Compendium of food additive specifications

Addendum 12

Joint FAO/WHO Expert Committee on Food Additives (JECFA)
63rd Meeting

Geneva, Italy, 8–17 June 2004

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Contents

Introduction

This volume contains specifications of identity and purity prepared at the 63rd meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), held in Geneva, 8-17 June 2004. These specifications should be considered only in conjunction with the report of the above meeting which will be printed in the WHO Technical Report Series. Toxicological monographs of the substances considered at the 63rd meeting of JECFA will be published in the WHO Food Additives Series.

The general principles applied in the elaboration of specifications established at the earlier JECFA sessions have been published in the Principles for the Safety Assessment of Food Additives and Contaminants in Food, WHO Environmental Health Criteria, No. 70, 1987. The specifications of identity and purity of food additives established by JECFA are meant to identify the substance that has been subject to biological testing, to ensure that the substance is of adequate degree of purity for safe use in food, and to reflect and encourage good manufacturing practices. These principles were last reaffirmed by the 59th session of JECFA in 2002.

The specifications are mainly established for the use of toxicologists and others concerned with the identity and purity of the substance. As agreed by JECFA at its 26th meeting, specifications may also be established prior to the eventual completion of toxicological evaluation, in certain cases, when the available toxicological data are inadequate or incomplete, and do not permit the establishment of full or temporary acceptable daily intakes (ADIs). References are made in individual specifications to some of the criteria that may be of interest in commerce, but they do not necessarily include all the requirements of interest to the commercial user. These specifications are not more stringent than is necessary to accomplish their purpose and should easily be attainable by the producing industries. The report of the 23rd meeting gives the reasons why certain specifications are designated as "tentative".

There were a total of 217 specifications (twenty food additives, uses other than flavouring agent; 197 flavouring agents) considered at the 63rd meeting: Specifications for 186 compounds were newly adopted, of which five remained tentative. 31 specifications were revised of which three remained tentative.

NOTE: Use of (FNP 5) in specifications refers to General Methods (Guide to JECFA Specifications), FAO Food and Nutrition Paper 5/Rev. 2 (1991).

Notes to the reader

On-line edition of the Compendium of food additive specifications

A consolidated edition of the *Compendium of food additive specifications* is now available at FAO's JECFA Web page at *http://www.fao.org/es/esn/jecfa/index_en.stm.* The edition is divided into two sections: one covering flavouring agents and the other covering all other food additives. Users can search by additive name or number (INS, JECFA No., FEMA, CAS). For additives other than flavouring agents, they can also search by functional use and purity criteria. Searches can also be conducted for all specifications designated as tentative. The analytical methods for food additives which are published as Guide to JECFA Specifications (FAO Food and Nutrition Paper 5/Rev. 2), can be accessed as well, even with a direct link from the single specification.

Limits for heavy metals in food additives

An explanatory note is available at the FAO Joint Secretariat's Web page. It should be noted that the revision of the limit test for heavy metals constitutes a change of the specifications in its own right. For a food additive the valid JECFA specification consists of the specification as originally published plus the modifications introduced by the revision of the heavy metal test. Modified specifications will be republished in a consolidated second edition of the *Compendium of food additive specifications* (FAO Food and Nutrition Paper 52).

Chemical and Technical Assessments (CTA)

The CTAs which were prepared at the 61st and 63rd meeting are published electronically at FAO's JECFA webpage http://www.fao.org/es/ESN/jecfa/chemical_assessment_en.stm.

Comments and feedback

The FAO Joint Secretariat to JECFA welcomes and encourages any feedback on this volume and the online edition of the Compendium. Suggestions on how the availability of the results of JECFA's work can be improved are welcome. Please send your comments to:

jecfa@fao.org

Joint FAO/WHO Expert Committee on Food Additives, 63rd Meeting, Geneva, 8–17 June 2004

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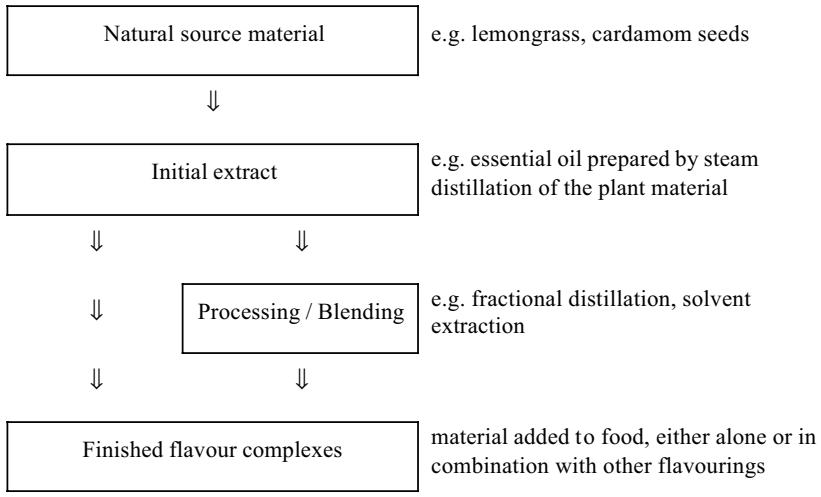
Section A: Principles governing the establishment and revision of specifications

Flavour complexes derived from natural sources

At this meeting, the Committee further considered a possible approach to the safety assessment of complex flavours derived from natural sources (usually from plant material) such as essential oils, oleoresins and solvent extracts. After considering the available data on three of the five flavour complexes originally included on the agenda – derived from essential oils of lemongrass, cardamom seed and bois de rose – the Committee defined the information that would be required in order to test the application of the revised Procedure for the Safety Evaluation of Flavouring Agents (Annex 1 Ref 131) which it had previously adopted for the safety evaluation of chemically-defined flavourings.

Background

Although these flavourings are typically named after the initial extract prepared from the source material, it is common practice for the initial extracts to be processed and refined in a variety of ways, to produce a range of flavour complexes with the specific properties desired for particular food applications. These processes might include distillation, concentration, solvent extraction and blending of extracts from different batches. Processing is generally carried out by flavour companies or, in certain cases, possibly by food manufacturers who use the finished flavours. The progression from source material to finished flavour is illustrated below:



The initial extracts are typically prepared from the plant material close to the point of production. Their composition may vary considerably at this level due to a variety of factors such as climate, geography, genotype and maturity of the source material. The flavour producer aims to supply flavour complexes with consistent technical and olfactory properties. This is primarily achieved by processing and blending to meet a target composition which is monitored by chemical analysis.

Although the finished flavour complexes are entirely derived from the original extract, using only physical processes such as those described above, their composition is likely to differ quantitatively from the initial extracts prepared directly from the source material.

The evaluation of finished flavour complexes is dependent upon:

(a) Information on the composition of the material that is added to food (and hence on the elaboration of a reliable specification that covers the range of finished flavour complexes that may be derived from the initial extracts);

(b) Safety evaluations of the individual components and congeneric groups

(c) Estimates of intake of the finished flavour complexes and, hence of the individual components.

Compositional data necessary to support the safety evaluation of a finished flavour complex

i. General considerations

The safety evaluations of finished flavour complexes derived from natural sources would be based on the revised Procedure, with particular consideration of the major components and of congeneric groups. The analytical data should be adequate to apply the revised Procedure.

Intake should be taken into account in determining the extent to which chemical characterisation and identification of individual components is necessary, beyond those necessary to define their flavour characteristics. In applying the Revised Procedure for the Safety Evaluation of Flavouring Agents the estimated intake of the individual agent is compared with appropriate thresholds of toxicological concern to determine whether or not the intake represents a safety concern. The same numerical thresholds can be applied to the intakes of individual identified components and combinations of components, such as occur in congeneric groups, which are present in finished flavour complexes derived from natural sources. The same intake thresholds can also be used as a basis for establishing analytical requirements as described below.

The human intake thresholds of toxicological concern are of two types: thresholds of 1800, 540 and 90 µg/person per day which are applied for structural classes I, II and III, respectively, and a general threshold of 1.5µg/person per day applicable to all structural classes. The thresholds for classes I, II and III are based on the lower 5th percentile NOEL for the structural class, from toxicological studies in animals, divided by the usual 100-fold safety (uncertainty) factor. The general threshold (step B5 of the Procedure) is a pragmatic value based on an estimate of the human intake associated with a lifetime risk of cancer of less than 1 in a million calculated by linear-extrapolation from animal studies (Report of 46th Meeting). Because of the assumptions used in the derivation of this threshold, it is considered to be sufficiently conservative to cover all types of toxicity. The Committee considered that these thresholds can provide the basis for a pragmatic approach to the development of limits of sensitivity for analytical methods, when linked to reliable and validated estimates of intake, which should be derived from long-term average poundage.

ii. Consideration of individual components

Identified components

Based on step B5 of the Procedure, the Committee concluded there would be no significant safety concern if the intake for an identified component in a finished flavour complex derived from natural sources were less than 1.5 µg/person per day. This threshold can be used to establish a general limit for analytical characterization for components in a finished flavour complex under (b) below, based on the estimated intake of the complex. For example, if the estimated daily intake of the finished flavour complex is 150 µg /person per day, then there would be no safety concern for any component present at <1%. Similarly, if the estimated daily intake of the finished flavour complex is 15 µg/person per day, then there would be no safety concern for any component present at <10%. For high volume finished flavour complexes the limit for analytical characterisation would be set at 0.1-0.5% (see (b) below). Because the threshold is based on lifetime carcinogenicity data, the % should be the average value of the analyses, and not the highest single value.

Unidentified components

The chromatographic analysis of a finished flavour complex is likely to reveal the presence of a large number of unidentified minor components. Previously the Committee has not considered the general threshold of 1.5 µg/person per day for unidentified components. The Committee recognised that application of the general threshold to an unidentified component could not provide the same reassurance of safety as for structurally defined compounds, but considered that it could be incorporated into a pragmatic approach for establishing analytical requirements for finished flavour complexes derived from natural sources. This threshold combined with the estimated intake of the complex can be used to define a limit for the percentage of a chromatographic peak above which structural characterization would be necessary. For example, if the estimated daily intake of the finished flavour complex is 150µg/person per day, then chemical characterization would be required for any component present >1%, so that safety evaluation of the component could be undertaken.

Product descriptions and specifications

A key part of the safety assessment will be the preparation of appropriate specifications covering the relevant finished flavour complexes. As with all food additive evaluations, the purpose of specifications for flavour complexes is to identify the material, to ensure that it meets the criteria for safe use, and to encourage good manufacturing practice. Specifications should reflect the materials used throughout the world and should take account of existing specifications drawn up at national or international level.

The Committee noted the existence of internationally agreed specifications prepared by the International Organization for Standardization (ISO) for over 100 essential oils obtained by steam distillation of plant materials. Essential oils and derived products are numerically the largest group of flavour complexes. ISO standards describe the oils and define the acceptable ranges for various parameters, including the methods for measuring these values. Many of these standards include ranges for the key chemical components, accompanied by typical gas chromatograms that can be used to confirm the identity of the oils. The Committee concluded that these standards need to be taken into account when setting specifications for food flavourings, particularly when selecting the parameters to be included and the associated analytical methods.

In order to develop specifications for flavour complexes added to food, and to provide the data necessary for the safety evaluation to proceed, the Committee requires a full description of the range of source materials and processing

conditions. Manufacturers should also provide the results of appropriate analyses carried out on samples of representative flavour complexes, accompanied by details of the analytical methods (including validation of the methods) and a full description of each sample, including the source materials and production processes. Manufacturers should also address the possible presence of undesirable compounds associated with the source material (or species with which it might be confused) and should provide sufficient information to differentiate the flavour complexes from other products with similar properties.

Standard information in the specifications for finished flavour complexes will include: descriptions of the source material(s), the derivation of the initial extract, and any subsequent processing stages; a physical description of the flavour complexes; information on solubility; and (for liquid products) specific gravity, refractive index and optical rotation.

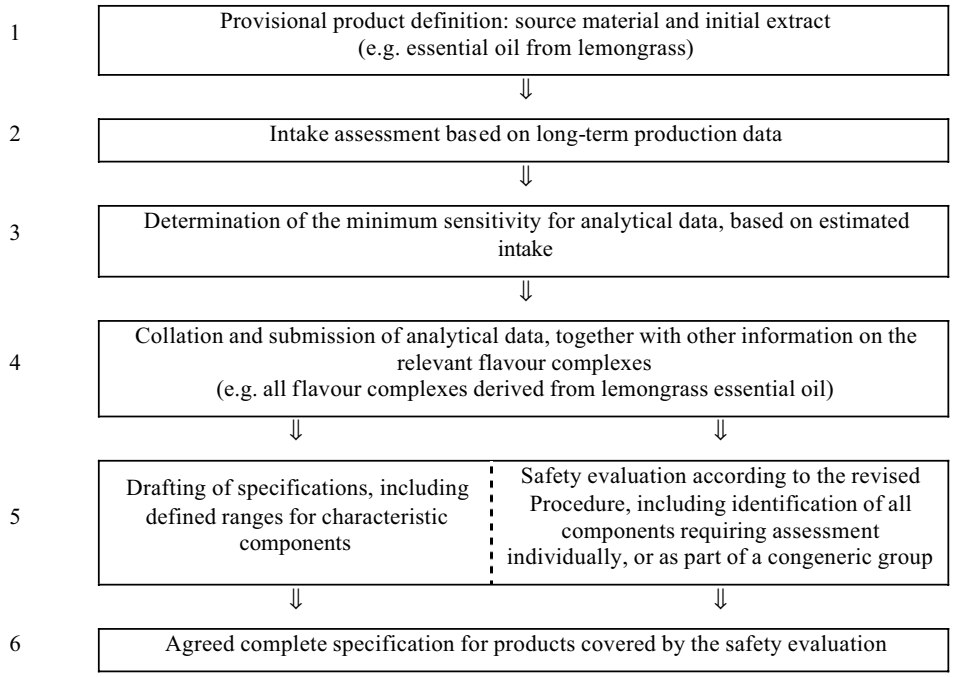
Specifications developed by the Committee will include the following information on composition, which is essential for the safety evaluation to proceed (see below).

(a) upper and lower concentrations of major characterising components, including all key constituents identified in relevant ISO standards and any other components considered to be critical for the organoleptical properties of the flavouring.

(b) a list of other components that may be present at or above a given level; the level will depend on the intake and the relevant threshold of toxicological concern (see above) in the revised Procedure for the Safety Evaluation of Flavouring Agents. Components present in the flavour complex at levels above 0.1-0.5% should be characterized if their estimated intake exceeds 1.5 µg/person per day. The need for more detailed characterization would be determined on a case-by-case basis depending on the nature of the starting material.

(c) upper limits for any other relevant components, including likely impurities and contaminants or potentially toxic components such as inherent toxins associated with any part of the source species or with related species with which it might be confused.

The overall scheme for evaluating finished flavour complexes is summarised in the following diagram:



The Committee requested data, in line with the above proposals, on examples of flavour complexes with a range of different constituents and representing different estimated intake levels in order to develop appropriate specifications and to evaluate the application of the revised Procedure to this type of flavouring agent. In particular, in the first detailed consideration of finished flavour complexes, quantitative data should be provided on the composition of representative samples of the selected flavour complexes, which allows the identification of all components present in the flavour complexes at levels above 0.1% and with an estimated intake of 1.5µg/day or more.

Determination of carotenoids

The Committee recognized that there is an increasing number of specifications for the analysis of members of the family of carotenoid compounds. Each specification prescribes the use of a different instrumental method of analysis. The Committee decided that it would be advantageous to consolidate and minimize the number of methods for the analysis of members of the carotenoid family and to publish them in FAO Food and Nutrition Paper, No. 5.

Revision of heavy metals and arsenic specifications

At its fifty-third meeting, the Committee agreed to implement the decision taken at its forty-ninth and fifty-first meetings, namely, to review and replace the limit test for heavy metals (as lead) and arsenic with, as appropriate, limits for the individual elements of concern in all existing specifications established by the Committee. In order to accomplish this, the Committee decided to review the existing specifications on the basis of functional use (e.g. antioxidant, preservative), and set a target of 5 years for completion of the task.

At its fifty-fifth and subsequent four meetings, the Committee reviewed all the specifications that had not been modified during previous meetings.

The principles adopted by the Committee in its reviews were as follows:

After removing the 'heavy metals (as lead)' specification, a maximum concentration of 2 mg/kg for lead and 1 mg/kg for cadmium and mercury would be established, except where there were data to support higher or lower maximum concentrations, or there were issues related to consumer exposure.

A limit for arsenic would only be included when the source from which the additive was prepared or the nature of the manufacturing method for the additive indicated that arsenic was likely to be a contaminant.

Section B: Specifications of certain food additives (uses other than as flavouring agents) and other substances

ACETIC ACID, GLACIAL

Prepared at 63rd JECFA (2004) and published in FNP 52 ADD 12 (2004) superseding specifications prepared at the 19th JECFA (1975), and published in FNP 52 (1992). Metal contaminants specifications amended at the 59th JECFA (2002). A group ADI 'not limited' for acetic acid and its potassium and sodium salts was established at the 17th JECFA (1973) and maintained at the 49th JECFA (1997).

SYNONYMS INS No. 260

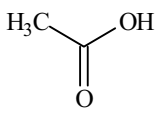
DEFINITION Acetic acid is manufactured by aerial oxidation of C5-C6 fractions of aliphatic hydrocarbons, and separation of the various acids by distillation. Also by oxidation of acetaldehyde, methanol and of butane or as the reaction product of methanol and carbon dioxide.

Chemical name Acetic acid, ethanoic acid

C.A.S. number 64-19-7

Chemical formula $C_2H_4O_2$

Structural formula



Formula weight 60.05

Assay Not less than 99.5%

DESCRIPTION Colourless liquid, having a pungent characteristic odour

FUNCTIONAL USES Acid, flavouring agent (see Flavouring agent specification, JECFA No. 81)

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Miscible with water, ethanol, glycerol and diethyl ether

Test for acid 1 in 3 aqueous solution is acidic

Test for acetate (FNP 5) Apply to a 1 in 3 solution of the sample
Passes test

PURITY

Solidification point (FNP 5) Not lower than 15.6º

Non-volatile residue (FNP 5) Not more than 0.01% after evaporation of 20 g of the sample and holding at 100° for 2 h.

Readily oxidizable substances Dilute 2 ml of the sample in a glass-stoppered container with 10 ml of water and add 0.1 ml of 0.1 N potassium permanganate. The pink colour does not change to brown within 30 min.

Lead (FNP5)	Not more than 0.5 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental methods."
METHOD OF ASSAY	Measure about 2 ml of the sample into a tared, glass-stoppered flask, and weigh accurately. Add 40 ml of water, then add phenolphthalein TS and titrate with 1 N sodium hydroxide. Each ml of 1 N sodium hydroxide is equivalent to 60.05 mg of $C_2H_4O_2$.

ALUMINIUM LAKES OF COLOURING MATTERS
GENERAL SPECIFICATIONS

Prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004) superseding specifications prepared at the 25th JECFA (1981), published in FNP 19 (1981) and FNP 52 (1992).

DEFINITION	Aluminium lakes are prepared under aqueous conditions by reacting aluminium oxide with colouring matter complying with purity criteria set out in the appropriate specification monograph. Undried aluminium oxide is usually freshly prepared by reacting aluminium sulfate or aluminium chloride with sodium carbonate or sodium bicarbonate or aqueous ammonia. Following lake formation, the product is filtered, washed with water and dried. Unreacted aluminium oxide may also be present in the final product.
Assay	Content of colouring matter shall be within the range specified by the vendor.
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water
Identification of colouring matter (FNP 5)	Dissolve the sample using the method described in Colouring matter, Procedure for Lakes under Methods for Food Colours. Use the identification test described in the appropriate colour specifications monograph.
PURITY	
Water-soluble chlorides and sulfates (FNP 5)	Not more than 2 % calculated as sodium salts. Use the procedure for Water-soluble chlorides and sulfates in aluminium lakes under Methods for Food Colours
Hydrochloric acid-insoluble matters (FNP 5)	Not more than 0.5 % Use the procedure for Hydrochloric acid-insoluble matters in lakes under Methods for Food Colours
Ether-extractable matter (FNP 5)	Not more than 0.2 % (Method II)
Arsenic (FNP 5)	Not more than 3 mg/kg (Method II)
Lead (FNP 5)	Not more than 5 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, “Instrumental Methods”.
METHOD OF ASSAY (FNP 5)	See Colouring matter, Total content by spectrophotometry, Procedure for Lakes under Methods for Food Colours

ALUMINIUM POWDER

Prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004) superseding specifications prepared at the 51st JECFA (1998), published in FNP 52 Add 6 (1998). The limited use of aluminium as a surface colourant for certain items of confectionery was not considered to present a hazard (21st JECFA, 1977).

SYNONYMS	CI Pigment Metal, CI (1975) No. 77000, INS No. 173
DEFINITION	Produced by grinding aluminium that may be carried out in the presence of edible vegetable oils and/or food grade fatty acids.
Chemical Name	Aluminium
C.A.S. number	7429-90-5
Chemical formula	Al
Atomic weight	26.98
Assay	Not less than 99.0 %
DESCRIPTION	Silvery grey powder
FUNCTIONAL USES	Colour (for surface only)
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water and in organic solvents, soluble in dilute hydrochloric acid.
Test for aluminium (FNP 5)	A sample dissolved in dilute hydrochloric acid passes test.
PURITY	
Loss on drying (FNP 5)	Not more than 0.5 % (105°)
Arsenic (FNP 5)	Not more than 3 mg/kg (Method II)
Lead (FNP 5)	Not more than 20 mg/kg Weigh 5 g of sample and transfer to a beaker. Add 50 ml concentrated hydrochloric acid and heat on a hot plate until totally dissolved. Dilute with water to 100 ml in a volumetric flask. Determine using an atomic absorption technique appropriate to the specified level.
METHOD OF ASSAY	Wash a small sample in hexane, repeating to remove traces of any associated oil or fatty acid. Transfer about 0.2 g of the sample, accurately weighed, to a 500 ml flask fitted with a rubber stopper carrying a 150 ml separating funnel, an inlet tube connected to a cylinder of carbon dioxide and an outlet tube dipping into a water-trap. Add 60 ml of freshly boiled and cooled water and disperse the sample, replace the air by carbon dioxide and add, by the separating funnel, 100 ml of a solution containing 56 g of ferric ammonium sulfate and 7.5 ml of sulfuric acid in freshly boiled and cooled water. While maintaining an atmosphere of carbon dioxide in the flask, heat to boiling and boil for 5 min. After the sample has dissolved, cool rapidly to 20°, and dilute to 250 ml with freshly boiled and cooled water. To 50 ml of this solution, add 15 ml of phosphoric acid and titrate with 0.1 N potassium permanganate. 1 ml of 0.1 N potassium permanganate is equivalent to 0.8994 mg of Al.

BENZOYL PEROXIDE

Prepared at the 63rd JECFA (2004), published in FNP 52 Add 12 (2004) superseding specifications prepared at the 55th JECFA (2000) and published in FNP 52 Add 8 (2000). Treatment of whey with benzoyl peroxide at a maximum concentration of 100 mg/kg does not pose a safety concern (63rd JECFA, 2004).

SYNONYMS Benzoyl superoxide, INS No. 928

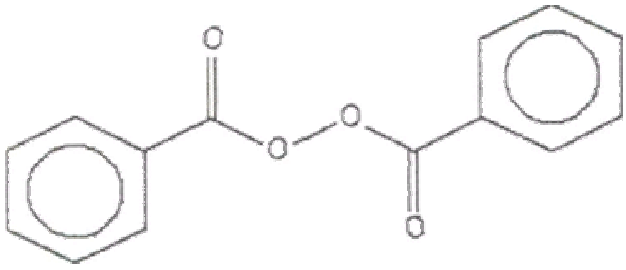
DEFINITION Benzoyl peroxide is manufactured by the reaction of benzoyl chloride, sodium hydroxide and hydrogen peroxide.

Chemical name Dibenzoyl peroxide

C.A.S. number 94-36-0

Chemical formula $C_{14}H_{10}O_4$

Structural formula



Formula weight 242.23

Assay Not less than 96.0%

DESCRIPTION Colourless, crystalline solid having a faint odour of benzaldehyde.
Caution: Benzoyl peroxide, especially in the dry form, is a dangerous, highly reactive, oxidizing material and has been known to explode spontaneously

FUNCTIONAL USES Bleaching agent

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Insoluble in water, slightly soluble in ethanol and soluble in ether.

Melting range (FNP 5) 103 - 106° with decomposition

Decomposition to benzoic acid To 0.5 g of the sample add 50 ml of 0.5 N ethanolic potassium hydroxide, heat gradually to boiling and continue boiling for 15 min. Cool and dilute with 200 ml of water. Add sufficient 0.5 N hydrochloric acid to make strongly acidic and extract with ether. Dry the ether solution over anhydrous sodium sulfate, and then evaporate to dryness on a steam bath. The benzoic acid so obtained melts between 121° and 123°.

PURITY

Lead (FNP5) — Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".

METHOD OF ASSAY — Dissolve about 250 mg of the sample, accurately weighed, in 15 ml of acetone in a 100-ml glass-stoppered bottle. Add 3 ml of 50% (w/v) potassium iodide solution and swirl for 1 min. Titrate immediately with 0.1 N sodium thiosulfate (without addition of starch as an indicator). Each ml of 0.1 N sodium thiosulfate is equivalent to 12.11 mg of $C_{14}H_{10}O_4$.

HEXOSE OXIDASE FROM *CHONDRUS CRISPUS* EXPRESSED IN *HANSENULA POLYMORPHA*

New specifications prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). An ADI "not specified" was established at the 63rd JECFA (2004).

SYNONYMS HOX

SOURCES Produced by a submerged fermentation of a pure culture of a non-pathogenic and nontoxigenic genetically modified strain of *Hansenula polymorpha* containing the hexose oxidase gene derived from *Chondrus crispus*. The enzyme is produced intracellularly and upon cell disruption is released into the fermentation broth and is subsequently separated from the yeast cells and subjected to ultrafiltration and diafiltration to obtain the concentrated hexose oxidase. It is then spray-dried onto a suitable food-grade carrier such as wheat starch.

ACTIVE PRINCIPLES Hexose oxidase

SYSTEMATIC NAMES AND NUMBERS D-hexose:oxygen 1-oxidoreductase; EC 1.1.3.5; CAS No. 9028-75-5

REACTIONS CATALYZED Oxidation of hexose sugars to their corresponding lactones and hydrogen peroxide

DESCRIPTION Off-white to brownish micro-granules

FUNCTIONAL USES Enzyme preparation.
Used in bread dough to strengthen the gluten network; in products like shredded cheese, potato chips, egg white powder and whey protein isolates to minimize Maillard reactions; in cottage cheese and tofu to facilitate curd formation and in products like ketchup, mayonnaise and salad dressings to scavenge oxygen.

GENERAL SPECIFICATIONS Must conform to the *General Specifications for Enzyme Preparations used in Food Processing* (FNP 52, current edition, including amendments).

CHARACTERISTICS

IDENTIFICATION

Hexose oxidase activity — The sample shows hexose oxidase activity
See description under TESTS

TESTS

Hexose oxidase activity

Principle

Hexose oxidase catalyses the formation of hydrogen peroxide and glucono-delta-lactone from glucose and oxygen. Hydrogen peroxide subsequently reacts with 2, 2'-azino-bis(3-ethylbenzthiazolin-6-sulfonic acid) (ABTS), resulting in the development of a green colour. This reaction is catalysed by the enzyme peroxidase. The colour intensity is measured spectrophotometrically at 405 nm. The activity unit HOX is defined as the amount of enzyme that catalyses the formation of 1 µmole of H_2O_2 per minute at 25 °.

Reagents

0.1M Phosphate buffer, pH 6.3: Dissolve 22.82 g $K_2HPO_4 \cdot 3H_2O$ in approx. 800 ml water. The pH is adjusted to 6.3 and to 1000 ml with water.

Reagent 1 (Glucose (55 mM) in 0.1 M phosphate buffer, pH 6.3): Dissolve 5.44 g glucose monohydrate ($C_2H_{12}O_6 \cdot H_2O$ D(+)) in 400 ml freshly made 0.1 M phosphate buffer. Adjust to pH 6.3 with conc. HCl. And to 500 ml with 0.1 M phosphate buffer.

Reagent 2 (ABTS stock solution): Weigh 500 mg ABTS into a 100 ml measuring flask and dilute to volume with water. Store in 1.5 ml volumes.

Reagent 3(Peroxidase (0.1 mg/mL) in 0.1 M phosphate buffer, pH 6.3):

Dissolve 10 mg peroxidase in 100 ml phosphate buffer. Store in 1.5 ml volumes.

Procedure

Substrate preparation: Pipette 1.0 ml Reagent 2 and 1.0 ml Reagent 3 into a 25 ml measuring flask and make up to volume with Reagent 1. The substrate is held for 30 min in a water bath at 25 °.

Standard curve for H_2O_2 assay: Dilute 0.2 ml H_2O_2 (concentration determined) with water to 1000 ml. This gives the control sample a peroxide concentration of approx. 2 µmol/ml.

