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FAO JECFA Monographs 10

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS

Joint FAO/WHO Expert Committee on Food Additives

73rd Meeting 2010

World Health Organization

Food and Agriculture Organization of the United Nations

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73rd Meeting 2010

FOOD AND AGRICULTURE ORGANIZATION OF THE UNITED NATIONS
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SPECIAL NOTE

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Geneva, 8 – 17 June, 2010

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INTRODUCTION

This volume of FAO JECFA Monographs contains specifications of identity and purity prepared at the 73rd meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), held in Geneva on 8 - 17 June 2010. The specifications monographs are one of the outputs of JECFA's risk assessment of food additives, and should be read in conjunction with the safety evaluation, reference to which is made in the section at the head of each specifications monograph. Further information on the meeting discussions can be found in the summary report of the meeting (see Annex 1), and in the full report which will be published in the WHO Technical Report series. Toxicological monographs of the substances considered at the meeting will be published in the WHO Food Additive Series.

Specifications monographs prepared by JECFA up to the 65th meeting, other than specifications for flavouring agents, have been published in consolidated form in the Combined Compendium of Food Additive Specifications which is the first publication in the series FAO JECFA Monographs. This publication consist of four volumes, the first three of which contain the specifications monographs on the identity and purity of the food additives and the fourth volume contains the analytical methods, test procedures and laboratory solutions required and referenced in the specifications monographs. FAO maintains an on-line searchable database of all JECFA specifications monographs from the FAO JECFA Monographs, which is available at: http://www.fao.org/ag/agn/jecfa-additives/search.html . The specifications for flavourings evaluated by JECFA, and previously published in FAO Food and Nutrition Paper 52 and subsequent Addenda, are included in a database for flavourings (flavouring agent) specifications which has been updated and modernized. All specifications for flavourings that have been evaluated by JECFA since its 44th meeting, including the 73rd meeting, are available in the new format online searchable database at the JECFA website at FAO: http://www.fao.org/ag/agn/jecfa-flav/search.html. The databases have query pages and background information in English, French, Spanish, Arabic and Chinese. Information about analytical methods referred to in the specifications is available in the Combined Compendium of Food Additive Specifications (Volume 4), which can be accessed from the query pages.

An account of the purpose and function of specifications of identity and purity, the role of JECFA specifications in the Codex system, the link between specifications and methods of analysis, and the format of specifications, are set out in the Introduction to the Combined Compendium, which is available in shortened format online on the query page, which could be consulted for further information on the role of specifications in the risk assessment of additives.

Chemical and Technical Assessments (CTAs) for some of the food additives have been prepared as background documentation for the meeting. These documents are available online at: http://www.fao.org/ag/agn/agns/jecfa_archive_cta_en.asp .

Contact and Feedback

More information on the work of the Committee is available from the FAO homepage of JECFA at: http://www.fao.org/ag/agn/agns/jecfa_index_en.asp . Readers are invited to address comments and questions on this publication and other topics related to the work of JECFA to:

jecfa@fao.org

SPECIFICATIONS FOR CERTAIN FOOD ADDITIVES

New and revised specifications

New (N) or revised (R) specifications monographs were prepared for the following food additives and these are provided in this publication:

Activated carbon (R)
Cassia gum (R)
Indigotine (R)
Steviol glycosides (R)
Sucrose esters of fatty acids (R)
Sucrose monoesters of lauric, palmitic or stearic acid (N, T)
Titanium dioxide (R)

In the specifications monographs that have been assigned a tentative status (T), there is information on the outstanding information and a timeline by which this information should be submitted to the FAO JECFA Secretariat.

New and revised INS numbers assigned to food additives by the Codex Alimentarius Commission at its 33rd session in 2010, (ALINORM 10/33/12, Appendix IX) and a correction for the INS number for Stannous chloride to No. 512, have been introduced in the corresponding JECFA food additive specifications monographs in the on-line database, as appropriate, and these are not reproduced in this publication.

