-D-Diastereomer, Ac: ***Diaaurantiamide acetate***
$C_{27}H_{28}N_2O_4$ 444.529
Mp 167°. Genus name misspelt as Acantophora in the paper.

[112924-28-4, 125276-43-9, 150881-04-2]

Maiti, B.C. *et al., Experientia*, 1976, **32**, 1166 (*deriv*)
Cox, R.E. *et al., JCS Perkin 1*, 1976, 578-580 (*deriv*)
McCorkindale, N.J. *et al., Tetrahedron*, 1978, **34**, 2791-2795 (*synth, ms, pmr, ir*)
Banerji, A. *et al., Phytochemistry*, 1981, **20**, 2217-2220 (*isol, synth, pmr, cmr, ms*)
Wahidulla, S. *et al., Phytochemistry*, 1991, **30**, 3323-3325 (*Aurantiamide acetate, Diaaurantiamide acetate, isol, Acanthophora*)
Banerji, A. *et al., Indian J. Chem., Sect. B*, 1993, **32**, 776-778 (*Benzoylaurantiamide*)
Ferreira, D.T. *et al., J. Braz. Chem. Soc.*, 1995, **6**, 323-326 (*Benzoylaurantiamide*)
Ragasa, C.Y. *et al., Philipp. J. Sci.*, 1998, **127**, 267-276 (*activity*)
Lu, H. *et al., Planta Med.*, 1999, **65**, 586 (*isol, activity, Asperglaucide*)
Hayashi, Y. *et al., JOC*, 2000, **65**, 8402-8405 (*synth*)
Isshiki, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 1195-1197 (*isol*)

Aurantiumal A-732

5-[(3,6-Dimethyl-6-formyl-2-hepteny-l)oxy]psoralen

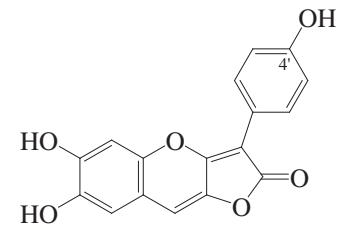


$C_{21}H_{22}O_5$ 354.402
Isol. from oil of grapefruit peel (*Citrus paradisi*). Cryst. (EtOAc/EtOH). Mp 134-136°. Prob. artifact.

Fisher, J.F. *et al., Tetrahedron*, 1966, **22**, 1489 (*isol*)
Fisher, J.F. *et al., J. Agric. Food Chem.*, 1979, **27**, 1334

Aurantricholide B A-733

6,7-Dihydroxy-3-(4-hydroxyphenyl)-2H-furo[3,2-b][1]benzopyran-2-one, 9CI [264923-56-0]



$C_{17}H_{10}O_6$ 310.262

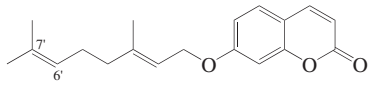
Pigment isol. from the mushroom *Suillus grevillei* (larch bolete). Unstable orange solid. Mp 320° dec. λ_{max} 204 (log ϵ 4.54); 267 (log ϵ 4.19); 416 (log ϵ 4.32) (MeOH).

4′-Deoxy: [264923-55-9] ***Aurantricholide A***
$C_{17}H_{10}O_5$ 294.263
Unstable orange solid. Mp 272° dec. λ_{max} 270; 412; 482 (MeOH).

Klostermeyer, D. *et al., Eur. J. Org. Chem.*, 2000, 603-609 (*isol, synth, pmr, cmr*)

Auraptene† A-734

*7-(3,7-Dimethyl-2,6-octadienyloxy)-2*H*-1-benzopyran-2-one, 9CI*. O-*Geranylumbelliferone. Feronialactone. 7-Geranyloxycoumarin* [495-02-3]



$C_{19}H_{22}O_3$ 298.381

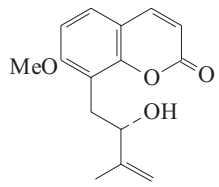
Not to be confused with Meranzin, M-257. Isol. from *Citrus aurantium* (Seville orange), bael fruit (*Aegle marmelos*) and grapefruit oil. Prisms (EtOH). Mp 68°. λ_{max} 252; 329 (MeOH) (Berdy).

*Δ7′-Isomer, 6′*R*-hydroxy:* [118584-19-3] *7-[(6-Hydroxy-3,7-dimethyl-2,7-octadienyl)oxy]-2*H*-1-benzopyran-2-one*
$C_{19}H_{22}O_4$ 314.38
Isol. from *Citrus hassaku* juice oil. Cryst. Mp 75°. $[\alpha]_D^{26}$ +10 (c, 1.0 in EtOH).

Kariyone, T. *et al., Chem. Pharm. Bull.*, 1953, **1**, 119-122 (*struct, synth, bibl*)
Coates, R.M. *et al., Tetrahedron*, 1970, **26**, 5699-5706 (*synth*)
Yamada, S. *et al., Tet. Lett.*, 1976, **29**, 2557-2560 (*6′R,7′-epoxide, synth, abs config*)
Masuda, T. *et al., Phytochemistry*, 1992, **31**, 1363-1366 (*6′-hydroxy*)

Auraptenol† A-735

*8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxy-2*H*-1-benzopyran-2-one, 9CI. 8-(2-Hydroxy-3-methyl-3-butenyl)-7-methoxycoumarin*



(*S*)–*form*

$C_{15}H_{16}O_4$ 260.289

(*S*)-*form* [1221-43-8]
Constit. of Seville bitter orange (*Citrus aurantium* ssp. *amara*) oil. Needles (EtOH). Mp 109-110°. $[\alpha]_D^{26}$ +14 (c, 1 in EtOH).

2′-Deoxy, 2′-hydroperoxy: [109741-39-1] ***Peroxyauraptenol***
$C_{15}H_{16}O_5$ 276.288
Prisms. Mp 114-116°. $[\alpha]_D$ +3.53 ($CHCl_3$).

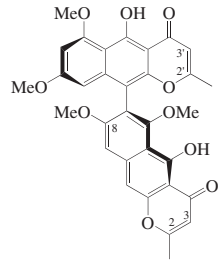
2′-Ketone: [19668-69-0] *7-Methoxy-8-(3-methyl-2-oxo-3-butenyl)-2*H*-1-benzopyran-2-one, 9CI*. ***Murrayone***. *Prangone*
$C_{15}H_{14}O_4$ 258.273
Mp 130°.

(±)-*form* [61235-25-4]
Cryst. (C_6H_6/hexane). Mp 109-110°.

Stanley, W.L. *et al., Tetrahedron*, 1965, **21**, 89 (*isol, struct*)
Lakshmi, M.V. *et al., Indian J. Chem.*, 1972, **10**, 564 (*Murrayone*)
Abyshev, A.Z. *et al., Khim. Prir. Soedin.*, 1974, **10**, 568; *Chem. Nat. Compd. (Engl. Transl.)*, 581 (*Murrayone*)
Raj, K. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 332 (*synth*)
Barik, B.R. *et al., Phytochemistry*, 1983, **22**, 792 (*abs config*)
Yamahara, J. *et al., Chem. Pharm. Bull.*, 1985, **33**, 1676 (*isol*)
Ito, C. *et al., Heterocycles*, 1987, **26**, 1731 (*Peroxyauraptenol*)

Aurasperone A A-736

*5,5′-Dihydroxy-6,6′,8,8′-tetramethoxy-2,2′-dimethyl-7,10′-bi-4*H*-naphtho[2,3-b]pyran-4,4′-dione, 9CI* [15085-74-2]



Absolute Configuration

$C_{32}H_{26}O_{10}$ 570.551
Metab. of *Aspergillus niger, Aspergillus awamori* and *Aspergillus fonsecaeus*. Isol. from *Aspergillus niger* infected mango fruits. Yellow plates ($CHCl_3$/propanol); needles (EtOH). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 207° (prisms), 290-291° (270°) (needles). $[\alpha]_D^{25}$ -242 (c, 1.0 in $CHCl_3$). λ_{max} 225 (ϵ 51286); 258 (ϵ 53700); 280 (ϵ 100000); 325 (ϵ 8700); 405 (ϵ 12900) (EtOH) (Berdy).

Di-Ac:
Pale yellow needles (EtOH aq.). Mp 320° dec. $[\alpha]_D^{25}$ -242 (c, 1.0 in $CHCl_3$).

O^8*-De-Me:* [92280-05-2] ***Dianhydroaurasperone C***
$C_{31}H_{24}O_{10}$ 556.525
Prod. by *Aspergillus niger*. λ_{max} 225 (ϵ 23000); 255 (ϵ 27000); 280 (ϵ 85000); 325 (ϵ 3700); 405 (ϵ 5800) (MeOH) (Berdy).

$O^{6'}$*-De-Me:* [67924-64-5] ***Aurasperone D***
$C_{31}H_{24}O_{10}$ 556.525
Mycotoxin from *Aspergillus niger* infected mango fruits. Microcryst. yellow solid. Mp 115°. Abs. config. not certain.

▶ DU3122000

O^6,$O^{6'}$*-Di-de-Me,* O^5,$O^{5'}$*-di-Me:* [71695-22-2] ***Isoaurasperone A***. *Isoaurasperone*
$C_{32}H_{26}O_{10}$ 570.551
Mycotoxin from *Aspergillus niger* infected mango fruits. Pale yellow solid. Mp 198-203°. Abs. config. not certain.

O^6,$O^{6'}$*-Di-de-Me,* O^5,$O^{5'}$*-di-Me, di-Ac:* Mp 148-151°.

2,3-Dihydro, 2ξ-hydroxy: [95272-15-4] ***Aurasperone E***. *Fonsecinone D* [71722-01-5]
$C_{32}H_{28}O_{11}$ 588.567
Isol. from *Aspergillus niger* infected mango fruits. Solid. Mp 166-170°. Abs. config. not certain. λ_{max} 229 (ϵ 38900); 255 (sh) (ϵ 41700); 280 (ϵ 70800); 320 (ϵ 14100); 328 (sh) (ϵ 14100); 403 (ϵ 9120) (95% EtOH) (Derep).

2,3-Dihydro, 2ξ-hydroxy, O^8*-de-Me:* ***Aurasperone F***
$C_{31}H_{26}O_{11}$ 574.54
Yellow powder. λ_{max} 213; 281; 320; 334; 406 (MeOH).

2′,3′-Dihydro, 2′ξ-hydroxy: [95152-76-4] ***Fonsecinone B***
$C_{32}H_{28}O_{11}$ 588.567
Mycotoxin prod. by *Aspergillus fonsecaeus*. Isol. from infected mango fruits. Amorph. Mp 172-173°. Abs. config. not certain. λ_{max} 229 (ϵ 38900); 255 (sh) (ϵ 41700); 280 (ϵ 70800); 320 (ϵ 14100); 328 (sh) (ϵ 14100); 403 (ϵ 9120) (95% EtOH) (Derep).

2′,3′-Dihydro, 2′ξ-hydroxy, O^8*-de-Me:* [940895-78-3] ***Nigerasperone C***
$C_{31}H_{26}O_{11}$ 574.54
Yellow powder. Mp 222-224°. $[\alpha]_D^{20}$ -11.5 (c, 0.34 in MeOH). Abs. config. not certain.

2,2′,3,3′-Tetrahydro, 2,2′-dihydroxy: [41689-67-2] ***Aurasperone B***
$C_{32}H_{30}O_{12}$ 606.582
Mycotoxin from *Aspergillus niger, Aspergillus awamori* and *Aspergillus fonsecaeus*. Yellow. Mp 186° dec. $[\alpha]_D^{25}$ +46.3 (c, 1.4 in $CHCl_3$). No stereochem. determined. λ_{max} 233; 280; 315; 331; 404 (MeOH) (Berdy).

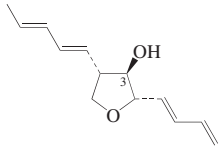
2,2′,3,3′-Tetrahydro, 2,2′-dihydroxy, O^8*-de-Me:* [41689-66-1] ***Aurasperone C***
$C_{31}H_{28}O_{12}$ 592.555
Mycotoxin pigment from *Aspergillus niger* and *Aspergillus awamori*. Yellow. Mp 185° dec. Similar to Fonsecinones.

Tamura, T. *et al., Agric. Biol. Chem.*, 1966, **30**, 107; 683 (*isol*)
Wang, P. *et al., Agric. Biol. Chem.*, 1966, **30**, 683-687 (*struct*)
Namiki, N. *et al., Agric. Biol. Chem.*, 1972, **36**, 2511 (*Aurasperone C, struct*)
Ghosal, S. *et al., Phytochemistry*, 1978, **17**, 689-694 (*Aurasperone D*)

Ghosal, S. *et al., J. Agric. Food Chem.*, 1979, **27**, 1347-1351 (*Aurasperone A, Aurasperone D, Isoaurasperone A*)
Ehrlich, K.C. *et al., Appl. Environ. Microbiol.*, 1984, **48**, 1-4 (*Dianhydroaurasperone C*)
Priestap, H. *et al., Tetrahedron*, 1984, **40**, 3617-3624 (*Fonsecinones, Aurasperone B*)
Koyama, K. *et al., Chem. Pharm. Bull.*, 1987, **35**, 4049-4055 (*abs config*)
Campos, F.R. *et al., Magn. Reson. Chem.*, 2005, **43**, 962-965 (*pmr, cmr*)
Bouras, N. *et al., Nat. Prod. Res.*, 2005, **19**, 653-659 (*Aurasperone F*)
Zhang, Y. *et al., J. Antibiot.*, 2007, **60**, 204-210 (*Nigerasperone C*)

Aureonitol A-737

2-(1,3-Butadienyl)tetrahydro-4-(1,3-pentadienyl)-3-furanol. 2-(1,3-Butadienyl)-3-hydroxy-4-(1,3-pentadienyl)tetrahydrofuran [71774-51-1]



Absolute Configuration

$C_{13}H_{18}O_2$ 206.284

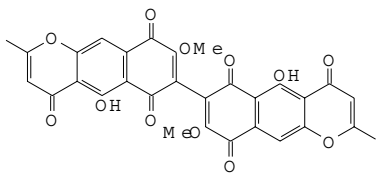
Absolute configuration finally confirmed in 2008. Cryst. Mp 64-65°. $[\alpha]_D^{27}$ -7.8 (c, 1 in $CHCl_3$). λ_{max} 235 (Et_2O).

Triepimer: **ent-*Aureonitol***
$C_{13}H_{18}O_2$ 206.284
Prod. by *Chaetomium globosum* growing on tomatoes. Semisolid. $[\alpha]_D^{25}$ +2.5 (c, 0.12 in $CHCl_3$). λ_{max} 249 (log ϵ 3.5); 275 (log ϵ 3.1) ($CHCl_3$).

Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 664-665 (*isol, pmr*)
Abraham, W.-R. *et al., Phytochemistry*, 1992, **31**, 2405-2408 (*isol, pmr, cmr*)
Marwah, R.G. *et al., Tetrahedron*, 2007, **63**, 8174-8180 (*isol, pmr, cmr, ms*)
Jervis, P.J. *et al., JOC*, 2008, **73**, 7616-7624 (*synth, !abs config*)
Kingsland, S.R. *et al., Aust. J. Chem.*, 2009, **62**, 269-274 (*isol, pmr, cmr*)

Aurofusarin A-738

[13191-64-5]



$C_{30}H_{18}O_{12}$ 570.465

Golden-yellow plates ($CHCl_3$). Mp 330°. λ_{max} 248 (ϵ 48977); 269 (ϵ 33113); 381 (ϵ 9795); 422 ($CHCl_3$). λ_{max} 249 (log ϵ 4.69); 267 (log ϵ 4.52); 372 (log ϵ 4.05) (dioxan).

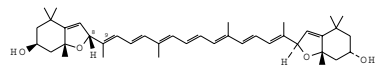
Di-Ac:
Yellow plates. Mp 330°.

Di-Me ether:
Yellow needles (MeOH). Mp 250-251° dec.

Baker, P.M. *et al., JCS(C)*, 1966, 2234-2237 (*struct*)
Birchall, G.R. *et al., JCS(C)*, 1966, 2237-2239 (*isol, struct*)
Gray, J.S. *et al., JCS(C)*, 1967, 2580-2587 (*struct*)
Shibata, S. *et al., Chem. Pharm. Bull.*, 1968, **16**, 405-410; 411-413 (*isol, uv, pmr, struct*)
Neuhof, T. *et al., Eur. J. Mass Spectrom.*, 2008, **14**, 329-333 (*anal, ms, chromatogr*)

Auroxanthin A-739

5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene-3,3′-diol [27785-15-5]



(8R,8′R)-form

$C_{40}H_{56}O_4$ 600.88

Isol. from *Viola tricolor, Lonicera japonica, Delonix regia* and other plants. Yellow cryst. (EtOH). Mp 203°. A *cis*-isomer was reported from *D. regia*.

3,3′-Dideoxy: [6821-09-6] *5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-carotene.* ***Aurochrome***
$C_{40}H_{56}O_2$ 568.881
Widespread carotenoid. Cryst.(C_6H_6/MeOH). Mp 185°.

3′-Deoxy: [73745-06-9] *5,8:5′,8′-Diepoxy-5,5′,8,8′-tetrahydro-β,β-caroten-3-ol.* ***Cryptochrome***
$C_{40}H_{56}O_3$ 584.881
Isol. from *Prunus persica* (peach) and fruits of *Averrhoa carambola*. Isol. only in trace amounts. λ_{max} 424; 456 (CS_2). λ_{max} 399; 424 (EtOH).

(8*R*,8′*R*)-*form* [95034-12-1]
λ_{max} 378; 398; 423 (no solvent reported).

(8*R*,8′*S*)-*form* [51921-06-3]
λ_{max} 378; 398; 423 (no solvent reported).

(8*S*,8′*S*)-*form* [51921-05-2]
λ_{max} 378; 398; 423 (no solvent reported).

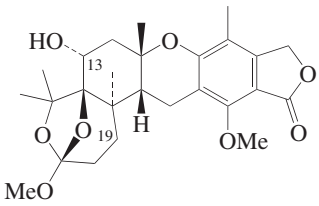
(8*R*,8′*R*,9*Z*)-*form* [95119-78-1]
λ_{max} 378; 398; 423 (no solvent reported).

[22350-65-8]

Karrer, P. *et al., Helv. Chim. Acta*, 1944, **27**, 1684; 1945, **28**, 427 (*struct*)
Goodwin, T.W. *et al., Biochem. J.*, 1956, **62**, 346 (*isol*)
Jungalwala, F.B. *et al., Biochem. J.*, 1962, **85**, 1 (*isol*)
Stobart, A.K. *et al., Phytochemistry*, 1967, **6**, 1467 (*isol*)
Gross, J. *et al., Phytochemistry*, 1983, **22**, 1479 (*Cryptochrome*)
Acemoglu, M. *et al., Helv. Chim. Acta*, 1984, **67**, 471 (*synth, uv, pmr, cmr*)
Märki-Fischer, E. *et al., Helv. Chim. Acta*, 1984, **67**, 2143 (*isol*)

Austalide B A-741

[81543-02-4]



Absolute Configuration

$C_{26}H_{34}O_8$ 474.55

Mycotoxin of the food storage mould *Aspergillus ustus*. Cryst. (C_6H_6/hexane). Mp 243-245°. $[\alpha]_D$ -46.2 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

13-Ac: [81543-01-3] ***Austalide A***
$C_{28}H_{36}O_9$ 516.587
Mycotoxin. Metab. of *Aspergillus ustus*. Cryst. ($CHCl_3$/MeOH). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 212-214°. $[\alpha]_D^{24}$ -84.4 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep). λ_{max} 207 (ϵ 17140); 222 (ϵ 35400) (MeOH) (Berdy).

19α-Hydroxy: [81543-06-8] ***Austalide F***
$C_{26}H_{34}O_9$ 490.549
Mycotoxin of *Aspergillus ustus*. Cryst. (Me_2CO). Mp 261-263°. $[\alpha]_D$ -57.7 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

19α-Hydroxy, 13-Ac: [81543-05-7] ***Austalide E***
$C_{28}H_{36}O_{10}$ 532.586
Mycotoxin. Metab. of *Aspergillus ustus*. Cryst. (Me_2CO). Mp 262-264°. $[\alpha]_D$ -123.6 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep).

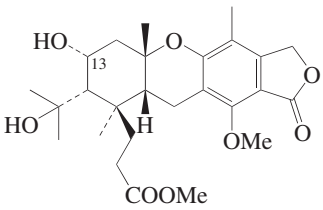
19α-Hydroxy, 19-Ac: [81543-04-6] ***Austalide D***
$C_{28}H_{36}O_{10}$ 532.586
Mycotoxin. Metab. of *Aspergillus ustus*. Cryst. (Me_2CO). Sol. MeOH, $CHCl_3$; poorly sol. H_2O, hexane. Mp 259-261°. $[\alpha]_D$ -73.4 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep). λ_{max} 207 (ϵ 17140); 222 (ϵ 35400) (MeOH) (Berdy).

19α-Hydroxy, di-Ac: [81543-03-5] ***Austalide C***
$C_{30}H_{38}O_{11}$ 574.624
Mycotoxin. Metab. of *Aspergillus ustus*. Amorph. $[\alpha]_D$ -99 (c, 1 in $CHCl_3$).

Horak, R.M. *et al., JCS Perkin 1*, 1985, 345-356 (*isol, struct, pmr*)
De Jesus, A.E. *et al., JCS Perkin 1*, 1987, 2253-2257 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393-394 (*biosynth, abs config*)
Paquette, L.A. *et al., JACS*, 1994, **116**, 2665-2666; 11323-11324 (*synth*)

Austalide H A-742

[96817-10-6]



Absolute Configuration

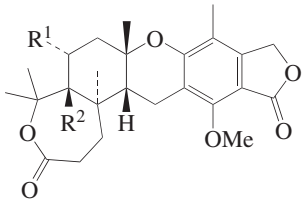
$C_{26}H_{36}O_8$ 476.566
Mycotoxin of the food storage mould (*Aspergillus ustus*). Glass. $[\alpha]_D^{24}$ -19.5 (c, 1.0 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

13-Ac: [96817-09-3] ***Austalide G***
$C_{28}H_{38}O_9$ 518.603
Mycotoxin prod. by *Aspergillus ustus*. Glass. $[\alpha]_D^{24}$ -100.2 (c, 1 in $CHCl_3$). λ_{max} 222 (ϵ 35400); 267 (ϵ 17100) (MeOH) (Derep).

Horak, R.M. *et al., JCS Perkin 1*, 1985, 363-367 (*isol, struct, pmr*)
De Jesus, A.E. *et al., JCS Perkin 1*, 1987, 2253-2257 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393-394 (*biosynth, abs config*)

Austalide I A-742a

[96817-08-2]



R^1 = OAc, R^2 = H
Absolute Configuration

$C_{27}H_{34}O_8$ 486.561
Mycotoxin from the food storage mould (*Aspergillus ustus*). Cryst. Mp 236-238°. $[\alpha]_D^{24}$ -132.6 (c, 1 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

Horak, R.M. *et al., JCS Perkin 1*, 1985, 363-367 (*Austalide I*)
De Jesus, A.E. *et al., JCS Perkin 1*, 1987, 2253-2257 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393-394 (*biosynth, abs config*)

Austalide J A-743

[87833-51-0]

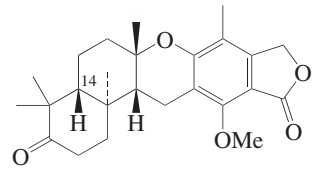
As Austalide I, A-740 with
R^1 = H, R^2 = OH

$C_{25}H_{32}O_7$ 444.524
Mycotoxin of the food storage mould (*Aspergillus ustus*). Cryst. (MeOH). Mp 284-286°. $[\alpha]_D^{24}$ -42.1 (c 1.0 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

Horak, R.M. *et al., JCS Perkin 1*, 1985, 363-367 (*isol, struct, pmr*)
De Jesus, A.E. *et al., JCS Perkin 1*, 1987, 2253-2257 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393-394 (*biosynth, abs config*)

Austalide K A-744

[87833-53-2]



Absolute Configuration

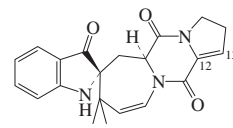
$C_{25}H_{32}O_5$ 412.525
Mycotoxin of the food storage mould (*Aspergillus ustus*). Glass. $[\alpha]_D^{24}$ -75.9 (c, 1.00 in $CHCl_3$). λ_{max} 223 (ϵ 28700); 269 (ϵ 16800) (MeOH) (Derep).

14β-Hydroxy: [87833-52-1] ***Austalide L***
$C_{25}H_{32}O_6$ 428.524
Mycotoxin prod. by *Aspergillus ustus*. Cryst. (C_6H_6/hexane). Mp 207-208°. $[\alpha]_D^{24}$ -71 (c, 1.00 in $CHCl_3$). λ_{max} 223 (ϵ 31200); 269 (ϵ 16600) (MeOH) (Derep).

Horak, R.M. *et al., JCS Perkin 1*, 1985, 363-367 (*isol, struct, pmr*)
De Jesus, A.E. *et al., JCS Perkin 1*, 1987, 2253-2257 (*biosynth*)
Dillen, J.L.M. *et al., Chem. Comm.*, 1989, 393-394 (*biosynth, abs config*)

Austamide A-745

[34427-31-1]



Absolute Configuration

$C_{21}H_{21}N_3O_3$ 363.415
Yellow amorph. solid. Sol. MeOH, $CHCl_3$. $[\alpha]_D^{20}$ +152 (c, 1 in EtOH). λ_{max} 234 (ϵ 26300); 256 (ϵ 2344); 282 (ϵ 8700); 392 (ϵ 2700) (EtOH) (Berdy).

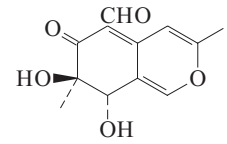
12S,13-Dihydro: [34506-79-1] ***12,13-Dihydroaustamide***
$C_{21}H_{23}N_3O_3$ 365.431
Cryst. (Me_2CO). Mp 235-238°. $[\alpha]_D^{22}$ +55 (c, 1.1 in $CHCl_3$). Fluorescent.

12ξ-Hydroxy, 12,13-dihydro: [59476-59-4] ***12,13-Dihydro-12-hydroxyaustamide***
$C_{21}H_{23}N_3O_4$ 381.43
Cryst. (MeOH). Mp 164-165°.

Coetzer, J. *et al., Acta Cryst. B*, 1973, **29**, 685 (*cryst struct*)
Steyn, P.S. *et al., Tetrahedron*, 1973, **29**, 107-120 (*isol, uv, ir, pmr, ms, struct, deriv*)
Steyn, P.S. *et al., Phytochemistry*, 1976, **15**, 355-356 (*dihydro*)
Harrison, D.M. *et al., Tet. Lett.*, 1981, **22**, 2501-2504 (*synth*)
Stocking, E.M. *et al., JACS*, 2000, **122**, 9089-9098 (*biosynth*)
Williams, R.M. *et al., Chem. Pharm. Bull.*, 2002, **50**, 711-740 (*rev, synth, biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 484

Austdiol A-746

*7,8-Dihydro-7,8-dihydroxy-3,7-dimethyl-6-oxo-6*H*-2-benzopyran-5-carboxaldehyde, 9CI* [53043-28-0]



Absolute configuration

$C_{12}H_{12}O_5$ 236.224
Toxic metab. of the food storage mould *Aspergillus ustus*. Yellow needles. Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 255° dec. $[\alpha]_D^{26}$ +160.3 (c, 1.25 in Py). λ_{max} 256 (ϵ 15135); 376 (ϵ 23990) (EtOH) (Berdy).

▶ Mutagenic activity (without metabolic activation). DJ2232000

Di-Ac:
Needles (C_6H_6/hexane). Mp 238-239° dec.

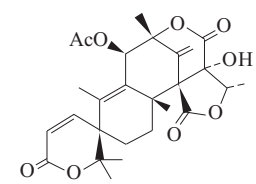
7-Epimer: [1227500-86-8] ***7-Epiaustdiol***
$C_{12}H_{12}O_5$ 236.224
Cryst. (EtOAc/MeOH). Mp 174-176°. $[\alpha]_D^{20}$ +116.1 (c, 0.1 in MeOH). λ_{max} 373 (log ϵ 4.1) (MeOH).

7-Epimer, 8-Me ether: [1227500-88-0] ***8-O-Methyl-7-epiaustdiol***
$C_{13}H_{14}O_5$ 250.251
Yellow powder. Mp 160-161°. $[\alpha]_D^{20}$ +115.5 (c, 0.1 in MeOH). λ_{max} 371 (log ϵ 4.33) (MeOH).

Vleggaar, R. *et al., JCS Perkin 1*, 1974, 45-49 (*isol, struct*)
Pohland, A.E. *et al., Pure Appl. Chem.*, 1982, **54**, 2219-2284 (*uv, ir, pmr, ms, cd*)
Colombo, L. *et al., JCS Perkin 1*, 1983, 2745-2749 (*biosynth*)
Lo Presti, L. *et al., Acta Cryst. C*, 2003, **59**, o199-o201 (*cryst struct*)
Liu, F. *et al., Planta Med.*, 2010, **76**, 185-189 (*7-Epiaustdiols*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 790

Austin, 9CI A-747

[61103-89-7]



Absolute configuration

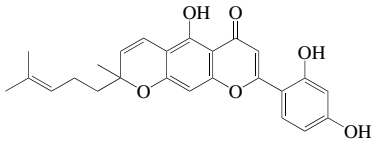
$C_{27}H_{32}O_9$ 500.544
Mycotoxin prod. by the food storage mould (*Aspergillus ustus*). Cryst. ($CHCl_3$/MeOH). Mp 298-300°. λ_{max} 243 (ϵ 11900) (EtOH) (Berdy).

O-*De-Ac:* [72040-27-8] ***Austinol***
$C_{25}H_{30}O_8$ 458.507
Metab. of *Emericella nidulans, Emericella dentata, Aspergillus variecolor* and *Aspergillus ustus*. Amorph.

Chexal, K.K. *et al., JACS*, 1976, **98**, 6748 (*cryst struct*)
Fukuyama, K. *et al., Chem. Pharm. Bull.*, 1980, **28**, 2270 (*cryst struct*)
Simpson, T.J. *et al., Chem. Comm.*, 1981, 1042 (*biosynth*)
Maebayashi, Y. *et al., Chem. Pharm. Bull.*, 1982, **30**, 1911 (*abs config*)
McIntyre, C.R. *et al., Chem. Comm.*, 1982, 781 (*biosynth*)
Simpson, T.J. *et al., JCS Perkin 1*, 1982, 2687 (*cmr*)
Simpson, T.J. *et al., Chem. Comm.*, 1984, 1242 (*biosynth*)
Ahmed, S.A. *et al., JCS Perkin 1*, 1989, 807 (*biosynth*)
Cole, R.J. *et al., Handbook of Toxic Fungal Metabolites*, Academic Press, 1981, 802

Australone A A-748

[196705-71-2]

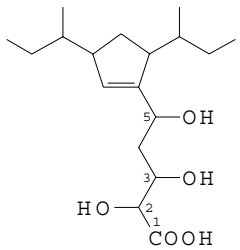


$C_{25}H_{24}O_6$ 420.461
Yellowish needles (hexane/Me_2CO). Mp 195-197°. $[\alpha]_D^{25}$ -36 (c, 0.05 in Me_2CO). λ_{max} 230 (log ϵ 4.4); 290 (log ϵ 4.44); 310 (sh) (log ϵ 4.24); 358 (log ϵ 4.42) (MeOH).

2,3-Dihydro: [123702-94-3] ***Kuwanol C***
$C_{25}H_{26}O_6$ 422.477
Constit. of *Morus alba* (white mulberry). Amorph. powder. $[\alpha]_D^{22}$ -10 (c, 0.31 in EtOH).

Hano, Y. *et al., Heterocycles*, 1989, **29**, 807-813 (*Kuwanol C*)
Ko, H.-H. *et al., J. Nat. Prod.*, 1997, **60**, 1008-1011 (*Australone A*)

Auxin a A-749



$C_{18}H_{32}O_5$ 328.448
Fraudulent work. Claimed to have been isolated from peanut oil and corn oil. Mp 196°. Almost certainly Cholic acid #HLJ07-V.

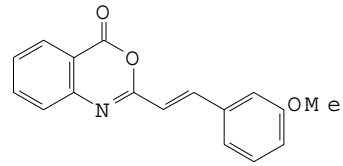
1,5-Lactone: Auxin a lactone
$C_{18}H_{30}O_4$ 310.433
Mp 173°. Almost certainly 1,4-Benzenediol.

2-Deoxy, 3-ketone: Auxin b
$C_{18}H_{30}O_4$ 310.433
Claimed isoln. from peanut and corn oils. Mp 183°.
Almost certainly Thiosemicarbazide.

Kögl, F. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1933, **214**, 241; 1934, **225**, 215
Mori, K. *et al., Annalen*, 1991, 775 (*bibl*)

Avenalumin II A-750

*2-[2-(3-Methoxyphenyl)ethenyl]-4*H*-3,1-benzoxazin-4-one, 9CI. 2-(3-Methoxycinnamoyl)-4*H*-3,1-benzoxazin-4-one* [78214-14-9]

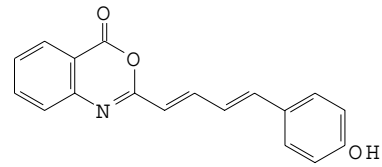


$C_{17}H_{13}NO_3$ 279.295
The proposed struct. illus. has been questioned (see Crombie *et al*). Phytoalexin from oat (*Avena sativa*) infected with rust fungus *Puccinia coronata*. Poorly sol. hexane. λ_{max} 317; 336 (MeOH) (Berdy).

Mayama, S. *et al., Physiol. Plant Pathol.*, 1981, **19**, 217 (*isol*)
Collins, F.W. *et al., Spectroscopy (Ottawa)*, 1985, **4**, 171 (*synth, ms*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)

Avenalumin III A-751

*2-[4-(4-Hydroxyphenyl)-1,3-butadienyl]-4*H*-3,1-benzoxazin-4-one, 9CI* [78214-15-0]

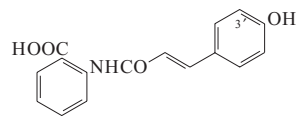


$C_{18}H_{13}NO_3$ 291.306
The proposed struct. illus. has been questioned (see Crombie *et al*). Phytoalexin isol. from oat (*Avena sativa*) infected with rust fungus (*Puccinia coronata*). Poorly sol. hexane.

Mayama, S. *et al., Physiol. Plant Pathol.*, 1981, **19**, 217 (*isol*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)

Avenanthramide D A-752

N-p-*Hydroxycinnamoylanthranilic acid. Dianthramide P* [115610-36-1]



(*E*)*–form*
$C_{16}H_{13}NO_4$ 283.283
Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, H_2O, C_6H_6. λ_{max} 218 (ϵ 19950); 329 (ϵ 29500) (MeOH) (Berdy). λ_{max} 213 (ϵ 26900); 314 (ϵ 12020); 371 (ϵ 32360) (MeOH/NaOH) (Berdy).

(E)-form
Isol. from the oat *Avena sativa*. Rods (Me_2CO aq.). Sol. MeOH, $CHCl_3$; poorly sol. H_2O. Mp 219°. λ_{max} 300; 329 (MeOH) (Berdy).

3′-Methoxy: [93755-77-2] ***Avenanthramide E***. N-*Feruloylanthranilic acid*
$C_{17}H_{15}NO_5$ 313.309
Isol. from the oat *Avena sativa*. Pale yellow needles (Me_2CO aq.). Sol. EtOAc, Et_2O, H_2O-Me_2CO; poorly sol. $CHCl_3$, H_2O, C_6H_6. Mp 235°. λ_{max} 211; 338 (MeOH) (Berdy). λ_{max} 219; 385 (MeOH/NaOH) (Berdy).

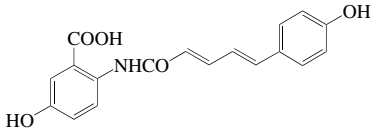
(Z)-form
Isol. from *Avena sativa* (oat).

3′-Methoxy: [116764-24-0] Z-*Avenanthramide E*
$C_{17}H_{15}NO_5$ 313.309
Isol. from oat (*Avena sativa*).

Collins, F.W. *et al., J. Chromatogr.*, 1988, **445**, 363 (*hplc*)
Ponchet, M. *et al., Phytochemistry*, 1988, **27**, 725
Collins, F.W. *et al., J. Agric. Food Chem.*, 1989, **37**, 60 (*isol, pmr, cmr, uv, ms*)
Crombie, L. *et al., Tet. Lett.*, 1990, **31**, 2647 (*synth*)
Ishihara, A. *et al., Phytochemistry*, 1999, **50**, 237-242 (*biosynth*)

Avenanthramide L A-753

[172549-38-1]

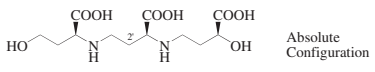


$C_{18}H_{15}NO_5$ 325.32
Isol. from oat, *Avena sativa*, inoculated with *Puccinia coronata* f.sp. *avenae*. Yellow cryst. Mp 267-269°. λ_{max} 355 (log ϵ 4.8) (MeOH).

Miyagawa, H. *et al., Biosci., Biotechnol., Biochem.*, 1995, **59**, 2305-2306 (*isol, uv, pmr*)
Ishihara, A. *et al., Phytochemistry*, 1999, **50**, 237-242 (*biosynth*)

Avenic acid A A-754

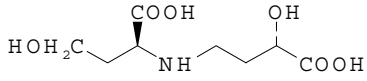
N-*[3-(3-Hydroxy-3-carboxypropylamino)-3-carboxypropyl]homoserine, 9CI* [76224-57-2]



$C_{12}H_{22}N_2O_8$ 322.314
Isol. from root washings of *Avena sativa* (oats). Mp 300°. $[\alpha]_D$ +16.4 (c, 0.11 in 2N HCl).

*2′*S*-Hydroxy:* [956358-62-6] ***2′-Hydroxyavenic acid A***
$C_{12}H_{22}N_2O_9$ 338.314
Fushiya, S. *et al., Tet. Lett.*, 1980, 3071 (*isol, struct*)
Fushiya, S. *et al., Chem. Lett.*, 1981, 909 (*synth*)
Ueno, D. *et al., New Phytol.*, 2007, **174**, 304-310 (*2′-Hydroxyavenic acid A*)

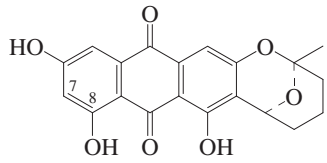
Avenic acid B **A-755**
N-*(3-Carboxy-3-hydroxypropyl)-*L*-homoserine, 9CI* [76224-58-3]



$C_8H_{15}NO_6$ 221.21
Constit. of the roots of *Avena sativa* (oats). Amorph. solid.
Fushiya, S. *et al., Chem. Lett.*, 1980, 1215 (*isol, pmr, cmr, synth*)
Ripperger, H. *et al., Heterocycles*, 1982, **17**, 447 (*rev*)

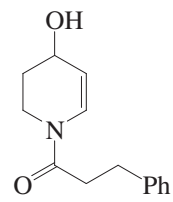
Avenothionin **A-756**
Peptides. Analogs of purothionins. Two avenothionins (α- and β-) have been characterised. They contain 45 AA residues including 8 cysteines. Isol. from oat (*Avena sativa*).
[79468-42-1, 79468-43-2]
Bekes, F. *et al., Cereal Chem.*, 1981, **58**, 360 (*isol*)

Averufin **A-757**
*3,4,5,6-Tetrahydro-7,9,11-trihydroxy-2-methyl-2,6-epoxy-2*H*-anthra[2,3-*b*]oxocin-8,13-dione, 9CI* [14016-29-6]



$C_{20}H_{16}O_7$ 368.342
Bright orange-red laths (Me_2CO). Sol. MeOH, C_6H_6, bases; poorly sol. H_2O. Mp 280-282° dec. $[\alpha]_D$ 0. λ_{max} 223 (ε 34700); 256 (sh) (ε 16300); 266 (ε 18300); 286 (sh) (ε 27200); 294 (ε 33000); 324 (ε 9530); 453 (ε 10750) (EtOH).
▶ Shows mutagenic activity. KC4150000
Tri-Ac: [74810-25-6]
$C_{26}H_{22}O_{10}$ 494.454
Yellow needles (EtOH). Mp 210-214°. $[\alpha]_D$ -14.9 (c, 0.424 in $CHCl_3$).
*8-Me ether: 8-*O*-Methylaverufin*
Orange solid. λ_{max} 223 (log ε 4.47); 290 (log ε 4.33); 309 (log ε 4.12); 446 (log ε 3.75) (MeOH).
6,8-Di-Me ether: [61470-56-2] ***6,8-Di-O-methylaverufin***. *Antibiotic SIPI 8917-I. SIPI 8917-I*
[79896-27-8]
$C_{22}H_{20}O_7$ 396.396
Prod. by rice inoculated with *Emericella foeniculicola* and from a fungal isolate SIPI-8917. Cryst. (Me_2CO). Mp 208-209°. λ_{max} 225; 250; 287; 313; 439 (MeOH).
Tri-Me ether: [15894-83-4]
$C_{23}H_{22}O_7$ 410.423
Yellow prisms. Mp 190-191°.
7-Methoxy: [95963-94-3] ***7-Methoxyaverufin***
$C_{21}H_{18}O_8$ 398.368
Yellow cryst. (Me_2CO). Mp 198-200° dec. λ_{max} 207; 226; 290; 320; 400 (MeOH).
Pusey, D.F.G. *et al., JCS*, 1963, 3542-3547 (*isol*)
Knight, J.A. *et al., JCS(C)*, 1967, 2328-2331 (*struct*)
Ando, K. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 2091-2096 (*cryst struct*)
Fitzell, D.C. *et al., J. Agric. Food Chem.*, 1975, **23**, 442-444 (*biosynth*)
Castonguay, A. *et al., Can. J. Chem.*, 1977, **55**, 1324-1332 (*synth*)
Gorst-Allman, C.P. *et al., JCS Perkin 1*, 1977, 2181-2188 (*cmr, biosynth*)
Steyn, P.S. *et al., JCS Perkin 1*, 1979, 451-459 (*pmr, 6,8-di-Me*)
Townsend, C.A. *et al., JACS*, 1981, **103**, 6885-6888; 1985, **107**, 270-271 (*synth, abs config*)
Simpson, T.J. *et al., Chem. Comm.*, 1982, 631-632; 632-634 (*biosynth*)
Sankawa, U. *et al., Heterocycles*, 1982, **19**, 1053-1058 (*biosynth*)
Kachholz, T. *et al., J. Nat. Prod.*, 1983, **46**, 499-506 (*biosynth*)
Koreeda, M. *et al., JOC*, 1985, **50**, 5426-5428 (*synth, abs config*)
O'Malley, G.J. *et al., JOC*, 1985, **50**, 5533-5537 (*synth*)
Maebayashi, Y. *et al., Maikotokishin (Tokyo)*, 1985, **21**, 36-37 (*6,8-Di-O-methylaverufin*)
Ahmad, V.U. *et al., Z. Naturforsch., B*, 1985, **40**, 319-320 (*7-methoxy, isol, uv, ir, pmr, ms*)
Chandler, I.M. *et al., Chem. Comm.*, 1987, 17-18 (*biosynth*)
Townsend, C.A. *et al., JCS Perkin 1*, 1988, 839-861 (*synth, bibl*)
Maskey, R.P. *et al., J. Antibiot.*, 2003, **56**, 459-463 (*8-O-Methylaverufin*)
Zhu, F. *et al., Youji Huaxue*, 2004, **24**, 1114-1117 (*marine, isol*)
Shao, C. *et al., Magn. Reson. Chem.*, 2008, **46**, 886-889 (*6,8-Di-O-methylaverufin*)

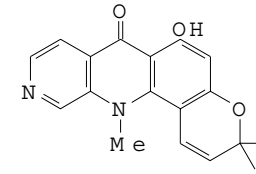
Awaine **A-758**
3-Phenylpropanoic acid 2,3-didehydro-4-hydroxypiperidide [593254-86-5]



$C_{14}H_{17}NO_2$ 231.294
Alkaloid from the aerial parts of *Piper methysticum* (kava). Oil.
Dragull, K. *et al., Phytochemistry*, 2003, **63**, 193-198 (*Awaine*)

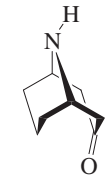
AX Peptides **A-759**
Peptides consisting of 46 amino acid residues including 8 cysteines. Isol. from leaves of *Beta vulgaris* infected with *Cercospora beticola*.
AX 1 [159075-61-3]
AX 2 [159075-62-4]
AX 3 [159075-63-5]
Eur. Pat., 1994, 612 847 (*isol*)
Kragh, K.M. *et al., Mol. Plant-Microbe Interact.*, 1995, **8**, 424-434 (*isol*)

Azaacridone A **A-760**
Azacridone A [150050-14-9]



$C_{18}H_{16}N_2O_3$ 308.336
First naturally occurring azaacridone alkaloid. Alkaloid from roots of *Citrus paradisi* (grapefruit). Light brown oil.
Takemura, Y. *et al., Chem. Pharm. Bull.*, 1993, **41**, 789 (*isol, uv, ir, pmr, struct*)
Scopton, A. *et al., Org. Lett.*, 2004, **6**, 3869-3871 (*synth*)

9-Azabicyclo[3.3.1]nonan-3-one, 9CI **A-761**
Granatonine. Norgranatan-3-one. Norpseudopelletierine [4390-39-0]



$C_8H_{13}NO$ 139.197
Found in pomegranate (*Punica granatum*) bark. Mp 123°.
▶ CL5593500
Picrate:
Cryst. (MeOH). Mp 216°.
N-*(Trifluoroacetyl):* [180406-55-7]
$C_{10}H_{12}F_3NO_2$ 235.206
Cryst. (Et_2O/hexane). Mp 70-73°.
N-*Benzoyl:* [36146-90-4]
$C_{15}H_{17}NO_2$ 243.305
Oil.
N-*(4-Methylbenzenesulfonyl):* [180406-57-9]
$C_{15}H_{19}NO_3S$ 293.386
Cryst. (EtOH). Mp 149-151°.
N-*Me:* [552-70-5] *9-Methyl-9-azabicyclo[3.3.1]nonan-3-one, 9CI. Granatan-3-one.* N*-Methylgranatonine. Pseudopelletierine. Ψ-Pelletierine*
$C_9H_{15}NO$ 153.224
Found in bark of pomegranate (*Punica granatum*). Prismatic plates

(petrol). V. sol. H_2O. Mp 62-64°. Bp 246°. Strong base.

N-*Me, oxime:* [6164-67-6]
$C_9H_{16}N_2O$ 168.238
Plates (Et_2O). Mp 128-129°.

N-*Me,* N-*oxide:*
$C_9H_{15}NO_2$ 169.223
Mp 160-162°.

N-*Me,* N-*oxide; hydrochloride:* Mp 224°.

N-*Benzyl:*
$C_{15}H_{19}NO$ 229.321
Mp 72°. $Bp_{0.005}$ 115-120°.

Org. Synth., Coll. Vol., 4, 1963, 816 (*synth, bibl*)
Chen, C.-Y. *et al., JCS(B)*, 1966, 539 (*conformn*)
Guthrie, R.D. *et al., JCS(C)*, 1966, 1207 (*ms, N-Me*)
Wiseman, J.R. *et al., JOC*, 1977, **42**, 629 (*synth, N-Me*)
Dupeyre, R.M. *et al., Bull. Soc. Chim. Fr.*, Part II, 1978, 612-620 (*synth, pmr, N-benzyl*)
Hill, R.K. *et al., Tetrahedron*, 1982, **38**, 1959 (*synth, N-Me*)
Neuhoefer, H. *et al., Pharmazie*, 1993, **48**, 389-391 (*isol*)
Momose, T. *et al., JCS Perkin 1*, 1997, 1307-1313 (*N-benzyl*)
Kirihara, M. *et al., Tetrahedron*, 1999, **55**, 2911-2926 (*derivs*)

8-Azabicyclo[3.2.1]octane-3,6-diol A-762

3,6-Dihydroxynortropane. 3,6-Nortropanediol

(3*S*,6*R*)-*form*

$C_7H_{13}NO_2$ 143.185

(3*S*,6*R*)-*form*
Alkaloid from the fruit of *Morus alba* (white mulberry). Powder. $[\alpha]_D$ -1.3 (c, 0.6 in H_2O).

(3*R,6*R**)-*form***
N-*Me:* see 8-Methyl-8-azabicyclo[3.2.1]octane-3,6-diol, #BBZ13-Q

3-O-*Tigloyl:* [65636-83-1] ***3-Tigloyloxynortropan-6-ol***
[65636-84-2]
$C_{12}H_{19}NO_3$ 225.287
Plates (EtOH) (as hydrochloride). Mp 289-290° (hydrochloride). Opt. rotn. not measured.

3-O-*Benzoyl:* ***3-Benzoyloxynortropan-6-ol***
$C_{14}H_{17}NO_3$ 247.293
Mp 225° (as picrate).

6-O-*Benzoyl, 3-(2-methylpropanoyl):* ***6-Benzoyloxy-3-isobutanoyloxynortropane***
$C_{18}H_{23}NO_4$ 317.384
Light brown powder. $[\alpha]_D^{25}$ -21.4 (c, 0.07 in MeOH). λ_{max} 232 (log ϵ 4.07); 275 (log ϵ 2.87) (MeOH).

3-O-*(3,4,5-Trimethoxybenzoyl):* ***3-(3,4,5-Trimethoxybenzoyloxy)nortropan-6-ol***
$C_{17}H_{23}NO_6$ 337.372
Prisms (EtOH aq.) (as picrate). Mp 201° (picrate).

6-O-E-*Cinnamoyl, 3*-O-*propanoyl:* ***6-trans-Cinnamoyloxy-3-propanoyloxynortropane***
$C_{19}H_{23}NO_4$ 329.395
Amorph. solid. $[\alpha]_D^{25}$ -23.1 (c, 0.31 in MeOH). λ_{max} 280 (log ϵ 4.37) (MeOH).

6-O-*(3,4,5-Trimethoxy-Z-cinnamoyl), 3*-O-*(2-methylpropanoyl):* ***3-Isobutanoyloxy-6-(3,4,5-trimethoxy-cis-cinnamoyloxy)nortropane***
$C_{23}H_{31}NO_7$ 433.5
Semisolid. $[\alpha]_D^{25}$ -25.2 (c, 0.07 in $CHCl_3$). λ_{max} 326 (log ϵ 4.43) (MeOH).

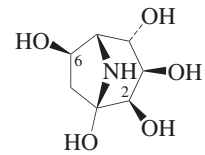
(3*R*,6*S*)-*form*
3β,6β-Dihydroxynortropane
Alkaloid from the fruit of *Morus alba* (white mulberry). $[\alpha]_D$ -8.2 (c, 0.34 in H_2O).

Di-O-*tigloyl:* [359723-70-9] *3,6-Ditigloyloxynortropane*
$C_{17}H_{25}NO_4$ 307.389

Evans, W.C. *et al., Phytochemistry*, 1978, **17**, 171 (*3-tiglate*)
Al-Said, M.S. *et al., Phytochemistry*, 1986, **25**, 851-853 (*3-benzoate*)
El-Iman, Y.M.A. *et al., Phytochemistry*, 1987, **26**, 2385-2389 (*3-trimethoxybenzoate*)
Zuanazzi, J.A.S. *et al., Biochem. Syst. Ecol.*, 2001, **29**, 819-825 (*ditiglate*)
Asano, N. *et al., J. Agric. Food Chem.*, 2001, **49**, 4208-4213 (*3β,6β-form*)
Kusano, G. *et al., Chem. Pharm. Bull.*, 2002, **50**, 185-192 (*Morus alba isolate*)
Khattak, K.F. *et al., Heterocycles*, 2003, **60**, 917-924 (*Erythroxylum moonii esters*)

8-Azabicyclo[3.2.1]octane-1,2,3,4,6-pentol A-763

1,2,3,4,6-Pentahydroxynortropane. 1,2,3,4,6-Nortropanepentol



(1*R* ,2*R* ,3*R* ,4*S* ,5*R* ,6*R*)-*form*

$C_7H_{13}NO_5$ 191.183

(1*R,2*R**,3*R**,4*S**,5*R**,6*R**)-*form*** [190957-44-9]
Calystegine C₂
Alkaloid from *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -40.6 (c, 0.32 in H_2O).

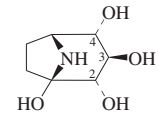
(1*R,2*S**,3*R**,4*S**,5*R**,6*R**)-*form*** [156705-04-3]
Calystegine C₁
Alkaloid from *Morus alba* (white mulberry) and *Lycium chinense* (Chinese boxthorn). Powder. $[\alpha]_D$ +23.1 (c, 0.8 in H_2O).

N-*Me:* [197449-07-3] **N-*Methylcalystegine C₁***
$C_8H_{15}NO_5$ 205.21
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +27.6 (c, 0.3 in H_2O).

Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369-376; 1997, **248**, 296-303 (*isol, pmr, cmr*)
Kato, A. *et al., Phytochemistry*, 1997, **45**, 425-429 (*Calystegine C_2*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Watson, A.A. *et al., Phytochemistry*, 2001, **56**, 265-295 (*rev*)
Dräger, B. *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)

8-Azabicyclo[3.2.1]octane-1,2,3,4-tetrol A-764

1,2,3,4-Tetrahydroxynortropane. 1,2,3,4-Nortropanetetrol



(1*R*,2*S*,3*R*,4*S*)-*form*

$C_7H_{13}NO_4$ 175.184

(1*R*,2*S*,3*R*,4*S*)-*form* [127414-85-1]
Calystegine B₂. *Nortropanoline*
Alkaloid from *Solanum tuberosum* (potato), *Solanum melongena* (aubergine). $[\alpha]_D$ +2.9 (c, 0.2 in H_2O). $[\alpha]_D$ +17.1 (c, 0.41 in H_2O) (synthetic).

N-*Me:* [184045-65-6] **N-*Methylcalystegine B₂***
$C_8H_{15}NO_4$ 189.211
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +22.2 (c, 0.22 in H_2O).

(1*S*,2*R*,3*S*,4*R*)-*form* [146275-92-5]
$[\alpha]_D$ -17.5 (c, 0.37 in H_2O).

4-O-α-D-*Galactopyranoside:* ***4-O-α-D-Galactopyranosylcalystegine B₂***
$C_{13}H_{23}NO_9$ 337.326
Alkaloid from the fruit of *Morus alba* (white mulberry). $[\alpha]_D$ +114.5 (c, 0.48 in H_2O).

(1*R*,2*R*,3*R*,4*S*)-*form* [178231-95-3]
Calystegine B₃
Powder. $[\alpha]_D$ +82.8 (c, 0.5 in H_2O).

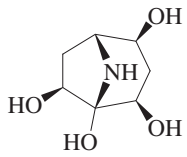
(1*R*,2*S*,3*R*,4*R*)-*form* [184046-85-3]
Calystegine B₄
Powder. $[\alpha]_D$ -63 (c, 0.65 in H_2O).

Goldmann, A. *et al., Phytochemistry*, 1990, **29**, 2125 (*isol*)
Ducrot, P.-H. *et al., Tet. Lett.*, 1990, **31**, 3879; 3883 (*pmr, cmr, struct, synth*)
Boyer, F.-D. *et al., Synlett*, 1992, 969 (*synth*)
Duclos, O. *et al., Tet. Lett.*, 1992, **33**, 8061 (*synth*)
Nash, R.J. *et al., Phytochemistry*, 1993, **34**, 1281 (*occur*)
Boyer, F.-D. *et al., Tetrahedron*, 1994, **50**, 10443 (*synth*)
Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369 (*Calystegine B_3*)
Asano, N. *et al., Carbohydr. Res.*, 1996, **284**, 169; **293**, 195 (*Calystegine B_3, Calystegine B_4*)
Goldmann, A. *et al., J. Nat. Prod.*, 1996, **59**, 1137
Souli&e, J. *et al., Tetrahedron*, 1996, **52**, 15137 (*synth*)
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*N-Methylcalystegine B_2*)

Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Asano, N. *et al., J. Agric. Food Chem.*, 2001, **49**, 4208-4213 (*4-Galactosylcalystegine B_2*)
Watson, A.A. *et al., Phytochemistry*, 2001, **56**, 265-295 (*rev*)
Bekkouche, K. *et al., Phytochemistry*, 2001, **58**, 455-462 (*occur*)
Boyer, F.-D. *et al., Tet. Lett.*, 2001, **42**, 1275-1277 (*Calystegine B_2, synth*)
Marco-Contelles, J. *et al., JOC*, 2002, **67**, 3705-3717 (*Calystegine B_2, synth*)
Skaanderup, P.R. *et al., JOC*, 2003, **68**, 2115-2122 (*Calystegine B_2 B_3 B_4, synth*)
Scholl, Y. *et al., Phytochemistry*, 2003, **62**, 325-332 (*biosynth*)
Dräger, B. *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)
Chen, Y.-L. *et al., Org. Biomol. Chem.*, 2007, **5**, 3330-3339 (*Calystegine A_3, synth*)
Moosophon, P. *et al., Eur. J. Org. Chem.*, 2010, 3337-3344 (*Calystegine B_4, synth*)

8-Azabicyclo[3.2.1]octane-1,2,4,7-tetrol A-765

1,2,4,7-Tetrahydroxynortropane. 1,2,4,7-Nortropanetetrol



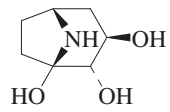
$C_7H_{13}NO_4$ 175.184

(1*R,2*R**,4*S**,7*S**)-*form*** [197565-91-6]
Calystegine B_5
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ +9.6 (c, 0.31 in H_2O).

Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*Calystegine B_5*)
Dräger, B. *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)

8-Azabicyclo[3.2.1]octane-1,2,3-triol A-766

1,2,3-Trihydroxynortropane. 1,2,3-Nortropanetriol



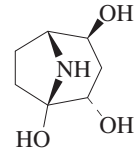
$C_7H_{13}NO_3$ 159.185

(1*R*,2*S*,3*R*)-*form* [131580-36-4]
Calystegine A_3
Alkaloid from *Solanum tuberosum* (potato). Powder. $[\alpha]_D$ -17.3 (c, 0.5 in H_2O).

Goldmann, A. *et al., Phytochemistry*, 1990, **29**, 2125-2127 (*isol*)
Ducrot, P.-H. *et al., Tet. Lett.*, 1990, **31**, 3879-3882; 3883-3886 (*pmr, cmr, struct, synth*)
Boyer, F.-D. *et al., Synlett*, 1992, 357-359 (*synth*)
Nash, R.J. *et al., Phytochemistry*, 1993, **34**, 1281 (*occur*)
Asano, N. *et al., Eur. J. Biochem.*, 1995, **229**, 369 (*isol, pmr, cmr*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Bekkouche, K. *et al., Phytochemistry*, 2001, **58**, 455-462 (*occur*)
Dräger, B, *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)
Monrad, R.N. *et al., Eur. J. Org. Chem.*, 2009, 3387-3395 (*synth*)

8-Azabicyclo[3.2.1]octane-1,2,4-triol A-767

1,2,4-Trihydroxynortropane. 1,2,4-Nortropanetriol



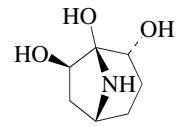
$C_7H_{13}NO_3$ 159.185

(1*R,2*S**,4*S**)-*form*** [197565-90-5]
Calystegine A_7
Alkaloid from the roots of *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -10.8 (c, 0.27 in H_2O).

Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*isol*)
Dräger, B. *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)
Csuk, R. *et al., Tetrahedron*, 2008, **64**, 9417-9422 (*synth*)

8-Azabicyclo[3.2.1]octane-1,2,7-triol A-768

1,2,7-Trihydroxynortropane. 1,2,7-Nortropanetriol



$C_7H_{13}NO_3$ 159.185

(1*R,2*R**,7*R**)-*form*** [177794-04-6]
Calystegine A_6
Alkaloid from and *Lycium chinense* (Chinese boxthorn). $[\alpha]_D$ -27.6 (c, 0.4 in H_2O).

Asano, N. *et al., Carbohydr. Res.*, 1996, **284**, 169-178 (*isol, pmr, cmr*)
Asano, N. *et al., Eur. J. Biochem.*, 1997, **248**, 296-303 (*isol*)
Schimming, T. *et al., Phytochemistry*, 1998, **49**, 1989-1995 (*occur*)
Dräger, B. *et al., Nat. Prod. Rep.*, 2004, **21**, 211-223 (*rev*)
Biastoff, S. *et al., Alkaloids (Academic Press)*, 2007, **64**, 49-102 (*rev*)

8-Azabicyclo[3.2.1]octan-3-ol, 9CI A-769

3-Hydroxynortropane. 3-Nortropanol

(1*RS*,3*RS*,5*SR*)-*form*

$C_7H_{13}NO$ 127.186

(1*RS*,3*SR*,5*SR*)-*form* [501-33-7]
exo-*form*. ***Nor-ψ-tropine***. *Norpseudotropine*
Alkaloid from the fruit of *Morus alba* (white mulberry). Cryst. (C_6H_6/pentane). Mp 134.5-135° (129-130°).
▶ LD_{50} (mus, orl) 227 mg/kg. RD0875000
Hydrochloride: [14383-51-8]
Cryst. Mp 280-282° dec.
▶ RD0600000
N-*Benzoyl:* [18470-33-2] ***Nortropacocaine***
$C_{14}H_{17}NO_2$ 231.294
Feathery cryst. (synthetic, as picrate). Mp 234° (picrate).
O-*Phenylacetyl:* [104086-62-6] ***Nortropan-3-yl phenylacetate***
$C_{15}H_{19}NO_2$ 245.321
N-*Me:* see 8-Methyl-8-azabicyclo[3.2.1]octan-3-ol, #CCB71-I

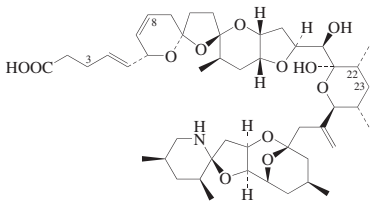
(1*RS*,3*RS*,5*SR*)-*form* [538-09-0]
endo-*form*. *Nortropeine*. *Tropigenin*. *Nortropenol*. *Nortropine*
▶ LD_{50} (mus, orl) 1420 mg/kg. RD0700000
Hydrochloride: [17366-48-2]
Cryst. Mp 200°.
O-*(2-Methylbutanoyl):* [537-28-0] ***Isoporoidine***
$C_{12}H_{21}NO_2$ 211.303
O-*(3-Methylbutanoyl):* [500-58-3] ***Poroidine***
$C_{12}H_{21}NO_2$ 211.303
Co-isol. with Isoporoidine, difficult to separate.
O-*Benzoyl:* ***3α-Benzoyloxynortropane***
$C_{14}H_{17}NO_2$ 231.294
Mp 232° (as picrate).
O-*(4-Methoxybenzoyl):* [76678-90-5] ***Merresectine A***
$C_{15}H_{19}NO_3$ 261.32
Yellow solid.
O-*(3,4-Dimethoxybenzoyl),* N-*propyl:* ***Conpropine***
$C_{19}H_{27}NO_4$ 333.427
Amorph. powder.
O-*Cinnamoyl*(E-*):* [126394-79-4] ***Nortropinyl cinnamate***
$C_{16}H_{19}NO_2$ 257.332
Yellow gum.
O-*Cinnamoyl,* N-*Ac:* [136945-63-6]
Needles (CH_2Cl_2/petrol). Mp 143°.

Barger, G. *et al., JCS*, 1937, 1820-1823 (*Poroidine, Isoporoidine*)
Werner, G. *et al., Annalen*, 1967, **708**, 210-217 (*synth*)
Kraiss, G. *et al., Tet. Lett.*, 1971, **12**, 57-58 (*synth*)

Chappell, G.S. *et al., J. Pharm. Sci.*, 1973, **62**, 414-419 (*nmr*)
Tufariello, J.J. *et al., JACS*, 1979, **101**, 2435-2442 (*synth*)
Al-Yahya, M.A.I. *et al., JCS Perkin 1*, 1979, 2130-2132 (*isol, Poroidine, Isoporoidine*)
El-Imam, Y.M.A. *et al., Phytochemistry*, 1985, **24**, 2285-2289 (*Nortropacocaine*)
Al-Said, M.S. *et al., JCS Perkin 1*, 1986, 957-959 (*phenylacetate*)
Al-Said, M.S. *et al., Phytochemistry*, 1986, **25**, 851-853 (*3-benzoyl*)
Arbain, D. *et al., Aust. J. Chem.*, 1991, **44**, 1013-1015 (*Nortropinyl cinnamate*)
Kusano, G. *et al., Chem. Pharm. Bull.*, 2002, **50**, 185-192 (*isol, pmr, cmr*)
Jenett-Siems, K. *et al., Phytochemistry*, 2005, **66**, 1448-1464 (*Merresectine A*)
Gapparov, A.M. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 2008, **44**, 743-744 (*Conpropine*)

Azaspiracid 1 A-770

Killarytoxin 3 [214899-21-5]



Absolute Configuration

$C_{47}H_{71}NO_{12}$ 842.077

Struct. finally confirmed in 2004. There are various errors in the assignment of CAS numbers to the minor congeners. Alkaloid from *Mytilus edulis* (blue mussel). Shellfish toxin. Amorph. solid. $[\alpha]_D^{20}$ -21 (c, 0.1 in MeOH).

Me ester: ***Azaspiracid 30***
$C_{48}H_{73}NO_{12}$ 856.104
Alkaloid from *Mytilus edulis* (blue mussel).

*3*R*-Hydroxy:* [629656-50-4] ***Azaspiracid 7***
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

*23*R*-Hydroxy:* [629656-53-7] ***Azaspiracid 8***
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

3,23-Dihydroxy: [1021443-12-8] ***Azaspiracid 14***
$C_{47}H_{71}NO_{14}$ 874.076
Alkaloid from *Mytilus edulis* (blue mussel).

21-Deoxy, 21,22-didehydro: ***Azaspiracid 26***
$C_{47}H_{69}NO_{11}$ 824.062
Alkaloid from *Mytilus edulis* (blue mussel).

8-Methyl: [265996-92-7] ***Azaspiracid 2***
$C_{48}H_{73}NO_{12}$ 856.104
Alkaloid from *Mytilus edulis* (blue mussel).

8-Methyl, Me ester: ***Azaspiracid 32***
$C_{49}H_{75}NO_{12}$ 870.131
Alkaloid from *Mytilus edulis* (blue mussel).

*8-Methyl, 3*R*-hydroxy:* [629656-62-8] ***Azaspiracid 11***
$C_{48}H_{73}NO_{13}$ 872.104
Alkaloid from *Mytilus edulis* (blue mussel).

*8-Methyl, 23*R*-hydroxy:* [629656-65-1] ***Azaspiracid 12***
$C_{48}H_{73}NO_{13}$ 872.104
Alkaloid from *Mytilus edulis* (blue mussel).

8-Methyl, 3,23-dihydroxy: [1021443-14-0] ***Azaspiracid 16***
$C_{48}H_{73}NO_{14}$ 888.103
Alkaloid from *Mytilus edulis* (blue mussel).