The following standard curve is prepared:

Approx. peroxide concentration (µmol/ml)	Dilution B (ml)	Water (ml)
0.000	0.0	20.0
0.050	0.5	19.5
0.100	1.0	19.0
0.200	2.0	18.0
0.400	4.0	16.0
0.600	6.0	14.0
0.800	8.0	12.0

Measuring the standard curve: Pipette 50 µl from each concentration (0-0.8 µmol/ml) into a disposable microcuvette and add 950 µl of substrate. Measure the absorbance after 5 min at 405 nm. Zero the spectrophotometer with the sample containing 0 µmol/ml peroxide.

Sample preparation

Make duplicate measurements of the activity. Weigh out the enzyme as follows:

Sample weight (g) = 31/expected activity per gram

Dissolve the samples in 100 ml volumetric flasks with phosphate buffer and mix on a magnetic stirrer for 20 min. Fill the flasks with buffer, and filter turbid samples through syringe filters (Cameo 25 A, 0.45µ or equivalent). Subsequent dilutions are made in phosphate buffer.

Measurement

Measure the samples within 30 min of the final dilution. Zero the spectrophotometer with a sample of buffer. Add 50 µl of diluted sample to a disposable microcuvette. Place the cuvette in the photometer, and when 950 µl substrate is added to the cuvette, start the measurement of optical density.

Measure the optical density at 405 nm at 5 second intervals for 1 minute. Plot the optical density as a function of time. Determine the slope (OD/min) of the curve for the interval 0.25 to 0.75 min. The maximal OD at which a linear response is obtained is approx. 2.0 because the amount of ABTS becomes a limiting factor at higher OD.

Calculations

The activity of powder samples is determined as follows:

$$HOX/g = \frac{D \cdot act \cdot 100}{Std.slope \cdot weight}$$

Where:

D =	Dilution
act =	slope in OD/min of the sample
weight =	grams of spray dried powder suspended in 100 ml K_2HPO_4 buffer
Std. slope =	slope in OD/µmol/ml of the standard curve

HYDROGEN PEROXIDE

Prepared at 63rd JECFA (2004) and published in FNP 52 ADD 12 (2004) superseding specifications prepared at the 29th JECFA (1985), published in FNP 52 (1992). No ADI was allocated by the 24th JECFA (1980) with comment "may be used only where better methods of milk preservation are not available". Small residues of hydrogen peroxide on food (which has been treated with antimicrobial washing solutions) at the time of consumption would not pose a safety concern (63rd JECFA, 2004).

DEFINITION	The principal method for the manufacture of hydrogen peroxide is the catalytic reduction by hydrogen of a substituted anthraquinone dissolved in a mixed aromatic hydrocarbon solvent, to anthraquinol. The hydrogenation catalyst is removed and the anthraquinol solution is subjected to aerial oxidation, to yield anthraquinone and hydrogen peroxide. The anthraquinone is recycled and the hydrogen peroxide, extracted with water, is purified and concentrated. The dilution of the concentrate is adjusted and a tin based stabilizer added.
Chemical name	Hydrogen peroxide
C.A.S. number	7722-84-1
Chemical formula	H_2O_2
Structural formula	H-O-O-H
Formula weight	34.01
Assay	Not less than the labelled concentration or within the range stated on the label
DESCRIPTION	An odourless, or nearly odourless, transparent and colourless liquid Caution: Powerful oxidizing agent. Avoid contact with eyes and skin.
FUNCTIONAL USES	Antimicrobial agent
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Miscible with water
Test for peroxide (FNP 5)	Passes test
Acidity	Acid to litmus
PURITY	
Non-volatile residue (FNP 5)	Not more than 60 mg/kg
Acidity	Not more than 0.03% (as sulfuric acid) Dilute 9 ml of the sample with 90 ml of carbon dioxide-free water, add methyl red TS, and titrate with 0.02 N sodium hydroxide. The volume of sodium hydroxide solution should not be more than 3 ml greater than the volume required for a blank test on 90 ml of water used for dilution.
Phosphate	Not more than 50 mg/kg See description under TESTS
Iron	Not more than 0.5 mg/kg See description under TESTS
Tin	Not more than 10 mg/kg See description under TESTS

Lead — Not more than 4 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental methods

TESTS

PURITY TESTS

Phosphate — Evaporate 400 mg of the sample to dryness on a steam bath. Dissolve the residue in 25 ml of approximately 0.5 N sulfuric acid. Add 1 ml of ammonium molybdate solution (500 mg of $(NH_4)_6Mo_7O_{24} \cdot 4H_2O$ in 10 ml of water) and 1 ml of p-methylaminophenol sulfate TS, and allow to stand for 2 h. Any blue colour produced should not exceed that of a control solution made the same way as the test solution, using 2.0 ml of Phosphate Standard Solution (20 µg PO_4) in an equal volume of solution containing equal quantities of reagents used in the test.

Iron — Evaporate 20 g of the sample to dryness on a steam bath with 10 mg of sodium chloride, dissolve the residue in 2 ml of hydrochloric acid, and dilute to 50 ml with water. Add about 40 mg of ammonium persulfate crystals and 10 ml of ammonium thiocyanate TS, and mix. Any red or pink colour does not exceed that produced by 1.0 ml of *Iron Standard Solution* (10 µg Fe) in an equal volume of solution containing the quantities of the reagents used in the test.

Tin — *Aluminium Chloride Solution*: Dissolve 8.93 g of aluminium chloride, $AlCl_3 \cdot 6H_2O$, in sufficient water to make 1000 ml.

Gelatin Solution: On the day of use, dissolve 100 mg of gelatin in 50 ml of boiled water that has been cooled to between 50° and 60°.

Tin Stock Solution: Dissolve 250.0 mg of lead-free tin foil in 10 to 15 ml of hydrochloric acid, and dilute to 250.0 ml with dilute hydrochloric acid (1 in 2).

Standard Solution
On the day of use, transfer 5.0 ml of Tin Stock Solution into a 100-ml volumetric flask, dilute to volume with water, and mix. Transfer 2.0 ml of this solution (100 µg Sn) into a 250-ml Erlenmeyer flask, and add 15 ml of water, 5 ml of nitric acid, and 2 ml of sulfuric acid.

Place a small stemless funnel in the mouth of the flask, and heat until strong fumes of sulfuric acid are evolved. Cool, add 5 ml of water, evaporate again to strong fumes, and cool. Repeat the addition of water and heating to strong fumes, then add 15 ml of water, heat to boiling, and cool. Dilute to about 35 ml with water, add 1 drop of methyl red TS and 2.0 ml of the Aluminium Chloride Solution, and mix. Make the solution just alkaline by the drop wise addition of stronger ammonia TS, stirring gently, and then add 0.1 ml in excess. (Caution: To avoid dissolving the aluminium hydroxide precipitate, do not add more than 0.1 ml in excess of the ammonia solution.) Centrifuge for about 15 min at 4000 rpm, and then decant the supernatant liquid as completely as possible without disturbing the precipitate. Dissolve the precipitate in 5 ml of dilute hydrochloric acid (1 in 2), add 1.0 ml of the Gelatin Solution, and dilute to 20.0 ml with a saturated solution of aluminium chloride.

Sample Solution
Transfer 10 g of the sample into a 250-ml Erlenmeyer flask, and add 15 ml of water, 5 ml of nitric acid, and 2 ml of sulfuric acid. Mix and heat gently on a hot plate to initiate and maintain a vigorous decomposition.

When decomposition is complete, place a small stemless funnel in the mouth of the flask, and continue as directed for the Standard Solution (above), beginning with "... and heat until strong fumes of sulfuric acid are evolved."

Procedure

Rinse a polarographic cell or other vessel with a portion of the Standard Solution, then add a suitable volume to the cell, immerse it in a constant temperature bath maintained at 35±0.2°, and deaerate by bubbling oxygen-free nitrogen or hydrogen through the solution for at least 10 min. Insert the dropping mercury electrode of a suitable polarograph, and record the polarogram from -0.2 to -0.7 V and at a sensitivity of 0.0003 μA per mm, using a saturated calomel reference electrode. In the same manner, record a polarogram of a portion of the Sample Solution at the same current sensitivity. The height of the wave produced by the Sample Solution is not greater than that produced by the Standard Solution at the same half-wave potential.

METHOD OF ASSAY

Accurately weigh a volume of the sample equivalent to about 300 mg of H_2O_2 into a 100-ml volumetric flask, dilute to volume with water, and mix thoroughly. To a 20-ml portion of this solution add 25 ml of diluted sulfuric acid TS, and titrate with 0.1 N potassium permanganate. Each ml of 0.1 N potassium permanganate is equivalent to 1.701 mg of H_2O_2.

1-HYDROXYETHYLIDENE-1,1-DIPHOSPHONIC ACID

New specifications prepared at 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). Levels of residue that are expected to remain on foods do not pose a safety concern (63rd JECFA, 2004).

SYNONYMS HEDP, ethane-1-hydroxy-1,1-diphosphonic acid, EHDP, editronic acid

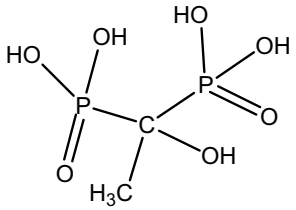
DEFINITION 1-Hydroxyethylidene-1,1-diphosphonic acid (HEDP) is manufactured commercially by the reaction of phosphorous acid with one or more acetylating agents; specifically acetic anhydride, acetyl chloride and/or acetic acid. The final product is typically a 60% solution of HEDP in water.

Chemical name 1-hydroxyethylidene-1,1-diphosphonic acid

C.A.S. number 2809-21-4

Chemical formula $CH_3C(OH)[PO(OH)_2]_2$

Structural formula



Empirical formula $C_2H_8O_7P_2$

Formula weight 205.02

Assay Total active acid 58 – 62%

DESCRIPTION Clear pale yellow liquid, free of suspended matter

FUNCTIONAL USES Sequestrant (for use in antimicrobial washing solutions)

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Miscible with water, phosphoric acid and ethylene glycol; soluble in most organic solvents

pH Not more than 2.0 (1% soln)

Specific gravity 1.430- 1.471 at 20º

Freezing point -25º

PURITY

Chloride Not more than 40 mg/kg
See description under TESTS

Phosphorous acid Not more than 4.0%
See description under TESTS

Acetic acid Not more than 1.0%
See description under TESTS

Iron (FNP 5)	Not more than 10 mg/kg Determine using an atomic absorption technique appropriate to the specified level
Arsenic (FNP 5)	Not more than 5 mg/kg
Lead (FNP 5)	Not more than 5 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental methods"

TESTS

PURITY TESTS

Chloride

Determine by potentiometric titration by placing 25 g of the sample, accurately weighed, into a titration vessel and adding sufficient water to cover the electrodes. Add 3 ml of concentrated nitric acid. Titrate with 0.005 mol/l silver nitrate to first inflection point and record the titre in ml (A). Calculate the chloride content (mg/kg) from:

Chloride (mg/kg) = [A x M x 3.55 x 10000] / W

where
M = concentration of silver nitrate solution (mol/l)
W = weight of sample taken (g)

Phosphorous acid

Determined by iodometric titration. Iodine oxidizes the phosphorous acid present to phosphate, excess iodine is determined and the Phosphorous acid calculated.

Buffer solution pH 7.3: Dissolve 138 g of sodium dihydrogen phosphate in 800 ml of water and adjust pH to 7.3 with 50% sodium hydroxide solution. Make up to 1000 ml with water.

Add 1.5 g of the sample to 20 ml of water in a 250 ml beaker. Add 50 ml of pH 7.3 phosphate buffer. Adjust pH to 7.3 using 50% sodium hydroxide. Transfer the solution to an iodine flask and add 25.0 ml of 0.1 N iodine. Stopper and swirl the solution and place in the dark immediately. After 15 min, remove the flask and add 5 ml acetic acid to flask. Titrate with 0.1 N sodium thiosulfate until a light straw yellow colour. Add starch indicator and continue titration until the end point "black to colourless" is observed and record the titre in ml (B). Repeat titration with a reagent blank determination omitting the sample and record the titre in ml (A).

Calculate the percentage of phosphorus acid from:

Phosphorous acid (%) = [(A-B) x N x E x 100] / [w x 1000]

where

N = normality of sodium thiosulfate solution
E = equivalent weight of H_3PO_3 (40.99)
w = weight of sample taken (g)

The accuracy has been determined as +/- 0.01% at phosphorous acid level of 1.28%

Acetic acid

Determine by ion chromatography using a Dionex ICE-ASI column with weak acid eluent. Set up the system in line with the instrument manufacturer's operation procedure.

The signal from the acetate ion is quantified against a calibration standard using Formic acid as the internal standard.
Equipment: Dionex ICE-AS1 column
Reagents: Acetic acid (analytical grade) and formic acid (analytical grade)
Procedure: Carry out the determination according to the instrument manufacturer's operation procedure

METHOD OF ASSAY

Place about 3 g of the sample, accurately weighed (w) into a beaker and add 100-150 ml of

water. Stir the solution with a magnetic stirrer (maintain throughout titration). Insert pH electrode(s) and record the pH value. Titrate with 1 mol/l sodium hydroxide and record pH (or millivolts) after every 1ml added. Stop the titration at pH 10. Plot the pH as a function of added sodium hydroxide and manually draw the titration curve. Two inflection points will be observed at around pH 3 and pH 8. Take only into account the inflection point at around pH 8. Trace the tangent to this inflection point in order to determine the end-point. Calculate the total active acid from

$$\text{Total active acid (\%)} = [A \times 206 \times N] / [30 \times w] - [1.676 \times P]$$

Where

A = ml of N NaOH from start of titration to end point at pH 8-85
N = concentration of sodium hydroxide used
P = concentration of phosphorous acid (%) (Determined as above)
1.676 = [MW of HEDP x 2] / [MW of phosphorous acid x 3]

Using auto-titration for end-point detection, accuracy has been determined as +/- 0.2% at total active acid level of 63.5%

HYDROXYPROPYL CELLULOSE

Revised specification prepared at the 63rd JECFA (2004) and published in FNP52 Add 12 (2004) superseding specifications prepared at the 29th JECFA (1985) and published in FNP 52. A group ADI "not specified" was established at the 29th JECFA (1985).

SYNONYMS Cellulose hydroxypropyl ether; modified cellulose; INS No. 463

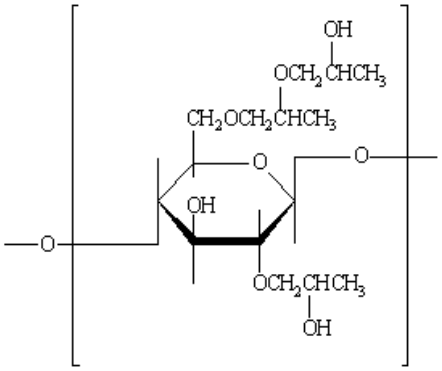
DEFINITION An ether of cellulose containing hydroxypropyl substitution prepared from cellulose by treatment with alkali and propylene oxide. The article of commerce can be specified further by viscosity.

Chemical names Hydroxypropyl ether of cellulose, cellulose hydroxypropyl ether

C.A.S. number 9004-64-2

Chemical formula $[C_6H_7O_2(OH)_X(OCH_2CHOHCH_3)_y(OCH_2CH[R_w]CH_3)_z]_n$
where
x + y + z = 3
y + z (1+w) = not greater than 4.6
R = A substituent comprising "w" hydroxypropoxy groups

Structural formula



One of many possible structural formulae for the repeating unit of a hydroxypropyl cellulose with molar substitution of 3.0 and a degree of polymerization of n, showing a monomeric hydroxypropyl substitution at C_2 and a dimeric hydroxypropyl substitution at C_6.

Formula weight Unsubstituted structural unit: 162.14
Trisubstituted structural unit: 336.37
Macromolecules: from about 30 000 (n about 100) up to about 1 million (n about 2500)

Assay Not more than 80.5% of hydroxypropoxy groups equivalent to not more than 4.6 hydroxypropyl groups per anhydroglucose unit on the dried basis

DESCRIPTION Slightly hygroscopic, white or off-white, almost odourless, granular or fibrous powder

FUNCTIONAL USES Emulsifier, thickener, stabiliser, binder, suspension agent, film coating

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Swells in water, producing a clear to opalescent, viscous colloidal solution; insoluble in ethanol; insoluble in ether

Foam formation	A 0.1% solution of the sample is shaken vigorously. A layer of foam appears. This test permits the distinction of sodium carboxymethyl cellulose from other cellulose ethers.
Precipitate formation	To 5 ml of a 0.5% solution of the sample, add 5 ml of a 5% solution of copper sulfate or of aluminium sulfate. No precipitate appears. This test permits the distinction of sodium carboxymethyl cellulose from other cellulose ethers.
Substituents	See description under METHOD OF ASSAY
PURITY	
Loss on drying (FNP 5)	Not more than 10.0% (105° to constant weight)
pH	Not less than 5.0 and not more than 8.0 (1 in 100 soln)
Sulfated ash	Not more than 0.5%. Test 1 g of the sample
Lead (FNP 5)	Not more than 2 mg/kg. Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental Methods"
Propylene chlorohydrins	Not more than 0.1 mg/kg See description under TESTS

TESTS

PURITY TESTS

Propylene chlorohydrins — Determine by gas liquid chromatography (FNP 5) using the following procedure:

Preparation of Standards

Stock Standard Solution: Weigh 0.1 g propylene chlorohydrin (C.A.S. No. 127-00-4, mixture of 1-Chloro-2-propanol-70% and 2-Chloro-1-propanol-30%) to the nearest 0.0001g and bring to a final volume of 100 ml with diethyl ether.

Working Standard Solution: Perform serial dilutions (in diethyl ether) of stock standard to achieve a working calibration range of 6-25 ng/ml.
Note: All standard solutions should be prepared with diethyl ether of the highest purity

Gas Chromatography

Gas Chromatograph with a Halogen Specific Detector, on-column injector, and linear column temperature programming.

Column:	30 m x 0.53 mm x 1 µm DB-WAX or equivalent.	
Temperature programming:	Initial Temperature	35°
	Initial Hold Time	7.0 min
	Ramp Rate	8.0°/min
	Final Temperature	200°
	Final Hold Time	5.0 min
	Inlet	200°
	Detector (XSD)	1000°
Flow rates:		
	Helium (carrier gas)	5 psi (column head pressure at 35°)
	Detector Make-up Gas (air)	40 psi
	Retention times (min):	
	1-Chloro-2-propanol	~11.7
	2-Chloro-1-propanol	~12.5

Procedure:
Weigh ~1 g of sample into a centrifuge tube and record weight to the nearest 0.01 g. Quantitatively add 5.0 ml diethyl ether to the sample and sonicate for 10 minutes. Centrifuge the sample to separate the mixture. Remove a portion of the diethyl ether extract for GC analysis.

Calculations:
Prepare a calibration curve by plotting the concentration (ng/ml) versus detector response (in a linear range of 6-25 ng/ml). From the linear regression of this curve, calculate ng/g using the following equation:

$$ng/g = (V \times (R-b)/m)/W$$

where:

R= detector response for the sample
b = y-intercept of the linear regression curve
m = slope of the linear regression curve
V= final volume (5.0 ml)
W= weight of the sample in grams

METHOD OF ASSAY

Determination of the hydroxypropoxy group content
Apparatus
The apparatus for hydroxypropoxy group determination is shown in the accompanying diagram. The boiling flask, D, is fitted with an aluminium foil-covered Vigreux column, E, on the sidearm and with a bleeder tube through the neck and to the bottom of the flask for the introduction of steam and nitrogen. A steam generator, B, is attached to the bleeder tube through Tube C, and a condenser, F, is attached to the Vigreux column. The boiling flask and steam generator are immersed in an oil bath, A, equipped with a thermo-regulator such that a temperature of 155° and the desired heating rate may be maintained. The distillate is collected in a 150 ml beaker, G, or other suitable container.

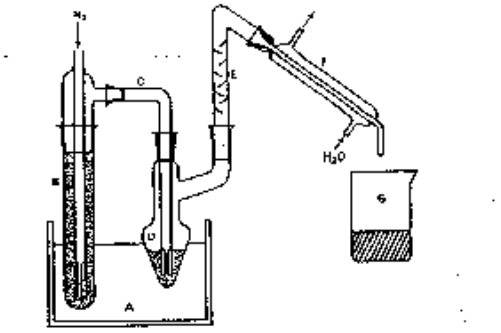


Figure Apparatus for Hydroxypropyl Determination

Procedure
Transfer about 100 mg of the sample, previously dried at 105° for 2 h and accurately weighed, into the boiling flash, and add 10 ml of chromium trioxide solution (60 g in 140 ml of water). Immerse the steam generator and the boiling flask in the oil bath (at room temperature) to the level of the top of the chromium trioxide solution. Start cooling water through the condenser and pass nitrogen gas through the boiling flask at the rate of one bubble per sec. Starting at room temperature, raise the temperature of the oil bath to 155° over a period of not less than 30 min, and maintain this temperature until the end of the determination. Distil until 50 ml of the distillate is collected. Detach the condenser from the Vigreux column, and wash it with water, collecting the washings in the distillate container. Titrate the combined washings and distillate with 0.02 N sodium hydroxide to a pH of 7.0, using a pH meter set at the

expanded scale.
NOTE: Phenolphthalein TS may be used for this titration, if it is also used for all standards and blanks.
Record the volume, V_a of the 0.02 N sodium hydroxide used. Add 500 mg of sodium bicarbonate and 10 ml of dilute sulfuric acid TS, and then after evolution of carbon dioxide has ceased, add 1 g of potassium iodide. Stopper the flask, shake the mixture, and allow it to stand in the dark for 5 min. Titrate the liberated iodine with 0.02 N sodium thiosulfate to the sharp disappearance of the yellow colour, confirming the end-point by the addition of a few drops of starch TS. Record the volume of 0.02 N sodium thiosulfate required as Y_a.
Make several reagent blank determinations, using only the chromium trioxide solution in the above procedure. The ratio of the sodium hydroxide titration (V_b) to the sodium thiosulfate titration (Y_b), corrected for variation in normalities, will give the acidity-to-oxidizing ratio, $V_b/Y_b = K$, for the chromium trioxide carried over in the distillation. The factor K should be constant for all determinations.
Make a series of blank determinations using 100 mg of methyl cellulose (containing no foreign material) in place of the sample, recording the average volume of 0.02 N sodium hydroxide required as V_m and the average volume of 0.02 N sodium thiosulfate required as Y_m.
Calculate the hydroxypropoxy group content of the sample, in mg, by the formula:

$$75.0 \times [N_1 (V_a - V_m) - k N_2 (Y_a - Y_m)]$$

where
N_1 = the exact normality of the 0.02 N sodium hydroxide solution
N_2 = the exact normality of the 0.02 N sodium thiosulfate solution
$k = V_b N_1 / Y_b N_2$

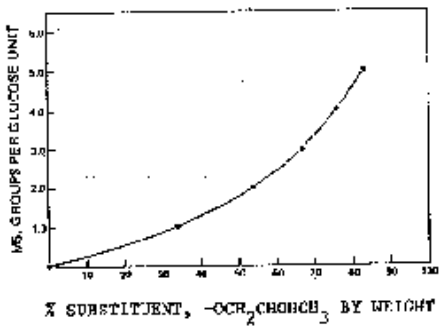


Chart for converting percentage of substitution, by weight, of hydroxypropoxy groups to molecular substitution per glucose unit.

Determination of the methoxy group

See Apparatus and Procedure in *Ethoxy and Methoxy Group Determination* and determine the content of methoxy group ($-OCH_3$).

Calculation

Calculate as percentage. Correct the % of methoxy groups thus determined by the formula:

$$A - (B \times 0.93 \times 31 / 75)$$

where

A = the total % of $-OCH_3$ groups determined
B = the % of $-OCH_2CHOHCH_3$ determined in the Method of Assay for Hydroxypropoxy group content
0.93 = an average obtained by determining, on a large number of samples, the propylene produced from the reaction of hydriodic acid with hydroxypropoxy groups during the Method of Assay for methoxy groups ($-OCH_3$).

HYDROXYPROPYLMETHYL CELLULOSE

Revised specification prepared at the 63rd JECFA (2004) and published in FNP52 Add 12 (2004) superseding specifications prepared at the 29th JECFA (1985) and published in FNP 52. A group ADI" not specified" was established at the 29th JECFA (1985).

SYNONYMS INS No. 464

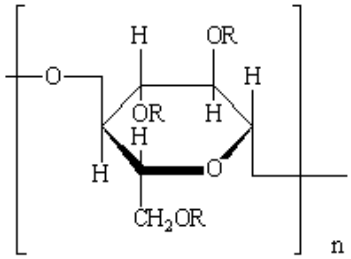
DEFINITION A methyl cellulose modified with a small number of 2-hydroxypropyl groups attached through ether links to anhydroglucose units of the cellulose. The article of commerce may be further specified by viscosity.

Chemical names Hydroxypropylmethyl cellulose, 2-hydroxypropyl ether of methyl cellulose

C.A.S. number 9004-65-3

Chemical formula $[C_6H_7O_2(OH)_x(OCH_3)_y(OCH_2CHOHCH_3)_z]_n$
where
z = 0.07 - 0.34
y = 1.12 - 2.03
x = 3-(z + y): (z + y = degree of substitution)

Structural formula



where R = H or CH_3 or $CH_2CHOHCH_3$

Formula weight Unsubstituted structural unit: 162.14
Structural unit with 1.19 degree of substitution: approx. 180
Structural unit with 2.37 degree of substitution: approx. 210
Macromolecules: from about 13,000 (n about 70) up to about 200,000 (n about 1000)

Assay Not less than 19% and not more than 30% of methoxy groups ($-OCH_3$) and not less than 3% and not more than 12% hydroxypropoxy groups ($-OCH_2CHOHCH_3$), on the dried basis

DESCRIPTION Hygroscopic white or off-white powder, or granules or fine fibres

FUNCTIONAL USES Emulsifier, thickening agent, stabiliser

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Swells in water, producing a clear to opalescent, viscous colloidal solution; insoluble in ethanol

Foam formation A 0.1% solution of the sample is shaken vigorously. A layer of foam appears. This test permits the distinction of sodium carboxymethyl cellulose from other cellulose ethers.

Precipitate formation To 5 ml of a 0.5% solution of the sample, add 5 ml of a 5% solution of copper sulfate or of aluminium sulfate. No precipitate appears. This test permits the distinction of sodium carboxymethyl cellulose from other cellulose ethers.

Substituents	See description under METHOD OF ASSAY
PURITY	
Loss on drying (FNP 5)	Not more than 10.0% (105° to constant weight)
pH	Not less than 5.0 and not more than 8.0 (1 in 100 soln)
Sulfated ash	Not more than 1.5% for products with viscosities of 50 centipoise or above, and not more than 3% for products with viscosities below 50 centipoise Test 1 g of the sample
Lead (FNP 5)	Not more than 2 mg/kg. Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental Methods"
Propylene chlorohydrins	Not more than 0.1 mg/kg See description under TESTS

TESTS

PURITY TESTS

Propylene chlorohydrins — Determine by gas liquid chromatography (FNP 5) using the following procedure:

Preparation of Standards

Stock Standard Solution: Weigh 0.1 g propylene chlorohydrin (C.A.S. No. 127-00-4, mixture of 1-Chloro-2-propanol-70% and 2-Chloro-1-propanol-30%) to the nearest 0.0001g and bring to a final volume of 100 ml with diethyl ether.

Working Standard Solution: Perform serial dilutions (in diethyl ether) of stock standard to achieve a working calibration range of 6-25 ng/ml.
Note: All standard solutions should be prepared with diethyl ether of the highest purity available

Gas Chromatography

Gas Chromatograph with a Halogen Specific Detector, on-column injector, and linear column temperature programming.

Column	30 m x 0.53 mm x 1 µm DB-WAX or equivalent.	
Temperature programming:	Initial Temperature	35°
	Initial Hold Time	7.0 min
	Ramp Rate	8.0°/min
	Final Temperature	200°
	Final Hold Time	5.0 min
	Inlet	200°
	Detector (XSD)	1000°
Flow rates:	Helium (carrier gas)	5 psi (column head pressure at 35°)
	Detector Make-up Gas (air)	40 psi
	Retention times (min):	
	1-Chloro-2-propanol	~11.7
	2-Chloro-1-propanol	~12.5

Procedure:

Weigh ~1 g of sample into a centrifuge tube and record weight to the nearest 0.01 g. Quantitatively add 5.0 ml diethyl ether to the sample and sonicate for 10 minutes. Centrifuge the sample to separate the mixture. Remove a portion of the diethyl ether extract for GC analysis.

Calculations:
Prepare a calibration curve by plotting the concentration (ng/ml) versus detector response (in a linear range of 6-25 ng/ml). From the linear regression of this curve, calculate ng/g using the following equation:

$$ng/g = (V \times (R-b)/m)/W$$

where:

R= detector response for the sample
b = y-intercept of the linear regression curve
m = slope of the linear regression curve
V= final volume (5.0 ml)
W= weight of the sample in grams

METHOD OF ASSAY

Determination of the hydroxypropoxy group content

Apparatus
The apparatus for hydroxypropoxy group determination is shown in the accompanying diagram. The boiling flask, D, is fitted with an aluminium foil-covered Vigreux column, E, on the sidearm and with a bleeder tube through the neck and to the bottom of the flask for the introduction of steam and nitrogen. A steam generator, B, is attached to the bleeder tube through Tube C, and a condenser, F, is attached to the Vigreux column. The boiling flask and steam generator are immersed in an oil bath, A, equipped with a thermo-regulator such that a temperature of 155° and the desired heating rate may be maintained. The distillate is collected in a 150 ml beaker, G, or other suitable container.