Minor editorial revisions and corrections to the limits and information relating to metals and arsenic as published in FAO JECFA Monographs 1 (2005, 2006), Combined Compendium of Food Additive Specifications, have been made to the following JECFA food additive specifications monographs in the on-line database and are not reproduced in this publication: Carotenes (Algae), Carotenes (Vegetable), Calcium silicate, Ferric ammonium citrate, Grape skin extract, Potassium carbonate, Trimagnesium phosphate and Trisodium phosphate. The corrected limits correspond to those agreed by the Committee and published in the reports of JECFA from the relevant meetings (57th, 59th and 63rd meetings of JECFA).

ACTIVATED CARBON

Prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010), superseding specifications prepared at the 37th JECFA (1990) and published in the Combined Compendium of Food Additive Specifications, FAO JECFA Monographs 1 (2005). No ADI was established at the 31st JECFA (1987).

SYNONYMS Activated charcoal, decolourizing carbon

DEFINITION A solid, porous, carbonaceous material prepared by carbonizing and activating organic substances. The raw materials, which include sawdust, peat, lignite, coal, cellulose residues, coconut shells, petroleum coke, etc., may be carbonized and activated at high temperature with or without the addition of inorganic salts in a stream of activating gases such as steam or carbon dioxide. Alternatively, carbonaceous matter may be treated with a chemical activating agent such as phosphoric acid or zinc chloride and the mixture carbonized at an elevated temperature, followed by removal of the chemical activating agent by water washing.

Chemical names Carbon

C.A.S. number 7440-44-0

Chemical formula C

Formula weight 12.01

DESCRIPTION Powder or granules, black, odourless

FUNCTIONAL USES Adsorbent, decolourizing agent

GENERAL SPECIFICATIONS Must conform to the latest edition of the JECFA General Specifications and Considerations for Enzyme Preparations Used in Food Processing.

CHARACTERISTICS

IDENTIFICATION

Solubility Adsorbent, decolourizing agent

Adsorption Place about 3 g of powdered sample in a glass-stoppered flask containing 10 ml of dilute hydrochloric acid (5%), boil for 30 s, and cool to room temperature. Add 100 ml of iodine TS, stopper, and shake vigorously for 30 sec. Filter through filter paper (Whatman No. 2 or equivalent), discarding the first portion of filtrate. Compare 50 ml of the filtrate with a reference solution prepared by diluting 10 ml of iodine to 50 ml with water, but not treated with carbon. The colour of the carbon treated iodine solution shall be lighter in colour than that of the reference solution, indicating the adsorptivity of the sample.

PURITY

Adsorption power	Not less than 90% and not more than 110% of the value stated on label. See description under TESTS
Loss on drying (Vol. 4)	Not more than 15% (120º, 4 h) (See Volume 4 under "GENERAL METHODS, Inorganic Components.")
Sulfide compounds	To 1.0 g of the sample in a conical flask add 5 ml of 1 N hydrochloric acid and 20 ml of water. Heat to boiling. The fumes released do not turn lead acetate paper brown. (Lead acetate paper is prepared by saturating filter paper with lead acetate TS and drying the paper at 100º).
Acid soluble substances	Not more than 3% To about 1 g of the sample, accurately weighed, add 25 ml of dilute nitric acid TS and boil for 5 min. Filter whilst hot through a sintered-glass filter (10) and wash with 10 ml of hot water. Evaporate the combined filtrate and washings to dryness on a water bath, add to the residue 1 ml of hydrochloric acid, evaporate to dryness again and dry the residue to constant weight at 103±2º.
Sulfated ash	Not more than 5% Heat a silica or platinum crucible to redness for 30 min, allow to cool in a desiccator and weigh. Accurately weigh about 1 g of sample in the crucible and add 2 ml of sulfuric acid TS. Heat at first on a water bath, then cautiously over a flame, then progressively to about 600º. Continue the incineration until all black particles have disappeared and allow the crucible to cool. Add a few drops of dilute sulfuric acid TS, heat and incinerate as before and allow to cool. Evaporate and incinerate carefully, allow to cool, weigh, and repeat the ignition for 15 min to constant weight.
Water extractable substances	Not more than 4% Transfer about 5 g of sample, accurately weighed, into a 250 ml flask provided with a reflux condenser and a Bunsen valve. Add 100 ml of water and several glass beads, and reflux for 1 h. Cool slightly, and filter through Whatman No 2 or equivalent filter paper, discarding the first 10 ml of filtrate. Cool the filtrate to room temperature, and pipet 25.0 ml into a tared dish. Evaporate the filtrate in the dish to incipient dryness on a hot plate never allowing the solution to boil. Dry for 1 h at 103±2º in a vacuum oven, cool and weigh. Calculate the percentage of water extractables in the filtrate, based on the sample weight and volume of sample taken for gravimetric measurement.
Alcohol soluble substances	Not more than 0.5% To 2.0 g of sample add 50 ml of ethanol (96 per cent) and boil under a reflux condenser for 10 min. Filter immediately, wash residue with 10 ml of warm ethanol and filter. Quantitatively transfer the combined filtrate into a tared beaker containing a few antibumping stones. Evaporate to dryness on a water bath and dry to a constant mass at 103±2º. The residue on evaporation weighs not more than 10 mg**.**
Alkali soluble coloured substances	To 0.25 g of sample add 10 ml of 2 N sodium hydroxide and boil for 1 min. Cool, filter and dilute the filtrate to 10 ml with water. Prepare a