8-Methyl, 21-deoxy, 21,22-didehydro: ***Azaspiracid 28***
$C_{48}H_{71}NO_{11}$ 838.089
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl: [265996-93-8] ***Azaspiracid 3***
$C_{46}H_{69}NO_{12}$ 828.051
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, Me ester: ***Azaspiracid 29***
$C_{47}H_{71}NO_{12}$ 842.077
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 3*R*-hydroxy:* [344422-49-7] ***Azaspiracid 4***
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 23*S*-hydroxy:* [344422-51-1] ***Azaspiracid 5***
$C_{46}H_{69}NO_{13}$ 844.05
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, 3,23-dihydroxy: [1021443-10-6] ***Azaspiracid 13***
$C_{46}H_{69}NO_{14}$ 860.049
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, 21-deoxy, 21,22-didehydro: ***Azaspiracid 25***
$C_{46}H_{67}NO_{11}$ 810.035
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, 8-methyl: [629656-47-9] ***Azaspiracid 6***
$C_{47}H_{71}NO_{12}$ 842.077
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, 8-methyl, Me ester: ***Azaspiracid 31***
$C_{48}H_{73}NO_{12}$ 856.104
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 8-methyl, 3*R*-hydroxy:* [629656-56-0] ***Azaspiracid 9***
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel).

*22-Demethyl, 8-methyl, 23*R*-hydroxy:* [629656-59-3] ***Azaspiracid 10***
$C_{47}H_{71}NO_{13}$ 858.077
Alkaloid from *Mytilus edulis* (blue mussel). Cahn-Ingold-Prelog priorities change at C-23.

22-Demethyl, 8-methyl, 3,23-dihydroxy: [1021443-13-9] ***Azaspiracid 15***
$C_{47}H_{71}NO_{14}$ 874.076
Alkaloid from *Mytilus edulis* (blue mussel).

22-Demethyl, 8-methyl, 21-deoxy, 21,22-didehydro: ***Azaspiracid 27***
$C_{47}H_{69}NO_{11}$ 824.062
Alkaloid from *Mytilus edulis* (blue mussel).

Carboxy: ***Azaspiracid 18***
$C_{48}H_{71}NO_{14}$ 886.087
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 3-hydroxy: [1021500-92-4] ***Azaspiracid 22***
$C_{48}H_{71}NO_{15}$ 902.087
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 8-methyl: [1021500-90-2] ***Azaspiracid 20***
$C_{49}H_{73}NO_{14}$ 900.114
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 8-methyl, 3-hydroxy: [1021500-94-6] ***Azaspiracid 24***
$C_{49}H_{73}NO_{15}$ 916.113
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 22-demethyl: [1021500-87-7] ***Azaspiracid 17***
$C_{47}H_{69}NO_{14}$ 872.06
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 22-demethyl, 3-hydroxy: [1021500-91-3] ***Azaspiracid 21***
$C_{47}H_{69}NO_{15}$ 888.06
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Carboxy, 22-demethyl, 8-methyl: ***Azaspiracid 19***
$C_{48}H_{71}NO_{14}$ 886.087
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

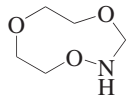
Carboxy, 22-demethyl, 8-methyl, 3-hydroxy: ***Azaspiracid 23***
$C_{48}H_{71}NO_{15}$ 902.087
Alkaloid from *Mytilus edulis* (blue mussel). Posn. of additional carboxy group not determined.

Satake, M. *et al., JACS*, 1998, **120**, 9967-9968 (*Azaspiracid 1*)
Ofuji, K. *et al., Nat. Toxins*, 1999, **7**, 99-102 (*Azaspiracids 2,3*)
Food Sci. Technol., Seafood and Freshwater Toxins, (ed. Botana, L.M.), Marcel Dekker, 2000, **103**,
Ofuji, K. *et al., Biosci., Biotechnol., Biochem.*, 2001, **65**, 740-742 (*Azaspiracids 4,5*)
James, K.J. *et al., Toxicon*, 2003, **41**, 277-283 (*isol, ms*)
Lehane, M. *et al., J. Chromatogr., A*, 2004, **1024**, 63-70 (*hplc-ms*)
Nicolaou, K.C. *et al., Chem. - Asian J.*, 2006, **1**, 245-263 (*synth*)
Nicolaou, K.C. *et al., JACS*, 2006, **128**, 2244-2257; 2258-2267; 2859-2872 (*synth, struct*)
Evans, D.A. *et al., JACS*, 2008, **130**, 16295-16309 (*synth*)

Twiner, M.J. *et al., Mar. Drugs*, 2008, **6**, 39-72 (*rev*)
Rehmann, N. *et al., Rapid Commun. Mass Spectrom.*, 2008, **22**, 549-558 (*isol, ms*)
McCarron, P. *et al., J. Agric. Food Chem.*, 2009, **57**, 160-169 (*Azaspiracids 1,3,6,9, formn*)
Ueoka, R. *et al., Toxicon*, 2009, **53**, 680-684 (*Azaspiracid 2, isol, pmr, ms*)
Furey, A. *et al., Toxicon*, 2010, **56**, 173-190 (*rev, tox*)

1-Aza-2,5,8-trioxacyclononane A-771

Hexahydro-1,4,7,2-trioxaazonine, 9CI



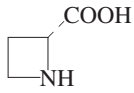
$C_5H_{11}NO_3$ 133.147

N-*Butyl:* [957466-26-1] ***Trigoxazonane***
$C_9H_{19}NO_3$ 189.254
Alkaloid from the roots of *Trigonella foenum-graecum* (fenugreek). Oil.

Evidente, A. *et al., Phytochemistry*, 2007, **68**, 2487-2492 (*isol, pmr, cmr, ms*)

2-Azetidinecarboxylic acid, 9CI A-772

Homoserine lactone (incorr.) [2517-04-6]



(*R*)-*form*

$C_4H_7NO_2$ 101.105

Early isolates before the struct. was clarified were referred to under the name Homoserine lactone. See 3-Aminodihydro-2(3*H*)-furanone, A-381.

(*S*)-*form* [2133-34-8]
Present in roots and leaves of *Convallaria majalis* (lily-of-the-valley). *Convallaria majalis* is banned by the FDA from food use in the USA. Cryst. (MeOH). Sol. H_2O. Mp >121° dec. $[\alpha]_D^{21}$ -121.7 (c, 0.5 in H_2O). Unstable in mineral acids.

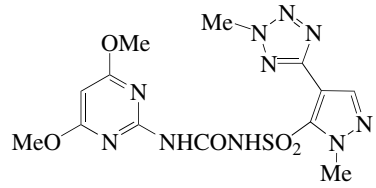
▶ Exp. reprod. and teratogenic effects. LD_{50} (mus, scu) 1000 mg/kg. CM4310500

N-*(3-Hydroxypropyl):* [91106-30-8]
Medicanine
$C_7H_{13}NO_3$ 159.185
Amino acid from seeds of *Medicago sativa* (alfalfa). Hygroscopic cryst. Mp 124-126° (synthetic). $[\alpha]_D$ -92.2 (c, 0.13 in H_2O) (natural). $[\alpha]_D$ -100.5 (c, 0.45 in H_2O) (synthetic).

Fushiya, S. *et al., Heterocycles*, 1984, **22**, 1039-1040 (*Medicanine*)

Azimsulfuron, ANSI, BSI A-773

N-*[[(4,6-Dimethoxy-2-pyrimidinyl)amino]carbonyl]-1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)-1*H*-pyrazole-5-sulfonamide, 9CI. 1-(4,6-Dimethoxy-2-pyrimidinyl)-3-[[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)pyrazol-5-yl]sulfonyl]urea. Gulliver™. IN-A8947. A 8947* [120162-55-2]



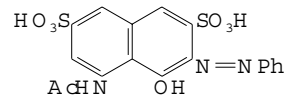
$C_{13}H_{16}N_{10}O_5S$ 424.399
Acetolactate synthase inhibitor. Post-emergence herbicide for control of *Echinochloa* spp., used esp. on rice. Solid. Mp 170°. pK_a 3.6.

▶ LD_{50} (rat, orl) >5000 mg/kg.

US Pat., 1988, (*(DuPont)*)4 746 353 (*synth, activity*)
Marquez, T. *et al., Brighton Crop Prot. Conf. - Weeds*, 1995, 65-72 (*activity*)
Barefoot, A.C. *et al., Brighton Crop Prot. Conf. - Weeds*, 1995, 713-718 (*metab*)
Pesticide Manual, 11th edn., 1997, 39; 63-65
Powley, C.R. *et al., J. Agric. Food Chem.*, 1998, **46**, 514-519 (*anal, hplc*)

Azorhodine 2G A-774

5-(Acetylamino)-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic acid, 9CI. C.I. Acid red 1. C.I. Food red 10. C.I. 18050. Brilliant acid red G. Fast crimson GR. Naphthazine rose 2G. Red 2G. Solar fast red 3G. Vopsider red ASTR G. E128. Many other names



$C_{18}H_{15}N_3O_8S_2$ 465.464
Strictly, the name Azorhodine 2G applies to the disodium salt. Colourant additive for food.

▶ QJ6030000

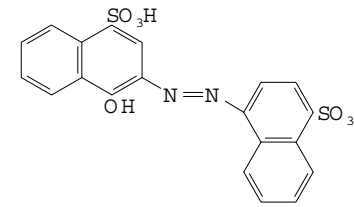
Di-Na salt: [3734-67-6]
$C_{18}H_{13}N_3O_8S_2$ 463.448
Dark red cryst. Sol. H_2O; sl. sol. EtOH; insol. Et_2O.

▶ QJ6030000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 984B (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 29
Popa, G. *et al., Zh. Anal. Khim.*, 1959, **14**, 322 (*detn, Pd*)
Mathur, J.N. *et al., Indian J. Appl. Chem.*, 1970, **33**, 209
Colour Index, *3rd Edn*, 1971, **4**, 4116 (*synth*)
Nemodruk, A.A. *et al., Zh. Anal. Khim.*, 1972, **27**, 326 (*detn, Fe*)

Azorubine A-775

4-Hydroxy-3-[(4-sulfo-1-naphthalenyl)azo]-1-naphthalenesulfonic acid, 9CI. Brilliant carmoisine. Carmoisine. Chromotrope FB. C.I. Chromotrope FB. Lissamine red W. Nacarat. C.I. Acid red 14. C.I. Food red 3. C.I. Mordant blue 79. E122. Many other names [3567-69-9]



$C_{20}H_{14}N_2O_7S_2$ 458.472
Strictly, the name Azorubine applies to the disodium salt. Food dye. Dark red cryst. powder (as Na salt). Na salt sol. H_2O; mod. sol. EtOH; insol. Me_2CO. CAS no. refers to Na salt.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 988C (*ir*)
Sigma-Aldrich Library of Stains, Dyes and Indicators, 204
Colour Index, *3rd Edn*, 1971, **4**, 4068 (*synth*)
Bosch Serrat, F. *et al., An. Quim.*, 1972, **68**, 155 (*detn, Mg*)
Bosch Serrat, F. *et al., Inf. Quim. Anal.*, 1973, **27**, 14 (*detn, Pd*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HJF500

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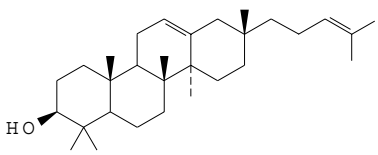
12,21-Baccharadien-3-ol B-1



$C_{30}H_{50}O$ 426.724

3β-*form* [160598-94-7]
Constit. of *Glycine max* (soybean). Cryst. Mp 133-135°.

Akihisa, T. *et al., Phytochemistry*, 1994, **37**, 1413 (*isol, pmr, cmr*)

Bacillolysin B-2

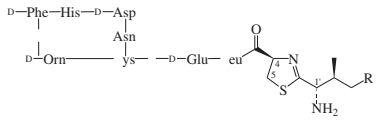
Bacillus metalloendopeptidase. Bacillus subtilis neutral proteinase. E.C. 3.4.24.28 [76774-43-1]

Enzyme, a peptidase of the thermolysin family with Zn and Ca as cofactors. Used for lactose redn. and flavour modification in dairy processing, for fortifying brewing malt proteins and for softening wheat gluten in baking.

Feder, J. *et al., Biochim. Biophys. Acta*, 1971, **251**, 74-78 (*isol*)
Pauptit, R.A. *et al., J. Mol. Biol.*, 1988, **199**, 525-537 (*cryst struct*)

Bacitracin, BAN, INN, JAN, USAN B-3

Bacilliquin. Ayfivin



Bacitracin A = = Ile, R = CH_3
B_1 = = Ile, R = H
B_2 = Val, = Ile, R = CH_3
B_3 = Ile, = Val, R = CH_3
D_1 = Val, = Ile, R = H
D_2 = Ile, = Val, R = H
D_3 = = Val, R = CH_3
= = Val, R = H

Cyclic peptide antibiotic. Nomenclature for minor components was revised in 1995. Permitted food additive for animal and human consumption. Sol. H_2O, $HCONH_2$, 2-propanol, Py, EtOH, MeOH; fairly sol. Me_2CO, butanol, dioxan; poorly sol. EtOAc, hexane. Coml. prod. contains small quantities of other components. λ_{max} 270 (ϵ) (12*M* HCl) (Derep). λ_{max} 252 (ϵ 3550) (EtOH) (Derep).

► Nephrotoxic effects and hypersensitivity reactions reported from therapeutic use (intramuscular administration). LD_{50} (rat, ipr) 190 mg/kg. LD_{50} (gpg, orl) 2000 mg/kg (Bacitracin) ; LD_{50} (mus, ivn) 360 mg/kg , LD_{50} (mus, ipr) 200-640 mg/kg , LD_{50} (mus, scu) 1300-2500 mg/kg. CP0350000

Bacitracin A [22601-59-8]
$C_{66}H_{103}N_{17}O_{16}S$ 1422.71
Permitted food additive for animal and human consumption. Hygroscopic amorph. powder. $[\alpha]_D^{23}$ +5 (c, 0.1 in 0.02*M* HCl).

1′-Deamino, 1′-oxo, 4,5-didehydro: [22601-63-4] ***Bacitracin F***
$C_{66}H_{98}N_{16}O_{17}S$ 1419.663
λ_{max} 288 (ϵ 3980) (EtOH) (Derep).
λ_{max} 289 (ϵ 4830) (MeOH).
Enantiomer: Enantiotracin A

Bacitracin B_1 [57762-79-5]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-64-7] ***Bacitracin H_1***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin B_2 [57762-78-4]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-54-3] ***Bacitracin H_2***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin B_3 [149146-32-7]
$C_{65}H_{101}N_{17}O_{16}S$ 1408.683

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-55-4] ***Bacitracin H_3***
$C_{65}H_{96}N_{16}O_{17}S$ 1405.636

Bacitracin D_1
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-62-5] ***Bacitracin I_1***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin D_2
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [167289-63-6] ***Bacitracin I_2***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin D_3 [144572-46-3]
$C_{64}H_{99}N_{17}O_{16}S$ 1394.656

1′-Deamino, 1′-oxo, 4,5-didehydro: [144572-52-1] ***Bacitracin I_3***
$C_{64}H_{94}N_{16}O_{17}S$ 1391.61

Bacitracin E
$C_{63}H_{97}N_{17}O_{16}S$ 1380.63

[1405-89-6, 1405-87-4]

Newton, G.G.F. *et al., Biochem. J.*, 1950, **47**, 257
Lockhart, I.M. *et al., Biochem. J.*, 1955, **61**, 534 (*struct*)
Weisiger, J.R. *et al., JACS*, 1955, **77**, 731; 3123 (*struct*)
Konigsberg, W. *et al., JOC*, 1962, **27**, 934 (*Bacitracin F, synth*)
Nussbaumer, P.A. *et al., Pharm. Acta Helv.*, 1965, **40**, 210 (*Bacitracin F, chromatog*)
Ressler, C. *et al., JACS*, 1966, **88**, 2025 (*struct*)
Galardy, R.E. *et al., Biochemistry*, 1971, **10**, 2429 (*conformn*)
Tsuji, K. *et al., J. Chromatogr.*, 1975, **112**, 663 (*chromatog*)
Hirotsu, Y. *et al., Pept. Chem.*, 1978, **16**, 171 (*Bacitracin F, synth*)
Storm, D.R. *et al., Antibiotics, Vol. 5*/*Part 1: Mechanism of Action of Antibacterial Agents*, (ed. Hahn, F.E.), Springer, 1979, 1-17 (*rev*)
Brewer, G.A. *et al., Anal. Profiles Drug Subst.*, 1980, **9**, 1 (*rev*)
Toscano, W.A. *et al., Pharmacol. Ther.*, 1982, **16**, 199 (*pharmacol, rev*)
Froeyshov, O. *et al., Drugs Pharm. Sci.*, 1984, **22**, 665 (*isol, props, rev*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 8368
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BAC 250
Pfeffer, S. *et al., FEBS Lett.*, 1991, **285**, 115 (*cryst struct*)
Ikai, Y. *et al., J. Antibiot.*, 1992, **45**, 1325 (*ms, struct*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 121
Ikai, Y. *et al., J. Antibiot.*, 1995, **48**, 233-242 (*isol, struct, abs config*)
Lee, J. *et al., JOC*, 1996, **61**, 3983 (*synth, pmr*)
Kimura, K. *et al., Biosci., Biotechnol., Biochem.*, 1997, **61**, 1754-1756 (*activity*)
McDougal, P.G. *et al., Bioorg. Med. Chem. Lett.*, 2003, **13**, 2239-2240 (*Enantiotracin A*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAC250

Bacteriocin 217 B-4

Peptide, MW *ca.* 7 kDa. Prod. by *Lactobacillus paracasei* ssp. *paracasei* BGBUK2-16 isol. from traditionally homemade white-pickled cheese.

Lozo, J. *et al., J. Food Prot.*, 2004, **67**, 2727-2734 (*isol*)

Bacteriocin AS 48 B-5

Antibiotic AS 48. AS 48 [101516-81-8]

Cyclic polypeptide containing 70 amino acids. Similar to mammalian NK-lysin. Antibacterial food preservative. Sol. H_2O; poorly sol. butanol, hexane. λ_{max} 280 (H_2O) (Berdy).

Galvez, A. *et al., Antimicrob. Agents Chemother.*, 1989, **33**, 437-441 (*isol*)
Samyn, B. *et al., FEBS Lett.*, 1994, **352**, 87-90 (*struct*)
Martinez-Bueno, M. *et al., J. Bacteriol.*, 1994, **176**, 6334-6339 (*struct, props*)
Abriouel, H. *et al., Appl. Environ. Microbiol.*, 1998, **64**, 4623-4626 (*activity*)
Langdon, C.M. *et al., J. Biomol. NMR*, 1998, **12**, 173-175 (*secondary struct*)
González, C. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 11221-11226 (*struct, activity*)
Sánchez-Barrena, M.J. *et al., J. Mol. Biol.*, 2003, **334**, 541-549 (*pmr, cryst struct*)
Maqueda, M. *et al., Curr. Protein Pept. Sci.*, 2004, **5**, 399-416 (*rev*)
Sánchez-Hidalgo, M. *et al., Cell. Mol. Life Sci.*, 2011, **68**, 2845-2857 (*rev*)

Bacteriocin 28b B-6

[148466-49-3]
[173432-00-3]

Peptide. Bacteriocin prod. by *Serratia marcescens* N28b.

Viejo, M.B. *et al., J. Gen. Microbiol.*, 1992, **138**, 1737-1743

Bacteriocin Bc48 B-7

[138635-52-6]

Protein; MW 80 kDa. Bacteriocin prod. by *Enterococcus faecalis* ssp. *liquefaciens* S-48 and its mutant strain B-48-28.

Lopez-Lara, I. *et al., Can. J. Microbiol.*, 1991, **37**, 769-774 (*isol*)
Martinez-Bueno, M. *et al., Plasmid*, 1992, **26**, 61-69

Bacteriocin C3603 B-8

[91315-24-1]

Basic protein. Prod. by *Streptococcus mutans* C3603.

Ikeda, T. *et al., Infect. Immun.*, 1982, **35**, 861-868 (*isol*)

Bacteriocin GM005 B-9

Tetrameric peptide. Prod. by *Lactobacillus* GM005 isol. from miso paste.

Onda, T. *et al., Int. J. Food Microbiol.*, 2003, **87**, 153-159 (*isol*)

Bacteriocin J46 B-10

J46 [173584-72-0]
[181232-45-1]

Polypeptide consisting of 27 amino acid residues. Prod. by *Lactococcus lactis* ssp. *cremoris* J46 isol. from fermented milk. Bacteriocin.

Huot, E. *et al., Anaerobe*, 1996, **2**, 137-145 (*Bacteriocin J46*)

Lasta, S. *et al., J. Antibiot.*, 2008, **61**, 89-93 (*synth, pmr, conformn*)

Bacteriocin PsVP-10 B-11

[212771-49-8]

Peptide. Prod. by *Pseudomonas* sp. R-10.

Hubert, E. *et al., J. Appl. Microbiol.*, 1998, **84**, 910-913 (*isol*)

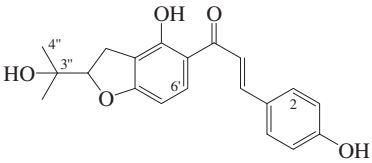
Bacteriocin TH14 B-12

Protein. Prod. by *Provotella intermedia* (*Bacteroides intermedius*).

Takada, K. *et al., J. Periodontol.*, 1991, **62**, 439-444 (*isol*)

Bakuchalcone B-13

1-[2,3-Dihydro-4-hydroxy-2-(1-hydroxy-1-methylethyl)-5-benzofuranyl]-2-propen-1-one, 9CI [84575-13-3]



$C_{20}H_{20}O_5$ 340.375
Pale yellow needles (Me_2CO/hexane). Mp 204-205°. λ_{max} 240 (log ϵ 3.8); 308 (log ϵ 3.7); 366 (log ϵ 4.3) (MeOH).

3′′-Deoxy: [929258-80-0] ***3′′-Deoxybakuchalcone***
$C_{20}H_{20}O_4$ 324.376

3′′-Deoxy, 3′′,4′′-didehydro: [894353-17-4] ***Artonin ZA***. *Lespecyrtin B_1*
[1103683-91-5 (Lespecyrtin B_1)]
$C_{20}H_{18}O_4$ 322.36
Constit. of the leaves of *Artocarpus heterophyllus* (jackfruit). Amorph. solid. $[\alpha]_D^{23}$ +34.1 (c, 1.5 in MeOH). λ_{max} 370 (log ϵ 4.47) (MeOH).

3′′-Deoxy, 3′′,4′′-didehydro, α,β-dihydro: [1103684-02-1] ***Lespecyrtin C_1***
$C_{20}H_{20}O_4$ 324.376
Amorph. solid. $[\alpha]_D^{23}$ +59.4 (c, 1.08 in MeOH). λ_{max} 220 (sh) (log ϵ 4.44); 241 (sh) (log ϵ 4.05); 288 (log ϵ 4.27) (MeOH).

4-Deoxy: [61235-35-6] ***Flemistrictin B***
$C_{20}H_{20}O_4$ 324.376
Orange-yellow needles (C_6H_6/hexane). Mp 135°. $[\alpha]_D^{26}$ -95.9 (c, 0.44 in EtOH).

6′-Hydroxy: ***Desmethylxanthohumol J***
$C_{20}H_{20}O_6$ 356.374
Constit. of hops (*Humulus lupulus*). Yellow-orange solid.

2-Hydroxy, 3′′-deoxy, 3′′,4′′-didehydro: [894353-18-5] ***Artonin ZB***
$C_{20}H_{18}O_5$ 338.359
Constit. of the leaves of *Artocarpus heterophyllus* (jackfruit).

6′-Methoxy, 3′′,4-dideoxy, 3′′,4′′-didehydro: ***Crassichalcone***
$C_{21}H_{20}O_4$ 336.387
Yellow oil. λ_{max} 215 (log ϵ 4.26); 348 (log ϵ 4.25) (MeOH).

Rao, J.M. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 339 (*Flemistrictin B, isol, struct, synth*)

Gupta, G.K. *et al., Phytochemistry*, 1982, **21**, 2149-2151 (*isol, synth, uv, pmr, ms*)

Gomez-Garibay, F. *et al., Phytochemistry*, 1999, **52**, 1159-1163 (*Crassichalcone*)

Chadwick, L.R. *et al., J. Nat. Prod.*, 2004, **67**, 2024-2032 (*Desmethylxanthohumol J*)

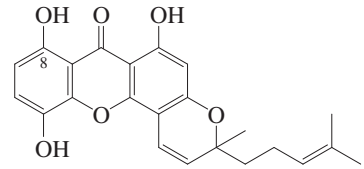
Yao, S. *et al., Zhongguo Tianran Yaowu*, 2005, **3**, 219-223 (*Artonins ZA,ZB*)

Agarwal, D. *et al., Indian J. Chem., Sect. B*, 2006, **45**, 2574-2579 (*3′′-Deoxybakuchalcone*)

Mori-Hongo, M. *et al., J. Nat. Prod.*, 2009, **72**, 63-71 (*Lespecyrtins B_1,C_1*)

Bangangxanthone A B-14

*6,8,11-Trihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3*H*,7*H*-pyrano[2,3-c]xanthen-7-one*



$C_{23}H_{22}O_6$ 394.423
CAS numbering shown.

(+)-*form*
Yellow needles. Mp 157-158°. $[\alpha]_D^{29}$ +25 (c, 0.03 in Me_2CO). λ_{max} 201 (log ϵ 4.22); 210 (log ϵ 4.03); 222 (log ϵ 4.12); 268 (log ϵ 4.4); 336 (log ϵ 4.08); 360 (log ϵ 3.92) (MeOH).

8-Deoxy: [35338-77-3] ***6,11-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3*H*,7*H*-pyrano[2,3-c]xanthen-7-one, 9CI***
$C_{23}H_{22}O_5$ 378.424
Constit. of the root bark of *Garcinia livingstonei* (imbe). Yellow plates. Mp 140-141°. No opt. rotn. reported. λ_{max} 250 (ϵ 31500); 266 (ϵ 30000); 308 (ϵ 9900); 329 (ϵ 11000); 370 (ϵ 3000) (MeOH) (Berdy).

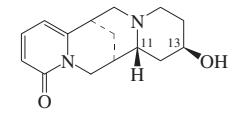
Locksley, H.D. *et al., JCS(C)*, 1971, 3804 (*deoxy, synth*)

Sordat-Diserens, I. *et al., Phytochemistry*, 1992, **31**, 313-316 (*deoxy, isol, pmr, cmr*)

Lannang, A.M. *et al., Phytochemistry*, 2005, **66**, 2351-2355 (*isol, pmr, cmr, ms*)

Baptifoline B-15

13-Hydroxyanagyrine. Alkaloid P3† [732-50-3]



Absolute Configuration

$C_{15}H_{20}N_2O_2$ 260.335
Alkaloid from *Caulophyllum thalictroides* (blue cohosh). Hexagonal or triangular plates (MeOH), needles (Me_2CO). Mp 210°. $[\alpha]_D$ -147.7 (-140) (EtOH). $[\alpha]_D^{16}$ -89.05 (c, 1.415 in H_2O).

Marion, L. *et al., JACS*, 1948, **70**, 3253; 3472 (*isol*)

Martin-Smith, M. *et al., Can. J. Chem.*, 1957, **35**, 37 (*struct*)

Bohlmann, F. *et al., Chem. Ber.*, 1958, **91**, 2189; 2194; 1962, **95**, 944 (*isol, struct, synth*)

Flom, M.S. *et al., J. Pharm. Sci.*, 1967, **56**, 1515 (*isol*)

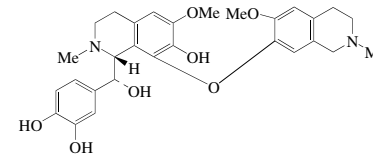
Monakhova, T.E. *et al., Khim. Prir. Soedin.*, 1973, **9**, 59; *Chem. Nat. Compd. (Engl. Transl.)*, 52 (*isol*)

Ohmiya, S. *et al., Phytochemistry*, 1974, **13**, 1016 (*isol*)

Kennelly, E.J. *et al., J. Nat. Prod.*, 1999, **62**, 1385-1389 (*isol, pmr, cmr*)

Bargustanine B-16

[169626-12-4]



$C_{29}H_{34}N_2O_7$ 522.597
Alkaloid from roots of *Berberis vulgaris* (barberry). Cryst. (MeOH). Mp 193-194°. $[\alpha]_D^{20}$ +114.2 (c, 0.3 in MeOH). λ_{max} 218 (sh) (log ϵ 4.85); 286 (log ϵ 3.98) (EtOH).

Karimov, A. *et al., Khim. Prir. Soedin.*, 1993, **29**, 44-47; *Chem. Nat. Compd. (Engl. Transl.)*, 1993, **29**, 35-38

Basrubrins B-17

Two proteins, α-Basrubrin (4.3 kDa) and β-Basrubrin (5 kDa). Isol. from seeds of the Ceylon spinach *Basella rubra*.

[389063-22-3, 389063-37-0]

Wang, H. *et al., Biochem. Biophys. Res. Commun.*, 2001, **288**, 765-770 (*isol*)

Wang, H. *et al., Peptides (N.Y.)*, 2004, **25**, 1204-1209 (*isol*)

Bass hepcidin B-18

Morone *Hepcidin* [452112-54-8]

Gly-Cys-Arg-Phe-Cys-Cys-Asn-Cys-Cys-Pro-Asn-Met-Ser-Gly-Cys-Gly-Val-Cys-Cys-Arg-Phe

$C_{86}H_{128}N_{29}O_{25}S_9$ 2256.731

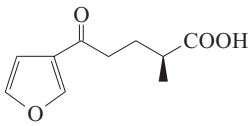
Struct. of reduced form shown. Isol. from

gills of the hybrid striped bass, (white bass (*Morone chrysops*) x striped bass (*Morone saxatilis*)).

Shike, H. *et al., Eur. J. Biochem.*, 2002, **269**, 2232-2237 (*isol*)

Batatic acid B-19

α-Methyl-δ-oxo-3-furanpentanoic acid, 9CI. 5-(3-Furanyl)-2-methyl-5-oxopentanoic acid [496-07-1]



(*S*)–*form*

$C_{10}H_{12}O_4$ 196.202

(*S*)-*form*

Obt. from sweet potato infected with *Ceratostomella fimbriata*. Poorly sol. hexane. Mp 88.5-89.5°. $[\alpha]_D^{10}$ +17.5 (EtOH).

2,4-Dinitrophenylhydrazone: Mp 154.5-155.5°.

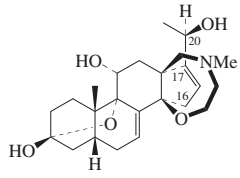
(±)-*form*

Mp 106-107°.

Kubota, T. *et al., Tetrahedron*, 1958, **4**, 68

Batrachotoxinin A B-20

[19457-37-5]



Absolute Configuration

$C_{24}H_{35}NO_5$ 417.544

Toxic principle of poison frogs and beetles. Constit. of skin and feathers of toxic New Guinea birds which feed on the insects, and which are eaten by certain tribes after careful preparation. Minor analogues listed in this entry are also present. Cryst. (hexane/Et_2O). Mp 222-224° (as carbonate salt) Mp 160-162° (synth).

▶ Very toxic. LD_{50} (mus, scu) 1 mg/kg. Avoid skin contact. CR4025000

O^{20}*-(2,4-Dimethyl-3-pyrrolecarboxylate):* [23509-16-2] ***Batrachotoxin***. *BTX*
$C_{31}H_{42}N_2O_6$ 538.683
Toxin found in skin of New Guinea birds which are eaten by some tribes after careful preparation. Noncryst.

▶ V. toxic, avoid skin contact. LD_{50} (mus, ipr) 0.002 mg/kg. LD_{50} (mus, scu) 0.002 mg/kg. Very toxic by intraperitoneal and subcutaneous routes. CR3990000

O^{20}*-(2-Ethyl-4-methyl-3-pyrrolecarboxylate):* [23509-17-3] ***Homobatrachotoxin***
$C_{32}H_{44}N_2O_6$ 552.709
Toxin found in skin of New Guinea birds which are eaten by some tribes after careful preparation. Noncryst.

▶ CR5075000

Daly, J.W. *et al., JACS*, 1965, **87**, 124-126 (*isol, ms, ir, pmr*)

Tokuyama, T. *et al., JACS*, 1969, **91**, 3931-3938 (*isol, ir, uv, pmr, ms, cryst struct, O^{20}-(4-bromobenzoyl)*)

Ger. Pat., 1973, (*(Ciba-Geigy A.G.)*)2 325 873 (*manuf, ir, revised pmr, ms*)

Imhof, R. *et al., Helv. Chim. Acta*, 1973, **56**, 139-162 (*partial synth*)

Witkop, B. *et al., Alkaloids (Academic Press)*, 1983, **21**, 219-223 (*pharmacol*)

Daly, J.W. *et al., Alkaloids: Chem. Biol. Perspect.*, 1986, **4**, 23 (*rev, pharmacol*)

Dumbacher, J.P. *et al., Science (Washington, D.C.)*, 1992, **258**, 799-801 (*Homobatrachotoxin, occur*)

Deligeorges, S. *et al., Recherches*, 1996, **284**, 50-51 (*Homobatrachotoxin, isol*)

Kurosu, M. *et al., JACS*, 1998, **120**, 6627-6628 (*synth*)

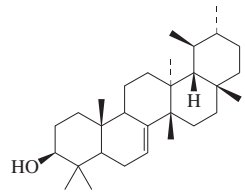
Weldon, P.J. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **21**, 12948-12949 (*rev*)

Dumbacher, J.P. *et al., Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 12970-12975; 2004, **101**, 15857-15860 (*occur, birds, insects*)

Pihko, A.J. *et al., Tetrahedron*, 2005, **61**, 8769-8807 (*synth, rev*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, BAR750

7-Baueren-3-ol B-21



3β-*form*

$C_{30}H_{50}O$ 426.724

3β-*form* [6466-94-0]
Ilexol. *Baurenol*. *Bauerenol*
Cryst. (Me_2CO). Mp 207-208°. $[\alpha]_D^{19}$ -20.7 (c, 0.7 in $CHCl_3$).

Ac: [17020-04-1]
$C_{32}H_{52}O_2$ 468.762
Constit. of *Adansonia digitata* (baobab). Cryst. ($CHCl_3$/hexane). Mp 290-292°. $[\alpha]_D^{24}$ -1.1 (c, 1 in $CHCl_3$).

Me ether: [11008-41-6]
$C_{31}H_{52}O$ 440.751
Constit. of *Saccharum officinarum* (sugar cane). Cryst. (EtOAc). Mp 212-215°. $[\alpha]_D$ -32 (c, 1.2 in $CHCl_3$).

3-Ketone: [6895-55-2] ***7-Bauren-3-one***. *Bauerenone*
$C_{30}H_{48}O$ 424.709
Cryst. (EtOAc). Mp 240°. $[\alpha]_D^{25}$ -47.5 (c, 1 in $CHCl_3$).

(3β,13β)-*form*

Ac: [309724-35-4] ***Mongolenin***
$C_{32}H_{52}O_2$ 468.762
Cryst. ($CHCl_3$). Mp 283-284°. $[\alpha]_D^{12}$ -33 (c, 0.2 in $CHCl_3$).

Bryce, T.A. *et al., Tetrahedron*, 1967, **23**, 1283 (*Me ether*)

Buckley, D.G. *et al., Chem. Ind. (London)*, 1971, 298 (*pmr*)

Fukuoka, M. *et al., Chem. Pharm. Bull.*, 1972, **20**, 974 (*isol, struct*)

Campello, J. de P. *et al., Phytochemistry*, 1975, **14**, 2300 (*ketone*)

Khan, M.R. *et al., Pak. J. Sci. Ind. Res.*, 1979, **22**, 301 (*cmr*)

Tinant, B. *et al., Bull. Soc. Chim. Belg.*, 1982, **91**, 117 (*cryst struct*)

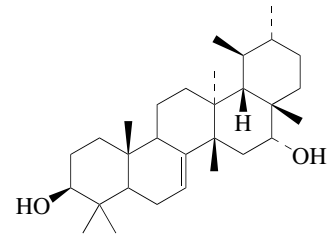
Chakravarty, A.K. *et al., Tetrahedron*, 1991, **47**, 2337 (*cmr*)

Shin, S.C. *et al., CA*, 1993, **119**, 266455w (*Ac*)

Yaoita, Y *et al., Nat. Med. (Tokyo)*, 1998, **52**, 273-275 (*pmr*)

Hu, J.-F. *et al., Nat. Prod. Lett.*, 2000, **14**, 211-215 (*Mongolenin*)

7-Baurene-3,16-diol B-22



$C_{30}H_{50}O_2$ 442.724

(3β,16α)-*form* [214351-30-1]
Constit. of *Tussilago farfara* (coltsfoot). Needles. Mp 282-285°. $[\alpha]_D^{28}$ -25.6 (c, 0.2 in Py).

Yaoita, Y. *et al., Nat. Med. (Tokyo)*, 1998, **52**, 273-275 (*isol, pmr, cmr*)

Bavaricins B-23

Peptides. Prod. by *Lactobacillus bavaricus*. Bacteriocins with potential food uses.

Bavaricin A [154213-77-1]
Prod. by *Lactobacillus bavaricus* MI401. MW 3500-4000; partial struct. reported.

Bavaricin MN [144376-92-1]
Prod. by *Lactobacillus bavaricus* MN. Struct. comprises 42 aminoacid residues, MW 4769.

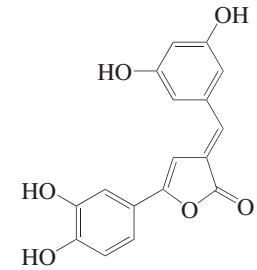
Larsen, A.G. *et al., J. Appl. Bacteriol.*, 1993, **75**, 113-122 (*Bavaricin A*)

Kaiser, A.L. *et al., J. Appl. Bacteriol.*, 1993, **75**, 536-540 (*Bavaricin MN*)

Kaiser, A.L. *et al., Appl. Environ. Microbiol.*, 1996, **62**, 4529-4535 (*Bavaricin MN*)

BE 23372M B-24

5-(3,4-Dihydroxyphenyl)-3-[(3,5-dihydroxyphenyl)methylene]-2(3H)-furanone [145588-13-2]



$C_{17}H_{12}O_6$ 312.278

Sol. MeOH, DMSO, Me_2CO; fairly sol. $CHCl_3$, EtOAc; poorly sol. hexane. λ_{max} 266 (ϵ 8800); 426 (ϵ 20400) (MeOH) (Derep).

(E)-form

Prod. by *Rhizoctonia solani* found on the bark of *Ginkgo biloba* (ginkgo). Red-orange solid. Mp 265-270° dec. λ_{max} 266 (ϵ 8800); 426 (ϵ 20400) (MeOH).

Japan. Pat., 1992, 4 275 284 (*isol, struct, activity*)

Okabe, T. *et al., J. Antibiot.*, 1994, **47**, 289-293; 294-296; 297 (*isol, struct, activity*)

Beijeran B-25

[→3)-α-D-GalA-(1→3)-β-L-Rha-(1→3)-α-D-Glc-6-Ac-(1→]

Exopolysaccharide prod. by *Azotobacter beijerinckii* YNM1. Proposed for use in food industries.

Ogawa, K. *et al., Carbohydr. Res.*, 1997, **300**, 41-45 (*conform*)

Yui, T. *et al., Carbohydr. Res.*, 1997, **304**, 341-345 (*struct*)

Bian, W. *et al., Carbohydr. Res.*, 2002, **337**, 305-314 (*Na salt, cryst struct*)

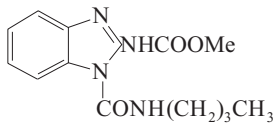
Benincasins B-26

Two arginine/glutamine-rich peptides (α- and β-Benincasins). Isol. from wax gourd seeds.

Ng, T.B. *et al., Peptides (N.Y.)*, 2003, **24**, 11-16 (*isol*)

Benomyl, ANSI, BSI, ISO, JMAF B-27

Methyl 1-[(butylamino)carbonyl]-1H-benzimidazol-2-ylcarbamate, 9CI. Methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate. Agrocit. Benlate. Fundazol. Fungochrom [17804-35-2]



$C_{14}H_{18}N_4O_3$ 290.321

Agricultural and horticultural systemic fungicide mainly used on rice and soybean. V. spar. sol. H_2O; sol. $CHCl_3$; less sol. other org. solvs. Dec. before melting.

▶ Toxic to freshwater fish and aquatic invertebrates. OES: long-term 10 mg m^{-3}; short-term 15 mg m^{-3}. Skin irritant. Can cause contact dermatitis. Exp. reprod. and teratogenic effects. DD6475000

[8068-35-7]

US Pat., 1966, 3 631 176

Tolkmith, H. *et al., Residue Rev.*, 1974, **53**, 99 (*rev*)

Bleidner, W.E. *et al., Anal. Methods Pestic. Plant Growth Regul.*, 1978, **10**, 157 (*rev, props, detn*)

Kirino, O. *et al., Agric. Biol. Chem.*, 1980, **44**, 35 (*activity*)

Cairns, T. *et al., Biomed. Mass Spectrom.*, 1983, **10**, 24 (*ms*)

Dangerous Prop. Ind. Mater. Rep., 1988, **8**, 45 (*rev*)

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A31

Hanson, D.J. *et al., Chem. Eng. News*, November 16, 1992, 4 (*rev, tox*)

Hanson, D.J. *et al., Chem. Eng. News*, April 6, 1992, 15 (*rev, tox*)

Pharmaceutical Manufacturing Encyclopaedia, 1997, No. 60

Handbook of Pesticide Toxicology, (eds. Hayes, W.J. et al), Academic Press, 1991, 1452

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAV575

Bentonite B-28

E558 [1302-78-9]

$Na_{0.33}[Al_{1.67}Mg_{0.33}Si_4O_{10}(OH)_2]$

$[Al_{1.67}H_2Mg_{0.33}Na_{0.33}O_{12}Si_4]$ 367.017

Rock containing Montmorillonite, M-992 and various other clay minerals. Widely distributed mineral. Used in foods as a colourant, pigment and stabiliser.

▶ CT9450000

van Olpen, H. *et al., Clay Colloid Chemistry*, 2nd Edn., Wiley, N. Y., 1977,

Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **5**, 238; 241; **6**, 193; 200 (*rev*)

Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 24-26

Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1536

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 242-243

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAV750

Benzaldehyde, USAN B-29

Benzenecarboxaldehyde. Formylbenzene. FEMA 2127 [100-52-7]

PhCHO

C_7H_6O 106.124

Found in plants, esp. in almond kernels. Also present in strawberry jam, leek, crispbread, cheese, black tea and several essential oils. Parent and derivs. (e.g. glyceryl acetal) are used as flavourings. Liq. with characteristic almond-type odour. V. spar. sol. H_2O; misc. org. solvs. d_4^{15} 1.05. Mp -26° Fp -56.9. Bp 178-179° Bp_{10} 62°. pK_a 14.9 (25°,hydrate, 1% EtOH). pK_a -6.9 (as base). Log P 1.5 (calc). Steam-volatile. Forms bisulfite compd. Slowly oxid. in air. Reduces $AgNO_3.NH_2$ but not Fehling's soln. λ_{max} 244; 280 (MeOH) (Berdy).

▶ Fl. p. 63°, autoignition temp. 190°. Violently oxid. by 90% HCOOOH. Skin irritant. May cause dermatitis. CNS depressant. LD_{50} (rat, orl) 1300 mg/kg. CU4375000

Di-Me acetal: [1125-88-8] *(Dimethoxymethyl)benzene. Dimethoxyphenylmethane. FEMA 2128*

$C_9H_{12}O_2$ 152.193

Constit. of rhubarb and potato. Used in perfumery and food flavouring. Moisture-sensitive liq. $d_4^{15.5}$ 1.03. Bp 198° Bp_{18} 87-89°. n_D^{20} 1.4930.

[3592-47-0, 932-90-1]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 104A (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 932B; **3**, 492A (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1283B; 1578B (*ir*)

Briner, E. *et al., Helv. Chim. Acta*, 1937, **20**, 293

Braude, E.A. *et al., JCS*, 1955, 3754 (*uv*)

Natalis, P. *et al., J. Phys. Chem.*, 1965, **69**, 2943 (*ms*)

Org. Synth., 1971, **51**, 11; 20; 31; 1974, **54**, 42; 1977, **56**, 36 (*synth*)

Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037 (*ir*)

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 693 (*rev, tox*)

Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)

Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 64 (*rev*)

Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1340

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 244; 245 (*use, occur*)

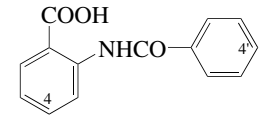
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2561; 2583

Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 106

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BAY500

2-Benzamidobenzoic acid B-30

2-(Benzoylamino)benzoic acid, 9CI. N-*Benzoylanthranilic acid.* ***Dianthramide B***†. *FEMA 4078* [579-93-1]



$C_{14}H_{11}NO_3$ 241.246

The naming system for dianthramides was changed in 1988. Flavouring ingredient. Cryst. (EtOH aq.) with fruity aroma. Sol. MeOH, EtOAc; poorly sol. H_2O. Mp 183-184°. Bp 341-342°. λ_{max} 207; 245; 314 (MeOH) (Berdy). λ_{max} 239; 281; 319 (MeOH/NaOH) (Berdy).

Zentmeyer, D.T. *et al., JOC*, 1949, **14**, 967-981 (*synth*)

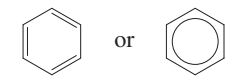
Hauteville, M. *et al., J. Het. Chem.*, 1988, **25**, 715 (*synth, ir, pmr*)

Lee, C.K. *et al., JOC*, 1989, **54**, 3744-3747 (*synth, uv, ir, pmr*)

Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 142 (*use, props*)

Benzene B-31

Cyclohexatriene. [6]Annulene [71-43-2]



C_6H_6 78.113

Used in processing of modified hop extract. May arise at low levels in soft drinks by decarbonylation of benzoic acid preservative in the presence of

Ascorbic acid, A-687 or Isoascorbic acid, I-96. Liq. V. spar. sol. H_2O; misc. most org. solvs. d_4^{20} 0.88. Mp 5.53°. Bp 80.8° (80.103°, 80.12°, 80.36°, 80.49°). n_D^{20} 1.5014. The name Benzene should not be confused with Benzol(e) (coml. products consisting mainly of benzene) or with Benzin(e) (obsolescent name for low-boiling petroleum spirit). The German name for Benzene is however Benzol. First isol. by Faraday in 1825. λ_{max} 184 (log ϵ 4.78); 202 (log ϵ 3.8); 240 (log ϵ 2); 246 (log ϵ 2.3); 253 (log ϵ 2.4); 260 (log ϵ 2.2) (heptane).

▶ Highly flammable, fl. p. -11°. Human carcinogen (IARC group 1). Direct skin contact with liq. causes erythema and vesiculation; prolonged contact can cause dermatitis. Acute exposure by ingestion or inhalation produces the symptoms of CNS depression, and depression of haematopoietic system. Prolonged or repeated exposure injures the bone marrow (often irreversibly) and depletes erythrocytes, leukocytes or platelets producing headache, fatigue, anorexia. More severe exposure is associated with development of pancytopenia and aplastic anaemia. Various forms of leukaemia are implicated in occup. exposures. MEL: long-term 5 ppm. CY1400000

Picrate: Mp 82-84°. Readily dissociates on exp. to air.

[1120-89-4, 1076-43-3, 34504-50-2]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 931A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 849A (*ir*)
Kekulé, A. *et al., Annalen*, 1866, **137**, 129; 1872, **162**, 77 (*struct*)
Ingold, C.K. *et al., Proc. R. Soc. London, A*, 1938, **169**, 149 (*struct*)
Rybicka, S.M. *et al., JCS*, 1950, 3671 (*props*)
Adv. Chem. Ser., 1955, **15**, 11 (***props***)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1969, **2**, 21; 125; 1972, **3**, 288; 1977, **6**, 364 (*use*)
Šantavý, F. *et al., Coll. Czech. Chem. Comm.*, 1972, **37**, 1825 (*uv*)
Newton, M.D. *et al., JACS*, 1974, **96**, 17 (*struct*)
Norbeck, J.M. *et al., JACS*, 1974, **96**, 3386 (*struct*)
Hancock, E.G. *et al., Benzene and its Industrial Derivatives*, Benn, Tonbridge and London, 1975, (*book*)
Obenland, S. *et al., JACS*, 1975, **97**, 6633
Cardinal, J.R. *et al., J. Phys. Chem.*, 1978, **82**, 1614 (*uv*)
Medved, M. *et al., Org. Mass Spectrom.*, 1979, **14**, 307 (*ms*)
Fielder, R.J. *et al., HSE Toxicity Review 4: Benzene*, HMSO, London, 1982,
Cooper, D.L. *et al., Nature (London)*, 1986, **323**, 699 (*struct*)
Kalf, G.F. *et al., Crit. Rev. Toxicol.*, 1987, **18**, 141 (*metab, box*)
Askoy, M. *et al., Benzene Carcinogenicity*, CRC Press, 1988, (*tox*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Takayanagi, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 2491 (*cryst struct, picrate*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, 73 (*rev, bibl*)
Snyder, R. *et al., Environ. Health Perspect.*, 1993, **100**, 293 (*tox, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1099
Environ. Health Perspect., Suppl. 6, 1996, **104**, (*rev, tox*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 247-248
Nyman, P.J. *et al., J. Agric. Food Chem.*, 2008, **56**, 571-576 (*detn, glc, beverages*)
IARC Monogr. (Web), http://monographs.iarc.fr
Snyder, C.A. *et al., Ethel Browning's Toxicity and Metabolism of Industrial Solvents, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1*, 1987, 3 (*rev, tox*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2149
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 103
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 107
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BBL250

Benzenecarbothioic acid, 9CI B-32

Thiobenzoic acid, 8CI. Monothiobenzoic acid [98-91-9]

PhCOSH⇔PhC(S)OH

C_7H_6OS 138.19

Yellow oil cryst. on chilling in ice. Mp 15-18° Mp 24°. pK_a 2.66 (H_2O).

▶ LD_{50} (rat, ipr) 350 mg/kg. DH6839000

SH-form

Me ester: [5925-68-8] S-*Methyl benzenecarbothioate.* S-*Methyl thiobenzoate. FEMA 3857*

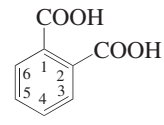
C_8H_8OS 152.217

Flavouring agent for foods. Yellow liq. Bp 210-212°. λ_{max} 234 (ϵ 4580) (CH_2Cl_2).

Org. Synth., Coll. Vol., 4, 1963, 924 (*synth*)
Mori, M. *et al., Int. J. Sulfur Chem., Part A*, 1972, **2**, 79 (*esters*)
Zhou, X. *et al., Synth. Commun.*, 1989, **19**, 3143 (*synth, pmr*)
Garcia, J. *et al., Synthesis*, 1989, 305 (*S-alkyl esters*)
Katritzky, A.R. *et al., Org. Prep. Proced. Int.*, 1995, **27**, 361 (*synth, Me ester, benzyl ester, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1217 (*S-Me ester*)
Thiel, V. *et al., Org. Biomol. Chem.*, 2010, 234-246 (*Me ester, synth, marine isol*)

1,2-Benzenedicarboxylic acid, 9CI B-33

Phthalic acid, 8CI. Alizarinic acid. Naphthalinic acid† *. Phthalinic acid* [88-99-3]



$C_8H_6O_4$ 166.133

Plates (H_2O). Sol. hot H_2O, alkalis; mod. sol. H_2O, EtOH; spar. sol. Et_2O. Mp 210° dec Mp 234°. pK_{a1} 2.95; pK_{a2} 5.41 (25°,H_2O). Forms anhydride at Mp. Frequent reports of the isol. of phthalate esters as nat. prods. are in prob. all cases erroneous because of their ubiquitous presence in solvs., laboratory plastics, etc. as plasticisers.

▶ Fl. p. 168°. Violent reaction on heating with $NaNO_2$. Skin and mucous membrane irritant. Low acute mammalian toxicity. TH9625000

Bis(2-ethylnonyl) ester: Bis(2-ethylnonyl) phthalate

$C_{30}H_{50}O_4$ 474.723

Reported as a nat. prod. from the red alga *Acanthophora spicifera*. Nat. occurrence doubtful in view of the widespread presence of phthalate esters in the environment.

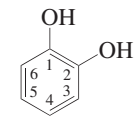
[4409-98-7, 10197-71-4, 79723-02-7, 131-15-7, 102904-15-4, 523-24-0, 15968-01-1, 3198-29-6]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 200D; 274A; 307B; 307C; 307D; 308A; 351D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1088A; 1274C; 1274A; 1275B; 1275A; 1275C; 1276A; 1276B; 1276C; 1277B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1375B; 1375C; 1375D; 1376A; 1376B; 1376C; 1376D; 1377A (*ir*)
Aldrich Library of NMR Spectra, **6**, 153B (*pmr*)
Registry of Mass Spectral Data, Wiley-Interscience, 543 (*ms*)
Sadtler Standard C-13 NMR Spectra, 979 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 1730 (*uv*)
Welcher, F.J. *et al., Organic Analytical Reagents*, Van Nostrand, N.Y., 1947, **2**, 75 (*use*)
Matsuda, S. *et al., CA*, 1958, **52**, 9995c (*esters, synth, props*)
Cross, B.E. *et al., JCS*, 1963, 2937-2943 (*isol*)
Toxicol. Ind. Health, 1987, **3**, 7; 99; 151; 165 (*esters, tox*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **18**, 991 (*rev*)
Wahidulla, S. *et al., Phytochemistry*, 1998, **48**, 1203-1206 (*isol, bis-2-ethylnonyl ester*)

1,2-Benzenediol, 9CI B-34

Pyrocatechol, 8CI. Catechol† *. 1,2-Dihydroxybenzene. Catechin (obsol.)*† [120-80-9]

[12385-08-9]



$C_6H_6O_2$ 110.112

Constit. of var. foodstuffs esp. coffee, cocoa, bread crust, roasted malt and beer. Needles (H_2O). Sol. H_2O, EtOH, Et_2O, C_6H_6, $CHCl_3$, Py. Mp 105°. Bp 240°. pK_{a1} 9.23; pK_{a2} 13 (25°). Log P 0.88 (calc). Sublimes. Steam-volatile.

▶ Explodes on contact with conc. HNO_3. Fl. p. 126/127°. Skin, eye and respiratory tract irritant. Prolonged or repeated exp. can also cause dermatitis. Cocarcinogen in exp. skin-painting studies. Possible human carcinogen (IARC 2B). LD_{50} (rat, orl) 260 mg/kg. LD_{50} (rbt, skn) 800 mg/

kg. Exp. reprod. effects. OES: long-term 5 ppm. UX1050000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1072B; 1072D; 1101B; 1172A; 1264B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 180C; 247C; 248A; 294C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1004D; 1005A; 1037A (*ir*)
Registry of Mass Spectral Data, Wiley, 128 (*ms*)
Sadtler Standard C-13 NMR Spectra, 4428 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 2572 (*uv*)
Org. Synth., Coll. Vol., 1, 1932, 149
Rosotte, R. *et al., Chim. Anal. (Paris)*, 1959, **41**, 229 (*detn, Ta*)
Ackermann, G. *et al., Talanta*, 1962, **9**, 1015 (*detn, Nb*)
Busev, A.I. *et al., Zh. Anal. Khim.*, 1968, **23**, 1348 (*detn, W*)
Gibalo, I.M. *et al., Zh. Anal. Khim.*, 1971, **26**, 1531 (*detn, Nb*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 996 (*rev*)
Lang, R. *et al., J. Agric. Food Chem.*, 2006, **54**, 5755-5762 (*occur, formn*)
IARC Monogr. (Web), http://monographs.iarc.fr

1,3-Benzenediol, 9CI B-35

Resorcinol, 8CI. 1,3-Dihydroxybenzene. Astriderm. Reso. Resorcin. Rezacuid. FEMA 3589 [108-46-3]
[12385-08-9]

$C_6H_6O_2$ 110.112
Present in roasted barley, cane molasses, coffee, beer and wine. Flavouring ingredient. Platelets (EtOH). Sol. Et_2O, H_2O, EtOH, C_6H_6; sl. sol. $CHCl_3$. Mp 111°. Bp 280°. pK_{a1} 9.3; pK_{a2} 11.06 (20°). Log P 0.81 (calc).

▶ Fl. p. 127°, autoignition temp. 608°. Skin and eye irritant. Possible skin sensitiser. Can cause restlessness, methaemoglobinaemia, convulsions and other systemic effects by skin absorption and ingestion. LD_{50} (rat, orl) 301 mg/kg. OES: long-term 10 ppm; short-term 20 ppm. VG9625000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1057B; 1104C; **2**, 300A; 312D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 212B; 300A; 1289A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 988B; 1039B; 1380C; 1380B (*ir*)
Registry of Mass Spectral Data, Wiley, 128 (*ms*)
Sadtler Standard C-13 NMR Spectra, 4428 (*cmr*)
Sadtler Standard Ultraviolet Spectra, 2572 (*uv*)
Kim, Y.C. *et al., Fundam. Appl. Toxicol.*, 1987, **9**, 409 (*metab*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **13**, 996 (*rev*)
Resorcinol: Its uses and derivatives, (ed. Dressler, H.), Plenum Press, New York, 1994, (***book***)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996,
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2420-2421
Durairaj, R.B. *et al., Resorcinol: Chemistry, Technology and Applications*, 2005, (***book***)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1791 (*use*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 501
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1092
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, HNH500; REA000; REF050; REA100; RDZ900

1,4-Benzenediol, 9CI B-36

Hydroquinone, 8CI, USAN. *1,4-Dihydroxybenzene. Hydroquinol. Quinol. Arctuvin. Eldopaque. Eldoquin. Pyrogentisinic acid. Pyrogentisic acid. Tecquinol* [123-31-9]
[12385-08-9]

$C_6H_6O_2$ 110.112
Needles (H_2O). Sol. MeOH. Mp 172°. Bp_{730} 285°. pK_{a1} 9.91; pK_{a2} 11.56 (20°). Log P 0.81 (calc). Component of Artra and Solaquin. λ_{max} 227; 295 (MeOH) (Berdy). λ_{max} 250 (ϵ 204) ($CHCl_3$) (Berdy).

▶ Fl. p. 165°, autoignition temp. 515°. Eye irritant. Prolonged or repeated exposure can cause corneal pigmentation and other damage to the eyes. Repeated skin contact produces irritation; sensitisation, dermatitis, and depigmentation. LD_{50} (rat, orl) 320 mg/kg. OES: long-term 2 mg m^{-3}; short-term 4 mg m^{-3}. Exp. carcinogen. MX3500000

O-*[5-O-Benzoyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* ***Cucurbitoside E***
$C_{24}H_{28}O_{12}$ 508.478
Constit. of the seeds of *Cucurbita moschata* (pumpkin). Amorph. powder. $[\alpha]_D^{25}$ -77 (c, 0.3 in MeOH). λ_{max} 225 (log ϵ 4.11); 284 (log ϵ 3.4) (MeOH).

Mono-Et ether: [622-62-8] *4-Ethoxyphenol. FEMA 3695*
$C_8H_{10}O_2$ 138.166
Isol. from Chinese star anise oil (*Illicium verum*). Food flavourant. Leaflets (H_2O) with sweet herbaceous odour. Sl. sol. H_2O; sol. C_6H_6, Me_2CO, EtOAc, EtOH. Mp 66-67°. Bp 246° Bp 246-247°. pK_{a1} 10.13 (25°).

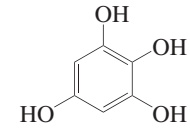
▶ SL3790000

[3225-30-7, 1122-95-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1079A; 1079B; 1079D; 1107D; 1169B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 254B; 255A; 255C; 304C; 411C; 1289B (*nmr*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, nos. 203; 205; 208
Tashiro, M. *et al., Synthesis*, 1979, 988-989 (*monoethers, synth, ir*)
Koike, K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 225-228 (*Cucurbitoside E*)

1,2,3,5-Benzenetetrol, 9CI, 8CI B-37

1,2,3,5-Tetrahydroxybenzene [634-94-6]



$C_6H_6O_4$ 142.111
Needles (H_2O). Mp 168-170° (165°).

1-Me ether, 2-O-[4-hydroxy-3,5-dimethoxybenzoyl-(→6)-β-D-glucopyranoside]:
$C_{22}H_{26}O_{13}$ 498.44
Constit. of *Rumex acetosa* (sorrel).

1,3-Di-Me ether, 2-O-β-D-glucopyranoside: [121748-12-7] *4-Hydroxy-2,6-dimethoxyphenyl glucoside.* ***Leonuriside A***
$C_{14}H_{20}O_9$ 332.307
Constit. of *Coix lachryma-jobi* (Job's tears) and *Prunus* sp. Needles (Me_2CO aq.). Mp 232-234°. $[\alpha]_D^{25}$ -44.4 (c, 0.2 in Me_2CO/MeOH).

1,3-Di-Me ether, 5-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [1124321-98-7]
$C_{20}H_{30}O_{14}$ 494.449
Constit. of wheat germ (*Triticum aestivum*). Powder. λ_{max} 204 (log ϵ 4.65); 226 (sh) (log ϵ 3.8); 280 (log ϵ 3.3) (MeOH/AcOH aq.).

1,3-Di-Me ether, 5-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [1124321-99-8]
$C_{26}H_{40}O_{19}$ 656.591
Constit. of wheat germ (*Triticum aestivum*). Powder. $[\alpha]_D^{24}$ -41.7 (c, 0.16 in H_2O). λ_{max} 204 (log ϵ 4.64); 226 (sh) (log ϵ 3.8); 280 (log ϵ 3.28) (MeOH/AcOH aq.).

1,2,3-Tri-Me ether, 5-O-β-D-glucopyranoside: [41514-64-1]
$C_{15}H_{22}O_9$ 346.333
Constit. of *Quillaja saponaria* (soap-bark tree). Needles (Et_2O/MeOH). Mp 201-203°. $[\alpha]_D^{20}$ -22.3 (c, 0.38 in MeOH).

1,2,3-Tri-Me ether, 5-O-[2,6-bis(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside]: [125288-23-5] *3,4,5-Trimethoxyphenyl 2,6-digalloylglucoside*
$C_{29}H_{30}O_{17}$ 650.546
Isol. from *Psidium guajava* (guava). Needles + $3H_2O$ (H_2O). Mp 269-271°. $[\alpha]_D^{26}$ -33.5 (c, 0.5 in Me_2CO).

1,2,3-Tri-Me ether, 5-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [87562-76-3] ***Kelampayoside A***
$C_{20}H_{30}O_{13}$ 478.449
Isol. from *Cinnamomum cassia* (Chinese cinnamon). Amorph. powder; needles (as hexa-Ac). Mp 132-134° (hexa-Ac). $[\alpha]_D^{25}$ -99.8 (c, 0.5 in MeOH) (-81.7). λ_{max} 205 (ϵ 42660); 225 (ϵ 12300); 275 (ϵ 3800) (MeOH).

1,2,3-Tri-Me ether, 5-Ac: [17742-46-0]
$C_{11}H_{14}O_5$ 226.229
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. (MeOH aq.). Mp 74°.

1,3,5-Tri-Me ether, Ac: [30225-90-2]
$C_{11}H_{14}O_5$ 226.229
Constit. of *Eucalyptus globulus* (Tasmanian blue gum). Cryst. (EtOH aq.). Mp 100°.

[67173-66-4, 68944-24-1, 108543-42-6, 87562-77-4]

Hattori, S. *et al., Acta Phytochim.*, 1931, **5**, 219-237 (*1,2,3-tri-Me ether, synth*)
Hue, R. *et al., Bull. Soc. Chim. Fr.*, 1970, 3617-3624 (*synth, Me ethers*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1982, **30**, 2061-2068 (*Trimethoxyphenyl galloylglucoside*)
Sargent, M.V. *et al., JCS Perkin 1*, 1982, 403-411 (*synth, 1,3,5-tri-Me ether*)
Miyamura, M. *et al., Phytochemistry*, 1983, **22**, 215-218 (*Trimethoxyphenyl apiofuranosylglucoside*)
Shimomura, H. *et al., Phytochemistry*, 1988, **27**, 644-646 (*isol, pmr, cmr*)
Otsuka, H. *et al., Phytochemistry*, 1989, **28**, 883-886; 1990, **29**, 3823-3825 (*Leonuriside A*)
Fuchino, H. *et al., Chem. Pharm. Bull.*, 1995, **43**, 1937-1942 (*tri-Me ether apiosylglucoside*)
Kitagawa, I. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1162-1167 (*Kelampayosides*)
Santos, G.G. *et al., Phytochemistry*, 1997, **44**, 1309-1312 (*Eucalyptus globulus constits*)
Sugaya, K. *et al., CA*, 1999, **130**, 279238e (*Leonuriside A*)
Duynstee, H.I. *et al., Tetrahedron*, 1999, **55**, 9881-9898 (*Kelampayosides, synth*)
Anke, J. *et al., Planta Med.*, 2006, **72**, 995 (*Rumex acetosa constit*)
Zhokhov, S.S. *et al., J. Nat. Prod.*, 2009, **72**, 656-661 (*wheat germ glucosides*)

Benzenethiol, 9CI B-38

Thiophenol. Phenyl mercaptan. Mercaptobenzene. FEMA 3616 [108-98-5]

PhSH

C_6H_6S 110.179
Flavouring agent. Constit. of cooked beef. Liq. with penetrating odour. d_4^{20} 1.08 d_4^{25} 1.97. Fp -14.8. Bp 169.5° Bp_{30} 77°. n_D^{20} 1.5893.

▶ Violent explosion has resulted during prep. from benzenediazonium chloride. Flammable, fl. p. 50 (rat, orl) 46 mg/kg. LD_{50} (rat, skn) 300 mg/kg. LC_{50} (rat, ihl) 33 ppm (4h exposure). OES: long-term 0.5 ppm. DC0525000

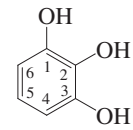
S-*Me:* see Methyl phenyl sulfide, M-392

[3111-52-2, 13133-62-5, 930-69-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1173A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 415A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1089A (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 504 (*synth, bibl*)
Adv. Chem. Ser., 1955, **15**, 325 (***props***)
Lawesson, S.-O. *et al., Acta Chem. Scand.*, 1966, **20**, 2325 (*ms*)
Wagner, A.W. *et al., Chem. Ber.*, 1966, **99**, 375 (*synth*)
Jenden, D.L. *et al., Anal. Chem.*, 1968, **40**, 125; 1972, **44**, 1879 (*use*)
Jones, I.W. *et al., JCS Perkin 2*, 1973, 1125 (*uv*)
Overman, L.E. *et al., Synthesis*, 1974, 59 (*synth*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1977, **6**, 585; 1979, **7**, 367; 1980, **8**, 420; 1981, **9**, 312; 447; 465; 1982, **10**, 281; 399; 1984, **11**, 57; 1986, **12**, 485; 505; 545; 1988, **13**, 297; 312; 1992, **16**, 372 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 248-249
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 137 (*use*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2200
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 110
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, PFL850

1,2,3-Benzenetriol, 9CI B-39

Pyrogallol, 8CI. 1,2,3-Trihydroxybenzene. Pyrogallic acid [87-66-1]



$C_6H_6O_3$ 126.112
Constit. of coffee, cocoa, bread crust, potato crisps, roasted malt and beer. Plates or needles. V. sol. H_2O, EtOH, Et_2O; sl. sol. $CHCl_3$, C_6H_6. Mp 133-134°. Bp 309° Bp_{12} 171.5°. pK_{a1} 9.28; pK_{a2} 11.34 (20°, μ = 0.1). Bitter taste. Readily absorbs O_2. λ_{max} 244; 267; 275 (MeOH) (Berdy).