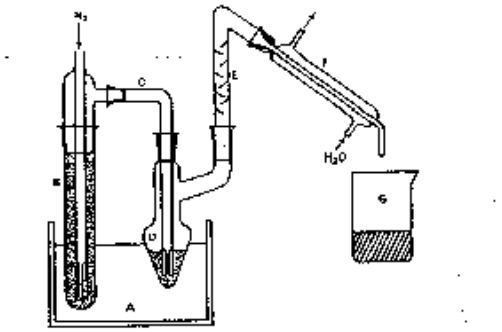


Figure Apparatus for Hydroxypropyl Determination

Procedure
Transfer about 100 mg of the sample, previously dried at 105° for 2 h and accurately weighed, into the boiling flash, and add 10 ml of chromium trioxide solution (60 g in 140 ml of water). Immerse the steam generator and the boiling flask in the oil bath (at room temperature) to the level of the top of the chromium trioxide solution. Start cooling water through the condenser and pass nitrogen gas through the boiling flask at the rate of one bubble per sec. Starting at room temperature, raise the temperature of the oil bath to 155° over a period of not less than 30 min, and maintain this temperature until the end of the determination. Distil until 50 ml of the distillate is collected. Detach the condenser from the Vigreux column, and wash it with water, collecting the washings in the distillate container. Titrate the combined washings and distillate with 0.02 N sodium hydroxide to a pH of 7.0, using a pH meter set at the expanded scale.
NOTE: Phenolphthalein TS may be used for this titration, if it is also used for all standards and blanks.
Record the volume, V_a of the 0.02 N sodium hydroxide used. Add 500 mg of sodium bicarbonate and 10 ml of dilute sulfuric acid TS, and then after evolution of carbon

dioxide has ceased, add 1 g of potassium iodide. Stopper the flask, shake the mixture, and allow it to stand in the dark for 5 min. Titrate the liberated iodine with 0.02 N sodium thiosulfate to the sharp disappearance of the yellow colour, confirming the end-point by the addition of a few drops of starch TS. Record the volume of 0.02 N sodium thiosulfate required as Y_a.

Make several reagent blank determinations, using only the chromium trioxide solution in the above procedure. The ratio of the sodium hydroxide titration (V_b) to the sodium thiosulfate titration (Y_b), corrected for variation in normalities, will give the acidity-to-oxidizing ratio, $V_b/Y_b = K$, for the chromium trioxide carried over in the distillation. The factor K should be constant for all determinations.

Make a series of blank determinations using 100 mg of methyl cellulose (containing no foreign material) in place of the sample, recording the average volume of 0.02 N sodium hydroxide required as V_m and the average volume of 0.02 N sodium thiosulfate required as Y_m.

Calculate the hydroxypropoxy group content of the sample, in mg, by the formula:

$$75.0 \times [N_1 (V_a - V_m) - k N_2 (Y_a - Y_m)]$$

where

N_1 = the exact normality of the 0.02 N sodium hydroxide solution
N_2 = the exact normality of the 0.02 N sodium thiosulfate solution
k = $V_b N_1 / Y_b N_2$

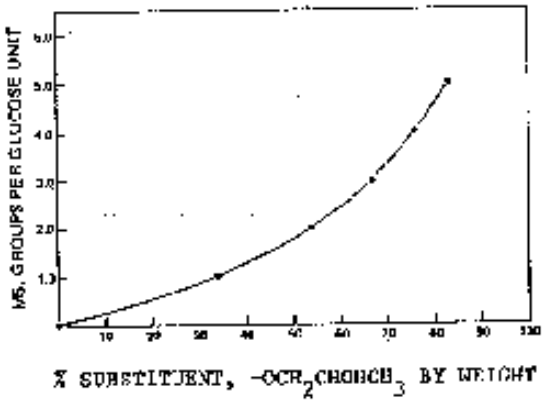


Chart for converting percentage of substitution, by weight, of hydroxypropoxy groups to molecular substitution per glucose unit.

Determination of the methoxy group

See Apparatus and Procedure in *Ethoxy and Methoxy Group Determination* and determine the content of methoxy group ($-OCH_3$).

Calculation

Calculate as percentage. Correct the % of methoxy groups thus determined by the formula:

$$A - (B \times 0.93 \times 31 / 75)$$

where

A = the total % of $-OCH_3$ groups determined
B = the % of $-OCH_2CHOHCH_3$ determined in the Method of Assay for Hydroxypropoxy group content
0.93 = an average obtained by determining, on a large number of samples, the propylene produced from the reaction of hydriodic acid with hydroxypropoxy groups during the Method of Assay for methoxy groups ($-OCH_3$).

IRON OXIDES

Specifications prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004), superseding specifications prepared at the 35th JECFA (1989) and published in FNP 52 (1992). An ADI of 0-0.5 mg/kg bw was established at the 53rd JECFA (1999).

SYNONYMS

Iron Oxide yellow: CI Pigment Yellow 42 and 43; CI(1975) No. 77492; INS No. 172 (iii)
Iron Oxide Red: CI Pigment Red 101 and 102; CI (1975) No. 77491; INS No. 172(ii)
Iron Oxide Black: CI Pigment Black 11; CI (1975) No. 77499; INS No. 172(i)

DEFINITION

Produced from ferrous sulfate by heat soaking, removal of water, decomposition, washing, filtration, drying and grinding.
They consist essentially of anhydrous and/or hydrated iron oxides; range of hues includes yellows, reds, browns and blacks. Food quality iron oxides are primarily distinguished from technical grades by the comparatively low levels of contamination by other metals; this is achieved by the selection and control of the source of the iron and/or by the extent of chemical purification during the manufacturing process.

Chemical names	Iron Oxide Yellow:	Hydrated ferric oxide, hydrated iron (III) oxide
	Iron Oxide Red:	Iron sesquioxide, anhydrous ferric oxide, anhydrous iron (III) oxide
	Iron Oxide Black:	Ferroso ferric oxide, iron (II,III) oxide
C.A.S. number	Iron Oxide Yellow:	51274-00-1
	Iron Oxide Red:	1309-37-1
	Iron Oxide Black:	1317-61-9
Chemical formula	Iron Oxide Yellow:	$FeO(OH) \cdot xH_2O$
	Iron Oxide Red:	Fe_2O_3
	Iron Oxide Black:	$FeO \cdot Fe_2O_3$
Formula weight	88.85	$FeO(OH)$
	159.70	Fe_2O_3
	231.55	$FeO \cdot Fe_2O_3$
Assay	Not less than 60% of iron	

DESCRIPTION

Yellow, red, brown or black powder

FUNCTIONAL USES

Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)

Insoluble in water and organic solvents; soluble in concentrated mineral acids

Water soluble matter (FNP 5)

Not more than 1.0%

PURITY

Loss on drying (FNP 5)

Iron Oxide Red : Not more than 1% (105°, 4 h)

Arsenic (FNP5)

Not more than 3 mg/kg (Method II)

See description under TESTS

Cadmium	Not more than 1 mg/kg
	See description under TESTS
Lead	Not more than 10 mg/kg
	See description under TESTS
Mercury (FNP 5)	Not more than 1 mg/kg
	Determine using an atomic absorption technique appropriate to the specified level. The selection of samples size and method of sample preparation may be based on principles of methods described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Arsenic, cadmium and lead	Weigh 5 g of the sample and transfer to a beaker. Add 50 ml concentrated hydrochloric acid and heat on a hot plate until totally dissolved. Dilute with water to 100 ml in a volumetric flask. Determine cadmium and lead using an atomic absorption technique appropriate to the specified level and arsenic using Method II of FNP 5.

METHOD OF ASSAY

Weigh accurately about 0.2 g of the sample, add 10 ml of 5 N hydrochloric acid and heat cautiously to boiling in a 200-ml conical flask until the sample has dissolved. Allow to cool, add 6 to 7 drops of 30% hydrogen peroxide solution and again heat cautiously to boiling until all the excess hydrogen peroxide has decomposed (about 2-3 min). Allow to cool, add 30 ml of water and about 2 g of potassium iodide and allow to stand for 5 min. Add 30 ml of water and titrate with 0.1 N sodium thiosulfate adding starch TS as the indicator towards the end of the titration. Each ml of 0.1 N sodium thiosulfate is equivalent to 5.585 mg of Fe (III).

LUTEIN FROM *TAGETES ERECTA*

New specifications prepared at the 63rd JECFA (2004) and published in FNP52 Add 12 (2004). A group ADI of 0 - 2 mg/kg bw for lutein from T. erecta *and synthetic zeaxanthin was established at the 63rd JECFA (2004).*

SYNONYMS Vegetable lutein; vegetable luteol; Bo-Xan (lutein)

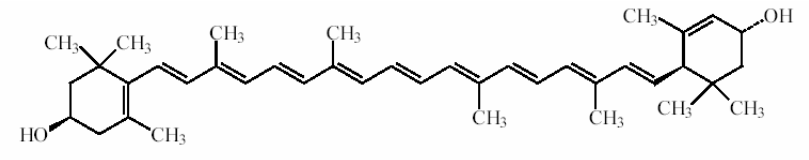
DEFINITION Lutein from *Tagetes erecta* L. is a purified extract of xanthophylls obtained from marigold oleoresin. The oleoresin is prepared from hexane extracts of marigold (*Tagetes erecta* L) flowers, saponified with potassium hydroxide in either methanol or propylene glycol. The resulting crystalline material contains lutein, and minor components including other carotenoids and waxes.

Chemical names β,ε-carotene-3,3'-diol; all-*trans*-lutein; 4',5'-didehydro-5',6'-dihydro-beta,beta-carotene-3,3'-diol (lutein)

C.A.S. number 127-40-2 (lutein)

Chemical formula $C_{40}H_{56}O_2$ (lutein)

Structural formula



Formula weight 568.88 (lutein)

Assay Not less than 80 % total carotenoids, not less than 70 % lutein

DESCRIPTION A free-flowing, orange-red powder

FUNCTIONAL USES Colour, nutrient supplement

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5) Insoluble in water, soluble in hexane

Spectrophotometry (FNP 5) A chloroform/ethanol (9:1) solution shows maximum absorbance at ca. 445 nm

Melting range 177 to 178º

Test for carotenoids (FNP 5) The colour of a solution of the sample in acetone disappears after successive addition of a 5% solution of sodium nitrite and 0.5 M of sulfuric acid.

PURITY

Moisture (FNP 5) Not more than 1.0%

Ash (FNP 5) Not more than 1.0%

Zeaxanthin	Not more than 9.0%. See description under METHOD OF ASSAY
Lead	Not more than 3 mg/kg. Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental Methods"
Hexane (FNP 5*)	Not more than 50 mg/kg
Methanol (FNP 5*)	Not more than 10 mg/kg
Propylene glycol	Not more than 1000 mg/kg Test as described for *Sucrose Esters of Fatty Acids* (FNP 52 Add 11 p 76)
Waxes	Not more than 14.0% See description under TESTS.

TESTS

PURITY TESTS

Waxes

Determine by gas chromatography using the following conditions:

Apparatus

GC equipped with an autosampler, a splitless injection system, flame ionization detector (FID), programmable column and detector flow rates.

GC column	DB5, 30 m x 0.25 mm ID with a 0.25 µm film thickness.
GC injector temperature:	280°
FID temperature:	300°
GC column initialtemperature:	50° (held for 2 min)
GC oven temperature increase rate:	13°/min
GC column final temperature:	300° (held for 8 min)
Carrier gas (Helium) flow rate:	1.0 ml/min
Injection mode:	splitless
Approximate run time:	30 min

Internal standard pentacosane (C25)

Calibration standards are prepared through the addition of absolute hydrocarbon standards to methylene chloride to provide hydrocarbon concentrations of 2.0, 10, 25, 50, 75, and 100 mg/kg.

Sample Preparation

Accurately weigh 200 mg of sample into a centrifuge tube and dissolve in exactly 20 ml of methylene chloride. Sonication or vortex mixing may be required to completely dissolve the product.

Centrifuge sample at 2500 rpm for 5 min if the sample appears turbid. Transfer 40 µl into 2 ml autosampler vial that contains 1.6 ml of methylene chloride and 20 µl of (5000 mg/kg) pentacosane for a final concentration of 50 mg/kg.

Sample Analysis

Autosampler injects a 1.0 µl aliquot of the solution onto the GC column.

Results

The approximate retention according to GC/FID times of nonacosane (C29), triacontane (C30), henitriacontane (C31), C32, triatriacontaine (C33), C34, C35, and the internal standard pentacosane (C25) are 18.6, 19.1, 19.6, 20.0, 20.5, 20.9, 21.4, and 16.3 minutes, respectively.

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* *Residual solvents, using head-space gas chromatography with flame ionization detection (FID)* – FNP 52 Addendum 11 (pp 165 f)

METHOD OF ASSAY

Determine the total carotenoid content and the content of lutein and zeaxantin by HPLC using the following conditions:

Reagents:

Hexane (HPLC grade)
Ethyl acetate (HPLC grade)
Ethyl alcohol
Toluene
Solvent Mixture: (10:6:7:7 hexane:ethanol:acetone:toluene v/v/v/v).

Standard Solution:

Weigh accurately about 1g lutein and transfer into 100 ml amber volumetric flask and dilute to mark with the Solvent Mixture.

Apparatus

UV/vis spectrophotometer

HPLC system with suitable diode array detector, autosampler, column oven, signal processor and degasser.

Analytical column: 3 µm silica, 4.6 mm x 250 mm.

Instrument Conditions

Oven temperature:	ambient
Mobile Phase:	70:30 (v:v) hexane/ethyl acetate (isocratic elution)
Flow Rate:	1.5 ml/min
Injection:	10 µl
Detection:	performed at 446 nm
Run Time:	approximately 40 min

Sample Preparation:

Weigh sample (range 27 to 33 mg) into a glass weighing funnel, wash crystals with heat into a 100 ml volumetric flask, dilute to the mark and stir for 10 min. Pipette 1 ml from flask into a second 100 ml volumetric flask, dilute to the mark with ethanol, mix by inversion for 20 seconds. Read samples in a spectrophotometer at 446 nm.

For HPLC, dry the samples down using nitrogen steam, dissolve solids in 70:30 hexane:ethyl acetate, add 0.5 ml to HPLC vials and measure at 446 nm.

Results

The retention times for lutein and zeaxanthin are approximately 7.7 and 8.1 min, respectively. The resolution between the HPLC peaks for lutein and xeazanthin ranged from 3.06 to 3.09.

Calculation

$$\text{Total carotenoids (\%)} = \frac{\text{Absorbance at 446 nm x 10000}}{\text{sample mass in g x 2550}}$$

Note: The factors 10000 and 2550 are the dilution factor and extinction value for a 1% solution, respectively.

Lutein (%) = total carotenoids x area % lutein

Zeaxanthin (%) = total carotenoids x area % zeaxanthin

MAGNESIUM SULFATE
(Tentative)

Information required on
- other functional uses of magnesium sulfate including their use levels, and
- the commercial use of anhydrous magnesium sulfate.

New tentative specifications prepared at 63rd JECFA (2004), published in FNP 52 Add 12 (2004). No safety evaluation undertaken.

SYNONYMS	Epsom salt (heptahydrate), INS No.518	
DEFINITION	Magnesium sulfate occurs naturally in sea water, mineral springs and in minerals such as kieserite and epsomite. It is recovered from them or by reacting sulfuric acid and magnesium oxide. It is produced with one or seven molecules of water of hydration or in a dried form containing the equivalent of between 2 and 3 waters of hydration.	
Chemical names	Magnesium sulfate	
C.A.S. number	Monohydrate: Heptahydrate: Dried:	14168-73-1 10034-99-8 15244-36-7
Chemical formula	Monohydrate: Heptahydrate: Dried:	$MgSO_4.H_2O$ $MgSO_4.7H_2O$ $MgSO_4.xH_2O$, where x is the average hydration value (between 2 and 3)
Formula weight	Monohydrate: Heptahydrate:	138.38 246.47
Assay	Not less than 99.0 % on the ignited basis	
DESCRIPTION	Colourless crystals, granular crystalline powder or white powder. Crystals effloresce in warm, dry air.	
FUNCTIONAL USES	Nutrient	
CHARACTERISTICS		
IDENTIFICATION		
Solubility (FNP 5)	Freely soluble in water, very soluble in boiling water, and sparingly soluble in alcohol.	
Test for Magnesium (FNP 5)	Passes test	
Test for Sulfate (FNP 5)	Passes test	
PURITY		
Loss on ignition (FNP 5)	Monohydrate: between 13.0 and 16.0 %; Heptahydrate: between 40.0 and 52.0 %, Dried: between 22.0 and 32.0 % (105°, 2hr, then 400° to constant weight)	
pH (FNP 5)	Between 5.5 and 7.5 (1 in 20 soln.)	
Chloride (FNP 5)	Not more than 0.03% Test 1g of the sample as described in FNP 5, “Chloride Limit Test” using 0.9 ml of 0.01 N hydrochloric acid in the control	
Arsenic (FNP 5)	Not more than 3 mg/kg (Method II)	

Iron (FNP 5)	Not more than 20 mg/kg Test as directed in FNP 5, "Iron Limited Test" using 1 ml of Iron Standard TS
Selenium (FNP 5)	Not more than 30 mg/kg Test 200 mg of the sample as described in FNP 5, "Selenium Limit Test (Method II)"
Lead (FNP 5)	Not more than 2mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the method described in FNP 5, "Instrumental Methods".
METHOD OF ASSAY	Accurately weigh about 0.5 g of the ignited sample, dissolve in 5 ml of hydrochloric acid TS (dilute), dilute with water to 100 ml, and mix. Transfer 50 ml of this solution into a 250-ml conical flask, add 10 ml of ammonia-ammonium chloride buffer TS and 0.1 ml of eriochrome black TS. Titrate with 0.05 mol/l disodium ethylenediaminetetraacetate until the red-purple solution changes to blue in colour. Each ml of 0.05 mol/l disodium ethylenediaminetetraacetate is equivalent to 12.04 mg of $MgSO_4$.

OCTANOIC ACID

New specifications prepared at 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). Small residues of octanoic acid on food (which has been treated with antimicrobial washing solutions) at the time of consumption would not pose a safety concern (63rd JECFA, 2004).

SYNONYMS	Caprylic acid
DEFINITION	Octanoic acid is manufactured from vegetable oils (coconut, palm, kernel, or palm stearene) by first refining the oil, followed by methyl transesterification and separation by distillation. The separated methyl octanoate is saponified and acidified to give octanoic acid.
Chemical name	Octanoic acid
C.A.S. number	124-07-2
Chemical formula	$CH_3(CH_2)_6CO_2H$
Formula weight	144.21
Assay	Not less than 95%
DESCRIPTION	Colourless oily liquid having a slight unpleasant odour
FUNCTIONAL USES	Antifoaming agent, surfactant. (Material for use as a flavouring agent is specified in FNP 52 Add 5, JECFA No. 99).
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Slightly soluble in water; soluble in most organic solvents
Infrared spectrum (FNP 5)	The infrared spectrum of a potassium bromide dispersion of the sample corresponds to the reference infrared spectrum in the Annex.
Acid value (FNP 5)	Between 366 and 396
PURITY	
Water (FNP 5)	Not more than 0.4% (Karl Fischer Method)
Sulfated ash (FNP 5)	Not more than 0.1% Test 10 g of the sample (Method II)
Unsaponifiable matter	Not more than 0.2% See description under TESTS
Iodine value (FNP 5)	Not more than 2.0
Decanoic acid	Not more than 3% See description under METHOD OF ASSAY
Lead (FNP 5)	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of the sample size and method of sample preparation may be based on the principles of the method described in FNP 5, “Instrumental methods”

TESTS

PURITY TESTS

Unsaponifiable matter

Weigh accurately 5.0 g of the sample into a 250 ml flask, add a solution of 2 g of potassium hydroxide in 40 ml of alcohol, and boil gently under a reflux condenser for 1 h or until saponification is complete. Transfer the contents of the flask to a glass-stoppered graduated extraction cylinder. Wash the flask with sufficient alcohol to make a volume of 40 ml in the cylinder, and complete the transfer with warm and then cold water until the total volume is 80 ml. Finally, wash the flask with a few ml of petroleum ether, add the washings to the cylinder, cool the contents of the cylinder to room temperature, and add 50 ml of petroleum ether.

Insert the stopper, shake the cylinder vigorously for at least 1 min, and allow both layers to become clear. Siphon the upper layer as completely as possible without removing any of the lower layer, collecting the ether fraction in a 500-ml separator. Repeat the extraction and siphoning at least six times with 50-ml portions of petroleum ether, shaking vigorously each time. Wash the combined extracts, with vigorous shaking, with 25-ml portions of 10% alcohol until the wash water is neutral to phenolphthalein, and discard the washings. Transfer the ether extract to a tared beaker, and rinse the separator with 10 ml of ether, adding the rinsings to the beaker. Evaporate the ether on a steam bath just to dryness, and dry the residue to constant weight, preferably at 75° to 80° under a vacuum of not more than 200 mm of Hg, or at 100° for 30 min. Cool in a desiccator, and weigh to obtain the uncorrected weight of unsaponifiable matter.

Determine the quantity of fatty acids in the residue as follows: Dissolve the residue in 50 ml of warm alcohol (containing phenolphthalein TS and previously neutralized with sodium hydroxide to a faint pink colour), and titrate with 0.02 N sodium hydroxide to the same colour. Each ml of 0.02 N sodium hydroxide is equivalent to 5.659 mg of fatty acids, calculated as oleic acid.

Subtract the calculate weight of fatty acids from the weight of the residue to obtain the corrected weight of unsaponifiable matter in the sample.

METHOD OF ASSAY

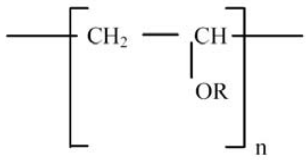
Determine using an appropriate gas chromatographic technique. The selection of sample size and method of sample preparation may be based on AOCS Method Cc 1-62 and Ce 1f-96 and follow the principles of the method described in FNP 5 "Instrumental methods". The percentage of octanoic acid is the area percent of the methyl octanoate peak.

Decanoic acid may be determined using the same gas chromatographic technique.

POLYVINYL ALCOHOL

New specifications prepared at the 61st JECFA (2003) and published in FNP 52 Add 11 (2003). An ADI of 50 mg/kg bw was established at 61st JECFA (2003).

Vinyl alcohol polymer, PVOH, INS No. 1203

DEFINITION	Polyvinyl alcohol is a synthetic resin prepared by the polymerization of vinyl acetate, followed by partial hydrolysis of the ester in the presence of an alkaline catalyst. The physical characteristics of the product depend on the degree of polymerization and the degree of hydrolysis.
Chemical names	Ethenol homopolymer
C.A.S. number	9002-89-5
Chemical formula	$(C_2H_3OR)_n$ where R=H or $COCH_3$ (randomly distributed)
Structural formula	

Where R=H or $COCH_3$ (randomly distributed)

DESCRIPTION	Odourless, translucent, white or cream-coloured granular powder.
FUNCTIONAL USES	Coating, binder, sealing agent and surface-finishing agent.
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Soluble in water, sparingly soluble in ethanol.
pH (FNP 5)	5.0 – 6.5 (1 in 5)
Infrared spectrum (FNP 5)	The infrared absorption spectrum of a potassium bromide dispersion of the sample corresponds to that of a poly vinyl alcohol standard (see Appendix).
Colour reaction A	Dissolve 0.01 g of the sample in 100 ml of water with warming and let the solution cool to room temperature. To 5 ml of the solution, add one drop of iodine TS and a few drops of boric acid solution (1 in 25). A blue colour is produced.
Colour reaction B	Dissolve 0.5 g of the sample in 10 ml of water with warming and let the solution cool to room temperature. Add 1 drop of iodine TS to 5 ml of solution and allow to stand. A dark red to blue colour is produced.
Precipitation reaction	Add 10 ml of ethanol to the remaining 5 ml of solution prepared for Colour reaction B. A white, turbid or flocculent precipitate is formed.
PURITY	
Loss on drying (FNP 5)	Not more than 5.0% (105°, 3 h)
Residue on ignition (FNP 5)	Not more than 1.0%
Water insoluble substances (FNP5)	Not more than 0.1% Substitute a 100-mesh screen for the sintered-glass filter specified in FNP 5

Particle size	Not less than 99.0% material to pass through a 100 mesh sieve Determine by sieving for 30 min 100g of sample through a 100 mesh sieve and weigh the material passing through the sieve.
Methanol and methyl acetate	Not more than 1.0 % of each See description under TESTS
Acid value	Not more than 3.0 See description under TESTS
Ester value	Between 125 and 153 mg KOH/g See description under TESTS
Degree of hydrolysis	Between 86.5 and 89.0% See description under TESTS
Viscosity	4.8 - 5.8 mPa•s (4% solution at 20º) See description under TESTS
Lead (FNP 5)	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Methanol and methyl acetate

Place 2.0 g of the sample into a 100 ml screw-cap bottle, and add a magnetic stirrer. Add 98 ml of water and 30 µl of acetone. Close the bottle tightly with the screw cap and heat in a water-bath, stirring continuously. Once the solution becomes clear, remove the bottle from the water bath and allow it to cool to room temperature.

Prepare a standard by taking 2 ml of a mixed solution of methanol and methyl acetate (1.2 % v/v solution), 98 ml of water and 30µl acetone; proceed as above starting from "close the bottle…Temperature".

GC Conditions:

Column:	Sunpak A (3.2 mm i.d. x 3 m) or equivalent
Column temperature:	160°
Injector temperature:	160°
Detector temperature:	160°

Inject 0.4 $\pm$ 0.1µl of the standard solution into the gas chromatograph and record the peak areas (PAs) for methanol, methyl acetate and acetone. Inject 0.4 $\pm$ 0.1 µl of the sample solution and record the peak areas (PAs) for methanol, methyl acetate, and acetone. Calculate the methanol and methyl acetate content using the formulae:

$$\text{Methanol (wt\%)} = \text{PA(methanol)/PA(acetone)} \times PR_1 \times 0.024 \times 100/2$$

$$\text{Methyl acetate (wt \%)} = \text{PA(methyl acetate)/ PA(acetone)} \times PR_2 \times 0.024 \times 100/2$$

where

0.024 = conversion factor to obtain the masses of methanol and methyl acetate added to 30 µl acetone (density = 0.8) for the methanol/methyl acetate standard;

PR_1 and PR_2 are the peak area ratios PA(acetone)/PA(methanol) and PA(acetone)/PA(methyl acetate), respectively, of the standard 1.2% methanol and methyl acetate aqueous solutions.

Acid value

Add 250 ml of water and a stir bar into a 500-ml round-bottom flask, attach a reflux condenser and begin heating in a boiling water bath. Add 10.0 g of the sample and continue heating for 30 minutes while stirring continuously. Remove the flask from the water-bath and continue stirring until the solution reaches room temperature. Take 50 ml

of the solution, add 1 ml of phenolphthalein TS and titrate with 0.05 M potassium hydroxide until the pink colour persists for 15 seconds; record the titre in ml (V). Calculate the acid value, A.

$$A = (56.1 \times V \times M)/W$$

Where

56.1 = the formula weight of KOH
M = molarity of the KOH solution
W = weight of sample (g).

Ester value

Accurately weigh about 1.0 g of sample into a 250-ml round-bottom flask, add 25 ml 0.5 M alcoholic potassium hydroxide, 25.0 ml of water and a few glass beads. Attach a condenser and allow the contents to reflux for 30 minutes in a boiling water-bath. Let cool to room temperature, remove the condenser, add 1 ml of phenolphthalein TS and titrate immediately with 0.5 M hydrochloric acid; record the titre in ml (V_1).

Carry out a blank test under the same conditions. Titrate with 0.5 M hydrochloric acid and record the titre in ml (V_2). Calculate the saponification value, S:

$$S = 56.1(V_2 - V_1) \times M/W$$

Where

56.1= formula weight of KOH
M = molarity of the hydrochloric acid solution
W = weight of the sample in (g).

Calculate the ester value, E:

$$E = S - A$$

Where

S = saponification value
A = acid value

Degree of hydrolysis

Convert the saponification value obtained during the determination of the ester value to the "dried basis" (S_{db}):

$$S_{db} = (S \times 100)/(100 - LOD)$$

Where

LOD= Loss on Drying.

The degree of hydrolysis is:

$$100 - [7.84\ S_{db}/(100 - 0.075\ S_{db})]$$

Viscosity

Calibration of *capillary-type* viscometers

An oil of known viscosity is used to determine the viscometer constant (k*)*.

Ostwald-Type Viscometer: Fill the tube with the exact amount of oil (adjusted to 20.0±0.1º), as specified by the manufacturer. Use either pressure or suction to adjust the meniscus of the column of liquid in the capillary tube to the level of the top graduation line. Allow the liquid to flow into the reservoir against atmospheric pressure by opening both the filling and capillary tubes. If either tube is not open, false values might be obtained. Record the time (seconds), for the liquid to flow from the upper mark to the lower mark of the capillary tube (efflux time).

Ubbelohde-Type Viscometer: Place a quantity of the oil (adjusted to 20.0 ± 0.1º) in the filling tube, and transfer to the capillary tube by gentle suction. Keep the air vent tube closed in order to prevent bubble formation in the liquid. Adjust the meniscus of the column of liquid in the capillary tube to the level of the top graduation line. Allow the liquid to flow into the reservoir against atmospheric pressure by opening both the filling and capillary tubes. If either tube is not open, false values might be obtained. Record the efflux time (seconds).