reference solution by mixing 1.90 ml of solution A (1% hydrochloric acid) and 0.10 ml of a solution B (9.6 ml of ferric chloride TS + 0.2 ml of cobaltous chloride TS + 0.2 ml of cupric sulfate TS). The colour of sample solution shall not be more intense than that of the reference solution.

Cyanogen compounds — Mix 5 g of sample with 50 ml of water and 2 g of tartaric acid. Distil the mixture, collecting 25 ml of distillate below the surface of a mixture of 2 ml of sodium hydroxide TS and 10 ml of water contained in a small flask placed in an ice bath. Dilute the distillate to 50 ml with water, and mix. Add 12 drops of ferrous sulfate TS to 25 ml of the diluted distillate, heat almost to boiling, cool, and add 1 ml of hydrochloric acid. No blue colour is produced.

Higher aromatic hydrocarbons — Extract 5 g of the sample with about 45 ml of cyclohexane in a continuous extraction apparatus for 2 h. Collect the extract and dilute to 50 ml with cyclohexane. Examine under ultraviolet light at 365 nm. The colour or fluorescence of the solution is not more intense than that of a 83 ng/ml solution of quinine prepared in 0.01N sulfuric acid, examined under the same conditions.

Arsenic (Vol. 4) — Not more than 3 mg/kg
Accurately weigh about 4 g of the sample into a conical flask, add 80 ml of 2 N hydrochloric acid, extra pure, and boil gently under reflux for 1 h, filter and wash the filter with 2 N hydrochloric acid. Cool and quantitatively transfer the filtrate into 100 ml volumetric flask and make up to volume with the same acid. Determine arsenic using atomic absorption hydride generation technique.

Lead (Vol. 4) — Not more than 5 mg/kg
Determine using an AAS/ICP-AES technique appropriate to the specified level using the solution prepared under arsenic.

Zinc (Vol.4) — Not more than 25 mg/kg
Determine using an AAS/ICP-AES technique appropriate to the specified level using the solution prepared under arsenic.

TESTS

PURITY TESTS

Adsorption power — To about 0.3 g of dried sample, accurately weighed, in a 100 ml ground-glass-stoppered conical flask, add 25.0 ml of a freshly prepared solution of 0.5 g of phenazone in 50 ml of water. Shake thoroughly for 15 min. Filter and reject the first 5 ml of filtrate. Pipette 10.0 ml of the filtrate into a conical flask, add 1.0 g of potassium bromide and 20 ml of dilute hydrochloric acid TS. Using 0.1 ml of ethoxychrysoidine solution as indicator, titrate with 0.1 N potassium bromate until the colour changes from reddish-pink to yellowish-pink. Titrate slowly (1 drop every 15 sec) towards the end of the titration. Carry out a blank titration using 10.0 ml of the phenazone solution.