▶ Stains skin and hair black. Skin and eye irritant. Skin absorption can cause methaemoglobinaemia, haemolysis and kidney damage. LD_{50} (mus, orl) 300 mg/kg. Exp. reprod. and teratogenic effects. UX2800000

1,3-Di-Me ether: [91-10-1] *2,6-Dimethoxyphenol. Syringol. FEMA 3137*
$C_8H_{10}O_3$ 154.165
Isol. from maple syrup and var. *Allium* spp. Flavouring ingredient. Spar. sol. H_2O; sol. EtOH, Et_2O. Mp 55-56°. Bp 262-267°.

▶ SL0900000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1046D; 1081C; 1083D; 1101C; 1103D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 193A; 258A; 261C; 295C; 299A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 975C; 1014A; 1017A; 1037D; 1038D (*ir*)
Shipchandler, M.T. *et al., JCS Perkin 1*, 1975, 1400 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **18**, 670 (*rev*)
Ollis, W.D. *et al., Phytochemistry*, 1978, **17**, 1383; 1401 (*3-Methoxy-1,2-benzenediol, 2,3-Dimethoxyphenol, isol*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 842-843 (*1,3-di-Me ether*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 451 (*1,3-di-Me ether*)
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 1088
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DOJ200; PPQ500

1,2,4-Benzenetriol, 9CI, 8CI B-40

1,2,4-Trihydroxybenzene. Hydroxyhydroquinone. Hydroxyquinol [533-73-3]

$C_6H_6O_3$ 126.112
Plates (Et_2O). Sol. H_2O. Mp 140.5° subl. pK_{a1} 9.08; pK_{a2} 11.82 (20°).

▶ LD_{50} (mus, scu) 120 mg/kg. DC4200000

2-Me ether, 1-O-[4-hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]: [1005452-03-8] ***6′-O-Vanilloylisotachioside***
$C_{21}H_{24}O_{11}$ 452.414
Constit. of the leaves of *Baccaurea ramiflora* (Burmese grape). Amorph. powder. $[\alpha]_D^{19}$ -29.8 (c, 0.56 in MeOH). λ_{max} 202 (log ε 4.46); 221 (log ε 4.2); 263 (log ε 3.82); 288 (log ε 3.69); 362 (log ε 2.47) (MeOH).

2-Me ether, 1-O-[4-hydroxy-3,5-dimethoxybenzoyl-(→6)-β-D-glucopyranoside]: [945259-61-0] ***Apinoside A***†
$C_{22}H_{26}O_{12}$ 482.44
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal).

2-Me ether, 1-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [1124322-01-5]
$C_{25}H_{38}O_{18}$ 626.564
Constit. of wheat germ (*Triticum aestivum*). Powder. λ_{max} 196 (log ε 4.57); 220 (log ε 3.83); 284 (log ε 3.4) (MeOH/AcOH aq.).

2-Me ether, 4-O-[4-hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]: [1005452-04-9] ***6′-O-Vanilloyltachioside***
$C_{21}H_{24}O_{11}$ 452.414
Constit. of the leaves of *Baccaurea ramiflora* (Burmese grape). Amorph. powder. $[\alpha]_D^{20}$ -22.4 (c, 0.58 in MeOH). λ_{max} 202 (log ε 4.27); 220 (log ε 4.05); 265 (log ε 3.63); 288 (log ε 3.53); 361 (log ε 2.38) (MeOH).

2-Me ether, 4-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [1124321-96-5]
$C_{19}H_{28}O_{13}$ 464.422
Constit. of wheat germ (*Triticum aestivum*). Powder. $[\alpha]_D^{24}$ -47.5 (c, 0.07 in H_2O). λ_{max} 196 (log ε 4.58); 220 (log ε 3.76); 284 (log ε 3.44) (MeOH/AcOH aq.).

2-Me ether, 4-O-[β-D-glucopyranosyl-(1→6)-β-D-glucopyranosyl-(1→6)-β-D-glucopyranoside]: [1124321-91-0]

$C_{25}H_{38}O_{18}$ 626.564
Constit. of wheat germ (*Triticum aestivum*). Powder. $[\alpha]_D^{24}$ -48.7 (c, 0.42 in H_2O). λ_{max} 196 (log ϵ 4.58); 220 (log ϵ 3.75); 284 (log ϵ 3.48) (MeOH/AcOH aq.).

*2-Me ether, 4-*O*-[β-*D*-glucopyranosyl-(1→6)-β-*D*-glucopyranosyl-(1→6)-β-*D*-glucopyranosyl-(1→6)-β-*D*-glucopyranoside]:* [1124321-94-3]
$C_{31}H_{48}O_{23}$ 788.706
Constit. of wheat germ (*Triticum aestivum*). Powder. λ_{max} 196 (log ϵ 4.56); 220 (log ϵ 3.73); 284 (log ϵ 3.45) (MeOH/AcOH aq.).

An, N. *et al., Yaoxue Xuebao*, 2006, **41**, 233-235 (*Apinoside A*)
Yang, X.-W. *et al., Planta Med.*, 2007, **73**, 1415-1417 (*6′-Vanilloyltachioside, 6′-Vanilloylisotachioside*)
Zhokhov, S.S. *et al., J. Nat. Prod.*, 2009, **72**, 656-661 (*wheat germ glucosides*)

1,3,5-Benzenetriol, 9CI B-41

1,3,5-Trihydroxybenzene. ***Phloroglucinol****. Phloroglucin. Dilospan S. Spasfon-Lyoc* [108-73-6]

$C_6H_6O_3$ 126.112
Leaflets or plates + $2H_2O$ (H_2O). Mod. sol. H_2O; sol. EtOH, Et_2O, Py, Me_2CO. Mp 117° (dihydrate) Mp 217-219° (anhyd.) (rapid heat) Mp 200-209° (slow heat). pK_{a1} 7.97; pK_{a2} 9.23 (20°). Log P 0.14 (calc). Forms polymers with aldehydes and with diamines; no coml. importance.

▶ Skin and eye irritant. LD_{50} (rat, orl) 5200 mg/kg. Exp. reprod. effects. SY1050000

O-*β-D-Glucopyranoside:* [28217-60-9]
Phlorin
$C_{12}H_{16}O_8$ 288.254
Isol. from thyme (*Thymus vulgaris*) and from citrus fruit. Proposed marker for adulteration of orange juice with peel. Cryst. Mp 231-233°. $[\alpha]_D^{22}$ -74.58.

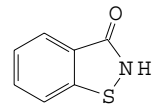
O-*[3,4,5-Trihydroxybenzoyl-(→6)-β-D-glucopyranoside]:* [94356-21-5] *3,5-Dihydroxyphenyl 1-*O*-(6-*O*-galloyl-β-D-glucopyranoside)*
$C_{19}H_{20}O_{12}$ 440.36
Isol. from commercial rhubarb (*Rheum* spp.). Needles + $1H_2O$ (H_2O). Mp 168-169°. $[\alpha]_D^{25}$ -41.2 (c, 0.59 in MeOH).

[6099-90-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1050B; 1085C; 1106D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 202B; 264A; 303B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 982A; 1018D; 1040D (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 455-457 (*synth*)
McKillop, A. *et al., Synth. Commun.*, 1974, **4**, 35-43 (*synth*)
Kashiwada, Y. *et al., Chem. Pharm. Bull.*, 1984, **32**, 3461-3471 (*6-galloylglucoside*)
Highet, R.J. *et al., JOC*, 1988, **53**, 2843-2844 (*tautom, props*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **19**, 792-799 (*rev, props, tox*)
Louche, L.M.-M. *et al., J. Agric. Food Chem.*, 1998, **46**, 4193-4197 (*Phlorin*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, PGR000; 1992, TKY250

1,2-Benzisothiazol-3(2*H*)-one, 9CI B-42

1,2-Benzisothiazolinone. 2-Thiobenzimide. Proxel [2634-33-5]



C_7H_5NOS 151.189
Industrial biocide. Present in can-end cements. Needles (EtOH aq.). Mp 157-158°.

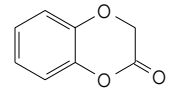
▶ DE4620000

S-*Oxide:* [14599-38-3]
$C_7H_5NO_2S$ 167.188
Cryst. (Me_2CO). Mp 157-158°.

S,S-*Dioxide:* see Saccharin, S-2

McKibben, M. *et al., JCS*, 1923, 170 (*synth*)
Reissert, A. *et al., Ber.*, 1928, **61**, 1680 (*props*)
Cavalca, L. *et al., Gazz. Chim. Ital.*, 1970, **100**, 629 (*cryst struct*)
Feichtinger, H. *et al., Chem. Ber.*, 1971, **104**, 1697 (*synth*)
Davis, M. *et al., Adv. Heterocycl. Chem.*, 1972, **14**, 43 (*rev*)
Japan. Pat., 1978, 78 37 862 (*synth*)
Szabó, J. *et al., Tetrahedron*, 1988, **44**, 2985 (*oxide, synth, cmr, pmr, ir*)

1,4-Benzodioxin-2(3*H*)-one B-43

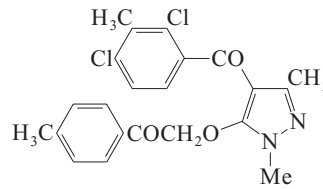


$C_8H_6O_3$ 150.134
Patented as food aroma and flavour enhancer. Yellow-white solid. Mp 55°. A synthesis giving a Mp of 135° was erroneous.

Sampson, P. *et al., J. Het. Chem.*, 1994, **31**, 1011 (*synth, pmr, cmr, bibl*)

Benzofenap, BSI B-44

*4-(2,4-Dichloro-3-methylbenzoyl)-1,3-dimethyl-5-[(4-methylbenzoyl)methoxy]-1*H*-pyrazole. 2-[4-(2,4-Dichloro-*m*-toluoyl)-1,3-dimethylpyrazol-5-yloxy]-4′-methylacetophenone. Yukawide. MY 71* [82692-44-2]

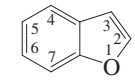


$C_{22}H_{20}Cl_2N_2O_3$ 431.317
Herbicide used on rice. Solid. Mp 133.1-133.5°.

Japan. Pat., 1986, (*(Mitsubishi)*)61 103 872 (*synth*)
Ikeda, K. *et al., Jpn. Pestic. Inf.*, 1991, **59**, 16 (*props*)
Pesticide Manual, 11th edn., 1997, No. 66 (*use*)

Benzofuran, 9CI B-45

Coumarone. Benzo[b]furan. Benzofurfuran. 1-Oxaindene. 1-Oxindene [271-89-6]



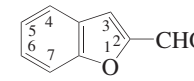
C_8H_6O 118.135
Maillard prod. present in roasted coffee aroma. Constit. of *Coix lachryma-jobi* (Job's tears) and *Gentiana lutea* (yellow gentian). Oil. d_{15}^{15} 1.08. Mp -27°. Bp_{735} 166.5-168° Bp_{80} 97.5-99°. n_D^{20} 1.5663. Steam-volatile. Stable to alkalis, polymerised by H_2SO_4. Dipole moment 0.79D.

▶ LD_{50} (mus, ipr) 500 mg/kg. Possible human carcinogen (IARC 2B). DF6423800

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 683B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 168C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1505A (*ir*)
Klarmann, B. *et al., JACS*, 1951, **73**, 4476 (*synth*)
Badger, G.M. *et al., JCS*, 1956, 3438 (*uv*)
Black, P.J. *et al., Aust. J. Chem.*, 1965, **18**, 353 (*pmr*)
Appleton, R.A. *et al., Phytochemistry*, 1971, **10**, 447-449 (*isol*)
Org. Synth., Coll. Vol., 5, 1973, 251 (*synth*)
Platzer, N. *et al., Bull. Soc. Chim. Fr.*, 1974, 905 (*cmr*)
Cagniant, P. *et al., Adv. Heterocycl. Chem.*, 1975, **18**, 337 (*rev*)
Kuster, T. *et al., Helv. Chim. Acta*, 1978, **61**, 1017 (*ms*)
Audit, M. *et al., Org. Magn. Reson.*, 1983, **21**, 698 (*pmr*)
Fraser, R.R. *et al., Can. J. Chem.*, 1985, **63**, 3505 (*cmr*)
Kreher, R.P. *et al., Chem. Ber.*, 1991, **124**, 645 (*bibl*)
IARC Monogr. (Web), http://monographs.iarc.fr
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCK250

2-Benzofurancarboxaldehyde, 9CI B-46

2-Formylbenzofuran. FEMA 3128 [4265-16-1]



$C_9H_6O_2$ 146.145
Flavouring ingredient. Needles. Mp 148-150°. Bp_{18} 135°. λ_{max} 209 (log ϵ 2.1); 243 (log ϵ 1.1); 260 (log ϵ 0.9); 300 (log ϵ 1) (MeOH).

Robba, M. *et al., Bull. Soc. Chim. Fr.*, 1977, 142 (*synth, pmr*)

Shiotani, S. *et al., J. Het. Chem.*, 1991, **28**, 1469 (*cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 249
Podea, P.V. *et al., Tetrahedron: Asymmetry*, 2008, **19**, 500-511 (*synth, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 701 (*use*)
Maulidiani, *et al., Nat. Prod. Commun.*, 2009, **4**, 1031 (*isol, pmr, cmr, ms*)

Benzoic acid, 9CI, USAN B-47

Benzenecarboxylic acid. E210. FEMA 2131 [65-85-0]

PhCOOH

$C_7H_6O_2$ 122.123

For salts see Benzoic acid salts, B-48. Widespread in plants esp. in essential oils and fruits, mostly in esterified form. Also present in butter, cooked meats, pork fat, white wine, black and green tea, mushroom and Bourbon vanilla. Used in foodstuffs as antimicrobial and flavouring agent and as preservative. In practical food preservation, the Na salt of benzoic acid is the most widely used form (see Benzoic acid salts, B-48). The antimicrobial activity comprises a wide range of microorganisms, particularly yeasts and moulds. Undissociated benzoic acid is more effective than dissociated, thus the preservative action is more efficient in acidic foodstuffs. Typical usage levels are 500-2000 ppm. Leaflets or needles (H_2O). Sol. MeOH, C_6H_6; fairly sol. hexane; v. spar. sol. H_2O. Mp 122°. Bp 249° Bp_{10} 133°. Log P 1.88 (calc). Steam-volatile. λ_{max} 228 (E1%/1cm 728); 273 (E1%/1cm 93.2); 300 (E1%/1cm 46.8) (MeOH) (Berdy).

▶ Fl. p. 121°, autoignition temp. 570°. Eye, skin and mucous membrane irritant. Hypersensitivity reactions reported. Low systemic toxicity. Detoxification in humans occurs by conjugation with amino acids (mainly glycine resulting in hippuric acid). DG0875000

Me ester: [93-58-3] *Methyl benzoate. FEMA 2683*
$C_8H_8O_2$ 136.15
Present in various flower oils, banana, cherry, pimento berry, ceriman (*Monstera deliciosa*), clove bud and stem, mustard, coffee, black tea, dill, starfruit and cherimoya (*Annona cherimola*). Used in flavourings. Liq. with fruity odour. d_{25}^{25} 1.09. Fp -12.3. Bp 199.6° Bp_{24} 96-98°.

▶ Fl. p. 83°. Skin and eye irritant. LD_{50} (rat, orl) 1350 mg/kg. DH3850000

Et ester: [93-89-0] *Ethyl benzoate. FEMA 2422*
$C_9H_{10}O_2$ 150.177
Found in various fruits, e.g. apple, banana, sweet cherry. Also present in milk, butter, wines, black tea, bourbon vanilla and fruit brandies. Flavouring agent. Liq. with aromatic/fruity odour. d_4^{25} 1.04. Fp -34. Bp 212.9° Bp_{10} 87.2°. n_D^{20} 1.5045.

▶ Fl. p. 88°, autoignition temp. 490°. Skin and eye irritant. LD_{50} (rat, orl) 2100 mg/kg. DH0200000

Propyl ester: [2315-68-6] *Propyl benzoate. FEMA 2931*
$C_{10}H_{12}O_2$ 164.204
Present in cherry and clove stem, also in butter. Flavouring ingredient. Liq. with balsamic, nutty odour and sweet fruity-nutty flavour. d_{15}^{15} 1.03. Fp -51–52. Bp 230°. n_D^{20} 1.5100.

Isopropyl ester: [939-48-0] *Isopropyl benzoate. FEMA 2932*
$C_{10}H_{12}O_2$ 164.204
Present in feijoa fruit (*Feijoa sellowiana*), apple, pear, cocoa and honey. Flavouring ingredient. d_{15}^{15} 1.02. Bp 218-219°.

▶ Fl. p. 89/99°. Skin and eye irritant. LD_{50} (rat, orl) 3730 mg/kg. DH3150000

2-Propenyl ester: see 2-Propen-1-ol, P-686

Benzyl ester: [120-51-4] ***Benzyl benzoate, USAN***. *Ascabin. Benylate. Vanzoate. FEMA 2138. Many other names*
$C_{14}H_{12}O_2$ 212.248
Contained in Peru balsam and Tolu balsam. Isol. from other plants e.g. *Jasminum* spp., ylang-ylang oil. Used in food flavouring. Leaflets with balsamic/almond flavour and sharp, pungent flavour. d^{18} 1.11. Mp 21° (19.5°). Bp 323-324° (316-317°) $Bp_{0.1}$ 80-82°. Log P 3.88 (uncertain value) (calc). Spar. steam-volatile.

▶ Fl. p. 148°, autoignition temp. 480°. Eye, mucous membrane, and possible skin irritant. Hypersensitivity reactions reported. LD_{50} (rat, orl) 500 mg/kg. DG4200000

[8000-95-1, 1079-02-3, 43019-90-5, 766-76-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 186A; 271B; 291B; 291C; 292D; 340A; 340B; 340C; 380D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1063B; 1199A; 1240A; 1240B; 1241A; 1241B; 1244A; 1337C; 1411A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 181D; 1322C; 1357D; 1358B; 1358A; 1358C; 1360A; 1389D; 1390A; 1390B (*ir*)
Jesson, J.P. *et al., Proc. R. Soc. London, A*, 1962, **268**, 68-78 (*Raman*)
Beynon, J.H. *et al., Z. Naturforsch., A*, 1965, **20**, 883-887 (*ms*)
Evans, H.B. *et al., J. Phys. Chem.*, 1968, **72**, 2552-2562 (*pmr*)
Morris, W.W. *et al., J. Assoc. Off. Anal. Chem.*, 1973, **56**, 1037-1064 (*Me ester, Et ester, ir*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1979, **17**, 715-722 (*rev, tox*)
Ullmann's Encycl. Ind. Chem., 5th Ed, VCH, Weinheim, 1985, **A3**, 555 (*rev*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493-1518 (*cmr*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BCL750; BCM000; EGR000; MHA500
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 103 (*rev*)
Tremblay, G.C. *et al., Pharmacol. Ther.*, 1993, **60**, 63-90 (*rev, pharmacol, tox*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 32-34; 38-39; 433-435
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1118; 1431
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 249; 263; 951; 1485; 1718; 2281; 2340; 2527 (*occur, props, esters*)
Indrayanto, G. *et al., Anal. Profiles Drug Subst.*, 1999, **26**, 1-46 (*rev*)
Sato, K. *et al., Bull. Chem. Soc. Jpn.*, 1999, **72**, 2287-2306 (*synth, pmr, cmr*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2511
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 107
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 117
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BBV250; SFB000; BCM000; IOD000; EGR000; BCQ250; BQK250; BDM500; BCL750; MHA750; PKW760

Benzoic acid salts B-48

Benzoates
Salts of Benzoic acid, B-47.

Na salt: [532-32-1] *Sodium benzoate. E211. FEMA 3025*
$C_7H_5NaO_2$ 144.105
Antimicrobial preservative in foods, e.g. margarine and artificially sweetened fruit preserves. Flavouring agent and adjuvant. Powder or flakes.

▶ DH6650000

K salt: [582-25-2] *Potassium benzoate. E212*
$C_7H_5KO_2$ 160.214
Preservative for margarines and wines. Cryst. + $3H_2O$.

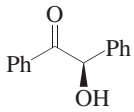
NH_4 salt: [1863-63-4] *Ammonium benzoate. Vulnoc AB*
$C_7H_9NO_2$ 139.154
Preservative. d 1.26. Mp 198°. Undergoes conversion to ammonium hydrogen benzoate on crystallisation from hot H_2O or on prolonged storage in the solid state.

Ca salt: [2090-05-3] *Calcium benzoate. E213*
$C_{14}H_{10}CaO_4$ 282.309
Preservative, used in margarine.

US Pat., 1929, 1 704 636 (*NH_4 salt, synth*)
Kirk-Othmer Encycl. Chem. Technol., 2nd edn., Wiley, 1963, **3**, 433 (*NH_4 salt, use, props*)
Adams, S.K. *et al., Inorg. Chim. Acta*, 1975, **12**, 163-166 (*ms, ir*)
Oxton, I.A. *et al., Can. J. Chem.*, 1977, **55**, 3831-3837 (*NH_4 salt, pmr, stability*)
Czech. Pat., 1982, 225 768 (*Ca salt, synth*)
Lewandowski, W. *et al., Can. J. Spectrosc.*, 1987, **32**, 41-45 (*synth, ir*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, 107 (*Ca salt, use, props*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 370-371; 2281-2282; 2527-2529 (*salts*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1840 (*Na salt*)

Benzoin, 8CI B-49

2-Hydroxy-1,2-diphenylethanone, 9CI. α-Hydroxybenzyl phenyl ketone. Benzoylphenylcarbinol. 2-Hydroxy-2-phenylacetophenone. FEMA 2132 [119-53-9]



(*R*)-*form*

$C_{14}H_{12}O_2$ 212.248
Flavouring ingredient.
▶ LD_{50} (rat, orl) 10,000 mg/kg. DI1590000

(*R*)-*form* [5928-66-5]
Needles. Mp 131-132.5°. $[\alpha]_D^{12}$ -117.5 (Me_2CO).

(*S*)-*form* [5928-67-6]
Needles. Mp 131-132.5°. $[\alpha]_D^{25}$ +118.4 (Me_2CO).

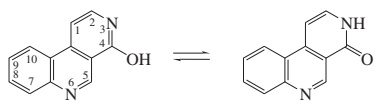
(±)-*form* [579-44-2]
Prisms (EtOH) with vanilla taste. Insol. H_2O; sol. Me_2CO, hot EtOH. Mp 133-134°. Bp_{768} 344° Bp_{12} 194°.

[441-38-3, 57794-28-2, 1459-20-7, 574-06-1, 8050-35-9]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 37B; 37C; 38C; 38B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 852C; 853A; 853C; 854A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1257C (*ir*)
Org. Synth., Coll. Vol., 1, 1932, 94 (*synth*)
Watson, M.B. *et al., Chem. Ind. (London)*, 1954, 658 (*abs config*)
Kenyon, J. *et al., JCS*, 1965, 435 (*resoln*)
Kreiser, W. *et al., Annalen*, 1971, **745**, 164 (*synth*)
Couvert, O. *et al., C. R. Seances Acad. Sci., Ser. C*, 1972, **274**, 296 (*pmr*)
Ohgo, Y. *et al., Chem. Lett.*, 1974, 1327 (*synth*)
Kudo, T. *et al., Bull. Chem. Soc. Jpn.*, 1975, **48**, 2969
Hakimelahi, G.H. *et al., Helv. Chim. Acta*, 1977, **60**, 342 (*synth*)
Haisa, M. *et al., Acta Cryst. B*, 1980, **36**, 2832 (*cryst struct*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 252
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 139 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCP250; MHE000; BCP500

Benzo[*c*][2,7]naphthyridin-4-ol B-50

Benzo[c][2,7]naphthyridin-4(3H)-one, 9CI. 4-Hydroxybenzo[c][2,7]naphthyridine. 2,9-Diazaphenanthren-1(2H)-one. ***Perlolidine****. Samoquasine A* [7344-61-8] [62574-41-8 (Samoquasine A)]



$C_{12}H_8N_2O$ 196.208
Samoquasine A finally shown to be identical with Perlolidine in 2008. Alkaloid from *Annona squamosa* (sugar apple). Mp 338-345° (332-334°). pK_{a1} 4.01; pK_{a2} 11.39 (18°). λ_{max} 239 (ε 50300); 243 (ε 49300); 252 (ε 45000); 322 (ε 11600); 337 (ε 13800) (EtOH aq.). λ_{max} 240 (ε 19400); 249 (ε 23500); 256 (ε 28000); 272 (ε 10700); 283 (ε 8800); 377 (ε 12200) (0.01M HCl). λ_{max} 237; 284; 325; 355 (0.01M NaOH).

OH-form

Me ether: [156780-62-0] *4-Methoxybenzo[c][2,7]naphthyridine*
$C_{13}H_{10}N_2O$ 210.235
Cryst. Mp 88° Mp 139-141°.

Et ether: [399039-97-5] *4-Ethoxybenzo[c][2,7]naphthyridine*
$C_{14}H_{12}N_2O$ 224.262
Beige cryst. Mp 104°.

Grimmett, R.E.R. *et al., N.Z. J. Sci. Technol., Sect. B*, 1943, **24**, 151 (*isol*)
White, E.P. *et al., N.Z. J. Sci. Technol., Sect. B*, 1946, **27**, 242
Powers, J.C. *et al., JACS*, 1968, **90**, 7102 (*synth, uv, ir, ms*)
Lalezari, I. *et al., J. Het. Chem.*, 1980, **17**, 1761 (*synth, ms*)
Bracher, F. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1989, **322**, 511 (*synth, pmr, ms*)
Rocca, P. *et al., JOC*, 1993, **58**, 7832 (*synth, pmr, ir*)
Björk, P. *et al., Heterocycles*, 1997, **44**, 237-253 (*synth, Me ether*)
Duvey, G. *et al., J. Het. Chem.*, 2001, **38**, 1039-1044 (*Me ether, Et ether*)
Yang, Y.-L. *et al., Tet. Lett.*, 2003, **44**, 319-322 (*isol, pmr, cmr*)
Timmons, C. *et al., JOC*, 2008, **73**, 9168-9170 (*Samoquasine A*)

Benzophenone, 8CI B-51

Diphenylmethanone, 9CI. Diphenyl ketone. Phenyl ketone. FEMA 2134 [119-61-9]

PhCOPh

$C_{13}H_{10}O$ 182.221
Present in grapes, cherimoya, mountain papaya, soursop and black tea. Flavouring and adjuvant agent. Permitted component (UV-stabilizer) of food contact rubber articles intended for repeated use. Rhombic prisms (stable form), monoclinic prisms (labile form) with apricot-peach taste. Insol. H_2O. d_4^{18} 1.11. Mp 48.5-49° (stable form) Mp 26° (labile form). Bp_{100} 224° Bp_{10} 157.6°.
▶ LD_{50} (mus, orl) 2895 mg/kg. DI9950000

[16592-08-8]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1264D; **2**, 58A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 884C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1265B (*ir*)
Adv. Chem. Ser., 1955, **15**, 354 (***props***)
Natlis, P. *et al., J. Phys. Chem.*, 1965, **69**, 2943 (*ms*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 873 (*rev, tox*)
Grimaud, M. *et al., Bull. Soc. Chim. Fr.*, 1974, 1935 (*uv*)
Groebal, B.T. *et al., Chem. Ber.*, 1977, **110**, 854 (*use*)
Loletta, M. *et al., Inorg. Chim. Acta*, 1977, **24**, 195 (*pmr, cmr*)
Abraham, R.J. *et al., JCS Perkin 2*, 1988, 1429 (*conformn*)
Zadel, G. *et al., Angew. Chem., Int. Ed.*, 1992, **31**, 1035 (*synth*)
Zhao, D. *et al., Synthesis*, 1994, 915 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 254-255
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 140 (*use, occur*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html, (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BCS250

Benzophenone synthase B-52

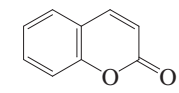
E.C. 2.3.1.151. Malonyl-CoA:3-hydroxybenzoyl-CoA malonyltransferase [175780-21-9]

Enzyme. Isol. from cell cultures of *Centaurium erythraea* (centaury). Also acts on benzoyl-CoA giving 2,4,6-Trihydroxybenzophenone, T-683.

Beerhues, L. *et al., FEBS Lett.*, 1996, **383**, 264-266 (*Centaurium erythraea*)
Liu, B. *et al., Plant J.*, 2003, **34**, 847-855 (*Hypericum androsaemum*)

2*H*-1-Benzopyran-2-one, 9CI B-53

Coumarin. Coumarinic anhydride. α-Benzopyrone. Cumarin [91-64-5]



$C_9H_6O_2$ 146.145
Occurs in sweet clover. Banned by FDA for use in food. Rhombic cryst. Sol. EtOH, MeOH, Et_2O; poorly sol. H_2O. Mp 70°. Bp 291°. Log P 1.41 (calc). Hydrol. by hot conc. alkalis. λ_{max} 273 (ε 10960); 307 (ε 5623) (MeOH) (Berdy).
▶ LD_{50} (rat, orl) 293 kg/kg. Exp. hepatotoxic with species differences between rodent/primate. Exp. teratogen.
GN4200000

Hydrazone: [5841-34-9]
Yellow cryst. (MeOH). Mp 85-86°.

Semicarbazone:
Light yellow cryst. (EtOH aq.). Mp 218-220°.

Di-Et acetal: [33871-81-7] *2,2-Diethoxy-2H-1-benzopyran*
$C_{13}H_{16}O_3$ 220.268
Liq. Bp_{10} 134-136° $Bp_{0.5}$ 104°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 322B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1311B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1386C (*ir*)
May, P. *et al., Perfum. Essent. Oil Res.*, 1925, **16**, 45 (*synth*)
Dean, F.M. *et al., Fortschr. Chem. Org. Naturst.*, 1952, **9**, 225 (*rev*)

Stoker, J.R. *et al., J. Biol. Chem.*, 1962, **237**, 2303 (*biosynth*)
Barnes, C.S. *et al., Aust. J. Chem.*, 1964, **17**, 975 (*ms*)
Sheinker, Yu.N. *et al., Dokl. Akad. Nauk SSSR, Ser. Khim.*, 1964, **158**, 1352 (*pmr*)
Abernethy, J.L. *et al., J. Chem. Educ.*, 1969, **46**, 561 (*rev*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 1318 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 385 (*rev, tox*)
Subbotin, O.A. *et al., Khim. Prir. Soedin.*, 1975, **11**, 458; *Chem. Nat. Compd. (Engl. Transl.)*, 1975, **11**, 476 (*cmr*)
IARC Monogr., 1976, **10**, 113; 1987, *Suppl. 7*, 61 (*rev, tox*)
Chan, K.K. *et al., Tetrahedron*, 1977, **33**, 899 (*nmr*)
Duddeck, H. *et al., Org. Magn. Reson.*, 1982, **20**, 55 (*cmr*)
Abu-Eittah, R.H. *et al., Can. J. Chem.*, 1985, **63**, 1173 (*uv*)
Ziegler, T. *et al., Chem. Ber.*, 1987, **120**, 373 (*synth*)
Sato, K. *et al., JCS Perkin 1*, 1987, 1753 (*synth*)
Ullmann's Encycl. Ind. Chem., 5th Ed., VCH, Weinheim, 1988, **A11**, 208 (*rev*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, CNV000
Nyquist, R.A. *et al., Appl. Spectrosc.*, 1990, **44**, 791 (*ir*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **7**, 647 (*rev*)
Zhou, C. *et al., Yingyong Huaxue*, 1992, **9**, 79 (***synth***)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1358
Sigma-Aldrich Library of Stains, Dyes and Indicators, 224
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, CNV000

4*H*-1-Benzopyran-4-one, 9CI B-54

Chromone. Benz-γ-pyrone. Benzopyrone [491-38-3]

$C_9H_6O_2$ 146.145
Isol from Ye Hao (*Carum carvi*). Needles (H_2O or petrol). Mp 59°. Sublimes. Steam-volatile.

▶ LD_{50} (mus, ipr) 91 mg/kg. GB7887000

Hydrochloride: Mp 101-102°.

Hydrobromide: Mp 175° (sinters at 169°).

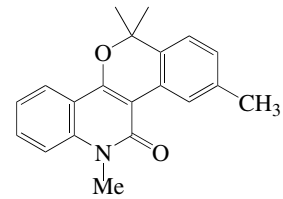
Oxime: [61348-46-7]
$C_9H_7NO_2$ 161.16
Cryst. Mp 130° (127°).

Phenylhydrazone: [34810-68-9]
Pale yellow cryst. (MeOH). Mp 112° (108-109°).

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 95D (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 93C (*ir*)
Schönberg, A. *et al., JACS*, 1950, **72**, 3396-3399 (*synth*)
Badawi, M.M. *et al., Chem. Ind. (London)*, 1966, 498-499 (*ms*)
Badawi, M.M. *et al., Indian J. Chem.*, 1967, **5**, 93-96 (*nmr*)
Kostka, K. *et al., Chem. Anal. (Warsaw)*, 1969, **14**, 1145 (*use*)
Griffiths, P.J.F. *et al., Spectrochim. Acta A*, 1972, **28**, 707-713 (*uv*)
Ellis, G.P. *et al., JCS Perkin 1*, 1981, 2557-2560 (*cmr*)
Shanker, Ch.G. *et al., Synthesis*, 1983, 310-311 (*synth*)
Szabó, V. *et al., Tetrahedron*, 1986, **42**, 4215-4222 (*oxime*)
Baba, K. *et al., Bot. Mag., Tokyo (Shokubutsugaki Zasshi)*, 1989, 216-221 (*occur*)
Aléman, C. *et al., JOC*, 1999, **64**, 1768-1769 (*struct*)

Benzosimuline B-55

[198336-58-2]

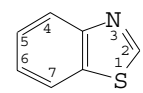


$C_{20}H_{19}NO_2$ 305.376
Alkaloid from the bark of *Zanthoxylum simulans* (Szechuan pepper). Oil. λ_{max} 210 (log ε 4.19); 233 (log ε 4.42); 250 (sh) (log ε 4.05); 268 (log ε 3.95); 310 (sh) (log ε 3.74); 320 (sh) (log ε 3.79); 331 (log ε 3.86); 346 (log ε 3.94); 365 (log ε 3.81) (EtOH).

Chen, I.-S. *et al., Phytochemistry*, 1997, **46**, 525-529 (*isol, uv, ir, pmr, cmr*)

Benzothiazole, 9CI B-56

[95-16-9]



C_7H_5NS 135.189
Isol. from cranberries. Sol. EtOH, CS_2, v. spar. sol. H_2O. Bp 223-225° Bp_{25} 119-120°. pK_a 1.2 (H_2O). Steam-volatile.

▶ Fl. p. 112°. LD_{50} (rat, orl) 466 mg/kg; LD_{50} (mus, orl) 900 mg/kg. DL0875000

Picrate: Mp 176°.

N-*Oxide:* [27655-38-5]
C_7H_5NOS 151.189
Prisms + $1H_2O$ (MeOAc or Et_2O). Mp 45-48°.

Methiodide: [2786-31-4]
Needles. Mp 210°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 699C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 200A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1511A (*ir*)
Reid, W. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1962, **295**, 143 (*synth*)
Ellis, B. *et al., Spectrochim. Acta*, 1965, **21**, 1881 (*uv*)
Anjou, K. *et al., Acta Chem. Scand.*, 1967, **21**, 2076-2082 (*isol*)
Takahashi, S. *et al., Chem. Pharm. Bull.*, 1970, **18**, 1176 (*oxide*)
Witanowski, M. *et al., Tetrahedron*, 1972, **28**, 637 (*nmr*)
Selva, A. *et al., Org. Mass Spectrom.*, 1974, **9**, 1161 (*ms*)
Diehl, P. *et al., Org. Magn. Reson.*, 1976, **8**, 155 (*pmr*)
Faure, R. *et al., Can. J. Chem.*, 1978, **56**, 46 (*cmr*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 274; 1990, **15**, 20 (*use*)
Angelelli, J.M. *et al., Spectrosc. Lett.*, 1980, **13**, 741 (*ir*)
Bakke, J.M. *et al., J. Chem. Ecol.*, 1983, **9**, 513
Bieräugel, H. *et al., Tetrahedron*, 1983, **39**, 3971 (*synth*)
Bordwell, F.G. *et al., JACS*, 1991, **113**, 985 (*deriv, synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDE500

2(3*H*)-Benzothiazolethione, 9CI B-57

2-Benzothiazolethiol. 2-Mercaptobenzothiazole. 2-Benzothiazolinethione. Accelerator M. Accel M. Captax. Kaptax. Pneumax MBT. Thiotax. Vulkacit M. Wobezit M [149-30-4]

$C_7H_5NS_2$ 167.255
NH-form predominates. Constit. of cranberries. Needles (MeOH aq.). Spar. sol. EtOH, Et_2O, AcOH; insol. H_2O; sol. alkalis. Mp 177-179°. Readily oxidised to the disulfide.

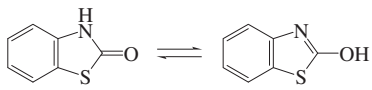
▶ LD_{50} (rat, orl) 100 mg/kg. Exp. carcinogen. Exp. reprod. and teratogenic effects. DL6475000

[155-04-4, 2492-26-4]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 701D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 204B; 204C (*nmr*)
Jacobson, P. *et al., Ber.*, 1891, **24**, 1403-1411
Welcher, J.F. *et al., Organic Analytical Reagents*, Van Nostrand, N.Y., 1948, **4**, 109 (*use*)
Morgan, K.I. *et al., JCS*, 1958, 854-858 (*uv*)
Chesick, J.P. *et al., Acta Cryst. B*, 1971, **27**, 1441-1444 (*cryst struct*)
DeJongh, D.C. *et al., Adv. Mass Spectrom.*, 1974, **6**, 99-103 (*ms*)
Fries, J. *et al., Organic Reagents for Trace Analysis*, E. Merck, Darmstadt, 1977, 302 (*use*)
Uher, M. *et al., Chem. Zvesti*, 1978, **32**, 486-492 (*tautom*)
Faure, R. *et al., Org. Magn. Reson.*, 1978, **11**, 617-627 (*cmr, tautom*)
Cristiani, F. *et al., Phosphorus Sulfur Relat. Elem.*, 1984, **20**, 231-240 (*ir*)
Radha, A. *et al., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.*, 1985, **171**, 225-228 (*cryst struct*)
Stierle, A.A. *et al., Tet. Lett.*, 1991, **32**, 4847-4848 (*Tedania ignis constit, isol*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDF000; SIG500; BHA750

2-Benzothiazolol B-58

*2(3*H*)-Benzothiazolone, 9CI. 2-Benzothiazolinone. 2-Hydroxybenzothiazole* [934-34-9]



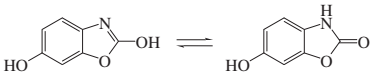
C_7H_5NOS 151.189

NH-form predominates. Isol. from *Cucumis sativus* (cucumber). Needles (EtOH). Mp 138-139°.

Yu, J.Q. *et al., J. Chem. Ecol.*, 1994, **20**, 21-31 (*Cucumis sativus constit*)

2,6-Benzoxazolediol B-59

*6-Hydroxy-2(3*H*)-benzoxazolone, 9CI. 6-Hydroxy-2-benzoxazolinone. 2,6-Dihydroxybenzoxazole* [78213-03-3]



$C_7H_5NO_3$ 151.121

Exists in *NH*-form. Needles (H_2O) or pale yellow cryst. Mp 288-292° (260°). λ_{max} 268; 302; 305; 340 (MeOH).

6-Me ether: [532-91-2] *2-Hydroxy-6-methoxybenzoxazole. 6-Methoxy-2(3*H*)-benzoxazolone. 6-Methoxy-2-benzoxazolinone. 6-Methoxy-2-benzoxazolol. MBOA.* ***Coixol***
$C_8H_7NO_3$ 165.148
Isol. from roots of *Coix lacryma jobi* (Job's tears) and from seedlings of wheat, corn and rye. Pink cryst. (MeOH aq.). Sol. bases, EtOH, Et_2O, C_6H_6; fairly sol. H_2O; poorly sol. hexane. Mp 160-161° (154-155°). λ_{max} 229; 286 (H_2O) (Berdy).

▶ DM5275200

NH-form

N,O-*Di-Ac:* [103853-98-1]
$C_{11}H_9NO_5$ 235.196
Solid ($CHCl_3$/petrol). Mp 194-196°.

N-*Me:* [359434-29-0]
$C_8H_7NO_3$ 165.148
Solid (EtOH). Mp 203-204°.

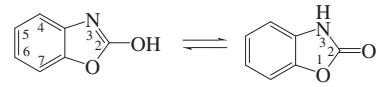
6-Me ether, N-*Ac:* [62655-08-7]
$C_{10}H_9NO_4$ 207.185
Needles. Mp 147.5°.

6-Me ether, N-*benzoyl:*
$C_{15}H_{11}NO_4$ 269.256
Needles. Mp 162-162.5°.

Koyama, T. *et al., Yakugaku Zasshi*, 1955, **75**, 699-701 (*6-Me ether*)
Beck, S.D. *et al., J. Agric. Food Chem.*, 1957, **5**, 933-935 (*6-Me ether, detn*)
Smissman, E.E. *et al., JACS*, 1957, **79**, 4697-4698 (*6-Me ether, isol, synth*)
Hietala, P.K. *et al., Acta Chem. Scand.*, 1958, **12**, 119-123 (*detn*)
Wahlroos, O. *et al., Acta Chem. Scand.*, 1958, **12**, 124-128 (*activity, 6-Me ether*)
List, P.H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1959, **292**, 452-456 (*6-Me ether*)
Zinner, H. *et al., Chem. Ber.*, 1960, **93**, 1331-1339 (*synth*)
Allen, E.H. *et al., JOC*, 1971, **36**, 2004-2005 (*6-Me ether*)
Richey, J.D. *et al., Agric. Biol. Chem.*, 1976, **40**, 2413-2416 (*6-Me ether, synth*)
Kubo, I. *et al., Experientia*, 1983, **39**, 355 (*6-Me ether, synth*)
Cole, E.R. *et al., Aust. J. Chem.*, 1986, **39**, 295-301 (*synth, ir, pmr*)
Sicher, D. *et al., Synthesis*, 1989, 875-876 (*6-Me ether*)
Maleski, R.J. *et al., J. Het. Chem.*, 1991, **28**, 1937-1939 (***synth***)
Bjostad, L.B. *et al., J. Chem. Ecol.*, 1992, **18**, 931-944 (*6-Me ether, isol*)
Hayashi, T. *et al., Phytochemistry*, 1994, **37**, 1611-1614 (*6-Me ether, occur*)
Venkateswarlu, Y. *et al., Biochem. Syst. Ecol.*, 1999, **27**, 519-520 (*6-Me ether, isol, activity*)
Delhomel, J.F. *et al., J. Het. Chem.*, 2001, **38**, 633-639 (*N-Me*)
Amer, M.E. *et al., J. Braz. Chem. Soc.*, 2004, **15**, 262-266 (*isol*)
Ray, S. *et al., Synth. Commun.*, 2010, **40**, 2377-2388 (*synth, ir, uv, pmr, cmr, ms, N,O-di-Ac*)

2-Benzoxazolol B-60

*2(3*H*)-Benzoxazolone, 9CI. 2-Benzoxazolinone, 8CI. 2-Hydroxybenzoxazole. BOA* [59-49-4]



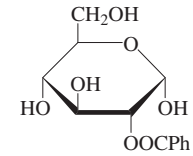
$C_7H_5NO_2$ 135.122

Tautomeric. *NH*-form predominates. Found in rye seedlings. Sol. bases, Et_2O; fairly sol. H_2O; poorly sol. hexane. Mp 141-142°. pK_{a1} 8.9 (23°). λ_{max} 270 (H_2O) (Berdy). λ_{max} 275 (EtOH) (Berdy).

▶ LD_{50} (rat, orl) 700 mg/kg. LD_{50} (mus, orl) 554 mg/kg. DM4905000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 698A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 198A (*nmr*)
Sandmeyer, T. *et al., Ber.*, 1886, **19**, 2650-2657 (*synth*)
Seidel, P. *et al., J. Prakt. Chem.*, 1890, **42**, 445-457 (*synth, Ph ether*)
Williams, R.T. *et al., Biochem. J.*, 1947, **41**, 1 (*synth*)
Thompson, M.L. *et al., Can. J. Chem.*, 1973, **51**, 3313 (*ms*)
Llinares, J. *et al., Can. J. Chem.*, 1979, **57**, 937 (*cmr, tautom*)
Yamato, M. *et al., Chem. Pharm. Bull.*, 1983, **31**, 3946 (*synth, Me ether, Et ether, benzyl ether, pmr*)
Maleski, R.J. *et al., J. Het. Chem.*, 1991, **28**, 1937 (***synth***)
Press, J.B. *et al., JOC*, 1992, **57**, 6335 (*synth*)
Patonay, T. *et al., Synth. Commun.*, 1994, **24**, 2507 (*synth*)
Wang, X. *et al., Eur. J. Org. Chem.*, 2005, 1675-1679 (*synth, pmr, cmr*)
El-Faham, A. *et al., J. Het. Chem.*, 2006, **43**, 599-606 (*synth, ir, pmr, cmr, ms*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDJ000

2-*O*-Benzoylglucose B-61



α-D-Pyranose-*form*

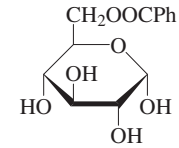
$C_{13}H_{16}O_7$ 284.265

D-*form* [63029-01-6]
Constit. of *Vaccinium vitis-idaea* (cowberry) and *Vaccinium macrocarpon* (cranberry).

Chaudhuri, R.K. *et al., Helv. Chim. Acta*, 1981, **64**, 2401-2404 (*isol, pmr, cmr*)
Heimhuber, B. *et al., Phytochemistry*, 1990, **29**, 2726-2727 (*isol, synth, nmr*)

6-*O*-Benzoylglucose B-62

Glucose 6-benzoate, 9CI. ***Vacciniin***



α-D-Pyranose-*form*

$C_{13}H_{16}O_7$ 284.265

D-*form* [14200-76-1]
Isol. from *Vaccinium* sp. (red whortleberries and cranberries). Amorph., cryst. hydrate (Me_2CO). Mp 104-106°. $[\alpha]_D$ +48 (EtOH).

[90-75-5, 130323-07-8]

Brigl, P. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1934, **229**, 117 (*isol, struct*)
Heimhuber, B. *et al., Phytochemistry*, 1990, **29**, 2726 (*isol, synth, pmr*)

Benzyl acetate B-63

FEMA 2135 [140-11-4]

$H_3CCOOCH_2Ph$

$C_9H_{10}O_2$ 150.177

Occurs in jasmine, apple, cherry, guava fruit and peel, wine grape, white wine, tea, plum, cooked rice, Bourbon vanilla, naranjilla fruit (*Solanum quitoense*), Chinese cabbage and quince. Flavouring agent. Liq. with jasmine odour and bitter, pungent taste. d_{25}^{25} 1.05. Bp 215.5-216° Bp_{102} 134°. n_D^{25} 1.4994.

▶ Skin irritant. LD_{50} (rat, orl) 2490 mg/kg. AF5075000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 277A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1201B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1335C (*ir*)
Merker, R.L. *et al., JOC*, 1961, **26**, 5180 (*synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 875 (*rev, tox*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1981, **9**, 82 (*use*)

Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BDX000
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 259-260 (*occur, props*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992,

Benzyl alcohol, BAN, INN, USAN B-64

Benzenemethanol, 9CI. Benzenecarbinol. Hydroxymethylbenzene. α-Hydroxytoluene. Phenylcarbinol. Phenylmethanol. Peruvin†. FEMA 2137 [100-51-6]

$PhCH_2OH$

C_7H_8O 108.14
Constit. of jasmine and other ethereal oils, both free and as esters. Also present in cherry, orange juice, mandarin peel oil, guava fruit, feijoa fruit, pineapple, leek, cinnamon, cloves, mustard, fermented tea, basil and red sage. Flavouring ingredient. Liq. Mod. sol. H_2O. d^{20} 1.05 d_{15}^{15} 1.05. Fp -15.2. Bp 205.3° Bp_{10} 93°. n_D^{20} 1.5396. pK_a 15.4 (25°).

▶ Fl. p. 93/96/101°, autoignition temp. 436°. Mixt. with 58% H_2SO_4 dec. explosively at 180°. Eye and skin irritant. Ingestion or inhalation can cause adverse gastrointestinal and CNS effects. LD_{50} (rat, orl) 1230 mg/kg. DN3150000

O-*[5-O-Benzoyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [1097040-08-8] ***Viscartin A***
$C_{25}H_{30}O_{11}$ 506.505
Constit. of *Cucurbita moschata* (pumpkin). Pale yellow solid. $[\alpha]_D^{23}$ -50 (c, 1.5 in MeOH). λ_{max} 201 (log ϵ 0.58); 227 (log ϵ 0.29); 274 (log ϵ 0.04) (MeOH).

O-*[4-Hydroxybenzoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [1190117-05-5]
$C_{25}H_{30}O_{12}$ 522.505
Constit. of the seeds of *Cucurbita moschata* (pumpkin). $[\alpha]_D^{24}$ -58 (c, 0.2 in MeOH). λ_{max} 258 (log ϵ 4.02) (MeOH).

O-*[α-L-Arabinofuranosyl-(1→6)-β-D-glucopyranoside]:* [88510-11-6]
$C_{18}H_{26}O_{10}$ 402.397
Isol. from wine grapes (*Vitis vinifera*) and tomatoes. $[\alpha]_D$ -39 (c, 0.02 in H_2O).

O-*[α-L-Arabinopyranosyl-(1→2)-β-D-glucopyranoside]:* [1256283-53-0]
$C_{18}H_{26}O_{10}$ 402.397
Constit. of the leaves of *Smallanthus sonchifolius* (yacon). Amorph. powder. $[\alpha]_D$ -75.1 (c, 1 in MeOH).

O-*[β-D-Xylopyranosyl-(1→6)-D-glucopyranoside]:* [130622-31-0] *Benzyl β-primeveroside*
$C_{18}H_{26}O_{10}$ 402.397
Aroma precursor from Oolong tea leaves (*Camellia sinensis*). Constit. of *Panax ginseng*. Cryst. (EtOH). Mp 188-189°. $[\alpha]_D^{20}$ -71.2 (c, 1 in H_2O).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [56775-64-5] *Benzyl gentiobioside*
$C_{19}H_{28}O_{11}$ 432.424
Constit. of tomato cell cultures (*Lycopersicon esculentum*, Solanaceae). $[\alpha]_D$ -76.2 (c, 0.01 in H_2O).

O-*[β-D-Glucopyranosyl-(1→3)-[β-D-xylopyranosyl-(1→2)]-β-D-glucopyranoside]:* [152502-28-8]
$C_{24}H_{36}O_{15}$ 564.539
Constit. of *Sesamum indicum* (sesame). Amorph. powder + $1\frac{1}{2}H_2O$. $[\alpha]_D^{22}$ -41.7 (c, 0.66 in MeOH). λ_{max} 207 (sh) (log ϵ 3.98); 227 (sh) (log ϵ 3.49) (MeOH).

O-*[β-D-Glucopyranosyl-(1→2)-[β-D-glucopyranosyl-(1→3)]-β-D-glucopyranoside]:* [81417-79-0] ***Zizybeoside II***
$C_{25}H_{38}O_{16}$ 594.566
Constit. of dried fruits of Chinese jujube (*Zizyphus jujuba*). Needles (MeOH aq.). Mp 237-238°. $[\alpha]_D^{26}$ -39 (c, 1.00 in H_2O).

O-*Sulfate:* [26687-85-4] ***Benzyl sulfate***
$C_7H_8O_4S$ 188.204
Constit. of various plant spp. Flavour component.

[20194-18-7]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1121D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 326B (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1046D (*ir*)
Truett, W.L. *et al., JACS*, 1951, **73**, 5913-5915 (*synth*)
Adv. Chem. Ser., 1955, **15**, 347 (*props*)
Aplin, R.T. *et al., Can. J. Chem.*, 1969, **47**, 1599-1601 (*ms*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 248 (*occur*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1973, **11**, 1011 (*rev, tox*)
Shapiro, M.J. *et al., JOC*, 1976, **41**, 3197-3201 (*cmr*)
Bastaert, G. *et al., C. R. Seances Acad. Sci., Ser. C*, 1980, **290**, 193 (*uv*)
Okamura, N. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3507-3514 (*Zizybeoside*)
Williams, P.J. *et al., Phytochemistry*, 1983, **22**, 2039-2041 (*6-arabinofuranosylglucoside*)
Schaefer, T. *et al., Can. J. Chem.*, 1989, **67**, 1015-1021 (*pmr, conformn*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BDX000; BDX500
Suzuki, N. *et al., Phytochemistry*, 1993, **34**, 729-732 (*Sesamum triglycoside*)
Guo, W. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 1532-1534 (*primeveroside*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1119
De Rosa, S. *et al., Phytochemistry*, 1996, **42**, 1031-1034 (*6-arabinosylglucoside*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 261-262 (*occur, props*)
Boss, B. *et al., Phytochemistry*, 1999, **50**, 219-225 (*Benzyl sulfate*)
Li, Y. *et al., Molecules*, 2008, **13**, 2500-2508 (*Viscartin A*)
Li, F.-S. *et al., Nat. Prod. Commun.*, 2009, **4**, 511-512 (*hydroxybenzoylapiosylglucoside*)
Zheng, X. *et al., Nat. Prod. Commun.*, 2009, **4**, 1201-1204 (*2-arabinosylglucoside*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2625
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 120; 121
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDX500

Benzyl butyl ether B-65

(Butoxymethyl)benzene, 9CI. 1-Benzyloxybutane. α-Butoxytoluene. FEMA 2139 [588-67-0]

$PhCH_2OCH_2CH_2CH_2CH_3$

$C_{11}H_{16}O$ 164.247
Constit. of the aroma of roasted cashew and some edible mushrooms. Flavouring agent. d_4^{20} 0.92. Bp_{15} 95-97° Bp_{10} 92°. n_D^{20} 1.4833.

Barluenga, J. *et al., Synthesis*, 1983, 53 (*synth, pmr, cmr*)
Li, J. *et al., CA*, 1987, **107**, 115303w (*synth*)
Jayalekshmy, A. *et al., ACS Symp. Ser.*, 1988, **409**, 355 (*occur*)
Motoi, M. *et al., Polym. J. (Tokyo)*, 1989, **21**, 987 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 264 (*use, occur*)

Benzyl ethyl ether B-66

(Ethoxymethyl)benzene, 9CI. Ethyl benzyl ether. FEMA 2144 [539-30-0]

$PhCH_2OEt$

$C_9H_{12}O$ 136.193
Present in cocoa, American cranberry, lychee and eucalyptus oil. Flavouring agent. Liq. with powerful fruity odour. d^{20} 0.95. Bp 189° Bp_{18} 78°. n_D^{20} 1.4955.

McKillop, A. *et al., Tetrahedron*, 1974, **30**, 2467 (*synth*)
Adcock, W. *et al., JOC*, 1976, **41**, 1498 (*cmr*)
Grandi, R. *et al., JOC*, 1976, **41**, 1755 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 267-268
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 149 (*use, occur*)
Sax, N.I. *et al., Dangerous Properties of Industrial Materials, 5th edn., Van Nostrand Reinhold*, 1979, 411

Benzyl formate B-67

Phenylmethyl formate. FEMA 2145 [104-57-4]

$HCOOCH_2Ph$

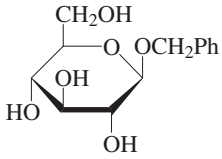
$C_8H_8O_2$ 136.15
Occurs in essential oils. Present in sour cherry, crowberry, *Vaccinium spp.* fruits, coffee, black tea, yellow passion fruit, *Ocimum basilicum* varieties and other foods. Used in perfumery and food flavouring. Liq. with fruity odour. Bp 203° Bp_{10} 83-84°. n_D^{20} 1.5404.

Be'hal, M.A. *et al., Ann. Chim. (Paris)*, 1900, **20**, 411 (*props*)
Bredereck, H. *et al., Chem. Ber.*, 1954, **87**, 726 (*synth*)
Suezawa, H. *et al., J. Phys. Org. Chem.*, 1993, **6**, 399 (*conformn*)
Suri, S.C. *et al., Synth. Commun.*, 1996, **26**, 1031 (*synth, ir, pmr, cmr, ms*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 268-269 (*props, occur*)

Benzyl glucopyranoside, 8CI B-68

Phenylmethyl glucopyranoside [34246-23-6]



α-D-*form*

$C_{13}H_{18}O_6$ 270.282

β-D-*form* [4304-12-5]
Constit. of *Ribes rubrum* (red currant) fruit and *Cucumis melo* var. *inodorus* (melon) and found in cell cultures of *Lycopersicon esculentum* (tomato). Needles (EtOAc/MeOH). Mp 123-125°. $[\alpha]_D^{25}$ -59.2 (c, 0.67 in MeOH).

6-O-*Malonyl:* [187340-52-9] ***Benzyl 6-malonylglucoside***
$C_{16}H_{20}O_9$ 356.329
Constit. of raspberries, strawberries, guava and green tea.

De Rosa, S. *et al., Phytochemistry*, 1996, **42**, 1031-1034 (*Lycopersicon esculentum constit*)
Withopf, B. *et al., J. Agric. Food Chem.*, 1997, **45**, 907-911 (*6-malonyl, detn*)
Schwarz, B. *et al., J. Agric. Food Chem.*, 2007, **55**, 1394-1404 (*Ribes rubrum constit*)
De Marino, S. *et al., Phytochem. Lett.*, 2009, **2**, 130-133 (*β-D-form, isol, melon, pmr, cmr*)

Benzyl glucosinolate B-69

*1-Thio-β-D-glucopyranose 1-[*N-*(sulfooxy)benzenethanimidate], 9CI*. ***Glucotropaeolin***. *Glucotropeolin*. *Phenylmethyl glucosinolate* [499-26-3]

$PhCH_2C(SGlc){=}NOSO_3H$

$C_{14}H_{19}NO_9S_2$ 409.437
Isol. from seeds of *Tropaeolum majus* (garden nasturtium), *Lepidium sativum* (garden cress) and other crucifers. Present in maca tubers (*Lepidium meyenii*).

K salt: [5115-71-9]
Amorph. powder.

Me_4N salt:
Cryst. Mp 188-189°. $[\alpha]_D^{28}$ -16.7 (H_2O).

Tetra-Ac:
Cryst. +1H_2O (EtOH aq.) (as K salt). Mp 197-199° dec. (K salt). $[\alpha]_D^{25}$ -19 (c, 0.5 in H_2O).

[92761-40-5, 117489-68-6]

Schultz, O.E. *et al., Z. Naturforsch., B*, 1952, **7**, 500; 1953, **8**, 151 (*isol*)
Schultz, O.E. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1955, **288**, 525 (*isol*)
Ettlinger, M.G. *et al., JACS*, 1957, **79**, 1764 (*synth*)
Benn, M.H. *et al., Can. J. Chem.*, 1963, **41**, 2836 (*synth*)
Underhill, E.W. *et al., Biochem. Biophys. Res. Commun.*, 1964, **14**, 425 (*biosynth*)
Fenwick, G.R. *et al., Biomed. Mass Spectrom.*, 1980, **7**, 410; 1981, **8**, 265 (*ms*)
Hanley, A.B. *et al., J. Sci. Food Agric.*, 1983, **34**, 869 (*isol*)
Cox, I.J. *et al., Carbohydr. Res.*, 1984, **132**, 323 (*pmr, cmr*)
Piacente, S. *et al., J. Agric. Food Chem.*, 2002, **50**, 5621-5625 (*isol, maca*)

Benzyl isothiocyanate B-70

(Isothiocyanatomethyl)benzene, 9CI. *Phenylmethyl isothiocyanate*. *Benzyl mustard oil*. *Tromocaps*. *Tromalyt active substance*. *Urogran*. *FEMA 4428* [622-78-6]

$PhCH_2NCS$

C_8H_7NS 149.216
Isol. from *Tropaeolum majus* (garden nasturtium) and *Lepidium sativum* (garden cress), also in other plants esp. in the Cruciferae. Potential nutraceutical. Flavouring ingredient. Pale yellow oil or orange-red cryst. Mp 41°. Bp 243° Bp_{12} 125-126°. Log P 3.2 (calc).

▶ Severe irritant. LD_{50} (mus, scu) 150 mg/kg. NX8250000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 465D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1552C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1422D (*ir*)
Hofmann, A.W. *et al., Ber.*, 1868, **1**, 201 (*synth*)
McKay, A.F. *et al., JACS*, 1959, **81**, 4328 (*synth, props*)
Kjaer, A. *et al., Acta Chem. Scand.*, 1963, **17**, 2143 (*ms*)
Tahahashi, K. *et al., Bull. Chem. Soc. Jpn.*, 1963, **36**, 108 (*pmr*)
Daxenbichler, M.E. *et al., J. Agric. Food Chem.*, 1964, **12**, 127 (*occur*)
Martin, D. *et al., Angew. Chem., Int. Ed.*, 1967, **6**, 168
Jochims, J.C. *et al., Angew. Chem., Int. Ed.*, 1967, **6**, 174 (*synth*)
Weuffen, W. *et al., Pharmazie*, 1967, **22**, 506; 510; 1968, **23**, 579 (*props*)
Lien, E.J. *et al., J. Med. Chem.*, 1968, **11**, 430 (*props*)
Molina, P. *et al., Synthesis*, 1982, 596 (*synth*)
Goerler, K. *et al., Xenobiotica*, 1982, **12**, 535 (*metab*)
Kim, S. *et al., JOC*, 1986, **51**, 2613 (*synth*)
Muthusamy, S. *et al., Org. Prep. Proced. Int.*, 1989, **21**, 228 (*synth*)
Pintao, A.M. *et al., Planta Med.*, 1995, **61**, 233 (*pharmacol*)
Hecht, S.S. *et al., Adv. Exp. Med. Biol.*, 1996, **401**, 1; 13 (*pharmacol, rev*)
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1678
Chen, X. *et al., Synthesis*, 2011, 3991-3996 (*synth, pmr, cmr*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*use, occur*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BEU250

Benzyl methyl disulfide B-71

Methyl phenylmethyl disulfide, 9CI. *FEMA 3504* [699-10-5]

$PhCH_2$-S-SMe

$C_8H_{10}S_2$ 170.299
Present in cocoa and roasted peanut. Flavouring ingredient. Mp 61-62°. $Bp_{0.2}$ 66° $Bp_{2.5}$ 105-110°. n_D^{24} 1.5996.

▶ JO0400000

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 432A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1103C (*ir*)
Armitage, D.A. *et al., JCS Perkin 1*, 1972, 680 (*synth*)
Harpp, D.N. *et al., JOC*, 1979, **44**, 4140 (*synth*)
Masui, M. *et al., Chem. Comm.*, 1984, 843 (*synth*)
Graber, D.R. *et al., JOC*, 1987, **52**, 4620 (*synth*)
Metzner, P. *et al., Synthesis*, 1994, 761 (*synth, pmr, cmr, ms*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1723-1724
Bewick, S.A. *et al., Aust. J. Chem.*, 2005, **58**, 218-223 (*synth, pmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1221 (*use, occur*)

Benzyl methyl sulfide, 8CI B-72

[(Methylthio)methyl]benzene, 9CI. *FEMA 3597* [766-92-7]

$PhCH_2SMe$

$C_8H_{10}S$ 138.233
Flavouring agent. Present in cooked pork. Liq. with powerful horseradish odour. d^{20} 1.03. Bp 199-201° Bp_{25} 80° Bp_4 70-72°. n_D^{20} 1.5632.

S-*Oxide (±):* [824-86-2] *[(Methylsulfinyl)methyl]benzene, 9CI. Benzyl methyl sulfoxide*
$C_8H_{10}OS$ 154.232
Cryst. (petrol). Mod. sol. H_2O, Et_2O, petrol, sol. EtOH, AcOH. Mp 54°.

S-*Oxide (S-):* [14090-81-4]
$C_8H_{10}OS$ 154.232
Oil. $[\alpha]_D^{20}$ +5 (c, 0.5 in $CHCl_3$).

S,S-*Dioxide:* [3112-90-1] *[(Methylsulfonyl)methyl]benzene. Benzyl methyl sulfone. DMIT*
$C_8H_{10}O_2S$ 170.232
Sol. H_2O. Mp 127°.

Thomson, T. *et al., JCS*, 1932, 69 (*synth, dioxide*)
Hünig, S. *et al., Annalen*, 1953, **579**, 23 (*oxide*)
Doerftel, K. *et al., J. Prakt. Chem.*, 1970, **312**, 701 (*ir*)
Russell, G.A. *et al., JOC*, 1979, **44**, 3990 (*synth*)
Youm, J.R. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2140 (*cmr*)
Luzzio, F.A. *et al., Synth. Commun.*, 1984, **14**, 209 (*synth*)
Fujisaki, S. *et al., Bull. Chem. Soc. Jpn.*, 1985, **58**, 2429 (*synth*)
Langler, R.F. *et al., Can. J. Chem.*, 1987, **65**, 2385 (*synth*)
Comasseto, J.V. *et al., J. Organomet. Chem.*, 1987, **334**, 329 (*synth, pmr*)
Lu, X. *et al., Synthesis*, 1987, 66 (*synth*)
Christophersen, C. *et al., Biochem. Syst. Ecol.*, 1989, **17**, 459 (*occur*)
Torisawa, Y. *et al., Tet. Lett.*, 1990, **29**, 1729 (*synth*)
Olah, G.A. *et al., Synthesis*, 1994, 277 (*synth, pmr, cmr*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 274

Kelly, P. *et al., Eur. J. Org. Chem.*, 2006, 4500-4509 (*oxide, S-form*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 156 (*use*)

Benzyl thiocyanate B-73

Phenylmethyl thiocyanate, 9CI. Benzyl rhodanide [3012-37-1]

$PhCH_2SCN$

C_8H_7NS 149.216
Isol. from *Lepidium sativum* (garden cress) as a benzyl glucosinolate (see Benzyl glucosinolate, B-69) degradation prod. Cryst. (petrol). Mp 41-42°.

▶ LD_{50} (mus, scu) 100 mg/kg. XK8155000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 465A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1550C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1422B (*ir*)
Footner, H.B. *et al., JCS*, 1925, **127**, 2887 (*synth*)
Gmelin, R. *et al., Acta Chem. Scand.*, 1959, **13**, 1474 (*isol*)
Bacon, R.G.R. *et al., JCS*, 1964, 5594 (*synth*)
Mravec, D. *et al., Coll. Czech. Chem. Comm.*, 1970, **35**, 3274 (*synth*)
Harpp, D.N. *et al., Synthesis*, 1979, 181 (*synth*)
Hasapis, H. *et al., Phytochemistry*, 1982, **21**, 1009 (*isol*)
Renwick, G.R. *et al., Crit. Rev. Food Sci. Nutr.*, 1983, **18**, 123 (*glucosinolates, rev*)
Kagabu, S. *et al., Chem. Pharm. Bull.*, 1991, **39**, 784 (*synth*)
Fujiki, K. *et al., Synth. Commun.*, 1999, **29**, 3289-3294 (*synth, ms*)
Renard, P.Y. *et al., Chem. Eur. J.*, 2002, **8**, 2910-2918 (*synth, ir, pmr*)
Yadav, L.D.S. *et al., Synth. Commun.*, 2011, **41**, 100-112 (*synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BFL000

Benzylamine, 8CI B-74

Benzenemethanamine, 9CI. α-Aminotoluene. Moringine [100-46-9]

$PhCH_2NH_2$

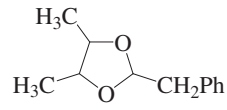
C_7H_9N 107.155
Alkaloid from *Moringa oleifera* (horseradish tree). d_4^{19} 0.98. Bp 185° Bp_{12} 90°. n_D^{20} 1.5401. pK_a 8.82 (20°, 60% dioxan aq.). Absorbs CO_2 from air.