The viscosity constant for *capillary-type* viscometers is given by:

$$k = v/dt,$$

Where, v is the known viscosity (mPa•s) of the oil used for viscometer calibration; d is the density (g/ml) of the liquid tested at 20º/20º; and t (seconds) is the efflux time.

Procedure:

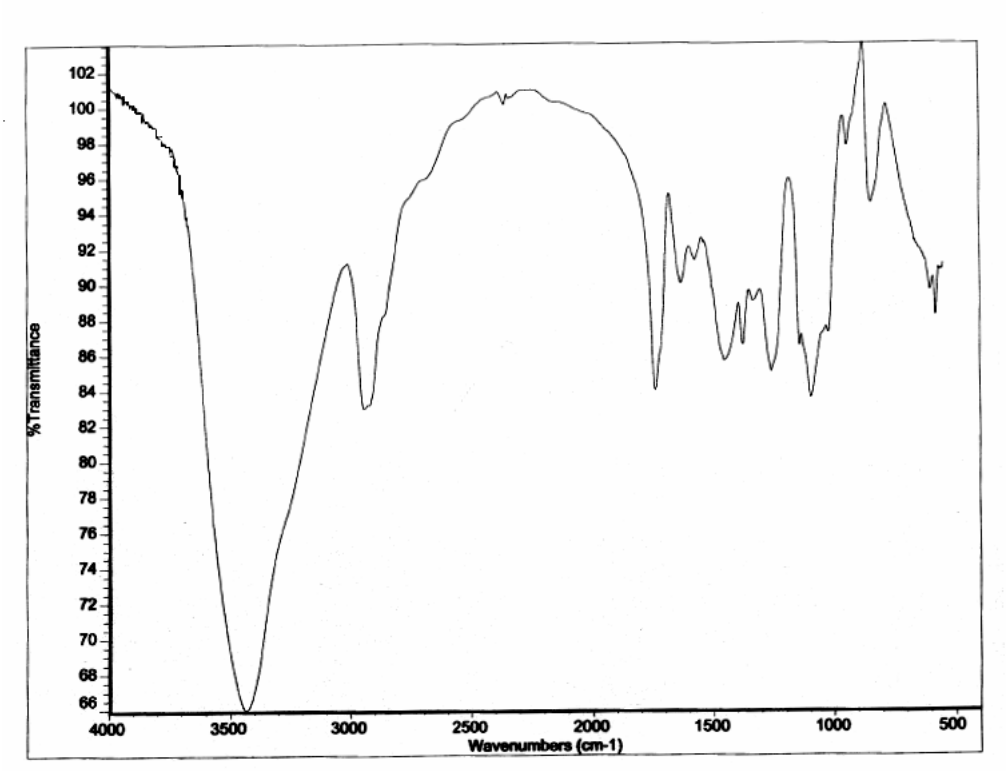
Weigh a quantity of undried sample equivalent to 6.00 g on the dried basis. Into a tared 250-ml flask containing a magnetic stir bar and approximately 140 ml of water, quickly (seconds) transfer the sample, while simultaneously stirring slowly and continuously. Once the sample appears thoroughly saturated, slowly increase the stirring rate to minimize the entrainment of air in the mixture. Heat the mixture to 90°, and maintain it at this temperature for approximately 5 minutes; discontinue heating and continue stirring for 1 hour. Add water in small amounts to attain a total mixture weight of 150 g, and resume stirring until the mixture appears homogenous. Filter the mixture through a tared 100-mesh screen into a 250 ml conical flask, cool the filtrate to about 15°, mix, and determine its viscosity at 20º using an appropriate viscometer (follow the manufacturer's instructions). NOTE: The temperature at which the viscosity measurement is made must be strictly controlled.

For measurements using *capillary-type* viscometers, the viscosity is given by:

$$v = kdt$$

where t is the efflux time for the sample solution and d is its density at 20º.

Appendix



POLYVINYL ALCOHOL

STEVIOL GLYCOSIDES
(Tentative)

Information required for commercially available products on

- analytical data on distribution and concentrations of all component steviol glycosides, including those that are not identified in these tentative specifications
- method of analysis for the determination of all component steviol glycosides, including those that are not identified in these tentative specifications
- the nature and concentration of the non-steviol glycosides fractions
- the quantities of residual solvents from purification steps of the manufacturing process
- the hydrolytic stability of the steviol glycosides in acidic foods and beverages

New tentative specifications prepared at the 63rd JECFA (2004), published in FNP 52 Add 12 (2004). A temporary ADI of 0-2 mg/kg bw (expressed as steviol) was established at the 63rd JECFA (2004).

DEFINITION

Steviol glycosides are obtained by extracting leaves of *Stevia rebaudiana* Bertoni with hot water followed by solvent purification of the water-soluble extract. Ion exchange resins may also be used during the purification process. Stevioside and rebaudioside A are the principal steviol glycosides of the specified material. Rebaudioside C and dulcoside A are secondary steviol glycosides**.** Other steviol glycosides may also be present.

Chemical name

The following are the chemical names for the principal and secondary steviol glycosides:
Stevioside: 13-[(2-O-β–D-glucopyranosyl-β–D-glucopyranosyl) oxy] kaur-16-en-18-oic acid β-D-glucopyranosyl ester

Rebaudioside A: 13-[(2-O-β –D-glucopyranosyl-3-O-β–D-glucopyranosyl-β-D-glucopyranosyl)oxy] kaur-16-en-18-oic acid β-D-glucopyranosyl ester

Rebaudioside C: 13-[(2-O-α–L-rhamnopyranosyl-3-O-β–D-glucopyranosyl-β-D-glucopyranosyl)oxy] kaur-16-en-18-oic acid β-D-glucopyranosyl ester

Dulcoside A: 13-[2-O-α–L-rhamnopyranosyl-β–D-glucopyranosyl]oxy] kaur-16-en-18-oic acid β-D-glucopyranosyl ester

C.A.S. number

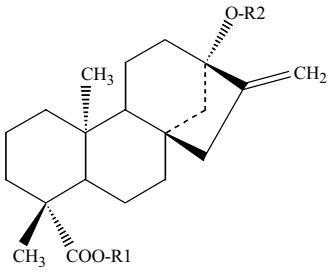
The following are the C.A.S. numbers for the principal and secondary steviol glycosides:
Stevioside: 57817-89-7
Rebaudioside A: 58543-16-1
Rebaudioside C: 63550-99-2
Dulcoside A: 64432-06-0

Chemical formula

The following are the chemical formulas for the principal and secondary steviol glycosides:
Stevioside: $C_{38}H_{60}O_{18}$
Rebaudioside A: $C_{44}H_{70}O_{23}$
Rebaudioside C: $C_{44}H_{70}O_{22}$
Dulcoside A: $C_{38}H_{60}O_{17}$

Structural formula

The following are the structural formulas for the principal and secondary steviol glycosides:



Compound name	R1	R2
Stevioside	β-Glc	β-Glc-β-Glc(2→1)
Rebaudioside A	β-Glc	β-Glc-β-Glc(2→1) | β-Glc(3→1)
Rebaudioside C	β-Glc	β-Glc-α-Rha(2→1) | β-Glc(3→1)
Dulcoside A	β-Glc	β-Glc-α-Rha(2→1)

Steviol (R1 = R2 = H) is the aglycone of the steviol glycosides.
Glc and Rha represent, respectively, glucose and rhamnose sugar moieties.

Formula weight

The following are the formula weights for the principal and secondary steviol glycosides:

Stevioside:	804.88	Rebaudioside C:	951.03
Rebaudioside A:	967.03	Dulcoside A:	788.88

Assay

Not less than 95% of total steviol glycosides. The sum of the percentages of stevioside and rebaudioside A is not less than 70%.

DESCRIPTION

White crystalline powder, odourless or having a slight characteristic odour. About 200-300 times sweeter than sucrose.

FUNCTIONAL USES

Sweetener

CHARACTERISTICS

IDENTIFICATION

Solubility (FNP 5)

Freely soluble in water and in ethanol

Stevioside and rebaudioside A

The material contains not less than 70% of stevioside and rebaudioside A as identified and determined in the Method of Assay.

PURITY

Ash (FNP 5)

Not more than 1%
Test 3 g of the sample (Method I)

Loss on drying (FNP 5)

Not more than 4% (105°, 3h)

Residual solvents

Information required

Arsenic (FNP 5) Not more than 1 mg/kg

Lead (FNP 5) Not more than 1 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental methods".

METHOD OF ASSAY Determine the percentages of the steviol glycosides by high pressure liquid chromatography (FNP 5).

Standards: Stevioside, >99.3% purity and rebaudioside A, >97% purity (available from Wako pure Chemical Industries, Ltd. Japan).

Mobile phase: Mix HPLC grade acetonitrile and water (80:20). Adjust the pH to 3.0 with phosphoric acid (85% reagent grade. Filter through 0.22 µm Millipore filter or equivalent.

Standard solution: Accurately weigh 50 mg of dried (105°, 3h) stevioside standard into a 100 ml volumetric flask and dilute to volume with mobile phase.

Sample solution: Accurately weigh 60 – 120 mg of the sample into a 100 ml volumetric flask. Dissolve in the mobile phase and dilute with the mobile phase to volume.

Conditions:

Column:	Supelcosil LC-NH2 or equivalent (length: 15 - 30 cm; inner diameter: 3.9 - 4.6 mm)
Mobile phase:	A 80:20 mixture of acetonitrile and water (see above)
Flow rate:	Adjust so that the retention time of stevioside is about 10 min.
Injection volume:	5 - 10 µl
Detector:	UV at 210 nm
Column temperature:	40°

Equilibrate the instrument by pumping mobile phase through it until a drift-free baseline is obtained. Record the chromatograms of the sample solution and of the standard solution.

The relative retention times of dulcoside A and rebaudioside C with respect to stevioside are 0.68 – 0.76 and 1.15 - 1.23, respectively. To obtain the retention time of rebaudioside A, use the rebaudioside A standard.

Measure the peak areas of stevioside, rebaudioside A, rebaudioside C and dulcoside A from the sample solution. Measure the peak area of stevioside from the standard solution.

Calculate the percentage of stevioside, dulcoside A, rebaudioside A and rebaudioside C from the formulas:

% stevioside =	[Ws/W] x [Aa/As] x 100
% dulcoside A =	[Ws/W] x Ab x [0.98/As] x 100
% rebaudioside A=	[Ws/W] x Ac x [1.20/As] x 100
% rebaudioside C =	[Ws/W] x Ad x [1.18/As] x 100

where

Ws =	weighed amount (mg) of stevioside in the standard solution
W =	weighed amount of sample (mg)
As =	Peak area of stevioside from the standard solution
Aa =	Peak area of stevioside from the sample solution
Ab =	Peak area of dulcoside A from the sample solution
Ac =	Peak area of rebaudioside A from the sample solution
Ad =	Peak area of rebaudioside C from the sample solution

The factors 0.98, 1.20, and 1.18 for, respectively, dulcoside A, rebaudioside A, and rebaudioside C are the ratios of their formula weights to that of the formula weight of stevioside.

Calculate (1) the % of steviol glycosides (sum the four percentages) and (2) the sum of the percentages for stevioside and rebaudioside A.

TITANIUM DIOXIDE

Prepared at the 63rd JECFA (2004), published in FNP 52 Add 12 (2004) superseding specifications prepared at the 39th JECFA (1992), published in FNP 52 Add 1 (1992). An ADI "not limited" was established at the 13th JECFA (1969).

SYNONYMS	Titanium dioxide, CI Pigment white 6, CI (1975) No. 77891, INS No. 171
DEFINITION	Titanium dioxide consists essentially of pure titanium dioxide which may be coated with small amounts of alumina and/or silica to improve the technological properties of the product. It is manufactured by digesting ilmenite ($FeTiO_3$) or ilmenite and titanium slag with sulfuric acid and the product is diluted with water or dilute acid. The resulting liquor is clarified by sedimentation to remove insoluble residues such as silica and iron is removed by crystallization (as $FeSO_4$. $7H_2O$) and filtration. The liquid is then hydrolyzed with alkali under controlled conditions to produce a precipitate of titanium dioxide. The product is filtered, washed, calcined and micronized.
C.A.S. number	13463-67-7
Chemical formula	TiO_2
Formula weight	79.88
Assay	Not less than 99.0% on the dried basis (on an aluminium oxide and silicon dioxide-free basis)
DESCRIPTION	Amorphous white powder
FUNCTIONAL USES	Colour
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Insoluble in water, hydrochloric acid, dilute sulfuric acid and organic solvents. Dissolves slowly in hydrofluoric acid and hot concentrated sulfuric acid.
Colour reaction	Add 5 ml sulfuric acid to 0.5 g of the sample, heat gently until fume of sulfuric acid appear, then cool. Cautiously dilute to about 100 ml with water and filter. To 5 ml of this clear filtrate, add few drops of hydrogen peroxide, an orange red colour appears immediately.
PURITY	
Loss on drying (FNP 5)	Not more than 0.5% (105°, 3 h)
Loss on ignition (FNP 5)	Not more than 1.0% (800 °) on dried basis
Aluminium oxide and/or silicon dioxide	Not more than 2%, either singly or combined See description under TESTS
Acid-soluble substances	Not more than 0.5% Not more than 1.5% for products containing alumina and/or silica. Suspend 5 g of the sample in 100 ml 0.5 N hydrochloric acid and on steam bath for 30 min with occasional stirring. Filter through a Gooch crucible fitted with a glass fibre filter paper. Wash with three 10-ml portions of 0.5 N hydrochloric acid, evaporate the combined filtrate and washings to dryness and ignite at a dull red heat to constant weight.

Water-soluble matter (FNP 5)	Not more than 0.5% Proceed as directed under acid soluble substances (above), using water in place of 0.5 N hydrochloric acid.
Impurities soluble in 0.5 N hydrochloric acid	
Antimony	Not more than 2 mg/kg See description under TESTS
Arsenic (FNP5)	Not more than 3 mg/kg (Method II) See description under TESTS
Cadmium	Not more than 1 mg/kg See description under TESTS
Lead	Not more than 10 mg/kg See description under TESTS
Mercury (FNP 5)	Not more than 1 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of samples size and method of sample preparation may be based on principles of methods described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Antimony, arsenic, cadmium and lead	Transfer 10.0 g of sample into a 250-mL beaker, add 50 mL of 0.5 *N* hydrochloric acid, cover with a watch glass, and heat to boiling on a hot plate. Boil gently for 15 min, then pour the slurry into a 100 to 150-mL centrifuge bottle, and centrifuge for 10 to 15 min, or until undissolved material settles. Decant the supernatant extract through a Whatman No. 4 filter paper, or equivalent, collecting the filtrate in a 100-mL volumetric flask and retaining as much as possible of the undissolved material in the centrifuge bottle. Add 10 mL of hot water to the original beaker, washing off the watch glass with the water, and pour the slurry into the centrifuge bottle. Form a slurry, using a glass stirring rod, and centrifuge. Decant through the same filter paper, and collect the washings in the volumetric flask containing the initial extract. Repeat the entire washing process two more times. Finally, wash the filter paper with 10 to 15 mL of hot water. Cool the contents of the flask to room temperature, dilute to volume with water, and mix. Determine antimony, cadmium and lead using an atomic absorption technique appropriate to the specified level and arsenic using Method II of FNP 5.
Aluminium oxide	Reagents and sample solutions 0.01 N Zinc sulfate: Dissolve 2.9 g of zinc sulfate ($ZnSO_4 \cdot 7H_2O$) in sufficient water to make 1000 ml. Standardize the solution as follows: Dissolve 500 mg of high-purity (99.9%) aluminium wire, accurately weighed, in 20 ml of concentrated hydrochloric acid, heating gently to effect solution, then transfer into a 1000-ml volumetric flask, dilute to volume with water, and mix. Transfer a 10 ml aliquot of this solution into a 500 ml Erlenmeyer flask containing 90 ml of water and 3 ml of concentrated hydrochloric acid, add 1 drop of methyl orange TS and 25 ml of 0.02 M disodium ethylenediaminetetraacetate (EDTA), and continue as directed below under Sample Solution C, beginning with "Add dropwise ammonia solution (1 in 5) until...". Calculate the titer T of zinc sulfate solution by the formula: $$T = \frac{18.896 \times W}{V}$$ where T = mg of Al_2O_3 per ml of zinc sulfate solution W = g of the aluminium wire V = ml of the zinc sulfate solution consumed in the second titration

18.896 factor derived as follows:

$$\frac{MW\ of\ Al_2O_3}{MW\ of\ Al}\ x\ 1000\ mg\ /\ kg\ x\ 10\ ml\ /\ 2$$

Sample Solution A

Fuse 1 g of the sample, accurately weighed, with 10 g of sodium bisulfate ($NaHSO_4 \cdot H_2O$) contained in a 250-ml high-silica glass Erlenmeyer flask. (Caution: Do not use more sodium bisulfate than specified, as an excess concentration of salt will interfere with the EDTA titration later on in the procedure.)

Begin heating at low heat on a hot plate, then gradually raise the temperature until full heat is reached. When spattering has stopped and light fumes of SO_3 appear, heat in the full flame of a Meker burner, with the flask tilted so that the fusion is concentrated at one end of the flask. Swirl constantly until the melt is clear (except for silica content), but guarding against prolonged heating to avoid precipitation of titanium dioxide. Cool, add 25 ml sulfuric acid solution (1 in 2) and then heat until the mass has dissolved and a clear solution results. Cool, and dilute to 120 ml with water.

Sample Solution B

Measure out 200 ml of approximately 6.25 M sodium hydroxide, and add 65 ml of it to Sample Solution A while stirring with a magnetic stirrer ; pour the remaining 135 ml of the alkali solution into a 500-ml volumetric flask.

Slowly, and with constant stirring, add the sample mixture to the alkali solution in the 500-ml volumetric flask, then dilute to volume with water, and mix. (Note: If the procedure is delayed at this point for more than 2 hours, store the contents of the volumetric flask in a polyethylene bottle.) Allow most of the precipitate to settle out (or centrifuge for 5 min) then filter the supernatant liquid through a very fine filter paper. Label the filtrate Sample Solution B.

Sample Solution C

Transfer 100 ml of the Sample Solution B into a 500-ml Erlenmeyer flask, add 1 drop of methyl orange TS, acidify with hydrochloric acid solution (1 in 2), and then add about 3 ml in excess. Add 25 ml of 0.02 M disodium ethylenediamine tetraacetate, and mix. [Note: If the approximate Al_2O_3 content is known, calculate the optimum volume of EDTA solution to be added by the formula (4 x % Al_2O_3) + 5.]

Add, dropwise, ammonia solution (1 in 5) until the colour is just completely changed from red to orange-yellow, the add 10 ml of ammonium acetate buffer solution (77 g of ammonium acetate plus 10 ml of glacial acetic acid, dilute to 1000 ml with water) and 10 ml of diammonium hydrogen phosphate solution (150 g of diammonium hydrogen phosphate in 700 ml of water, adjusted to pH 5.5 with a 1 in 2 solution of hydrochloric acid, then dilute to 1000 ml with water). Boil for 5 min, cool quickly to room temperature in a stream of runnig water, add 3 drops of xylenol orange TS, and mix. If the solution is purple, yellow-brown, or pink, bring the pH to 5.3 - 5.7 by the addition of acetic acid; at the desired pH a pink colour indicates that not enough of the EDTA solution has been added, in which case another 100 ml of Sample Solution B should be taken and treated as directed from the beginning of the description of "Sample Solution C", except that 50 ml, rather than 25 ml, of 0.02 M disodium ethylenediamine tetraacetate should be used.

Procedure

Titrate Sample Solution C with 0.01 N zinc sulfate to the first yellow-brown or pink end-point colour that persists for 5-10 sec.

Caution:

This titration should be performed quickly near the end-point by adding rapidly 0.2 ml increments of the titrant until the first colour change occurs; although the colour will fade in 5-10 sec, it is the true end-point. Failure to observe the first colour change will result in an incorrect titration. The fading end-point does not occur at the second end-point. This first titration should require more than 8 ml of titrant, but for more accurate work a titration of 10-15 ml is desirable.

Add 2 g of sodium fluoride, boil the mixture for 2-5 min, and cool in a stream of running water. Titrate the EDTA (which is released by fluoride from its aluminium

complex) with 0.01 N zinc sulfate to the same fugitive yellow-brown or pink end-point as described above.

Calculation:

Calculate the percentage of aluminium oxide (Al_2O_3) in the sample taken by the formula:

$$\%\ of\ Al_2O_3 = \frac{V\ x\ T}{2\ x\ S}$$

where

V = ml of 0.01 N zinc sulfate consumed in the second titration
T = the titer of the zinc sulfate solution, determined previously
S = g of the sample taken

Silicon dioxide

Fuse 1 g of the sample, accurately weighed, with 10 g of sodium bisulfate ($NaHSO_4 \cdot H_2O$) contained in a 250-ml high-silica glass Erlenmeyer flask. Heat gently over a Meker burner, while swirling the flask, until decomposition and fusion are complete and the melt is clear, except for the silica content, and then cool.

Caution:

Do not overheat the contents of the flask at the beginning, and heat cautiously during fusion to avoid spattering.

To the cold melt add 25 ml of sulfuric acid solution (1 in 2), and heat very carefully and very slowly until the melt is dissolved. Cool, and carefully add 150 ml of water, pouring very small portions down the sides of the flask, with frequent swirling, to avoid over-heating and spattering. Allow the contents of the flask to cool, and then filter through fine ashless filter paper, using a 60 degree gravity funnel. Wash out all the silica from the flask onto the filter paper with sulfuric acid solution (1 in 10). Transfer the filter paper and its contents into a platinum crucible, dry in an oven at 120^0, and then heat the partly covered crucible over a Bunsen burner. To prevent flaming of the filter paper, heat first the cover from above, and then the crucible from below.

When the filter paper is consumed, transfer the crucible to a muffle furnace and ignite at 1000^o for 30 min. Cool in a desiccator, and weigh. Add 2 drops of sulfuric acid (1 in 2) and 5 ml of concentrated hydrofluoric acid (sp.gr. 1.15), and carefully evaporate to dryness, first on a low-heat hot plate (to remove the HF) and then over a Bunsen burner (to remove the H_2SO_4). Take precautions to avoid spattering, especially after removal of the HF. Ignite at 1000^o for 10 min, cool in a desiccator, and weigh again. Record the difference between the two weights as the content of SiO_2 in the sample.

METHOD OF ASSAY

Transfer about 300 mg of the sample, previously dried at 105^o for 3 h and accurately weighed, into a 250-ml beaker, add 20 ml of sulfuric acid and 7 to 8 g of ammonium sulfate, and mix. Heat on a hot plate until fumes of sulfuric acid appear, and continue heating over a strong flame until the sample dissolves or it is apparent that the undissolved residue is siliceous matter. Cool, cautiously dilute with 100 ml of water, and stir. Heat carefully to boiling while stirring, allow the insoluble matter to settle, and filter. Transfer the entire residue to the filter, and wash thoroughly with cold dilute sulfuric acid TS. Dilute the filtrate with water to 200 ml, and cautiously add about 10 ml of stronger ammonia TS to reduce the acid concentration to about 5% by volume of sulfuric acid.

Prepare a zinc amalgam Jones reductor column in a 25 cm glass tube, placing a pledget of glass wool in the bottom of the tube and filling the constricted portion of the tube with zinc amalgam prepared as follows:

Add to 30 mesh zinc to a 2% mercuric chloride solution, using about 10 min, 100 ml of the solution for each 100 g of zinc. After about 10 min, decant the solution from the zinc, the wash the zinc with water by decantation. Transfer the zinc amalgam to the reductor tube, wash the column with 100-ml portions of dilute sulfuric acid TS until 100 ml of the washing does not decolourize 1 drop of 0.1 N potassium permanganate.

Place 50 ml of ferric ammonium sulfate TS in a 500-ml suction flask, and add 0.1 N potassium permanganate until a faint pink colour persists for 5 min. Attach the Jones reductor tube containing the Zinc amalgam column to the neck of the flask, and pass 50 ml of dilute sulfuric acid TS through the tube at a rate of about 30 ml per min. Pass the prepared titanium solution through the column at the same rate, followed by 100 ml each of dilute sulfuric acid TS and water. During these operations, keep the tube filled with solution or water above the upper level of the amalgam column. Gradually release the suction, wash down the outlet tube and the sides of the receiver, and titrate immediately with 0.1 N potassium permanganate. Perform a blank determination, substituting 200 ml of dilute sulfuric acid (1 in 20) for the sample solution, and make any necessary correction. Each ml of 0.1 N potassium permanganate is equivalent to 7.990 mg of TiO_2.

XYLANASE FROM *BACILLUS SUBTILIS* EXPRESSED IN *BACILLUS SUBTILIS*

Ne e a e a e a e E FA (2004) a e FNP 2 A 12 (2004). A ADI e e a e a e a e E FA (2004).

SYNONYMS

Beta-1,4-D-xylan xylanohydrolase; endo-1,4-beta-xylanase; beta-D-xylanase; beta-xylanase

SOURCES

Produced by pure culture fermentation of a nonpathogenic and nontoxigenic genetically modified strain of *Ba* containing the xylanase gene derived from *B.* . The enzyme is secreted to the fermentation broth which is subsequently separated from the bacterial cells and subjected to ultrafiltration to obtain the concentrated xylanase. The concentrated enzyme is either dried on a suitable carrier (e.g., starch and salt) or formulated as a liquid product using food grade compounds for stabilization and preservation. The dried product can be prepared either as a free-flowing microgranulate or tablets.

ACTIVE PRINCIPLES

Xylanase

SYSTEMATIC NAMES AND NUMBERS

1,4-beta-D-xylan xylanohydrolase; EC 3.2.1.8; CAS No. 9025-57-4

REACTIONS CATALYZED

Endohydrolysis of 1,4-beta-D-xylosidic linkages in xylans and arabinoxylans

DESCRIPTION

Brownish liquid, off-white microgranulate or tablets.

FUNCTIONAL USES

Enzyme preparation.
Used in baked goods and pasta to increase dough stability.

GENERAL SPECIFICATIONS

Must conform to the General Specifications for Enzyme Preparations used in Food Processing (FNP 52, current edition, including amendments).

CHARACTERISTICS

IDENTIFICATION

Xylanase activity

The sample shows endo-xylanase activity
See description under TESTS

TESTS

Xylanase activity

Principle

Xylanase samples are incubated with azurine-crosslinked wheat arabinoxylan substrate. Xylanase hydrolyses the substrate to water-soluble fragments with the concomitant change in colour. The reaction is terminated after a designated time and the optical density (OD) of the reaction mixture is measured at 590 nm (OD_{590}). Xylanase activity is calculated based on the rate of release of the azurine dye. One xylanase unit (XU) is defined as the amount of enzyme that increases the OD_{590} at a rate of one OD per 10 minutes under standard conditions (pH=5.00; 40^{o}).

Apparatus

Spectrophotometer
Magnetic stirrer
Thermostatic water bath
Whatman No. 1 filter paper
Test tubes (15 ml)

Reagents

Citric acid monohydrate
Disodium hydrogen phosphate dihydrate

TRIS (tris (hydroxyl methyl) amino methane)
Sodium hydroxide
Substrate (azurine-crosslinked wheat arabinoxylan: Xylazyme tablets from Megazyme, Ireland)

Note: a new batch of the substrate should be compared with a previous batch by analyzing the same enzyme preparation using both substrates. If a difference in enzymatic activity is noted, an appropriate correction factor should be calculated and applied to the results obtained with the new batch of the substrate.

Reagent solutions

ction buff r (McIlvaine buffer, pH 5.00): Dissolve 10.19 g of citric acid monohydrate and 18.33 g disodium hydrogen phosphate dihydrate in 850 ml distilled water in a 1000 ml volumetric flask. Adjust the pH to 5.00 using either 0.1M citric acid monohydrate or 0.2M disodium hydrogen phosphate dihydrate. Add water to 1000 ml. The buffer can be stored for up to 6 months at 2-5^{o}.

top solution (2% w/v TRIS, pH 12.0): Dissolve 20 g of TRIS in 850 ml distilled water in a 1000 ml volumetric flask. Adjust the pH to 12.0 with 5M NaOH. The solution can be stored for up to six months at 2-5^{o}.

Test sample solutions

Accurately weigh a quantity of the enzyme preparation that would give an OD increase within the range of 0.3 – 1.2 in a 100 ml volumetric flask. Add 60 ml of the reaction buffer. Stir the solution using a magnetic stirrer for 10 minutes. Remove the magnet and add the reaction buffer to volume. Transfer the enzyme solution to a glass beaker and let it stand for 5 minutes or until the precipitate settles. Use clear solution for analysis.

Blank

Pre-heat 1.0 ml reaction buffer at 40.0^{o} for 5 minutes. Add one Xylazyme tablet. After exactly 10 minutes at 40.0^{o}, add 10.0 ml stop solution and filter the sample through Whatman No.1 filter.

Procedure

1) Prepare 3 test tubes for each test sample. Pipette 1 ml of the reaction buffer to each tube and add 50, 75, and 100 microliters of the test sample solution.
2) Pre-heat all test sample solutions at 40.0o for 5 minutes.
3) Add one Xylazyme tablet to each tube. Do not stir.
4) After 10 minutes (±1 sec.), terminate the reaction by adding 10 ml stop solution.
5) Filter all solutions through Whatman No. 1 filter paper.
6) Measure OD of each test sample solution against the blank at 590 nm.