Calculate adsorption power from:

$$[235.3 (a - b)]/[d \times m]$$

where

a is the volume (ml) of 0.1 N potassium bromate consumed by the blank;

b is the volume (ml) of 0.1 N potassium bromate consumed by the test solution;

m is the mass (g) of dried sample; and

d is the value stated on the label.

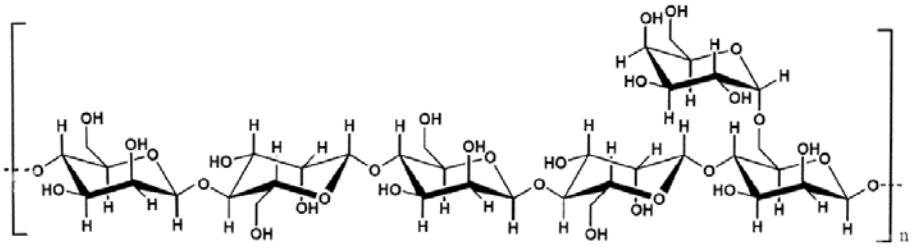
CASSIA GUM

Prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010), superseding tentative specifications prepared at the 71st JECFA (2009) and published in FAO JECFA Monographs 7 (2009). An ADI "not specified" was established at the 71st JECFA (2009).

SYNONYMS INS 427

DEFINITION Primarily the ground purified endosperm of the seeds of *Cassia tora* and *Cassia obtusifolia*, (Fam. *Leguminsae*) containing less than 0.05% of Cassia occidentalis. It consists mainly of high molecular weight (approximately 200,000-300,000) polysaccharides composed of galactomannans; the mannose: galactose ratio is about 5:1. The structural formula for cassia gum galactomannan is given below. The seeds are dehusked and degermed by thermal mechanical treatment followed by milling and screening of the endosperm. The ground endosperm is further purified by extraction with isopropanol.

Structural formula



Assay Not less than 75% of galactomannan

DESCRIPTION Pale yellow to off-white, odourless free-flowing powder

FUNCTIONAL USES Thickener, emulsifiier, foam stabilizer, moisture retention agent and texturizing agent.

CHARACTERISTICS

IDENTIFICATION

Solubility
Insoluble in ethanol
Disperses well in cold water forming colloidal solutions.

Gel formation with borate
Add sufficient amounts of sodium borate TS to an aqueous dispersion of the sample sufficient to raise the pH to above 9; a gel is formed.

Gel formation with xanthan gum
Passes test
See description under tests

Gum constituents (Vol. 4)
Proceed as directed under Gum Constituents Identification (Vol. 4) using 100 mg of sample instead of 200 mg and 1-10 µl of the hydrolysate instead of 1-5 µl. Use galactose and mannose as reference standards. These constituents should be present.

Viscosity	Less than 500 mPas (25º, 2h) (1% solution) See description under TESTS
pH (Vol. 4)	5.5-8.0 (1%)
PURITY	
Loss on drying (Vol. 4)	Not more than 12% (105º , 5 h)
Total ash (Vol. 4)	Not more than 1.2%
Acid-insoluble matter (Vol. 4)	Not more than 2.0%
Protein (Vol. 4)	Not more than 7.0% Proceed as directed under Nitrogen Determination (Kjeldahl Method; Vol. 4). The percent of nitrogen in the sample multiplied by 6.25 gives the percent of protein in the sample.
Crude fat	Not more than 1% See description under TESTS
Starch	To a 1 in 10 dispersion of the sample add a few drops of iodine TS; no blue colour is produced.
Anthraquinones	Not more than 0.5 mg/kg See description under TESTS
Residual solvents	Isopropanol: Not more than 1.0% See description under TESTS
Lead (Vol. 4)	Not more than 1 mg/kg Determine using an AAS/ICP-AES 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 Volume 4 (under "General Methods, Metallic Impurities").
Microbiological criteria (Vol. 4)	Total plate count: Not more than 5,000 cfu/g Yeast and mould: Not more than 100 cfu/g *E. coli*: Negative in 1 g *Salmonella*: Negative in 25 g

TESTS

IDENTIFICATION TESTS

Gel formation with xanthan gum	Weigh 1.5 g of the sample and 1.5 g of xanthan gum and blend them. Add this blend with (rapid stirring) into 300 ml water at 80º in a 400 ml beaker. Stir until the mixture is dissolved and continue stirring for an extra 30 min after dissolution (maintain the temperature above 60º during the stirring process). Discontinue stirring and allow the mixture to cool at room temperature for at least 2 h.