▶ Fl. p. 63°. Reacts violently with *N*-haloimides. Corrosive and irritating to all tissues. DP1488500

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1266B; 1266C; 1274C; 1274A; 1274D; 1275A; 1279B; **2**, 366B (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 565B; 565C; 581B; 582A; 582B; 582C; 589A; 1385A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1163A; 1165D; 1166B; 1166C; 1167D (*ir*)
Chen, A.L. *et al., J. Am. Pharm. Assoc.*, 1931, **20**, 339 (*isol, derivs*)
Chakravarti, R.N. *et al., CA*, 1955, **50**, 16891f (*isol*)
Leyson, R. *et al., Spectrochim. Acta*, 1963, **19**, 243 (*ir*)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1967, **1**, 51; 1975, **5**, 479; 1980, **8**, 70; 1982, **10**, 26 (*use*)
Witanowski, M. *et al., Can. J. Chem.*, 1969, **47**, 1321 (*N-15 nmr*)
Egli, R.A. *et al., Helv. Chim. Acta*, 1970, **53**, 47 (*synth*)
Aihara, A. *et al., Bull. Chem. Soc. Jpn.*, 1972, **45**, 1942 (*pmr*)
Lichter, R.L. *et al., JACS*, 1972, **94**, 2495 (*N-15 nmr*)
Shapiro, M.J. *et al., JOC*, 1976, **41**, 3197 (*cmr*)
Kostyanovsky, R.G. *et al., Org. Mass Spectrom.*, 1976, **11**, 237 (*ms*)
Knights, R.J. *et al., Anal. Biochem.*, 1977, **77**, 106 (*use*)
Bastaert, G. *et al., C. R. Seances Acad. Sci., Ser. C*, 1980, **290**, 193 (*uv*)
Bradamante, S. *et al., JOC*, 1980, **45**, 105 (*cmr*)
Elmore, D.T. *et al., Acta Cryst. C*, 1992, **48**, 1331 (*cryst struct*)
Bretherick, L. *et al., Handbook of Reactive Chemical Hazards, 4th edn., Butterworths*, 1990, 2631
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 122
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BDY000; DQQ000; DQP800

2-Benzyl-4,5-dimethyl-1,3-dioxolane B-75

Phenylacetaldehyde 2,3-butylene glycol acetal. FEMA 2875 [5468-06-4]

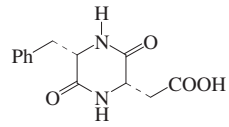


$C_{12}H_{16}O_2$ 192.257
Flavouring ingredient for baked goods, puddings, candies and nonalcoholic beverages. Viscous liq. with floral-earthy odour and fruity flavour. Bp_{10} 118°.

Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1653 (*use*)

5-Benzyl-3,6-dioxo-2-piperazineacetic acid B-76

3,6-Dioxo-5-(phenylmethyl)-2-piperazineacetic acid, 9CI. 5-Benzyldiketopiperazine-2-acetic acid. Cyclo(aspartylphenylalanyl). Cyclo(phenylalanylaspartyl) [55102-13-1]



(2*S*,5*S*)-*form*

$C_{13}H_{14}N_2O_4$ 262.265

(2*S*,5*S*)-*form* [5262-10-2]
L-cis-*form*
Degradn. product of Aspartame, A-694. Constit. of roasted cocoa nibs. Gelatinous needles (AcOH). Mp 256-258°.

[130856-96-1, 130856-97-2, 109062-52-4, 156769-20-9, 108147-50-8]

Davey, J.M. *et al., JCS(C)*, 1966, 555-566 (*synth*)
Hutchinson, S.A. *et al., Food Res. Int.*, 1999, **15**, 249-261 (*formn*)
Stark, T. *et al., J. Agric. Food Chem.*, 2005, **53**, 7222-7231 (*isol, ms*)

3-Benzyl-4-heptanone B-77

3-(Phenylmethyl)-4-heptanone, 9CI. Benzyl dipropyl ketone (incorr.). Morellone. FEMA 2146 [7492-37-7]

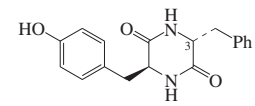
$H_3CCH_2CH(CH_2Ph)COCH_2CH_2CH_3$

$C_{14}H_{20}O$ 204.311
Used in food flavouring (plum/peach). No phys. props. reported.

Eur. Pat., 1989, 373 993 (*synth*)

3-Benzyl-6-(4-hydroxybenzyl)-2,5-piperazinedione, 8CI B-78

Cyclo(phenylalanyltyrosyl)



(3*R*,6*S*)-*form*

$C_{18}H_{18}N_2O_3$ 310.352

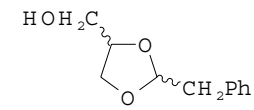
(3*R*,6*S*)-*form* [25582-20-1]
Cryst. (MeOH aq.). Mp 271-273° (as hydrate). $[\alpha]_D^{25}$ +1.4 (c, 0.48 in DMF).

(3*S*,6*S*)-*form* [5147-17-1]
Constit. of the roots of *Panax notoginseng* (sanchi). Cryst. (DMF aq.). Mp 300-302°. $[\alpha]_D^{25}$ -159 (c, 0.14 in DMF).

Blaha, K. *et al., Coll. Czech. Chem. Comm.*, 1969, **34**, 4000-4005; 1970, **35**, 619-643 (*synth, ord*)
Oya, M. *et al., Pept. Chem.*, 1977, **15**, 55-60 (*synth*)
Yamazaki, T. *et al., Biopolymers*, 1991, **31**, 1513-1528 (*conformn*)
Tan, N. *et al., Yunnan Zhiwu Yanjiu*, 2003, **25**, 366-368 (*isol*)

2-Benzyl-4-hydroxymethyl-1,3-dioxolane B-79

Phenylacetaldehyde glyceryl acetal. Acetal CD. FEMA 2877. 2-Benzyl-1,3-dioxolane-4-methanol, 9CI [5694-72-4]



$C_{11}H_{14}O_3$ 194.23
Mixt. with 5-Hydroxy-2-benzyl-1,3-dioxane, H-446 is used as a flavouring ingredient. No phys. props. reported.

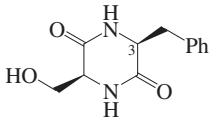
[29895-73-6]

Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1976, **14**, 829

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2180-2181

3-Benzyl-6-hydroxymethyl-2,5-piperazinedione B-80

3-(Hydroxymethyl)-6-(phenylmethyl)-2,5-piperazinedione, 9CI. Cyclo(phenylalanylseryl). Cyclo(serylphenylalanyl) [57287-86-2]



(3*S*,6*S*)-*form*

$C_{12}H_{14}N_2O_3$ 234.254

(3*R*,6*S*)-*form* [69176-06-3]
Cryst. (MeOH). $[\alpha]_D^{20}$ -10.2 (c, 1 in DMF).

(3*S*,6*R*)-*form* [35591-01-6]
Cryst. (MeOH). Mp 258-268° dec. $[\alpha]_D^{20}$ +11.2 (c, 1 in DMF).

(3*S*,6*S*)-*form* [35591-00-5]
L-L-form. (-)-cis-*form*
Constit. of roasted cocoa nibs. Cryst. (EtOAc). Mp 235-240° dec. (244-246°). $[\alpha]_D^{25}$ -56 (c, 0.2 in MeOH). $[\alpha]_D^{20}$ -105 (c, 1 in DMF).

Kirby, G.W. *et al., JCS Perkin 1*, 1978, 1336-1338; 1991, 1283-1290 (*isol, synth, biosynth*)
Qin, W. *et al., Zhongcaoyao*, 1995, **26**, 3-6 (*isol*)
Stark, T. *et al., J. Agric. Food Chem.*, 2005, 7222-7231 (*L,L-form, isol, ms*)
Isaka, M. *et al., Org. Lett.*, 2005, **7**, 2257-2260 (*isol, pmr, cmr*)

2-Benzylidene-1-heptanol B-81

2-(Phenylmethylene)-1-heptanol, 9CI. 2-Pentyl-3-phenyl-2-propen-1-ol. α-Pentylcinnamyl alcohol. α-Amylcinnamyl alcohol. FEMA 2065 [101-85-9] [184900-07-0]

$PhCH{=}C(CH_2OH)(CH_2)_4CH_3$

$C_{14}H_{20}O$ 204.311
Flavouring ingredient. Liq. with light floral odour. Bp_{12} 162° Bp_5 141-143°. *E/Z*-form unspecified.

Phenylurethane: Bp 61-62°.

Formyl: [7493-79-0] *α-Amylcinnamyl formate. FEMA 2066*
$C_{15}H_{20}O_2$ 232.322
Flavouring ingredient. Liq. with sweet, herbaceous somewhat green odour. Bp 277°.

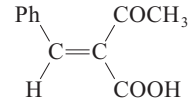
Ac: [7493-78-9] *α-Amylcinnamyl acetate. FEMA 2064*
$C_{16}H_{22}O_2$ 246.349
Flavouring ingredient. Liq. with somewhat fruity flavour. d_4^{20} 1. Bp_2 125-128°. n_D^{20} 1.5356.

3-Methylbutanoyl: [7493-80-3] *α-Amylcinnamyl isovalerate. FEMA 2067*
$C_{19}H_{28}O_2$ 288.429
Flavouring ingredient. Liq. with mild fruity, somewhat spicy flavour. Bp_4 171°.

Bogert, M.T. *et al., JACS*, 1931, **53**, 1605-1609 (*synth*)
Mastagli, P. *et al., C. R. Hebd. Seances Acad. Sci.*, 1937, **204**, 1656-1658 (*synth*)
Mastagli, P. *et al., Annalen*, 1938, **10**, 281-377 (*synth*)
Pansevich-Kolyada, V.I. *et al., CA*, 1967, **68**, 2746a; 1968, **71**, 12892w (*Ac, synth*)
Opdyke, D.L.J. *et al., Food Cosmet. Toxicol.*, 1974, **12**, 817; 1976, **14**, 677 (*tox, use, Ac*)
Konings, A.W.T. *et al., Chem.-Ztg.*, 1990, **114**, 1-5 (*synth*)
Dallacker, F. *et al., Chem.-Ztg.*, 1990, **114**, 1-5 (*synth*)
Choi, J. *et al., Tet. Lett.*, 1996, **37**, 1057-1060 (*Z-form, synth*)
Lutz, C. *et al., JOC*, 1997, **62**, 7895-7898 (*E,S-form, synth, pmr, cmr*)
Mosciano, G. *et al., Perfum. Flavor.*, 1997, **22**, 47-50 (*Ac, use, props*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 86-89 (*use, esters, props*)

2-Benzylidene-3-oxobutanoic acid B-82

3-Oxo-2-(phenylmethylene)butanoic acid, 9CI. 2-Acetyl-3-phenylacrylic acid. α-Acetylcinnamic acid [4361-81-3]



(*E*)-*form*

$C_{11}H_{10}O_3$ 190.198
Prisms (C_6H_6). Mp 103-110° (appears to refer to a mixt. of geom. isomers).

(*E*)-*form* [70083-47-5]
Cryst. Mp 100°.

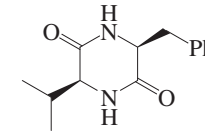
Et ester: [15802-62-7] *FEMA 4597* [620-80-4]
$C_{13}H_{14}O_3$ 218.252
Flavouring ingredient. Cryst. Mp 46°. *E/Z*- Stereochem. not specified by FEMA.

(*Z*)-*form* [70083-46-4]
Et ester: [15802-63-8] [620-80-4]
Flavouring ingredient. Cryst. (EtOH). Mp 60°. $Bp_{0.9}$ 125-126°.

Danion-Bougot, R. *et al., Bull. Soc. Chim. Fr.*, 1968, 2526 (*esters*)
Kato, T. *et al., Chem. Pharm. Bull.*, 1978, **26**, 3877 (*synth*)
Al-Hassan, S.S. *et al., JCS Perkin 1*, 1980, 2645 (*ester*)
Adachi, I. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3235 (*ester*)
Tanikaga, R. *et al., Bull. Chem. Soc. Jpn.*, 1988, **61**, 3211 (*ester*)
Zoeller, J.R. *et al., JOC*, 1990, **55**, 319 (*ester, bibl*)
Coté, M.L. *et al., Acta Cryst. C*, 1996, **52**, 2612-2614 (*E-form, synth, cryst struct*)
The Good Scents Company, (*Et ester, use*)

3-Benzyl-6-isopropyl-2,5-piperazinedione B-83

3-(1-Methylethyl)-6-(phenylmethyl)-2,5-piperazinedione, 9CI. Cyclo(phenylalanylvalyl). Cyclo(valylphenylalanyl) [14474-71-6] [55904-04-6, 55904-03-5]



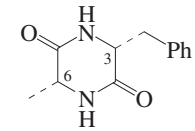
$C_{14}H_{18}N_2O_2$ 246.308

(3*S*,6*S*)-*form* [35590-86-4]
L,L-form
Constit. of the roots of *Panax notoginseng* (sanchi). Isol. from cocoa.

Oya, M. *et al., Pept. Chem.*, 1977, **15**, 55-60 (*synth*)
Kanmera, T. *et al., Int. J. Pept. Protein Res.*, 1980, **16**, 280-290 (*synth*)
Van der Greef, J. *et al., J. Chromatogr.*, 1987, **394**, 77-88 (*cocoa, isol*)
Yamazaki, T. *et al., Biopolymers*, 1991, **31**, 1513-1528 (*conformn*)
Tan, N. *et al., Yunnan Zhiwu Yanjiu*, 2003, **25**, 366-368 (*Panax, isol*)
Stark, T. *et al., J. Agric. Food Chem.*, 2005, **53**, 7222-7231 (*isol, synth, pmr, cmr, ms*)
Cabrera, G.M. *et al., J. Nat. Prod.*, 2006, **69**, 1806-1808 (*Paecilomyces, isol*)

3-Benzyl-6-methyl-2,5-piperazinedione B-84

3-Methyl-6-(phenylmethyl)-2,5-piperazinedione, 9CI. Cyclo(phenylalanylalanyl). Cyclo(alanylphenylalanyl) [14474-78-3]



(3*R*,6*R*)-*form*

$C_{12}H_{14}N_2O_2$ 218.255

(3*R*,6*R*)-*form* [23927-15-3]
D-D-form. (-)-cis-*form*
Mp 266-268°. $[\alpha]_D$ -60 (H_2O).

(3*R*,6*S*)-*form* [23927-18-6]
D-L-form. (-)-trans-*form*
Mp 253-255°. $[\alpha]_D$ -80 (H_2O).

(3*S*,6*R*)-*form* [15136-19-3]
L-D-form. (+)-trans-*form*
Mp 253-256°. $[\alpha]_D$ +80.1 (H_2O).

(3*S*,6*S*)-*form* [15180-22-0]
L-L-form. (+)-cis-*form*
Constit. of the roots of *Panax notoginseng* (sanchi). Constit. of cocoa nibs. Cryst. (MeOH). Mp 290-291° dec. (sealed tube). $[\alpha]_D^{19}$ +63 (c, 0.95 in AcOH).

Vul'fson, N.S. *et al., Khim. Geterotsikl. Soedin.*, 1966, 614 (*ms*)
Westley, J.W. *et al., Anal. Chem.*, 1968, **40**, 1888 (*chromatog, pmr*)
Slater, G.P. *et al., Chem. Ind. (London)*, 1969, 1092 (*synth*)
White, E.P. *et al., N.Z. J. Sci.*, 1972, **15**, 178 (*isol*)
Pickenhagan, W. *et al., Helv. Chim. Acta*, 1975, **58**, 1078 (*synth*)
Izumiya, N. *et al., JACS*, 1977, **99**, 8346 (*synth*)
Tan, N. *et al., Yunnan Zhiwu Yanjiu*, 2003, **25**, 366-368 (*Panax, isol*)
Stark, T. *et al., J. Agric. Food Chem.*, 2005, **53**, 7222-7321 (*L,L-form, isol, ms*)

2-Benzyl-3-oxobutanoic acid B-85

2-Benzylacetoacetic acid. 2-Acetyl-3-phenylpropanoic acid [2382-58-3]

$H_3CCOCH(COOH)CH_2Ph$

$C_{11}H_{12}O_3$ 192.214

(±)-*form*

Oil with aromatic smell. Spar. sol. H_2O. Bp_{13} 156-162°. Decarboxylates on warming.

Me ester: [3666-82-8]
$C_{12}H_{14}O_3$ 206.241
Bp_5 145°.

Et ester: [620-79-1] *FEMA 2416*
$C_{13}H_{16}O_3$ 220.268
Flavouring ingredient. Insol. H_2O, misc. EtOH, Et_2O. d^{25} 1.06. Bp 276° Bp_{18} 164°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 280A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1216B (*nmr*)
Ceresole, M. *et al., Ber.*, 1882, **15**, 1871 (*synth*)
Rupe, H. *et al., Annalen*, 1920, **426**, 33 (*resoln*)
Kabachnik, M.I. *et al., Tetrahedron*, 1961, **12**, 76 (*ester*)
Kazankova, M.A. *et al., Zh. Obshch. Khim.*, 1965, **35**, 1447 (*ester*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 943 (*Et ester*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 563 (*Et ester*)

1-Benzyloxy-1-(2-methoxyethoxy)ethane B-86

Benzyl methoxyethyl acetal. Acetaldehyde benzyl β-methoxyethyl acetal. FEMA 2148 [7492-39-9]

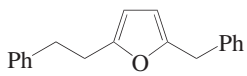
$MeOCH_2CH_2OCH(CH_3)OCH_2Ph$

$C_{12}H_{18}O_3$ 210.272
Flavouring ingredient. Liq. with sweet, green, fruity odour. Bp_{10} 161-162°.

Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 156 (*use*)

2-Benzyl-5-(2-phenylethyl)-furan B-87

2-(2-Phenylethyl)-5-(phenylmethyl)furan [26171-91-5]



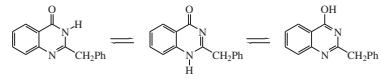
$C_{19}H_{18}O$ 262.351
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal).

3″-Methoxy, 4″-hydroxy: [1041740-13-9] *2-(4-Hydroxy-3-methoxybenzyl)-5-(2-phenylethyl)furan.* ***Alpinoid D***
$C_{20}H_{20}O_3$ 308.376
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal). Yellow cryst. Mp 70-72°. λ_{max} 202 (log ϵ 4.43); 227 (log ϵ 4.1); 279 (log ϵ 3.36) (MeOH).

Mavoungou-Gomes, L. *et al., C. R. Seances Acad. Sci., Ser. C*, 1970, **270**, 750-753 (*synth*)
Sun, Y. *et al., Planta Med.*, 2008, **74**, 427-431 (*Alpinoid D*)
An, N. *et al., Food Chem.*, 2010, **119**, 513-517 (*Alpinoid D*)

2-Benzyl-4(3*H*)-quinazolinone B-88

*2-(Phenylmethyl)-4(3*H*)-quinazolinone, 9CI. **Glycosminine**. Glycophymine. 2-Benzyl-4-hydroxyquinazoline. 2-(Phenylmethyl)-4-quinazolinol* [4765-56-4]



$C_{15}H_{12}N_2O$ 236.273
Specific inhibitor of serine protease and human leucocyte elastase. Cryst. (MeOH, EtOH, $CHCl_3$ or C_6H_6). Mp 254-256° (248-249°).

OH-form

Me ether: [72361-61-6] *4-Methoxy-2-(phenylmethyl)quinazoline. 2-Benzyl-4-methoxyquinazoline.* ***Glycophymoline***
$C_{16}H_{14}N_2O$ 250.299
Cryst. (C_6H_6/MeOH). Mp 165°.

1*H*-form

N-*Me:* [6873-15-0] *1-Methyl-2-(phenylmethyl)-4(1*H*)-quinazolinone. 2-Benzyl-1-methyl-4(1*H*)-quinazolinone.* ***Arborine***. *Glycosine*
$C_{16}H_{14}N_2O$ 250.299
Major alkaloid from *Ruta graveolens* (rue). Cryst. (MeOH/$CHCl_3$). Mp 161-162° (155-156°).

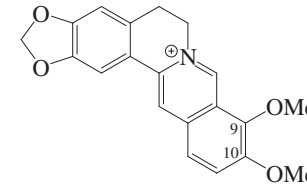
N-*Me, hydrochloride:*
Cryst. + $2H_2O$ (H_2O). Mp 215° dec. (partial melting at 106-108°).

N-*Me, picrate:*
Yellow needles (EtOH). Mp 172-173°.

Chakravarti, D. *et al., Tetrahedron*, 1961, **16**, 224-250 (*Arborine, uv, ir, pmr, struct*)
Pakrashi, S.C. *et al., Tetrahedron*, 1963, **19**, 1011 (*uv, ir, pmr, ms, struct, synth*)
Pakrashi, S.C. *et al., Indian J. Chem.*, 1968, **6**, 472 (*synth*)
O'Donovan, D.G. *et al., JCS(C)*, 1970, 2466-2470 (*biosynth*)
Patel, V.S. *et al., J. Indian Chem. Soc.*, 1972, **49**, 59 (*uv*)
Kametani, T. *et al., JACS*, 1977, **99**, 2306-2309 (*synth, ir, pmr*)
Rhee, R.P. *et al., JOC*, 1977, **42**, 3650 (*synth, ir, pmr*)
Sarkar, M. *et al., Phytochemistry*, 1977, **16**, 2007 (*isol, uv, ir, ms, synth*)
Kametani, T. *et al., Heterocycles*, 1978, **9**, 1585 (*synth*)
Bhattacharyya, J. *et al., Heterocycles*, 1979, **12**, 929; 1980, **14**, 1469 (*uv, ir, pmr, cmr*)
Naik, N.R. *et al., J. Indian Chem. Soc.*, 1979, **56**, 708-711 (*synth, uv, ir*)
Sarkar, M. *et al., Phytochemistry*, 1979, **18**, 694 (*Glycophymoline*)
Yamato, M. *et al., Chem. Pharm. Bull.*, 1981, **29**, 3124 (*synth*)
Chakraborty, D.P. *et al., Synthesis*, 1981, 977-979 (*synth*)
Teshima, T. *et al., J. Biol. Chem.*, 1982, **257**, 5085 (*pharmacol*)
Ganjian, I. *et al., Synth. Commun.*, 1984, **14**, 33 (*synth, pmr*)
Johne, S. *et al., Alkaloids (Academic Press)*, 1986, **29**, 129-140 (*Arborine, rev, pharmacol*)
Uozumi, Y. *et al., JACS*, 1989, **111**, 3725 (*synth, ir, pmr, ms*)
Muthukrishnan, J. *et al., Phytochemistry*, 1999, **50**, 249-254 (*Arborine, isol, pmr, cmr*)

Berberine B-89

5,6-Dihydro-9,10-dimethoxybenzo[g]-1,3-benzodioxolo[5,6-a]quinolizinium(1+), 9CI. Umbellatine†. Berbericine. Natural yellow 18. C.I. 75160. Majarine [2086-83-1]



$C_{20}H_{18}NO_4^{\oplus}$ 336.366
Log P -0.4 (uncertain value) (calc).

▶ Adverse human effects including reduced body temperature. Can cause death by central paralysis. LD_{50} (mus, orl) 329 mg/kg. DR9870000

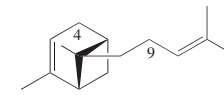
O^9-*De-Me:* [17388-19-1] ***Berberrubine***. *Chileninone*
$C_{19}H_{16}NO_4^{\oplus}$ 322.34
Alkaloid from *Berberis vulgaris* (barberry). Deep red amorph. solid (as chloride).

[79236-58-1 (Berberine cation)]

Späth, E. *et al., Monatsh. Chem.*, 1929, **52**, 117-128 (*Berberrubine, struct*)
Gharbo, S.A. *et al., J. Nat. Prod.*, 1973, **36**, 349-351 (*Berberrubine, activity*)
Siwon, J. *et al., Planta Med.*, 1981, **41**, 65-68 (*Berberrubine, occur*)
Valencia, E. *et al., Tetrahedron*, 1984, **40**, 3957-3962 (*Berberrubine, struct*)
Shamma, M. *et al., J. Nat. Prod.*, 1986, **49**, 398-405 (*Berberrubine, struct*)

α-Bergamotene B-90

Bergamotene [13474-59-4]
[17699-05-7]



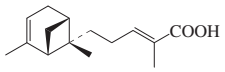
$C_{15}H_{24}$ 204.355
Constit. of oils of carrot (*Daucus carota*), bergamot (*Citrus bergamia*), also lime (*Citrus aurantifolia*), citron (*Citrus medica*) and cottonseed oil (*Gossypium hirsutum*). Oil. d^{20} 0.86. $[\alpha]_D^{20}$ -44.1 ($CHCl_3$). n_D^{20} 1.4904.

9-Oxo, 4ξ-β-D-glucopyranosyloxy: [1151862-03-1] ***Curvifloruside D***
$C_{21}H_{32}O_7$ 396.48
Powder. $[\alpha]_D^{20}$ -30 (c, 0.35 in MeOH). λ_{max} 227 (MeOH).

Kováts, E. *et al., Helv. Chim. Acta*, 1963, **46**, 2705-2731 (*pmr, ms, struct*)
Larsen, S.D. *et al., JACS*, 1977, **99**, 8015-8020 (*synth*)
Kulkarni, Y.S. *et al., JOC*, 1985, **50**, 2809-2810 (*synth*)
Snider, B.B. *et al., JOC*, 1988, **53**, 4508-4515 (*synth*)

Lai, G.-F. *et al., Helv. Chim. Acta*, 2009, **92**, 470-480 (*Curvifloruside D*)

α-Bergamotenoic acid B-91



(*E*)-*form*

$C_{15}H_{22}O_2$ 234.338

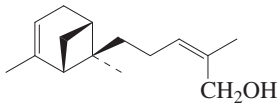
(*E*)-*form* [114248-38-3]
Cryst. (pentane). Mp 59-60°. $[\alpha]_D^{23}$ -46.3 (c, 1.3 in $CHCl_3$).

(*Z*)-*form* [124439-27-6]
Flavouring ingredient. Constit. of East Indian sandalwood oil. Oil.

Coates, R.M. *et al., JOC*, 1988, **53**, 2186-2192 (*isol*)
Nikiforov, A. *et al., Annalen*, 1990, 119-121 (*isol, pmr*)
Mori, K. *et al., Synthesis*, 1994, 417-421 (*synth*)

α-Bergamotenol B-92

[88034-74-6]



$C_{15}H_{24}O$ 220.354
Constit. of the famine food *Santalum album* (sandalwood). Flavouring ingredient. Oil. $[\alpha]_D$ -55.6 (c, 0.39 in $CHCl_3$).

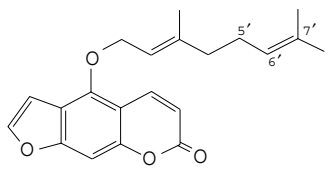
*(*E*)-Isomer, aldehyde:* [65336-62-1] ***α-Bergamotenal***
$C_{15}H_{22}O$ 218.338
Constit. of the roots of *Saussurea lappa* (costus). Oil. $Bp_{0.01}$ 70-75°. $[\alpha]_D$ -46.7 (neat).

[176777-61-0, 176777-60-9, 176777-62-1, 65336-63-2]

Maurer, B. *et al., Helv. Chim. Acta*, 1977, **60**, 2177-2190 (*α-Bergamotenal*)
Brunke, E.J. *et al., Dev. Food Sci.*, 1988, **18**, 819-831 (*rev*)
Pant, A.K. *et al., J. Essent. Oil Res.*, 1992, **4**, 9-13 (*isol*)
Yu, J.G. *et al., Yaoxue Xuebao*, 1993, **28**, 840-844 (*isol*)
Chapuis, C. *et al., Helv. Chim. Acta*, 1998, **81**, 153-162 (*abs config*)
Alizadeh, B.H. *et al., Biosci., Biotechnol., Biochem.*, 2002, **66**, 1415-1418 (*synth, pmr, cmr*)

Bergamottin B-93

*4-[(3,7-Dimethyl-2,6-octadienyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. Bergaptol geranyl ether. 5-Geranyloxypsoralen. Bergaptin* [7380-40-7]



$C_{21}H_{22}O_4$ 338.402
Constit. of bergamot oil. Also from lemon oil and oils of other *Citrus* spp. and carrot (*Daucus carota*). Cryst. (Et_2O/petrol). Mp 59-61° (54°).

*6′*R*,7′-Epoxide:* [105866-30-6] ***Epoxybergamottin***
$C_{21}H_{22}O_5$ 354.402
Constit. of grapefruit (*Citrus paradisi*) peel oil. Cryst. (EtOAc/hexane). Mp 82.5-83.5°.

*6′,7′-Dihydro, 6′*R*,7′-dihydroxy:* [71339-34-9] *4-[(6,7-Dihydroxy-3,7-dimethyl-2-octenyl)oxy]-7*H*-furo[3,2-*g*][1]benzopyran-7-one.* ***6′,7′-Dihydroxybergamottin (incorr.)***
[51956-35-5]
$C_{21}H_{24}O_6$ 372.417
Isol. from *Citrus macroptera* whole fruits, a non-commercial sp. of the South Pacific. Cryst. Mp 104-106°. $[\alpha]_D$ +12.7 ($CHCl_3$).

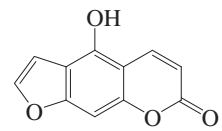
*6′,7′-Dihydro, 6′,7′-dihydroxy, 6′*R*,7′-octylidene:* [1181223-79-9] *6′,7′-Dihydroxybergamottin octanal acetal*
$C_{29}H_{38}O_6$ 482.616
Constit. of grapefruit peel (*Citrus paradisi*). Amorph. powder. λ_{max} 251 (log ϵ 4.17); 260 (sh); 268 (sh); 310 (log ϵ 4.05) (MeOH).

*6′,7′-Dihydro, 6′,7′-dihydroxy, 6′*R*,7′-decylidene:* [1181223-80-2] *6′,7′-Dihydroxybergamottin decanal acetal*
$C_{31}H_{42}O_6$ 510.669
Constit. of grapefruit peel (*Citrus paradisi*). Amorph. powder. λ_{max} 251 (log ϵ 4.14); 260 (sh); 267 (sh); 314 (log ϵ 4.15) (MeOH).

Späth, E. *et al., Ber.*, 1937, **70**, 2272-2276 (*Bergamottin*)
Chatterjee, A. *et al., JCS*, 1961, 2246-2247 (*Bergamottin, synth*)
Bates, R.B. *et al., Tet. Lett.*, 1963, 1683-1686 (*Bergamottin, config*)
Dreyer, D.L. *et al., Phytochemistry*, 1973, **12**, 3011-3013 (*6′,7′-dihydro-6′,7-dihydroxy*)
Tatum, J.H. *et al., Phytochemistry*, 1979, **18**, 500-502 (*Epoxybergamottin*)
Bellevue, F.H. *et al., Bioorg. Med. Chem. Lett.*, 1997, **7**, 2593-2598 (*synth, 6′,7′-dihydroxy*)
César, T.B. *et al., J. Nat. Prod.*, 2009, **72**, 1702-1704 (*octylidene, decylidene*)

Bergaptol B-94

*4-Hydroxy-7*H*-furo[3,2-*g*][1]benzopyran-7-one, 9CI. 4-Hydroxypsoralen* [486-60-2]



$C_{11}H_6O_4$ 202.166
Present in various citrus spp. Needles (EtOAc). Mp 277-278°.

O-*β-D-Glucopyranoside:* [131623-13-7] *Bergaptol glucoside*
$C_{17}H_{16}O_9$ 364.308
Needles (MeOH). Mp 254-256°.

O-*[α-L-Rhamnopyranosyl-(1→6)-β-D-glucopyranoside]: Bergaptol rutinoside*
$C_{23}H_{26}O_{13}$ 510.451
Mp 240-242°. $[\alpha]_D^{25}$ +150 (c, 0.5 in MeOH). λ_{max} 222; 251; 258; 266; 308 (MeOH).

O-*[β-D-Glucopyranosyl-(1→6)-β-D-glucopyranoside]:* [958243-11-3] *Bergaptol gentiobioside*
$C_{23}H_{26}O_{14}$ 526.45
$[\alpha]_D^{20}$ -5 (c, 0.1 in MeOH).

Me ether: [484-20-8] *4-Methoxy-7*H*-furo[3,2-*g*]benzopyran-7-one.* ***Bergapten****. Heraclin. Majudin. 5-Methoxypsoralen (obsol.)*
$C_{12}H_8O_4$ 216.193
Major constit. of bergamot oil (*Citrus bergamia*). Present in celery, esp. the outer leaves, and other common grocery vegetables. Implicated in photodermatitis among grocery workers. Needles (EtOH). Sol. MeOH, Et_2O; poorly sol. H_2O. Mp 188°. Log P 2.3 (calc). Pastinacin was impure Bergapten. λ_{max} 222 (ϵ 22600); 250 (ϵ 16500); 310 (ϵ 13600) (MeOH) (Berdy). λ_{max} 220 (ϵ 14100); 242 (ϵ 8000); 268 (ϵ 10700); 310 (ϵ 9100) (EtOH) (Berdy).

▶ Skin photosensitiser. Probable human carcinogen (IARC 2A). LD_{50} (mus, orl) 8100 mg/kg. LV1300000

O-*(2-Hydroxy-3-methyl-3-butenyl):* see Pabulenol, P-1

O-*(3,6,6-Trimethyl-7-oxo-2-heptenyl):* see Aurantiumal, A-732

O-*(3,7-Dimethyl-2,6-octadienyl):* see Bergamottin, B-93

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1321A (*nmr*)
Baetcke, E. *et al., Ber.*, 1912, **45**, 3705 (*struct*)
Glatfelder, A. *et al., Helv. Chim. Acta*, 1920, **3**, 541; 1921, **4**, 718 (*synth*)
Socias, L. *et al., Ber.*, 1934, **67**, 59 (*isol*)
Kubiczek, G. *et al., Ber.*, 1937, **70**, 1253 (*synth*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, no. 1369 (*occur, deriv*)
Austin, D.J. *et al., Phytochemistry*, 1973, **12**, 1657 (*biosynth*)
Boyd, R.K. *et al., Can. J. Chem.*, 1979, **57**, 1995 (*ms*)
Duddeck, H. *et al., Phytochemistry*, 1979, **18**, 139 (*cmr*)
Gu, Z. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2498 (*deriv*)
Ginderow, D. *et al., Acta Cryst. C*, 1991, **47**, 2144 (*cryst struct*)
Diawara, M.M. *et al., J. Agric. Food Chem.*, 1995, **43**, 723-727 (*occur*)
McNeely, W. *et al., Drugs*, 1998, **56**, 667-690 (*rev, Me ether*)
Masuda, T. *et al., Phytochemistry*, 1998, **47**, 13-16 (*Bergapten, isol, pmr, cmr*)
Kawaii, S. *et al., J. Agric. Food Chem.*, 1999, **47**, 4073 (*activity*)
Oliva, A. *et al., J. Chem. Ecol.*, 1999, **25**, 519-526 (*activity*)
Caceres, A. *et al., Fitoterapia*, 2001, **72**, 376-381 (*rutinoside*)
Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, J. Wiley, 2002, **83**, 1-619 (*rev*)

Murray, R.D.H. *et al., Prog. Chem. Org. Nat. Prod.*, 2002, **83**, 1-619 (*rev*)
Oda, K. *et al., Heterocycles*, 2005, **65**, 1985-1988 (*Bergapten, synth*)
Zhao, Y. *et al., Yaoxue Xuebao*, 2007, **42**, 1070-1073 (*gentiobioside*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, MFN275

Bervulcine B-95

$C_{18}H_{19}NO_3$ 297.353

Struct. unknown. Alkaloid from *Berberis vulgaris* (barberry). Mp 125-126° dec. $[\alpha]_D^{24}$ -185 (c, 0.2 in $CHCl_3$).

Hydroiodide:
Prisms (H_2O). Mp 236° dec.

Methiodide:
Cryst. (H_2O). Mp 269° dec.

Picrate:
Fine needles (MeOH). Mp 188-190° dec.

Döpke, W. *et al., Naturwissenschaften*, 1963, **50**, 595

Betaine B-96

Carboxy-N,N,N-*trimethylmethanaminium hydroxide inner salt, 9CI. (Carboxymethyl)trimethylammonium. Glycine betaine. Glycocoll betaine. Lycine. Abromine. Oxyneurine. Rubrine C. FEMA 4223* [107-43-7]

$Me_3N^{\oplus}CH_2COO^{\ominus}$

$C_5H_{11}NO_2$ 117.147

Dietary additive. Deliquescent scales or cryst.; cryst. + 1H_2O (H_2O). pK_a 3.84 (free acid). Dec. at *ca.* 310° (293-4°) with isom. to Me_2NCH_2COOMe.

▶ LD_{50} (mus, scu) 10800 mg/kg. DS5900000

Monohydrate: [17146-86-0] *Trimethylglycine hydroxide*
Cryst. Loses water at 100° to form inner salt.

Hydrochloride: [590-46-5] *Betaine hydrochloride, USAN. Lycine hydrochloride. Achyin. Acidin. Acidol. Acinorm. Acipepsol. Aciventral forte. Euacid. Muriat. Pepsacid. Pluchine*
Needles. Mp 243-244° dec. $[\alpha]_D^{20}$ -29.51 (H_2O).

▶ BP3136000

Aspartate (1:1): [52921-08-1] *Hepastyl. Somabet. Somatyl*

Picrate:
Yellow prisms (H_2O). Mp 181-182°.

[590-47-6]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 482B; 496B (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 563D; 588C (*ir*)
Stoltzenberg, H. *et al., Hoppe-Seyler's Z. Physiol. Chem.*, 1914, **92**, 445-494 (*synth*)
Edsall, J.T. *et al., JACS*, 1943, **65**, 1767-1770 (*synth, spectra*)
Guggenheim, M. *et al., Die Biogenen Amine*, 4th Ed., S. Karger, Basle, 1951, 240 (*occur*)
Gautier, J.A. *et al., C. R. Hebd. Seances Acad. Sci.*, 1955, **241**, 884-886 (*synth*)
Leifer, A. *et al., JACS*, 1957, **79**, 5098-5101 (*struct, ir*)
US Pat., 1957, 2 800 502 (*synth*)
Fr. Pat., 1964, M2462 (*salt*)
Dasgupta, B. *et al., Experientia*, 1967, **23**, 989-991; 1968, **24**, 882; 1970, **26**, 477-478 (*isol*)
West, M.E. *et al., J. Pharm. Pharmacol.*, 1967, **19**, 197-198 (*Rubrine C, isol, ir, pmr*)
Motohashi, N. *et al., Chem. Pharm. Bull.*, 1976, **24**, 1737-1741 (*cmr*)
Venkatasubramanian, K. *et al., Indian J. Phys., A*, 1984, **88A**, 40-49 (*Rubrine C, cryst struct*)
Larsen, C. *et al., Biomed. Environ. Mass Spectrom.*, 1988, **17**, 187-191 (*ms*)
Haussuehl, S. *et al., Z. Kristallogr.*, 1989, **188**, 311-320 (*derivs, cryst struct*)
Chevalier, Y. *et al., J. Phys. Chem.*, 1990, **94**, 1768-1774 (*conformn*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1553
Merck Index, 13th edn., 2001, No. 1182 (*props, bibl*)
Blunden, G. *et al., Phytochemistry*, 2001, **58**, 451-454 (*occur*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, GHA050

Betaine homocysteine *S*-methyltransferase B-97

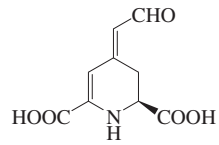
E.C. 2.1.1.5. Trimethylammonioacetate:L-homocysteine S-*methyltransferase. BHMT* [9029-78-1]

Methyltransferase enzyme. Isol. from pig liver.

Klee, W.A. *et al., Biochim. Biophys. Acta*, 1961, **54**, 157-164 (*mammalian liver*)
Skiba, W.E. *et al., J. Biol. Chem.*, 1982, **257**, 14944-14948 (*human liver*)
Lee, K.H. *et al., Arch. Biochem. Biophys.*, 1992, **292**, 77-86 (*rat liver*)
Garrow, T.A. *et al., J. Biol. Chem.*, 1996, **271**, 22831-22838 (*pig liver*)
Bose, N. *et al., Acta Cryst. D*, 2001, **57**, 431-433 (*cryst struct*)

Betalamic acid B-98

1,2,3,4-Tetrahydro-4-(oxoethylidene)-2,6-pyridinedicarboxylic acid [18766-66-0]



Absolute Configuration

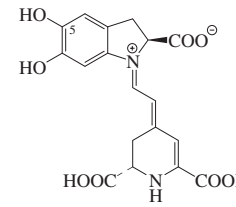
$C_9H_9NO_5$ 211.174

Precursor of betalains pigments in plants of the Centrospermae. Detected in *Beta vulgaris* (beetroot). Yellow soln. in H_2O at pH 9, or amorph. green residue. Sensitive to air, acids and strong alkali. Various protected derivs. known. λ_{max} 430 (no solvent reported).

Kimler, L. *et al., Chem. Comm.*, 1971, 1329 (*isol, synth, struct*)
Döpp, H. *et al., Chem. Ber.*, 1973, **106**, 3473 (*synth, uv*)
Büchi, G. *et al., JOC*, 1977, **42**, 2192 (*synth*)
Hilpert, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1547 (*synth*)
Fischer, N. *et al., Helv. Chim. Acta*, 2004, **55**, 649-658 (*biosynth*)

Betanidin B-99

*2-Carboxy-1-[(2,6-dicarboxy-2,3-dihydro-4(1*H*)-pyridinylidene)ethylidene]-2,3-dihydro-5,6-dihydroxy-1*H*-indolium hydroxide inner salt* [2181-76-2]



Absolute Configuration

$C_{18}H_{16}N_2O_8$ 388.333

Cryst. (as hydrochloride). Forms cryst. K and NH_4 salts. Shows rapid *E*/*Z* isom. in soln. λ_{max} 271 (ϵ 8530); 295 (sh) (ϵ 7170); 544 (ϵ 51000) (no solvent reported) (hydrochloride).

5-O-β-D-Glucopyranoside: [7659-95-2] ***Betanin***. *Phytolaccanin. C.I. Natural Red 33. E 162*
$C_{24}H_{26}N_2O_{13}$ 550.475
Red pigment from beetroot, *Beta vulgaris* var. *rubra* and other Centrospermae. Used as a food dye.

▶ US7968100

5-O-(6-O-Sulfo-β-D-glucopyranoside): [13798-16-8] ***Prebetanin***
$C_{24}H_{26}N_2O_{16}S$ 630.539
Pigment from beetroot *Beta vulgaris*.

5-O-(4-O-Malonyl-β-D-glucopyranoside): ***Phyllocactin II***
$C_{27}H_{28}N_2O_{16}$ 636.522
Constit. of the fruit peel of *Hylocereus ocamponis*.

5-O-[β-D-Apiofuranosyl-(1→2)-β-D-glucopyranoside]:
$C_{29}H_{34}N_2O_{17}$ 682.591
Constit. of the fruit peel of *Hylocereus ocamponis*.

5-O-[4-Hydroxy-3-methoxy-E-*cinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:* [290313-64-3] [178885-00-2]
$C_{39}H_{42}N_2O_{20}$ 858.762
Pigment from *Phytolacca americana* (pokeberry).

5-O-[4-Hydroxy-3,5-dimethoxy-E-*cinnamoyl-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{40}H_{44}N_2O_{21}$ 888.788
Constit. of the fruit peel of *Hylocereus ocamponis*.

5-O-[β-D-Glucopyranosyl-(1→2)-4-O-malonyl-β-D-glucopyranoside]: [951659-92-0]
$C_{33}H_{38}N_2O_{21}$ 798.664
Constit. of the fruit of *Mammillaria* spp. Tentative struct. assigned.

5-O-[β-D-Glucopyranosyl-(1→2)-6-O-malonyl-β-D-glucopyranoside]: [951676-55-4] ***Mammillarinin***
$C_{33}H_{38}N_2O_{21}$ 798.664

Constit. of the fruit of *Mammillaria* spp.

5-O-*[β-D-Glucuronopyranosyl-(1→2)-β-D-glucopyranoside]:* [15167-84-7] ***Amaranthin***. *Amarantin* [11033-33-3]
$C_{30}H_{34}N_2O_{19}$ 726.601
Pigment from *Amaranthus caudatus* (love-lies-bleeding) and *Amaranthus tricolor* (Chinese spinach).

6-O-*[4-Hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranoside]:* [143022-02-0] ***Gomphrenin II***
$C_{33}H_{32}N_2O_{15}$ 696.62
Pigment from the fruits of *Basella rubra* (Malabar spinach).

14,15-Didehydro, 5-O-*β-D-glucopyranoside:* [71199-29-6] ***Neobetanin***
$C_{24}H_{24}N_2O_{13}$ 548.459
Present in roots of red beet (*Beta vulgaris* ssp. *vulgaris* var. *conditiva*). Also in flowers of Barbary fig (*Opuntia ficus-indica*). Prob. artifact. λ_{max} 267; 306; 470 (no solvent reported). λ_{max} 298; 365 (H_2O).

15-Epimer: [4934-32-1] ***Isobetanidin***
$C_{18}H_{16}N_2O_8$ 388.333
Minor congener of Betanidin. Epimeric at the piperidine COOH group.

15-Epimer, 5-O-*β-D-glucopyranoside:* [15121-53-6] ***Isobetanin***
$C_{24}H_{26}N_2O_{13}$ 550.475
Minor congener of Betanin, e.g. from beetroot and *Amaranthus* spp.

15-Epimer, 5-O-*(4*-O-*malonyl-β-D-glucopyranoside):* ***Isophyllocactin II***
$C_{27}H_{28}N_2O_{16}$ 636.522
Constit. of the fruit peel of *Hylocereus ocamponis.*

15-Epimer, 5-O-*[3-hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranoside]:* ***Isohylocerenin***
$C_{30}H_{34}N_2O_{17}$ 694.602
Constit. of the fruit of *Hylocereus ocamponis* and *Hylocereus polyrhizus.*

15-Epimer, 5-O-*[β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{29}H_{34}N_2O_{17}$ 682.591
Constit. of the fruit peel of *Hylocereus ocamponis.*

15-Epimer, 5-O-*[4-hydroxy-3-methoxy*-E-*cinnamoyl-(→3)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{39}H_{42}N_2O_{20}$ 858.762
Pigment from *Phytolacca americana* (pokeberry).

15-Epimer, 5-O-*[4-hydroxy-3,5-dimethoxy*-E-*cinnamoyl-(→5)-β-D-apiofuranosyl-(1→2)-β-D-glucopyranoside]:*
$C_{40}H_{44}N_2O_{21}$ 888.788
Constit. of the fruit peel of *Hylocereus ocamponis.*

15-Epimer, 5-O-*[β-D-glucopyranosyl-(1→2)-4*-O-*malonyl-β-D-glucopyranoside]:* [951659-95-3]
$C_{33}H_{38}N_2O_{21}$ 798.664
Constit. of the fruit of *Mammillaria* spp. Tentative struct. assigned.

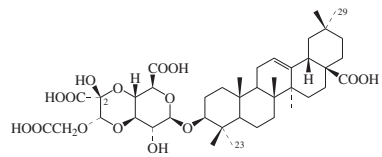
15-Epimer, 5-O-*[β-D-glucopyranosyl-(1→2)-6*-O-*malonyl-β-D-glucopyranoside]:* ***Isomammilarinin***
$C_{33}H_{38}N_2O_{21}$ 798.664
Constit. of the fruit of *Mammillaria* spp.

15-Epimer, 6-O-*[4-hydroxy*-E-*cinnamoyl-(→6)-β-D-glucopyranoside]:* [143062-65-1] ***Isogomphrenin II***
$C_{33}H_{32}N_2O_{15}$ 696.62
Pigment from the fruits of *Basella rubra* (Malabar spinach).

Piattelli, M. *et al., Ann. Chim. (Rome)*, 1966, **56**, 1060 (*Amaranthin*)
Wyler, H. *et al., Helv. Chim. Acta*, 1967, **50**, 545-560; 1984, **67**, 1793-1800 (*Prebetanin*)
Hilpert, H. *et al., Helv. Chim. Acta*, 1984, **67**, 1547-1561 (*synth*)
Alard, D. *et al., Phytochemistry*, 1985, **24**, 2383-2385 (*Neobetanin*)
Schliemann, W. *et al., Phytochemistry*, 1996, **42**, 1039-1046 (*Phytolacca americana constits*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 241 (*Betanin, use*)
Cai, Y. *et al., J. Agric. Food Chem.*, 2001, **49**, 1971 (*bibl, Gomphrenin II, Celosianin I, Isocelosianins, Isogomphrenin II*)
Wybraniec, S. *et al., J. Agric. Food Chem.*, 2007, **55**, 8138-8143 (*Mammillaria constits*)

Betavulgaroside II B-100

[168010-05-7]



$C_{41}H_{60}O_{15}$ 792.916
Complex glycoside of 3-Hydroxy-12-oleanen-28-oic acid, H-872. Constit. of *Beta vulgaris* (sugar beet). Cryst. Mp 173-174°. $[\alpha]_D$ +70.1 (MeOH).

28-O-*β-D-Glucopyranosyl ester:* [158511-55-8] ***Betavulgaroside I***. *Achyranthoside B*
$C_{47}H_{70}O_{20}$ 955.058
Constit. of *Beta vulgaris* (sugar beet). Cryst. Mp 215-217°. $[\alpha]_D$ +49.5 (MeOH).

2″-Me ether, 28-O-*β-D-glucopyranosyl ester:* [158511-54-7] ***Achyranthoside A***
$C_{48}H_{72}O_{20}$ 969.085
$[\alpha]_D$ +64.3 (MeOH) (as tri-Me ester).

23-Hydroxy, 28-O-*β-D-glucopyranosyl ester:* [354552-00-4] ***Basellasaponin A***
$C_{47}H_{70}O_{21}$ 971.057
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 228-230°. $[\alpha]_D^{24}$ +30.1 (c, 0.1 in MeOH). Complex glycoside of Hederagenin.

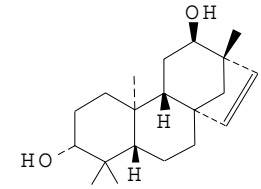
23-Aldehyde, 28-O-*β-D-glucopyranosyl ester:* [354552-02-6] ***Basellasaponin B***
$C_{47}H_{68}O_{21}$ 969.042
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 226-228°. $[\alpha]_D^{26}$ +57.4 (c, 0.1 in MeOH). Complex glycoside of Gypsogenin.

23-Carboxylic acid, 28-O-*β-D-glucopyranosyl ester:* [354552-04-8] ***Basellasaponin C***
$C_{47}H_{68}O_{22}$ 985.041
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 230-232°. $[\alpha]_D^{25}$ +42.1 (c, 0.1 in MeOH). Complex glycoside of Gypsogenic acid.

29-Carboxylic acid, 28-O-*β-D-glucopyranosyl ester:* [354552-06-0] ***Basellasaponin D***
$C_{47}H_{68}O_{22}$ 985.041
Constit. of *Basella rubra* (Malabar spinach). Cryst. (MeOH aq.). Mp 215-217°. $[\alpha]_D^{27}$ +24 (c, 0.1 in MeOH). Complex glycoside of Serratagenic acid.

Ida, Y. *et al., Tet. Lett.*, 1994, **35**, 6887 (*Achyranthosides, isol, pmr, cmr, cryst struct*)
Yoshikawa, M. *et al., Chem. Pharm. Bull.*, 1996, **44**, 1212-1217 (*Betavulgarosides*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 1999, **47**, 1717-1724 (*abs config*)
Murakami, T. *et al., Chem. Pharm. Bull.*, 2001, **49**, 776-779 (*Basellasaponins*)

15-Beyerene-3,12-diol B-101



$C_{20}H_{32}O_2$ 304.472

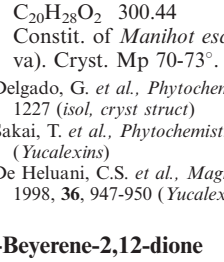
(*ent*-3β,12α)-*form* [88047-95-4] ***15-Stachene-3α,12β-diol***
Cryst. Mp 204-205°. $[\alpha]_D^{25}$ +8.73 (c, 0.126 in MeOH).

12-Ketone: [119626-51-6] ent-*3β-Hydroxy-15-beyeren-12-one.* ***Yucalexin B14***
$C_{20}H_{30}O_2$ 302.456
Constit. of *Manihot esculenta* (cassava).

3,12-Diketone: [88048-00-4] ent-*15-Beyerene-3,12-dione.* ***Yucalexin B6***
$C_{20}H_{28}O_2$ 300.44
Constit. of *Manihot esculenta* (cassava). Cryst. Mp 70-73°.

Delgado, G. *et al., Phytochemistry*, 1983, **22**, 1227 (*isol, cryst struct*)
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769 (*Yucalexins*)
De Heluani, C.S. *et al., Magn. Reson. Chem.*, 1998, **36**, 947-950 (*Yucalexin B16, pmr, cmr*)

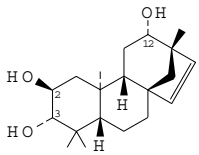
15-Beyerene-2,12-dione B-102



$C_{20}H_{28}O_2$ 300.44

ent-form [64657-12-1]
Yucalexin B7
Constit. of cassava roots (*Manihot esculenta*).
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769

15-Beyerene-2,3,12-triol B-103



(ent-2α,3β,12β)

$C_{20}H_{32}O_3$ 320.471

(*ent*-2α,3β,12β)-*form*
Needles (EtOH aq.). Mp 218-221.5°. $[\alpha]_D$ -11 (c, 1.86 in $CHCl_3$).

2-Ketone: [119626-53-8] ent-*3β,12β-Dihydroxy-15-beyeren-2-one.* ***Yucalexin B18***
$C_{20}H_{30}O_3$ 318.455
Constit. of *Manihot esculenta* (cassava root). $[\alpha]_D^{26}$ -9.4 (c, 0.17 in $CHCl_3$).

12-Ketone: [119626-55-0] ent-*2α,3β-Dihydroxy-15-beyeren-12-one.* ***Yucalexin B22***
$C_{20}H_{30}O_3$ 318.455
Constit. of cassava roots (*Manihot esculenta*).

2,12-Diketone: [35470-61-2] ent-*3β-Hydroxy-15-beyerene-2,12-dione.* ***Yucalexin B9***
$C_{20}H_{28}O_3$ 316.439
Constit. of cassava root *Manihot esculenta*. Mp 163-165.5°. $[\alpha]_D$ -329 ($CHCl_3$). $[\alpha]_D^{23}$ -73.9 (c, 0.83 in $CHCl_3$). Bitter taste. Large discrepancy in opt. rotn. of the two isolates.

Triketone: [50719-31-8] ent-*15-Beyerene-2,3,12-trione.* ent-*2-Hydroxy-1,15-beyeradiene-3,12-dione.* ***Yucalexin B5***
$C_{20}H_{26}O_3$ 314.424
Constit. of cassava roots *Manihot esculenta*. Prisms. Mp 170-173°. $[\alpha]_D$ -374 (c, 2.3 in $CHCl_3$). Exists as an enol form.

(*ent*-3β,12α)-*form*

2-Ketone: [119679-04-8] ent-*3β,12α-Dihydroxy-15-beyeren-2-one.* ***Yucalexin B20***
$C_{20}H_{30}O_3$ 318.455
Constit. of cassava *Manihot esculenta*.

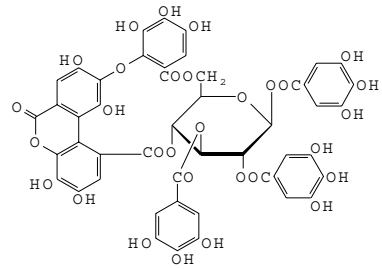
(2α,3β,12β)-*form*

Triketone: [413609-13-9] ***2-Hydroxy-1,15-beyeradiene-3,12-dione***. *15-Beyerene-2,3,12-trione*
$C_{20}H_{26}O_3$ 314.424
Oil. $[\alpha]_D^{25}$ -22.4 (c, 0.53 in $CHCl_3$). Exists as enol-form.

Triketone, 2-enol acetate: [413609-12-8] ***2-Acetoxy-1,15-beyeradiene-3,12-dione***
$C_{22}H_{28}O_4$ 356.461
Cryst. (MeOH). Mp 136-138°. $[\alpha]_D^{25}$ -294.2 (c, 2.1 in $CHCl_3$).
Piacenza, L.P.L. *et al., JCS Perkin 1*, 1979, 1004-1012 (*Androstachys johnsonii constit*)
Sakai, T. *et al., Phytochemistry*, 1988, **27**, 3769-3779 (*Manihot esculenta constits*)
Anjaneyulu, A.S.R. *et al., J. Nat. Prod.*, 2002, **65**, 382-385 (*Excoecaria agallocha constits*)

Bicornin B-104

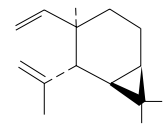
[124854-12-2]



$C_{48}H_{32}O_{30}$ 1088.763
Constit. of *Trapa bicornis* (horn nut). Amorph. powder. $[\alpha]_D$ +4.7 (MeOH).
Yoshida, T. *et al., Chem. Pharm. Bull.*, 1989, **37**, 2655 (*struct, pmr, cmr*)

Bicycloelemene B-105

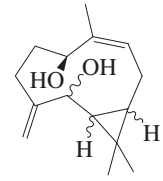
3-Ethenyl-3,7,7-trimethyl-2-(1-methylethenyl)bicyclo[4.1.0]heptane, 9CI. 2-Isopropenyl-3-methyl-3-vinylbicyclo[4.1.0]heptane [32531-56-9]



$C_{15}H_{24}$ 204.355
Constit. of peppermint oil. Oil. $[\alpha]_D^{20}$ -34.
Ulahov, R. *et al., Coll. Czech. Chem. Comm.*, 1967, **32**, 808 (*isol*)
Takeda, K. *et al., Chem. Comm.*, 1971, 308 (*struct*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1976, **14**, 852 (*synth*)

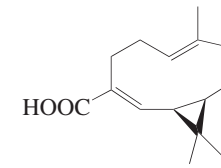
4(15),9-Bicyclogermacradiene-1,5-diol B-106

Baynol A [353453-03-9]



$C_{15}H_{24}O_2$ 236.353
Constit. of *Laurus nobilis* (bay laurel).
Matsuda, H. *et al., CA*, 2001, **135**, 164690g (*isol*)

1(10),4-Bicyclogermacradien-15-oic acid B-107



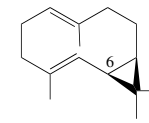
$C_{15}H_{22}O_2$ 234.338

(1(10)*E*,4*E*)-*form* [310396-79-3]
Madolin P
Cryst. (MeOH). Mp 174-176°. $[\alpha]_D$ +48 (c, 0.142 in $CHCl_3$). λ_{max} 250 (MeOH).

(1(10)*E*,4*Z*)-*form* [1247014-34-1]
Volvalerenic acid A
Constit. of *Valeriana officinalis* var. *latifolia* (valerian). Amorph. solid. $[\alpha]_D^{23}$ +117 (c, 0.26 in MeOH). λ_{max} 262 (log ϵ 4.1) (MeOH).
Wu, T.-S. *et al., Biol. Pharm. Bull.*, 2000, **23**, 1216-1219 (*Madolin P*)
Wang, P.-C. *et al., J. Nat. Prod.*, 2010, **73**, 1563-1567 (*Volvalerenic acid A*)

Bicyclogermacrene B-108

[24703-35-3]

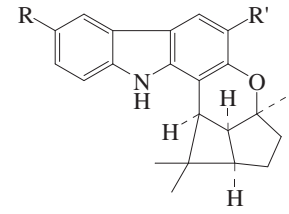


$C_{15}H_{24}$ 204.355
Constit. of the peel oil of *Citrus junos* (yuzu). Oil. $[\alpha]_D$ +61 ($CHCl_3$).

6-Epimer: [169276-07-7] ***Isolepidozene***
$C_{15}H_{24}$ 204.355
Oil. $[\alpha]_D$ -50 (c, 0.05 in $CHCl_3$).
Nishimura, K. *et al., Tetrahedron*, 1973, **29**, 271 (*isol, struct*)
McMurry, J.E. *et al., JOC*, 1987, **52**, 4885 (*synth*)
Ihara, M. *et al., JOC*, 1994, **59**, 8092 (*synth*)
Hardt, I.H. *et al., Phytochemistry*, 1995, **40**, 605 (*Isolepidozene*)

Bicyclomahanimbicine B-109

*1,2,2*a,*10,10*c,*11,11*a,*11*b-*Octahydro-2*a,*7,11,11-tetramethyl-3-oxa-10-azacyclobut[3,4]indeno[5,6-*a*]fluorene, 9CI* [28613-80-1]



R = CH_3, R' = H

$C_{23}H_{25}NO$ 331.457

Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Mp 218° dec. Probably an artifact. Also obt. by shaking a sol. of Mahanimbicine, M-35 with ion-exchange resin (H^+).

Kureel, S.P. *et al., Chem. Ind. (London)*, 1970, 958 (*uv, ir, pmr, struct, synth*)

Bicyclomahanimbine **B-110**

*1,2,2*a,*10,10*c,*11,11*a,*11*b-*Octahydro-2*a,*4,11,11-tetramethyl-3-oxa-10-azacyclobut[3,4]indeno[5,6-*a*]fluorene, 9CI*
[31077-94-8]

As Bicyclomahanimbicine, B-109 with R = H, R′ = CH_3

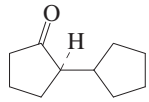
$C_{23}H_{25}NO$ 331.457
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Mp 145°. $[\alpha]_D^{23}$ -1.23 ($CHCl_3$). Probably an artifact. Also obt. readily from Mahanimbine, B-109.

N-*Me:* Mp 156°.

Kureel, S.P. *et al., Tet. Lett.*, 1969, 3857 (*uv, ir, pmr, ms*)
Bandaranayake, W.M. *et al., JCS Perkin 1*, 1974, 998 (*struct*)

[1,1′-Bicyclopentyl]-2-one, 9CI **B-111**

2-Cyclopentylcyclopentanone [4884-24-6]



(*R*)-*form*

$C_{10}H_{16}O$ 152.236

(*R*)-*form* [2865-81-8]
$[\alpha]_D^{22}$ +90.6 (c, 1.1 in dioxan). $[\alpha]_D^{23}$ +86.6 (c, 1.1 in $CHCl_3$) (53% ee).

(*S*)-*form* [2866-71-9]
$[\alpha]_D^{22}$ -91.1 (c, 1 in dioxan).

(±)-*form* [3063-68-1]
FEMA 4514
Flavour and fragrance ingredient. d_{22} 0.98. Bp_2 82-83°. n_D^{24} 1.4773.

Oxime:
$C_{10}H_{17}NO$ 167.25
Mp 78-79°.

2,4-Dinitrophenylhydrazone:
Mp 158-159°.

Semicarbazone:
Cryst. (EtOH). Mp 210°.

Mayer, R. *et al., Chem. Ber.*, 1956, **89**, 1443-1454 (*synth*)
Varech, D. *et al., Bull. Soc. Chim. Fr.*, 1965, 1662-1669 (*synth, config*)
Kirk, D.N. *et al., JCS Perkin 1*, 1976, 2171-2177 (*cd*)
Eur. Pat., 1980, 16 650 (*(±)-form, synth, use*)
Gurkova, S.N. *et al., Zh. Strukt. Khim.*, 1985, **26**, 183-185; *J. Struct. Chem. (Engl. Transl.)*, 1985, **26**, 821-823 (*Ge complex, cryst struct*)
Yanagisawa, A. *et al., Tetrahedron*, 1998, **54**, 10253-10264 (*R-form*)
The Good Scents Company, (*use*)

Bifidocin B **B-112**

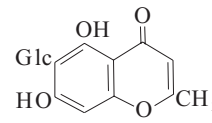
[204402-16-4]

Polypeptide containing 36 amino acids. Bacteriocin prod. by *Bifidobacterium bifidum* NCFB 1454.

Yildirim, Z. *et al., J. Food Prot.*, 1998, **61**, 47-51 (*isol*)
Yildirim, Z. *et al., J. Appl. Microbiol.*, 1999, **86**, 45-54 (*isol, struct*)

Biflorin† **B-113**

*6-β-D-Glucopyranosyl-5,7-dihydroxy-2-methyl-4*H*-1-benzopyran-4-one, 9CI*
[89701-85-9]



$C_{16}H_{18}O_9$ 354.313
Constit. of *Eugenia caryophyllata* (clove). Cryst. Mp 300-303° dec. $[\alpha]_D^{28}$ +24.4 (c, 0.34 in Py).

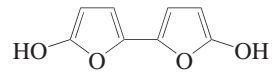
*2′-*O*-(3,4,5-Trihydroxybenzoyl):* ***Kunzeachromone C***
$C_{23}H_{22}O_{13}$ 506.419
Fine needles (MeOH). Mp 212-214°. $[\alpha]_D^{23}$ -87 (c, 1 in MeOH). λ_{max} 210 (log ϵ 4.73); 258 (log ϵ 4.45); 274 (log ϵ 4.23) (MeOH).

*2′,3′-Bis-*O*-(3,4,5-trihydroxybenzoyl):* ***Kunzeachromone D***
$C_{30}H_{26}O_{17}$ 658.525
Pale yellow amorph. powder. $[\alpha]_D^{23}$ -23 (c, 1 in MeOH). λ_{max} 215 (log ϵ 4.74); 259 (log ϵ 4.33); 277 (log ϵ 4.72) (MeOH).

Ghosal, S. *et al., Phytochemistry*, 1983, **22**, 2591
Zhang, Y. *et al., Phytochemistry*, 1997, **45**, 401 (*isol, pmr, cmr*)
Ito, H. *et al., J. Nat. Prod.*, 2004, **67**, 411-415 (*Kunzeachromones*)

[2,2′-Bifuran]-5,5′-diol **B-114**

5,5′-Dihydroxy-2,2′-bifuran



$C_8H_6O_4$ 166.133

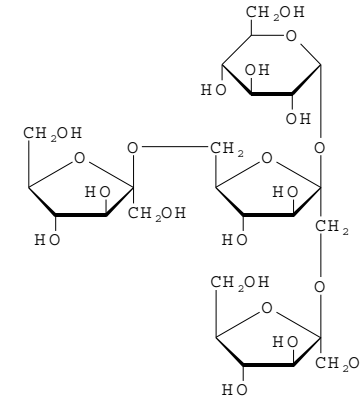
Bis(2-methylpropyl) ether: [1253591-85-3] *5,5′-Bis(2-methylpropoxy)-2,2′-bifuran*
$C_{16}H_{22}O_4$ 278.347
Oil.

Dibutyl ether: [1035897-79-0] *5,5′-Dibutoxy-2,2′-bifuran*
$C_{16}H_{22}O_4$ 278.347
Constit. of *Chrysanthemum coronarium* (chop-suey greens). Amorph. yellow powder. λ_{max} 241; 274 ($CHCl_3$).

Song, M.-C. *et al., Arch. Pharmacal Res.*, 2008, **31**, 573-578 (*dibutyl ether*)
Liu, J. *et al., Chin. Chem. Lett.*, 2010, **21**, 70-72 (*bis-2-methylpropyl ether*)

Bifurcose **B-115**

1-β-D-Fructofuranosyl-(2→1)-[β-D-fructofuranosyl-(2→6)]-β-D-fructofuranosyl α-D-glucopyranoside. 1,6-Kestotetraose
[3568-31-8]

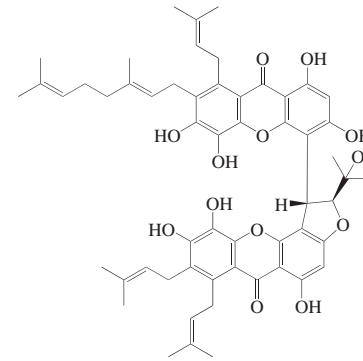


$C_{24}H_{42}O_{21}$ 666.583
A fructan. Isol. from barley (*Hordeum vulgare*) and *Panicum miliaceum* (proso millet). Cryst. Mp 156°. $[\alpha]_D^{20}$ +8.8 (H_2O).