Calculations

Perform linear regression on OD_{590} as a function of test sample volumes (in milliliters) used in the analysis. Calculate the activity of the enzyme preparation in xylanase units (XU) per gram (g) using the following equation:

$$\text{——} = \frac{V}{W}$$

Where:

S = Slope obtained from linear regression of the OD_{590} as a function of sample volume in ml
V = Volume of the volumetric flask used to prepare the test sample solution in ml (multiplied by further dilutions, if applicable)
W = Weight of the enzyme preparation in grams

XYLANASE (RESISTANT TO XYLANASE INHIBITOR) FROM *BACILLUS SUBTILIS* CONTAINING A MODIFIED XYLANASE GENE FROM *BACILLUS SUBTILIS*

New specifications prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). An ADI "not specified" was established at the 63rd JECFA (2004).

SYNONYMS Beta-1,4-D-xylan xylanohydrolase; endo-1,4-beta-xylanase; beta-D-xylanase; beta-xylanase

SOURCES Produced by pure culture fermentation of a nonpathogenic and nontoxigenic genetically modified strain of *Bacillus subtilis* containing the xylanase gene derived from *B. subtilis* and modified to encode xylanase that is resistant to the xylanase inhibitor present in flour. The enzyme is secreted to the fermentation broth which is subsequently separated from the bacterial cells and subjected to ultrafiltration to obtain the concentrated xylanase. The concentrated enzyme is either dried on a suitable carrier (e.g., starch and salt) or formulated as a liquid product using food grade compounds for stabilization and preservation. The dried product can be prepared either as a free-flowing microgranulate or tablets.

ACTIVE PRINCIPLES Xylanase

SYSTEMATIC NAMES AND NUMBERS 1,4-beta-D-xylan xylanohydrolase; EC 3.2.1.8; CAS No. 9025-57-4

REACTIONS CATALYZED Endohydrolysis of 1,4-beta-D-xylosidic linkages in xylans and arabinoxylans

DESCRIPTION Brownish liquid, off-white microgranulate or tablets.

FUNCTIONAL USES Enzyme preparation.
Used in baked goods and pasta to increase dough stability.

GENERAL SPECIFICATIONS Must conform to the General Specifications for Enzyme Preparations used in Food Processing (FNP 52, current edition, including amendments).

CHARACTERISTICS

IDENTIFICATION

Xylanase activity — The sample shows endo-xylanase activity
See description under TESTS

TESTS

Xylanase activity

Principle

Xylanase samples are incubated with azurine-crosslinked wheat arabinoxylan substrate. Xylanase hydrolyses the substrate to water-soluble fragments with the concomitant change in colour. The reaction is terminated after a designated time and the optical density (OD) of the reaction mixture is measured at 590 nm (OD_{590}). Xylanase activity is calculated based on the rate of release of the azurine dye. One xylanase unit (XU) is defined as the amount of enzyme that increases the OD_{590} at a rate of one OD per 10 minutes under standard conditions (pH=5.00; 40^{o}).

Apparatus

Spectrophotometer
Magnetic stirrer
Thermostatic water bath
Whatman No. 1 filter paper
Test tubes (15 ml)

Reagents

Citric acid monohydrate
Disodium hydrogen phosphate dihydrate

TRIS (tris (hydroxyl methyl) amino methane)
Sodium hydroxide
Substrate (azurine-crosslinked wheat arabinoxylan: Xylazyme tablets from Megazyme, Ireland)

Note: a new batch of the substrate should be compared with a previous batch by analyzing the same enzyme preparation using both substrates. If a difference in enzymatic activity is noted, an appropriate correction factor should be calculated and applied to the results obtained with the new batch of the substrate.

Reagent solutions

Reaction buffer (McIlvaine buffer, pH 5.00): Dissolve 10.19 g of citric acid monohydrate and 18.33 g disodium hydrogen phosphate dihydrate in 850 ml distilled water in a 1000 ml volumetric flask. Adjust the pH to 5.00 using either 0.1M citric acid monohydrate or 0.2M disodium hydrogen phosphate dihydrate. Add water to 1000 ml. The buffer can be stored for up to 6 months at 2-5°.

Stop solution (2% w/v TRIS, pH 12.0): Dissolve 20 g of TRIS in 850 ml distilled water in a 1000 ml volumetric flask. Adjust the pH to 12.0 with 5M NaOH. The solution can be stored for up to six months at 2-5°.

Test sample solutions

Accurately weigh a quantity of the enzyme preparation that would give an OD increase within the range of 0.3 – 1.2 in a 100 ml volumetric flask. Add 60 ml of the reaction buffer. Stir the solution using a magnetic stirrer for 10 minutes. Remove the magnet and add the reaction buffer to volume. Transfer the enzyme solution to a glass beaker and let it stand for 5 minutes or until the precipitate settles. Use clear solution for analysis.

Blank

Pre-heat 1.0 ml reaction buffer at 40.0° for 5 minutes. Add one Xylazyme tablet. After exactly 10 minutes at 40.0°, add 10.0 ml stop solution and filter the sample through Whatman No.1 filter.

Procedure

1) Prepare 3 test tubes for each test sample. Pipette 1 ml of the reaction buffer to each tube and add 50, 75, and 100 microliters of the test sample solution.
2) Pre-heat all test sample solutions at 40.0° for 5 minutes.
3) Add one Xylazyme tablet to each tube. Do not stir.
4) After 10 minutes (±1 sec.), terminate the reaction by adding 10 ml stop solution.
5) Filter all solutions through Whatman No. 1 filter paper.
6) Measure OD of each test sample solution against the blank at 590 nm.

Calculations

Perform linear regression on OD_{590} as a function of test sample volumes (in milliliters) used in the analysis. Calculate the activity of the enzyme preparation in xylanase units (XU) per gram (g) using the following equation:

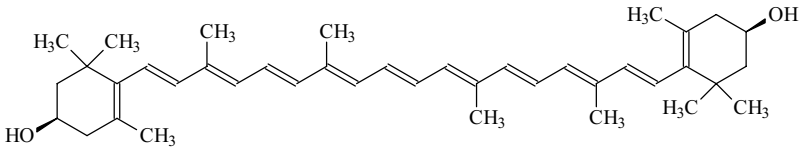
$$\frac{XU}{g} = S\frac{V}{W}$$

Where:

S = Slope obtained from linear regression of the OD_{590} as a function of sample volume in ml
V = Volume of the volumetric flask used to prepare the test sample solution in ml (multiplied by further dilutions, if applicable)
W = Weight of the enzyme preparation in grams

ZEAXANTHIN (SYNTHETIC)

New specifications prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004). A group ADI of 0 – 2 mg/kg bw for lutein and synthetic zeaxanthin was established at the 63rd JECFA (2004).

DEFINITION	These specifications apply to synthetic all-trans isomer of zeaxanthin that is produced by the Wittig reaction from the raw materials that are commonly used in the production of other carotenoids with application in foods. Minor quantities of cis-zeaxanthins and byproducts 12'-apo-zeaxanthinal, parasiloxanthin diatoxanthin and triphenyl phosphine oxide may be present in the final product.
Chemical Names	(all-E)-1,1'-(3,7,12,16-Tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis[2,6,6-trimethylcyclohexene-3-ol]; 3R,3'R-β,β-Carotene-3,3'-diol
C.A.S. number	144-68-3
Chemical formula	$C_{40}H_{56}O_2$
Structural formula	
Formula weight	568.89
Assay	Not less than 96.0% and not more than 101.0%
DESCRIPTION	Orange-red crystalline powder, with little or no odour
FUNCTIONAL USES	Colour, nutrient supplement
CHARACTERISTICS	
IDENTIFICATION	
Solubility (FNP 5)	Sparingly soluble in ethanol, practically insoluble in water
Test for carotenoid	The colour of the solution of the sample in acetone disappears after successive additions of a 5 % solution of sodium nitrite and 1N sulfuric acid.
Spectrophotometry (FNP 5)	An ethanol solution of the sample shows maximum absorption at 450 to 454 nm
PURITY	
Loss on drying (FNP 5)	Not more than 0.2 % (80° under reduced pressure for 18 h in the presence of P_2O_5)
cis-Zeaxanthins	Not more than 2.0 % See description under METHOD OF ASSAY
12'-Apo-zeaxanthinal, diatoxanthin, parasiloxanthin	Not more than 1.0 % See description under METHOD OF ASSAY
Triphenyl phosphine oxide (TPPO)	Not more than 100 mg/kg See description under TESTS
Lead (FNP 5)	Not more than 2 mg/kg Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, "Instrumental Methods".

TESTS

PURITY TESTS

Triphenyl phosphine oxide (TPPO)

Determine by HPLC using the following conditions:

Calibration solution:

10 mg/l TPPO (99 %) in tetrahydrofuran.

Test solution:

Dissolve 950 to 1000 mg of sample in 100 ml of tetrahydrofuran.

Mobile phase:

Isopropanol : hexane (1 : 20.2)

Apparatus:

Column:	Stainless steel; 150 x 4.6 mm
Stationary phase:	Supelcosil LC-Si, 5 µm or similar
Pump:	Flow 1.5 ml/min; pressure 35 to 40 bar
Detector:	UV 210 nm
Injection:	50 µl

Results:

Run time: 10 min
The retention time for TPPO is approximately 8.1 min.

Calculation:

$$\% \text{ TPPO} = \frac{A_s \times W_c \times 0.99 \times 100 \times 100}{A_c \times W_s \times 1000}$$

Where

A_s = peak area of the sample solution
A_c = peak area of the calibration solution
W_c = weight of TPPO (99 %) in mg
W_s = weight of the sample in mg

METHOD OF ASSAY

The HPLC method of assay is designed to determine *trans*-zeaxanthin, *cis*-zeaxanthins and zeaxanthin related impurities: 12'-apo-zeaxanthinal, parasiloxanthin and diatoxanthin.

Calibration solutions:

Solution 1: Accurately weigh 34 to 36 mg of 12'-apo-zeaxanthinal and dissolve in 100 ml of tetrahydrofuran.

*Solution 2:*Accurately weigh 34 to 36 mg of diatoxanthin and dissolve in 100 ml of tetrahydrofuran.

*Solution 3:*Accurately weigh 69.0 to 71.0 mg of zeaxanthin. Add 50 ml of tetrahydrofuran, 1 ml of calibration solution 1, and 1 ml of calibration solution 2. Bring to volume (100 ml) with 48 ml tetrahydrofuran.

Test solution:

Accurately weigh 69.0 to 71.0 mg of sample and dissolve in 100 ml of tetrahydrofuran.

Mobile phase:

In a 2000 ml volumetric flask containing a small quantity of hexane, add 400 ml of ethyl acetate, 20 ml of 2-methoxyethanol, and 2.0 ml of *N*-ethyldiisopropylamine. Bring to volume with hexane.

Apparatus:

Column:	Stainless steel; 250 x 4 mm
Column temperature:	25°
Stationary phase:	Spherisorb Si, 3 µm or similar
Pump:	Flow 1.0 ml/min; pressure 85 bar
Detector:	VIS 450 nm
Injection:	2.0 µl
Run time:	35 min

Results:

The retention times for *trans*-zeaxanthin and *cis*-zeaxanthins are approximately 17.7 and 24.4 to 25.8 min, respectively.

The retention times for the by-products 12'-apo-zeaxanthinal, parasiloxanthin, and diatoxanthin are approximately 8.2, 17.0, and 20.5 min, respectively.

For *trans*-zeaxanthin, *cis*-zeaxanthins, and parasiloxanthin perform external standardization with the zeaxanthin response factor.

For 12'-apo-zeaxanthinal perform external standardization with the 12'-apo-zeaxanthinal response factor.

For diaxanthin perform external standardization with the diaxanthin response factor.

Substance	Response Factor	Relative Response factor related to *trans*-Zeaxanthin at 450 nm
trans-Zeaxanthin	$4.671e^{-10}$	1
12'-Apo-zeaxanthinal	$1.134e^{-9}$	2.428
Diatoxanthin	$5.588e^{-10}$	1.962
Parasiloxanthin	$4.671e^{-10}$	1
cis-Zeaxanthins	$4.671e^{-10}$	1

Calculation:

$$\% \text{ substance to be determined} = \frac{A_s \times RFi \times 100}{W_s}$$

Where:

As = peak area of the substance to be determined in the test solution
RFi = response factor of the substance to be determined in the test solution
Ws = weight of the sample in mg

with: $$RFi = \frac{W_r \times C_r}{A_r \times 100}$$

Where

Wr = weight of the reference substance from the calibration in mg
Cr = content of the reference substance in percent
Ar = peak area of the reference substance from the calibration

ZEAXANTHIN-RICH EXTRACT FROM *TAGETES ERECTA*
(Tentative)

Information is required on the non-zeaxanthin components in total carotenoids and on the composition of the non-carotenoid components by end of 2006.

New specifications prepared at the 63rd JECFA (2004) and published in FNP 52 Add 12 (2004).

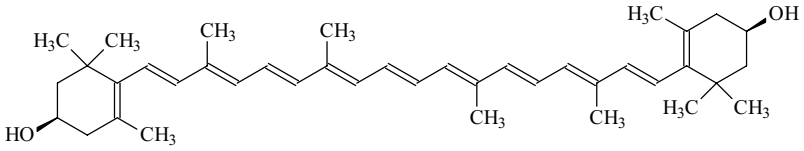
DEFINITION These specifications apply to zeaxanthin rich extract from red flowers of *Tagetes erecta* L. obtained with hexane extraction and subsequent purification of oleoresin by saponification, crystallization and washing of separated crystals alternatively in hexane and methanol to achieve desired purity. Beside zeaxanthin which is the main colouring principle, other carotenoids can be contained in various amounts, as well as fats, oils and waxes originating from the plant material.

Chemical Names (all-E)-1,1'-(3,7,12,16-Tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaene-1,18-diyl)bis[2,6,6-trimethylcyclohexene-3-ol]; 3R,3'R-β,β-Carotene-3,3'-diol

C.A.S. number 144-68-3 (Zeaxanthin)

Chemical formula $C_{40}H_{56}O_2$ (Zeaxanthin)

Structural formula



Formula weight 568.89 (Zeaxanthin)

Assay Not less than 30 % of total carotenoids (as zeaxanthin) and not less than 65 % of zeaxanthin in total carotenoids

DESCRIPTION Orange-red crystalline powder, with little or no odour

FUNCTIONAL USES Colour, nutrient supplement

CHARACTERISTICS

IDENTIFICATION

Test for carotenoid The colour of the solution of the sample in acetone disappears after successive additions of a 5 % solution of sodium nitrite and 1N sulfuric acid.

Spectrophotometry (FNP 5) A solution of the sample in chloroform/ethanol (1:9) shows maximum absorption at ca. 453 nm

PURITY

Residual solvents Hexane and methanol, not more than 50 mg/kg, singly or in combination
See description in FNP 52 addendum 11, section E

Lead (FNP 5) Not more than 2 mg/kg
Determine using an atomic absorption technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on the principles of the methods described in FNP 5, “Instrumental Methods”.

METHOD OF ASSAY

Total carotenoids (as zeaxanthin)

Proceed as directed in FNP 5 under Colouring Matters, Total Content by Spectrophotometry, Procedure 2, using the following conditions:

w = amount (g) to obtain adequate absorbance

$V_1 = V_2 = V_3 = 100$ ml

$v_1 = v_2 = 10$ ml

$A^{1\%}_{1cm} = 2540$

$\lambda_{max} = 453$ nm

Zeaxanthin in total carotenoids

Determine by reverse phase HPLC using the following conditions:

Column:	C18, 5 µm (4.6 x 250 mm)
Flow:	0.6 ml/min
Wave length:	453 nm
Injection volume:	10 µl
Column temperature:	ambient
Injector temperature:	10°
Run time:	15 min
Mobile phase:	acetonitrile/water/chloroform (82:2:15)

Sample preparations:

Weight a sample containing approximately 7 to 9 mg of zeaxanthin (determined according to theoretical content) into a 100 ml volumetric flask. Dissolve and bring to volume with chloroform. Place 1 ml of the resultant solution into volumetric flask and dilute to 25 ml using the mobile phase solution as a diluent.

Zeaxanthin as a % of total carotenoids equals:

$$\frac{A_1 \times 100}{A_1 + A_2}$$

where

A_1 = area of the trans- zeaxanthin peak

A_2 = area of trans-lutein peak

Identification of the peak areas corresponding to trans-zeaxanthin and trans-lutein is verified by comparison of the retention times with standards.

Section C: Limits[1] for heavy metals in the specifications of certain food additives (uses other than as flavouring agents) [mg/kg]

Additive name	INS		As	Pb	Cd	Hg
Aluminium ammonium sulfate	523		-	3	-	-
Ammonium chloride	510		-	2	-	-
Ammonium hydrogen carbonate	503	(ii)	-	2	-	-
Azodicarbonamide	927	a	-	2	-	-
Bees wax	901		-	2	-	-
Benzoic acid	210		-	2	-	-
Benzyl alcohol	-		-	2	-	-
Butan-1,3-diol	-		-	2	-	-
Butan-1-ol	-		-	2	-	-
Butan-2-ol	-		-	2	-	-
Butyl *p*-hydroxybenzoate	-		-	2	-	-
Calcium acetate	263		-	2	-	-
Calcium benzoate	213		-	2	-	-
Calcium carbonate	170		3	3	-	-
Calcium chloride	509		-	2	-	-
Calcium cyclamate	952		-	1	-	-
Calcium hydrogen phosphate	341	(ii)	3	4	-	-
Calcium sulfate	516		-	2	-	-
Candelilla wax	902		-	2	-	-
Castor oil	1503		-	2	-	-
Chlorine	925		-	2	-	1
Citranaxanthin	-		-	2	-	-
Cyclodextrin, beta-	459		-	1	-	-
Cyclohexane	-		-	2	-	-
Dammar gum	-		-	2	-	-
Diethyl tartrate	-		-	2	-	-
Diethylene glycol monoethyl ether	-		-	2	-	-
Dimethyl dicarbonate	242		-	2	-	-
Diphenyl	-		-	2	-	-
Edible gelatin	-		1	1.5	0.5	0.15
Ferric ammonium citrate	-		-	2	-	-
Glycerol	422		-	2	-	-
Glycerol diacetate	-		-	2	-	-
Heptanes	-		-	2	-	-
Hexamethylene tetramine	239		-	2	-	-
Isoamyl acetate	-		-	2	-	-
Isobutanol	-		-	2	-	-
Isopropyl acetate	-		-	2	-	-
Lactic acid	270		-	2	-	-
Light petroleum	-		-	2	-	-
Lysozyme hydrochloride	1105		-	2	-	-
Magnesium carbonate	504	(i)	-	2	-	-
Magnesium chloride	511		-	2	-	-
Magnesium hydrogen phosphate	343	(ii)	3	4	-	-
Magnesium lactate	329		-	2	-	-
Methanol	-		-	2	-	-
Mineral oil (high viscosity)	905		-	1	-	-
Monoglyceride citrate	-		-	2	-	-
Nisin	234		-	1	-	-
Norhydroguaiaretic acid	-		-	2	-	-
Pentapotassium triphosphate	451	(ii)	3	4	-	-
Phenyl phenol, *o*-	231		-	2	-	-
Polyvinylpolypyrrolidone, Insoluble	1202		-	2	-	-
Polyvinylpyrrolidone	1201		-	2	-	-
Potassium acetate	261		-	2	-	-
Potassium benzoate	212		-	2	-	-
Potassium bromate	924	a	-	2	-	-

[1] See *Notes to the reader* (page v).

Additive name	INS		As	Pb	Cd	Hg
Potassium chloride	508		-	2	-	-
Potassium dihydrogen phosphate	501	(ii)	3	4	-	-
Potassium iodate	917		-	2	-	-
Potassium nitrate	252		-	2	-	-
Potassium nitrite	249		-	2	-	-
Potassium sodium L(+) tartrate	337		-	2	-	-
Potassium sulfate	515	(i)	-	2	-	-
Propan-1-ol	-		-	2	-	-
Propylene glycol	1520		-	2	-	-
Sodium benzoate	211		-	2	-	-
Sodium carboxy methyl cellulose	466		-	2	-	-
Sodium cyclamate	952		-	1	-	-
Sodium diacetate	262	(ii)	-	2	-	-
Sodium nitrate	251		-	2	-	-
Sodium nitrite	250		-	2	-	-
Sodium *o*-phenyl phenol	232		-	2	-	-
Sodium percarbonate	-		-	2	-	-
Sodium thiocyanate	-		-	2	-	-
Sorbic acid	200		-	2	-	-
Sucralose	955		-	1	-	-
Tannic acid	181		-	2	-	-
Tartaric acid, DL-	-		-	2	-	-
Toluene	-		-	2	-	-
Triacetin	1518		-	2	-	-
Trichlorotrifluoroethane, 1,1,2-	-		-	2	-	-
Urea	927	b	-	2	-	-

Section D: Specifications of certain flavouring agents

At its 44th meeting JECFA considered a new approach to the safety evaluation of flavouring agents. This approach incorporates a series of criteria whose use enables the evaluation of a large number of these agents in a consistent and timely manner. At the current meeting of the Committee specifications of identity and purity were prepared or revised for 197 flavouring agents.

Information on specifications for flavouring agents is given on the following tables under the following headings, most of which are self-explanatory:

Name; Chemical name (Systematic name); Synonyms; Flavour and Extract Manufacturers' Association of the United States (FEMA) No; FLAVIS (FL) No; Chemical Abstract Service Registry (CAS) No; Molecular weight; Chemical formula; Physical form/odour; Solubility; Solubility in ethanol, Boiling point (for information only); Identification test (ID); Assay min% (Gas chromatographic (GC) assay of flavouring agents); Acid value max; Refractive index (at 20º, if not otherwise stated); Specific gravity (at 25º, if not otherwise stated)

The field called "Other requirements" contains three types of entry:

- Items in normal type are additional requirements, such as further purity criteria or other tests
- Items contained in square brackets are provided for information, for example the typical isomer composition of the flavouring agent. These are not considered to be requirements.
- Substances listed after "SC:" are secondary constituents which have been taken into account in the safety evaluation of the named flavouring agent. If the commercial product contains less than 95% of the named compound, it is a requirement that the major part of the product (i.e. not less than 95%) is accounted for by the sum of the named compound and one or more of the secondary constituents.

The field called "JECFA" contains the number of the meeting at which the specifications were prepared and the status of the specification. R means "specifications revised", S means "existing specifications maintained", S,T means "existing tentative specifications maintained, (further information required)", N means "new specifications", and N,T means "new tentative specifications, (further information required)".

The last column indicates the data (information) required for the tentative specifications. Abbreviations for "data required" are as follows: A=assay minimum, A(e)=equivalence factor for assay, A(m)=details of assay method, BP=boiling point, ID=identity test, Low assay=quantitative information on by-products, RI=refractive index, SG=specific gravity. A(e) is an equivalence factor to convert an assay obtained by aldehyde / ketone determination, ester determination, total alcohols determination, or titration determination to the % value which would be obtained if GC had been used for the assay (FNP 5).

The infrared and other spectra, used for identification and comparison purposes, are provided from page 97 onwards (copies for certain spectra may be obtained from the FAO Joint Secretariat or from FEMA, Suite 925, 1620 I Street, N.W., Washington DC, USA).

A comprehensive index listing all names, chemical names, and synonyms is added on page 120.

Note on spectra: only spectra which were submitted to the 63rd meeting are reproduced in this volume. The reader is referred to previous Addenda for copies of spectra of revised specifications.
Spectra for 1419-1425, 1426, 1428-1434, 1437-1439 are reproduced with permission of http://webbook.nist.gov/chemistry.

No	Name chemical name / synonyms	FEMA / FL / CAS numbers	Formula M.W.	Physical form / odour	Solubility / solubility in ethanol	B.P. (°C)	ID test / assay min	A.V.	Ref. index / *Sp. gravity*	Other requirements	JECFA	Data required
53	**Citronellyl formate** 3,7-Dimethyl-6-octen-1-yl formate	2314 09.078 105-85-1	C11 H20 O2 184.28	colourless liquid/strong, fruity, floral odour	soluble in alcohol, most fixed oils; slightly soluble in propylene glycol; insoluble in glycerol, water 1 ml in 3 ml 80% alcohol remains in soln to 10 ml	235	IR 90	3	1.443-1.452 0.890-0.903	SC: citronellol; Min assay includes formate esters of geraniol, nerol and rhodinol	63rd/R	
55	**Neryl formate** 2-cis-3,7-Dimethyl-2,6-octadien-1-yl formate	2776 09.212 2142-94-1	C11 H18 O2 182.26	colourless to pale yellow liquid/sweet, herbaceous, green, rose odour	insoluble in water 1ml in 10 ml 70% alcohol	215 - 225	IR 90	-	1.456-1.458 0.916-0.917 (15°)	SC: geraniol, nerol; Min assay includes formate esters of citronellol, geraniol and rhodinol	63rd/R	
68	**Rhodinyl butyrate** 3,7-Dimethyl-7-octen-1-yl butanoate	2982 141-15-1	C14 H26 O2 226.36	colourless to yellowish or greenish liquid/fruity, rose odour	- 1ml in 8ml 80% alcohol; 1ml in 1ml 90% alcohol	137 (13 mm Hg)	IR 85	1	1.446-1.456 0.880-0.895 (20°/20°)	SC: rhodinol	63rd/R	
399	**Methyl-beta-ionone** 5-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-4-penten-3-one beta-Cyclocitrylidene butanone; beta-n-Methylionone; Raldeine; beta-Cetone	2712 07.010 127-43-5	C14 H22 O 206.33	colourless to yellow liquid	- -	238-242	IR 88	-	1.503-1.508 0.930-0.935	SC: alpha- and beta-isomethylionone; Min assay includes cis and trans isomers of alpha-, beta- and gamma-methylionone	63rd/R	
471	**2,8-Dithianon-4-ene-4-carboxaldehyde** 5-(Methylthio)-2-(methylthiomethyl)-2-pentenal	3483 12.065 59902-01-1	C8 H14 OS2 190.32	-	slightly soluble in water -	104-105 (10 mmHg)	NMR 98	-	1.557-1.567 1.105-1.107		63rd/R	
504	**S-Methyl benzothioate** (S)-Methyl thiobenzoate Methanethiol, benzoate	3857 12.150 5925-68-8	C8 H8 OS 152.21	colourless to pale yellow liquid	soluble in oil and alcohol -	121-122 (22 mm Hg)	NMR 95	-	1.574-1.580 0.826-0.836		63rd/R	
557	**1-Mercapto-2-propanone** 1-Mercapto-2-propanone Mercaptoacetone	3856 12.143 24653-75-6	C3 H6 OS 90.14	colourless to pale yellow liquid	soluble in oil and alcohol -	47-49 (19 mm Hg)	NMR 98	-	1.455-1.465 0.817-0.847		63rd/R	
570	**Propenyl propyl disulfide** Propenyl propyl disulfide Propyl propenyl disulfide	3227 12.044 5905-46-4	C6 H12 S2 148.28	colourless liquid with odour of cooked onions	- -	78-80 (13 mm Hg)	92 (mixture of cis and trans)	-	1.522-1.532 0.972-0.978	SC: dipropyl disulfide	63rd/R	

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605	**1,3-Nonanediol acetate (mixed esters)** Mixture of 3-Acetoxynonyl acetate, 3-Hydroxynonyl acetate and 1-(2-Hydroxyethyl)heptyl acetate 3-Hexyl-1,3-propanediol acetate, mixed esters; Nonane diacetate	2783 09.225 1322-17-4	C11 H22 O3 / C13 H26	colourless to pale yellow, slightly oily liquid with floral odour similar to jasmine	slightly soluble in water; soluble in alcohol and oils 1 ml in 1 ml 95% alcohol	275-276	IR 95 (total of 2 monoesters and diester)	1.0	1.441-1.453 0.964-0.978		63rd/R	
615	**Butyl ethyl malonate** Propanedioic acid, butyl ethyl ester Ethyl butyl malonate	2195 09.441 17373-84-1	C9 H16 O4 188.22	-	- -	222	NMR 98	-	1.025-1.035 1.048-1.054		63rd/R	
628	**Ethyl aconitate (mixed esters)** 1-Propene-1,2,3-tricarboxylic acid, ethyl ester Ethyl 2-carboxyglutaconate; Ethyl 1-propene-1,2,3-tricarboxylate	2417 09.510 1321-30-8	C8 H14 O6	colourless, oily liquid with sweet, fruity, winey odour and taste	slightly soluble in water; soluble in alcohol -	260; 172 (18 mm Hg)	NMR 95	-	1.457 at 14.5°C 1.096 at 25°C		63rd/R	
631.2	**3-Methyl-2-oxobutanoic acid, sodium salt** Sodium 3-methyl-2-oxobutyrate Sodium, alpha-ketoisovalerate; Butanoic acid, 3-methyl-2-oxo-, sodium salt; Sodium 3-methyl-2-oxobutanoate	3869 08.051 3715-29-6	C5 H7 O3 Na 138.10	-	- -	n/a	NMR 99	-	n/a n/a		63rd/S, T	A(m)
632.2	**3-Methyl-2-oxopentanoic acid, sodium salt** Sodium 3-methyl-2-oxovalerate Valeric acid, 3-methyl-2-oxo-, sodium salt	3870 08.093 3715-31-9	C6 H9 O3 Na 152.10	-	- -	n/a	NMR 99	-	n/a n/a		63rd/S, T	A(m)
633.2	**4-Methyl-2-oxopentanoic acid, sodium salt** Sodium 4-methyl-2-oxovalerate Valeric acid, 4-methyl-2-oxo, sodium salt; Sodium 4-methyl-2-ketopentanoate; Sodium 4-methyl-2-oxopentanoate	3871 08.052 4502-00-5	C6 H9 O3 Na 152.10	-	- -	n/a	NMR 99	-	n/a n/a		63rd/S, T	A(m)

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919	**Glyceryl monooleate** 2,3-Dihydroxypropyl 9-octadecenoate Monoolein	2526 111-03-5	C21 H40 O4 356.54	pale yellow viscous oily liquid with a faint fatty odour	insoluble in water; soluble in hot organic solvents soluble in hot alcohol	250 (8 mmHg)	NMR 65; total 95% mono-/di-/tri-glycerides	-	1.462-1.468 0.925-0.935	complies with purity criteria for Mono- and diglycerides in FNP52 SC: Di- and tri-glycerides; Glycerol; 9-Octadecenoic acid	63rd/R	
1203	**Ammonium isovalerate** Ammonium 3-methylbutyrate Isovaleric acid, ammonium salt	2054 16.001 7563-33-9	C5 H13N O2 119.16	Deliquescent colourless crystals; sharp, cheesy, yet somewhat sweet aroma	Soluble in water, oils soluble	n/a	NMR 98	3	n/a n/a	mp: 72°	63rd/R	
1218	**4-Ethyloctanoic acid** 4-Ethyloctanoic acid -	3800 08.079 16493-80-4	C10 H20 O2 172.27	Liquid; fruity, floral aroma	Slightly soluble in water; soluble in hexane soluble	110° (1 mm Hg)	NMR IR 99		1.430-1.439 0.898-0.908		63rd/R	
1263	**Isoeugenyl phenylacetate** 2-Methoxy-4-propenylphenyl phenylacetate 4-Propenylguaiacyl phenylacetate; 2-Methoxy-4-(1-propen-1-yl)phenyl phenylacetate	2477 09.710 120-24-1	C18 H18 O3 282.34	Yellow viscous liquid; sweet vanilla, clove-like and honey aroma	Insoluble in water soluble	268 (17 mmHg)	NMR 95	1	1.575-1.577 1.113-1.117		63rd/R	
1273	**Ethyl 5-hexenoate** Ethyl 5-hexenoate -	3976 54653-25-7	C8 H14 O2 142.2	Colourless liquid; fruity aroma	insoluble in water; soluble in most non-polar solvents soluble	181-182°	NMR MS IR 95	1	1.430-1.439 0.902-0.912		63rd/R	
1291	**3-Mercapto-2-methylpentan-1-ol (racemic)** 3-Mercapto-2-methylpentanol -	3996 227456-27-1	C6 H14 O S 134.24	Clear liquid; onion like aroma	Slightly soluble in water; soluble in organic solvents soluble	50° (0.5 mm Hg)	NMR IR 99	1	1.480-1.490 0.985-0.995		63rd/R	
1296	**spiro[2,4-Dithia-1-methyl-8-oxabicyclo(3.3.0)octane-3,3'-(1'-oxa-2'-methyl)-cyclopentane]** spiro[2,4-Dithia-1-methyl-8-oxabicyclo(3.3.0)octane-3,3'-(1'-oxa-2'-methyl)-cyclopentane] 2',3-Dimethyl-3',4-dioxa-2,8-dithiabi-cyclo[3.3.0]octanespirocyclopentane	3270 15.007 38325-25-6	C10 H16 O2 S2 232.36	colourless to pale yellow liquid	Insoluble in water; soluble in non-polar solvents soluble	135-140° (3 mm Hg)	NMR IR MS 95		1.559-1.565 1.200-1.208		63rd/R	

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1301	**Indole** Indole 1-Benzazole; Benzopyrrole; 1-Benzo(b)pyrrole; 2,3-Benzopyrrole	2593 14.007 120-72-9	C8 H7 N 117.15	White lustrous, flakey crystalline solid; Unpleasant odour at high concentration, odour becomes floral at higher dilutions	Soluble in fixed oils and propylene glycol; Insoluble in glycerol Soluble	-	NMR 97%	NA	- -	mp: 51-54°	63rd/N	
1302	**6-Methylquinoline** 6-Methylquinoline p-Methylquinoline; p-Toluquinoline	2744 14.042 91-62-3	C10 H9 N 143.19	Colourless oily liquid; Pungent heavy quinoline-like odour	Soluble in benzene and ether; Slightly soluble in water Soluble	259°	NMR 98%	1.0	1.611-1.617 1.060-1.066		63rd/N	
1303	**Isoquinoline** Isoquinoline 2-Azanaphthalene; 2-Benzazine; Benzo(c)pyridine; 3,4-Benzopyridine	2978 14.001 119-65-3	C9 H7 N 129.16	Colourless liquid, hygroscopic platelets when solid; Heavy-sweet balsamic, herbaceous aroma	Slightly soluble in water Soluble	242-243°	NMR 97%	1.0	1.621-1.627 1.097-1.103	mp: 27-29°	63rd/N	
1304	**Skatole** 3-Methylindole 3-Methyl-4,5-benzopyrrole; beta-Methylindole; 3-Methylindole	3019 14.004 83-34-1	C9 H9 N 131.18	White scales or powder; Mothball, putrid, decayed, faecal odour, jasmine-like or fruity upon dilution	Soluble in boiling water Soluble	-	NMR 97%	NA	- -	mp: 95-97°	63rd/N	
1305	**1-Ethyl-2-acetylpyrrole** 2-Acetyl-1-ethylpyrrole 1-Ethyl-2-acetylazole; 1-(N-Ethylpyrrol-2-yl)ethanone	3147 14.045 39741-41-8	C8 H11 N O 137.18	Colourless to yellowish liquid; Warm, nutty, ethereal aroma	Soluble in fixed oils and propylene glycol Soluble	209-211°	NMR 98%	1.0	1.550-1.556 1.052-1.058		63rd/N	
1306	**1-Methyl-2-acetylpyrrole** 2-Acetyl-1-methylpyrrole Methyl 1-methylpyrrol-2-yl ketone; 1-Methylpyrrol-2-yl methyl ketone	3184 14.046 932-16-1	C7 H9 N O 123.16	Colourless to yellowish liquid; Earthy aroma	- Soluble	200-202°	NMR 98%	1.0	1.539-1.545 1.037-1.043		63rd/N	
1307	**Methyl 2-pyrrolyl ketone** 2-Acetylpyrrole 2-Acetylpyrrole; Methyl pyrrolyl ketone; 2-Pyrrolyl methyl ketone	3202 14.047 1072-83-9	C6 H7 N O 109.13	Light beige to yellowish fine crystals; Bready, walnut, licorice-like aroma	Soluble in water and ether Soluble	-	NMR 97%	NA	- -	mp: 87-93°	63rd/N	
1308	**2-Pyridinemethanethiol** 2-Pyridine methanethiol 2-Pyridylmethanethiol; 2-Pyridyl methyl mercaptan	3232 14.030 2044-73-7	C6 H7 NS 125.20	Colourless to yellow liquid; Pungent sulferous aroma	Soluble	57-58° (0.6 mm Hg)	NMR 98%	1.0	1.573-1.580 1.150-1.157		63rd/N	

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1309	**2-Acetylpyridine** 2-Acetylpyridine 2-Acetopyridine; Methyl 2-pyridyl ketone	3251 14.038 1122-62-9	C7 H7 N O 121.14	Colourless to yellow liquid; Tobacco-like, popcorn, heavy-oily-fatty aroma	Soluble in ether and acids Soluble	189-193°	NMR 97%	1.0	1.518-1.524 1.077-1.084		63rd/N	
1310	**N-Furfurylpyrrole** 1-Furfurylpyrrole 1-(2-furfuryl)pyrrole; 1-Furfuryl-1H-pyrrole	3284 13.134 1438-94-4	C9 H9 N O 147.18	Colourless to yellow liquid; Vegetable, earthy-green aroma	- Soluble	76-78° (1 mm Hg)	NMR 98%	1.0	1.529-1.536 1.078-1.084		63rd/N	
1311	**2-(2-Methylpropyl)pyridine** 2-(2-Methylpropyl)pyridine Isobutylpyridine	3370 14.058 6304-24-1	C9 H13 N 135.21	Colourless to yellow liquid; Sharp aroma	Insoluble in water Soluble	181°	NMR 97%	1.0	1.480-1.486 0.894-0.900		63rd/N	
1312	**3-(2-Methylpropyl)pyridine** 3-(2-Methylpropyl)pyridine 3-Isobutylpyridine; 3-(2-Butyl)pyridine	3371 14.059 14159-61-6	C9 H13 N 135.21	Colourless liquid; Sharp penetrating aromatic aroma	Insoluble in water Soluble	68-68.5° (8 mm Hg)	NMR 97%	1.0	1.488-1.494 0.898-0.904		63rd/N	
1313	**2-Pentylpyridine** 2-Pentylpyridine 2-Amylpyridine	3383 14.060 2294-76-0	C10 H15 N 149.24	Colourless to yellow liquid;	Insoluble in water Soluble	102-107°	NMR 97%	1.0	1.485-1.491 0.895-0.901		63rd/N	
1314	**Pyrrole** Pyrrole Azole; Divinyleneimine; Imidole	3386 14.041 109-97-7	C4 H5 N 67.09	Colourless to yellowish liquid; Nutty, sweet, warm, ethereal aroma	Soluble in most fixed oils; Slightly soluble in water Soluble	130-131°	IR 98%	1.0	1.507-1.510 0.955-0.975		63rd/N	
1315	**3-Ethylpyridine** 3-Ethylpyridine beta-Ethylpyridine; beta-Lutidine	3394 14.061 536-78-7	C7 H9 N 107.16	Colourless to brownish liquid; Tobacco aroma	Soluble in ether; Slightly soluble in water Soluble	166°	NMR 98%	1.0	1.499-1.505 0.951-0.957		63rd/N	
1316	**3-Acetylpyridine** 3-Acetylpyridine Methyl 3-pyridyl ketone; beta-Acetylpyridine; 1-(3-pyridinyl)ethanone	3424 14.039 350-03-8	C7 H7 N O 121.14	Colourless to yellow liquid; Sweet, nutty, popcorn-like aroma	Soluble in acids,alcohol, ether, and water Soluble	230°	NMR 97%	1.0	1.530-1.540 1.103-1.112		63rd/N	
1317	**2,6-Dimethylpyridine** 2,6-Dimethylpyridine 2,6-Lutidine	3540 14.065 108-48-5	C7 H9 N 107.16	Colourless oily liquid; Diffusive minty aroma, nutty, coffee-like	Soluble in water; Slightly soluble in fat Soluble	143-145°	MS 99%	1.0	1.495-1.501 0.917-0.923		63rd/N	
1318	**5-Ethyl-2-methylpyridine** 5-Ethyl-2-methylpyridine 2-Ethyl-5-methylpyridine; 5-Ethyl-2-picoline	3546 14.066 104-90-5	C8 H11 N 121.18	Colourless liquid; Sharp penetrating aromatic aroma	Slightly soluble in water and fat Soluble	172-175°	NMR 97%	1.0	1.495-1.502 0.917-0.923		63rd/N	

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1319	**2-Propionylpyrrole** 2-Propionylpyrrole Ethyl 2-pyrrolyl ketone; 1-(2-Pyrrolyl)-1-propanone	3614 14.068 1073-26-3	C7 H9 N O 123.16	White crystalline solid; Rubbur, leathery, quinoline-type aroma	Slightly soluble in water; Insoluble in fats Soluble	-	NMR 99%	NA	- -	mp: 43-45°	63rd/N	
1320	**Methyl nicotinate** Methyl 3-pyridinecarboxylate 3-carbomethoxypyridine; Methyl 3-pyridinecarboxylate	3709 14.071 93-60-7	C7 H7 N O2 137.14	White crystalline solid; Fresh caramelic nutty, mild tobacco aroma	Soluble in fat; Slightly soluble in water Soluble	-	NMR 98%	NA	- -	mp: 38-43°	63rd/N	
1321	**2-(3-Phenylpropyl)pyridine** 2-(3-Phenylpropyl)pyridine	3751 14.072 2110-18-1	C14 H15 N 197.28	Colourless liquid;	Soluble in fat; Insoluble in water Soluble	142-143° (1 mm Hg)	NMR 97%	1.0	1.558-1.563 1.012-1.018		63rd/N	
1322	**2-Propylpyridine** 2-Propylpyridine 1-(2-Pyridyl)propane; 2-n-Propylpyridine; Conyrine	4065 14.143 622-39-9	C8 H11 N 121.20	Colourless liquid; Tobacco, nutty aroma	Slightly soluble in water Soluble	169-171°	NMR 98%	1.0	1.490-1.496 0.907-0.917		63rd/N	
1323	**Camphene** Camphene 2,2-Dimethyl-3-methylenenorbornane; 3,3-Dimethyl-2-methylenenorcamphane; 2,2-Dimethyl-3-methylenebicyclo[2.2.1]heptane	2229 01.009 79-92-5	C10 H16 136.24	Colourless crystalline solid; mild, oil-camphoraceous aroma	Insoluble in water; soluble in oils Soluble	-	NMR 80%	<1.0	- -	SC: C15H24 terpene hydro-carbons (eg. Valencene); Minimum assay value may inclu-de traces of limonene, myr-cene, alpha and beta pinene and other common C10H16 ter-penes; mp: 52°	63rd/N	
1324	**beta-Caryophyllene** 4,11,11-Trimethyl-8-methylene-bicyclo[7.2.0]undec-4(trans)-ene caryophyllene; (E)-caryophylene; trans-caryophyllene;	2252 01.007 87-44-5	C15 H24 204.36	Colourless to slightly yellow oily liquid; woody-spicy, dry, clove-like aroma	Insoluble in water; soluble in oils, ether Soluble	256°	IR 80%	<1.0	1.498-1.504 0.899-0.908	SC: C15H24 terpene hydrocarbons (eg. Valencene)	63rd/N	
1325	**p-Cymene** 1-Isopropyl-4-methylbenzene cymene; p-isopropyltoluene; p-methylcumene; 1-methyl-4-isopropylbenzene	2356 01.002 99-87-6	C10 H14 134.22	Colourless to pale yellow mobile liquid; citrusy aroma reminiscent of lemon	Insoluble in water; soluble in oils Soluble	177°	IR 97%	<1.0	1.484-1.491 0.853-0.855		63rd/N	

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1326	**d-Limonene** p-Mentha-1,8-diene (+)-p-Mentha-1,8-diene; 1,8(9)-p-Menthadiene; 4-Isopropenyl-1-methyl-1-cyclohexene; Hesperidine	2633 01.045 5989-27-5	C10 H16 136.24	Colourless mobile liquid; fresh, light, sweet, citrusy aroma	Insoluble in water, propylene glycol; slightly Soluble in glycerol; Soluble in oils Soluble	175-177°	IR 96% (sum of d/l isomers)	<1.0	1.471-1.477 0.838-0.843	Sp.rotation +96 to +104° (25°); Compounds present above 0.5%: linalool, myrcene	63rd/N,T	
1327	**Myrcene** 7-Methyl-3-methyleneocta-1,6-diene 7-Methyl-3-methylene-1,6-octadiene; 2-Methyl-6-methylene-2,7-octadiene; 3-Methylene-7-methyl-1,6-octadiene	2762 01.008 123-35-3	C10 H16 136.24	Colourless or very pale straw-coloured mobile liquid; sweet balsamic aroma	Insoluble in water; soluble in oils Soluble	166-167°	NMR 90%	<1.0	1.466-1.471 0.789-1.793	SC: C15H24 terpene hydrocarbons (eg. Valencene); Minimum assay value may include traces of limonene, alpha and beta pinene and other common C10H16 terpenes	63rd/N	
1328	**alpha-Phellandrene** p-Mentha-1,5-diene p-mentha-1,5-diene; 5-isopropyl-2-methyl-1,3-cyclohexadiene; menthadiene; dihydro-p-cymene	2856 01.006 99-83-2	C10 H16 136.24	Colourless to slightly yellow, mobile liquid; peppery, woody, herbaceous aroma	Insoluble in water; soluble in oils Soluble	175°	IR 95%	<1.0	1.471-1.477 0.845-0.855		63rd/N	
1329	**alpha-Pinene** 2,6,6-Trimethyl-bicyclo[3.1.1]hept-2-ene 2-Pinene; 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene;	2902 01.004 80-56-8	C10 H16 136.24	Colourless mobile liquid; warm, resinous, pine-like aroma	Insoluble in water; soluble in oils Soluble	155°	NMR 97%	<1.0	1.462-1.468 0.855-0.860	Minimum assay value may include traces of limonene, beta pinene and other common C10H16 terpenes	63rd/N	
1330	**beta-Pinene** 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane 2(10)-Pinene; 6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane; pseudopinene; 6,6-Dimethyl-2-methylene-norpinane	2903 01.003 127-91-3	C10 H16 136.24	Colourless mobile liquid; dry woody, resinous piney aroma	Insoluble in water; soluble in oils Insoluble	163-166°	NMR 97%	<1.0	1.476-1.482 0.867-0.871	Minimum assay value may include traces of limonene, alpha pinene and other common C10H16 terpenes	63rd/N	
1331	**Terpinolene** p-Mentha-1,4(8)-diene p-Mentha-1,4(8)-diene; 4-Isopropylidene-1-methylcyclohexene; Isoterpinene;	3046 01.005 586-62-9	C10 H16 136.24	Colourless or very pale straw-coloured oily liquid; sweet-piney, oily, pleasant aroma	Insoluble in water; soluble in oils Soluble	183-185°	NMR 95%	<1.0	1.474-1.484 0.872-0.882		63rd/N	

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1332	**Biphenyl** Biphenyl diphenyl; bibenzene; phenylbenzene	3129 01.013 92-52-4	C12 H10 154.21	White to light brown leaflet solid, Pungent green aroma, rose-like upon dilution	Insoluble in water Soluble	254°	NMR 99%	<1.0	- -	mp: 69°	63rd/N	
1333	**p,alpha-Dimethylstyrene** 1-Isopropenyl-4-methylbenzene 1-methyl-4-(1-methylethenyl)benzene; 1-methyl-4-isopropenylbenzene; 1-p-tolyl-1-methylethylene; 4-isopropenyltoluene	3144 01.010 1195-32-0	C10 H12 132.20	Colourless mobile liquid; citrusy-lemon like aroma	Insoluble in water; soluble in oils Soluble	186-189°	NMR 97%	<1.0	1.532-1.535 0.846-0.854		63rd/N	
1334	**4-Methylbiphenyl** 4-Methyl-1,1'-biphenyl 1-methyl-4-phenylbenzene; 4-methyldiphenyl; 4-phenyltoluene; p-methylbiphenyl	3186 01.011 644-08-6	C13 H12 168.24	White solid	Insoluble in water Soluble	-	NMR 98%	<1.0	- -	mp: 49-50°	63rd/N	
1335	**1-Methylnaphthalene** 1-Methylnaphthalene alpha-Methylnaphthalene	3193 01.014 90-12-0	C11 H10 142.20	Colourless to slightly pale yellow liquid; Earthy, phenolic aroma	Insoluble in water; Soluble in oils Soluble	241-245°	NMR 97%	<1.0	1.612-1.618 1.020-1.025		63rd/N	
1336	**Bisabolene** 6-Methyl-2-(4-methylcyclohex-3-enylidene)hept-5-ene 2-heptene, 2-methyl-6-(4-methyl-3-cyclohexen-1-ylidene)-; g-bisabolene	3331 01.016 495-62-5	C15 H24 204.36	Colourless slightly viscous oil; pleasant, warm sweet-spicy-balsamic aroma	Insoluble in water; soluble in oils Insoluble	262°	NMR 97%	<1.0	1.493-1.497 0.850-0.858		63rd/N	
1337	**Valencene** 1,2-Dimethyl-9-isopropylene-bicyclo[4.4.0]dec-5-ene 4.beta.H,5.alpha.-Eremophila-1(10),11-diene	3443 01.017 4630-07-3	C15 H24 204.36	Colourless to pale yellow oily liquid	Insoluble in water; soluble in oils Insoluble	123° (11mm Hg)	NMR 94%	<1.0	1.498-1.508 0.914-0.919	SC: Other sesquiterpenes	63rd/N	
1338	**3,7-Dimethyl-1,3,6-octatriene** 3,7-Dimethylocta-1,3(trans),6-triene beta-Ocimene; Ocimene; trans-beta-Ocimene	3539 01.018 13877-91-3	C10 H16 136.24	Colourless to straw-coloured mobile liquid; warm herbaceous aroma	Insoluble in water; soluble in oils Soluble	177°	NMR 80%	<1.0	1.478-1.491 0.801-0.805	SC: cis-beta-Ocimene	63rd/N	

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1339	**p-Mentha-1,3-diene** p-Mentha-1,3-diene alpha-Terpinene; 1-Isopropyl-4-methyl-1,3-cyclohexadiene; Terpilene; 1-Methyl-4-(1-methylethyl)-1,3-cyclohexadiene	3558 01.019 99-86-5	C10 H16 136.24	Colourless oily liquid; refreshing, lemony-citrus aroma	Insoluble in water; soluble in most fixed oils Soluble	173°	NMR 89%	<1.0	1.475-1.480 0.833-0.838	SC: 1,4- and 1,8-cineole; Minimum assay value may include traces of limonene, alpha and beta pinene and other common C10H16 terpenes	63rd/N	
1340	**p-Mentha-1,4-diene** p-Mentha-1,4-diene gamma-Terpinene; 1-Isopropyl-4-methyl-1,4-cyclohexadiene; 1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene	3559 01.020 99-85-4	C10 H16 136.24	Colourless oily liquid; refreshing, herbaceous-citrusy aroma	Insoluble in water; soluble in most fixed oils Soluble	182°	NMR 95%	<1.0	1.472-1.478 0.841-0.845	Minimum assay value may include traces of limonene, alpha and beta pinene and other common C10H16 terpenes	63rd/N	
1341	**1,3,5-Undecatriene** Undeca-1,3,5-triene	3795 01.061 16356-11-9	C11 H18 150.26	Colourless to pale yellow liquid; fruity, green, pineapple, tropical spruce needle aroma	slightly soluble in water; soluble in fats Soluble	80-81° (12 mm Hg)	NMR 94% (sum of cis/trans isomers)	<1.0	1.510-1.518 0.788-0.796	SC: 2,4,6-undecatriene (Z,Z,E)	63rd/N	
1342	**d-3-Carene** 3,7,7-trimethyl-bicyclo-[4.1.0] hept-3-ene 3-carene; (+)-3-carene	3821 01.029 13466-78-9	C10 H16 136.24	Colourless to light pale liquid; fruity aroma	Insoluble in water; soluble in benzene, pet ether Slightly soluble	169-174°	NMR 92%	<1.0	1.468-1.478 0.860-0.868	SC: beta-pinene, limonene, myrcene, p-cymene	63rd/N	
1343	**Farnesene (alpha and beta)** 3,7,11-Trimethyldodeca-1,3,6,10-tetraene and 3-Methylene-7,11-dimethyldodeca-1,6,10-triene	3839 01.040 502-61-4	C15 H24 204.36	Colourless to pale green-yellow liquid; fruity aroma	Insoluble in water; soluble in benzene, pet ether Slightly soluble	53-57° (1 mm Hg)	NMR 38% alpha + 29% beta (sum of cis/trans isomers)	<1.0	1.490-1.500 0.834-0.845	SC: bisabolene, up to 10% other isomers (valencene, bourbonene, cadinene, guaiene)	63rd/N	
1344	**1-Methyl-1,3-cyclohexadiene** 1-Methyl-1,3-cyclohexadiene 2,3-Dihydrotoluene	1489-56-1	C7 H10 94.16	Colourless oily liquid; Light fruity aroma	Insoluble in water; soluble in most fixed oils Soluble	118-120°	NMR 95%	<1.0	1.446-1.452 0.846-0.853		63rd/N	

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1345	**beta-Bourbonene** 2-Methyl-8-methylene-5-isopropyl-tricyclo[5.3.0.0(2.6)]decane 1,2,3,3a,3b.beta.,4,5,6,6a.beta.,6b.alpha.-Decahydro-1.alpha.-isopropyl-3a.alpha.-methyl-6-methylene-cyclobuta[1,2:3,4]dicyclopentene; (-)-beta-Bourbonene	01.024 5208-59-3	C15 H24 204.36	Colourless to yellow oily liquid; Woody aroma	Insoluble in water; soluble in most fixed oils Soluble	121° (11 mm Hg)	NMR 96%	<1.0	1.500-1.507 0.899-0.908	Minimum assay value may include traces of other C15H24 compounds (cadinene, guaiene, farnesene)	63rd/N	
1346	**Cadinene (mixture of isomers)** 1,2,4a,5,8,8a-hexahydro-1-isopropyl-4,7-dimethylnaphthalene Cadina-3,9-diene	29350-73-0	C15 H24 204.36	Colourless, slightly viscous liquid; usually bearing the aroma of the oil from which it is derived	Insoluble in water Soluble	124° (9 mm Hg)	NMR 96% (alpha + beta)	<1.0	1.506-1.512 0.919-0.925		63rd/N	
1347	**Guaiene** 2,8-Dimethyl-5-isopropylidene-bicyclo[5.3.0] dec-1(7)-ene Guaia-1(5),7(11)-diene; beta-Guaiene; beta-Guajene	01.026 88-84-6	C15 H24 204.36	Mobile greenish-yellow liquid; Earthy, spicy aroma	Insoluble in water, propylene glycol; Soluble in oils Soluble	118° (2 mm Hg)	NMR 96%	<1.0	1.503-1.509 0.912-0.918	Minimum assay value may include traces of other C15H24 compounds (cadinene, farnesene, valencene)	63rd/N	
1348	**Butyl 2-decenoate** Butyl dec-2-enoate Butyl decylenate	2194 09.235 7492-45-7	C14 H26 O2 226.36	Colourless liquid; Powerful, fatty, fruity aroma	Soluble in most fixed oils; Insoluble in water Soluble	119-120° (20 mm Hg)	NMR 98%	2.0	1.444-1.451 0.877-0.883		63rd/N	
1349	**2-Decenal** Dec-2-enal 2-Decen-1-al; Decenaldehyde; Decylenic aldehyde; 3-Heptyl acrolein	2366 05.076 3913-71-1	C10 H18 O 154.25	Colourless to slightly yellow liquid; Powerful waxy, orange aroma	Soluble in most fixed oils; Insoluble in water Soluble	229°	IR 92% (sum of cis/trans isomers)	10.0	1.452-1.458 0.836-0.846	SC: 2-Decenoic acid	63rd/N	
1350	**2-Dodecenal** 2-Dodecenal 2-Dodecen-1-al; n-Dodecen-2-al; 3-Nonyl acrolein	2402 05.037 4826-62-4	C12 H22 O 182.31	Colourless to slightly yellow liquid; Fatty, citus-like aroma	Soluble in most fixed oils; Insoluble in water Soluble	272°	IR 93% (sum of cis/trans isomers)	10.0	1.454-1.460 0.839-0.849	SC: 2-Dodecenoic acid	63rd/N	
1351	**Ethyl acrylate** Ethyl prop-2-enoate Ethyl propenoate; Ethyl 2-propenoate; Acrylic acid ethyl ester; Ethyl acrylic ester	2418 09.037 140-88-5	C5 H8 O2 100.12	Colourless mobile liquid; lachrymator/intense, harsh, fruity aroma	Soluble in ether and oils; Slightly soluble water Soluble	99-101°	IR 97%	5.0	1.403-1.409 0.916-0.919		63rd/N	