Schlubach, H.H. *et al., Annalen*, 1958, **614**, 126; 1963, **665**, 191; 1964, **677**, 165 (*isol*)

Bigarcinenone A **B-116**

[1073496-49-7]



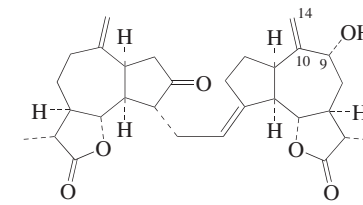
Relative Configuration

$C_{56}H_{62}O_{13}$ 943.098
Constit. of the bark of famine food *Garcinia xanthochymus.* Amorph. yellow powder. $[\alpha]_D$ -1.3 (c, 0.3 in Me_2CO). λ_{max} 238 (log ϵ 4.38); 281 (log ϵ 4.09); 324 (log ϵ 4.12); 343 (log ϵ 4.14) (MeOH).

Zhong, F.-F. *et al., Helv. Chim. Acta*, 2008, **91**, 1695-1703 (*isol, pmr, cmr, ms*)

Biguaiascorzolide A **B-117**

[1178553-45-1]



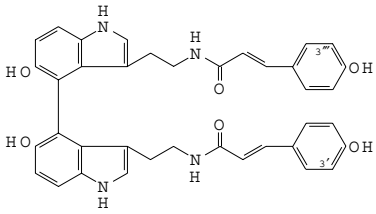
$C_{30}H_{38}O_6$ 494.627
Constit. of *Scorzonera austriaca*. Gum.

9-Ketone, 10α,14-dihydro: [1178553-46-2] ***Biguaiascorzolide B***
$C_{30}H_{38}O_6$ 494.627
Constit. of *Scorzonera austriaca*. Gum. $[\alpha]_D^{20}$ -15 (c, 0.36 in $CHCl_3$).

Zhu, Y. *et al., Food Chem.*, 2009, **114**, 1316-1320 (*Biguaiascorzolides A,B*)

4,4″-Bi[*N*-4-hydroxycinnamoylserotonin] B-118

*4,4″-Bis(*N-p-*coumaroylserotonin)*



$C_{38}H_{34}N_4O_6$ 642.71

(*E,E*)-*form* [175702-01-9]
Isol. from safflower (*Carthamus tinctorius*) oil cake. Powder. Mp 180-182°. λ_{max} 221 (ε 43000); 294 (ε 35000); 305 (ε 34700) (MeOH).

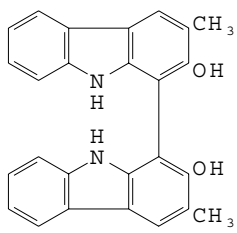
3′-Methoxy: [175702-02-0] ***4-[*N-*(*p-*Coumaroyl)serotonin-4″-yl]*-N-*feruloylserotonin***
$C_{39}H_{36}N_4O_7$ 672.736
From *Carthamus tinctorius* oil cake. Powder. Mp 179-181°. λ_{max} 221 (ε 70500); 292 (ε 51000); 309 (ε 52700) (MeOH).

3′,3‴-Dimethoxy: [175702-03-1] ***4,4″-Bi[*N-*(4-hydroxy-3-methoxycinnamoyl)serotonin]***. *4,4″-Bis(*N-*feruloyl)-serotonin*
$C_{40}H_{38}N_4O_8$ 702.762
From *Carthamus tinctorius* oil cake. Mp 158-160°. λ_{max} 289 (ε 35400); 317 (ε 38800) (MeOH).

Zhang, H.-L. *et al., Chem. Pharm. Bull.*, 1997, **45**, 1910-1914 (*isol, uv, ir, pmr, cmr*)

1,1′-Bi[2-hydroxy-3-methylcarbazole] B-119

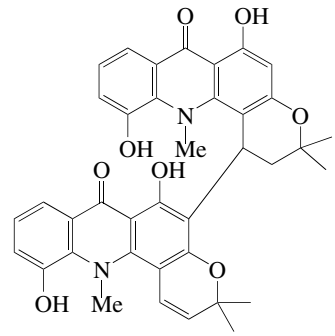
*3,3′-Dimethyl-[1,1′-bi-9*H*-carbazole]-2,2′-diol, 9CI* [155519-83-8]



$C_{26}H_{20}N_2O_2$ 392.456
Alkaloid from roots of *Murraya koenigii* (curryleaf tree). Oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)
Knölker, H.J. *et al., Synlett*, 1996, 737 (*synth*)

Bi[5-hydroxynoracronycine] B-120

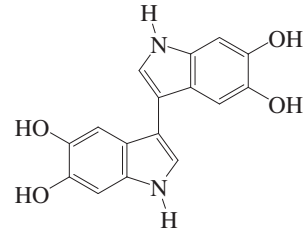


$C_{38}H_{34}N_2O_8$ 646.695
Alkaloid from the roots of *Citrus paradisi* (grapefruit). Yellow cubes (Me_2CO). Mp 207-209°. Racemic. λ_{max} 202; 231; 271; 290 (sh); 345 (sh) (EtOH).

Takemura, Y. *et al., Chem. Pharm. Bull.*, 1998, **46**, 693-696 (*isol, synth, uv, ir, pmr, cmr, ms*)

3,3′-Bi-1*H*-indole-5,5′,6,6′-tetrol B-121

*5,5′,6,6′-Tetrahydroxy-3,3′-bi-1*H*-indole* [390401-91-9]

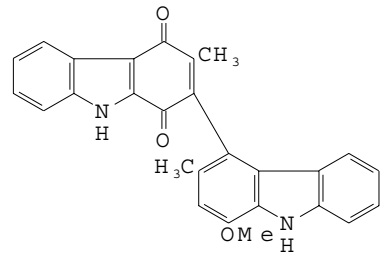


$C_{16}H_{12}N_2O_4$ 296.282
The synthesis in 2004 suggests that the struct. needs revision. Constit. of beetroot peel, *Beta vulgaris*.

Kujala, T. *et al., Z. Naturforsch., C*, 2001, **56**, 714-718 (*isol, pmr, cmr, ms*)
Mee, S.P.H. *et al., Tetrahedron*, 2004, **60**, 3695-3712 (*synth*)

Bikoeniquinone A B-122

*1′-Methoxy-3,3′-dimethyl-[2,4′-bi-9*H*-carbazole]-1,4-dione, 9CI* [155519-84-9]

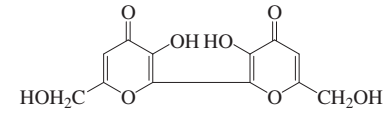


$C_{27}H_{20}N_2O_3$ 420.467
Alkaloid from roots of *Murraya koenigii* (curryleaf tree) (Rutaceae). Orange oil.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096 (*isol, uv, ir, pmr, ms, struct*)

Bikojic acid B-123

*6,6′-Bis(5-hydroxy-2-hydroxymethyl-4*H*-pyran-4-one). BGY-F*



$C_{12}H_{10}O_8$ 282.206
Dimer of 5-Hydroxy-2-(hydroxymethyl)-4*H*-pyran-4-one, H-641. Found in cotton lint associated with aflatoxin contamination in cotton seed *Gossypium hirsutum*. Bright greenish-yellow fluorescent compd.

Zeringue, H.J. *et al., Phytochemistry*, 1999, **52**, 1391-1397

Bile salt sulfotransferase B-124

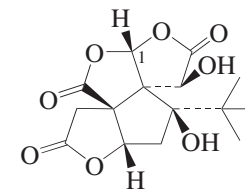
E.C. 2.8.2.14. 3′-Phosphoadenylyl-sulfate:glycolithocholate sulfotransferase. Glycolithocholate sulfotransferase. Bile acid:3′-phosphoadenosine-5′-phosphosulfate sulfotransferase†*. Bile acid sulfotransferase I. BAST I* [65802-92-8]

Sulfotransferase enzyme. Isol. from pig, rabbit. Acceptor substrates incl. both conjugated and unconjugated bile salts. Human enzyme activity range pH 5.5-10.5. Labile at 4°, but at -30°, in ethylene glycol, can be stored for at least 3 months.

Chen, L.-J. *et al., Biochim. Biophys. Acta*, 1977, **480**, 219-227; 1978, **522**, 443-451 (*rat*)
Loeoef, L. *et al., Biochim. Biophys. Acta*, 1978, **530**, 451-460; 1980, **617**, 192-204 (*human*)
Chen, L.-J. *et al., Methods Enzymol.*, 1981, **77**, 213-218 (*mammals*)
Chen, L.J. *et al., Arch. Biochem. Biophys.*, 1985, **241**, 371-379 (*human*)
Barnes, S. *et al., J. Lipid Res.*, 1986, **27**, 1111-1123 (*rhesus monkey*)
Macrides, T.A. *et al., Comp. Biochem. Physiol., B: Comp. Biochem.*, 1994, **107**, 461-469 (*shark*)
Russell, D.W. *et al., Annu. Rev. Biochem.*, 2003, **72**, 137-174 (*rev*)

Bilobalide A B-125

Bilobalide [33570-04-6]

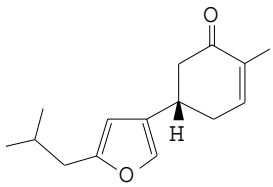


$C_{15}H_{18}O_8$ 326.302
Unusual cyclopentanoid sesquiterpene. Constit. of leaves of *Ginkgo biloba* (ginkgo). Cryst. (H_2O). Mp 300°. $[\alpha]_D^{20}$ -66.6. Log P -3.25 (uncertain value) (calc). Component of commercially available *Ginkgo biloba* extract (GBE).

Weinges, K. *et al., Annalen*, 1969, **724**, 214-216; 1972, **759**, 158-172 (*isol, pmr, ms*)
Nakanishi, K. *et al., JACS*, 1971, **93**, 3544-3546 (*struct*)
Corey, E.J. *et al., JACS*, 1987, **109**, 7534-7536 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1988, **29**, 3423-3426 (*synth*)
Crimmins, M.T. *et al., JACS*, 1992, **114**, 5445-5447; 1993, **115**, 3146-3155 (*synth*)
Atzori, C. *et al., Antimicrob. Agents Chemother.*, 1993, **37**, 1492-1496 (*antibacterial activity*)
Bruno, C. *et al., Planta Med.*, 1993, **59**, 302-307 (*neoroprotectant activity*)
Van Beek, T. *et al., J. Nat. Prod.*, 1997, **60**, 735-738 (*isol*)
Cartayrade, A. *et al., Plant Physiol. Biochem. (Paris)*, 1997, **35**, 859-868; 869-879 (*biosynth*)
Song, W. *et al., Zhongguo Yaoli Xuebao (Acta Pharmacol. Sin.)*, 2000, **21**, 415-420 (*activity*)
Stromgaard, K. *et al., Angew. Chem., Int. Ed.*, 2004, **43**, 1640-1658 (*rev*)
Jaracz, S. *et al., Phytochemistry*, 2004, **65**, 2897-2902 (*isol*)
Nakanishi, K. *et al., Bioorg. Med. Chem.*, 2005, **13**, 4987-5000 (*rev*)
van Beek, T.A. *et al., Bioorg. Med. Chem.*, 2005, **13**, 5001-5012 (*rev*)
Shi, C. *et al., Apoptosis*, 2010, **15**, 715-727 (*activity*)

Bilobanone B-126

2-Methyl-5-[5-(2-methylpropyl)-3-furanyl]-2-cyclohexen-1-one, 9CI



$C_{15}H_{20}O_2$ 232.322

(*S*)-*form* [17015-33-7]
Constit. of *Ginkgo biloba* (ginkgo). Oil. $Bp_{0.09}$ 118-122° (bath). $[\alpha]_D$ +6.7.

Oxime: Mp 64-65°.

Semicarbazone: Mp 142-144°.

1ξ-Alcohol: ***Bilobanol***
$C_{15}H_{22}O_2$ 234.338

Irie, H. *et al., Chem. Comm.*, 1967, 678 (*struct*)
Büchi, G. *et al., JOC*, 1969, **34**, 857 (*synth*)
Hegde, S.E. *et al., JOC*, 1982, **47**, 3148 (*synth*)
Traditional Chinese Medicines, (ed. Milne, G.A.), Ashgate, 1999, 651 (*Bilobanol*)

Biochanin C B-127

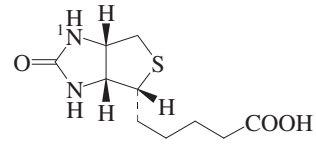
$C_{16}H_{13}N_3O_4$ 311.296

Struct. unknown. Isol. from seeds of *Cicer arietinum* (chickpea). Large prisms (EtOH or H_2O). Sol. H_2O. Mp 315°. Conts. one OMe group, unsatd. to Br_2.

Siddiqui, S. *et al., J. Sci. Ind. Res.*, 1945, **4**, 68-70
Warsi, S.A. *et al., Pak. J. Sci. Res.*, 1951, **3**, 85-88

Biotin, INN, USAN B-128

*Hexahydro-2-oxo-1*H*-thieno[3,4-*d*]imidazole-4-pentanoic acid, 9CI. Vitamin H. Coenzyme R. Vitamin B_7. Factor S*† [58-85-5]
[22879-79-4]



$C_{10}H_{16}N_2O_3S$ 244.314
Present in many foods; particularly rich sources include yeast, eggs, liver, certain fish (e.g. mackerel, salmon, sardines), soybeans, cauliflower and cow peas. Dietary supplement. Isol. from various higher plant sources, e.g. sweet corn seedlings and radish leaves. Fine needles (H_2O). Sol. H_2O. Mp 232-233°. $[\alpha]_D^{20}$ +91 (c, 1 in 0.1*M* NaOH). Log P -0.18 (calc).

▶ Shows exp. reproductive effects.

S-*Oxide:* [3376-83-8] *Biotin sulfoxide*
$C_{10}H_{16}N_2O_4S$ 260.313
Polymorphic plates (H_2O). Mp 238° part. dec. $[\alpha]_D^{20}$ -39.5 (c, 1.01 in 0.1*M* NaOH).

Me ester: [608-16-2]
$C_{11}H_{18}N_2O_3S$ 258.341
Cryst. Mp 166.5°. $[\alpha]_D^{15}$ +82 (c, 0.45 in MeOH).

Succinimidoyl ester: [35013-72-0]
$C_{14}H_{19}N_3O_5S$ 341.387
Cryst. (2-propanol). Mp 196-198°.

Amide: [6929-42-6] *Biotinamide*
$C_{10}H_{17}N_3O_2S$ 243.329
Rosettes (MeOH or H_2O). Mp 242-244°. $[\alpha]_D^{23}$ +80 (c, 2.5 in EtOH).

N^1-*Benzyl:* [76335-62-1] N-*Benzylbiotin. γ-Biotin*
$C_{17}H_{22}N_2O_3S$ 334.438
Needles (MeOH aq.). Mp 183-184°. Originally descr. as a natural vitamin under the name γ-biotin and descr. as *N*-phenylbiotin. Later shown to be an artifact with no vitamin activity.

[10406-89-0]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 809C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1317C (*nmr*)
Harris, S.A. *et al., JACS*, 1944, **66**, 1756-1757 (*synth, resoln*)
Wolf, D.E. *et al., JACS*, 1951, **73**, 4142-4144 (*amide, synth*)
Jansen, A.B.A. *et al., JCS*, 1962, 4909-4914; 1964, 1530-1531 (*γ-Biotin*)
Trotter, J. *et al., Biochemistry*, 1966, **5**, 713-714 (*cryst struct, abs config*)
Green, N.M. *et al., JCS(C)*, 1970, 1330-1333 (*cd, ord*)
De Titta, G.T. *et al., JACS*, 1976, **98**, 1920-1926 (*cryst struct*)
Marx, M. *et al., JACS*, 1977, **99**, 6754-6756 (*synth, bibl*)
Ohrui, H. *et al., Agric. Biol. Chem.*, 1978, **42**, 865-868 (*synth*)
Vasilevskis, J. *et al., JACS*, 1978, **100**, 7423-7424 (*synth, bibl*)
Uskokovic, M.R. *et al., Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley*, 1978, **24**, 41 (*rev*)
Baggiolini, E.G. *et al., JACS*, 1982, **104**, 6460-6462 (*synth*)
Whitney, R.A. *et al., Can. J. Chem.*, 1983, **61**, 1158-1160 (*synth*)
Bonjour, J.-P. *et al., Handbook of Vitamins*, (ed. Machlin, L.J.), M. Dekker, New York, 1984, 403 (*rev*)
Dakshinamurti, K. *et al., Ann. N.Y. Acad. Sci.*, (Eds.), 1985, **447**, (*book*)
Bentley, R. *et al., Trends Biochem. Sci.*, 1985, **10**, 51-56 (*rev, abs config*)
Al-Hakim, A.H. *et al., Nucleic Acids Res.*, 1986, **14**, 9965-9976 (*succinimidoyl ester*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 1715
Lee, H.L. *et al., Tetrahedron*, 1987, **43**, 4887-4903 (*synth*)
Corey, E.J. *et al., Tet. Lett.*, 1988, **29**, 57-60 (*synth*)
Lewis, R.J. *et al., Food Additives Handbook*, Van Nostrand Reinhold International, New York, 1989, BGD100
Senuma, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 882-887 (*rev, synth*)
Parameswaran, K.N. *et al., Org. Prep. Proced. Int.*, 1990, **22**, 119-121 (*succinimidoyl ester, synth*)
Alcázar, V. *et al., Tetrahedron*, 1990, **46**, 1057-1062 (*synth*)
Bihovsky, R. *et al., Tetrahedron*, 1990, **46**, 7667-7676 (*synth*)
De Titta, G.T. *et al., JACS*, 1994, **116**, 6485-6493 (*cryst struct, nmr*)
Moolenaar, M.J. *et al., Angew. Chem., Int. Ed.*, 1995, **34**, 2391-2393 (*synth*)
Deroose, F.D. *et al., JOC*, 1995, **60**, 321-330 (*synth, bibl*)
Nicolaou, K.C. *et al., Classics in Total Synthesis, Targets, Strategies, Methods*, VCH, 1996, 285 (*bibl, synth*)
De Clercq, P.J. *et al., Chem. Rev.*, 1997, **97**, 1755-1792 (*rev, synth*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1336
Chen, F.-E. *et al., Synthesis*, 2000, 2004-2008; 2003, 2155-2160 (*synth, ir, pmr, ms*)
Mori, Y. *et al., Heterocycles*, 2002, **58**, 125-127 (*synth*)
Seki, M. *et al., JOC*, 2002, **67**, 5527-5536 (*synth*)
Shimizu, T. *et al., Yakugaku Zasshi*, 2003, **123**, 43-52 (*synth*)
Seki, M. *et al., Chem. Eur. J.*, 2004, **10**, 6102-6110 (*synth*)
Kimura, M. *et al., Tet. Lett.*, 2004, **45**, 1635-1637 (*synth, bibl*)
Chavan, S.P. *et al., Tetrahedron*, 2005, **61**, 9273-9280 (*synth*)
Roje, S. *et al., Phytochemistry*, 2007, **68**, 1904-1921 (*biosynth, rev*)
Seki, M. *et al., Stud. Nat. Prod. Chem.*, 2008, **34**, 265-307 (*rev, prodn*)
Huang, J. *et al., Tetrahedron: Asymmetry*, 2008, **19**, 1436-1443 (*synth*)
Xiong, F. *et al., Tetrahedron: Asymmetry*, 2010, **21**, 665-669 (*synth*)
Chen, X.-X. *et al., Chem. Pharm. Bull.*, 2011, **59**, 488-491 (*synth*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, VSU100

Biotin synthase B-129

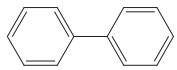
E.C. 2.8.1.6. Dethiobiotin:sulfur sulfurtransferase. BioB [80146-93-6]
[204794-88-7, 215108-34-2, 179608-56-1, 209603-31-6, 174764-24-0, 153554-27-9]

Sulfurtransferase enzyme. Isol. from lavender oil. An Fe-S enzyme. Radical intermeds. are formed by hydrogen atom transfer from dethiobiotin to the adenosyl radical.

Baldet, P. *et al., Eur. J. Biochem.*, 1993, **217**, 479-485 (*Lavandula vera*)
Flint, D.H. *et al., Methods Enzymol.*, 1997, **279**, 349-356 (*Escherichia coli*)
Bui, T.S. *et al., Methods Enzymol.*, 1997, **279**, 356-362 (*Bacillus sphaericus*)
Ugulava, N.B. *et al., Biochemistry*, 2001, **40**, 8343-8351; 8352-8358; 2003, **42**, 2708-2719 (*Escherichia coli*)
Berkovitch, F. *et al., Science (Washington, D.C.)*, 2004, **303**, 76-79 (*cryst struct*)

Biphenyl, 8CI, BSI, ISO B-130

1,1′-Biphenyl, 9CI. Bibenzene. Diphenyl. Phenylbenzene. Carolid AL. E230. FEMA 3129 [92-52-4]



$C_{12}H_{10}$ 154.211

Fungistat, esp. for citrus fruits. Used as food preservative and flavouring agent. Detected in bilberry, wine grape, carrot, peas, rum, potato, bell pepper, tomato, butter, milk, smoked fatty fish, cocoa, coffee, roast peanuts, olive, buckwheat and tamarind. Generally, the fruit packaging is impregnated with biphenyl, which evaporates into the air space surrounding the fruit. Some biphenyl is absorbed by the fruit skins. Monoclinic cryst. with faint pleasant odour. Mp 71°. Bp 254-255° Bp_{22} 145° $Bp_{0.2}$ 70-78°. Planar in the cryst. state at -233°, dihedral angle 10° in cryst. state >-233°, 25° in molten state, 32° in soln., 42° in gas phase.

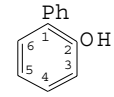
▶ Fl. p. 113°, autoignition temp. 540°. Eye and mucous membrane irritant. Prolonged or repeated skin contact may cause sensitisation and dermatitis. Occup. exposure causes changes to central and peripheral nervous systems, and gastrointestinal disturbances. LD_{50} (rat, orl) 3280 mg/kg. OES: long-term 0.2 ppm; short-term 0.6 ppm. DU8050000

[8004-13-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 948A (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 28C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 871B (*ir*)
Forrest, J. *et al., JCS*, 1960, 574 (*synth*)
Brownlee, R.T.C. *et al., JACS*, 1968, **90**, 1757 (*ir*)
Laseter, J.L. *et al., Org. Mass Spectrom.*, 1970, **4**, 599 (*ms*)
Nordén, B. *et al., Acta Chem. Scand.*, 1972, **26**, 429 (*uv*)
Kamezawa, N. *et al., J. Magn. Reson.*, 1973, **11**, 88 (*pmr*)
Schulman, E.M. *et al., JOC*, 1974, **39**, 2686 (*cmr*)
Charbonneau, G.P. *et al., Acta Cryst. B*, 1976, **32**, 1420; 1977, **33**, 1586 (*cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **7**, 782 (*rev*)
Takagi, K. *et al., Chem. Lett.*, 1979, 917 (*synth*)
Cook, I.B. *et al., Aust. J. Chem.*, 1989, **42**, 1493 (*cmr*)
Pesticide Manual, 9th edn., 1991, 1010
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A166
Bock, H. *et al., Chem. Eur. J.*, 1995, **1**, 557 (*bibl, conformn*)
Mukhopadhyay, S. *et al., Org. Process Res. Dev.*, 2002, **6**, 297-300 (*synth, pmr*)
Moglie, Y. *et al., Synth. Commun.*, 2008, **38**, 3861-3874 (*synth, ir, pmr, cmr, ms*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 163 (*use, props, occur*)
Maji, M.S. *et al., Synthesis*, 2009, 2467-2470 (*synth, pmr, cmr*)
Darweesh, A.F. *et al., Synthesis*, 2010, 3163-3173 (*synth, pmr, ms*)
Kaboudin, B. *et al., Synthesis*, 2011, 91-96 (*synth, pmr, cmr*)
Chemical Hazards of the Workplace, 3rd edn., (eds. Proctor, N.H. et al), Van Nostrand Reinhold, 1991, 113
Luxon, S.G. *et al., Hazards in the Chemical Laboratory, 5th edn., Royal Society of Chemistry*, 1992, 134
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BGE000

2-Biphenylol, 8CI B-131

2-Hydroxybiphenyl. 2-Phenylphenol, BSI, ISO. Orthophenylphenol. Orthoxenol. o-Xenol. Dowicide 1. nvalon OP. Manusept. Nectryl. Nipacide OPP. Rotoline. Stellisept. Torsite. E231. FEMA 3959 [90-43-7] [1322-20-9]



$C_{12}H_{10}O$ 170.21

Antifungal agent, preservative. Used for post-harvest control of storage disease in apples, citrus fruit, stone fruit, tomatoes, cucumber and peppers through the use of impregnated wrapping materials or by direct application in a wax. Used in food seasonings. Inhibitory to a wider range of moulds than Biphenyl, B-130. The practical way of treatment is to immerse citrus fruit in an alkaline aq. soln. of the parent compd. or its Na salt. Needles (petrol). Mp 56°. Bp 275° Bp_{14} 145°. pK_{a1} 10.01 (20°).

▶ Eye and skin irritant. LD_{50} (mus, orl) 1050 mg/kg. Exp. carcinogen. Exp. teratogenic effects. Fl. p. 107°. DV5775000

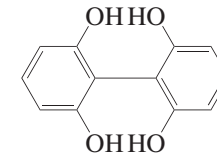
Na salt: [132-27-4] *Dowicide A. Natriphene. E232*
[6152-33-6]
Agricultural fungicide, disinfectant, food preservative, mould inhibitor for apples. Tetrahydrate. Sol. H_2O.

▶ Possible human carcinogen (IARC 2B). DV7700000

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1057A; 1059D; 1115D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 212A; 215C; 317A (*nmr*)
Hirsch, R. *et al., Ber.*, 1890, **23**, 3705 (*synth*)
Musso, H. *et al., Chem. Ber.*, 1959, **92**, 3101 (*ir*)
Trible, M.T. *et al., JACS*, 1969, **91**, 379 (*pmr*)
Drapala, T. *et al., Pol. J. Chem. (Rocz. Chem.)*, 1974, **48**, 965 (*ir, uv*)
Asabe, Y. *et al., Bunseki Kagaku (Jpn. Anal.)*, 1975, **24**, 160 (*use*)
Robbiani, R. *et al., Angew. Chem., Int. Ed.*, 1977, **16**, 120 (*ms*)
Lotjonen, S. *et al., Finn. Chem. Lett.*, 1978, 260 (*cmr*)
Reitz, R.H. *et al., Chem. Biol. Interact.*, 1983, **43**, 99 (*Na salt*)
IARC Monogr., 1983, **30**, 329; 1987, *Suppl. 7*, 70 (*rev, tox*)
Perrin, M. *et al., Acta Cryst. C*, 1987, **43**, 980 (*cryst struct*)
Roshchina, E.N. *et al., Zh. Prikl. Khim.*, 1989, **62**, 1295 (*synth*)
Nakagawa, Y. *et al., Biochem. Pharmacol.*, 1992, **43**, 159 (*tox*)
Lambert, A.C. *et al., Mutat. Res.*, 1994, **322**, 243 (*tox*)
Nakagawa, Y. *et al., Cancer Lett.*, 1996, **101**, 227 (*tox*)
Pesticide Manual, 11th edn., 1997, No. 567
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1670 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BGJ250; PEG000; BGJ750

2,2′,6,6′-Biphenyltetrol B-132

2,2′,6,6′-Tetrahydroxybiphenyl. 2,2′-Biresorcinol [4371-35-1]



$C_{12}H_{10}O_4$ 218.209

Isol. from Pu-er tea (*Camellia sinensis* var. *assamica*). Cryst. (EtOH). Mp 191-192° (244°).

2,2′-Di-Me ether (S-): [154052-02-5]
$C_{14}H_{14}O_5$ 262.262
$[\alpha]_D$ -144 (c, 0.77 in $CHCl_3$).

Tetra-Me ether: [19491-10-2] *2,2′,6,6′-Tetramethoxybiphenyl*
$C_{16}H_{18}O_4$ 274.316
Mp 175°.

Simada, T. *et al., CA*, 1933, **27**, 4595 (*synth*)
v. Arendonk, A.M. *et al., JACS*, 1933, **55**, 4227 (*synth*)
Lettré, H. *et al., Chem. Ber.*, 1952, **85**, 346 (*synth*)
Wünsche, Ch. *et al., Tetrahedron*, 1968, **24**, 3407 (*ms*)
Lindsten, G. *et al., JOC*, 1987, **52**, 547 (*synth, pmr, ms*)
Sanfilippo, C. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 3267-3270 (*2,2′-di-Me ether, resoln, S-form*)
Zhou, Z.-H. *et al., J. Agric. Food Chem.*, 2005, **53**, 8614-8617 (*isol*)
Govender, S. *et al., Org. Biomol. Chem.*, 2007, **5**, 2433-2440 (*tetra-Me ether*)

2,3′,4′,5′-Biphenyltetrol B-133

2,3′,4′,5′-Tetrahydroxybiphenyl

$C_{12}H_{10}O_4$ 218.209

Mp 150-151.5°.

3′,5′-Di-Me ether: [98211-57-5] *2,4′-Dihydroxy-3′,5′-dimethoxybiphenyl*. ***2′-Hydroxyaucuparin***
$C_{14}H_{14}O_4$ 246.262
Constit. of *Malus* x *domestica* cv. Liberty.

*3′,5′-Di-Me ether, 2-*O*-β-D-glucopyranoside:* [221662-15-3] ***Fortuneanoside C***
$C_{20}H_{24}O_9$ 408.404
Constit. of *Malus* x *domestica* cv. Liberty. $[\alpha]_D^{17}$ -36.1 (c, 0.39 in MeOH). λ_{max} 205 (log ϵ 4.17); 269 (log ϵ 3.47); 286 (sh) (log ϵ 3.45) (MeOH).

2,3′,5′-Tri-Me ether: [3810-90-0] *2,6-Dimethoxy-4-(2-methoxyphenyl)phenol. 4-Hydroxy-2′,3,5-trimethoxybiphenyl*. ***2-Methoxyaucuparin***
$C_{15}H_{16}O_4$ 260.289
Mp 120-122° Mp 206-207° (178-180°) subl. λ_{max} 268 (ϵ 12590); 288 (MeOH) (Berdy). λ_{max} 265 (ϵ 12500); 286 (ϵ 9600) (EtOH) (Berdy). λ_{max} 304 (MeOH/NaOH) (Berdy).

3′,4′,5′-Tri-Me ether: [1188276-87-0] *2-(3,4,5-Trimethoxyphenyl)phenol. 2-Hydroxy-3′,4′,5′-trimethoxybiphenyl*
$C_{15}H_{16}O_4$ 260.289
Viscous oil. λ_{max} 266 (log ϵ 4.2); 292 (log ϵ 4.3) (MeOH).

Tetra-Me ether: 2,3′,4′,5′-Tetramethoxybiphenyl
$C_{16}H_{18}O_4$ 274.316
Cryst. (MeOH aq.). Mp 71.5-72°.

Norin, T. *et al., Acta Chem. Scand.*, 1963, **17**, 1151-1156; 1157-1159 (*Methoxyaucuparin*)
Malterud, K.E. *et al., Z. Naturforsch., B*, 1985, **40**, 83 (*2′-Hydroxyaucuparin*)
Kokubun, T. *et al., Phytochemistry*, 1995, **40**, 57-59 (*Sorbus aucuparia constits*)
Borejsza-Wysocki, W. *et al., Phytochemistry*, 1999, **50**, 231-235 (*Malus constit*)
Dai, Y. *et al., J. Nat. Prod.*, 2006, **69**, 1022-1024 (*Fortuneanoside C*)
Kim, K.H. *et al., J. Nat. Prod.*, 2009, **72**, 2061-2064 (*3′,4′,5′-tri-Me ether*)

3,4,4′,5-Biphenyltetrol B-134

3,4,4′,5-Tetrahydroxybiphenyl
$C_{12}H_{10}O_4$ 218.209

3,4′-Di-Me ether: [130364-26-0] *3,4-Dihydroxy-4′,5-dimethoxybiphenyl*. ***Rhaphiolepsin***
$C_{14}H_{14}O_4$ 246.262
Genus name given as Rhaphiolepsis. λ_{max} 265 (ϵ 13800) (EtOH) (Derep).

*3,4′-Di-Me ether, 5-*O*-β-D-glucopyranoside:* ***Kakispyrol***
$C_{20}H_{24}O_9$ 408.404
Constit. of the leaves of *Diospyros kaki* (Japanese persimmon). Needles. Mp 195-197°.

3,5-Di-Me ether: 4,4′-Dihydroxy-3,5-dimethoxybiphenyl. ***Garcibiphenyl C***
$C_{14}H_{14}O_4$ 246.262
Oil. λ_{max} 206 (log ϵ 4.66); 264 (log ϵ 4.11) (MeOH). λ_{max} 207 (log ϵ 4.85); 281 (log ϵ 4.08) (MeOH/KOH).

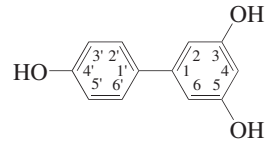
3,4,5-Tri-Me ether: [131189-45-2] ***4′-Hydroxy-3,4,5-trimethoxybiphenyl***. *3,4,5-Trimethoxy-4′-biphenylol*
$C_{15}H_{16}O_4$ 260.289
Cryst. ($CHCl_3$). Mp 142-143°.

3,4′,5-Tri-Me ether: [54961-04-5] *4-Hydroxy-3,4′,5-trimethoxybiphenyl*. ***4′-Methoxyaucuparin***
$C_{15}H_{16}O_4$ 260.289
Mp 99° (synthetic). λ_{max} 268 (ϵ 13500) (EtOH) (Derep). λ_{max} 267 (ϵ 13800) (MeOH) (Berdy). λ_{max} 298 (MeOH/NaOH) (Berdy).

Cotterill, P.J. *et al., JCS Perkin 1*, 1974, 2423 (*4′-Methoxyaucuparin*)
Watanabe, K. *et al., Agric. Biol. Chem.*, 1990, **54**, 1861 (*4′-Methoxyaucuparin, Rhaphiolepsin*)
Cardona, M.L. *et al., Phytochemistry*, 1990, **29**, 3003 (*isol, pmr*)
Kokubun, T. *et al., Phytochemistry*, 1995, **40**, 57 (*4′-Methoxyaucuparin*)
Chen, G. *et al., J. Asian Nat. Prod. Res.*, 2005, **7**, 265-268 (*Kakispyrol*)
Chen, J.-J. *et al., Planta Med.*, 2006, **72**, 473-477 (*Garcibiphenyl C*)

3,4′,5-Biphenyltriol B-135

3,4′,5-Trihydroxybiphenyl [74276-54-3]



$C_{12}H_{10}O_3$ 202.209
Constit. of *Trifolium repens* (white clover). Characterised as the tri-Me ether.

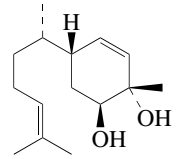
3-Me ether: [856451-92-8] *3-(4-Hydroxyphenyl)-5-methoxyphenol. 3,4′-Dihydroxy-5-methoxybiphenyl*. ***Garcibiphenyl A***
$C_{13}H_{12}O_3$ 216.236
Oil. λ_{max} 207 (log ϵ 4.53); 225 (sh) (log ϵ 4.25); 263 (log ϵ 4.11) (MeOH).

3,5-Di-Me ether: 4-(3,5-Dimethoxyphenyl)phenol. 4′-Hydroxy-3,5-dimethoxybiphenyl
$C_{14}H_{14}O_3$ 230.263
Powder. λ_{max} 210; 227; 265 (MeOH).

Tri-Me ether: [54960-97-3] *3,4′,5-Trimethoxybiphenyl*
$C_{15}H_{16}O_3$ 244.29
Plates (MeOH). Mp 61-62°.

Scheinmann, F. *et al., JCS Perkin 1*, 1974, 2423 (*synth, tri-Me ether, uv, pmr*)
Ghosal, S. *et al., J. Chem. Res., Synop.*, 1988, 196 (*isol, uv, ir, pmr*)
Dall'Acqua, S. *et al., Chem. Pharm. Bull.*, 2002, **50**, 1499-1501 (*3,5-di-Me ether*)
Chen, J.-J. *et al., Planta Med.*, 2004, **70**, 1195-1200 (*Garcibiphenyl A*)
Kitamura, Y. *et al., Tetrahedron*, 2007, **63**, 10596-10602 (*tri-Me ether*)

1,10-Bisaboladiene-3,4-diol B-136



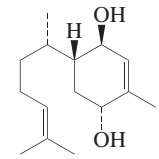
(3*S*,4*S*,6*R*,7*S*)-*form*

$C_{15}H_{26}O_2$ 238.369

(3*S*,4*S*,6*R*,7*S*)-*form* [129673-87-6]
Constit. of *Curcuma longa* (turmeric). Viscous oil. $[\alpha]_D$ -31.7 (c, 0.23 in MeOH).

(3*S*,4*S*,6*S*,7ξ)-*form*
Oil.
Zdero, C. *et al., Phytochemistry*, 1987, **26**, 1999-2006 (*isol, pmr*)
Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*isol, pmr, cmr*)
Sy, L.-K. *et al., Phytochemistry*, 1997, **45**, 537 (*isol, pmr, cmr*)

2,10-Bisaboladiene-1,4-diol B-137



(1*S*,4*R*,6*R*,7*S*)-*form*

$C_{15}H_{26}O_2$ 238.369

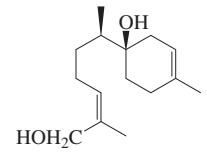
(1*S*,4*R*,6*R*,7*S*)-*form* [192709-64-1]
Constit. of *Curcuma longa* (turmeric). Needles (hexane). Mp 126.5-129°. $[\alpha]_D$ +5 (MeOH).

1-Ketone: [73695-95-1] ***4-Hydroxy-2,10-bisaboladien-1-one***. *4-Hydroxy-1-bisabolone*
$C_{15}H_{24}O_2$ 236.353
Oil. $[\alpha]_D^{24}$ -15.2 (c, 0.64 in $CHCl_3$).

(1ξ,4ξ,6ξ,7ξ)-*form* [947170-89-0]
Oil. $[\alpha]_D^{23}$ -15 (c, 0.13 in $CHCl_3$).

1-Ketone: [942606-26-0]
Oil. $[\alpha]_D^{23}$ -28.6 (c, 0.81 in $CHCl_3$).
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 1889-1892 (*Chrysothamnus nauseosus constit*)
Ohshiro, M. *et al., Phytochemistry*, 1990, **29**, 2201-2205 (*Curcuma longa constit*)
Todorova, M. *et al., Phytochemistry*, 2007, **68**, 1722-1730 (*Achillea collina constit*)

2,10-Bisaboladiene-6,12-diol B-138



(6*R*,7*R*,10*Z*)-*form*

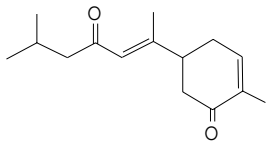
$C_{15}H_{26}O_2$ 238.369

(6*R*,7*R*,10*Z*)-*form* [872880-55-2]
Constit. of *Santalum album* (sandalwood). Oil. $[\alpha]_D^{20}$ -5.2 (c, 1 in $CHCl_3$).

(6*R*,7*S*,10*Z*)-*form* [189371-57-1]
Constit. of *Santalum album* (sandalwood). Oil. $[\alpha]_D^{25}$ -84.6 (c, 1.2 in $CHCl_3$). $[\alpha]_D^{20}$ -72.5 (c, 1 in $CHCl_3$). Stereochem. revised in 2005.
Alpha, T. *et al., Phytochemistry*, 1997, **44**, 1519-1522 (*Santalum austrocaledonicum constit*)
Kim, T.H. *et al., J. Nat. Prod.*, 2005, **68**, 1805-1808 (*Santalum album constits*)

3,7-Bisaboladiene-2,8-dione B-139

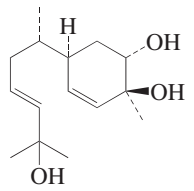
10,11-Dihydro-6-oxoatlantone [57095-92-8]



$C_{15}H_{22}O_2$ 234.338
Constit. of *Ginkgo biloba* (ginkgo).

Irie, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1892

4,9-Bisaboladiene-2,3,11-triol B-140



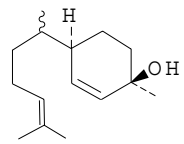
$C_{15}H_{26}O_3$ 254.369

(2*S*,3*S*,6*R*,7*S*,9*E*)-*form* [1253190-34-9]
Curculonone D
Constit. of *Curcuma longa* (turmeric).
Oil. $[\alpha]_D^{25}$ -30.5 (c, 0.12 in $CHCl_3$).

Chen, J.-J. *et al., Food Chem.*, 2010, **119**, 974-980 (*Curculonone D*)

1,10-Bisaboladien-3-ol B-141

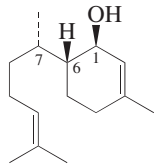
Zingiberenol [58334-55-7]



$C_{15}H_{26}O$ 222.37
Constit. of *Zingiber officinale*, isol. by glc. Oil.

Terhune, S.J. *et al., Can. J. Chem.*, 1975, **53**, 3285 (*isol*)
Paquette, L.A. *et al., Tet. Lett.*, 1982, **23**, 131 (*synth*)

2,10-Bisaboladien-1-ol B-142



(1*R* ,6*R* ,7*S*)-*form*
Relative Configuration

$C_{15}H_{26}O$ 222.37
Absolute stereochemical information is incomplete and some opt. rotns. are contradictory.

(6*R*,7*R*)-*form*

1-Ketone: [72441-71-5] ***2,10-Bisaboladien-1-one***
[173829-64-6]
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D^{24}$ -7.9 (c, 3.7 in $CHCl_3$). $[\alpha]_D$ +16 (c, 4 in $CHCl_3$). $[\alpha]_D$ +26 (neat).

(6*R*,7*S*)-*form*

1-Ketone: [61432-71-1]
Oil. $Bp_{0.1}$ 120°. $[\alpha]_D^{24}$ -37 (c, 3.7 in $CHCl_3$).

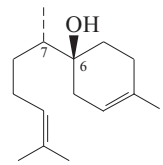
1-Ketone, 10ξ,11-epoxide: [1253190-33-8]
10,11-Epoxy-2-bisabolen-1-one. ***Curculonone C***
$C_{15}H_{24}O_2$ 236.353
Constit. of *Curcuma longa* (turmeric).
Oil. $[\alpha]_D^{25}$ -44.6 (c, 0.12 in $CHCl_3$). λ_{max} 234 (log ϵ 4.03) (MeOH).

(1*R*,6*R*,7*S*)-*form* [178456-52-5]
Sesquipiperitol
Oil. $[\alpha]_D^{22}$ -19 (c, 6.3 in hexane).

*1-Ketone, 2*R*,3*S*-epoxide:* [61432-72-2]
2,3-Epoxy-10-bisabolen-1-one. *2,3-Epoxy-2,3-dihydro-1-bisabolone*
$C_{15}H_{24}O_2$ 236.353
Oil. $Bp_{0.1}$ 125°. $[\alpha]_D^{24}$ +117 (c, 6.35 in $CHCl_3$).

Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 3366-3370 (*Stevia purpurea constits*)
Ghisalberti, E.M. *et al., Aust. J. Chem.*, 1979, **32**, 1627-1630 (*synth, abs config*)
Abegaz, B. *et al., J. Nat. Prod.*, 1983, **46**, 424-426 (*6R,7S-ketone, isol*)
Cool, L.G. *et al., Phytochemistry*, 1996, **42**, 1015-1019 (*Sesquipiperitol*)
Weyerstahl, P. *et al., Flavour Fragrance J.*, 1999, **14**, 15-28 (*Lantana camara constits*)
Reina, M. *et al., J. Nat. Prod.*, 2002, **65**, 448-453 (*Senecio palmensis constit*)
Hagiwara, H. *et al., JCS Perkin 1*, 2002, 895-900 (*synth*)
US Pat., 2004, 6 787 674 (*6R,7R-ketone, isol, activity*)
Chen, J.-J. *et al., Food Chem.*, 2010, **119**, 974-980 (*Curculonone C*)

2,10-Bisaboladien-6-ol B-143



(6*S*,7*S*)–*form*

$C_{15}H_{26}O$ 222.37

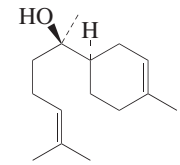
(6*S*,7*S*)-*form* [15352-77-9]
β-Bisabolol
Constit. of *Gossypium hirsutum* (cotton) oil and other essential oils. Oil. Bp_2 121-122°. $[\alpha]_D^{20}$ +7.16 (c, 0.28 in $CHCl_3$). $[\alpha]_D^{20}$ +23.3 ($CHCl_3$).

(6*R*,7*S*)-*form*
6*-epi-*β-Bisabolol
Constit. of bergamot oil. $[\alpha]_D^{20}$ -57 (c, 0.1 in $CHCl_3$).

Minyard, J.P. *et al., JOC*, 1968, **33**, 909 (*isol*)
Takaoka, D. *et al., Phytochemistry*, 1976, **15**, 425 (*isol*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1986, **69**, 698 (*abs config*)
Fráter, G. *et al., Helv. Chim. Acta*, 1989, **72**, 653 (*synth*)

2,10-Bisaboladien-7-ol B-144

6-Methyl-2-(4-methyl-3-cyclohexen-1-yl)-5-hepten-2-ol, 8CI



(6*R*,7*R*)-*form*

$C_{15}H_{26}O$ 222.37
Log P 4.66 (calc).

(6*R*,7*R*)-*form* [23178-88-3]
(+)-α-Bisabolol. *Bisabolol*
Constit. of essential oil of *Populus balsamifera* (balsam poplar). Oil. Bp_{12} 154-156°. $[\alpha]_D^{23}$ +53.8 (c, 2.6 in $CHCl_3$).
▶ LD_{50} (rat, orl) 14850 mg/kg. MJ9685000

7-O-*β*-D-*Fucopyranoside:* [84847-68-7]
$C_{21}H_{36}O_5$ 368.512
Oil. $[\alpha]_D$ -20.6 (c, 1 in $CHCl_3$).

(6*R*,7*S*)-*form* [76738-75-5]
6-Epi-α-bisabolol
Syrup. $[\alpha]_D^{23}$ +67.4 (MeOH).

(6*S*,7*R*)-*form* [78148-59-1]
Anymol. *7-Epi-α-Bisabolol*
Oil. Bp_1 114°. $[\alpha]_D$ -69 (c, 1.3 in EtOH).

p-*Phenylazophenylurethane:*
Orange needles (petrol). Mp 103-103.5°. $[\alpha]_D$ -7 (c, 1 in $CHCl_3$).

7-O-*Lyxopyranoside:* [258337-41-6]
$C_{20}H_{34}O_5$ 354.486

(6*S*,7*S*)-*form* [23089-26-1]
(-)-α-Bisabolol. *Levomenol, INN. FEMA 4666*
Isol. from essential oil of *Matricaria chamomilla* (German chamomile). Flavour and fragrance ingredient.
Yellowish oil with sweetish odour.
d_4^{20} 0.92. Bp_{12} 153°. $[\alpha]_D^{24}$ -68.4 (c, 1.16 in EtOH). n_D^{20} 1.4936.
Log P 4.66 (calc).
▶ LD_{50} (rat) 0.014 mg/kg.

(6ξ,7ξ)-*form*
O-*(6-Deoxy-β-*D*-altropyranoside):*
[79197-22-1]
$C_{21}H_{36}O_5$ 368.512
Gum. $[\alpha]_D^{24}$ -6.5 (c, 1 in $CHCl_3$).
Config. unknown.

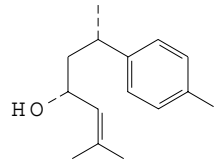
[515-69-5]

Šorm, F. *et al., Coll. Czech. Chem. Comm.*, 1951, **16**, 626 (*isol*)
O'Brien, K.G. *et al., Aust. J. Chem.*, 1953, **6**, 166; 1954, **7**, 298 (*Anymol*)
Yakovlev, V. *et al., Arzneim.-Forsch.*, 1969, **19**, 615 (*pharmacol, tox*)
Sampath, V. *et al., Indian J. Chem.*, 1969, **7**, 1060 (*isol*)
Kergomard, A. *et al., Tetrahedron*, 1977, **33**, 2215 (*synth*)
Schwartz, M.A. *et al., JOC*, 1979, **44**, 953 (*synth, abs config*)

Rustaiyan, A. *et al., Phytochemistry*, 1981, **20**, 1429 (*deoxyaltroside*)
Babin, D. *et al., Tetrahedron, Suppl.*, No. 1, 1981, 1 (*synth, abs config*)
San Feliciano, A. *et al., Phytochemistry*, 1982, **21**, 2115-2116 (*fucoside*)
Khan, V.A. *et al., Khim. Prir. Soedin.*, 1985, **21**, 575; *Chem. Nat. Compd. (Engl. Transl.)*, 1985, **21**, 575 (*isol, cmr*)
Ohloff, G. *et al., Helv. Chim. Acta*, 1986, **69**, 698 (*isol*)
Titova, T.F. *et al., Khim. Prir. Soedin.*, 1987, **23**, 460; *Chem. Nat. Compd. (Engl. Transl.)*, 1987, **23**, 386 (*isol*)
O'Donnell, G.W. *et al., Aust. J. Chem.*, 1989, **42**, 2021 (*bibl, isol, deriv*)
Carman, R.M. *et al., Aust. J. Chem.*, 1989, **42**, 2035; 2041 (*cryst struct, bibl, synth*)
Wu, C.-L. *et al., Phytochemistry*, 1992, **31**, 4213 (*pmr, cmr*)
Chen, X.-J. *et al., JOC*, 1993, **58**, 5528 (*synth*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1383
Nemoto, H. *et al., Tet. Lett.*, 1993, **34**, 4939 (*synth*)
Hashidoko, Y. *et al., Phytochemistry*, 1994, **35**, 325 (*6-Epi-α-bisabolol*)
Roth, L. *et al., Roth Collection of Natural Product Data*, VCH, Weinheim, 1995,
Meng, J.C. *et al., Spectrosc. Lett.*, 1999, **32**, 1005-1012 (*lyxopyranoside*)
Hashidoko, Y. *et al., Biosci., Biotechnol., Biochem.*, 2000, **64**, 907-910 (*isol, pmr, cmr*)
Piochon, M. *et al., Phytochemistry*, 2009, **70**, 228-236 (*synth*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*use*)

1,3,5,10-Bisabolapentaen-9-ol B-145

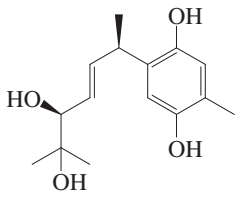
Bisacumol [120710-98-7]



$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{25}$ +14.8 (c, 1 in $CHCl_3$).

Uehara, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 237 (*isol, pmr, cmr*)
Kamal, A. *et al., Tetrahedron: Asymmetry*, 2009, **20**, 1267-1271 (*resoln, pmr, ir*)

1,3,5,8-Bisabolatetraene-1,4,10,11-tetrol B-146



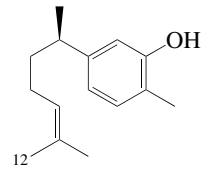
$C_{15}H_{22}O_4$ 266.336

(7*R*,8*E*,10*S*)-*form* [497931-68-7]
Helibisabonol B
Constit. of sunflowers. Oil. $[\alpha]_D^{25}$ -7.2 (c, 0.1 in Me_2CO).

Macías, F.A. *et al., Phytochemistry*, 2002, **61**, 687-692 (*isol, pmr, cmr*)

1,3,5,10-Bisabolatetraen-2-ol B-147

5-(1,5-Dimethyl-4-hexenyl)-2-methylphenol, 9CI. ***Xanthorrhizol*** [30199-26-9]



$C_{15}H_{22}O$ 218.338
Constit. of rhizomes of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{20}$ -52.5. λ_{max} 275 (ϵ 1900) (EtOH) (Derep).

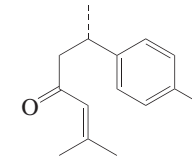
12-Acetoxy: ***12-Acetoxyxanthorrhizol***. *13-Acetoxyxanthorrhizol*
$C_{17}H_{24}O_3$ 276.375
Oil. $[\alpha]_D$ -76.5 (c, 0.52 in $CHCl_3$).

10,11-Epoxide: [364373-61-5] *10,11-Epoxy-1,3,5-bisabolatrien-2-ol.* ***10,11-Epoxyxanthorrhizol***. *12,13-Epoxyxanthorrhizol (incorr.)*
$C_{15}H_{22}O_2$ 234.338
Oil. $[\alpha]_D$ -0.13 (c, 0.54 in MeOH). Mixt. of 10-epimers. λ_{max} 272 (ϵ 2317) (MeOH).

Rimpler, H. *et al., Z. Naturforsch., B*, 1970, **25**, 995 (*isol, struct*)
Mane, R.B. *et al., Indian J. Chem.*, 1974, **12**, 938 (*synth*)
John, T.K. *et al., Indian J. Chem., Sect. B*, 1985, **24**, 35 (*synth*)
Rane, R.K. *et al., Indian J. Chem., Sect. B*, 1987, **26**, 572 (*synth*)
Garcá, G.E. *et al., J. Nat. Prod.*, 1987, **50**, 1055 (*synth*)
Joseph-Nathan, P. *et al., J. Nat. Prod.*, 1988, **51**, 1116-1128 (*cmr*)
Mendoza, G.V. *et al., J. Nat. Prod.*, 1993, **56**, 2073-2076 (*12-Acetoxyxanthorrhizol*)
Aguilar, M.I. *et al., Phytochemistry*, 1993, **33**, 1161-1163 (*cmr*)
Meyers, A.I. *et al., JOC*, 1997, **62**, 5219-5221 (*synth*)
Pat. Coop. Treaty (WIPO), 2000, 00 67 711
Hwang, J.-K. *et al., Planta Med.*, 2000, **66**, 196 (*Xanthorrhizol, isol, activity*)
Aguilar, M.I. *et al., Nat. Prod. Lett.*, 2001, **15**, 93-101 (*10,11-Epoxyxanthorrhizol*)
Rukayadi, Y. *et al., J. Antimicrob. Chemother.*, 2006, **57**, 1231-1234 (*activity*)
Rukayadi, Y. *et al., Lett. Appl. Microbiol.*, 2006, **42**, 400-404 (*activity*)
Ehara, T. *et al., Chem. Pharm. Bull.*, 2007, **55**, 1361-1364 (*synth*)
Marcoux, D. *et al., JOC*, 2009, **74**, 8939-8955 (*synth*)
Montiel, L.E. *et al., Helv. Chim. Acta*, 2010, **93**, 1261-1273 (*synth*)
Du, Z. *et al., Nat. Prod. Commun.*, 2011, **6**, 167-169 (*synth*)

1,3,5,10-Bisabolatetraen-9-one B-148

2-Methyl-6-(4-methylphenyl)-2-hepten-4-one, 9CI. **ar-*Turmerone***. *Dehydroturmerone*
[98524-10-8 (non-stereospecific), 38142-58-4 ((±)-form)]



(*S*)-*form*

$C_{15}H_{20}O$ 216.322

(*S*)-*form* [532-65-0]
Constit. of essential oil from *Curcuma longa* (turmeric) and *Curcuma amada* (mango-ginger). Pale yellow oil. Sol. C_6H_6, hexane. d^{20} 0.957. Bp_{10} 159-160°. $[\alpha]_D^{20}$ +82.21. Poss. artifact arising from aromatisation of 2,5,10-Bisabolatrien-9-one, B-163. λ_{max} 275 (ϵ 15700) (MeOH) (Berdy).

Semicarbazone:
Cryst. (C_6H_6). Mp 106°.

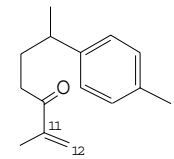
10,11-Dihydro: [4179-20-8] *2-Methyl-6-(4-methylphenyl)-4-heptanone. 1,3,5-Bisabolatrien-9-one. Dihydro*-ar-*turmerone*
$C_{15}H_{22}O$ 218.338
Oil. Bp_1 115°. $[\alpha]_D$ +31 (c, 7.2 in $CHCl_3$).

(*R*)-*form* [1141-54-4]
$[\alpha]_D^{25}$ -67.8 (c, 1 in $CHCl_3$).

Rupe, H. *et al., Helv. Chim. Acta*, 1936, **19**, 569-581 (*isol, struct*)
Honwad, V.K. *et al., Tetrahedron*, 1964, **20**, 2921-2925 (*abs config*)
Grieco, P.A. *et al., JOC*, 1973, **38**, 2909-2910 (*synth*)
Kashima, C. *et al., Bull. Chem. Soc. Jpn.*, 1979, **52**, 1735-1737 (*synth, pmr*)
Gosselin, P. *et al., JOC*, 1979, **44**, 2807-2809 (*synth*)
Meyers, A.I. *et al., Tet. Lett.*, 1979, **20**, 2749-2752 (*synth*)
Su, H.C.F. *et al., J. Agric. Food Chem.*, 1982, **30**, 290-292 (*isol*)
El Jazouli, M. *et al., Chem. Comm.*, 1985, 1598-1599 (*synth*)
Motoyoshiya, J. *et al., JOC*, 1985, **50**, 1326-1327 (*synth*)
Strunz, G.M. *et al., Can. J. Chem.*, 1992, **70**, 1317 (*synth*)
Ferreira, L.A. *et al., Toxicon*, 1992, **30**, 1211-1218 (*pharmacol*)
Kitahara, T. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 1137-1140 (*synth*)
Fuganti, C. *et al., JCS Perkin 1*, 1999, 279-282 (*synth*)
Mori, K. *et al., Tetrahedron: Asymmetry*, 2005, **16**, 685-692 (*R-form, synth*)
Kamal, A. *et al., Tetrahedron: Asymmetry*, 2009, **20**, 1267-1271 (*R-form, S-form, synth*)

1,3,5,11-Bisabolatetraen-10-one B-149

2-Methyl-6-(4-methylphenyl)-1-hepten-3-one [76760-39-9]



$C_{15}H_{20}O$ 216.322

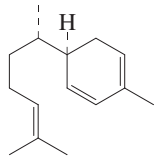
Props. and registry nos. refer to racemates which were obt. synthetically.
Constit. of oil of *Cinnamomum cassia* (Chinese cinnamon). Oil. $Bp_{0.01}$ 71-74°.

11,12-Dihydro: [76760-40-2] *1,3,5-Bisabolatrien-10-one. 2-Methyl-6-(4-methylphenyl)-3-heptanone*
$C_{15}H_{22}O$ 218.338
Constit. of oil of *Cinnamomum cassia* (Chinese cinnamon). Oil. $Bp_{0.01}$ 90°.

Thomas, A.F. *et al., Helv. Chim. Acta*, 1980, **63**, 1615 (*isol, struct, ms, synth*)

1,3,10-Bisabolatriene B-150

Zingiberene [495-60-3]



Absolute Configuration

$C_{15}H_{24}$ 204.355
Constit. of ginger oil. Also from wild thyme (*Thymus serpyllum*), long pepper (*Piper longum*) and kua (*Curcuma zedoaria*). Oil. Bp_{11} 128-130°. $[\alpha]_D^{27}$ -61.7 ($CHCl_3$).

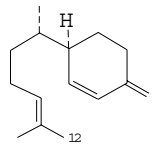
Nitrosochloride:
Cryst. Mp 93-94°.

7-Epimer: ***7-Epizingiberene***
$C_{15}H_{24}$ 204.355
Oil. $[\alpha]_D^{26}$ -76.1 ($CHCl_3$).

Eschenmoser, A. *et al., Helv. Chim. Acta*, 1950, **33**, 171 (*isol, struct*)
Arigoni, D. *et al., Helv. Chim. Acta*, 1954, **37**, 881 (*abs config*)
Joshi, G.D. *et al., Indian J. Chem.*, 1965, **3**, 91 (*synth*)
Soffer, M.D. *et al., Tet. Lett.*, 1985, **26**, 3543 (*cryst struct*)
Bhonsle, J.B. *et al., Indian J. Chem., Sect. B*, 1994, **33**, 313 (*synth, bibl*)
Breedon, D.C. *et al., Tetrahedron*, 1994, **50**, 11123 (*isol, cmr, pmr*)
Millar, J.G. *et al., J. Nat. Prod.*, 1998, **61**, 1025-1026 (*isol*)

1,3(15),10-Bisabolatriene B-151

3-(1,5-Dimethyl-4-hexenyl)-6-methylenecyclohexene, 9CI. ***β-Sesquiphellandrene*** [20307-83-9]



$C_{15}H_{24}$ 204.355
Constit. of the oil of ginger (*Zingiber officinale*). Oil. Bp_1 90°. $[\alpha]_D^{20}$ -3.99 (neat).

Nitrosite:
Cryst. (Me_2CO). Mp 88-90° dec. $[\alpha]_D^{20}$ +29 (c, 1.5 in $CHCl_3$).

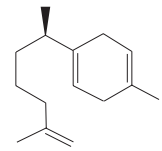
10ξ,11ξ-Epoxide: [80442-54-2] ***10,11-Epoxy-1,3(15)-bisaboladiene****. 10,11-Epoxy-β-sesquiphellandrene*
$C_{15}H_{24}O$ 220.354
Oil.

12-Oxo: [71939-69-0] *1,3(15),10-Bisabolatrien-12-al. 12-Oxo-β-sesquiphellandrene*
$C_{15}H_{22}O$ 218.338
Oil. $[\alpha]_D$ -9.3 (c, 0.15 in $CHCl_3$).

Connell, D.W. *et al., Aust. J. Chem.*, 1966, **19**, 283 (*β-Sesquiphellandrene*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 677 (*12-Oxo-β-sesquiphellandrene*)
Bohlmann, F. *et al., Phytochemistry*, 1981, **20**, 1887 (*Epoxybisaboladiene*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1999, **82**, 1427-1433 (*synth*)

2,5,11-Bisabolatriene B-152

1-(1,5-Dimethyl-5-hexenyl)-4-methyl-1,4-cyclohexadiene, 9CI. ***β-Curcumene*** [451-56-9]



(*R*)–*form*

$C_{15}H_{24}$ 204.355

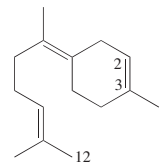
(R)-form [28976-67-2]
Constit. of the essential oil of *Curcuma amada* (mango-ginger) and *Curcuma xanthorrhiza* (Java turmeric). Liq. Bp_{19} 142°. $[\alpha]_D$ -48.2. The abs. config is as in CA but does not appear to be explicitly stated in the lit.

(S)-form
$Bp_{2.2}$ 98-100°. $[\alpha]_D^{20}$ +26.7.

Naves, Y.-R. *et al., Bull. Soc. Chim. Fr.*, 1951, 987
Jain, M.K. *et al., Indian J. Chem.*, 1964, **2**, 39 (*isol*)

2,6,10-Bisabolatriene B-153

4-(1,5-Dimethyl-4-hexenylidene)-1-methylcyclohexene, 9CI. ***γ-Bisabolene****. α-Bisabolene (obsol.)†. γ-Limene* [495-62-5]



(*E*)-*form*

$C_{15}H_{24}$ 204.355
Flavouring ingredient used singly or as mixed isomers. Component of FEMA 3331. See also 2,7,10-Bisabolatriene, B-154.

(E)-form [53585-13-0]
Oil. $[\alpha]_D^{24}$ -18.8 (c, 1 in $CHCl_3$).

2,3-Epoxide: [75744-73-9] *2,3-Epoxy-6,10-bisaboladiene.* ***γ-Bisabolene-2,3-epoxide***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D$ +37.3 (c, 2.2 in $CHCl_3$).
Called γ-Bisabolene 8,9-epoxide in the reference.

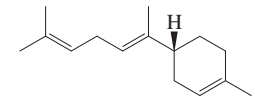
12-Hydroxy: 2,6,10-Bisabolatrien-12-ol. ***12-Hydroxy-γ-bisabolene***
$C_{15}H_{24}O$ 220.354
Oil.

(Z)-form [13062-00-5]
Constit. of oil of myrrh and oil of lime. Oil.

Vig, O.P. *et al., Indian J. Chem.*, 1970, **8**, 955 (*synth*)
Giraudi, E. *et al., Recherches*, 1974, **19**, 205 (*synth*)
Overton, K.H. *et al., Chem. Comm.*, 1976, 105 (*biosynth*)
Wolinsky, J.E. *et al., JOC*, 1976, **41**, 697 (*struct*)
Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **80**, 1997 (*isol*)
Suzuki, T. *et al., Chem. Lett.*, 1980, 1267 (*epoxide*)
Buss, A.D. *et al., Tet. Lett.*, 1983, **24**, 111 (*synth*)
Anastasis, P. *et al., Can. J. Chem.*, 1984, **62**, 2079 (*biosynth, bibl*)
Look, S.A. *et al., Experientia*, 1984, **40**, 931 (*12-Hydroxy-γ-bisabolene*)
Vig, O.P. *et al., Indian J. Chem., Sect. B*, 1989, **28**, 617 (*synth, deriv*)
Anastasia, L. *et al., Eur. J. Org. Chem.*, 2001, 3039-3043 (*synth, pmr, cmr*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 165 (*FEMA 3331, use*)

2,7,10-Bisabolatriene B-154

4-(1,5-Dimethyl-1,4-hexadienyl)-1-methylcyclohexene, 9CI. ***α-Bisabolene***†. *α-Limene. FEMA 3331* [17627-44-0]



(*R,E*)-*form*

$C_{15}H_{24}$ 204.355
Not the same as 2,6,10-Bisabolatriene, B-153 which has been renamed (formerly α-Bisabolene). The FEMA number refers to mixed bisabolenes including 2,7(14),10-Bisabolatriene, B-155 and 2,6,10-Bisabolatriene, B-153.
Flavouring ingredient isol. from bisabol myrrh and other natural sources, e.g. lemon, bergamot.

(R,E)-form [70286-31-6]
Oil. $[\alpha]_D^{20}$ +54.3 (c, 1 in EtOH).

(R,Z)-form [70286-33-8]
Oil. $[\alpha]_D^{20}$ -12 (c, 1 in EtOH).

(S,E)-form [70286-32-7]
Oil. $[\alpha]_D^{20}$ -38.9 (c, 1 in EtOH).

(S,Z)-form [58845-44-6]
Constit. of oil of Opopanax. Oil. Bp_{12} 155-157°. $[\alpha]_D^{20}$ +8 (c, 1 in EtOH).

(ξ,E)-form [25532-79-0]
Oil. Abs. config. not detd., no opt. rotn. given.