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1352	**Ethyl 2-nonynoate** Ethyl 2-nonynoate Ethyl octyne carbonate	2448 09.157 10031-92-2	C11 H18 O2 182.26	Colourless oily liquid; Green, violet-like aroma	Soluble in oils; Insoluble in water Soluble	226-227°	NMR 96%	2.0	1.450-1.456 0.901-0.907		63rd/N	
1353	**2-Hexenal** 2-Hexenal 2-Hexen-1-al; beta-Propyl acrolein; alpha-beta-Hexylenealdehyde; Leaf aldehyde	2560 05.189 6728-26-3	C6 H10 O 98.14	Pale yellow to colourless oily liquid; Strong fruity, green, vegetable-like aroma	Soluble in propylene glycol and most fixed oils; Very slightly soluble in water Soluble	47° (17mm Hg)	NMR 92% (sum of cis/trans isomers)	10.0	1.443-1.449 0.841-0.848	SC: 2-Hexenoic acid	63rd/N	
1354	**2-Hexen-1-ol** Hex-2-enol gamma-Propyl allyl alcohol; Leaf alcohol	2562 02.020 2305-21-7	C6 H12 O 100.16	Almost colourless liquid; Strong, fruity-green aroma	Soluble in propylene glycol and most fixed oils; Very slightly soluble in water Soluble	158-160	IR 95% (sum of cis/trans isomers)	2.0	1.437-1.442 0.836-0.841		63rd/N	
1355	**2-(E)Hexen-1-yl acetate** Hex-2-enyl acetate 2-Hexenyl ethanoate; 1-Acetoxy-2-hexene; Hex-2-enyl acetate	2564 09.196 2497-18-9	C8 H14 O2 142.20	Colourless to pale yellow liquid; Powerful green, fruity aroma	Very slightly soluble in water; Soluble in oils Soluble	165-166°	IR 90%	1.0	1.424-1.430 0.890-0.897	SC: (Z)-2-Hexenyl acetate	63rd/N	
1356	**Methyl 2-nonynoate** Methyl 2-nonynoate Methyl octine carbonate; Methyl octyne carbonate	2726 09.156 111-80-8	C10 H16 O2 168.24	Colourless oily liquid; Peach, violet aroma	Soluble in oils; Insoluble in water Soluble	121-122° (20 mm Hg)	NMR 97%	1.0	1.445-1.451 0.913-0.916		63rd/N	
1357	**Methyl 2-octynoate** Methyl 2-octynoate Methyl heptine carbonate; Methyl heptyne carbonate; methyl-n-hept-1-yne-1-carboxylate	2729 09.158 111-12-6	C9 H14 O2 154.21	Colourless to slightly yellow liquid; Powerful, unpleasant odour. Violet like when diluted.	Soluble in most fixed oils; Slightly soluble in propylene glycol; Insoluble in water, glycerin Soluble	215-217°	IR 95%	1.0	1.443-1.449 0.919-0.924		63rd/N	
1358	**Methyl 2-undecynoate** Methyl 2-undecynoate Methyl decine carbonate; Methyl decyne carbonate	2751 09.239 10522-18-6	C12 H20 O2 196.29	Colourless oily liquid; Powerful, waxy, green, floral aroma	Insoluble in water Soluble	230°	NMR 97%	1.0	1.443-1.449 0.915-0.921 (20°)		63rd/N	
1359	**2-Tridecenal** Tridec-2-enal 3-Decylacrolein; Tridecen-2-al-1	3082 05.078 7774-82-5	C13 H24 O 196.33	Colourless or slightly yellowish liquid; Oily, citus aroma	Soluble in most fixed oils; Insoluble in water Soluble	115-118° (10 mm Hg)	IR 92% (sum of cis-trans isomers)	5.0	1.455-1.461 0.842-0.862	SC: 2-Tridecenoic acid	63rd/N	
1360	**trans-2-Heptenal** Hept-2(trans)-enal beta-Butylacrolein; 2-Heptenic aldehyde	3165 05.150 18829-55-5	C7 H12 O 112.17	Colourless mobile liquid; Pungent green, somewhat fatty aroma	Soluble in oils; Insoluble in water Soluble	165-167°	IR 97%	5.0	1.428-1.434 0.857-0.863		63rd/N	

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1361	**trans-2-Hexenoic acid** Hex-2(trans)-enoic acid Acrylic, beta-propylacrylic acid; Hexen-2-oic acid	3169 08.054 13419-69-7	C6 H10 O2 114.14	Colourless needle-like crystals; Fatty acrid musty aroma/sweet on dilution	Soluble in ether, propylene glycol, and most fixed oils; Slightly soluble in water Soluble	-	NMR 97%	NA	- -	mp: 33-37°	63rd/N	
1362	**2-Nonenal** Non-2-enal 2-Nonen-1-al; 3-Hexyl acrolein; Heptylidene acetaldehyde; Iris aldehyde	3213 05.171 2463-53-8	C9 H16 O 140.22	White to slightly yellow liquid; Powerful, penetrating fatty, violet aroma	Soluble in most fixed oils; Insoluble in water Soluble	88-90° (12 mm Hg)	IR 92% (sum of cis/trans isomers)	10.0	1.454-1.460 0.855-0.865	SC: 2-Nonenoic acid	63rd/N	
1363	**2-Octenal** Oct-2-enal 2-Octen-1-al; 2-Pentyl acrolein; alpha-Amyl acrolein	3215 05.060 2363-89-5	C8 H14 O 126.20	Colourless to slightly yellow liquid; Fatty, green aroma	Slightly soluble in water; Soluble in most fixed oils Soluble	84-86° (19 mm Hg)	IR 92% (sum of cis/trans isomers)	10.0	1.449-1.455 0.835-0.845	SC: 2-Octenoic acid, ethyl octanoate	63rd/N	
1364	**2-Pentenal** Pent-2-enal 2-Ethylacrylic aldehyde; beta-Ethylacrolein	3218 05.102 764-39-6	C5 H8 O 84.11	Colourless to light yellow liquid; Pungent green, fruity aroma	Insoluble in water; soluble in PG, in most fixed oils Soluble	124°	NMR 98%	5.0	1.440-1.447 (21°) 0.850-0.856 (21°)		63rd/N	
1365	**trans-2-Nonen-1-ol** Non-2(trans)-en-1-ol (E)-2-Nonen-1-ol; trans-2-Nonenol	3379 02.090 31502-14-4	C9 H18 O 142.23	White liquid; Fatty, violet aroma	Insoluble in water Soluble	105° (12 mm Hg)	IR 95%	1.0	1.444-1.448 0.835-0.845		63rd/N	
1366	**2-Undecenal** 2-Undecenal 2-Undecen-1-al; Undecen-2-al; 3-Octylacrolein; Undecylenic aldehyde	3423 05.109 2463-77-6	C11 H20 O 168.27	Colourless to very pale straw coloured liquid; Fresh, fruity, orange peel aroma	Soluble in oils; Insoluble in water Soluble	115° (10 mm Hg)	NMR 98% (sum of cis/trans isomers)	6.0	1.452-1.459 0.837-0.847		63rd/N	
1367	**trans-2-Octen-1-yl acetate** Oct-2-enyl acetate E-2-Octenyl acetate; trans-2-Octenyl acetate	3516 09.276 3913-80-2	C10 H18 O2 170.25	Colourless liquid; Fruity aroma	Soluble in fats; Insoluble in water Soluble	88-89° (8 mm Hg)	NMR 97%	2.0	1.430-1.436 0.894-0.900		63rd/N	
1368	**trans-2-Octen-1-yl butanoate** Oct-2(trans)-enyl butyrate trans-2-Octen-1-yl butyrate	3517 09.277 84642-60-4	C12 H22 O2 198.30	Colourless liquid; Fruity aroma	Soluble in fats; Insoluble in water Soluble	112-113° (8 mm Hg)	NMR 96%	2.0	1.433-1.439 0.890-0.896		63rd/N	
1369	**cis-2-Nonen-1-ol** Non-2(cis)-en-1-ol (Z)-2-Nonenyl alcohol	3720 02.112 41453-56-9	C9 H18 O 142.23	Colourless liquid; Melon aroma	Soluble in oils and common organic solvents; Slightly soluble in water Soluble	96° (10 mm Hg)	NMR 96%	1.0	1.447-1.453 0.841-0.847		63rd/N	

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1370	**(E)-2-Octen-1-ol** Oct-2-en-1-ol 2-(E)-Octanol; (E)-2-Octenyl alcohol	3887 02.192 18409-17-1	C8 H16 O 128.21	Clear colourless liquid; Meaty, roasted aroma	Soluble in hexane, triacetin; Insoluble in water Soluble	88° (11 mm Hg)	NMR 96%	1.0	1.445-1.452 0.847-0.853		63rd/N	
1371	**(E)-2-Butenoic acid** But-2-enoic acid (E)-Crotonic acid	3908 08.072 107-93-7	C4 H6 O2 86.09	Off-white powder; Harsh, pungent, acrylic odour	Slightly soluble in water Soluble	-	NMR 98%	NA	- -	mp: 71-73°	63rd/N	
1372	**(E)-2-Decenoic acid** Dec-2(cis)-enoic acid	3913 08.073 334-49-6	C10 H18 O2 170.25	Colourless liquid; Peach-orange, slightly waxy aroma	Soluble in oils Soluble	161-162° (15 mm Hg)	NMR 97%	NA	1.456-1.466 0.923-0.933		63rd/N	
1373	**(E)-2-Heptenoic acid** trans-2-Heptenoic acid	3920 08.123 10352-88-2	C7 H12 O2 128.18	Colourless liquid; Disagreeable rancid aroma	Soluble in oils Soluble	224-228°	NMR 97%	NA	1.447-1.157 0.968-0.978		63rd/N	
1374	**(Z)-2-Hexen-1-ol** Hex-2(cis)-enol (Z)-2-Hexenol; cis-beta-gamma-Hexenol	3924 02.156 928-94-9	C6 H12 O 100.16	Colourless liquid; Green aroma	Soluble in fats; Insoluble in water Soluble	65° (0.5 mm Hg)	NMR 92%	2.0	1.437-1.445 0.845-0.853	SC: (E)-2-Hexen-1-ol	63rd/N	
1375	**trans-2-Hexenyl butyrate** Hex-2-enyl butyrate (E)-Hex-2-enyl butyrate; (E)-Hexenyl butanoate; trans-2-Hexenyl butanoate	3926 09.396 53398-83-7	C10 H18 O2 170.25	Colourless liquid; Fruity, green aroma	Soluble in fats; Insoluble in water Soluble	190°	NMR 95%	2.0	1.429-1.435 0.882-0.888		63rd/N	
1376	**(E)-2-Hexenyl formate** Hex-2-enyl formate trans-2-Hexenyl formate;	3927 09.397 53398-78-0	C7 H12 O2 128.18	Colroless liquid; Fruity, green aroma	Soluble in fats; Insoluble in water Soluble	75° (10 mm Hg)	NMR 97%	3.0	1.420-1.424 0.915-0.925		63rd/N	
1377	**trans-2-Hexenyl isovalerate** Hex-2-enyl 3-methylbutanoate (E)-Hex-2-enyl 3-methylbutanoate	3930 09.399 68698-59-9	C11 H20 O2 184.28	Colourless liquid; Fruity-buttery aroma	Soluble in fats; Insoluble in water Soluble	105° (20 mm Hg)	NMR 96%	3.0	1.425-1.435 0.875-0.885		63rd/N	
1378	**trans-2-Hexenyl propionate** Hex-2(trans)-enyl propionate (E)-2-Hexenyl propanoate	3932 09.395 53398-80-4	C9 H16 O2 156.23	Colourless liquid; Fruity, ripe apple-pear aroma	Soluble in fats; Insoluble in water Soluble	91° (20 mm Hg)	NMR 95%	3.0	1.426-1.433 0.885-0.895		63rd/N	
1379	**trans-2-Hexenyl pentanoate** Hex-2(trans)-enyl valerate (E)-Hex-2-enyl valerate; trans-2-Hexenyl valerate	3935 56922-74-8	C11 H20 O2 184.28	Colourless liquid; Fruity, winey, apple/pear aroma	Soluble in fats; Insoluble in water Soluble	70° (1 mm Hg)	NMR 93%	3.0	1.431-1.438 0.873-0.879	SC: Propanoic acid, 2-Hexenol	63rd/N	

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1380	**(E)-2-Nonenoic acid** Non-2-enoic acid	3954 08.101 14812-03-4	C9 H16 O2 156.22	Colourless liquid; Fatty aroma	Soluble in oils Soluble	131-132° (2 mm Hg)	NMR 97%	NA	1.456-1.464 0.930-0.940		63rd/N	
1381	**(E)-2-Hexenyl hexanoate** Hex-2-enyl hexanoate trans-2-Hexenyl caproate	3983 09.398 53398-86-0	C12 H22 O2 198.31	Colourless liquid; Green fruity aroma	Soluble in most fixed oils; Insoluble in water Soluble	125° (25 mm Hg)	IR 93%	3.0	1.432-1.446 0.875-0.885	SC: Hexanoic acid, 2-Hexenol	63rd/N	
1382	**(Z)-3- & (E)-2-Hexenyl propionate** Hex-3(cis)-enyl propionate and Hex-2-(trans)-enyl propionate Propanoic acid, cis-3, trans-2-hexenyl ester; Green note propionate	3778 09.564 33467-74-2	C9 H16 O2 156.23	Clear colourless liquid; Green fruity aroma	Insoluble in water Soluble	169-178°	NMR 47% of (Z)-3-isomer 49% of (E)-2- isomer	3.0	1.458-1.466 0.857-0.867		63rd/N	
1383	**(E)-2-Hexenal diethyl acetal** 1,1-Diethoxyhex-2(cis)-ene (E)-1,1-Diethoxy-2-hexene; Leafaldehyde diethyl acetal	4047 06.031 67746-30-9	C10 H20 O2 172.27	Colourless liquid; Fruity aroma	Soluble in most fixed oils; Insoluble in water Soluble	76-77° (15 mm Hg)	IR 97%	1.0	1.418-1.426 0.843-0.849		63rd/N	
1384	**2-Undecen-1-ol** Undec-2-en-1-ol 1-Hydroxy-2-undecene; 2-Undecenol	4068 02.210 37617-03-1	C11 H22 O 170.30	White to slightly yellow liquid; Fruity, fatty aroma	Soluble in most fixed oils; Insoluble in water Soluble	100-102° (2 mm Hg)	IR 95%	1.0	1.447-1.453 0.838-0.848		63rd/N	
1385	**Borneol** 1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol 2-Bornanol;Borneo camphor; Bornyl alcohol; 2-Camphanol	2157 02.016 507-70-0	C10 H18 O 154.25	White to off-white crystals; piney camphoraceous aroma	Slightly soluble in proylene glycol; Very slightly soluble in water; Insoluble in vegatable oils Soluble	-	IR 97%	NA	- -	mp: 202°; Minimum assay value may include isoborneol and other isomers of borneol as well as trace amounts of fenchyl alcohol and other C10H18O compounds	63rd/N	
1386	**Isoborneol** 1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol exo-2-Bornanol; exo-2-Camphanol; iso-Camphol; iso-Bornyl alcohol	2158 02.059 124-76-5	C10 H18 O 154.25	White to off-white crystals; piney camphoraceous aroma	Slightly soluble in proylene glycol; Very slightly soluble in water; Insoluble in vegatable oils Soluble	-	IR 92%	NA	- -	SC: Borneol; mp: 212-214°	63rd/N	

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1387	**Bornyl acetate** 1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-yl acetate Borneol acetate; Bornyl acetic ether; Bornyl ethanoate; 2-Camphanyl acetate	2159 09.017 76-49-3	C12 H20 O2 196.29	Colourless liquid, semicrystaline mass to white crystaline solid; Sweet herbaceous, piney aroma	Slightly soluble in water; Insoluble in glycerin, propylene glycol Soluble	226°	IR 98%	1.0	1.462-1.466 0.981-0.985	mp: 25°; Minimum assay value may include isobornyl acetate and other bornyl acetate isomers	63rd/N	
1388	**Isobornyl acetate** 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl acetate Isoborneol acetate; exo-2-Bornyl acetate; Isobornyl ethanoate	2160 09.218 125-12-2	C12 H20 O2 196.29	Colourless to very pale straw coloured liquid; Camphoraceous, piney, balsamic aroma	Soluble in most fixed oils; Slightly soluble in propylene glycol; Insoluble in water, glycerin Soluble	227°	IR 97%	1.0	1.462-1.465 0.979-0.984	Minimum assay value may include small amounts of bornyl acetate	63rd/N	
1389	**Bornyl formate** 1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-yl formate Bornyl methanoate; 2-Camphanyl formate; endo-2-Bornyl formate; Borneol formate	2161 09.082 7492-41-3	C11 H18 O2 182.26	Colourless liquid; Green, earthy refreshing aroma	Soluble in oils; Slightly soluble in water Soluble	106-108° (21 mm Hg)	NMR 95%	<1.0	1.466-1.472 1.007-1.013 (20°)		63rd/N	
1390	**Isobornyl formate** 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl formate exo-2-Bornyl formate; Bornyl (iso) formate; exo-2-Camphanyl formate; Isobornyl methanoate	2162 09.176 1200-67-5	C11 H18 O2 182.26	Colourless liquid; Green, earthy, herbaceouos-camphoraceous, piney aroma	Soluble in oils; Slightly soluble in water Soluble	94-95° (15 mm Hg)	NMR 96%	<1.0	1.469-1.473 1.011-1.017	Minimum assay value may include small amounts of bornyl formate	63rd/N	
1391	**Isobornyl propionate** 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl propanoate iso-Bornyl propionate; Bornyl (iso) propionate; exo-2-Bornyl propionate; exo-2-Camphanyl propionate	2163 09.131 2756-56-1	C13 H22 O2 210.32	Colourless oily liquid; Soft-turpentine aroma	Soluble in water, oils Soluble	245°	NMR 97%	<1.0	1.461-1.465 0.968-0.971	Minimum assay value may include small amounts of bornyl propionate	63rd/N	
1392	**Bornyl valerate** 1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-yl pentanoate Bornyl n-pentanoate; Bornyl n-valerate; Bornyl valerianate	2164 09.153 7549-41-9	C15 H26 O2 238.37	Colourless liquid; Fruity, herbaceous-camphoraceous aroma	Soluble in oils, Insoluble in water Soluble	136-137° (12 mm Hg)	NMR 96%	<1.0	1.459-1.465 0.957-0.963	Minimum assay value may include small amounts of isobornyl valerate	63rd/N	

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1393	**Bornyl isovalerate (endo-)** 1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-yl 3-methylbutanoate Bornyl iso-pentanoate; Bornyl iso-valerianate; Bornyl 3-methylbutanoate; Iso-Valeric acid, 2-bornyl ester	2165 09.456 76-50-6	C15 H26 O2 238.37	Colourless liquid; Warm, herbaceous, slightly earthy-green aroma	Soluble in oils, Insoluble in water Soluble	260°	NMR 97%	1.0	1.458-1.461 0.944-0.947		63rd/N	
1394	**Isobornyl isovalerate** 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl 3-methylbutanoate Isobornyl isopentanoate; iso-Bornyl iso-pentanoate; iso-Bornyl iso-valerianate; iso-Bornyl 3-methylbutanoate	2166 09.457 7779-73-9	C15 H26 O2 238.37	Colourless liquid; Herbaceouos-camphoraceous warm, and slightly green-woody aroma	Soluble in oils, Insoluble in water Soluble	266-269°	NMR 96%	1.0	1.463-1.469 0.900-0.906		63rd/N	
1395	**d-Camphor** dl-Bornan-2-one 2-Bornanone; 2-Camphanone; Formosa camphor; Laurel camphor	2230 07.006 464-49-3	C10 H16 O 152.24	White to gray translucent crystals or fused mass; Warm, minty, almost ethereal diffusive aroma	Soluble in oils, water Soluble	-	IR 96%	NA	- -	mp: 174-179°	63rd/N	
1396	**d-Fenchone** 1,3,3-Trimethyl-bicyclo[2.2.1]heptan-2-one 2-Fenchanone; d-1,3,3-Trimethyl-2-norbornanone; d-1,3,3-Trimethyl-2-norcamphanone	2479 07.159 4695-62-9	C10 H16 O 152.24	Colourless to pale yellow liquid; Camphoraceous aroma	Soluble in propylene glycol, vegetable oils; Insoluble in water Soluble	192°	IR 97% of C10H16O	<1.0	1.460-1.467 0.940-0.948	Minimum assay value may include small amounts of d-camphor	63rd/N	
1397	**Fenchyl alcohol** 1,3,3-trimethyl-bicyclo{2.2.1]heptan-2-ol 2-Fenchanol; Fenchol; 1,3,3-Trimethyl-2-norbornanol	2480 02.038 1632-73-1	C10 H18 O 154.25	White to pale yellow crystals; Camphoraceous aroma	Soluble in vegetable oils; Very slightly soluble in water Soluble	-	IR 97% of C10H18O	NA	- -	mp: 35-40°; Minimum assay value may include small amounts of borneol and isoborneol	63rd/N	
1398	**Nootkatone** 4,4a,5,6,7,8- Hexahydro-4,4a-dimethyl-6-(1-methylene-ethyl)-2(3H)-naphthalenone 4,4a,5,6,7,8-Hexahydro-6-iso-propenyl-4,4a-dimethyl-2(3H)-naphthalenone	3166 07.089 4674-50-4	C15 H22 O 218.35	Colourless to pale yellow or orange coloured oily liquid; Powerful fruity sweet, citrusy, grapefruit peel oil like aroma	Soluble in oils; Slightly soluble in water Soluble	73-103° (0.8 mm Hg)	NMR 93%	3.0	1.510-1.523 1.003-1.032	SC: Dihydronootkatone	63rd/N	
1399	**1,3,3-Trimethyl-2-norbornanyl acetate** 1,3,3-trimethyl-bicyclo[2.2.1]heptan-2-yl acetate Fenchyl acetate	3390 09.269 13851-11-1	C12 H20 O2 196.29	Colourless mobile liquid; Mild, sweet, fir oil type aroma	Soluble in oils; Slightly soluble in water Soluble	220°	NMR 98%	1.0	1.456-1.462 0.973-0.979		63rd/N	

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1400	**Methyl jasmonate** Methyl 3-oxo-2-pent-2-enyl-1-cyclopentylacetate Methyl (2-pent-2-enyl-3-oxo-1-cyclopentyl)acetate	3410 09.521 1211-29-6	C13 H20 O3 224.30	Colourless oily liquid; Powerful floral-herbaceous, sweet aroma	Soluble in oils; Slightly soluble in water Soluble	94° (0.05 mm Hg)	NMR 99%	1.0	1.470-1.476 1.017-1.023		63rd/N	
1401	**Cycloheptadeca-9-en-1-one** Cycloheptadec-9-en-1-one Cycloheptadenen-9-one-1; 9-Cycloheptadecen-1-one; Civetone; Civettone	3425 07.110 542-46-1	C17 H30 O 250.43	White or colourless crystalline mass; Musky aroma	Soluble in oils; Slightly soluble in water Soluble	-	NMR 99%	NA	- -	mp: 32°	63rd/N	
1402	**3-Methyl-1-cyclopentadecanone** 3-Methylcyclopentadecan-1-one Methylexaltone; d,l-Muscone	3434 07.111 541-91-3	C16 H30 O 238.42	Colourless or opaque crystalline mass; Soft, sweet, tenacious musk aroma	Soluble in oils; Slightly soluble in water Soluble	-	NMR 98%	NA	- -	mp: 33°	63rd/N	
1403	**2(10)-Pinen-3-ol** 3-Hydroxy-6,6-dimethyl-2-methylene-bicyclo[3.1.1]heptane Pinocarveol	3587 02.100 5947-36-4	C10 H16 O 152.24	Viscous, light yellow oil; Warm, woody-balsamic aroma	Soluble in oils; Insoluble in water Soluble	210°	NMR 95%	<1.0	1.445-1.451 0.977-0.983		63rd/N	
1404	**Verbenol** 4,6,6-Trimethyl-bicyclo[3.1.1]hept-3-en-2-one 2-Pinen-4-ol	3594 02.101 473-67-6	C10 H16 O 152.24	White to slightly yellow solid; Balsamic aroma	Very slightly soluble in water Soluble	-	NMR 95%	<1.0	- -	mp: 63-67°	63rd/N	
1405	**7-Methyl-4,4a,5,6-tetrahydro-2(3H)-naphthalenone** 4,4a,5,6-Tetrahydro-7-methylnapthalen-2(3H)-one	3715 07.136 34545-88-5	C11 H14 O 162.23	Light yellow crystaline powder; Sweet coumarin-like aroma	Soluble in ether, fat; Insoluble in water Soluble	-	IR 99%	<1.0	- -	mp: 36-37°	63rd/N	
1406	**3-Methyl-2-(n-pentanyl)-2-cyclopenten-1-one** 3-Methyl-2-pentylcyclopent-2-en-1-one Dihydrojasmone; 3-Methyl-2-pentyl-cyclopent-2-en-1-one	3763 07.140 1128-08-1	C11 H18 O 166.26	Colourless liquid; celery, herbacous, spicy aroma	Soluble in fats; Very slightly soluble in water Soluble	79° (0.19 mm Hg)	NMR 99%	<1.0	1.676-1.682 0.911-0.917		63rd/N	

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1407	**Dihydronootkatone** 1,2,6-Trimethyl-9-isopropylene-bicyclo[4.4.0]decan-4-one 1,10-Dihydronootkatone; 4b,H,5a-Eremophil-11-en-2-one	3776 07.153 20489-53-6	C15 H24 O 220.36	Colourless liquid; Citrus like green aroma	Soluble in ethers, fats; Very slightly soluble in water Soluble	100-104° (0.07 mm Hg)	NMR 90%	<1.0	1.502-1.508 0.975-0.988	SC: Nootkatone	63rd/N	
1408	**3-L-Menthoxypropane-1,2-diol** 3-(1-Menthoxy)propane-1,2-diol 3-l-(p-Menthane-3-yloxy)-1,2-propanediol	3784 02.224 87061-04-9	C13 H26 O3 230.35	Colourless liquid; Minty, vanilla aroma	Soluble in fat; Very slightly soluble in water Soluble	121-125° (0.25 mm Hg)	NMR 99%	1.0	1.472-1.476 0.989-0.999		63rd/N	
1409	**beta-Ionyl acetate** 4-(2,2,6-Trimethylcyclohex-1-enyl)but-3-en-2-yl acetate	3844 09.305 22030-19-9	C15 H24 O2 236.35	Colourless liquid; Natural raspberry aroma	Soluble in fats; Insoluble in water Soluble	120° (2 mm Hg)	NMR 92%	1.0	1.474-1.484 0.934-0.944	SC: acetic acid, beta-Ionol	63rd/N	
1410	**alpha-Isomethylionyl acetate** 3-Methyl-4-(2,6,6-trimethylcyclohex-2-enyl)but-3-en-2-yl acetate	3845 68555-61-3	C16 H26 O2 250.38	Colourless liquid; Vetivert-violet aroma	Soluble in hexane; Insoluble in water Soluble	90° (1 mm Hg)	NMR 95%	1.0	1.465-1.475 0.925-0.935		63rd/N	
1411	**3-(l-Menthoxy)-2-methylpropane-1,2-diol** (l)-2-Methyl-3-[5-methyl-2-(1-methylethyl)cyclohexyl]oxy-1,2-propanediol	3849 195863-84-4	C14 H28 O3 244.36	Colourless liquid; minty, cool aroma	Soluble in hexane; Slightly soluble in water Soluble	124° (0.4 mm Hg)	NMR 99%	1.0	1.468-1.474 0.978-0.984 (20°)		63rd/N	
1412	**Bornyl butyrate** 1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-yl butanoate Bornyl butanoate; Butyric acid, 2-bornyl ester	3907 09.319 13109-70-1	C14 H24 O2 224.34	Colourless liquid; Herbaceous aroma	Soluble in oils; Slightly soluble in water Soluble	247°	MS 97%	1.0	1.462-1.469 0.981-0.991		63rd/N	
1413	**D,L-Menthol(+/-)-propylene glycol carbonate** 2-Hydroxypropyl menthane-3-yl carbonate	3992 09.843 156324-82-2	C14 H26 O4 270.36	Clear colourless liquid; Menthol-like aroma	Soluble in most fixed oils, isooctanol, propylene glycol; Insoluble in water Soluble	140-143°	NMR 87%	2.0	1.455-1.461 1.011-1.017	SC: 1-(Hydroxymethyl) ethyl menthane-3-yl carbonate ("d,l-Menthol 2-propylene glycol carbonate")	63rd/N	
1414	**L-Monomenthyl glutarate** (L)-Monomenthane-3-yl glutarate Pentadienoic acid, mono[5 methyl-2-1(1-methylethyl)cyclohexyl]ester, [1L]; [1R(-)] monomenthyl glutarate	4006 220621-22-7	C15 H26 O4 270.36	Clear viscous liquid; Minty, menthol-like aroma	Soluble in propylene glycol, ethyl acetate; Insoluble in water Soluble	>300°	NMR 72%	1.0	1.465-1.471 0.894-0.900 (20°)	SC: dimenthyl glutarate; glutaric acid	63rd/N	