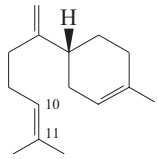
[70286-16-7, 29837-07-8, 70332-15-9]

Delay, F. *et al., Helv. Chim. Acta*, 1979, **62**, 369-377 (*synth, bibl*)
Scheffrahn, R.H. *et al., J. Chem. Ecol.*, 1983, **9**, 1293-1305 (*S,Z-form, isol, pmr*)
Sullivan, B.W. *et al., JOC*, 1986, **51**, 5134-5136 (*R,E-form, isol*)

Vig, O.P. *et al., J. Indian Chem. Soc.*, 1987, **64**, 756-757 (*synth*)
Buss, A.D. *et al., JCS Perkin 1*, 1987, 2569-2577 (*synth*)
Zdero, C. *et al., Phytochemistry*, 1991, **30**, 1161-1163 (*Athanasia constit*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 283-284 (*use, props*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 165 (*FEMA 3331, use*)

2,7(14),10-Bisabolatriene B-155

1-Methyl-4-(5-methyl-1-methylene-4-hexenyl)cyclohexene, 9CI. ***β-Bisabolene****. β-Limene* [21902-26-1]



(*R*)–*form*

$C_{15}H_{24}$ 204.355
Flavouring ingredient used singly or as mixed isomers. Component of FEMA 3331. See also 2,7,10-Bisabolatriene, B-154.

(*R*)-*form* [20377-48-4]
$[\alpha]_D$ +75. n_D^{20} 1.4879.

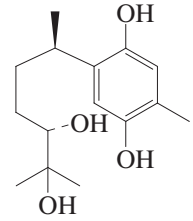
2β,3β-Epoxide: [733766-73-9] ***2,3-Epoxy-7(14),10-bisaboladiene***
$C_{15}H_{24}O$ 220.354
Oil. $[\alpha]_D^{25}$ +43.5 (c, 2.7 in $CHCl_3$). λ_{max} 214 (log ϵ 2.08) (EtOH).

(*S*)-*form* [495-61-4]
Constit. of the essential oils of bergamot, lemon, wild carrot, guava and many other fruits. Oil. $Bp_{10.5}$ 129-130°. $[\alpha]_D^{20}$ -84.4.

10ξ,11ξ-Epoxide: [88861-98-7] ***10,11-Epoxy-2,7(14)-bisaboladiene***
$C_{15}H_{24}O$ 220.354
Oil. $Bp_{0.1}$ 120°. $[\alpha]_D^{24}$ -89 (c, 11.1 in $CHCl_3$).

Pentegova, V.A. *et al., Coll. Czech. Chem. Comm.*, 1961, **26**, 1362-1372 (*R-form, isol*)
Manjarrez, A. *et al., JOC*, 1966, **31**, 348-349 (*synth*)
Andersen, N.H. *et al., Phytochemistry*, 1970, **9**, 1325-1340 (*R-form, isol*)
Vig, O.P. *et al., J. Indian Chem. Soc.*, 1971, **48**, 993-999 (*synth*)
Crawford, R.J. *et al., JACS*, 1972, **94**, 4298-4306 (*synth*)
Jeffs, P.W. *et al., J. Nat. Prod.*, 1974, **37**, 315-317 (*isol, Muricea*)
Miyazawa, M. *et al., Phytochemistry*, 1977, **16**, 1054-1057 (*S-form, occur*)
Andersen, N.H. *et al., Phytochemistry*, 1977, **16**, 1731-1751 (*S-form, occur*)
Scheffrahn, R.H. *et al., J. Chem. Ecol.*, 1983, **9**, 1293-1305 (*R-form, isol*)
Sakane, S. *et al., JACS*, 1983, **105**, 6154-6155 (*synth*)
Bohlmann, F. *et al., Phytochemistry*, 1983, **22**, 2243-2252 (*10,11-epoxide*)
Sakurai, H. *et al., Tetrahedron*, 1983, **39**, 883-894 (*synth*)
Nabeta, K. *et al., Agric. Biol. Chem.*, 1986, **50**, 2915-2916 (*biosynth*)
Nabeta, K. *et al., Biosci., Biotechnol., Biochem.*, 1993, **57**, 792-798 (*biosynth*)
Tabanca, N. *et al., Planta Med.*, 2003, **69**, 933-938 (*2,3-epoxide*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 165 (*FEMA 3331, use*)

1,3,5-Bisabolatriene-1,4,10,11-tetrol B-156

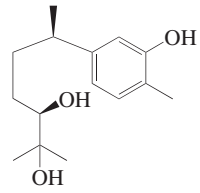


$C_{15}H_{24}O_4$ 268.352

(7*R*,10*S*)-*form* [497931-67-6]
Helibisabonol A
Constit. of sunflowers. Oil. $[\alpha]_D^{25}$ -44.9 (c, 0.1 in Me_2CO).

Macías, F.A. *et al., Phytochemistry*, 2002, **61**, 687-692 (*isol, pmr, cmr*)
Sirat, H.M. *et al., Tet. Lett.*, 2007, **48**, 457-460 (*synth*)

1,3,5-Bisabolatriene-2,10,11-triol B-157



(7*R*,10*R*)-*form*

$C_{15}H_{24}O_3$ 252.353

(7*R*,10*R*)-*form* [923602-51-1]
Constit. of *Curcuma xanthorrhiza* (Java turmeric).

(7*R*,10*S*)-*form* [923602-50-0]
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{25}$ -73.8 (c, 0.14 in MeOH). λ_{max} 273 (ϵ 3200) (MeOH).

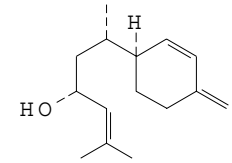
(7*R*,10ξ)-*form* [364373-62-6]
Oil. $[\alpha]_D$ -27.4 (c, 0.26 in MeOH). Mixt. of 10-epimers. λ_{max} 273 (ϵ 3577) (MeOH).

*10-*O*-[β-L-Arabinopyranosyl-(1→2)-β-D-glucopyranoside]:* [180869-58-3]
$C_{26}H_{42}O_{12}$ 546.611

Aguilar, M.I. *et al., Nat. Prod. Lett.*, 1995, **7**, 155; 2001, **15**, 93-101 (*isol, pmr, cmr*)
Matsuura, H. *et al., Nat. Prod. Res.*, 2007, **21**, 328-333 (*Curcuma xanthorrhiza constits*)
Sirat, H.M. *et al., Tet. Lett.*, 2007, **48**, 457-460 (*synth*)

1,3(15),10-Bisabolatrien-9-ol B-158

Bisacurol [120681-80-3]



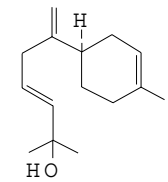
$C_{15}H_{24}O$ 220.354
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D$ -8.6 (c, 0.33 in MeOH).

Ketone: [87440-60-6] ***1,3(15),10-Bisabolatrien-9-one. Curlone****. β-Turmerone* [82508-14-3]
$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma longa* (turmeric). Oil. $[\alpha]_D$ -0.03 (c, 2.16 in $CHCl_3$).

Golding, B.T. *et al., Chem. Comm.*, 1982, 363 (*β-Turmerone*)
Kiso, Y. *et al., Phytochemistry*, 1983, **22**, 596 (*Curlone*)
Uehara, S. *et al., Chem. Pharm. Bull.*, 1989, **37**, 237 (*isol, pmr, cmr*)
Golding, B.T. *et al., JCS Perkin 1*, 1992, 1519 (*struct*)
Kreiser, W. *et al., Helv. Chim. Acta*, 1999, **82**, 1610-1639 (*synth, bibl*)

2,7(14),9-Bisabolatrien-11-ol B-159

Helianthol A

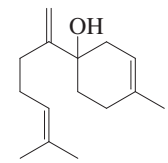


$C_{15}H_{24}O$ 220.354

(*R*)-*form* [72916-06-4]
Constit. of essential oil of *Helianthus tuberosus* (Jerusalem artichoke). Oil. $[\alpha]_D^{20}$ +61 (c, 0.3 in EtOH).

Miyazawa, M. *et al., Phytochemistry*, 1983, **22**, 1040

2,7(14),10-Bisabolatrien-6-ol B-160



$C_{15}H_{24}O$ 220.354

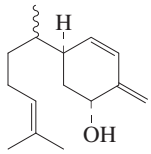
(+)-*form* [72916-05-3]
Helianthol B
Constit. of *Helianthus tuberosus* (Jerusalem artichoke).

(-)-*form* [947137-44-2]
Oil. $[\alpha]_D^{20}$ -2.5 (c, 0.04 in $CHCl_3$). λ_{max} 285 (log ϵ 2.29) ($CHCl_3$).

Kameoka, H. *et al., CA*, 1980, **92**, 116234 (*Helianthol B*)

Kladi, M. *et al., Tetrahedron*, 2007, **63**, 7606-7611 (*(-)-form*)

3(15),4,10-Bisabolatrien-2-ol B-161



(2*R* ,6*R* ,7ξ)-*form*

$C_{15}H_{24}O$ 220.354

(2*R*,6*R*,7ξ)-*form* [56144-26-4]
cis-*β*-*Sesquiphellandrol*
Constit. of oil of ginger (*Zingiber officinale*).

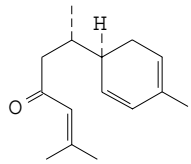
(2*R*,6*S*,7ξ)-*form* [56144-27-5]
trans-*β*-*Sesquiphellandrol*
Constit. of oil of ginger (*Zingiber officinale*).

(2ξ,6ξ,7ξ)-*form* [55853-55-9]
Sesquiphellandrol
Constit. of ginger (*Zingiber officinale*).

Bednarczyk, A.A. *et al., J. Agric. Food Chem.*, 1975, **23**, 499-501 (*β-Sesquiphellandrols*)
Sakamura, F. *et al., Phytochemistry*, 1986, **25**, 1333-1335 (*Sesquiphellandrol*)

1,3,10-Bisabolatrien-9-one B-162

2-Methyl-6-(4-methyl-2,4-cyclohexadien-1-yl)-2-hepten-4-one, 9CI. ***α-Turmerone*** [82508-15-4]

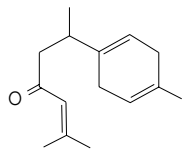


$C_{15}H_{22}O$ 218.338
Constit. of turmeric (*Curcuma longa*). Oil.

Golding, B.T. *et al., Chem. Comm.*, 1982, 363
Golding, B.T. *et al., JCS Perkin 1*, 1992, 1519 (*struct*)

2,5,10-Bisabolatrien-9-one B-163

Turmerone*. Tumerone* [56485-42-8]

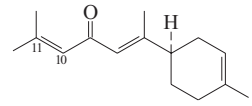


$C_{15}H_{22}O$ 218.338
Oil. Bp_{10} 125-126°. Unstable in air and light, dimerising and isomerising to 1,3,10-Bisabolatrien-9-one, B-162.

Mima, H. *et al., Yakugaku Zasshi*, 1959, **79**, 644 (*isol, struct, uv*)
Malingre, Th.M. *et al., Pharm. Weekbl.*, 1975, **110**, 601
Su, H.C.F. *et al., J. Agric. Food Chem.*, 1982, **30**, 290-292 (*isol*)
Kamal, A. *et al., Tetrahedron: Asymmetry*, 2009, **20**, 1267-1271 (*synth*)

2,7,10-Bisabolatrien-9-one B-164

2-Methyl-6-(4-methyl-3-cyclohexen-1-yl)-2,5-heptadien-4-one, 9CI. ***Atlantone****. α-Atlantone*



(*E*)–*form*

$C_{15}H_{22}O$ 218.338

(*E*)-*form* [26294-59-7]
Oil. Bp_1 142-145° (bath). $[\alpha]_D$ +1.2 (c, 0.83 in $CHCl_3$). n_D^{30} 1.5342.

10,11-Dihydro: [57130-01-5] *2,7-Bisabolad-ien-9-one.* ***10,11-Dihydroatlantone***
Isol. from heartwoods of *Ginkgo biloba* (ginkgo). Oil. Opt. inactive. Interconverts with the (*Z*)-form on standing.

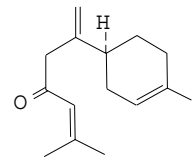
(*Z*)-*form* [56192-70-2]
Oil. n_D^{30} 1.5228.

10,11-Dihydro: [57130-00-4]
Found in *Ginkgo biloba* (ginkgo). Oil. Opt. inactive.

Pande, B.S. *et al., Tetrahedron*, 1971, **27**, 841 (*isol, struct*)
Babler, J.H. *et al., JOC*, 1974, **39**, 1656 (*synth*)
Plattier, M. *et al., Recherches*, 1974, **19**, 131 (*Dihydroatlantone*)
Irie, H. *et al., Chem. Pharm. Bull.*, 1975, **23**, 1892 (*Dihydroatlantone*)
Adams, D.R. *et al., JCS Perkin 1*, 1975, 1741 (*synth*)
Motoyoshiya, J. *et al., JOC*, 1985, **50**, 1326 (*synth*)
Manville, J.F. *et al., Phytochemistry*, 1989, **28**, 3073 (*pmr, cmr*)
Friesen, R.W. *et al., JOC*, 1996, **61**, 7202 (*synth*)

2,7(14),10-Bisabolatrien-9-one B-165

β-Atlantone [38331-79-2]

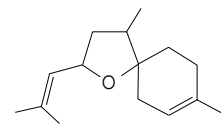


$C_{15}H_{22}O$ 218.338
Constit. of *Curcuma xanthorrhiza* (Java turmeric). Oil. $[\alpha]_D^{26}$ -48.8 (c, 0.12 in EtOH). λ_{max} 242 (ϵ 10900) (EtOH) (Derep).

Crawford, R.J. *et al., JACS*, 1972, **94**, 4298 (*synth*)
Itokawa, H. *et al., Chem. Pharm. Bull.*, 1985, **33**, 3488 (*isol*)

Bisabolene oxide B-166

[38970-57-9]



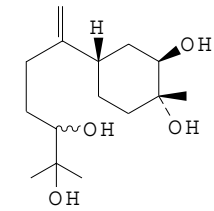
$C_{15}H_{24}O$ 220.354

Struct. shown to be incorrect by synth.
Constit. of *Gossypium hirsutum* (cotton). Oil.

Hedin, P.A. *et al., Phytochemistry*, 1972, **11**, 2118
Buchmann, B. *et al., Tetrahedron*, 1984, **40**, 3393 (*synth*)

7(14)-Bisabolene-2,3,10,11-tetrol B-167

[122470-42-2]

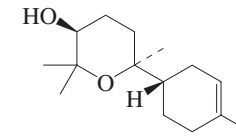


$C_{15}H_{28}O_4$ 272.384
Mycotoxin of *Fusarium sambucinum*. Glass.

Sanson, D.R. *et al., JOC*, 1989, **54**, 4313 (*isol*)

α-Bisabolol oxide A B-168

7,11-Epoxy-2-bisabolen-10-ol [22567-36-8]



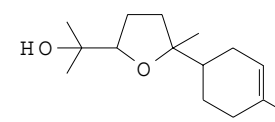
$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Liq. Bp 156-158°. $[\alpha]_D^{20}$ -41.7 (c, 0.22 in CCl_4). Log P 3.74 (calc).

10-Ketone: [22567-38-0] *7,11-Epoxy-2-bisabolen-10-one.* ***Bisabolone oxide A***
$C_{15}H_{24}O_2$ 236.353
Constit. of chamomile oil. Oil. $[\alpha]_D$ -6.2.

Sampath, V. *et al., Indian J. Chem.*, 1969, **7**, 100 (*struct*)
Schilcher, H. *et al., Planta Med.*, 1973, **23**, 132-144 (*chamomile constit*)
Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 189-196 (*α-Bisabolol oxide A, struct*)
Motl, O. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1977, **310**, 210-215 (*chamomile constits*)
Flaskamp, E. *et al., Z. Naturforsch., B*, 1981, **36**, 1023-1030 (*abs config*)
Adam, K.-P. *et al., Phytochemistry*, 1998, **48**, 953-959 (*biosynth*)
Orav, A. *et al., Nat. Prod. Res.*, 2010, **24**, 48-55 (*Chamomilla recutita constit*)

α-Bisabolol oxide B B-169

[26184-88-3]

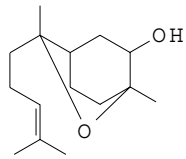


$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Liq. Log P 3.6 (calc).

Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, 309
Orav, A. *et al., Nat. Prod. Res.*, 2010, **24**, 48-55 (*Chamomilla recutita constit*)

α-Bisabolol oxide C B-170

[59861-08-4]

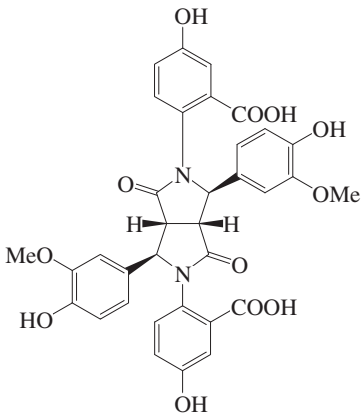


$C_{15}H_{26}O_2$ 238.369
Constit. of *Matricaria chamomilla* (German chamomile). Cryst. (EtOH). Mp 99-100°.

Schilcher, H. *et al., Arch. Pharm. (Weinheim, Ger.)*, 1976, **309**, 189

Bisavenanthramide B_1 B-171

[939790-85-9]



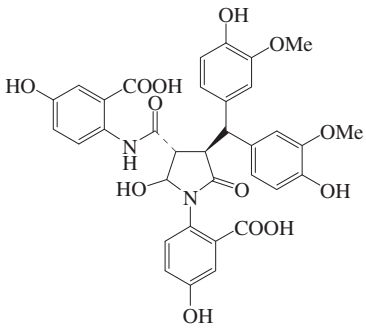
Relative Configuration

$C_{34}H_{28}N_2O_{12}$ 656.601
Isol. from elicited oat leaves (*Avena sativa*). Amorph. solid. Racemic. λ_{max} 210 (log ϵ 4.83); 233 (sh) (log ϵ 4.44); 285 (log ϵ 4.04); 300 (sh) (log ϵ 3.84) (MeOH).

Okazaki, Y. *et al., JOC*, 2007, **72**, 3830-3839 (*isol, pmr, cmr, ms*)

Bisavenanthramide B_2 B-172

[939790-86-0]

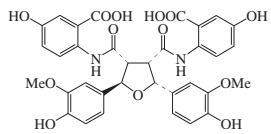


$C_{34}H_{30}N_2O_{13}$ 674.617
Isol. from elicited oat leaves (*Avena sativa*). Yellowish solid. Racemic. λ_{max} 204 (log ϵ 5.04); 265 (log ϵ 4.23); 317 (log ϵ 3.07) (MeOH).

Okazaki, Y. *et al., JOC*, 2007, **72**, 3830-3839 (*isol, pmr, cmr, ms*)

Bisavenanthramide B_5 B-173

[939790-89-3]

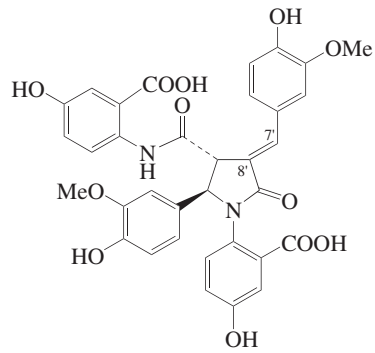


Relative Configuration

$C_{34}H_{30}N_2O_{13}$ 674.617
Isol. from elicited oat leaves (*Avena sativa*). Yellow solid. λ_{max} 204 (log ϵ 4.79); 224 (log ϵ 4.51); 263 (log ϵ 4.19); 328 (log ϵ 3.75) (MeOH).

Okazaki, Y. *et al., JOC*, 2007, **72**, 3830-3839 (*isol, pmr, cmr, ms*)

Bisavenanthramide B_6 B-174



$C_{34}H_{28}N_2O_{12}$ 656.601
Isol. from elicited oat leaves (*Avena sativa*). Racemic. λ_{max} 204 (log ϵ 4.61); 265 (log ϵ 4.31); 329 (log ϵ 4.45) (MeOH).

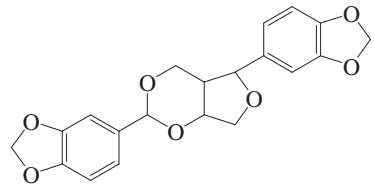
7′,8′α-Dihydro, 7′ξ-hydroxy (1): [939790-87-1] ***Bisavenanthramide B_3***
$C_{34}H_{30}N_2O_{13}$ 674.617
Isol. from elicited oat leaves (*Avena sativa*). Yellowish solid. Racemic. C-7′ epimer of B_4. λ_{max} 205 (log ϵ 4.76); 225 (sh) (log ϵ 4.42); 267 (log ϵ 3.98); 319 (log ϵ 3.49) (MeOH).

7′,8′α-Dihydro, 7′ξ-hydroxy (2): [939790-88-2] ***Bisavenanthramide B_4***
$C_{34}H_{30}N_2O_{13}$ 674.617
Isol. from elicited oat leaves (*Avena sativa*). Yellowish solid. Racemic. C-7′ epimer of B_3. λ_{max} 204 (log ϵ 4.87); 225 (sh) (log ϵ 4.59); 262 (log ϵ 4.19); 319 (log ϵ 3.67) (MeOH).

Okazaki, Y. *et al., Tetrahedron*, 2004, **60**, 4765-4771 (*isol, pmr, cmr, ms*)
Okazaki, Y. *et al., JOC*, 2007, **72**, 3830-3839 (*isol, pmr, cmr, ms*)

1,5-Bis(1,3-benzodioxol-5-yl)tetrahydro-4*H*-furo[3,4-*d*][1,3]dioxane B-175

3,7-Bis(3,4-methylenedioxyphenyl)-2,4,8-trioxabicyclo[4.3.0]nonane [877881-03-3]

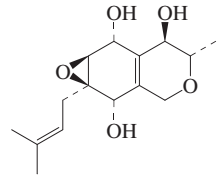


$C_{20}H_{18}O_7$ 370.358
Isol. from tea seed oil (*Camellia oleifera*). Cryst.

Lee, C.-P. *et al., J. Agric. Food Chem.*, 2006, **54**, 779-784 (*isol, pmr, cmr*)

Bisbynin B-176

1a,3,5,6,7,7a-Hexahydro-5-methyl-1a-(3-methyl-2-butenyl)-2H-oxireno[g][2]benzopyran-2,6,7-triol, 9CI [163365-14-8]

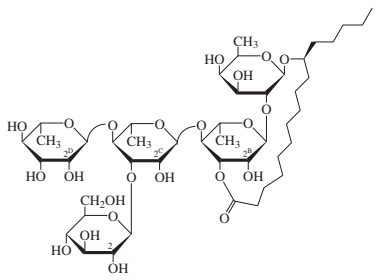


Relative Configuration

$C_{15}H_{22}O_5$ 282.336
Isol. from seeds of *Oryza sativa* (rice). Cryst. (CH_2Cl_2/MeOH). Sol. MeOH. Mp 144°.

De Silva, L.B. *et al., Tet. Lett.*, 1995, **36**, 1997 (*isol, pmr, cryst struct*)

Bis(deacyl)operculin V B-177



$C_{46}H_{80}O_{23}$ 1001.124

$2^C,4^D$-Bis(2S-methylbutanoyl): [882691-12-5] ***Murucoidin V***
$C_{56}H_{96}O_{25}$ 1169.359
Amorph. powder. Mp 148-150°. $[\alpha]_D$ -29 (c, 0.14 in MeOH).

2^C-Decanoyl: [1072160-34-9] ***Batatinoside VI***
$C_{56}H_{98}O_{24}$ 1155.376
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 142°. $[\alpha]_D$ -58 (c, 0.1 in MeOH).

*2^C-Decanoyl, 4^D-(2*S*-methylbutanoyl):* [156885-09-5] ***Stoloniferin IV***
$C_{61}H_{106}O_{25}$ 1239.493
Powder + $1H_2O$. Mp 112-120° dec. $[\alpha]_D$ -65.6 (c, 1.2 in MeOH).

*2^C-Dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [1035597-11-5] ***Murucoidin XI***
$C_{63}H_{110}O_{25}$ 1267.547
Powder. Mp 156-158°. $[\alpha]_D$ -50 (c, 0.32 in MeOH).

$2^C,4^D$-Didodecanoyl: [132625-00-4] ***Operculin V***
$C_{70}H_{124}O_{25}$ 1365.735
Powder (MeOH aq.). Mp 108-111° dec. $[\alpha]_D^{18}$ -53.8 (c, 2.6 in MeOH).

$2^C,4^D$-Dihexadecanoyl: [162666-30-0] ***Tuguajalapin IX***
$C_{78}H_{140}O_{25}$ 1477.949
Powder. Mp 77-80°. $[\alpha]_D$ -27.4 (c, 1.2 in $CHCl_3$).

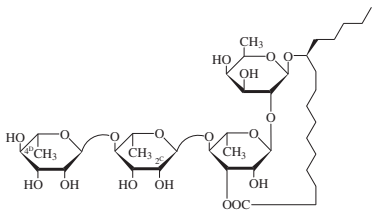
$2^C,4^D,6^E$-Trihexadecanoyl: [162666-21-9] ***Tuguajalapin I***
$C_{94}H_{170}O_{26}$ 1716.361
Powder. Mp 84-89°. $[\alpha]_D^{27}$ -36.3 (c, 1.7 in $CHCl_3$).

6^E-Octadecanoyl, $2^C,4^D$-dihexadecanoyl: [162666-29-7] ***Tuguajalapin IV***
$C_{96}H_{174}O_{26}$ 1744.415
Powder. Mp 78-85°. $[\alpha]_D^{21}$ -44.7 (c, 3.5 in $CHCl_3$).

*3^C-Deglucosyl, 2^C-decanoyl, 4^D-(2*S*-methylbutanoyl):* ***Stoloniferin XI***
$C_{55}H_{96}O_{20}$ 1077.351
Powder + ½ H_2O. Mp 105-110°. $[\alpha]_D$ -81.3 (c, 1.1 in MeOH).

Ono, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2986-2991 (*Operculin V*)
Noda, N. *et al., Chem. Pharm. Bull.*, 1994, **42**, 2011-2016 (*Tuguajalapins*)
Noda, N. *et al., Phytochemistry*, 1994, **36**, 365-371; 1998, **48**, 837-841 (*Stoloniferins*)
Chérigo, L. *et al., J. Nat. Prod.*, 2006, **69**, 595-599; 2008, **71**, 1037-1045 (*Murucoidins V,XI*)
Escalante-Sánchez, E. *et al., J. Agric. Food Chem.*, 2008, **56**, 9423-9428 (*Batatinoside VI*)

Bis(deacyl)operculin XI B-178



$C_{40}H_{70}O_{18}$ 838.982

2^C-Decanoyl: [1072160-30-5] ***Batatinoside II***
$C_{50}H_{88}O_{19}$ 993.234
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 107-110°. $[\alpha]_D$ -89.2 (c, 0.13 in MeOH).

*2^C-Dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [943861-63-0] ***Pescaprein V***
$C_{57}H_{100}O_{20}$ 1105.405
Powder. Mp 140-142°. $[\alpha]_D$ -57 (c, 0.1 in MeOH).

$2^C,4^D$-Didodecanoyl: [139638-42-9] ***Operculin XI***
$C_{64}H_{114}O_{20}$ 1203.593
Powder (Et_2O/hexane). Mp 105-113°. $[\alpha]_D^{22}$ -62.7 (c, 0.9 in MeOH).

*2^D-Dodecanoyl, 3^C-(2*S*-methylbutanoyl):* [943861-64-1] ***Pescaprein VI***
$C_{57}H_{100}O_{20}$ 1105.405
Powder. Mp 136-138°. $[\alpha]_D$ -17 (c, 0.1 in MeOH).

*3^C-Dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [1137253-85-0] ***Murucoidin XIV***
$C_{57}H_{100}O_{20}$ 1105.405
Powder. Mp 125-127°. $[\alpha]_D$ -60 (c, 0.47 in MeOH).

$3^C,4^D$-Didodecanoyl: [139638-43-0] ***Operculin XII***
$C_{64}H_{114}O_{20}$ 1203.593
Powder (Et_2O/hexane). Mp 107-116°. $[\alpha]_D^{22}$ -33 (c, 0.8 in MeOH).

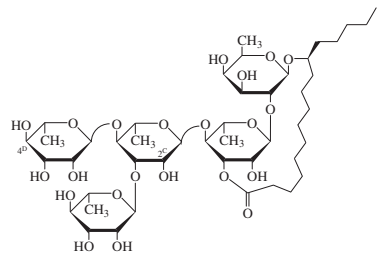
4^D-Dodecanoyl: [1072160-31-6] ***Batatinoside III***
$C_{52}H_{92}O_{19}$ 1021.287
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 88-90°. $[\alpha]_D$ -23 (c, 0.1 in MeOH).

2^D-E-Cinnamoyl, 4^D-dodecanoyl, 2^C-decanoyl: [1255952-66-9] ***Ipomotaoside C***
$C_{71}H_{116}O_{21}$ 1305.685
Constit. of the aerial parts of *Ipomoea batatas* (sweet potato). Powder. Mp 105-107°. $[\alpha]_D^{25}$ -37.4 (c, 3.1 in MeOH). λ_{max} 230 (log ϵ 3.98); 237 (log ϵ 4.03); 244 (log ϵ 3.88) (MeOH).

2^D-E-Cinnamoyl, 4^D-dodecanoyl, 3^C-decanoyl: [1255952-67-0] ***Ipomotaoside D***
$C_{71}H_{116}O_{21}$ 1305.685
Constit. of the aerial parts of *Ipomoea batatas* (sweet potato). Powder. Mp 106-108°. $[\alpha]_D^{25}$ -18.3 (c, 3.1 in MeOH). λ_{max} 230 (log ϵ 3.98); 237 (log ϵ 4.03); 244 (log ϵ 3.88) (MeOH).

Ono, M. *et al., Chem. Pharm. Bull.*, 1992, **40**, 1400-1403 (*Operculins XI,XII*)
Escobedo-Martinez, C. *et al., J. Nat. Prod.*, 2007, **70**, 974-978 (*Pescapreins V,VI*)
Escalante-Sánchez, E. *et al., J. Agric. Food Chem.*, 2008, **56**, 9423-9428 (*Batatinosides II,III*)
Chérigo, L. *et al., Phytochemistry*, 2009, **70**, 222-227 (*Murucoidin XIV*)
Yoshikawa, K. *et al., J. Nat. Prod.*, 2010, **73**, 1763-1766 (*Ipomotaosides C,D*)

Bis(deacyl)stoloniferin I B-179



$C_{46}H_{80}O_{22}$ 985.125

*2^C-(2*S*-Methylbutanoyl):* [1146541-53-8] ***Batataoside IV****. Batatoside IV*
$C_{51}H_{88}O_{23}$ 1069.242

Constit. of the roots of *Ipomoea batatas* (sweet potato). Amorph. powder. $[\alpha]_D^{20}$ -38 (c, 0.5 in MeOH).

*2^C-(2*S*-Methylbutanoyl), 4^D-(2-methylpropanoyl):* [1035597-07-9] ***Murucoidin IX***
$C_{55}H_{94}O_{24}$ 1139.333
Powder. Mp 156-158°. $[\alpha]_D$ -74 (c, 0.07 in MeOH).

*$2^C,4^D$-Bis(2*S*-methylbutanoyl):* [156848-77-0] ***Stoloniferin I***
$C_{56}H_{96}O_{24}$ 1153.36
Powder + ½H_2O. Mp 143-148° dec. $[\alpha]_D$ -85.4 (c, 10.9 in MeOH).

2^C-Decanoyl: [943861-66-3] ***Pescaprein VII***
$C_{56}H_{98}O_{23}$ 1139.376
Isol. from the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 134-136°. $[\alpha]_D$ -72 (c, 0.1 in MeOH).

2^C-Decanoyl, 4^D-(2-methylpropanoyl): [156848-78-1] ***Stoloniferin II***
$C_{60}H_{104}O_{24}$ 1209.467
Powder + 1½H_2O. Mp 138-143° dec. $[\alpha]_D$ -74.7 (c, 1 in MeOH).

*2^C-Decanoyl, 4^D-(2*S*-methylbutanoyl):* [156848-79-2] ***Stoloniferin III***
$C_{61}H_{106}O_{24}$ 1223.494
Powder + 1½H_2O. Mp 139-144° dec. $[\alpha]_D$ -72.5 (c, 1.6 in MeOH).

2^C-Decanoyl, 4^D-hexanoyl: [943861-70-9] ***Pescaprein IX***
$C_{62}H_{108}O_{24}$ 1237.521
Powder. Mp 123-124°. $[\alpha]_D$ -53 (c, 0.1 in MeOH).

2^C-Dodecanoyl: ***Pescaprein I***
$C_{58}H_{102}O_{23}$ 1167.43
Isol. from the roots of *Ipomoae batatas* (sweet potato). Amorph. powder. Mp 131-133°. $[\alpha]_D$ -65 (c, 0.06 in MeOH).

2^C-Dodecanoyl, 4^D-(2-methylpropanoyl): ***Pescaprein II***
$C_{62}H_{108}O_{24}$ 1237.521
Amorph. powder. Mp 120-123°. $[\alpha]_D$ -81 (c, 0.19 in MeOH).

*2^C-Dodecanoyl, 4^D-(2*S*-methylbutanoyl):* ***Pescaprein III***
$C_{63}H_{110}O_{24}$ 1251.548
Amorph. powder. Mp 121-123°. $[\alpha]_D$ -70 (c, 0.43 in MeOH).

2^C-Dodecanoyl, 4^D-hexanoyl: ***Pescaprein IV***
$C_{64}H_{112}O_{24}$ 1265.574
Amorph. powder. Mp 120-122°. $[\alpha]_D$ -60 (c, 0.81 in MeOH).

4^D-Dodecanoyl, 2^C-(2-methylpropanoyl): [943861-68-5] ***Pescaprein VIII***
$C_{62}H_{108}O_{24}$ 1237.521
Powder. Mp 110-112°. $[\alpha]_D$ -17 (c, 0.1 in MeOH).

*4^D-Dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [1072160-32-7] ***Batatinoside IV***
$C_{63}H_{110}O_{24}$ 1251.548
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 123-125°. $[\alpha]_D$ -51.8 (c, 0.1 in MeOH).

*2^C-(8*R*-Hydroxydodecanoyl), 4^D-(2*S*-methylbutanoyl):* [1035597-09-1] ***Murucoidin X***
$C_{63}H_{110}O_{25}$ 1267.547

Powder. Mp 128-130°. $[\alpha]_D$ -53 (c, 0.15 in MeOH).

2^D-E-*Cinnamoyl, 2^C-(2-methylbutanoyl), 3^D-(2-methylpropanoyl):* [1020196-42-2] ***Batatoside A***
$C_{64}H_{100}O_{25}$ 1269.479
Constit. of the tubers of *Ipomoea batatas* (sweet potato). Amorph. powder. Mp 122-124°. $[\alpha]_D^{25}$ -11.6 (c, 0.55 in MeOH). λ_{max} 280 (log ϵ 4.17) (MeOH).

2^D-E-*Cinnamoyl, 2^C-dodecanoyl, 4^D-decanoyl:* [1146541-55-0] ***Batataoside V.*** *Batatoside V*
$C_{77}H_{126}O_{25}$ 1451.827
Constit. of the roots of *Ipomoea batatas* (sweet potato). Amorph. powder. $[\alpha]_D^{25}$ -28.1 (c, 0.5 in MeOH). λ_{max} 204 (log ϵ 4.06); 217 (log ϵ 4.07); 280 (log ϵ 4.18) (MeOH).

2^D-E-*Cinnamoyl, 3^D-dodecanoyl, 2^C-(2-methylbutanoyl):* [1020196-76-2] ***Batatoside C***
$C_{72}H_{116}O_{25}$ 1381.693
Constit. of the tubers of *Ipomoea batatas* (sweet potato). Amorph. powder. Mp 109-111°. $[\alpha]_D^{25}$ -22 (c, 0.55 in MeOH). λ_{max} 280 (log ϵ 4.27) (MeOH).

3^D-E-*Cinnamoyl, 2^C-butanoyl, 4^D-(2-methylpropanoyl):* [1020196-59-1] ***Batatoside B***
$C_{63}H_{98}O_{25}$ 1255.452
Constit. of the tubers of *Ipomoea batatas* (sweet potato). Amorph. powder. Mp 119-121°. $[\alpha]_D^{25}$ -12.1 (c, 0.5 in MeOH). λ_{max} 280 (log ϵ 4.37) (MeOH).

3^D-E-*Cinnamoyl, 2^C-(2*S*-methylbutanoyl), 4^D-(2-methylpropanoyl):* [1072028-60-4] ***Batataoside I***
$C_{64}H_{100}O_{25}$ 1269.479
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder (MeOH). Mp 123-125°. $[\alpha]_D^{25}$ -26.9 (c, 0.4 in MeOH).

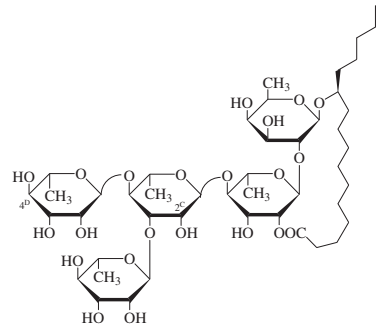
3^D-E-*Cinnamoyl, 4^D-dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [943153-71-7] ***Batatinoside I***
$C_{72}H_{116}O_{25}$ 1381.693
Constit. of *Ipomoea batatas* var. *batatas* (sweet potato).

*3^E-[*E-*Cinnamoyl-(→2)-4*-O-*dodecanoyl-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→3)][2*S*-methylbutanoyl-(→2)]-α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl-(1→11)-11-hydroxyhexadecanoyl], 3^D*-E-*cinnamoyl, 4^D-dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [943153-59-1] ***Batatin I***
$C_{144}H_{232}O_{50}$ 2763.387
Constit. of *Ipomoea batatas* var. *batatas* (sweet potato). Powder. Mp 117-120°. $[\alpha]_D$ -38 (c, 1 in MeOH).

*3^E-[*E-*Cinnamoyl-(→3)-4*-O-*dodecanoyl-α-L-rhamnopyranosyl-(1→4)-[α-L-rhamnopyranosyl-(1→3)][2*S*-methylbutanoyl-(→2)]-α-L-rhamnopyranosyl-(1→4)-α-L-rhamnopyranosyl-(1→2)-β-D-fucopyranosyl-(1→11)-11-hydroxyhexadecanoyl], 3^D*-E-*cinnamoyl, 4^D-dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [943153-60-4] ***Batatin II***
$C_{144}H_{232}O_{50}$ 2763.387
Constit. of *Ipomoea batatas* var. *batatas* (sweet potato). Powder. Mp 124-130°. $[\alpha]_D$ -33 (c, 0.1 in MeOH).

Noda, N. *et al., Phytochemistry*, 1994, **36**, 365-371; 1998, **48**, 837-841 (*Stoloniferins*)
Pereda-Miranda, R. *et al., J. Nat. Prod.*, 2005, **68**, 226-230; 2007, **70**, 974-978 (*Pescapreins*)
Escalante-Sánchez, E. *et al., J. Nat. Prod.*, 2007, **70**, 1029-1034 (*Batatins I,II, Batatinoside I*)
Yin, Y.-Q. *et al., Chem. Pharm. Bull.*, 2008, **56**, 1670-1674 (*Batataosides IV,V*)
Yin, Y. *et al., J. Agric. Food Chem.*, 2008, **56**, 2363-2368 (*Batatosides A,B,C*)
Escalante-Sánchez, E. *et al., J. Agric. Food Chem.*, 2008, **56**, 9423-9428 (*Batatinoside IV*)
Yin, Y.-Q. *et al., J. Asian Nat. Prod. Res.*, 2008, **10**, 233-238 (*Batataoside I*)
Chérigo, L. *et al., J. Nat. Prod.*, 2008, **71**, 1037-1045 (*Murucoidins IX,X*)

Bis(deacyl)stoloniferin VIII B-180



$C_{46}H_{80}O_{22}$ 985.125

2^C-(2*S*-*Methylbutanoyl):* [882691-08-9] ***Murucoidin I***
$C_{51}H_{88}O_{23}$ 1069.242
Isol. from the roots of *Ipomoea batatas* (sweet potato). Amorph. powder. Mp 154-156°. $[\alpha]_D$ -46 (c, 0.12 in MeOH).

2^C-(2*S*-*Methylbutanoyl), 4^D-(2-methylpropanoyl):* [882691-09-0] ***Murucoidin II***
$C_{55}H_{94}O_{24}$ 1139.333
Amorph. powder. Mp 155-157°. $[\alpha]_D$ -55 (c, 0.1 in MeOH).

*2^C,4^D-Bis(2*S*-methylbutanoyl):* [882691-10-3] ***Murucoidin III***
$C_{56}H_{96}O_{24}$ 1153.36
Amorph. powder. Mp 150-153°. $[\alpha]_D$ -42 (c, 0.2 in MeOH).

*2^C-Octanoyl, 4^D-(2*S*-methylbutanoyl):* [212072-42-9] ***Stoloniferin VIII***
$C_{59}H_{102}O_{24}$ 1195.44
Powder + $1^1/_2$ H_2O.

2^C-Decanoyl: [1072160-33-8] ***Batatinoside V***
$C_{56}H_{98}O_{23}$ 1139.376
Constit. of the roots of *Ipomoea batatas* (sweet potato).

*2^C-Decanoyl, 4^D-(2*S*-methylbutanoyl):* [212072-43-0] ***Stoloniferin IX***
$C_{61}H_{106}O_{24}$ 1223.494
Powder + $1H_2O$. Mp 132-139°. $[\alpha]_D$ -53.7 (c, 1.3 in MeOH).

*2^C-Dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [212072-44-1] ***Stoloniferin X***
$C_{63}H_{110}O_{24}$ 1251.548
Powder + $1H_2O$. Mp 122-127°. $[\alpha]_D$ -44.2 (c, 1.4 in MeOH).

*4^D-Dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [151310-52-0] ***Simonin III***
$C_{63}H_{110}O_{24}$ 1251.548
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 127-132°. $[\alpha]_D$ -37.5 (c, 1 in MeOH).

4^D-Dodecanoyl, 2^C-octanoyl: [151310-54-2] ***Simonin V***
$C_{66}H_{116}O_{24}$ 1293.628
Constit. of *Ipomoea batatas* (sweet potato). Powder. Mp 115-116°. $[\alpha]_D$ -35.2 (c, 1 in MeOH).

4^D-Dodecanoyl, 2^C-decanoyl: [151310-53-1] ***Simonin IV***
$C_{68}H_{120}O_{24}$ 1321.682
Constit of *Ipomoea batatas* (sweet potato). Powder. Mp 123-125°. $[\alpha]_D$ -43.3 (c, 1 in MeOH).

2^D-E-*Cinnamoyl, 2^C-(2*S*-methylbutanoyl), 4^D-(2-methylpropanoyl):* [1107648-22-5]
$C_{64}H_{100}O_{25}$ 1269.479
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 133-137°. $[\alpha]_D$ -20.7 (c, 1.1 in MeOH).

2^D-E-*Cinnamoyl, 2^C-decanoyl, 4^D-(2-methylpropanoyl):* [1100362-79-5] ***Pescaprein XIII***
$C_{69}H_{110}O_{25}$ 1339.613
Amorph. powder. $[\alpha]_D^{20}$ -18 (c, 0.14 in MeOH). λ_{max} 201 (log ϵ 4.1); 279 (log ϵ 3.8) (MeOH).

2^D-E-*Cinnamoyl, 2^C-decanoyl, 4^D-(2*S*-methylbutanoyl):* [1100362-76-2] ***Pescaprein XI***
$C_{70}H_{112}O_{25}$ 1353.64
Amorph. powder. $[\alpha]_D^{20}$ -12 (c, 0.15 in MeOH). λ_{max} 201 (log ϵ 4.5); 279 (log ϵ 3.8) (MeOH).

2^D-E-*Cinnamoyl, 4^D-decanoyl, 2^C-(2-methylpropanoyl):* [1107648-23-6]
$C_{69}H_{110}O_{25}$ 1339.613
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 105-109°. $[\alpha]_D$ -12.5 (c, 0.1 in MeOH).

2^D-E-*Cinnamoyl, 2^C-dodecanoyl, 4^D-(2-methylpropanoyl):* [1100362-81-9] ***Pescaprein XV***
$C_{71}H_{114}O_{25}$ 1367.667
Amorph. powder. $[\alpha]_D^{20}$ -13 (c, 0.13 in MeOH). λ_{max} 200 (log ϵ 4); 280 (log ϵ 3.9) (MeOH).

2^D-E-*Cinnamoyl, 2^C-dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [1100362-86-4] ***Pescaprein XVII***
$C_{72}H_{116}O_{25}$ 1381.693
Amorph. powder. $[\alpha]_D^{20}$ -6 (c, 0.17 in MeOH). λ_{max} 201 (log ϵ 3.9); 280 (log ϵ 3.9) (MeOH).

2^D-E-*Cinnamoyl, 4^D-dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [1107648-25-8]
$C_{72}H_{116}O_{25}$ 1381.693
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder. Mp 118-121°. $[\alpha]_D$ -10.8 (c, 2.3 in MeOH).

3^D-E-*Cinnamoyl, 2^C-(2*S*-methylbutanoyl), 4^D-(2-methylpropanoyl):* [1072028-62-6] ***Bataiaoside II***
$C_{64}H_{100}O_{25}$ 1269.479
Constit. of the roots of *Ipomoea batatas* (sweet potato). Powder (MeOH). Mp 115-117°. $[\alpha]_D^{25}$ -31.5 (c, 0.5 in MeOH). λ_{max} 280 (log ϵ 3.47) (MeOH).

3^D-E-*Cinnamoyl, 2^C,4^D-bis(2*S*-methylbutanoyl):* [1146541-51-6] ***Bataiaoside III***. *Batatoside III*
$C_{65}H_{102}O_{25}$ 1283.506
Constit. of the roots of *Ipomoea batatas* (sweet potato). Amorph. powder. $[\alpha]_D^{25}$ -18.7 (c, 0.4 in MeOH). λ_{max} 204 (log ϵ 4.28); 217 (log ϵ 4.25); 280 (log ϵ 4.33) (MeOH).

3^D-E-*Cinnamoyl, 2^C-decanoyl, 4^D-(2-methylpropanoyl):* [1100362-78-4] ***Pescaprein XII***
$C_{69}H_{110}O_{25}$ 1339.613
Amorph. powder. $[\alpha]_D^{20}$ -15 (c, 0.13 in MeOH). λ_{max} 201 (log ϵ 4.7); 279 (log ϵ 3.9) (MeOH).

3^D-E-*Cinnamoyl, 2^C-decanoyl, 4^D-(2*S*-methylbutanoyl):* [1100362-75-1] ***Pescaprein X***
$C_{70}H_{112}O_{25}$ 1353.64
Amorph. powder. $[\alpha]_D^{20}$ -17 (c, 0.14 in MeOH). λ_{max} 201 (log ϵ 4.2); 279 (log ϵ 3.9) (MeOH).

3^D-E-*Cinnamoyl, 2^C-dodecanoyl, 4^D-(2-methylpropanoyl):* [1100362-80-8] ***Pescaprein XIV***
$C_{71}H_{114}O_{25}$ 1367.667
Amorph. powder. $[\alpha]_D^{20}$ -26 (c, 0.14 in MeOH). λ_{max} 200 (log ϵ 4.3); 279 (log ϵ 4.2) (MeOH).

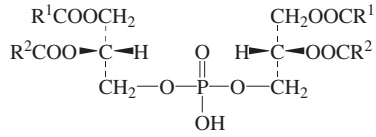
3^D-E-*Cinnamoyl, 2^C-dodecanoyl, 4^D-(2*S*-methylbutanoyl):* [1100362-85-3] ***Pescaprein XVI***
$C_{72}H_{116}O_{25}$ 1381.693
Amorph. powder. $[\alpha]_D^{20}$ -20 (c, 0.14 in MeOH). λ_{max} 201 (log ϵ 4.1); 279 (log ϵ 4) (MeOH).

*4^A-Epimer, 6^A-hydroxy, 4^D-dodecanoyl, 2^C-(2*S*-methylbutanoyl):* [151310-51-9] ***Simonin II***
$C_{63}H_{110}O_{25}$ 1267.547
Constit. of *Ipomoea batatas* (sweet potato). Powder. Mp 121-123.5°. $[\alpha]_D$ -27.8 (c, 1 in MeOH).

Noda, N. *et al., Chem. Pharm. Bull.*, 1992, **40**, 3163-3168 (*Simonins II-V*)
Noda, N. *et al., Phytochemistry*, 1994, **36**, 365-371 (*Stoloniferins VIII-X*)
Chérigo, L. *et al., J. Nat. Prod.*, 2006, **69**, 595-599 (*Murucoidins I-III*)
Noda, N. *et al., Chem. Pharm. Bull.*, 2008, **56**, 1607-1610 (*sweet potato glycosides*)
Yin, Y.-Q. *et al., Chem. Pharm. Bull.*, 2008, **56**, 1670-1674 (*Batataoside III*)
Escalante-Sánchez, E. *et al., J. Agric. Food Chem.*, 2008, **56**, 837-841 (*Batatinoside V*)
Yin, Y.-Q. *et al., J. Asian Nat. Prod. Res.*, 2008, **10**, 233-238 (*Batataoside II*)
Tao, H. *et al., J. Nat. Prod.*, 2008, **71**, 1998-2003 (*Pescapreins X-XVII*)

Bis(diacylglycero)phosphonic acids B-181

Bis(phosphatidic) acids. Bis(1,2-diacylglycero)-3-phosphate



An undefined mixt. has been isol. from soya bean.

Bis(ditetradecanoylglycero)phosphonic acid
[105380-97-0]
Phosphinicobis[oxy-3,1,2-propanetriyl] tetradecanoate, 9CI. Bis(1,2-ditetradecanoylglycero)-3-phosphate. Bis(dimyristoylglycero)phosphonic acid
[83818-31-9, 99759-77-0, 63988-25-0]
$C_{62}H_{119}O_{12}P$ 1087.589
Mp 49-50°. $[\alpha]_D^{22}$ +7.5 (c, 4 in C_6H_6).

Bis(dihexadecanoylglycero)phosphonic acid
[84905-98-6]
Phosphinicobis[oxy-3,1,2-propanetriyl] hexadecanoate, 9CI. Bis(1,2-dihexadecanoylglycero)-3-phosphate. Bis(dipalmitoylglycero)phosphonic acid
[21289-05-4]
$C_{70}H_{135}O_{12}P$ 1199.803
Cryst. (toluene/Me_2CO). Mp 62-63°. $[\alpha]_D^{23}$ +6.7 (c, 4 in C_6H_6).

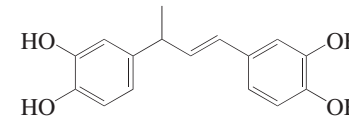
Bis(dioctadecanoylglycero)phosphonic acid
[105380-98-1]
Phosphinicobis[oxy-3,1,2-propanetriyl] octadecanoate, 9CI. Bis(1,2-dioctadecanoylglycero)-3-phosphate. Bis(distearoylglycero)phosphonic acid
[62438-23-7]
$C_{78}H_{151}O_{12}P$ 1312.017
Cryst. (Me_2CO). Mp 69.5-70.5°. $[\alpha]_D^{24}$ +6.2 (c, 4 in C_6H_6).

Bis(9*Z*-octadecenoylglycero)phosphonic acid
[17708-93-9]
Phosphinicobis[oxy-3,1,2-propanetriyl] 9-octadecenoate, 9CI. Olein 1,2-dihydrogen phosphate, 8CI. Bis(oleoylglycero)-phosphonic acid
$C_{78}H_{143}O_{12}P$ 1303.954
$[\alpha]_D$ +6.1 (c, 10 in $CHCl_3$).

Baer, E. *et al., J. Biol. Chem.*, 1952, **198**, 853-859 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl*)
Baer, E. *et al., Arch. Biochem. Biophys.*, 1958, **78**, 294-305 (*dioctadecanoyl, dioleoyl*)
Baer, E. *et al., Prog. Chem. Fats Other Lipids*, 1963, **6**, 31-86 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl, dioleoyl, synth, rev*)
Bioorg. Khim., 1977, **3**, 76-82 (*dioctadecanoyl*)
Stearns, E.M. *et al., Lipids*, 1977, **12**, 451-454 (*isol*)
Ramirez, F. *et al., Tetrahedron*, 1977, **33**, 599-608 (*ditetradecanoyl, dihexadecanoyl, dioctadecanoyl*)
Dang Quoc Quan, *et al., Lipids*, 1982, **17**, 798-802 (*ditetradecanoyl*)
Dang Quoc Quan, *et al., Chem. Phys. Lipids*, 1983, **33**, 33-40 (*dihexadecanoyl, synth, nmr*)

1,3-Bis(3,4-dihydroxyphenyl)-1-butene B-182

4,4′-(3-Methyl-1-propene-1,3-diyl)-bis[1,2-benzenediol], 9CI



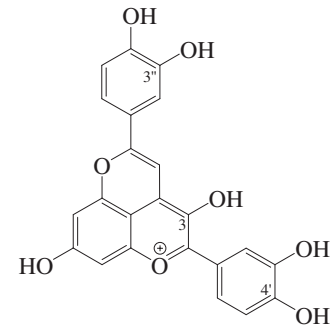
$C_{16}H_{16}O_4$ 272.3

Dihydro: [119773-33-0] *1,3-Bis(3,4-dihydroxyphenyl)butane. 4,4′-(1-Methyl-1,3-propanediyl)bis[1,2-benzenediol], 9CI*
$C_{16}H_{18}O_4$ 274.316
Bitter tasting constit. of espresso coffee.

(E)-form [143122-88-7]
Bitter tasting constit. of espresso coffee. No phys. props. reported.
Rizzi, G. *et al., J. Agric. Food Chem.*, 1992, **40**, 1666-1670 (*ms*)
Frank, O. *et al., J. Agric. Food Chem.*, 2007, **55**, 1945-1954 (*isol, dihydro, pmr, cmr, uv*)

2,5-Bis(3,4-dihydroxyphenyl)-3,8-dihydroxypyrano[4,3,2-*de*]-1-benzopyrylium(1+) B-183

Cyanidin-4-vinylcatechol



$C_{23}H_{15}O_8^{\oplus}$ 419.367

3-O-*[β-D-Xylopyranosyl-(1→2)-β-D-galactopyranoside]:*
$C_{34}H_{33}O_{17}^{\oplus}$ 713.625
Constit. of black carrot juice (*Daucus carota* ssp. *sativus* var. *atrorubens*).

3-O-*[4-Hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-galactopyranoside]:*
$C_{50}H_{51}O_{25}^{\oplus}$ 1051.938
Constit. of black carrot juice (*Daucus carota* ssp. *sativus* var. *atrorubens*).

3-O-*[4-Hydroxy-3,5-dimethoxycinnamoyl-(1→6)-β-D-galactopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-galactopyranoside]:*
$C_{51}H_{53}O_{26}^{\oplus}$ 1081.964

Constit. of black carrot juice (*Daucus carota* ssp. *sativus* var. *atrorubens*).

3′′-Me ether, 3-O-[β-D-xylopyranosyl-(1→2)-β-D-galactopyranoside]:
$C_{35}H_{35}O_{17}^{\oplus}$ 727.651
Constit. of black carrot juice (*Daucus carota* ssp. *sativus* var. *atrorubens*).

3′′-Me ether, 3-O-[4-hydroxy-3-methoxycinnamoyl-(→6)-β-D-glucopyranosyl-(1→6)-[β-D-xylopyranosyl-(1→2)]-β-D-galactopyranoside]:
$C_{51}H_{53}O_{25}^{\oplus}$ 1065.965
Constit. of black carrot juice (*Daucus carota* ssp. *sativus* var. *atrorubens*).

Schwarz, M. *et al., J. Agric. Food Chem.*, 2004, **52**, 5095-5101 (*isol, struct*)

1,2-Bis(3,4-dihydroxypheny-l)ethylene B-184

4,4′-(1,2-Ethenediyl)bis[1,2-benzenediol], 9CI. 3,3′,4,4′-Stilbenetetrol. 3,3′,4,4′-Tetrahydroxystilbene [133084-84-1]

$C_{14}H_{12}O_4$ 244.246

(*E*)-*form* [136273-05-7]
Mp 241° dec.

3-O-β-D-Glucopyranoside: [113231-13-3]
$C_{20}H_{22}O_9$ 406.388

3,3′-Di-Me ether: [7329-69-3] *1,2-Bis(4-hydroxy-3-methoxyphenyl)ethylene. 4,4′-Dihydroxy-3,3′-dimethoxystilbene* [137219-46-6, 4957-27-1]
$C_{16}H_{16}O_4$ 272.3
Constit. of the leaves of *Ginkgo biloba* (ginkgo). Cryst. (EtOH aq. or CH_2Cl_2/MeOH). Mp 212-215°. λ_{max} 224; 239 (sh); 309 (sh); 338; 350 (sh) (MeOH).

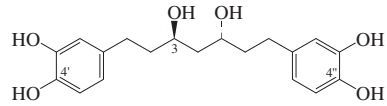
Tetra-Me ether: [18513-98-9] *1,2-Bis(3,4-dimethoxyphenyl)ethylene. 3,3′,4,4′-Tetramethoxystilbene*
$C_{18}H_{20}O_4$ 300.354
Pale yellow cryst. Mp 157° (149-152°).

Bis(methylene)ether: [76306-40-6] *3,4:3′,4′-Bis(methylenedioxy)stilbene*
$C_{16}H_{12}O_4$ 268.268
Prisms (CH_2Cl_2). Mp 214-215°.

[136273-06-8]

Talvitie, A. *et al., Finn. Chem. Lett.*, 1987, **14**, 43 (*isol, deriv*)
Gierer, J. *et al., J. Wood Chem. Technol.*, 1991, **11**, 171 (*synth*)
Thakkar, K. *et al., J. Med. Chem.*, 1993, **36**, 2950 (*synth, pmr*)
Chi, J. *et al., CA*, 1997, **127**, 231887b (*isol, 3,3′-di-Me ether*)
Hajdu, Z. *et al., J. Nat. Prod.*, 1998, **61**, 1298-1299 (*3,3′-di-Me ether*)
Wyatt, P. *et al., JCS Perkin 1*, 2001, 279-297 (*bismethylene ether, pmr, cmr*)
Ferré-Filmon, K. *et al., Eur. J. Org. Chem.*, 2005, 3319-3325 (*E-form, synth, pmr, 3,3′-di-Me ether*)
Vedernikov, A.I. *et al., Zh. Org. Khim.*, 2005, **41**, 864-875; *Russ. J. Org. Chem. (Engl. Transl.)*, 2005, **41**, 843-854 (*tetra-Me ether*)
Velder, J. *et al., Synthesis*, 2006, 273-278 (*E-form, tetra-Me ether*)

1,7-Bis(3,4-dihydroxy-phenyl)-3,5-heptanediol B-185



(3*R*,5*R*)-*form*

$C_{19}H_{24}O_6$ 348.395

(3*R*,5*R*)-*form*
Viscous syrup. $[\alpha]_D^{23}$ +4 (c, 0.1 in MeOH). λ_{max} 283 (log ε 3.79) (MeOH).

3-Ketone, 3′′-Me ether: [1022082-07-0] *1-(3,4-Dihydroxyphenyl)-5-hydroxy-7-(4-hydroxy-3-methoxyphenyl)-3-heptanone*
$C_{20}H_{24}O_6$ 360.406
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal). Yellow oil. $[\alpha]_D^{20}$ -6.6 (c, 0.15 in $CHCl_3$).

3-Ketone, 3′,3′′-di-Me ether: [100667-55-8] *5-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)-3-heptanone.* ***5-Epihexahydrocurcumin***
[36062-05-2 (unspecified stereochem), 93559-28-5 (deleted reg. number)]
$C_{21}H_{26}O_6$ 374.433
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal). Needles (C_6H_6). Mp 90-91°. $[\alpha]_D$ -10 (c, 0.28 in $CHCl_3$). λ_{max} 227 (log ε 4.36); 281 (log ε 4.05) (EtOH).

3,5-Diketone, 3′,3′′-di-Me ether: [36062-04-1] *1,7-Bis(4-hydroxy-3-methoxyphenyl)-3,5-heptanedione.* ***1,2,6,7-Tetrahydrocurcumin***
$C_{21}H_{24}O_6$ 372.417
Constit. of ginger (*Zingiber officinale*). Cryst. (petrol or Et_2O/hexane). Mp 95-96°. Enolised β-diketone.

(3*S*,5*S*)-*form*

3′,3′′-Di-Me ether: [112494-41-4] *1,7-Bis(4-hydroxy-3-methoxyphenyl)-3,5-heptanediol.* ***Octahydrocurcumin***
$C_{21}H_{28}O_6$ 376.449
Constit. of the rhizomes of ginger (*Zingiber officinale*) and Java turmeric (*Curcuma xanthorrhiza*). Needles. Mp 136°. $[\alpha]_D$ -18.5 (c, 0.26 in EtOH). λ_{max} 228 (log ε 3.81); 281 (log ε 3.48) (EtOH).

3′,3′′-Di-Me ether, 3,5-di-Ac:
$C_{25}H_{32}O_8$ 460.523
Constit. of the rhizomes of ginger (*Zingiber officinale*). Oil. $[\alpha]_D^{26}$ +7 (c, 0.68 in $CHCl_3$).

3-Ketone, 3′,3′′-di-Me ether: [39886-84-5] ***Hexahydrocurcumin***
$C_{21}H_{26}O_6$ 374.433
Constit. of the rhizomes of *Alpinia officinarum* (lesser galangal) and *Zingiber officinale* (ginger). Needles (C_6H_6). Mp 87°. $[\alpha]_D$ +9 ($CHCl_3$). λ_{max} 227 (log ε 4.36); 281 (log ε 4.05) (EtOH).

3-Ketone, 3′,3′′-di-Me ether, 5-Ac: [718638-99-4]
$C_{23}H_{28}O_7$ 416.47
Constit. of the rhizomes of ginger (*Zingiber officinale*). Oil. $[\alpha]_D^{25}$ +3 (c, 0.6 in $CHCl_3$).

(3*RS*,5*SR*)-*form*
meso-*form*

3′,3′′-Di-Me ether: [135413-63-7]
Constit. of rhizomes of ginger (*Zingiber officinale*). Oil. λ_{max} 228 (log ε 3.81); 281 (log ε 3.48) (EtOH).

3′,3′′-Di-Me ether, 3-Ac:
$C_{23}H_{30}O_7$ 418.486
Constit. of the rhizomes of ginger (*Zingiber officinale*). Oil. $[\alpha]_D^{24}$ +6 (c, 0.56 in $CHCl_3$).

3′,3′′-Di-Me ether, 3,5-di-Ac: [135308-87-1]
Constit. of rhizomes of ginger (*Zingiber officinale*). Oil. λ_{max} 227 (sh) (log ε 3.72); 281 (log ε 3.4) (EtOH).

(3*R*,5*R*)-*form*

3,5-Di-Ac:
$C_{23}H_{28}O_8$ 432.469
Constit. of rhizomes of ginger (*Zingiber officinale*). Oil. $[\alpha]_D^{25}$ +1.5 (c, 1.3 in EtOH). Indexed incorrectly by CA. λ_{max} 223 (log ε 4.07); 283 (log ε 3.7) (EtOH).

(3ξ,5ξ)-*form*

3′-Me ether, 3,5-di-Ac:
$C_{24}H_{30}O_8$ 446.496
Constit. of rhizomes of ginger (*Zingiber officinale*). Oil. λ_{max} 225 (sh) (log ε 3.9); 282 (log ε 3.6) (EtOH).

5′-Methoxy, 3-ketone, 3′,3′′-di-Me ether: 5-Hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-3-heptanone
$C_{22}H_{28}O_7$ 404.459
Constit. of the rhizomes of *Zingiber officinale* (ginger). Not obt. pure.

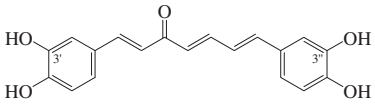
5′′-Methoxy, 3-ketone, 3′,3′′-di-Me ether: 5-Hydroxy-7-(4-hydroxy-3,5-dimethoxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-3-heptanone
$C_{22}H_{28}O_7$ 404.459
Constit. of the rhizomes of *Zingiber officinale* (ginger). Not obt. pure.

[93604-02-5]

Roughley, P.J. *et al., JCS Perkin 1*, 1973, 2379-2388 (*Tetrahydrocurcumin, synth, pmr*)
Kikuzaki, H. *et al., Chem. Pharm. Bull.*, 1991, **39**, 120-122 (*Hexahydrocurcumin, Zingiber officinale constits*)
Kikuzaki, H. *et al., Phytochemistry*, 1991, **30**, 3647-3651 (*Zingiber officinale constits*)
Yamahara, J. *et al., Yakugaku Zasshi*, 1992, **112**, 645-655 (*3′,3′′-di-Me ethers*)
Mazumder, A. *et al., J. Med. Chem.*, 1997, **40**, 3057-3063 (*Tetrahydrocurcumin, synth*)
Girija, C.R. *et al., Acta Cryst. C*, 2004, **60**, o611-o613 (*Tetrahydrocurcumin, cryst struct*)
Ma, J.P. *et al., Chin. Chem. Lett.*, 2004, **15**, 1306-1308 (*3-ketone 3′,3′′-di-Me Ac*)
Ma, J. *et al., Phytochemistry*, 2004, **65**, 1137-1143 (*Zingiber officinale constits*)
Jolad, S.D. *et al., Phytochemistry*, 2004, **65**, 1937-1954 (*Tetrahydrocurcumin, isol*)

An, N. *et al., Fitoterapia*, 2008, **79**, 27-31 (*3-ketone 3′′-Me ether*)

1,7-Bis(3,4-dihydroxyphenyl)-1,4,6-heptatrien-3-one B-186



$C_{19}H_{16}O_5$ 324.332

3′,3′′-Di-Me ether: ***1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,4,6-heptatrien-3-one***
$C_{21}H_{20}O_5$ 352.386
Constit. of the rhizomes of *Curcuma longa*. Yellow powder. Mp 128-129°. λ_{max} 267 (log ϵ 3.54); 406 (log ϵ 3.84) (MeOH).

1,2,6,7-Tetrahydro: [41137-87-5] *1,7-Bis(3,4-dihydroxyphenyl)-4-hepten-3-one.* ***Hirsutenone****. Hirsutanone (incorr.)*
$C_{19}H_{20}O_5$ 328.364
The name Hirsutanone, used in CA, is apparently incorrect.

1,2,6,7-Tetrahydro, 3′-Me ether: [138870-93-6] ***7-(3,4-Dihydroxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one***
$C_{20}H_{22}O_5$ 342.391
Constit. of the rhizomes of ginger *Zingiber officinale*. Oil. λ_{max} 222 (log ϵ 4.2); 282 (log ϵ 3.7) (EtOH).

1,2,6,7-Tetrahydro, 3′,3′′-di-Me ether: [128700-97-0] *1,7-Bis(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one.* ***Gingerenone A***
$C_{21}H_{24}O_5$ 356.418
Constit. of *Zingiber officinale* (ginger). Oil.

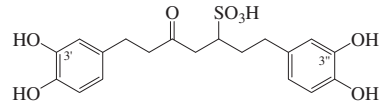
1,2,4,5,6,7-Hexahydro: 1,7-Bis(3,4-dihydroxyphenyl)-3-heptanone. ***Muricarpone B***
$C_{19}H_{22}O_5$ 330.38
Syrup.

5′-Methoxy, 1,2,6,7-tetrahydro, 3′,3′′-di-Me ether: [128700-99-2] *1-(4-Hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one.* ***Isogingerenone B***
$C_{22}H_{26}O_6$ 386.444
Constit. of *Zingiber officinale* (ginger).

5′′-Methoxy, 1,2,6,7-tetrahydro, 3′,3′′-di-Me ether: [128700-98-1] *7-(4-Hydroxy-3,5-dimethoxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-4-hepten-3-one.* ***Gingerenone B***
$C_{22}H_{26}O_6$ 386.444
Constit. of *Zingiber officinale* (ginger).