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1415	**L-Menthyl methyl ether** 1-Isopropyl-2-methoxy-4-methylcyclohexane 1-Isopropyl-2-methoxy-4-methylcyclohexane; 2-Isopropyl-5-methylcyclohexyl methyl ether	4054 1565-76-0	C11 H22 O 170.30	Clear colourless liquid; Minty aroma	Soluble in heptane; Slightly soluble in triacetin; Insoluble in water Soluble	81° (10.5 mm Hg)	NMR 99%	NA	1.441-1.447 0.856-0.862		63rd/N	
1416	**p-Menthane-3,8-diol** p-Menthane-3,8-diol 2-(2'Hydroxypropan-2'-yl)-5-methylcyclohexanol; 2-Hydroxy-alpha,alpha,4-trimethylcyclohexane methanol	4053 42822-86-6	C10 H20 O2 172.27	Opaque white crystals; Minty, herbaceous, Eucalyptus-like aroma	Slightly soluble in water Soluble	-	IR 99%	NA	- -	mp: 34-35°	63rd/N	
1418	**beta-Alanine** 3-Aminopropanoic acid 3-Aminopropanoic acid; beta-Aminopropionic acid	3252 17.001 107-95-9	C3 H7 N O2 89.09	Colourless needles;	Soluble in water; Insoluble in ether and acetone Slightly soluble	-	NMR 97%	NA	- -	mp: 202-207°	63rd/N	
1419	**L-Cysteine** L-Cysteine alpha-Amino-beta-mercaptopropionic acid; 2-Amino-3-mercaptopropionic acid; L-beta-Mercaptoalanine; alpha-Amino-beta-thiolpropionic acid	3263 17.033 52-90-4	C3 H7 N O2S 121.16	White crystals; Sulferous aroma	Very soluble in water and acetic acid; Insoluble in ether, acetone and benzene Soluble	-	MS 98%	NA	- -	mp: 240°; Sp.rotation = +6.9 to +8.5° (30°)	63rd/N	
1420	**L-Glutamic acid** L-Glutamic acid L-2-Aminopentanedioic acid; Aminoglutaric acid, 1-aminopropane-1,3-dicarboxylic acid	3285 56-86-0	C5 H9 N O4 147.13	White free-flowing, crystalline powder; Yeasty, bread-like aroma	Slight soluble in water and ether Insoluble	-	IR 98%	NA	- -	mp: 247-249°; Sp.rotation = +30 to +32° (22°, 6N HCl); Complies with purity criteria for L-Glutamic acid (FNP 52 p 693)	63rd/N	
1421	**Glycine** Glycine Aminoacetic acid; Glycoll; Aminoethanoic acid	3287 17.034 56-40-6	C2 H5 N O2 75.07	White crystalline powder; odourless	Soluble in water; Slightly soluble in ether Slightly soluble	-	IR 98%	NA	- -	mp: 245°	63rd/N	
1422	**DL-Isoleucine** 2-Amino-3-methylpentanoic acid DL-2-Amino-3-methylvaleric acid; alpha-Amino-beta-methylvaleric acid	3295 17.010 443-79-8	C6 H13 N O2 131.17	White crystalline powder; odourless	Soluble in water; Insoluble in ether Insoluble	-	IR 98%	NA	- -	mp: 290-292°	63rd/N	

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1423	**L-Leucine** L-Leucine 2-Aminoisobutylacetic acid; L-2-Amino-4-methylvaleric acid; alpha-Aminoisocaproic acid; 2-Amino-4-methylpentanoic acid	3297 17.012 61-90-5	C6 H13 N O2 131.17	Small white lustrous plates or crystalline powder; odourless	Soluble in water, acetic acid, dilute HCl, and alkaline hydroxides and carbonates Slightly soluble	-	IR 98%	NA	- -	mp: 293-295°; Sp. rotation = -9.5 to -11.5° (20°)	63rd/N	
1424	**DL-Methionine** 2-Amino-4-(methylthio)butanoic acid DL-2-amino-4-(methylthio)butyric acid; 2-Amino-4-(methylthio)butanoic acid; 2-Amino-g-(methylthio)butyric acid	3301 17.014 59-51-8	C5 H11 N O3 S 149.21	White crystalline platelets or powder; Characteristic aroma	Soluble in water; Insoluble in ether Soluble	-	MS 98%	NA	- -	mp: 281°	63rd/N	
1425	**L-Proline** Pyrrolidine-2-carboxylic acid L-Pyrrolidiencarboxylic acid	3319 17.019 147-85-3	C5 H9 N O2 115.13	White crystals or crystalline powder; odourless	Soluble in water; Insoluble in ether Soluble	-	NMR 98%	NA	- -	mp: 220-222°; Sp.rotation = -80 to -82° (20°)	63rd/N	
1426	**DL-Valine** 2-Amino-3-methylbutanoic acid alpha-Aminoisovaleric acid; 2-Amino-3-methylbutanoic acid; 2-Amino-3-methylbutyric acid	3444 17.023 516-06-3	C5 H11 N O2 117.15	White crystalline powder; odourless	Soluble in water; Insoluble in ether Insoluble	-	MS 98%	NA	- -	mp: 295°	63rd/N	
1427	**DL-(3-Amino-3-carboxypropyl)dimethylsufoniu m chloride** S-Methylmethioninesulphonium chloride DL-Methylmethionine sulfonium chloride;dl-(3-Amino-3-carboxypropyl)dimethylsulfonium chloride; Vitamin U	3445 17.015 1115-84-0	C6 H14 N O2 S Cl 199.70	White crystalline powder;; characteristic cabbage taste and aroma	Soluble in water; Insoluble in fat Soluble	-	NMR 98%	NA	- -	mp: 139°	63rd/N	
1428	**L-Phenylalanine** L-Phenylalanine L-alpha-Amino-beta-phenylpropionic acid; Aminohydrocinnamic acid; L-2-Amino-3-phenylpropionic acid	3585 17.018 63-91-2	C9 H11 N O2 165.19	Colourless or white platelike crystals or crystalline powder; odourless	Soluble in water; Slightly soluble in dilute mineral acid and alkali hydroxide solutions Slightly soluble	-	MS 98%	NA	- -	mp: 270-275°; Sp.rotation = -17.6 to -18.6° (20°)	63rd/N	
1429	**L-Aspartic acid** 2-Aminobutanedioic acid L-Aminosuccininc acid; 2-Aminobutanedioic acid	3656 17.005 56-84-8	C4 H7 N O4 133.10	White crystals or crystalline powder; odourless	Slightly soluble in water; Insoluble in ether Insoluble	-	MS 98%	NA	- -	mp: 270-271°; Sp.rotation = +12.2 to +13.3° (25°, 5N HCl)	63rd/N	

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1430	**L-Glutamine** L-Glutamine L-Aminoglutaramic acid; Glutamic acid-5-amide	3684 17.007 56-85-9	C5 H10 N2 O3 146.15	White crystals or crystalline powder; odourless	Soluble in water and ether Insoluble	-	IR 98%	NA	- -	mp: 190-192°; Sp.rotation = +15.5 to +16.5° (25°, 1N HCl)	63rd/N	
1431	**L-Histidine** L-Histidine L-alpha-Amino-4(or 5)-imidazolepropionic acid; 2-Amino-3(4-imidasyl)propionic acid	3694 17.008 71-00-1	C6 H9 N3 O2 155.16	White crystals or crystalline powder; odourless	Soluble in water; Insoluble in ether Slightly soluble	-	MS 98%	NA	- -	mp: 282°; Sp.rotation = +37.5 to +39.5° (25°)	63rd/N	
1432	**DL-Phenylalanine** DL-Phenylalanine DL-alpha-Amino-beta-phenylproionic acid, 2-Aminohydrocinnamic acid	3726 17.017 150-30-1	C9 H11 N O2 165.19	White crystalline platelets; odourless	Soluble in water and dilute mineral acid and alkali hydroxide solutions Slightly soluble	-	MS 98%	NA	- -	mp: 271-273°	63rd/N	
1434	**L-Tyrosine** L-Tyrosine L-beta-(p-Hydroxyphenyl)alanine	3736 17.022 60-18-4	C9 H11 N O3 181.19	Colourless silky needles or white crystalline powder; odourless	Soluble in water and dilute mineral acid and alkali hydroxide solutions Slightly soluble	-	IR 98%	NA	- -	mp: 342-344°; Sp.rotation = -4.5 to -5.5° (2°, 5N HCl)	63rd/N	
1435	**Taurine** 2-Aminoethanesulfonic acid 2-Aminoethanesulfonic acid	3813 16.056 107-35-7	C2 H7 N O3 S 125.15	White to cream coloured crystaline solid;	Soluble in water Soluble	-	NMR 98%	NA	- -	mp: >300°	63rd/N	
1437	**DL-Alanine** DL-Alanine DL-Aminopropanoic acid; (S)-2-Aminopropanoic acid; DL-2-Aminopropanoic acid;DL-2-Aminopropionic acid	3818 17.024 302-72-7	C3 H7 N O2 89.09	White crystalline powder; odourless	Solublein water Slightly soluble	-	MS 98%	NA	- -	mp: 198°	63rd/N	
1438	**L-Arginine** L-Arginine L-2-Aminoguanidinovaleric acid, (S)-2-Amino-5-guanidinovaleric acid	3819 17.003 74-79-3	C6 H14 N4 O2 174.20	White crystals or crystalline powder; odourless	Soluble in water; Insoluble in ether Slightly soluble	-	MS 98%	NA	- -	mp: 222°; Sp rotation = +15 to +17° (20°, 6N HCl)	63rd/N	
1439	**L-Lysine** L-Lysine (S)2,6-Diaminocaproic acid; L-2,6-Diaminohexanoic acid; a,e-Diaminocaproic acid	3847 17.026 56-87-1	C6 H14 N2 O2 146.19	White crystals or crystalline powder; odourless	Soluble in water Slightly soluble	-	MS 97%	NA	- -	mp: 215°; Sp.rotation = +12.5 to +13.5° (23°, 6N HCl)	63rd/N	

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1440	**2-Hexyl-4-acetoxytetrahydrofuran** 4-Acetoxy-2-hexyl-tetrahydrofuran	2566 10039-39-1	C12 H22 O3 214.31	Colourless liquid; Sweet floral-fruity aroma	Slightly soluble in water Soluble	121-126° (1 mm Hg)	NMR 97%	5.0	1.465-1.475 0.952-0.961		63rd/N	
1441	**2-(3-Phenylpropyl)tetrahydrofuran** 2-(3-Phenylpropyl)tetrahydrofuran 2-Hydrocinnamyl tetrahydrofuran	2898 13.007 3208-40-0	C13 H18 O 190.28	Colourless to pale straw-yellow liquid; Sweet, fruity aroma	Very slightly soluble in water Soluble	105-107° (1 mm Hg)	NMR 98%	1.0	1.511-1.516 0.975-0.983		63rd/N	
1442	**Tetrahydrofurfuryl acetate** Tetrahydrofurfuryl acetate Furfuryl alcohol, tetrahydro-, acetate; 2-(Acetoxymethyl)oxolane; 2-(Acetoxymethyl)tetrahydrofuran	3055 13.166 637-64-9	C7 H12 O3 144.20	Colourless liquid; Honey, maple, bready aroma	Soluble in water, ether, chloroform Soluble	194-195° (753 mm Hg)	NMR 97%	4.0	1.435-1.440 1.058-1.064		63rd/N	
1443	**Tetrahydrofurfuryl alcohol** Tetrahydrofurfuryl alcohol 2-(Hydroxymethyl)tetrahydrofuran; Tetrahydro-2-furancarbinol; Tetrahydro-2-furanmethanol; Tetrahydro-2-furylmethanol	3056 13.020 97-99-4	C5 H10 O2 102.15	Clear colourless liquid; Mild, warm oily caramel aroma	Soluble in water, fats Soluble	178-179°	IR 99%	3.0	1.449-1.455 1.050-1.052		63rd/N	
1444	**Tetrahydrofurfuryl butyrate** Tetrahydrofurfuryl butyrate Butyric acid, tetrahydrofurfuryl ester	3057 13.048 2217-33-6	C9 H16 O3 172.23	Colourless liquid; Heavy sweet aroma reminiscent of apricot and pineapple	Insoluble in water Soluble	227°	NMR 97%	4.0	1.446-1.452 1.007-1.013		63rd/N	
1445	**Tetrahydrofurfuryl propionate** Tetrahydrofurfuryl propionate Furfuryl alcohol, tetrahydro-, propionate; Propionic acid, tetrahydrofurfuryl ester	3058 13.049 637-65-0	C8 H14 O3 158.20	Colourless liquid; Fruity, earthy, phenolic, medicinal aroma	Insoluble in water Soluble	207°	NMR 97%	4.0	1.435-1.441 1.037-1.043		63rd/N	
1446	**4-Hydroxy-2,5-dimethyl-3(2H)-furanone** 4-Hydroxy-2,5-dimethylfuran-3(2H)-one Furaneol; Strawberry furanone; 2,5-Dimethyl-3-hydroxy-4-oxo-4,5-dihydrofuran; 2,5-Dimethyl-4,5-dihydrofuran-3-ol-4-one	3174 13.010 3658-77-3	C6 H8 O3 128.13	Colourless to white solid; Fruity caramel or burnt pineapple aroma	Soluble in oil; Insoluble in water Soluble	-	IR 98%	3.0	- -	mp: 78-80°	63rd/N	
1447	**Tetrahydrofurfuryl cinnamate** Tetrahydrofurfuryl 3-phenylprop-2-enoate	3320 13.060 65505-25-1	C14 H16 O3 232.28	Colourless slightly viscous liquid; Sweet persistent balmy vinous aroma	Soluble in oils; Insoluble in water Soluble	>300°	NMR 95%	3.0	1.593-1.600 1.107-1.113		63rd/N	

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1448	**2-Methyltetrahydrofuran-3-one** 4,5-Dihydro-2-methylfuran-3(2H)-one Dihydro-2-methyl-3(2H)-furanone; 2-Methyl-2H-furan-3-one; 2-Methyl-3-ketotetrahydrofuran; 2-Methyl-3-oxotetrahydrofuran	3373 13.042 3188-00-9	C5 H8 O2 100.12	Colourless liquid; Wintergreen-like aroma	Slightly soluble in oils Soluble	139°	NMR 97%	1.0	1.534-1.537 1.180-1.185		63rd/N	
1449	**2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone** 2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone 2-Ethyl-5-methyl-4,5-dihydrofuran-3-ol-4-one; 2-Methyl-4-hydroxy-5-ethylfuran-3-one; 4-hydroxy-2-methyl-5-ethyl-2,3-dihydrofur-3-one; Homofuraneol	3623 13.084 27538-09-6	C7 H10 O3 142.15	Yellow liquid; Sweet fruity caramel, butter scotch aroma	Soluble in water; Insoluble in fats Soluble	103° (15 mm Hg)	NMR 96%	4.0	1.509-1.514 1.133-1.143		63rd/N	
1450	**4-Hydroxy-5-methyl-3(2H)-furanone** 4-Hydroxy-5-methylfuran-3(2H)-one 4-Hydroxy-5-methyl-2,3-dihydrofuran-3-one; 5-Methyl-4-hydroxy-2,3-dihydrofuran-3-one; 5-Methyl-4-hydroxy-3(2H)-furanone	3635 13.085 19322-27-1	C5 H6 O3 114.10	Colourless to white solid; Fruity caramel or burnt pineapple aroma	Soluble in water; Slightly soluble in fats Soluble	-	NMR 97%	4.0	- -	mp: 126-133°	63rd/N	
1451	**2,5-Dimethyl-4-methoxy-3(2H)-furanone** 2,5-Dimethyl-4-methoxyfuran-3(2H)-one 2,5-Dimethyl-4-methoxy-2,3-dihydro-3-furanone; 2,5-Dimethyl-4-methyoxy-2H-furan-3-one; 4-Methoxy-2,5-dimethyl-3(2H)-furanone; Mesifuran	3664 13.089 4077-47-8	C7 H10 O3 142.15	Colourless liquid; Sweet, carmellic, burnt sugar, aroma	Soluble in fats; Insoluble in water Soluble	61-63° (0.3 mm Hg)	NMR 97%	3.0	1.475-1.481 1.091-1.097		63rd/N	
1452	**2,2-Dimethyl-5-(1-methylpropen-1-yl)tetrahydrofuran** 2,2-Dimethyl-5-(1-methylprop-1-enyl)tetrahydrofuran Ocimen quintoxide	3665 13.090 7416-35-5	C10 H18 O 154.25	Colourless liquid; Citrus aroma	Soluble in fats; Slightly soluble in water Soluble	65° (10 mm Hg)	NMR 98%	2.0	1.446-1.451 0.858-0.865		63rd/N	
1453	**2,5-Diethyltetrahydrofuran** 2,5-Diethyltetrahydrofuran	3743 13.095 41239-48-9	C8 H16 O 128.22	Colourless liquid; Powerful diffusive sweet-herbaceous carmellic aroma	Soluble in oils; Insoluble in water Soluble	116°	NMR 97%	1.0	1.401-1.407 0.827-0.833		63rd/N	

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1454	**cis,trans-2-Methyl-2-vinyl-5-(2-hydroxy-2-propyl)tetrahydrofuran** 5-(1-hydroxy-1-isopropyl)-2-methyl-2-vinyl tetrahydrofuran Linalool oxide; 2-Furanmethanol, 5ethenyltetrahydro-, a,a-, 5-trimethyl, cis-; Tetrahydro-alpha,alpha,5-trimethyl-5-vinylfurfuryl alcohol; cis-alpha,alpha,5-Trimethyl-5-vinyltetrahydrofurfuryl alcohol	3746 13.140 5989-33-3	C10 H18 O2 170.25	Colourless to slightly yellow liquid; Powerful sweet-woody penetrating aroma with floral undertones	Soluble in oils Soluble	188°	NMR 95%	3.0	1.451-1.456 0.932-0.942		63rd/N	
1455	**5-Isopropenyl-2-methyl-2-vinyltetrahydrofuran (cis and trans mixture)** 2-(1-Methylene-ethyl)-5-methyl-5-vinyltetrahydrofuran trans-5-Ethenyltetrahydro-a,a-5-trimethyl-2-furanmethanol; Tetrahydro-a,a-5-trimethyl-5-vinylfurfuryl alcohol-; (E)-Furanoid linalool oxide; trans-Furanoid linalool oxide	3759 13.097 13679-86-2	C10 H16 O 152.24	Colourless liquid; Pungent herbaceous, green, camphoraceous, piney aroma	Soluble in oils Soluble	58° (13 mm Hg)	NMR 97%	2.0	1.449-1.454 0.874-0.878		63rd/N	
1456	**4-Acetoxy-2,5-dimethyl-3(2H)furanone** 4-Acetoxy-2,5-dimethylfuran-3(2H)-one Furaneol acetate; 3(2H)-Furanone, 4-hydroxy-2,5-dimethyl-, acetate	3797 13.099 4166-20-5	C8 H10 O4 170.17	Colourless to pale yellow liquid; Faint caramel aroma	Slightly soluble in water Soluble	243°	NMR 85%	5.0	1.476-1.480 1.159-1.167	SC: 4-hydroxy-2,5-dimethyl-3(2H)-furanone	63rd/N	
1457	**(+/-)-2-(5-Methyl-5-vinyl-tetrahydrofuran-2-yl)propionaldehyde** 2-(5-Methyl-5-vinyl-tetrahydrofuran-2-yl)propionaldehyde Lilac aldehyde	4058 51685-39-3	C10 H16 O2 168.24	Clear colourless liquid; Floral aroma reminiscent of lilac	Insoluble in water Soluble	56-60° (1.2-1.4 mm Hg)	NMR 90% (sum of +/- isomers)	5.0	1.450-1.459 0.951-0.961 (20°)	SC: 6-hydroxy-2,6-dimethyl-2,7-octadienal	63rd/N	
1458	**Ethyl 4-phenylbutyrate** Ethyl 4-phenylbutyrate Butyric acid, 4-phenyl- ethyl ester; Ethyl 4-phenylbutanoate	2453 09.728 10031-93-3	C12 H16 O2 192.26	Colourless slightly oily liquid; Fruity, floral aroma	Soluble in oils; Insoluble in water Soluble	141-144° (12 mm Hg)	NMR 97%	1.0	1.489-1.495 0.986-0.992		63rd/N	

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1459	**beta-Methylphenethyl alcohol** 2-Phenylpropan-1-ol 1-Hydroxy-2-phenylpropane; 2-Phenyl-1-propanol; 2-Phenylpropanol; 2-Phenylpropyl alcohol	2732 02.073 1123-85-9	C9 H12 O 136.19	Colourless liquid; Sweet floral lilac, hyacinth type aroma	Soluble in oils; Slightly soluble in water Soluble	219°	NMR 98%	1.0	1.523-1.530 0.971-0.978		63rd/N	
1460	**2-Methyl-4-phenyl-2-butyl acetate** 1,1-Dimethyl-3-phenylpropyl acetate 2-Butanol, 2-methyl-4-phenyl-, acetate; Dimethylphenethylcarbinol acetate; Dimethylphenethyl carbinyl acetate	2735 09.029 103-07-1	C13 H18 O2 206.29	Colourless liquid; Jasmine and hyacinth-like aroma with a slight rosey undertone	Soluble in oils; Insoluble in water Soluble	244°	NMR 97%	1.0	1.488-1.490 0.986-0.990 (15°)		63rd/N	
1461	**2-Methyl-4-phenyl-2-butyl isobutyrate** 1,1-Dimethyl-3-phenylpropyl 2-methylpropanoate Isobutyric acid, 1,1-dimethyl-3-phenylpropyl ester	2736 09.484 10031-71-7	C15 H22 O2 234.34	Colourless liquid; Peculiar fruity-juicy, tea-like and herbaceous, richly sweet aroma	Soluble in oils; Insoluble in water Soluble	250°	NMR 96%	1.0	1.475-1.485 0.949-0.959		63rd/N	
1462	**2-Methyl-4-phenylbutyraldehyde** 2-Methyl-4-phenylbutyraldehyde alpha-Methylbenzenebutanal; 2-Methyl-4-phenylbutanal	2737 05.046 40654-82-8	C11 H14 O 162.23	Colourless oily liquid; Earthy musty but sweet floral aroma	Soluble in oils; Insoluble in water Soluble	253°	NMR 95%	3.0	1.506-1.510 0.968-0975		63rd/N	
1463	**3-Methyl-2-phenylbutyraldehyde** 3-Methyl-2-phenylbutyraldehyde alpha-Isopropylphenylacetaldehyde; 3-Methyl-2-phenylbutanal	2738 05.097 2439-44-3	C11 H14 O 162.23	Colourless oily liquid; Green fruity aroma	Soluble in oils; Insoluble in water Soluble	238°	NMR 97%	3.0	1.495-1.501 0.972-0.982		63rd/N	
1464	**Methyl 4-Phenylbutyrate** Methyl 4-phenylbutyrate Butyric acid, 4-phenyl-, methyl ester; Methyl 4-Phenylbutanoate	2739 09.729 2046-17-5	C11 H14 O2 178.23	Colourless liquid; Powerful, sweet, fruity, honey, floral aroma	Soluble in oils; Slightly soluble in water Soluble	149-151° (10 mm Hg)	NMR 97%	1.0	1.483-1.489 0.996-1.002		63rd/N	
1465	**2-Methyl-3-(p-isopropylphenyl) propionaldehyde** 2-Methyl-3-(4-isopropylphenyl)propanal alpha-Methyl-p-isopropylcinnamaldehyde; 3-(4-Isopropylphenyl)-2-methylpropanal; Cyclamal; Cyclamen aldehyde	2743 05.045 103-95-7	C13 H18 O 190.29	Colourless to pale yellow liquid; Strong floral aroma	Soluble in most fixed oils; Insoluble in propylene glycol, glycerin, water Soluble	270°	IR 90%	5.0	1.503-1.508 0.946-0.952	SC: 2-Methyl-3-(p-isopropylphenyl) propionic acid, 3-Methyl-3-(p-isopropylphenyl) propionaldehyde	63rd/N	

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1466	**2-Methyl-3-tolylpropionaldehyde (mixed o-,m-, p-)** 2-Methyl-3-(2,3 or 4-methylphenyl)propanal 2-Methyl-3-(4-methylphenyl)propanal; 3-(4-Methylphenyl)2-methylpropanal; p,a-Dimethylhydrocinnamaldehyde	2748 05.134 41496-43-9	C11 H14 O 162.23	Colourless oily liquid; Intensly sweet, fruity balsamic aroma	Soluble in oils; Slightly soluble in water Soluble	232-249°	NMR 95%	5.0	1.519-1.525 0.991-0.997		63rd/N	
1467	**2-Phenylpropionaldehyde** 2-Phenylpropanal alpha-Formylethylbenzene; 2-Phenylpropanal; 2-Phenylpropanaldehyde; Cumene aldehyde	2886 05.038 93-53-8	C9 H10 O 134.18	Colourless to pale yellow liquid; Intense, green, floral aroma reminiscent of hyacinth	Soluble in most fixed oils; Slightly soluble in propylene glycol; Insoluble in glycerin Soluble	202-205°	IR 95%	5.0	1.515-1.520 0.998-1.006		63rd/N	
1468	**2-Phenylpropionaldehyde dimethyl acetal** 1,1-Dimethoxy-2-phenylpropane alpha-Methylphenacetaldehyde dimethyl acetal; 2-Phenylpropanal dimethyl acetal	2888 06.030 90-87-9	C11 H16 O2 180.25	Colourless to slightly yellow liquid; Strong, warm, spicy aroma reminiscent of walnut	Soluble in ether; Insoluble in water Soluble	240-241°	IR 95%	1.0	1.492-1.497 0.989-0.994		63rd/N	
1469	**2-Phenylpropyl butyrate** 2-Phenylpropyl butyrate beta-Methylphenethyl butyrate; alpha-Phenylpropyl alcohol butyric ester; 2-Phenylpropyl n-butyrate	2891 09.057 80866-83-7	C13 H18 O2 206.29	Colourless liquid; Sweet, fruity, rum, apricot aroma	Soluble in oils; Slightly soluble in water Soluble	268-272°	NMR 98%	2.0	1.485-1.491 0.988-0.994		63rd/N	
1470	**2-Phenylpropyl isobutyrate** 2-Phenylpropyl 2-methylpropanoate 2-Phenylpropylisobutyrate; Hydrocinnamyl isobutyrate	2892 09.485 65813-53-8	C13 H18 O2 206.29	Colourless liquid; Fruity floral aroma	Soluble in oils; Insoluble in water Soluble	258°	NMR 97%	2.0	1.482-1.488 0.971-0.977		63rd/N	
1471	**2-(p-Tolyl)propionaldehyde** 2-(4-Methylphenyl)propanal a,4-Dimethylbenzeneacetaldehyde; 2-(p-Tolyl)propanal; 2-(p-Methylphenyl)propanal; 2-(p-Methylphenyl)propionaldehyde	3078 05.043 99-72-9	C10 H12 O 148.21	Colourless oily liquid; Intense, sweet, refreshing aroma similar to peppermint	Soluble in oils; Insoluble in water Soluble	222-224°	NMR 95%	5.0	1.513-1.517 0.979-0.985		63rd/N	
1472	**5-Methyl-2-phenyl-2-hexenal** 5-Methyl-2-phenylhex-2-enal 2-Hexenal, 5-methyl-2-phenyl-; 2-Phenyl-5-methylhex-2-enal; Cocal	3199 05.099 21834-92-4	C13 H16 O 188.27	Colourless to slightly yellow liquid; Cocoa-like aroma	Soluble in oils; Insoluble in water Soluble	96-100° (0.7 mm Hg)	NMR 96%	10.0	1.531-1.536 0.970-0.976		63rd/N	

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1473	**4-Methyl-2-phenyl-2-pentenal** 4-Methyl-2-phenylpent-2-enal 2-Pentenal, 4-methyl-2-phenyl-; 2-Phenyl-4-methylpent-2-enal	3200 05.100 26643-91-4	C12 H14 O 174.24	Colourless to slightly yellow liquid; Cocoa-like aroma	Soluble in oils; Insoluble in water Soluble	96° (0.7 mm Hg)	NMR 95%	10.0	1.533-1.539 0.980-0.986		63rd/N	
1474	**2-Phenyl-2-butenal** 2-Phenylbut-2(trans)-enal alpha-Phenylcrotonaldehyde; 2-Phenyl-2-butenal; 2-Phenylcrotonaldehyde	3224 05.062 4411-89-6	C10 H10 O 146.19	Colourless to slightly yellow liquid; green, floral, woody	Soluble in oils; Insoluble in water Soluble	177° (15 mm Hg)	NMR 97%	5.0	1.558-1.564 1.031-1.037		63rd/N	
1475	**Ethyl 2-ethyl-3-phenylpropanoate** Ethyl 2-ethyl-3-phenylpropionate alpha-Ethylhydrocinnamic acid ethyl ester; Ethylbenzylbutanoate	3341 09.802 2983-36-0	C13 H18 O2 206.29	Colourless liquid; green, floral aroma	Soluble in oils; Insoluble in water Soluble	72° (0.09 mm Hg)	IR 99%	1.0	1.483-1.489 0.972-0.979		63rd/N	
1476	**2-Phenyl-4-pentenal** 2-Phenylpent-4-enal 4-Pentenal, 2-Phenyl	3519 05.115 24401-36-3	C11 H12 O 160.22	Straw-coloured liquid; Fruity floral aroma	Soluble in oils; Insoluble in water Soluble	95° (3 mm Hg)	NMR 99%	5.0	1.524-1.529 0.999-1.006		63rd/N	
1477	**2-Methyl-4-phenyl-2-butanol** 2-Methyl-4-phenylbutan-2-ol 1,1,Dimethyl-3-phenylpropanol; 2-(2-phenylethyl)-2-propanol; 2-Methyl-4-phenyl-2-butanol; Dimethylphenethylcarbinol	3629 02.108 103-05-9	C11 H16 O 164.25	Colourless liquid; Lily, rose sweetness aroma	Soluble in fats; Slightly soluble in water Soluble	144° (85 mm Hg)	NMR 97%	2.0	1.506-1.512 0.960-0.966		63rd/N	
1478	**2-Oxo-3-phenylpropionic acid** 2-Oxo-3-phenylpropionic acid 3-Phenyl-2-oxopropanoic acid; 3-Phenylpyruvic acid	3892 08.109 156-06-9	C9 H8 O3 164.16	White crystalline powder	Soluble in water Soluble	-	NMR 98%	NA	- -	mp: 158-160°	63rd/N	
1479	**Sodium 2-oxo-3-phenylpropionate** Sodium 2-oxo-3-phenylpropionate Sodium 3-phenylpyruvate	3892 114-76-1	C9 H7 O3 Na 188.14		- -	-	NMR [req.]	NA	- -		63rd/N, T	ID