Terazawa, M. *et al., Mokuzai Gakkaishi*, 1973, **19**, 45-46 (*Hirsutenone*)
Endo, K. *et al., Phytochemistry*, 1990, **29**, 797-799 (*Gingerenones*)
Kikuzaki, H. *et al., Phytochemistry*, 1991, **30**, 3647-3651 (*tetrahydro-3′-Me ether*)
Venkateswarlu, S. *et al., Indian J. Chem., Sect. B*, 2001, **40**, 495-497 (*synth*)
Martin-Cordero, C. *et al., Phytochemistry*, 2001, **58**, 567-569 (*Hirsutenone*)
Park, S.-Y. *et al., J. Nat. Prod.*, 2002, **65**, 1227-1231 (*di-Me ether*)
Giang, P.M. *et al., Chem. Pharm. Bull.*, 2005, **54**, 139-140 (*Muricarpone B*)

1,7-Bis(3,4-dihydroxyphenyl)-5-oxo-3-heptanesulfonic acid B-187
Shogasulfonic acid C



$C_{19}H_{22}O_8S$ 410.444
Constit. of the rhizomes of *Zingiber officinale* (ginger). Pale yellow oil. $[\alpha]_D^{21}$ -5.6 (c, 0.25 in MeOH).

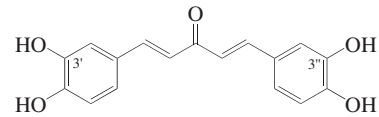
3′-Me ether: ***Shogasulfonic acid B***
$C_{20}H_{24}O_8S$ 424.471
Constit. of the rhizomes of *Zingiber officinale* (ginger). Pale green oil. $[\alpha]_D^{21}$ -1 (c, 1.6 in MeOH).

3′,3′′-Di-Me ether: 1,7-Bis(4-hydroxy-3-methoxyphenyl)-5-oxo-3-heptanesulfonic acid. ***Shogasulfonic acid A***
$C_{21}H_{26}O_8S$ 438.498
Constit. of the rhizomes of *Zingiber officinale* (ginger). Pale yellow powder. Mp 205° dec. $[\alpha]_D^{21}$ -0.5 (c, 2 in MeOH).

5′-Hydroxy, 3′,3′′-di-Me ether: ***Shogasulfonic acid D***
$C_{21}H_{26}O_9S$ 454.497
Constit. of the rhizomes of *Zingiber officinale* (ginger). Pale yellow cryst. Mp 154-158°. $[\alpha]_D^{21}$ -0.3 (c, 1 in MeOH).

Hori, Y. *et al., Phytochemistry*, 2003, **62**, 613-617 (*isol, pmr, cmr*)

1,5-Bis(3,4-dihydroxyphenyl)-1,4-pentadien-3-one B-188



$C_{17}H_{14}O_5$ 298.295

(E,E)-form

3′,3′′-Di-Me ether: [131359-25-6] *1,5-Bis(4-hydroxy-3-methoxyphenyl)-1,4-pentadien-3-one, 9CI*
$C_{19}H_{18}O_5$ 326.348
Constit. of the rhizomes of *Curcuma domestica* (turmeric). Yellow powder ($CHCl_3$/hexane). Mp 82-83°.

Tetra-Me ether: [39777-59-8] *1,5-Bis(3,4-dimethoxyphenyl)-1,4-pentadien-3-one. Diveratrylideneacetone*
$C_{21}H_{22}O_5$ 354.402
Yellow needles. Mp 83-85° (95-100°).

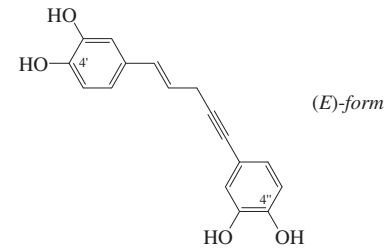
Bis(methylene ether): [614-66-4] *1,5-Bis(1,3-benzodioxol-5-yl)-1,4-pentadien-3-one, 9CI. 1,5-Bis(3,4-methylenedioxyphenyl)-1,4-pentadien-3-one*
$C_{19}H_{14}O_5$ 322.317
Mp 198-200° (185°).

3′-Deoxy, 3′′-Me ether: [148625-88-1] *1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one*
$C_{18}H_{16}O_4$ 296.322
Constit. of the rhizomes of *Curcuma domestica* (turmeric). Yellow powder ($CHCl_3$/hexane). Mp 161.5-162.5°.

[38552-39-5, 2150-50-7]

Wattanasin, S. *et al., Synthesis*, 1980, 647 (*synth*)
Masuda, T. *et al., Phytochemistry*, 1993, **32**, 1557-1560 (*isol, synth, pmr, cmr*)
Butcher, R.J. *et al., Acta Cryst. E*, 2007, **63**, o3115 (*tetra-Me ether, cryst struct*)

1,5-Bis(3,4-dihydroxyphenyl)-1-penten-4-yne B-189
4,4′-(1-Penten-4-yne-1,5-diyl)bis-1,2-benzenediol, 9CI. Rooperol [83644-00-2]



(*E*)-*form*

$C_{17}H_{14}O_4$ 282.295
Solid (EtOAc). Mp 154-156°.

Tetra-Ac: [83654-15-3]
$C_{25}H_{22}O_8$ 450.444
Unstable oil.

Tetra-Me ether: [96851-31-9]
$C_{21}H_{22}O_4$ 338.402
Pale yellow liq.

4′-O-β-D-Glucopyranoside: [125187-33-9] ***Obtuside A***
$C_{23}H_{24}O_9$ 444.437
Cryst. (EtOAc). $[\alpha]_D^{20}$ -43 (c, 0.4 in MeOH).

4′′-O-β-D-Glucopyranoside: [125187-34-0] ***Obtuside B***
Brown powder. $[\alpha]_D^{20}$ -59 (c, 0.5 in MeOH).

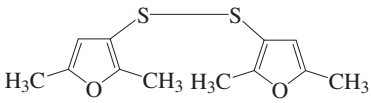
4,4′-Di-O-β-D-glucopyranoside: [83643-94-1] ***Hypoxoside***
$C_{29}H_{34}O_{14}$ 606.579
Isol. from *Hypoxis hemerocallidea* (African potato) corms. Cryst. (EtOH). Sol. MeOH, butanol. Mp 149-151°. $[\alpha]_D^{20}$ -73.5 (c, 0.9 in MeOH). λ_{max} 247; 257; 287 (MeOH) (Berdy).
▶ LD_{50} (mus, ipr) 1000 - 2000 mg/kg.

Marini-Bettolo, G.B. *et al., Tetrahedron*, 1982, **38**, 1683 (*isol, ms, pmr, cmr, derivs*)
Drewes, S. *et al., Phytochemistry*, 1984, **23**, 1313; 1988, **27**, 1101; 1989, **28**, 153 (*synth, ir, cmr, pmr*)
US Pat., 1987, 4 644 085 (*props*)
Galeffi, C. *et al., Planta Med.*, 1989, **55**, 318 (*monoglucosides, uv, pmr*)

Nair, V.D.P. *et al., J. Agric. Food Chem.*, 2006, **54**, 2816-2821 (*Hypoxoside, isol*)

Bis(2,5-dimethyl-3-furanyl) disulfide B-190

3,3′-Dithiobis[2,5-dimethylfuran], 9CI, 8CI. FEMA 3476 [28588-73-0]



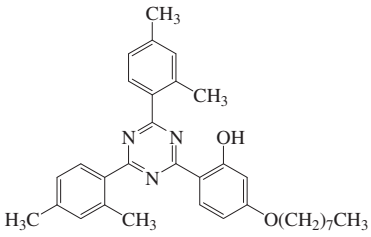
$C_{12}H_{14}O_2S_2$ 254.373

Synthetic meat flavouring agent. Yellow liq.

US Pat., 1977, 4 020 175 (*synth, use*)
Huber, U.A. *et al., Helv. Chim. Acta*, 1993, **76**, 2528-2536 (*synth, pmr*)

2-[4,6-Bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-5-(octyloxy)-phenol, 9CI B-191

2-[4,6-Di-(2,4-xylyl)-s-triazin-2-yl]-5-(octyloxy)phenol, 8CI. Cysorb UV-1164 [2725-22-6]



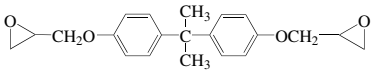
$C_{33}H_{39}N_3O_2$ 509.69

FDA permitted light stabiliser for food-contact olefinic polymers. Mp 83.5-84°.

Swiss Pat., 1969, 480 091 (*use, synth*)
Carrott, M.J. *et al., Analyst (London)*, 1998, **123**, 1827-1833 (*detn, ms*)
Fed. Regist., 2000, **65**, 26 746-26 747 (*use*)

2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane, 8CI B-192

2,2′-[(1-Methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane, 9CI. 2,2-[Bis(4-glycidyloxyphenyl)]propane. Bisphenol A diglycidyl ether. DGEBA. BADGE [1675-54-3]



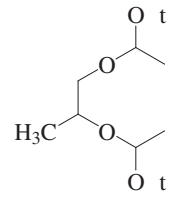
$C_{21}H_{24}O_4$ 340.418

Potential food contaminant arising from its use in epoxy resin coatings for cans, concrete vats and tanks, etc. d^{21} 1.16. Mp 43°. $Bp_{0.75}$ 225-249° (lit quotes a pressure range). n_D^{20} 1.5703.

Bring, A. *et al., Chem. Listy*, 1956, **50**, 1198-1199 (*synth*)
Rozentuler, S.M. *et al., Zh. Prikl. Khim.*, 1973, **46**, 2731-2734 (*synth*)
Sorokin, V.P. *et al., Polimery (Warsaw)*, 1977, **22**, 315-316 (*synth*)
Lin, S.C. *et al., J. Polym. Sci., Polym. Chem. Ed.*, 1979, **17**, 3095-3119 (*synth*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **9**, 730-755 (*rev*)
Chem. Technol. Epoxy Resins, 1993, (ed. Ellis, B.), Blackie, 1993, (*rev*)
Losada, P.P. *et al., J. Agric. Food Chem.*, 1997, **45**, 3493-3500 (*anal, bibl*)

1,2-Bis(1-ethoxyethoxy)propane B-193

4,6,9-Trimethyl-3,5,8,10-tetraoxadodecane. FEMA 3534 [67715-79-1]



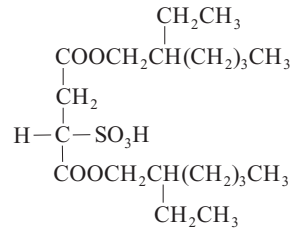
$C_{11}H_{24}O_4$ 220.308

Flavouring agent and adjuvant. Aldehyde generator used for enhancing the flavour of orange drinks. Liq. d_4^{25} 0.92. $Bp_{0.04}$ 47°. n_D^{20} 1.4112. Hydrolyses to acetaldehyde under aq. acidic conditions.

Oser, B.L. *et al., Food Technol. (Chicago)*, 1978, **32**, 60-62; **32(2)**, 64-66; 68-70 (*use*)
US Pat., 1981, 4 280 011 (*synth, use*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 411 (*use*)

1,4-Bis(2-ethylhexyl) sulfosuccinate, 8CI B-194

1,4-Bis(2-ethylhexyl) sulfobutanedioate, 9CI [10041-19-7]



$C_{20}H_{38}O_7S$ 422.582

Log P 6.12 (uncertain value) (calc).

Na salt: [577-11-7] ***Docusate sodium, BAN, INN****. Dioctyl sodium sulfosuccinate. Complemix. Dulcodos. Dyoctol. Klyx. Milkinol. Molcer. Nonit. Normax. Soliwax. Solovet. Waxsol. Willoderm. Alcopol O. Gemtex SC. Humifen WT 27G. Karawet DOSS. Lankropol KO 2. Pelex OT. Vatsol OT. Warcowet 060. Wetaid SR. Many other names*

Anionic surfactant used as wetting/dispersing/emulsifying agent in food processing. Hog/poultry scald agent. Used in cheeses, salad dressings, cocoa and dairy products. Waxy solid. Sol. H_2O, org. solvs. Doubtless a mixt. of diastereoisomers.

▶ Skin and severe eye irritant. LD_{50} (rat, orl) 1900 mg/kg. WN0525000

[128-49-4, 7491-09-0]

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 799A (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 897D (*ir*)
Averbakh, K.O. *et al., Zh. Prikl. Khim.*, 1968, **41**, 2307 (*synth*)
Koenig, H. *et al., Fresenius' Z. Anal. Chem.*, 1970, **251**, 225 (*nmr*)
Ahuja, S. *et al., Anal. Profiles Drug Subst.*, 1973, **2**, 199; 1983, **12**, 713 (*revs*)
Nelan, A.A.M. *et al., Bull. Soc. Chim. Belg.*, 1979, **8**, 31 (*synth, props*)
Moriarty, K.J. *et al., Gut*, 1985, **26**, 1008 (*pharmacol*)
Negwer, M. *et al., Organic-Chemical Drugs and their Synonyms, 6th edn., Akademie-Verlag*, 1987, 6012 (*synonyms*)
Handbook of Pharmaceutical Excipients, 2nd edn., (eds. Wade, A. *et al*), American Pharmaceutical Association/Pharmaceutical Press, 1994, 173-175
Martindale, The Extra Pharmacopoeia, 31st edn., Pharmaceutical Press, 1996, 1216
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 883-887 (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DJL000

Bis(2-ethylhexyl)phthalate esterase B-195

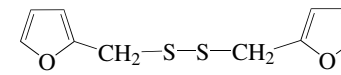
E.C. 3.1.1.60. Bis(2-ethylhexyl)phthalate acylhydrolase. DEHP esterase [92480-02-9]

Carboxylic ester hydrolase enzyme. Isol. from wheat. Also acts on 4-nitrophenyl esters (C_6-C_8). Purified wheat enzyme at 4° has $t_{1/2}$ of 1 day.

Krell, H.W. *et al., Eur. J. Biochem.*, 1984, **143**, 57-62 (*wheat*)
Krell, H.W. *et al., J. Agric. Food Chem.*, 1986, **34**, 194-198 (*wheat*)

Bis(2-furanylmethyl) disulfide B-196

2,2′-[Dithiobis(methylene)]bisfuran, 9CI. 2,2′-(Dithiodimethylene)difuran. Difurfuryl disulfide. Furfuryl disulfide. FEMA 3146 [4437-20-1]



$C_{10}H_{10}O_2S_2$ 226.32

Flavour component of roasted coffee, roasted sesame seeds and cooked meats. Flavouring ingredient. Liq. with a powerful sulfide aroma. d 1.23. Mp 10-11°. $Bp_{0.5}$ 112-115°.

Tressl, R. *et al., J. Agric. Food Chem.*, 1981, **29**, 1078-1082 (*occur*)
Gasser, U. *et al., Z. Lebensm.-Unters. -Forsch.*, 1988, **186**, 489-494; 1990, **190**, 3-8 (*occur*)
Nakamura, S. *et al., Agric. Biol. Chem.*, 1989, **53**, 1891-1899 (*occur*)
Firouzabadi, H. *et al., Bull. Chem. Soc. Jpn.*, 1992, **65**, 1131-1134 (*synth*)
Choi, J. *et al., JOC*, 1995, **60**, 3266-3267 (*synth*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 898-899
Iranpoor, N. *et al., Synthesis*, 1999, 49-50 (*synth*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 524 (*use*)

Bis(2-furanylmethyl) sulfide B-197

2,2′-(Thiodimethylene)difuran, 9CI. Furfuryl sulfide. Difurfuryl sulfide. FEMA 3238 [13678-67-6]

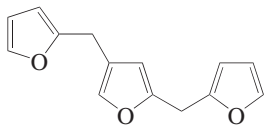
$C_{10}H_{10}O_2S$ 194.254
Present in coffee. Flavouring ingredient. Mp 31-32°. Bp_{14} 135-143°. n_D^{20} 1.5560.

S,S-*Dioxide:* [186685-62-1] *Bis(2-furanylmethyl) sulfone*
$C_{10}H_{10}O_4S$ 226.253
Cryst. Mp 72°.

Stoll, M. *et al., Helv. Chim. Acta*, 1967, **50**, 628 (*synth, ir, ms*)
Gol'dfarb, Ya.L. *et al., Izv. Akad. Nauk SSSR, Ser. Khim.*, 1967, 2509; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1967, 2387 (*synth*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2780
Rozen, S. *et al., JOC*, 1997, **62**, 1457-1462 (*dioxide*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1902 (*use*)

2,4-Bis(2-furanylmethyl)furan B-198

2,4-Difurfurylfuran. FEMA 4095 [64280-32-6]

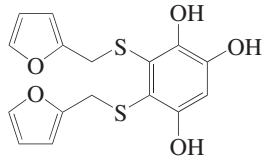


$C_{14}H_{12}O_3$ 228.247
Tentatively identified in licorice. Flavouring agent. Solid with floral, fruity odour. Mp 153°.

Frattini, C. *et al., J. Agric. Food Chem.*, 1977, **25**, 1238-1241 (*FEMA 4095, occur, glc*)
The Good Scents Company, (*FEMA 4095, use*)

5,6-Bis[(2-furanylmethyl)thio]-1,2,4-benzenetriol, 9CI B-199

5,6-Bis[(2-furanylmethyl)thio]-2-hydroxyhydroquinone [923267-64-5]

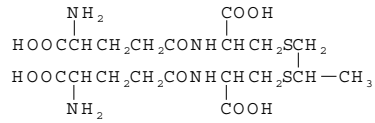


$C_{16}H_{14}O_5S_2$ 350.416
Constit. of brewed coffee. No phys. props. reported.

Mueller, C. *et al., J. Agric. Food Chem.*, 2006, **54**, 10076-10085; 2007, **55**, 4095-4102 (*isol, synth, pmr, cmr*)

N,N′-Bis(γ-glutamyl)-3,3′-(1,2-propylenedithio)dialanine B-200

N,N′-*[Propylenebis[thio(1-carboxyethylene)]]diglutamine*

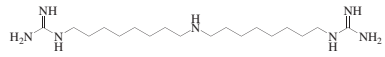


$C_{19}H_{32}N_4O_{10}S_2$ 540.615
Constit. of chives (*Allium schoenoprasum*). Cryst. (Me_2CO aq.).

Matikkala, E.J. *et al., Acta Chem. Scand.*, 1963, **17**, 1799 (*isol*)

Bis(8-guanidinooctyl)amine B-201

N,N‴-*(Iminodi-8,1-octanediyl)bisguanidine, 9CI. Iminoctadine* [13516-27-3]



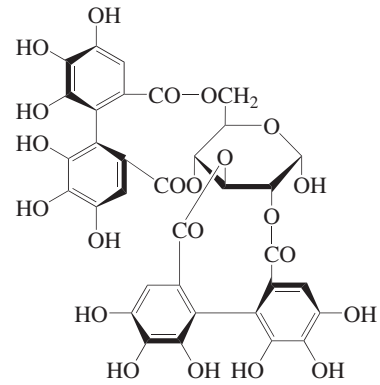
$C_{18}H_{41}N_7$ 355.569
Agricultural fungicide. Component of Guazatine, BSI.

▶ MF3624100

Acetate (1:3): [57520-17-9] *Panoctine* [39202-40-9]
Agricultural fungicide. Cryst. Sol. H_2O. Mp 140°.

▶ LD_{50} (rat, orl) 300 mg/kg. MF3624000
UK Pat., 1964, 1 114 155
Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A223
Pesticide Manual, 13th edn., 2003, 422; 459
Dreassi, E. *et al., J. Agric. Food Chem.*, 2007, **55**, 6850-6856 (*detn, hplc, ms*)

2,3:4,6-Bis(hexahydroxydiphenoyl)glucose B-202



$C_{34}H_{24}O_{22}$ 784.55

(*S,S*)$_{axial}$-*form* [7045-42-3]
Pedunculagin. *Juglanin*†
Amorph. sandy solid. $[\alpha]_D^{25}$ +106 (c, 2 in MeOH). Isol. as an equilibrated mixt. of α- and β-anomers.

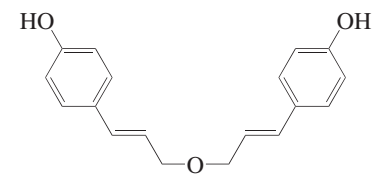
(*S,S*)$_{axial}$-α-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [82262-94-0] *1*-O-*Galloyl-2,3;4,6-bis-(S)-hexahydroxydiphenoyl-α-D-glucopyranose.* ***Potentillin***
$C_{41}H_{28}O_{26}$ 936.657
Isol. from *Rubus* spp. Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{20}$ +108 (c, 0.7 in EtOH). λ_{max} 222 (ε 64600); 258 (ε 35500) (MeOH) (Derep).

(*S,S*)$_{axial}$-β-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [79786-00-8] *1*-O-*Galloyl-2,3;4,6-bis-(S)-hexahydroxydiphenoyl-β-D-glucopyranose.* ***Casuarictin***. *1*-O-*Galloylpedunculagin*
$C_{41}H_{28}O_{26}$ 936.657
Isol. from *Corylus heterophylla* (Siberian filbert), blackberry and raspberry. Off-white amorph. powder + $6H_2O$ or light brown amorph. powder + $1H_2O$. $[\alpha]_D^{20}$ +35 (c, 0.2 in MeOH).

(2,3-*R*:4,6-*S*)$_{axial}$-β-D-pyranose-*form*
1-O-*(3,4,5-Trihydroxybenzoyl):* [121153-23-9] *1*-O-*Galloyl-2,3(R)-4,6(S)-bis(hexahydroxydiphenoyl)-β-D-glucopyranose.* ***Cuspinin***
$C_{41}H_{28}O_{26}$ 936.657
Off-white amorph. powder + $5H_2O$. $[\alpha]_D^{24}$ -18.2 (c, 0.9 in Me_2CO).

Schmidt, O.T. *et al., Annalen*, 1965, **690**, 150-162 (*Pedunculagin*)
Gupta, R.K. *et al., JCS Perkin 1*, 1982, 2525-2534 (*galloyl derivs*)
Okuda, T. *et al., JCS Perkin 1*, 1983, 1765-1772 (*ir, uv, cd, pmr, cmr*)
Okuda, T. *et al., Chem. Pharm. Bull.*, 1984, **32**, 2165-2173 (*Potentillin*)
Nonaka, G. *et al., Chem. Pharm. Bull.*, 1989, **37**, 50-53 (*Cuspinin*)
Ishimatea, M. *et al., Phytochemistry*, 1989, **28**, 3179-3184 (*1-Galloylpedunculagin*)
Feldman, K.S. *et al., JOC*, 1996, **61**, 2606-2612 (*Pedunculagin, synth, pmr, cmr*)
Lee, S.-H. *et al., Yakhak Hoechi*, 1997, **41**, 524-529 (*activity*)
Khanbabaee, K. *et al., Eur. J. Org. Chem.*, 2003, 2128-2131 (*synth*)

Bis(4-hydroxycinnamyl) ether B-203



$C_{18}H_{18}O_3$ 282.338

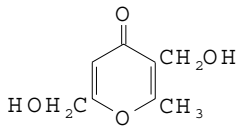
(*E,E*)-*form*
Di-Ac: [1179522-35-0] *Bis(4-acetoxycinnamyl) ether*
$C_{22}H_{22}O_5$ 366.413
Constit. of the rhizomes of *Alpinia*

galanga (greater galangal). Powder. Mp 92.5°. λ_{max} 203 (log ϵ 4.2); 255 (log ϵ 3.9) (MeOH).

Zhu, X.-L. *et al., Chin. J. Nat. Med.*, 2009, **7**, 19-20 (*Alpinia galanga ether*)

3,6-Bis(hydroxymethyl)-2-methyl-4*H*-pyran-4-one B-204

Herierin III [131123-56-3]



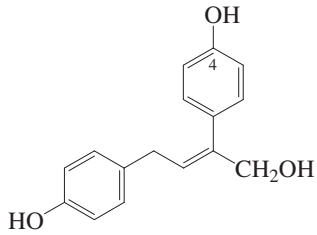
$C_8H_{10}O_4$ 170.165

Constit. of *Hericium erinaceum* (lions mane). Cryst. Mp 122-123°.

Qian, F. *et al., Yaoxue Xuebao*, 1990, **25**, 522-525 (*isol, pmr*)

2,4-Bis(4-hydroxyphenyl)-2-buten-1-ol B-205

4,4′,9-Trihydroxy-7,9′-dinorlign-8(8′)-ene



$C_{16}H_{16}O_3$ 256.301

7,9′-Dinorlignan.

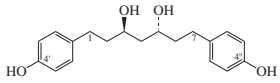
(E)-form

4-O-β-D-Glucopyranoside: ***Squadinorlignoside***
$C_{22}H_{26}O_8$ 418.443
Constit. of the stems of *Annona squamosa* (sugar apple). Syrup. λ_{max} 195; 225 (sh); 274 (MeCN).

Yang, Y.-L. *et al., Helv. Chim. Acta*, 2005, **88**, 2731-2737 (*isol, pmr, cmr*)

1,7-Bis(4-hydroxyphenyl)-3,5-heptanediol, 9CI B-206

Hannokinol [79120-40-4]



(3*R*,5*R*)-*form*

$C_{19}H_{24}O_4$ 316.396

Evidence for abs. config. various isolates of Hannokinol and its derivs. is incomplete and sometimes contradictory.

(3R,5R)-form [408324-76-5]

Isol. from *Amomum tsao-ko* (tsao-ko) fruits. $[\alpha]_D$ +4 (c, 0.10 in MeOH). $[\alpha]_D$ +11.4 (c, 0.38 in MeOH). λ_{max} 279 (log ϵ 3.5) (MeOH).

4′-Deoxy: [112494-44-7] ***1-(4-Hydroxyphenyl)-7-phenyl-3,5-heptanediol***
$C_{19}H_{24}O_3$ 300.397
Constit. of *Alpinia officinarum* (lesser galangal). Needles. Mp 109-111°. $[\alpha]_D$ +8.3 (c, 0.4 in $CHCl_3$). λ_{max} 215 (ϵ 8000); 225 (ϵ 8500); 275 (ϵ 1500) (EtOH).

(3RS,5SR)-form [79055-11-1]

meso-*form*

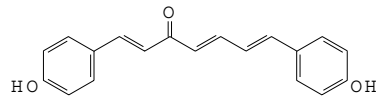
Isol. from *Amomum tsao-ko* (tsao-ko) fruits. Oil.

[56973-64-9]

Uehara, S. *et al., Chem. Pharm. Bull.*, 1987, **35**, 3298-3304 (*4′-deoxy*)

Martin, T.S. *et al., J. Am. Oil Chem. Soc.*, 2000, **77**, 667-673 (*Amomum tsao-ko constits*)

1,7-Bis(4-hydroxyphenyl)-1,4,6-heptatrien-3-one B-207



$C_{19}H_{16}O_3$ 292.334

(all-E)-form [149732-52-5]

Constit. of the rhizomes of *Curcuma domestica* (turmeric) and *Etlingera elatior*. Yellow powder. λ_{max} 245 (log ϵ 4.06); 395 (log ϵ 4.58) (EtOH).

1,2,4,5-Tetrahydro: [1251830-57-5] *1,7-Bis(4-hydroxyphenyl)-6-hepten-3-one*
$C_{19}H_{20}O_3$ 296.365
Yellowish oil. λ_{max} 201 (log ϵ 4.86); 262 (log ϵ 3.05) (MeOH).

Hexahydro: [130233-83-9] *1,7-Bis(4-hydroxyphenyl)-3-heptanone.* ***Acerogenin G***
$C_{19}H_{22}O_3$ 298.381
Amorph. powder.

Hexahydro, 4′′-O-β-D-glucopyranoside: [130233-82-8] ***Aceroside X***
$C_{25}H_{32}O_8$ 460.523
Needles. Mp 120-121°. $[\alpha]_D^{21}$ -29.7 (c, 1 in EtOH).

Hexahydro, 4′′-O-[β-D-apiofuranosyl-(1→6)-β-D-glucopyranoside]: [130233-81-7] ***Aceroside IX***
$C_{30}H_{40}O_{12}$ 592.639
Amorph. powder. $[\alpha]_D$ -63.5 (c, 1 in EtOH).

Nagai, M. *et al., Chem. Pharm. Bull.*, 1990, **38**, 1506-1508 (*Acerosides*)

Nakayama, R. *et al., Phytochemistry*, 1993, **33**, 501-502 (*isol, pmr*)

Inoue, T. *et al., Yakugaku Zasshi*, 1993, **113**, 181-197 (*rev*)

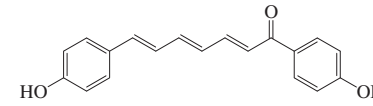
Bae, C.-I. *et al., Yakhak Hoechi*, 1997, **41**, 559-564 (*isol, activity*)

Jang, M.K. *et al., Arch. Pharmacal Res.*, 2004, **27**, 1220-1225 (*isol, pmr, cmr*)

Mohamad, H. *et al., J. Nat. Prod.*, 2005, **68**, 285-288 (*isol*)

Li, J. *et al., J. Nat. Prod.*, 2010, **73**, 1667-1671 (*Bis-4-hydroxyphenyl-6-hepten-3-one*)

1,7-Bis(4-hydroxyphenyl)-2,4,6-heptatrien-1-one B-208



$C_{19}H_{16}O_3$ 292.334

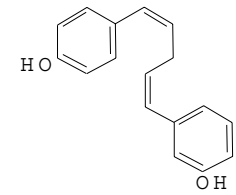
(all-E)-form

Constit. of the rhizomes of *Etlingera elatior* (torch ginger). Yellow powder. λ_{max} 395 (log ϵ 4.51) (MeOH).

Mohamad, H. *et al., J. Nat. Prod.*, 2005, **68**, 285-288 (*isol, pmr, cmr*)

1,5-Bis(4-hydroxyphenyl)-1,4-pentadiene B-209

*Di-(*p*-hydroxystyryl)methane*



$C_{17}H_{16}O_2$ 252.312

(1Z,4Z)-form

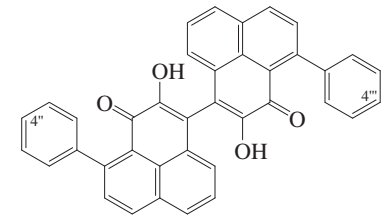
Constit. of *Alpinia galanga* (greater galangal) rhizomes.

Di-Ac:
Cryst. (C_6H_6/petrol). Mp 140-142°.

Barik, B.R. *et al., Phytochemistry*, 1987, **26**, 2126,

3,3′-Bis[2-hydroxy-9-phenyl-1*H*-phenalen-1-one] B-210

*2,2′-Dihydroxy-9,9′-diphenyl-[3,3′-bi-1*H*-phenalene]-1,1′-dione, 9CI.* ***3,3′-Bisanigorufone***



$C_{38}H_{22}O_4$ 542.589

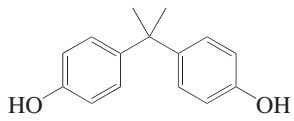
Constit. of the rhizomes of *Musa acuminata* (dwarf banana). Orange solid.

4′′,4′′′-Dihydroxy: [190372-82-8] *2,2′-Dihydroxy-9,9′-bis(4-hydroxyphenyl)-[3,3′-bi-1*H*-phenalene]-1,1′-dione. 3,3′-Bis[2-hydroxy-9-(4-hydroxyphenyl)-1*H*-phenalen-1-one].* ***3,3′-Bis(4′′-hydroxyanigorufone)***
$C_{38}H_{22}O_6$ 574.588
Constit. of *Musa acuminata* (dwarf banana). Orange-red cryst. (EtOH). Mp 205-210°. λ_{max} 215; 244; 274; 310; 369; 429 (MeOH).

Hoelscher, D. *et al., Phytochemistry*, 1997, **45**, 87-91 (*4′′,4′′′-dihydroxy*)
Otalvaro, F. *et al., Phytochemistry*, 2002, **60**, 61-66 (*isol, pmr, cmr*)

2,2′-Bis(4-hydroxyphenyl)-propane B-211

4,4′-(1-Methylethylidene)bisphenol, 9CI. 4,4′-Isopropylidenediphenol, 8CI. 1,1′-(1-Methylethylidene)bisphenylol, 9CI. Diphenylolpropane. Bisphenol A. Dian. Ipognox 88. Parabis. BPA [80-05-7]



$C_{15}H_{16}O_2$ 228.29
Potential food contaminant arising from its use in reusable polycarbonate food containers such as water carboys and kitchen utensils and as a coating for metal food containers. Banned in the EU for use in baby bottles. Sol. EtOH; sl. sol. CCl_4; insol. H_2O. Mp 156-157°. Bp_{13} 250-252°.

▶ Skin and eye irritant. LD_{50} (rat, orl) 3250 mg/kg. Exp. reprod. and teratogenic effects. SL6300000

Di-Ac: [10192-62-8]
$C_{19}H_{20}O_4$ 312.365
Cryst. Mp 79.5-81.5°.

Bis(2-methyl-2-propenoyl): [3253-39-2] *Bisphenol A dimethacrylate*
$C_{23}H_{24}O_4$ 364.44
Mp 72-74°.

Dibenzoyl: [2297-14-5]
$C_{29}H_{24}O_4$ 436.506
Cryst. (EtOH). Mp 153.5°.

Di-Me ether: [1568-83-8] *2,2-Bis(4-methoxyphenyl)propane*
$C_{17}H_{20}O_2$ 256.344
Mp 59-61.5°. Bp_5 190°.

Di-Et ether: [16079-00-8] *2,2-Bis(4-ethoxyphenyl)propane*
$C_{19}H_{24}O_2$ 284.397
Mp 49-50°.

Bis(1,1,2,2-tetrafluoroethyl) ether: [1544-19-0] *1,1′-(1-Methylethylidene)bis[4-(1,1,2,2-tetrafluoroethoxy)benzene]*
$C_{19}H_{16}F_8O_2$ 428.321
$Bp_{0.9}$ 136°. n_D^{25} 1.4640.

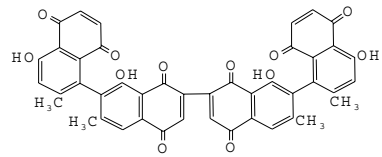
Di-2-propenyl ether: [3739-67-1] *1,1′-(1-Methylethylidene)bis[4-(2-propenyloxy)benzene]. 2,2-Bis(*p*-allyloxy)phenylpropane*
$C_{21}H_{24}O_2$ 308.419
Bp_5 120-125°. n_D^{20} 1.5648.

Bis(oxiranylmethyl) ether: see 2,2-Bis[4-(2,3-epoxypropoxy)phenyl]propane, B-192

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1119A; **2**, 316B (*ir, dipropenoyl*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 322C; 1296C (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1046A (*ir*)
v. Braun, J. *et al., Annalen*, 1929, **472**, 1 (*synth*)
England, D.C. *et al., JACS*, 1960, **82**, 5116 (*bis(tetrafluoroethyl) ether*)
UK Pat., 1963, 923 774 (*di-2-propenyl ether*)
Takenaka, J. *et al., Kogyo Kagaku Zasshi*, 1967, **70**, 2081 (*synth*)
Bilik, I.M. *et al., Zh. Prikl. Khim.*, 1967, **40**, 636 (*synth*)
Encyclopedia of Polymer Science and Engineering, 2nd edn., Wiley-Interscience, New York, 1986, **6**, 322; 1988, **11**, 648 (*rev, polymers*)
Hileman, B. *et al., Chem. Eng. News*, March 24, 1997, 37 (*rev, tox*)
Biles, J.E. *et al., J. Agric. Food Chem.*, 1997, **45**, 3541-3544 (*anal*)
Portada, T. *et al., Acta Cryst. E*, 2008, **64**, o262 (*dibenzoyl, synth, cryst struct*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BLD500

Bisisodiospyrin B-212

[30276-87-0]



$C_{44}H_{26}O_{12}$ 746.682
Constit. of roots of *Diospyros lotus* (date plum). Orange prisms. Mp 320°. $[\alpha]_D^{21}$ -678 (c, 0.14 in $CHCl_3$). λ_{max} 257 (log ϵ 4.69) and 444 nm (4.25).

Tetra-Me ether: Mp 223° dec.

Natori, S. *et al., Chem. Pharm. Bull.*, 1971, **19**, 2308; 2314 (*isol, struct*)
van der Vijver, L.M. *et al., Phytochemistry*, 1974, **13**, 2322 (*isol*)
Lillie, T.J. *et al., JCS Perkin 1*, 1977, 355 (*struct*)

Bis(4-isothiocyanatobutyl) disulfide B-213

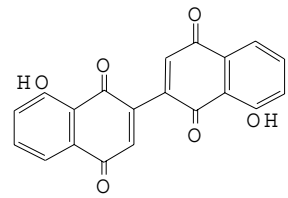
Isothiocyanic acid dithiobis(tetramethylene) ester, 9CI [18729-71-0]

$SCN(CH_2)_4–S–S–(CH_2)_4NCS$
$C_{10}H_{16}N_2S_4$ 292.514
Constit. of salad rocket (*Eruca sativa*). Thick yellow oil.

Vinkler, E. *et al., Acta Pharm. Hung.*, 1968, **38**, 6-14 (*synth*)
Cerny, M.S. *et al., J. Agric. Food Chem.*, 1996, **44**, 3835-3839 (*isol, nmr, ms, synth*)

3,3′-Bisjuglone B-214

8,8′-Dihydroxy[2,2′-binaphthalene]-1,1′,4,4′-tetrone, 9CI. 3,3′-Bijuglone [61836-43-9]

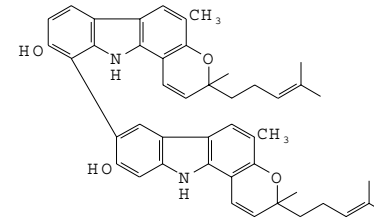


$C_{20}H_{10}O_6$ 346.295
Constit. of *Juglans regia* (walnut). Orange cryst. (C_6H_6). Mp 270° dec.

Babu, M.H. *et al., Phytochemistry*, 1978, **17**, 2042-2043 (*isol, uv, ir, ms, struct*)
Laatsch, H. *et al., Annalen*, 1980, 1321-1347 (*synth*)
Tanoue, Y. *et al., Tetrahedron*, 2002, **58**, 99-104 (*synth, pmr, cmr*)

Bismahanine B-215

[155519-87-2]

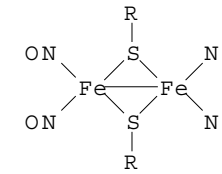


$C_{46}H_{48}N_2O_4$ 692.896
Alkaloid from the stem bark of *Murraya koenigii* (curryleaf tree). Oil. λ_{max} 224 (log ϵ 4.75); 245 (log ϵ 4.78); 298 (log ϵ 4.69); 331 (log ϵ 4.2); 342 (sh) (log ϵ 4.18); 359 (sh) (log ϵ 4.05) (MeOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096-2100 (*Bismahanine*)
Tachibana, Y. *et al., J. Agric. Food Chem.*, 2003, **51**, 6461-6467 (*Murraya koenigii constits, activity*)

Bis(μ-methanethiolato)tetranitrosyldiiron, 10CI B-216

Bis(μ-methylthio)tetranitrosyldiiron. Roussin's red methyl ester. Roussin's red [16071-96-8]



R = Me

$C_2H_6Fe_2N_4O_4S_2$ 325.92
Exists as an interconverting mixt. of *syn* and *anti* isomers in soln. Isol. from pickled vegetables consumed in Linxian, China. Fine red-brown or red-black needles (pentane). Mp 92-93° (88-89°). Ir ν_{NO} 1780vs, 1755vs cm^{-1} ($CHCl_3$).

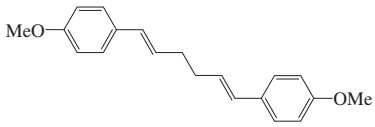
▶ Carcinogenic. NO4740000

[88643-72-5, 88643-17-8]

Li, M.-H. *et al., CA*, 1981, **94**, 25956; 18661; 133390 (*isol, tox*)
Beck, W. *et al., Chem. Ber.*, 1981, **114**, 3184 (*synth, ir, pmr*)
Seyferth, D. *et al., Organometallics*, 1986, **5**, 539 (*synth, pmr, cmr, ir, ms*)
Glidewell, C. *et al., Polyhedron*, 1988, **7**, 1371 (*reactions, epr*)
Liu, J. *et al., Carcinogenesis (London)*, 1989, **10**, 617-620 (*isol, tox*)

1,6-Bis(4-methoxyphenyl)-1,5-hexadiene B-217

1,1′-(1,5-Hexadiene-1,6-diyl)bis[4-methoxybenzene], 9CI. ***Ocimin***



$C_{20}H_{22}O_2$ 294.393

(E,E)-form [72448-90-9]

Neolignan from essential oil of *Ocimum americanum* (wild basil). Fluorescent flakes (EtOAc). Mp 170-171°.

Thappa, R.K. *et al., Phytochemistry*, 1979, **18**, 1242
Desai, D.G. *et al., Indian J. Chem., Sect. B*, 1982, **21**, 491 (*synth*)
Khasnis, D.S. *et al., Org. Prep. Proced. Int.*, 1991, **23**, 126 (*synth*)
Ornelas, M.A. *et al., Synth. Commun.*, 1999, **29**, 1401-1403 (*synth*)
Kadam, A.J. *et al., Indian J. Chem., Sect. B*, 2000, **39**, 628 (*synth*)

Bis(3-methylbutyl) disulfide B-218

Dithiobis[3-methylbutane]. Isopentyl disulfide, 8CI. Diisopentyl disulfide. Di(3-methylbutyl) disulfide. Isoamyl disulfide. FEMA 4575 [2051-04-9]

$(H_3C)_2CHCH_2CH_2$-S-S-$CH_2CH_2CH(CH_3)_2$

$C_{10}H_{22}S_2$ 206.416

Flavouring ingredient. Liq. with onion-like odour. Bp 250° Bp_{12} 123.5-124°.

Decker, Q.W. *et al., JOC*, 1957, **22**, 145 (*synth, uv*)
Chorbadjiev, S. *et al., J. Prakt. Chem.*, 1977, **319**, 1036 (*synth*)
Gupta, D. *et al., Can. J. Chem.*, 1981, **59**, 543 (*ms*)
Andersen, K.K. *et al., Tetrahedron*, 1982, **38**, 1965 (*occur*)
Wood, W.F. *et al., J. Chem. Ecol.*, 1991, **17**, 1415 (*occur*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*use*)

Bis(3-methylbutyl) trisulfide, CAS B-219

Diisoamyl trisulfide. Diisopentyl trisulfide. FEMA 4580 [955371-64-9]

$(H_3C)_2CHCH_2CH_2$-S-S-S-$CH_2CH_2CH(CH_3)_2$

$C_{10}H_{22}S_3$ 238.482

Flavouring ingredient. Liq. with sulfurous, garlic odour. Bp_1 89-91°.

US Pat., 1961, 3 013 970 (*FEMA 4580, use*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*FEMA 4580, use*)

Bis(methyldithio)methane B-220

2,3,5,6-Tetrathiaheptane. Methylenebis[methyl disulfide] [103439-78-7]

MeS-S-CH_2-S-SMe

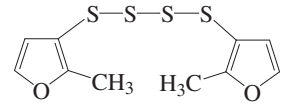
$C_3H_8S_4$ 172.36

Constit. of the mushroom *Lentinus edodes* (shiitake).

Chen, C.C. *et al., J. Agric. Food Chem.*, 1986, **34**, 830-833 (*isol, ms*)
Barbosa, L.C.A. *et al., Fitoterapia*, 1999, **70**, 152-156 (*isol*)

Bis(2-methyl-3-furanyl)tetrasulfide B-221

3,3′-Tetrathiobis[2-methylfuran], 9CI, 8CI. FEMA 3260 [28588-76-3]



$C_{10}H_{10}O_2S_4$ 290.452

Flavouring agent for meat products and baked goods. No phys. props. reported.

US Pat., 1977, 4 020 175 (*synth, use*)
Moran, E.J. *et al., Drug Chem. Toxicol.*, 1980, **3**, 249-258 (*tox*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1276 (*use*)

Bis(1-methylpropyl) disulfide, 9CI B-222

sec-*Butyl disulfide, 8CI. Di*-sec-*butyl disulfide. FEMA 4578* [5943-30-6] [91840-98-1]

$H_3CCH_2CH(CH_3)SSCH(CH_3)CH_2CH_3$

$C_8H_{18}S_2$ 178.362

Flavouring ingredient. Liq. with strong odour. Bp_{12} 120°.

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 431B (*nmr*)
Aldrich Library of Infrared Spectra, 3rd edn., 1981, 158C (*ir*)
Lanum, W.J. *et al., J. Chem. Eng. Data*, 1969, **14**, 93 (*ms, ir, props*)
Cohen, V.I. *et al., Helv. Chim. Acta*, 1976, **59**, 840 (*synth*)
Rajanikanth, B. *et al., Phytochemistry*, 1984, **23**, 899-900 (*isol, ms*)
Min, Z. *et al., Planta Med.*, 1987, **53**, 300-302 (*isol*)
The Good Scents Company, http://www.thegoodscentscompany.com/search.html (*use*)

Bis(methylthio) selenide B-223

SeS-*Methyl methanesulfeno(selenothioperoxoate), 13CI. [Selenobis(thio)]bismethane, 9CI. 2,4-Dithia-3-selenapentane* [41884-44-0]

Me–S–Se–S–Me

$C_2H_6S_2Se$ 173.161

Constit. of *Allium* sp.

Cai, X.-J. *et al., J. Agric. Food Chem.*, 1994, **42**, 2081 (*occur*)

Bis(methylthio)methane, 9CI B-224

Bismethylmercaptomethane. Formaldehyde dimethylmercaptal. 2,4-Dithiapentane. Truffle sulfide. FEMA 3878 [1618-26-4]

$MeSCH_2SMe$

$C_3H_8S_2$ 108.228

Odorous constit. of white truffle (*Tuber magnatum*); volatile component of some cheeses and boiled beef aroma. Also found in milk, fish oils, shiitake mushroom, truffles, prawns and lobster. Important off-flavour component of foods. Used in seasonings. Oily liq. with mustard-like odour. d_4^{20} 1.06. Bp 142-143° $Bp_{11.5}$ 41°. n_D^{23} 1.5340.

S,S-*Dioxide:* [20163-71-7] *Methyl (methylthio)methyl sulfone. (Methylsulfonyl)(methylthio)methane, 9CI*
$C_3H_8O_2S_2$ 140.227
Cryst. (Et_2O). Mp 50-51.2°.

S,S′-*Dioxide, (±)-:*
$C_3H_8O_2S_2$ 140.227
Mp 92-94°.

S,S′-*Dioxide* (meso-)*:* [54267-12-8] *Bis(methylsulfinyl)methane*
$C_3H_8O_2S_2$ 140.227
Mp 46-49°.

S,S,S′,S′-*Tetraoxide:* [1750-62-5] *Bis(methylsulfonyl)methane, 9CI*
$C_3H_8O_4S_2$ 172.226
Mp 145°.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 264D (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 426A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 347D (*ir*)
Böhme, H. *et al., Ber.*, 1941, **74**, 1667 (*synth*)
Schoenberg, A. *et al., Chem. Ber.*, 1967, **100**, 778 (*synth*)
Fiecchi, A. *et al., Tet. Lett.*, 1967, 1681 (*isol, sulfone*)
Sloot, D. *et al., J. Agric. Food Chem.*, 1975, **23**, 356 (*isol*)
Ogura, K. *et al., Bull. Chem. Soc. Jpn.*, 1980, **53**, 1414 (*dioxide, synth, pmr, ir*)
Freeman, D.J. *et al., Chem. Ind. (London)*, 1986, 877 (*isol*)
Castro, A. *et al., JOC*, 1992, **57**, 3496-3499 (*sulfone, synth, pmr, cmr*)
Bellesia, F. *et al., Flavour Fragrance J.*, 1996, **11**, 239-243 (*isol, truffle*)
Merck Index, 13th edn., 2001, No. 1255 (*bibl*)
Kouokam, J.C. *et al., Phytochemistry*, 2002, **60**, 403-407 (*isol*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 1412 (*use, occur*)

Bis[(methylthio)methyl] disulfide, 9CI B-225

2,4,5,7-Tetrathiaoctane [85544-38-3]

Me^2SCH_2-^{4}S-^{5}S-CH_2^7SMe

$C_4H_{10}S_4$ 186.387

Pale yellow oil. Bp_4 112-120° $Bp_{0.02}$ 83.2-85.8°.

2-Oxide: [155994-66-4] ***Methylsulfinylmethyl (methylthiomethyl) disulfide***
$C_4H_{10}OS_4$ 202.386

4-Oxide: [448948-84-3] *2,4,5,7-Tetrathiaoctane 4-oxide.* ***Marasmicin***
$C_4H_{10}OS_4$ 202.386
Yellow oil. λ_{max} 206 (log ϵ 4.03); 232 (sh) (MeCN).

2,2-Dioxide: [143113-67-1] ***Methylsulfonylmethyl(methylthiomethyl) disulfide***
$C_4H_{10}O_2S_4$ 218.386
Needles (Et_2O). Mp 59-60° (55°).

2,7-Dioxide: [244171-21-9] ***Bis[(methylsulfinyl)methyl] disulfide***
$C_4H_{10}O_2S_4$ 218.386

4,4-Dioxide: [211430-59-0]
$C_4H_{10}O_2S_4$ 218.386
Oil.

2,2,7,7-Tetraoxide: [74963-70-5] ***Bis(methylsulfonylmethyl) disulfide***
$C_4H_{10}O_4S_4$ 250.385
Isol. from the edible shiitake mushroom (*Lentinus edodes*).

Altamura, M.R. *et al., JOC*, 1963, **28**, 2438-2440 (*synth*)
Grossert, J. *et al., Can. J. Chem.*, 1980, **58**, 1106-1110 (*tetraoxide, struct*)
Hase, T.A. *et al., Synth. Commun.*, 1982, **12**, 947-950 (*synth*)
Takazawa, H. *et al., Yakugaku Zasshi*, 1982, **102**, 489-491 (*tetraoxide, isol*)
Weissflog, E. *et al., Phosphorus Sulfur Relat. Elem.*, 1983, **15**, 27-32 (*synth*)
Böhme, H. *et al., Sulfur Lett.*, 1984, **2**, 151-159 (*synth*)
Burton, S.G. *et al., Planta Med.*, 1992, **58**, 295-296 (*isol, ir, pmr*)
Kubota, K. *et al., Biosci., Biotechnol., Biochem.*, 1994, **58**, 430-431; 644-646 (*isol, synth*)
Block, E. *et al., JOC*, 1994, **59**, 2273-2275 (*tetraoxide, synth*)
Lim, H. *et al., Phytochemistry*, 1998, **48**, 787-790 (*4,4-dioxide, isol*)
Barbosa, L.C.A. *et al., Fitoterapia*, 1999, **70**, 152-156 (*2-oxide, 2,7-dioxide*)
Kubec, R. *et al., Phytochemistry*, 2002, **60**, 21-25 (*Marasmicin, isol, struct*)
Kouokam, J.C. *et al., Phytochemistry*, 2002, **60**, 403-407 (*2-oxide*)
Griffiths, R. *et al., Aust. J. Chem.*, 2005, **58**, 128-136 (*activity*)
Bewick, S.A. *et al., Aust. J. Chem.*, 2005, **58**, 218-223 (*tetraoxide, activity*)

Bis(methylthiomethyl) sulfide B-226

Thiobis[methylthiomethane], 9CI. 2,4,6-Trithiaheptane. FEMA 4214 [6540-86-9]

MeS-CH_2-S-CH_2-SMe

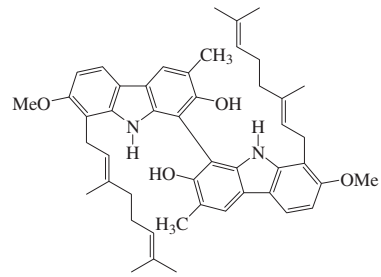
$C_4H_{10}S_3$ 154.321
Flavouring agent. Occurs in white truffle and cooked petai beans (*Parka speciosa*). Oil with roasted sulfurous odour. $Bp_{0.3}$ 41-44°.

4,4-Dioxide: Bis(methylthiomethyl) sulfone
$C_4H_{10}O_2S_3$ 186.32

Fehr, F. *et al., Chem. Ber.*, 1958, **91**, 996 (*synth*)
Welti, D. *et al., JCS*, 1962, 4372 (*synth, ir*)
Ohsaku, M. *et al., J. Mol. Struct.*, 1977, **42**, 31 (*ir*)
Schmidt, M. *et al., Z. Anorg. Allg. Chem.*, 1978, **445**, 167 (*synth, ir, pmr*)
Grossert, J.S. *et al., Can. J. Chem.*, 1981, **59**, 326 (*synth, ms, pmr, cmr*)
Kouokam, J.S. *et al., Phytochemistry*, 2002, **60**, 403-407 (*Scorodophloeus zenkeri constit*)
Frerot, E. *et al., Flavour Fragrance J.*, 2008, **23**, 434-440 (*cooked petai bean constit*)
The Good Scents Company, (*use*)

Bismurrayafoline E B-227

[252350-80-4]

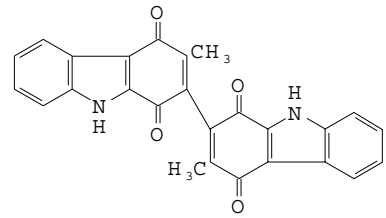


$C_{48}H_{56}N_2O_4$ 724.981
Alkaloid from the leaves of *Murraya koenigii* (curryleaf tree). Gum.

Nutan, M.T.H. *et al., Fitoterapia*, 1999, **70**, 130-133 (*Bismurrayafoline E*)
Tachibana, Y. *et al., J. Agric. Food Chem.*, 2001, **49**, 5589-5594 (*Bismurrayafoline E, activity*)

Bismurrayaquinone A B-228

3,3′-Dimethyl-[2,2′-bi-1H-carbazole]-1,1′,4,4′(9H,9′H)-tetrone, 9CI [155519-86-1]

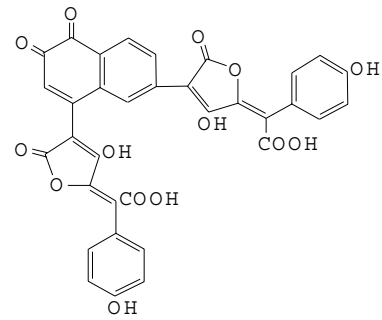


$C_{26}H_{16}N_2O_4$ 420.423
Alkaloid from roots of *Murraya koenigii* (curryleaf tree). Orange powder.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 2096-2100 (*Bismurrayaquinone A*)
Bringmann, G. *et al., Tetrahedron*, 1995, **51**, 9353-9360 (*synth*)
Murphy, W.S. *et al., JCS Perkin 1*, 1998, 4115-4119 (*synth*)
Konkol, L.C. *et al., Angew. Chem., Int. Ed.*, 2011, **50**, 9931-9934 (*synth*)

Bisnorbadioquinone A B-229

[90295-70-8]

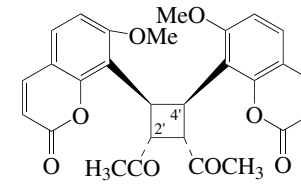


$C_{34}H_{18}O_{14}$ 650.508
Isol. from higher fungus *Xerocomus badius* (kostanjevka).

Steffan, B. *et al., Angew. Chem., Int. Ed.*, 1984, **23**, 445 (*isol, uv, pmr*)

Bisosthenon B-230

[123672-84-4]



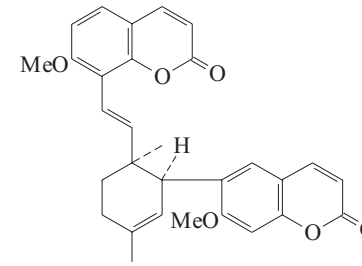
$C_{28}H_{24}O_8$ 488.493
Prisms. Mp 234-237°.

2′,4′-Diepimer: ***Bisosthenon B***
$C_{28}H_{24}O_8$ 488.493
Constit. of *Citrus paradisi* (grapefruit). Oil. $[\alpha]_D$ +24.5 (c, 0.1 in $CHCl_3$). λ_{max} 206; 265 (sh); 326 (EtOH).

Ito, C. *et al., Chem. Pharm. Bull.*, 1990, **38**, 2102
Takemura, Y. *et al., Heterocycles*, 1997, **45**, 1169 (*Bisosthenon B*)

Bisparasin B-231

[153178-05-3]

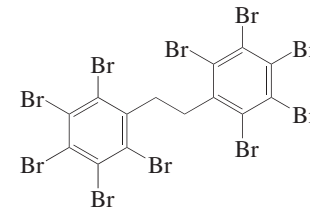


$C_{30}H_{28}O_6$ 484.548
Oil. Racemic.

Ito, C. *et al., Chem. Pharm. Bull.*, 1993, **41**, 1657 (*isol, pmr, cmr, struct*)

1,2-Bis(pentabromophenyl)ethane B-232

1,1′-(1,2-Ethanediyl)bis[2,3,4,5,6-pentabromobenzene], 9CI. Decabromodiphenylethane. DBDPE. DeBDethane [84852-53-9]



$C_{14}H_4Br_{10}$ 971.226
Environmental contaminant. Mp 349.1° (340°).

Kierkgaard, A. *et al., Environ. Sci. Technol.*, 2004, **38**, 3247-3253 (*detn, occur*)
Koeppen, R. *et al., Acta Cryst. E*, 2007, **63**, o585-o586 (*cryst struct, bibl*)

3′(2′),5′-Bisphosphate nucleotidase B-233

E.C. 3.1.3.7. Adenosine-3′(2′),5′-bisphosphate 3′(2′)-phosphohydrolase. 3′-Phosphoadenylylsulfate 3′-phosphatase. Phosphoadenylate 3′-nucleotidase. DPNPase [9025-83-6]

Phosphoric monoester hydrolase enzyme. Isol. from rabbit. Enzyme inhibited by $Na^{\oplus}$ and $Li^{\oplus}$. Also acts on 3′-phosphoadenylyl sulfate and on the corresp. 2′-phosphates.

Brunngraber, E.G. *et al., J. Biol. Chem.*, 1958, **233**, 472-477 (*rabbit*)
Ramaswarmy, S.G. *et al., J. Biol. Chem.*, 1987, **262**, 10044-10047 (*guinea pig*)
Ribeiro, J.M. *et al., Biochimie*, 1990, **72**, 227-234 (*rat*)
Quintero, F.J. *et al., Plant Cell*, 1996, **8**, 529-537 (*Arabidopsis thaliana*)
Yenush, L. *et al., FEBS Lett.*, 2000, **467**, 321-325 (*human*)

Bisphosphoglycerate phosphatase B-234

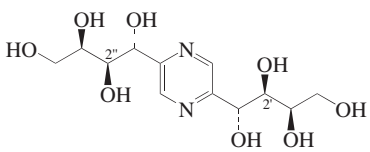
E.C. 3.1.3.13. 2,3-Bisphospho-D-glycerate 2-phosphohydrolase. 2,3-Diphosphoglyceric acid phosphatase [9033-04-9]

Phosphoric monoester hydrolase enzyme. Isol. from cow, pig, rabbit. Human enzyme activity range pH 4.0-10.0. At 4°, stable for 1 month, but kept for long-term storage when frozen.

Rapoport, S. *et al., J. Biol. Chem.*, 1951, **189**, 683-694 (*rat, rabbit*)
Harkness, D.R. *et al., Arch. Biochem. Biophys.*, 1970, **138**, 208-219 (*human*)
Diederich, D. *et al., Biochim. Biophys. Acta*, 1970, **212**, 441-449 (*mammals*)
Rose, Z.B. *et al., J. Biol. Chem.*, 1970, **245**, 3232-3241 (*human*)
Ramponi, G. *et al., Methods Enzymol.*, 1975, **42**, 409-426 (*rev*)
Harkness, D.R. *et al., Eur. J. Biochem.*, 1977, **78**, 343-351 (*jungle fowl*)
Pons, G. *et al., Biochim. Biophys. Acta*, 1982, **842**, 56-61 (*pig*)

2,5-Bis(1,2,3,4-tetrahydroxybutyl)pyrazine B-235

1,1′-(2,5-Pyrazinediyl)bis-1,2,3,4-butanetetrol, 9CI [68538-87-4]
[220145-43-7, 220145-46-0, 220145-47-1, 220145-44-8, 220145-45-9]



(1′*R*,1″*R*,2′*R*,2″*R*,3′*R*,3″*R*)-*form*

$C_{12}H_{20}N_2O_8$ 320.299

(1′*R*,1″*R*,2′*R*,2″*R*,3′*R*,3″*R*)-*form* [13121-64-7]
D-lyxo-*form*
Beige powder. Mp 109°.

(1′*R*,1″*R*,2′*S*,2″*S*,3′*R*,3″*R*)-*form* [13185-73-4]
D-arabino-*form*. D-*Fructosazine*
Present in ammonia caramels and soy sauce. Needles (EtOH). Mp 237°. $[\alpha]_D^{20}$ -84.1 (c, 1 in H_2O).

Octa-Ac: [13051-88-2]
Mp 174°. $[\alpha]_D^{11}$ -7.2 (c, 1 in $CHCl_3$).

(1′*R*,1″*R*,2′*S*,2″*S*,3′*S*,3″*S*)-*form* [41093-14-5]
L-xylo-*form*. L-*Sorbosazine*
Needles (EtOH). Mp 175-177°. $[\alpha]_D^{20}$ -27 (c, 0.1 in H_2O).

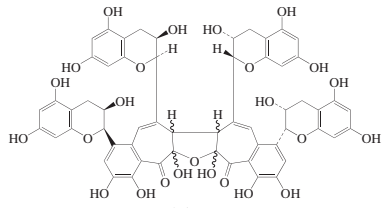
(1′ξ,1″ξ,2′ξ,2″ξ,3′ξ,3″ξ)-*form*
2′,2″-Bis-O-*(2-acetamido-2-deoxy-β-D-glucopyranoside):* [165956-47-8] Vibrio alginolyticus *Pyrazine. VAPY*
$C_{28}H_{46}N_4O_{18}$ 726.687
Powder. Sol. MeOH, H_2O. λ_{max} 275 (H_2O).

[68510-02-1]

Fujii, S. *et al., JOC*, 1966, **31**, 2239-2241 (*synth, fructosazine*)
Tsuchida, H. *et al., Agric. Biol. Chem.*, 1973, **37**, 2571-2578 (*Fructosazine, synth, uv, ir*)
Teglia, M.C. *et al., Carbohydr. Res.*, 1973, **26**, 377-384 (*synth, Sorbosazine*)
Tsuchida, H. *et al., Dev. Food Sci.*, 1986, **13**, 85-94 (*occur*)
Tsuchida, H. *et al., CA*, 1990, **113**, 229877r (*occur*)
Sumoto, K. *et al., Bull. Chem. Soc. Jpn.*, 1991, **39**, 792-794 (*Frucosazine, synth, ir, pmr, cmr*)
Yanai, T. *et al., J. Ferment. Bioeng.*, 1995, **80**, 406-407 (*VAPY*)
Japan. Pat., 1995, 95 118 286 (*VAPY*)
Pat. Coop. Treaty (WIPO), 1999, 9 903 842 (*synth, lyxo-form*)

Bistheaflavin A B-236

[353288-91-2]



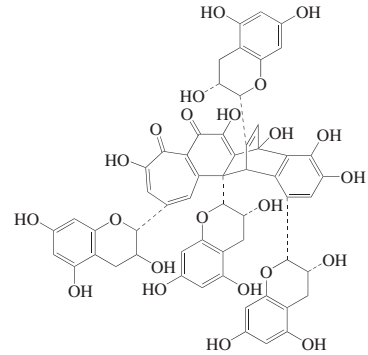
Relative Configuration

$C_{58}H_{48}O_{25}$ 1145.002
Pigment from oxidative dimerisation of Theaflavin, T-433 in tea fermentation. Red-brown powder + $6H_2O$. $[\alpha]_D^{15}$ -48.3 (c, 0.12 in MeOH). λ_{max} 255 (log ϵ 4.36); 274 (sh) (log ϵ 4.26); 320 (log ϵ 3.81) (MeOH).

Tanaka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 5785-5789 (*isol, pmr, cmr*)

Bistheaflavin B B-237

[384330-53-4]



Relative Configuration

$C_{57}H_{46}O_{23}$ 1098.977
Pigment from oxidative dimerisation of Theaflavin, T-433 in tea fermentation. Red-brown powder + $6H_2O$. $[\alpha]_D^{15}$ -72.8 (c, 0.06 in MeOH). λ_{max} 274 (log ϵ 4.1); 378 (log ϵ 3.7) (MeOH).

Tanaka, T. *et al., J. Agric. Food Chem.*, 2001, **49**, 5785-5789 (*isol, pmr, cmr*)

N,N′-Bis(2,2,2-trichloro-1-hydroxyethyl)urea, 9CI, 8CI B-238

Dicloralurea, BSI, INN, ISO, USAN. *SKF 1995. DCU, WSSA. Crag Herbicide 2* [116-52-9]

$Cl_3CCH(OH)NHCONHCH(OH)CCl_3$

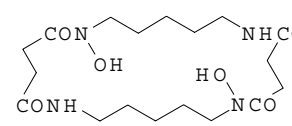
$C_5H_6Cl_6N_2O_3$ 354.83
Vet. food additive, inhibits methane production in herbicide ruminants. Growth stimulant. Herbicide, now supersededLog P 2.86 (calc).

▶ Skin irritant. LD_{50} (rat, orl) 6400 mg/kg. YS2787000

US Pat., 1973, (*(SmithKline French)*)3 733 417 (*use*)
Partis, M.D. *et al., J. Chromatogr.*, 1983, **259**, 189 (*hplc*)
Pesticide Manual, 9th edn., 1991, No. 4170
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, DGQ200

Bisucaberin B-239

6,17-Dihydroxy-1,6,12,17-tetraazacyclodocosane-2,5,13,16-tetrone, 9CI [112972-60-8]



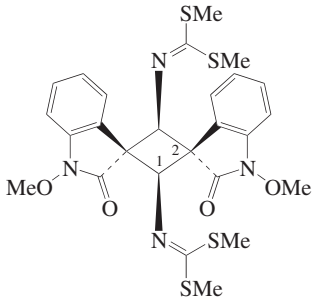
$C_{18}H_{32}N_4O_6$ 400.474
Isol. from the salmon pathogen *Vibrio salmonicida*. Cryst. Sol. DMSO; fairly sol. MeOH; poorly sol. EtOH, hexane, H_2O. Mp 180° dec. λ_{max} 215 (ϵ 5740) (MeOH) (Derep). λ_{max} 215 (ϵ 5700) (MeOH/HCl).

Kameyama, T. *et al., J. Antibiot.*, 1987, **40**, 1664-1676; 1671-1676 (*isol, pmr, cmr*)
Bergeron, R.J. *et al., Tetrahedron*, 1989, **45**, 4939-4944 (*synth*)

Hou, Z. *et al., Inorg. Chem.*, 1998, **37**, 6630-6637 (*struct*)
Winkelmann, G. *et al., BioMetals*, 2002, **15**, 153-160 (*isol, ms*)
Kadi, N. *et al., Chem. Comm.*, 2008, 5119-5121 (*biosynth*)

Biswasalexin A_1 B-240

[1207609-95-7]



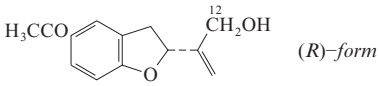
$C_{26}H_{28}N_4O_4S_4$ 588.796
Dimer of Wasalexin A, W-2. Achiral (centre of symmetry). Isol. from the leaves of *Thellungiella halophila* (salt cress) elicited with uv radiation. λ_{max} 229 (log ϵ 4.49) (CH_2Cl_2).

1,2-Diepimer: [1207609-96-8] ***Biswasalexin A_2***
$C_{26}H_{28}N_4O_4S_4$ 588.796
Isol. from the leaves of *Thellungiella halophila* (salt cress) elicited with uv radiation. λ_{max} 230 (log ϵ 4.62) (CH_2Cl_2).

Pedras, M.S.C. *et al., Phytochemistry*, 2009, **70**, 2010-2016 (*Biswasalexins A_1, A_2*)

Bitalin A B-241

1-[2,3-Dihydro-2-[1-(hydroxymethyl)ethenyl]-5-benzofuranyl]ethanone, 9CI. 5-Acetyl-2,3-dihydro-2-(1-hydroxy-2-propen-2-yl)benzofuran. 3′-Hydroxytremetone [34428-28-9]



(*R*)–*form*

$C_{13}H_{14}O_3$ 218.252
Numbering systems vary. Called 12-Hydroxytremetone in the lit.

(*R*)-*form* [35844-67-8]
Constit. of *Helichrysum italicum* (curry plant). Liq. $[\alpha]_D$ -61.2 (c, 2 in $CHCl_2$).

Angeloyl: [65580-28-1]
$C_{18}H_{20}O_4$ 300.354

(*S*)-*form* [78548-83-1]

β-D-Glucopyranoside:
$C_{19}H_{24}O_8$ 380.394
Constit. of *Helichrysum italicum* (curry plant). Mp 155°. $[\alpha]_D$ -53 (c, 0.1 in MeOH). λ_{max} 233; 287 (MeOH).

Ac: [134236-63-8] ***12-Acetyloxytremetone***
$C_{15}H_{16}O_4$ 260.289

*4-Hydroxy-*E*-cinnamoyl:* [158414-61-0] ***12-p-Coumaroyloxytremetone***
$C_{22}H_{20}O_5$ 364.397

Aldehyde: [70360-18-8] *5-Acetyl-2,3-dihydro-α-methylene-2-benzofuranacetaldehyde, 9CI.* ***12-Oxotremetone***
$C_{13}H_{12}O_3$ 216.236

12-Carboxylic acid, Me ester:
$C_{14}H_{14}O_4$ 246.262
Amorph. solid. $[\alpha]_D^{20}$ +8 (c, 0.36 in MeOH). λ_{max} 226; 285 (MeOH).

(±)-*form* [66614-28-6]
Bp_3 103-105° (bath).

(ξ)-*form*

2-Methylpropanoyl:
$C_{17}H_{20}O_4$ 288.343

2-Methylbutanoyl:
$C_{18}H_{22}O_4$ 302.369

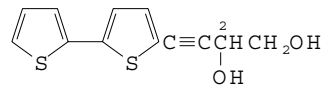
2-Methyl-2-butenoyl:
$C_{18}H_{20}O_4$ 300.354

[35844-68-9]

Bohlmann, F. *et al., Tet. Lett.*, 1970, **11**, 3575-3576 (*2-methylpropanoyl*)
Garcia de Quesada, T. *et al., Phytochemistry*, 1972, **11**, 446-449 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1977, **16**, 1973-1981; 1979, **18**, 1403-1405 (*2-methylbutanoyl, 2-methylbutenoyl, 4-hydroxycinnamoyl*)
Bohlmann, F. *et al., Phytochemistry*, 1979, **18**, 179-181; 668-671 (*12-Oxotremetone*)
Kawase, Y. *et al., Chem. Lett.*, 1980, **9**, 1581-1584 (*synth, abs config*)
Le Van, N. *et al., Phytochemistry*, 1981, **20**, 485-487 (*isol*)
Zapesochnaya, G.G. *et al., Chem. Nat. Compd. (Engl. Transl.)*, 1990, **26**, 342-343 (*isol*)
Zdero, C. *et al., Phytochemistry*, 1992, **31**, 155-157 (*angeloyl*)
Nieto, M. *et al., An. Asoc. Quim. Argent. (1921-2001)*, 1994, **82**, 105-109 (*Parastrephia lepidophylla derivs*)
Sala, A. *et al., J. Nat. Prod.*, 2001, **64**, 1360-1362 (*glucoside*)
Schmidt, T.J. *et al., Planta Med.*, 2003, **69**, 258-268 (*12-carboxylic acid Me ester*)
Ohgiya, T. *et al., Chem. Lett.*, 2004, **33**, 1084-1085 (*synth*)

4-[2,2′-Bithiophen-5-yl]-3-butyne-1,2-diol, 9CI B-242

5-(3,4-Dihydroxy-1-butynyl)-2,2′-bithiophene [1211-45-6]



$C_{12}H_{10}O_2S_2$ 250.342
Cryst. (CCl_4/Et_2O). Mp 102°. $[\alpha]_D$ +11 (c, 2.55 in $CHCl_3$) (c, 2.55 in Et_2O).

1-Ac: [95910-62-6] *5-(4-Acetoxy-3-hydroxy-1-butynyl)-2,2′-bithiophene.* ***α-Tertiophene***
$C_{14}H_{12}O_3S_2$ 292.379
Oil.

2-Ac: [1687-88-3] ***5-(3-Acetoxy-4-hydroxy-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{12}O_3S_2$ 292.379
Oil.

Di-Ac: [1233-95-0] ***5-(3,4-Diacetoxy-1-butynyl)-2,2′-bithiophene***
$C_{16}H_{14}O_4S_2$ 334.416
Oil. $[\alpha]_D$ +119 (c, 0.89 in $CHCl_3$). $[\alpha]_{Hg}^{25}$ +183 (c, 0.89 in Et_2O).

1-O-(3-Methylbutanoyl): [58930-56-6] ***5-(3-Hydroxy-4-isovaleryloxy-1-butynyl)-2,2′-bithiophene***
$C_{17}H_{18}O_3S_2$ 334.459
Oil.

1-O-(3-Methylbutanoyl), 2-Ac: [253268-01-8] *5-(3-Acetoxy-4-isovaleryloxy-1-butynyl)-2,2′-bithiophene*
$C_{19}H_{20}O_4S_2$ 376.497

2-O-(3-Methylbutanoyl): ***5-(4-Hydroxy-3-isovaleryloxy-1-butynyl)-2,2′-bithiophene***
$C_{17}H_{18}O_3S_2$ 334.459

2-Ketone, Ac: [1222-83-9] ***5-(4-Acetoxy-3-oxo-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{10}O_3S_2$ 290.363
Isol. from *Tagetes erecta* (African marigold). Cryst. (CCl_4). Mp 68°.

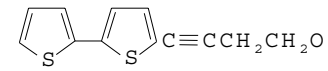
1-Deoxy, 1-chloro: [1020-03-7] ***5-(4-Chloro-3-hydroxy-1-butynyl)-2,2′-bithiophene.*** *1-Chloro-4-[5-(3-thienyl)-2-thienyl]-3-butyn-2-ol, 8CI*
$C_{12}H_9ClOS_2$ 268.787
Isol. from *Tagetes minuta* (Mexican marigold). Solid. Mp 55°.

1-Deoxy, 1-chloro, Ac: [96850-15-6] ***5-(3-Acetoxy-4-chloro-1-butynyl)-2,2′-bithiophene***
$C_{14}H_{11}ClO_2S_2$ 310.824
Yellow oil.

Bohlmann, F. *et al., Chem. Ber.*, 1965, **98**, 155; 876 (*isol, uv, ir, pmr, ord, struct, biosynth*)
Atkinson, R.E. *et al., JCS*, 1965, 7109 (*deriv*)
Bohlmann, F. *et al., Chem. Ber.*, 1976, **109**, 901 (*3-methylbutanoyl*)
Bohlmann, F. *et al., Planta Med.*, 1984, **50**, 192; 1985, **51**, 77 (*isol, derivs*)
Pensl, R. *et al., Z. Naturforsch., C*, 1985, **40**, 3 (*isol, biosynth*)
Chang, C.-T. *et al., Planta Med.*, 1990, **56**, 533
Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)
Lin, Y.-L. *et al., Chin. Pharm. J. (Taipei)*, 1999, **51**, 201-211 (*isol, activity*)

4-[2,2′-Bithiophen-5-yl]-3-butyn-1-ol, 9CI B-243

4-[5-(2-Thienyl)-2-thienyl]-3-butyn-1-ol, 8CI. 5-(4-Hydroxy-1-butynyl)-2,2′-bithiophene [1137-87-7]



$C_{12}H_{10}OS_2$ 234.342
Constit. of the roots of *Tagetes minuta* (Mexican marigold), *Tagetes* spp. Cryst. (Et_2O/petrol or CCl_4). Mp 68°.

Ac: [1219-28-9]
$C_{14}H_{12}O_2S_2$ 276.38
Isol. from *Tagetes* spp. Oil. $Bp_{0.001}$ 115°.

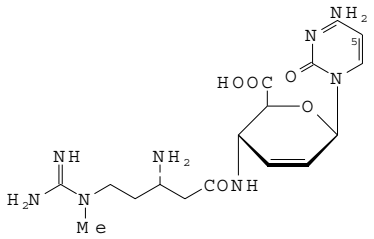
3-Methylbutanoyl: [61102-15-6]
$C_{17}H_{18}O_2S_2$ 318.46
Oil.

Bohlmann, F. *et al., Chem. Ber.*, 1962, **95**, 2945; 1964, **97**, 2125
Atkinson, R.E. *et al., JCS*, 1965, 7109 (*isol*)
Bohlmann, F. *et al., Phytochemistry*, 1976, **15**, 1309 (*isol*)
Rossi, R. *et al., Tetrahedron*, 1984, **40**, 2773 (*synth*)

Kagan, J. *et al., Prog. Chem. Org. Nat. Prod.*, 1991, **56**, 87 (*rev*)

Blasticidin S B-244

Cytovirin. NSC 91770. A 83094C. Antibiotic 21544. Antibiotic A 83094C. Bla-S [2079-00-7]



$C_{17}H_{26}N_8O_5$ 422.443

Nucleoside-type antibiotic. Contact fungicide used against rice blast disease in Japan. Needles (H_2O). Mp 235° (252-253°) dec. $[\alpha]_D^{11}$ +108.4 (c, 1 in H_2O). pK_{a1} 2.4; pK_{a2} 4.6; pK_{a3} 8; pK_{a4} 0. λ_{max} 275 (ε 14800) (0.1*N* HCl) (Derep). λ_{max} 266 (ε 11400) (0.1*N* NaOH) (Derep). λ_{max} 231 (ε 8900); 268 (ε 7000) (H_2O) (Derep).

▶ LD_{50} (rat, orl) 16 mg/kg. LD_{50} (rat, skn) 3100 mg/kg. EC4900000

Hydrochloride: [3513-03-9]
Mp 229° dec.

Hydrochloride (1:2): Mp 195° dec.

Me ester, hydrochloride (1:3): [3930-66-3]
Mp 206-208.5° dec.

N-*De-Me:* [63257-29-4] ***Demethylblasticidin S***
$C_{16}H_{24}N_8O_5$ 408.416
Sol. H_2O. λ_{max} 274 (H_2O). λ_{max} 274 (ε 12900) (HCl) (Berdy). λ_{max} 267 (ε 9200) (NaOH).

▶ LD_{50} (mus, orl) 35 mg/kg. MP8930000

3″-N-*Leucyl:* [19018-47-4] ***Leucylblasticidin S***. *Sch 36606. Antibiotic Sch 36606*
$C_{23}H_{37}N_9O_6$ 535.602
Needles (H_2O). Sol. H_2O; fairly sol. MeOH, DMSO; poorly sol. $CHCl_3$, hexane. Mp 252° dec. λ_{max} 269 (ε 8000) (H_2O). λ_{max} 276 (ε 11000) (HCl).

5-Fluoro: [102865-76-9] *Fluoroblasticidin S*
$C_{17}H_{25}FN_8O_5$ 440.433
Powder. Sol. H_2O; poorly sol. butanol, hexane. Mp 225-227°. λ_{max} 280 (ε 13500); 282 (ε 8020) (HCl). λ_{max} 275 (ε 5500) (NaOH) (Berdy). λ_{max} 276 (ε 12000) (H_2O).

5-Hydroxymethyl: [123067-52-7] ***5-Hydroxymethylblasticidin S***. *A 83094B. Antibiotic A 83094B*
$C_{18}H_{28}N_8O_6$ 452.469
Mp 225° dec. λ_{max} 279 (ε 11000) (0.01*M* HCl) (Derep). λ_{max} 272 (ε 8000) (H_2O) (Derep). λ_{max} 272 (pH 7 buffer).

Yonehara, H. *et al., J. Antibiot., Ser. A*, 1963, **16**, 195-202 (*isol*)
Otake, N. *et al., Tet. Lett.*, 1965, **6**, 1411-1419 (*struct*)
Fox, J.J. *et al., Tet. Lett.*, 1966, **1**, 897-904 (*struct*)
Yonehara, H. *et al., Tet. Lett.*, 1966, **7**, 3785-3791 (*abs config*)
Seto, H. *et al., Tet. Lett.*, 1966, **7**, 3793-3799 (*biosynth*)
Misato, T. *et al., Antibiotics, Vol. 1: Mechanism of Action*, (eds. Gottlieb, D. *et al*), Springer, 1967, 434-439 (*rev*)
Seto, H. *et al., Agric. Biol. Chem.*, 1968, **32**, 1299-1305 (*Leucylblasticidin S*)
Seto, H. *et al., J. Antibiot.*, 1977, **30**, 1022-1024 (*Demethylblasticidins*)
Swaminathan, V. *et al., Biochim. Biophys. Acta*, 1981, **655**, 335-341 (*cryst struct*)
Yonehara, H. *et al., Drugs Pharm. Sci.*, 1984, **22**, 651-663 (*rev*)
Japan. Pat., 1985, (*(Asahi glass)*)60 123 486 (*Fluoroblasticidin S*)
Probhakaran, P.C. *et al., Tet. Lett.*, 1986, **27**, 3815-3818 (*biosynth*)
Kawashima, A. *et al., Agric. Biol. Chem.*, 1987, **51**, 1183-1184 (*Fluoroblasticidin S*)
Dallwag, H. *et al., J. Antibiot.*, 1988, **41**, 1145-1147 (*Leucylblasticidin S*)
Isono, K. *et al., J. Antibiot.*, 1988, **41**, 1711-1739 (*rev*)
Larsen, S.H. *et al., J. Antibiot.*, 1989, **42**, 470-471 (*5-Hydroxymethylblasticidin S*)
Zhang, Q. *et al., Tetrahedron*, 2000, **56**, 693-701 (*biosynth*)
Ichikawa, Y. *et al., Chem. Eur. J.*, 2004, **10**, 3241-3251 (*synth, ir, pmr, cmr*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 11th edn., J. Wiley*, 2004, BLX500

Bleomycin hydrolase B-245

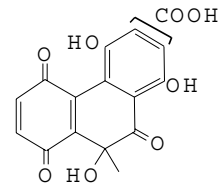
*E.C. 3.4.22.40. Aminopeptidase C (*Lactococcus lactis*)* [53096-17-6]

Cysteine endopeptidase enzyme. Isol. from *Saccharomyces cerevisiae* (baker's yeast), and from rabbit. Human enzyme activity range pH 6.0-8.0.

Nishimura, C. *et al., Biochemistry*, 1987, **26**, 1574-1578 (*rabbit*)
Sebti, S.M. *et al., Biochemistry*, 1989, **28**, 6544-6548 (*mammals*)
Broemme, D. *et al., Biochemistry*, 1996, **35**, 6706-6714 (*human, activity*)
Mistou, M.Y. *et al., Biochim. Biophys. Acta*, 1998, **1383**, 63-70 (*Lactococcus lactis*)
O'Farrel, P. *et al., Structure Fold. Des.*, 1999, **15**, 619-627 (*human, cryst struct*)
Zimny, J. *et al., J. Biol. Chem.*, 2006, **281**, 22485-22492 (*Saccharomyces cerevisiae*)

Blighinone B-246

[20544-62-1]



$C_{16}H_{10}O_8$ 330.25
Quinone from the fruit pulp of *Blighia sapida* (akee apple). Lemon-yellow cryst. (Py). Mp 360° dec.

Tri-Ac:
Cryst. (Py). Mp 340-344° dec.

Tri-Me ether:
Cryst. (Py). Mp 348-350°.

Garg, H.S. *et al., Tet. Lett.*, 1968, 1549

Blue copper proteins B-247

Type 1 Copper proteins

$[CuN_2S_2]$

A group of metalloproteins which have a single Cu atom at the active site and three characteristic props.: intense blue colour at *ca*. 600 nm, unusually narrow hyperfine coupling in the epr spectrum of the $Cu^{2\oplus}$ protein, and high reduction potentials (range 184-680 mV).

Amicyanin
Contains 106 amino acids.

Azurin
Contains 128 or 129 amino acids.

Cucumber basic protein
Plantacyanin. CBP
Isol. from cucumber. Contains 96 amino acids.

Plastocyanin
There are a number of Plastocyanins, each containing between 97 and 104 amino acids.

Pseudoazurin
Contains 123 amino acids.

Rusticyanin
Contains 144 amino acids.

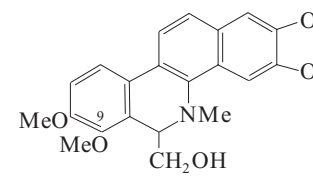
Stellacyanin
Contains 107 amino acids.

Umecyanin
Isol. from roots of horseradish. Contains 125 amino acids.

Lappin, A.G. *et al., Met. Ions Biol. Syst.*, (Ed. Sigel, H.), Vol. 13, Marcel Dekker, N.Y., 1981, 15 (*rev*)
Copper Proteins Copper Enzymes, (Ed. Lontie, R.), CRC Press, Boca Raton, 1984, (*book*)
Dooley, D.M. *et al., Life Chem. Rep.*, 1987, **5**, 91 (*rev*)
Latour, J.M. *et al., Bull. Soc. Chim. Fr.*, 1988, 508 (*rev*)
Ryden, L. *et al., Prog. Clin. Biol. Res.*, 1988, **274**, 349 (*rev*)
Guss, J.M. *et al., Sciences (N.Y.)*, 1988, 241; 806 (*cryst struct*)
Sykes, A.G. *et al., Adv. Inorg. Chem.*, 1991, **36**, 377 (*rev*)
Gross, E.L. *et al., Adv. Photosynth.*, 1996, **4**, 413-429 (*rev, Plastocyanin*)
Donaire, A. *et al., JACS*, 2002, **124**, 13698-13708 (*Pseudoazurin, Rusticyanin, pmr, struct*)
Dennison, C. *et al., JACS*, 2004, **126**, 2481-2489 (*Umecyanin, pmr, struct*)
Ralle, M. *et al., JACS*, 2004, **126**, 7244-7256 (*Azurin, spectra*)
Zhang, Y. *et al., JACS*, 2008, **130**, 3814-3823 (*quantum pmr*)
Lipton, A.S. *et al., JACS*, 2009, **131**, 13992-13999 (*Azurin, Cu-65 nmr*)

Bocconoline B-248

12,13-Dihydro-1,2-dimethoxy-12-methyl[1,3]benzodioxolo[5,6-c]phenanthridine-13-methanol, 9CI. 8-Hydroxymethyldihydrochelerythrine [32906-88-0]



$C_{22}H_{21}NO_5$ 379.412
Probably an artifact. Pillars (MeOH). Mp 232-233° (215-218°, 221-222°).

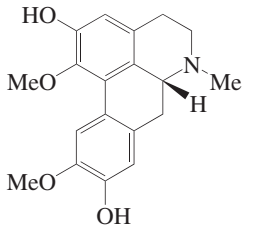
O^9-*De-Me:* ***7,8-Dihydro-8-hydroxymethylfagaridine***
$C_{21}H_{19}NO_5$ 365.385
Solid. Poss. artifact.

Deoxy: [159465-79-9] ***8-Methyldihydrochelerythrine***
$C_{22}H_{21}NO_4$ 363.412
Alkaloid from root bark of *Zanthoxylum simulans* (Szechuan pepper). Needles (MeOH). Mp 203-205°.

Tani, C. *et al., Yakugaku Zasshi*, 1962, **82**, 755 (*isol*)
Ishii, H. *et al., Tet. Lett.*, 1971, 2429 (*uv, ir, pmr, ms, struct*)
Novák, V. *et al., Coll. Czech. Chem. Comm.*, 1974, **39**, 3352 (*isol, uv*)
Ishii, H. *et al., Chem. Pharm. Bull.*, 1978, **26**, 166 (*uv, ir, pmr, ms, struct, synth*)
Itokawa, H. *et al., Phytochemistry*, 1978, **17**, 839 (*isol, uv, ir, pmr, ms*)
Castedo, L. *et al., Heterocycles*, 1981, **16**, 533 (*occur*)
Boulware, R.J. *et al., J. Nat. Prod.*, 1981, **44**, 200 (*7,8-Dihydro-8-hydroxymethylfagaridine*)
Chen, I.S. *et al., J. Nat. Prod.*, 1994, **57**, 1206 (*8-Methyldihydrochelerythrine*)

Boldine B-249

*5,6,6*a*,7-Tetrahydro-1,10-dimethoxy-6-methyl-4*H*-dibenzo[*de*,*g*]quinoline-2,9-diol, 9CI. 2,9-Dihydroxy-1,10-dimethoxyaporphine* [476-70-0]



(*R*)-*form*

$C_{19}H_{21}NO_4$ 327.379
Log P 2.42 (uncertain value) (calc).
▶ CE0750000

(*R*)-*form*

N-*De-Me:* [142794-65-8] ***(-)-Laurolitsine***
$C_{18}H_{19}NO_4$ 313.352
Solid. $[\alpha]_D^{27}$ -162 (c, 0.01 *M* in MeOH).

(*S*)-*form*

Alkaloid from *Sassafras* and the leaves of *Peumus boldus* (boldo). Flavouring ingredient. Mp 161-163°. $[\alpha]_D^{13}$ +111 (c, 1.03 in EtOH). λ_{max} 220 (log ϵ 4.6); 283 (log ϵ 4.21); 304 (log ϵ 4.23) (EtOH).
▶ LD_{50} (mus, orl) 450 mg/kg. CE0750000

Hydrochloride: [16625-69-7]
Cryst. (MeOH/Et_2O). Mp 218-222° dec. $[\alpha]_D^{20}$ +118 (c, 0.1 in EtOH).

N-*Oxide(*R*-):* [937018-76-3] ***Boldine*** **N^{β}-*oxide***
$C_{19}H_{21}NO_5$ 343.379

N-*Me:* [73892-20-3] **N-*Methylboldine***
$C_{20}H_{24}NO_4^{\oplus}$ 342.414
Cryst. (MeOH/Et_2O) (as chloride). Mp 252-255° dec. (chloride).

N-*De-Me:* [5890-18-6] *2,9-Dihydroxy-1,10-dimethoxynoraporphine.* ***Laurolitsine****. Norboldine*
$C_{18}H_{19}NO_4$ 313.352
Alkaloid from *Sassafras* and the leaves of *Peumus boldus* (boldo). Flavouring ingredient. Mp 138-140°. $[\alpha]_D$ +101 (c, 0.69 in EtOH).
▶ RB5935000

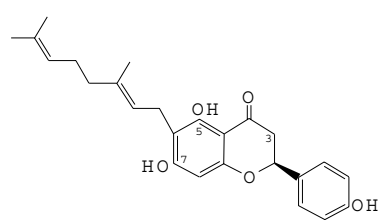
N-*De-Me,* N-*Ac:* **N-*Acetylnorboldine***
Mp 255-260°. $[\alpha]_D$ +370 (c, 0.11 in $CHCl_3$).

N-*De-Me,* N-*methoxycarbonyl:* **N-*Methoxycarbonylnorboldine***
$C_{20}H_{21}NO_6$ 371.389
Alkaloid from *Litsea cubeba* (mountain pepper). Cryst. (MeOH). Mp 140-142°. $[\alpha]_D^{20}$ +269.2 (c, 0.19 in MeOH). λ_{max} 194 (log ϵ 4.19); 216 (log ϵ 4.36); 283 (log ϵ 3.89); 303 (log ϵ 3.88) (MeOH).

Späth, E. *et al., Ber.*, 1933, **66**, 904-914 (*isol, struct*)
Nakasato, T. *et al., Chem. Pharm. Bull.*, 1959, **7**, 780-784 (*Laurolitsine*)
Johns, S.R. *et al., Aust. J. Chem.*, 1967, **20**, 1277-1281 (*Laurolitsine*)
Tewari, S. *et al., Phytochemistry*, 1972, **11**, 1149-1152 (*Boldine, Laurolitsine, isol, pmr, uv, ms*)
Kupchan, S.M. *et al., Chem. Comm.*, 1976, 91-92 (*synth*)
Bhakuni, D.S. *et al., JCS Perkin 1*, 1977, 706-709 (*biosynth*)
Bremner, J.B. *et al., Aust. J. Chem.*, 1978, **31**, 313-320 (*N-Methylboldine*)
Saxena, N.K. *et al., J. Indian Chem. Soc.*, 1979, **56**, 1020-1023 (*N-Methylboldine*)
Ringdahl, B. *et al., J. Nat. Prod.*, 1981, **44**, 80-85 (*cd*)
Atta-ur-Rahman, *et al., Fitoterapia*, 1991, **62**, 261-265 (*(-)-Laurolitsine*)
Asencio, M. *et al., Acta Cryst. C*, 1996, **52**, 1581-1583 (*cryst struct*)
Martindale, The Complete Drug Reference, 32nd edn., Pharmaceutical Press, 1999, 1554
Lee, S.-S. *et al., J. Nat. Prod.*, 2007, **70**, 637-642 (*N-oxide*)
Gan, L.-S. *et al., Nat. Prod. Commun.*, 2009, **4**, 43-46 (N-*Acetylnorboldine*)
Feng, T. *et al., Planta Med.*, 2009, **75**, 76-79 (*N-Methoxycarbonylnorboldine*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 10th edn., J. Wiley*, 2000, DNZ100

Bonannione A B-250

6-Geranyl-4′,5,7-trihydroxyflavanone. 6-Geranylnaringenin. Mimulone [97126-57-3]



$C_{25}H_{28}O_5$ 408.493
Isol. from the fruit of *Artocarpus communis* (breadfruit). Cryst. (C_6H_6/petrol). Mp 120-122°. $[\alpha]_D$ -8.2 (c, 0.4 in $CHCl_3$). λ_{max} 228 (log ϵ 4.42); 292 (log ϵ 4.31); 334 (log ϵ 3.7) (MeOH). λ_{max} 329 (MeOH/NaOH) (Berdy).

4′-Me ether: 6-Geranyl-5,7-dihydroxy-4′-methoxyflavanone. ***4′-O-Methylbonannione A***
$C_{26}H_{30}O_5$ 422.52
Pale yellow solid. Mp 133-136°. $[\alpha]_D$ -3.2 (c, 0.15 in MeOH). λ_{max} 296 (log ϵ 1.97) (MeOH).

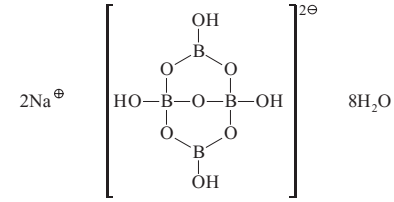
*3*R*-Hydroxy:* [96917-35-0] ***Bonanniol A***
$C_{25}H_{28}O_6$ 424.493
Amorph. solid. $[\alpha]_D^{18}$ +11.1 (c, 0.7 in $CHCl_3$).

*3*R*-Hydroxy, 5-Me ether:* [96917-37-2] ***Bonanniol B***
$C_{26}H_{30}O_6$ 438.519
Amorph. solid. $[\alpha]_D^{18}$ +33 (c, 0.1 in $CHCl_3$).

Bruno, M. *et al., Heterocycles*, 1985, **23**, 1147-1153 (*isol, pmr, cmr*)
Wollenweber, E. *et al., Phytochemistry*, 1989, **28**, 3493-3496 (*isol, cmr, pmr*)
Phillips, W.R. *et al., J. Nat. Prod.*, 1996, **59**, 495-497 (*isol, pmr, cmr*)
Wang, Y. *et al., J. Nat. Prod.*, 2001, **64**, 196-199 (*synth*)
Murphy, B.T. *et al., J. Nat. Prod.*, 2005, **68**, 417-419 (*4′-O-Methylbonannione A*)
Zhang, Y. *et al., Chin. J. Chem.*, 2011, **29**, 521-524 (*synth*)
Lin, J.-A. *et al., J. Agric. Food Chem.*, 2011, **59**, 105-111 (*isol, activity*)

Borax†, 11CI, 10CI, 9CI, 8CI B-251

Borax decahydrate. Boron sodium oxide ($B_4Na_2O_7$) decahydrate. Boron sodium oxide decahydrate. Boric acid disodium salt decahydrate. Disodium tetraborate decahydrate. Sodium borate, JAN, USAN. Tincal. E 285 [1303-96-4]
[13840-56-7]



$B_4H_{20}Na_2O_{17}$ 381.371
Also formulated as $Na_2O.2B_2O_3.10H_2O$. Listed in the EAFUS Food Additive Database (Jan. 2001) but with no current reported use. Historically used as a food preservative since *ca*. 1800, common in butter/margarine. Now limited to preservation of caviar. Mineral supplement. Colourless monoclinic cryst. Sol. H_2O (2 g per 100 cm^3 at 0°, 170 g per 100 cm^3 at 100°) MeOH, polyols; spar. sol. Me_2CO, EtOAc, EtOH. Stable in aq. soln. up to 61°, then dehydrates to Disodium tetraborate pentahydrate - complex dehydration reactions depend somewhat on sample's history.

► VZ2275000

Mineral-*form*

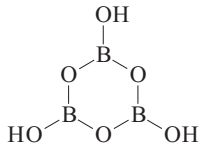
Colourless or white to greyish, greenish or bluish cryst.

[12322-85-9, 71377-02-1, 61028-24-8, 12447-40-4, 1344-90-7]

Theimer, O. *et al., Monatsh. Chem.*, 1950, **81**, 301 (*Raman*)
Nies, N.P. *et al., J. Chem. Eng. Data*, 1967, **12**, 303 (*synth*)
Thomas, G. *et al., J. Chim. Phys. Phys.-Chim. Biol.*, 1972, **69**, 1154 (*thermal anal*)
Levy, H.A. *et al., Acta Cryst. B*, 1978, **34**, 3502 (*nd, cryst struct*)
Kirk-Othmer Encycl. Chem. Technol., 3rd edn., Wiley, 1978, **4**, 80 (*manuf, uses, tox*)
Kochergin, V.P. *et al., Russ. J. Inorg. Chem. (Engl. Transl.)*, 1979, **24**, 1641 (*pmr, B-11 nmr*)
Nies, N.P. *et al., Mellor Compr. Treat. Inorg. Theor. Chem.*, 1980, 356 (*rev, bibl*)
Janda, R. *et al., Spectrochim. Acta A*, 1980, **36**, 997 (*ir, Raman*)
Turner, G.L. *et al., J. Magn. Reson.*, 1986, **67**, 544 (*B-11 nmr*)
Sigma-Aldrich Library of Chemical Safety Data, 1988, **2**, 3155C (*haz*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 290-291 (*props*)
Pesticide Manual, 15th edn., 2009, No. 93 (*borates*)
Food-Info, (*use*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, SFE500; SFF000

Boric acid (HBO_2), 11CI, 10CI B-252

Boric acid†. *Metaboric acid. E284* [13460-50-9]



α–*form* (*trimer*)

BHO_2 43.818

Common product of hydrolysis and pyrolysis of many boron compds. Three cryst. forms known. Preservative, acidity control agent, mineral supplement. Rarely used in foodstuffs.

Kracek, F.C. *et al., Am. J. Sci.*, 1938, **35**, 143 (*B_2O_3-H_2O phase diagram, synth*)
Silver, A.H. *et al., J. Chem. Phys.*, 1960, **32**, 959 (*B-11 nmr, α-form, β-form*)
Bray, P.J. *et al., J. Chem. Phys.*, 1961, **35**, 435 (*B-11 nmr, γ-form*)
Zachariasen, W.H. *et al., Acta Cryst.*, 1963, **16**, 380; 385 (*cryst struct, γ-form, β-form*)
Peters, C.R. *et al., Acta Cryst.*, 1964, **17**, 229 (*cryst struct, α-form*)
Bertoluzza, A. *et al., J. Mol. Struct.*, 1980, **64**, 123 (*ir, Raman*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1980, **5*l*A**, 224 (*rev, bibl*)

Boric acid (H_3BO_3), 9CI, 8CI, INN, JAN, USAN B-253

Boric acid†. *Boracic acid. Orthoboric acid* [10043-35-3]

$B(OH)_3$

BH_3O_3 61.833

Common product of hydrol. of many boron compds. containing B–Hal, OR, SR, H, NR_2 etc. bonds. Food contaminant deriving from paper and paperboard in contact with food. V. limited use as an antibacterial agent in caviar. Pearly scales or powder. Mod. sol. hot H_2O, v. spar. sol. cold H_2O. Mp 171° (often indefinite owing to gradual dehydration on heating). ΔH_f° -1094.3 kJ mol^{-1}.

► Acute exposure affects the gastrointestinal tract, CNS, skin, liver and kidneys. Symptoms of chronic intoxication include anorexia, gastrointestinal disturbances, debility, confusion, dermatitis, menstrual disorders, anaemia, convulsions and alopecia. Exp. reprod. and teratogenic effects. LD_{50} (rat, orl) 3000-4000 mg/kg. ED4550000

Mineral-*form*

Sassolite

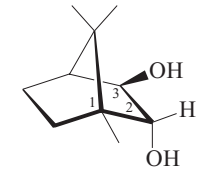
White to grey soft pearly triclinic cryst.

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 1246A (*ir*)
Zachariasen, W.H. *et al., Acta Cryst.*, 1954, **7**, 305 (*cryst struct*)
Sciarra, E. *et al., J. Am. Pharm. Assoc., Sci. Ed.*, 1960, **49**, 116 (*tox*)
Craven, B.M. *et al., Acta Cryst.*, 1966, **20**, 214 (*nd*)
Nöth, H. *et al., NMR Spectroscopy of Boron Compounds (NMR Basic Principles and Progress)*, Springer Verlag, 1978, (*B-11 nmr*)
Mellor Compr. Treat. Inorg. Theor. Chem., 1980, **5**, 224 (*rev, bibl*)
Butler, L.G. *et al., J. Magn. Reson.*, 1981, **42**, 120 (*nqr*)
Janda, R. *et al., Spectrochim. Acta A*, 1981, **36**, 997 (*ir, Raman*)
Houlsby, R.D. *et al., Antimicrob. Agents Chemother.*, 1986, **29**, 803 (*pharmacol*)
Gmelin Handbook Inorg. Chem., Syst. No. 13, *3rd Suppl.*, 1987, **2**, 96 (*rev, bibl*)
Kirk-Othmer Encycl. Chem. Technol., 4th edn., Wiley, 1991, **4**, 365 (*manuf, props, uses*)
Treinen, K.A. *et al., Toxicol. Appl. Pharmacol.*, 1991, **107**, 325 (*tox*)
Heindel, J.J. *et al., Fundam. Appl. Toxicol.*, 1992, **18**, 266 (*tox*)
Von Burg, R. *et al., J. Appl. Toxicol.*, 1992, **12**, 149 (*tox, rev*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1343
Encyclopedia of Reagents for Organic Synthesis, (ed. Paquette, L.A.), Wiley, 1995, **1**, 644-645 (*use*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 291-292
Stokinger, H.E. *et al., Patty's Ind. Hyg. Toxicol. (3rd Rev. edn.)*, Vol. 2, Wiley, 1980, **2B**, 2984 (*tox*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMC000

2,3-Bornanediol, 8CI B-254

1,7,7-Trimethylbicyclo[2.2.1]heptane-2,3-diol, 9CI. 2,3-Camphanediol

[45980-02-7, 30128-51-9, 56614-57-4, 38226-15-2, 30226-61-0, 56614-58-5, 64911-69-9, 13837-85-9, 30128-49-5]



(1*R*,2*R*,3*R*)–*form*

$C_{10}H_{18}O_2$ 170.251

(1*R*,2*R*,3*R*)-*form* [68738-11-4]

(+)-endo,exo-*form*

Cryst. (C_6H_6/petrol). Mp 254-256°. $[\alpha]_D$ +15 (c, 1.5 in EtOH).

2-Ac: [61586-52-5] ***Vulgarole***†

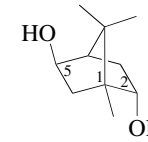
$C_{12}H_{20}O_3$ 212.288

Constit. of oil of *Artemisia vulgaris* (mugwort). Thick oil. Rel. config. only detd., could be the enantiomer.

Nano, G.M. *et al., Planta Med.*, 1976, **30**, 211-215 (*Vulgarole*)

2,5-Bornanediol B-255

1,7,7-Trimethylbicyclo[2.2.1]heptane-2,5-diol. 5-Hydroxyborneol



(1*R*,2*S*,5*R*)-*form*

$C_{10}H_{18}O_2$ 170.251

(1*R*,2*S*,4*R*,5*R*)-*form* [32751-73-8]

2-O-β-D-Glucopyranoside: [117615-23-3] ***Amomumoside***

$C_{16}H_{28}O_7$ 332.393

Amorph. powder. $[\alpha]_D^{20}$ -12.6 (c, 0.6 in MeOH).

2,5-Di-O-β-D-glucopyranoside: [870722-04-6] ***Zingiberoside A***

$C_{22}H_{38}O_{12}$ 494.535

Constit. of *Zingiber officinale* rhizome. Powder. Mp 136-139° dec. $[\alpha]_D^{21}$ -40.7 (c, 1.27 in MeOH).

2-O-[3S-Hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranoside]: [870722-06-8] ***Zingiberoside C***

$C_{22}H_{36}O_{11}$ 476.52

Constit. of *Zingiber officinale* rhizome. Oil. $[\alpha]_D^{21}$ -1.3 (c, 2.27 in MeOH).

2-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [870722-05-7] ***Zingiberoside B***

$C_{21}H_{36}O_{11}$ 464.509

Constit. of *Zingiber officinale* rhizome. Oil. $[\alpha]_D^{21}$ -50.5 (c, 1 in MeOH).

Me ester, 2-O-[3S-hydroxy-3-methylglutaroyl-(→6)-β-D-glucopyranoside]: [870555-73-0]

$C_{23}H_{38}O_{11}$ 490.547

Constit. of *Zingiber officinale* rhizome. Oil. $[\alpha]_D^{20}$ -14.3 (c, 0.4 in MeOH).

(1*S*,2*R*,4*S*,5*S*)-*form* [64911-68-8]

Angelicoidenol

[64854-31-5]

Cryst. ($CHCl_3$). Mp 255-257°. $[\alpha]_D^{25}$ -16.12 (c, 0.46 in MeOH).

2-O-β-D-Glucopyranoside: [118374-08-6]
$C_{16}H_{28}O_7$ 332.393
Amorph. powder. $[\alpha]_D^{20}$ -26.3 (c, 1 in MeOH).

2-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [217969-13-6]
$C_{21}H_{36}O_{11}$ 464.509
Amorph. powder. $[\alpha]_D^{22}$ -49 (c, 1.7 in MeOH).

2-O-E-Cinnamoyl: [934362-36-4]
$C_{19}H_{24}O_3$ 300.397
Oil.

2-O-E-Cinnamoyl, 5-Ac: [934362-37-5]
$C_{21}H_{26}O_4$ 342.434
Oil.

2-O-(4-Hydroxy-E-cinnamoyl): [934362-38-6]
$C_{19}H_{24}O_4$ 316.396
Oil.

2-O-(4-Hydroxy-Z-cinnamoyl): [934362-39-7]
$C_{19}H_{24}O_4$ 316.396
Oil.

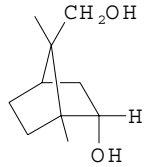
(1*R,2*S**,4*R**,5*R**)-*form*** [10359-41-8]

[10359-43-0, 10359-42-9]

Marquet, A. *et al., Bull. Soc. Chim. Fr.*, 1967, 128 (*synth*)
Allen, M.S. *et al., Can. J. Chem.*, 1979, **57**, 733 (*synth*)
Mahmood, U. *et al., Phytochemistry*, 1983, **22**, 774-776 (*Angelicoidenol*)
Gunawardana, Y.A.G.P. *et al., J. Nat. Prod.*, 1988, **51**, 142 (*isol, cmr, pmr*)
Inoshiri, S. *et al., Phytochemistry*, 1988, **27**, 2869-2871 (*Berchemia racemosa constits*)
Ahmed, A.A. *et al., Phytochemistry*, 1991, **30**, 1207 (*isol*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1595-1598 (*glycosides*)
Hori, Y. *et al., Heterocycles*, 2005, **65**, 2357-2367 (*Zingiberosides A-C*)
Lu, Z.-Q. *et al., J. Asian Nat. Prod. Res.*, 2006, **8**, 187-192 (*Conocephalum conicum esters*)

2,9-Bornanediol B-256

Vicodiol [128898-66-8]



$C_{10}H_{18}O_2$ 170.251
Cryst. ($CHCl_3$/hexane). Mp 242-244°. $[\alpha]_D$ -17 (c, 1 in $CHCl_3$).

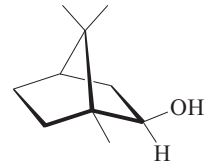
2-O-β-D-Glucopyranoside: [827038-27-7]
$C_{16}H_{28}O_7$ 332.393
Isol. from thyme. Amorph. powder. $[\alpha]_D^{23}$ -48 (c, 1.7 in MeOH).

2-O-[β-D-Apiofuranosyl-(1→6)-β-D-glucopyranoside]: [217969-26-1]
$C_{21}H_{36}O_{11}$ 464.509
Amorph. powder. $[\alpha]_D^{22}$ -61.9 (c, 1.2 in MeOH).

Vasanth, S. *et al., J. Nat. Prod.*, 1990, **53**, 354 (*isol, pmr, cmr, cryst struct*)
Kitajima, J. *et al., Chem. Pharm. Bull.*, 1998, **46**, 1595-1598 (*glycoside*)
Kitajima, J. *et al., Phytochemistry*, 2004, **65**, 3279-3287 (*2-glucoside*)

2-Bornanol B-257

1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol. 2-Hydroxybornane. Bingpian [10385-78-1]



(1*R*,2*R*)–*form*

$C_{10}H_{18}O$ 154.252
Both Borneol and Isoborneol and their acetates and formates are used as flavouring agents.

(1*R*,2*R*)-*form* [10334-13-1]
(-)-Isoborneol. *β-Camphol. Isocamphol. FEMA 2158*
Flavouring agent. Cryst. (petrol). Mp 212° (sealed tube). $[\alpha]_D^{20}$ -32.3 (MeOH).

(1*R*,2*S*)-*form* [464-43-7]
(+)-Borneol. *(+)-Bornyl alcohol. Borneo camphor. FEMA 2157*
Constit. of *Curcuma aromatica* and other plants. Cryst. (petrol). Mp 208°. Bp 212°. $[\alpha]_D^{20}$ +37.7 (c, 5 in EtOH).
▶ ED7060000

Formyl: [7492-41-3] *Bornyl formate. FEMA 2161*
$C_{11}H_{18}O_2$ 182.262
Flavouring agent. Liq. d^{20} 1.01. Bp_{21} 106-108°. n_D^{20} 1.4689.

Butanoyl: [13109-70-1] *Bornyl butyrate. FEMA 3907*
$C_{14}H_{24}O_2$ 224.342
Flavouring agent. d^{18} 0.97. Bp_{22} 141-143°. n_D^{18} 1.4638.

Pentanoyl: [7549-41-9] *Bornyl valerate. FEMA 2164*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Bp 249°. n_D^{20} 1.4615.

3-Methylbutanoyl: [76-50-6] *Bornyl isovalerate. FEMA 2165*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Oil. d^{18} 0.95. Bp_{26} 151-152°. n_D^{18} 1.4605.

(1*S*,2*R*)-*form* [464-45-9]
(-)-Borneol. *Linderol. Ngai camphor. FEMA 2157*
Constit. of *Blumea balsamifera* (sambong). Cryst. (petrol). Mp 208-209°. Bp 212°. $[\alpha]_D^{20}$ -37.74 (c, 5 in EtOH).
▶ Skin irritant. LD_{50} (rat, orl) 5800 mg/kg.
DT5095000

Ac: [5655-61-8] *(-)-Bornyl acetate. FEMA 4080*
$C_{12}H_{20}O_2$ 196.289
Isol. from carrot, rosemary and sage. Flavouring agent. Sol. MeOH, Et_2O; fairly sol. H_2O. Mp 27-29°. Bp 223-224° Bp_{14} 103°. $[\alpha]_D^{20}$ -38.1 (neat).

E-*Cinnamoyl:* [6330-67-2] ***Bornyl cinnamate***
[400763-27-1, 77942-64-4]
$C_{19}H_{24}O_2$ 284.397
Constit. of the roots of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Pale yellow oil.

O-*(3,4-Methylenedioxy-E-cinnamoyl):* [400771-30-4]
$C_{20}H_{24}O_4$ 328.407
Constit. of the roots of *Piper methysticum* (kava). FDA advises against use of kava in food due to potential risk of severe liver damage (2002). Needles (MeOH). Mp 138-140°.

(1*S*,2*S*)-*form* [16725-71-6]
(+)-Isoborneol. FEMA 2158
Flavouring agent. Cryst. (petrol). Mp 214°. $[\alpha]_D$ +33.89 (EtOH).

(1*RS*,2*RS*)-*form* [6627-72-1]
(±)-Isoborneol
Plates (petrol). Prac. insol. H_2O. Mp 212° (sealed tube).

Formyl: [1200-67-5] *Isobornyl formate. FEMA 2162*
$C_{11}H_{18}O_2$ 182.262
Flavouring agent. d^{18} 1. Bp_{20} 110°. n_D^{20} 1.4717.

Propanoyl: [2756-56-1] *Isobornyl propionate. FEMA 2163*
$C_{13}H_{22}O_2$ 210.316
Flavouring agent. Oil. $d^{15.5}$ 0.98. Bp 245°. n_D^{20} 1.4640.

3-Methylbutanoyl: [7779-73-9] *Isobornyl isovalerate. FEMA 2166*
$C_{15}H_{26}O_2$ 238.369
Flavouring agent. Liq.

(1*RS*,2*SR*)-*form* [24393-70-2]
(±)-Borneol. FEMA 2157
Flavouring agent. Mp 210-215° subl.
▶ Fl. p. 66°.

Ac: [125-12-2] *FEMA 2159*
Flavour and fragrance ingredient. Liq. or solid. Mp 26-29°. Bp 228-231°.

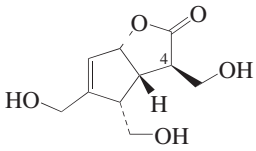
[16868-11-4, 507-70-0, 124-76-5]

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 169B; 169C; 631C (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 251A; 251B; 954A (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 246A; 246B; 660A (*ir, Ac*)
Karrer, W. *et al., Konstitution und Vorkommen der Organischen Pflanzenstoffe, 2nd edn., Birkhuser Verlag*, 1972, nos. 312; 313 (*occur*)
Oratani, T. *et al., Agric. Biol. Chem.*, 1974, **38**, 1961-1964 (*resoln*)
Gream, G.E. *et al., Aust. J. Chem.*, 1974, **27**, 567-587 (*(+)-Borneol, (-)-Isoborneol, synth*)
Helmchen, G. *et al., Tet. Lett.*, 1974, 1527-1530 (*abs config*)
Bohlmann, F. *et al., Org. Magn. Reson.*, 1975, **7**, 426-432 (*cmr*)
Tadesa, K. *et al., Agric. Biol. Chem.*, 1976, **40**, 1069-1073 (*biosynth*)
Stothers, J.B. *et al., Can. J. Chem.*, 1976, **54**, 1211-1221 (*cmr, biosynth*)
Yamaguchi, S. *et al., Tet. Lett.*, 1977, 89 (*config, pmr*)
Jonsson, S. *et al., J. Chem. Ecol.*, 1988, **14**, 713-721 (*occur*)
Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 1409
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 292-297; 1435-1440
Wu, D. *et al., J. Agric. Food Chem.*, 2002, **50**, 701-705 (*cinnamoyl ester, methylenedioxycinnamoyl ester*)
Fenaroli's Handbook of Flavor Ingredients, 6th edn., (ed. Burdock, G.A.), CRC Press, 2009, 169-175; 975-979 (*use, props, occur, esters*)

Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMD000; IHY000; NCQ820

Borreriagenin B-258

Morindacin [249916-07-2]
[877265-21-9 (Morindacin)]



$C_{10}H_{14}O_5$ 214.218

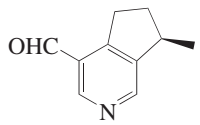
Struct. of Morindacin revised in 2006. Foam or syrup. $[\alpha]_D^{25}$ -1.3 (c, 0.79 in MeOH). $[\alpha]_D^{26}$ +2 (c, 0.2 in MeOH) (Morindacin). λ_{max} 210 (no solvent reported).

4-Epimer: [909389-73-7] ***4-Epiborreriagenin***
$C_{10}H_{14}O_5$ 214.218
Constit. of the fruit of *Morinda citrifolia* (noni). Powder. $[\alpha]_D^{27}$ -5 (c, 0.2 in MeOH). λ_{max} 197; 242 (MeOH).

Vieira, I.J.C. *et al., Org. Lett.*, 1999, **1**, 1169-1171 (*Borreriagenin*)
Kamiya, K. *et al., Chem. Pharm. Bull.*, 2005, **53**, 1597-1599 (*Morindacin, isol*)
Samoylenko, V. *et al., J. Agric. Food Chem.*, 2006, **54**, 6398-6402 (*4-Epiborreriagenin*)
Schripsema, J. *et al., Org. Lett.*, 2006, **8**, 5337-5340 (*struct*)

Boschniakine B-259

Indicaine†



(*R*)-*form*

$C_{10}H_{11}NO$ 161.203

(*R*)-*form* [18070-40-1]
Alkaloid from *Plantago psyllium* (African plantain). Bp_3 80-90°. $[\alpha]_D^{20}$ +21 (c, 0.98 in $CHCl_3$).

Picrate: Mp 126-128° Mp 156° (dimorph.).

Semicarbazone: Mp 217-220° (210-224°).

N-*Et:* [32152-74-2] ***Indicainine***
$C_{12}H_{16}NO^{\oplus}$ 190.264
Mp 125-127° (as picrate). $[\alpha]_D^{30}$ +14.2 (c, 1.9 in $CHCl_3$) (picrate). The correctness of the struct. has been questioned (D. Gross *et al*).

Carboxylic acid: [21857-97-6] ***Boschniakinic acid***. *Plantagonine*
$C_{10}H_{11}NO_2$ 177.202
Alkaloid from *Plantago psyllium* (African plantain). Mp 218-220°. $[\alpha]_D$ +38.6 (+ 30.8). λ_{max} 271 (log ϵ 3.5) (MeOH).

(*S*)-*form*
Carboxylic acid: [21913-34-8]
Mp 218-220°. $[\alpha]_D$ -30.1.

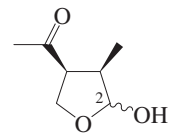
(±)-*form*
Carboxylic acid: Mp 226-227°.

(ξ)-*form*
Carboxylic acid, Me ester: [94054-29-2]
Deoxyrhexifoline
$C_{11}H_{13}NO_2$ 191.229
$[\alpha]_D^{20}$ -18 (c, 0.3 in $CHCl_3$) (synthetic). Abs. config. of natural product not detd. due to paucity of material. The *S*-enantiomer was synthesised as a foam.

Sakan, T. *et al., Tetrahedron*, 1967, **23**, 4635-4652 (*Boschniakine, Boschniakinic acid, uv, ir, synth, struct*)
Torssell, K. *et al., Acta Chem. Scand.*, 1968, **22**, 2715 (*struct*)
Dickinson, E.M. *et al., Tetrahedron*, 1969, **25**, 1523 (*pmr*)
Khakimdzhanov, S. *et al., Khim. Prir. Soedin.*, 1971, **7**, 126-127; *Chem. Nat. Compd. (Engl. Transl.)*, 1971, **7**, 121 (*Indicainine*)
Gross, D. *et al., Z. Chem.*, 1973, **13**, 296 (*ms*)
Cordell, G.A. *et al., Alkaloids (Academic Press)*, 1977, **16**, 431 (*rev*)
Roby, M.R. *et al., J. Nat. Prod.*, 1984, **47**, 846-853 (*Deoxyrhexifoline*)
Ranarivelo, Y. *et al., Heterocycles*, 1990, **31**, 1727-1731 (*(-)-Deoxyrhexifoline, synth*)
Ho, H.-Y. *et al., J. Chem. Ecol.*, 1993, **19**, 39-46 (*Megacrania, isol*)
Lin, L.-C. *et al., Chin. Pharm. J. (Taipei)*, 2004, **56**, 77-85 (*Boschniakinic acid, isol, pmr, cmr*)
Fu, J.-J. *et al., Helv. Chim. Acta*, 2007, **90**, 2151-2155 (*isol, pmr, cmr*)
Robert, N. *et al., Tetrahedron*, 2007, **63**, 3702-3706 (*synth*)

Botryodiplodin B-260

1-(Tetrahydro-5-hydroxy-4-methyl-3-furanyl)ethanone, 9CI. 4-Acetyl-2-hydroxy-3-methyltetrahydrofuran [27098-03-9]



Absolute Configuration

$C_7H_{12}O_3$ 144.17

Exists as a mixt. of anomeric forms in soln. Mycotoxin prod. by *Botryodiplodia theobromae*, *Penicillium carneoluteus* and from *Penicillium roquefortii* infected corn silage. Cryst. (Et_2O). Sol. H_2O, Me_2CO, MeOH, EtOH, Et_2O; fairly sol. C_6H_6, hexane, $CHCl_3$. Mp 50-52°. $[\alpha]_D^{25}$ -70 (c, 0.12 in MeOH). λ_{max} 278 (ϵ 25) ($CHCl_3$) (Berdy).

▶ LD_{50} (mus, ipr) 40-50 mg/kg. OB6005000

Ac:
Cryst. (Et_2O). Mp 45-47°. $[\alpha]_D$ -104 (c, 0.09 in $CHCl_3$).

2-O-(2-Phenylethyl): [948039-58-5] ***2-(2-Phenylethoxy)botryodiplodin***
$C_{15}H_{20}O_3$ 248.321
Oil. $[\alpha]_D^{25}$ +13.3 (c, 0.75 in $CHCl_3$).

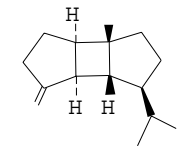
[95976-07-1, 95976-08-2, 81738-55-8]

McCurry, P.M. *et al., JACS*, 1973, **95**, 5824-5825 (*synth, stereochem*)

Wilson, S.R. *et al., JOC*, 1975, **40**, 3309-3311 (*synth*)
Sakai, K. *et al., Tet. Lett.*, 1979, **20**, 2365-2368 (*synth, abs config*)
Moreau, S. *et al., JOC*, 1982, **47**, 2358-2359 (*isol, cryst struct*)
Renauld, F. *et al., Tetrahedron*, 1984, **40**, 1823-1834 (*biosynth*)
Kurth, M.J. *et al., JOC*, 1985, **50**, 1840-1845 (*synth*)
Rehnberg, N. *et al., Acta Chem. Scand.*, 1990, **44**, 377-383 (*synth*)
Dulcere, J.P. *et al., Nat. Prod. Rep.*, 1992, **1**, 209-212 (*synth*)
Villar, F. *et al., Tet. Lett.*, 1999, **40**, 3375-3378 (*synth*)
Andrey, O. *et al., Tet. Lett.*, 2003, **44**, 7901-7904 (*synth*)
Nouguier, R. *et al., Tetrahedron: Asymmetry*, 2003, **14**, 3005-3018 (*synth*)
De Buyck, L. *et al., Tet. Lett.*, 2006, **47**, 7759-7762 (*synth*)
Cabedo, N. *et al., J. Agric. Food Chem.*, 2007, **55**, 6977-6983 (*isol, activity, bibl*)
Ramezani, M. *et al., J. Nat. Prod.*, 2007, **70**, 128-129 (*isol, pmr, cmr*)
Shier, W.T. *et al., Toxin Rev.*, 2007, **26**, 343-386 (*rev*)
Lewis, R.J. *et al., Sax's Dangerous Properties of Industrial Materials, 8th edn., Van Nostrand Reinhold*, 1992, BMK290

4(15)-Bourbonene B-261

β-Bourbonene [5208-59-3]



$C_{15}H_{24}$ 204.355
Flavouring agent. Oil. $[\alpha]_D^{20}$ -92.12.

ent-form [68036-15-7]
(+)-β-Bourbonene

7-Epimer: [92998-16-8] ***(+)-β-Epibourbonene***
$C_{15}H_{24}$ 204.355
Oil. $[\alpha]_D$ +94 (c, 1.02 in $CHCl_3$).

Křepinský, J. *et al., Tet. Lett.*, 1966, **7**, 359-367 (*struct*)
Krepinský, J. *et al., Tet. Lett.*, 1966, **7**, 3209-3214 (*abs config*)
White, J.D. *et al., JACS*, 1968, **90**, 6171-6177 (*synth*)
Naya, Y. *et al., Experientia*, 1978, **34**, 984-986 (*Ceroplastes ceriferus constit*)
Tomioka, K. *et al., Tet. Lett.*, 1982, **23**, 3401-3404 (*synth*)
Gopichand, Y. *et al., J. Nat. Prod.*, 1984, **47**, 607-614 (*Eunicea succinea constit*)
Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 298-299
Bülow, N. *et al., Phytochemistry*, 2000, **55**, 141-168 (*biosynth, pmr, cmr*)

Bovicins B-262

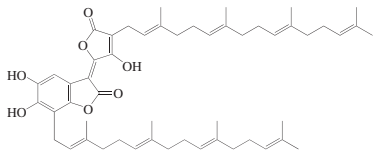
Lantibiotics.

Bovicin 255 [332091-52-8]
Peptide. Prod. by rumen *Streptococcus* LRC0255.

Bovicin HC5 [497259-32-2]
Peptide, MW *ca.* 2440 Da. Prod. by *Streptococcus bovis* HC5.

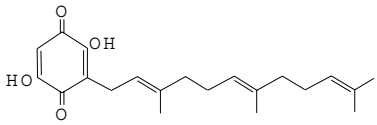
Bovicin HJ50 [757977-34-7]
Peptide. Isol. from *Streptococcus bovis* HJ50.
Whitford, W.F. *et al., Appl. Environ. Microbiol.*, 2001, **67**, 569-574 (*Bovicin 255, isol*)
Mantovani, H.C. *et al., Microbiology (Reading, U.K.)*, 2002, **148**, 3347-3352 (*Bovicin HC5, isol*)
Xiao, H. *et al., Microbiology (Reading, U.K.)*, 2004, **150**, 103-108 (*Bovicin HJ50, isol*)
Mantovani, H.C. *et al., Antimicrob. Agents Chemother.*, 2008, **52**, 2247-2249 (*HC5, props*)
Ni, J. *et al., Appl. Environ. Microbiol.*, 2011, **77**, 407-415 (*HJ50, biosynth*)
Lin, Y. *et al., Microbiol. Res.*, 2011, **166**, 146-154 (*HJ50, struct*)

Bovilactone 4.4 **B-263**
2,11-Bis(geranylgeranyl)gomphilactone [79839-34-2]



$C_{52}H_{70}O_7$ 807.121
Isol. from *Suillus bovinus* (amitake mushroom). Brownish oil. λ_{max} 275 (log ϵ 4.06); 382 (log ϵ 3.92); 460 (log ϵ 3.95) (MeOH).
Mühlbauer, A. *et al., Tet. Lett.*, 1998, **39**, 5167-5170 (*biosynth*)
Lang, M. *et al., Eur. J. Org. Chem.*, 2008, 3544-3551 (*biosynth, pmr, cmr*)

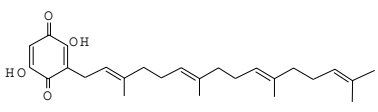
Boviquinone 3 **B-264**
2,5-Dihydroxy-3-(3,7,11-trimethyl-2,6,10-dodecatrienyl)cyclohexadiene-1,4-dione, 9CI. 3-Farnesyl-2,5-dihydroxy-1,4-benzoquinone. Helveticone [32916-10-2]



$C_{21}H_{28}O_4$ 344.45

(*E*,*E*)-*form* [34198-83-9]
Pigment from *Chroogomphus rutilus* (pine spike cap). Yellow cryst. (petrol). Mp 98-100°. λ_{max} 287 (log ϵ 4.33) (EtOH).
Beaumont, P.C. *et al., JCS(C)*, 1971, 2582-2585 (*isol, struct*)
Esser, F. *et al., Z. Naturforsch., B*, 1971, **26**, 336-338 (*isol, ir, uv, pmr, ms*)
Mühlbauer, A. *et al., Tet. Lett.*, 1998, **39**, 5167-5170 (*biosynth*)

Boviquinone 4 **B-265**
3-Geranylgeranyl-2,5-dihydroxy-1,4-benzoquinone. Bovinone [28129-52-4]



$C_{26}H_{36}O_4$ 412.568
Metab. of *Suillus bovinus*. Yellow cryst. (AcOH). Sol. MeOH, C_6H_6; poorly sol. H_2O. Mp 84-85°. λ_{max} 287 (ϵ 20500) (EtOH). λ_{max} 324 (EtOH/NaOH).
Beaumont, P.C. *et al., JCS(C)*, 1969, 2398-2403 (*isol*)
Mühlbauer, A. *et al., Tet. Lett.*, 1998, **39**, 5167-5170 (*biosynth*)
Lang, M. *et al., Eur. J. Org. Chem.*, 2008, 3544-3551 (*isol, biosynth, pmr, cmr*)

Brachyurin **B-266**
E.C. 3.4.21.32. Collagenolytic protease. Crab protease I. Crab protease II [848900-32-3]
Serine endopeptidase enzyme. Isol. from various crustaceans, e.g. crab, shrimp; also from fish, e.g. cod. Filefish (*Novoden modestrus*) enzyme activity range pH 6.5-8.5. Crab enzyme (*Carcinus maenas*) stable for over 1 month at r.t.
Grant, G.A. *et al., Methods Enzymol.*, 1981, **80**, 722-734 (*fiddler crab*)
Lu, P.J. *et al., Biol. Chem. Hoppe-Seyler*, 1990, **371**, 851-859 (*shrimp*)
Kristjansson, M.M. *et al., Comp. Biochem. Physiol., B: Biochem. Mol. Biol.*, 1995, **110**, 707-717 (*cod*)
Roy, P. *et al., Comp. Biochem. Physiol., B: Biochem. Mol. Biol.*, 1996, **115**, 87-95 (*crab, stability*)
Kim, S.K. *et al., J. Biochem. Mol. Biol.*, 2002, **35**, 165-171 (*filefish, activity*)
Rudenskaya, G.N. *et al., Russ. J. Bioorg. Chem. (Engl. Transl.)*, 2003, **29**, 101-111 (*rev*)

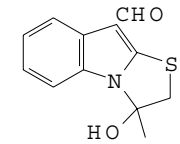
***Oncorhynchus mykiss* Bradykinin-related peptides** **B-267**
Arg-Arg-Pro-Pro-Gly-Trp-Ser-Pro-Leu-Arg
Struct. of Trout[Arg0]BK shown. Isol. from plasma of the rainbow trout *Oncorhynchus mykiss*.

Trout[Arg0]BK [178062-07-2]
Cod[Arg0]BK
$C_{55}H_{88}N_{20}O_{12}$ 1221.427
Also isol. from plasma of the Atlantic cod *Gadus morhua*.

Trout[Lys0]BK [152273-88-6]
$C_{55}H_{88}N_{18}O_{12}$ 1193.414
Conlon, J.M. *et al., FEBS Lett.*, 1993, **334**, 75-78 (*isol*)
Conlon, J.M. *et al., Peptides (N.Y.)*, 1996, **17**, 531-537 (*isol*)
Platzack, B. *et al., Am. J. Physiol.*, 1997, **272**, R710-R717 (*isol*)

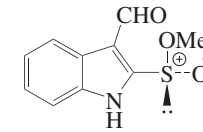
Branched-chain amino acid transaminase **B-268**
E.C. 2.6.1.42. Branched-chain amino-acid:2-oxoglutarate aminotransferase. Branched-chain amino acid aminotransferase. Transaminase B. BCAT [9054-65-3]
Aminotransferase enzyme. Isol. from pig. Also acts on L-isoleucine and L-valine.
Taylor, R.T. *et al., J. Biol. Chem.*, 1966, **241**, 4396-4405 (*pig heart*)
Aki, K. *et al., Biochim. Biophys. Acta*, 1968, **159**, 276-284 (*rat liver*)
Aki, K. *et al., J. Biochem. (Tokyo)*, 1969, **65**, 539-544 (*hog brain*)
Jenkins, W.T. *et al., Methods Enzymol., Part A*, 1970, **17**, 802-807 (*pig heart*)
Aki, K. *et al., Methods Enzymol., Part A*, 1970, **17**, 807-811 (*pig heart*)
Aki, K. *et al., Methods Enzymol., Part A*, 1970, **17**, 811-814 (*hog brain*)
Kawagishi, S. *et al., Arch. Oral Biol.*, 1983, **28**, 303-306 (*rat submandibular gland*)
Korpela, T.K. *et al., Methods Enzymol.*, 1988, **166**, 269-274 (*pig heart*)
Kamitori, S. *et al., J. Biochem. (Tokyo)*, 1989, **105**, 671-672 (*Escherichia coli*)
Wallin, R. *et al., J. Biol. Chem.*, 1990, **265**, 6019-6024 (*rat heart*)

Brassicanal B **B-269**
2,3-Dihydro-3-hydroxy-3-methylthiazolo[3,2-a]indole-9-carboxaldehyde, 9CI [126654-63-5]



$C_{12}H_{11}NO_2S$ 233.29
Exists in CD_3OD as an equilibrium mixt. of the hemiaminal (illus.) and open-chain keto form. Alkaloid from Chinese cabbage *Brassica campestris* ssp. *pekinensis* inoculated with *Pseudomonas cichorii*. Mp 169-170°. $[\alpha]_D$ 0. λ_{max} 207 (ϵ 25800); 220 (ϵ 25400); 252 (ϵ 24100); 277 (ϵ 14200); 315 (ϵ 11700) (MeOH) (Berdy).
Monde, K. *et al., Chem. Lett.*, 1990, 209 (*isol, uv, ir, pmr, cmr, ms, struct*)

Brassicanal C **B-270**
Methyl 3-formyl-1H-indole-2-sulfinate, 9CI [137761-23-0]



$C_{10}H_9NO_3S$ 223.252
Alkaloid from *Brassica oleracea* (cabbage) inoculated with *Pseudomonas cichorii*. Mp 150-151°. $[\alpha]_D$ -13.3 (c, 1.04 in MeOH) (natural). $[\alpha]_D$ -231 (c, 0.2 in MeOH) (synthetic). λ_{max} 215 (ϵ 18300); 247 (ϵ 13600); 309 (ϵ 9400) (MeOH).
Monde, K. *et al., Phytochemistry*, 1991, **30**, 2915-2917 (*isol, uv, ir, pmr, cmr, ms*)
Pedras, M.S.C. *et al., Phytochemistry*, 2006, **67**, 1503-1509 (*synth*)
Taniguchi, T. *et al., Org. Biomol. Chem.*, 2008, 4399-4405 (*ecd, vcd, abs config*)

Brassinin **B-271**
Methyl (1H-indol-3-ylmethyl)carbamodithioate, 9CI [105748-59-2]