A firm, viscoelastic gel forms after the temperature drops below 40º, but no such gel forms in a 1% control solution of cassia gum or xanthan gum alone prepared in a similar manner.

Viscosity

Weigh 5 g of the sample in a plastic dish and 495 g of distilled water at 20º in a 1000 ml beaker. Add a magnetic bar and place the beaker on the agitation plate. Adjust the speed of agitation to 750 rpm. Introduce quickly the 5 g of sample in the water and cover the beaker with a watch glass. Keep the temperature at 90º for 15 min. Cool the solution at 25º (the cooling must be ±1.5º) in a water bath and measure the viscosity after 2 h at 25º using a RVT Brookfield Spindle 1, speed 20 rpm. Repeat the procedure with a sample of 5 g of carob (locust) bean gum.

(Note: The viscosity of the cassia gum (150 - 500 mPas) must be less than 50% that of carob bean gum (2000 - 3500 mPas))

PURITY TESTS

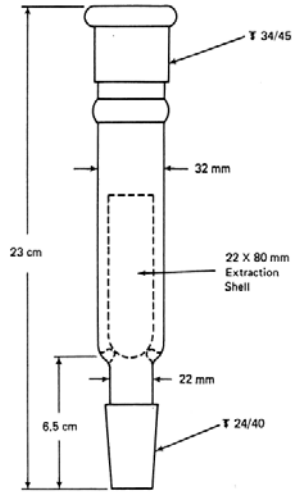
Crude fat

Apparatus

The apparatus consisting of a Butt-type extractor, as shown below, having a standard-taper 34/45 female joint at the upper end, to which is attached a Friedrichs- or Hopkins-type condenser, and a 24/40 male joint at the lower end, to which is attached a 125-ml Erlenmeyer flask.

Procedure

Transfer about 10 g of the sample, previously ground to 20-mesh or finer and accurately weighed, to a 15-cm filter paper, roll the paper tightly around the sample, and place it in a suitable extraction shell. Plug the top of the shell with cotton previously extracted with hexane, and place the shell in the extractor. Attach the extractor to a dry 125-ml Erlenmeyer flask containing about 50 ml of hexane and to a water-cooled condenser, apply heat to the flask to produce 150 to 200 drops of condensed solvent per min, and extract for 16 h. Disconnect the flask, and filter the extract to remove any insoluble residue. Rinse the flask and filter with a few ml of hexane, combine the washings and filtrate in a tared flask, and evaporate on a steam bath until no odor of solvent remains. Dry in a vacuum for 1 h at 100°, cool in a desiccator, and weigh.



Butt-Type Extractor for fat determination.

NOTE: The method for crude fat is referenced from the Food Chemicals Codex, 6th Edition, 2008, p. 1163.
Reprinted with permission from the US Pharmacopeia, 12601 Twinbrook Parkway, Rockville, MD USA 20852.

Anthraquinones

Principle

The antraquinones are extracted with acetonitrile and determined by High Performance Liquid Chromatography (Vol. 4) using the conditions below.
NOTE: Samples and standards should be protected from light.

Standards

Emodin (EMO), Aloe-emodin (AEM), Physcion (PHY) or 1,8-dihydroxy-3-methoxy-6-methyl-anthraquinone, Rhein (RHE) and Chrysophanic acid (CHR).
Internal standard: Danthrone (DAN) or 1,8-dihydroxy anthroquinone.

Use HPLC grade methanol for the solutions.

Stock standard solutions (100 mg/l): For each of the specific anthraquinone standards and for the internal standard: accurately weigh about 1 mg (±0.01 mg) of the standard. Transfer to 10 ml volumetric flasks with about 5 ml of methanol, sonicate for 15 min and dilute to volume with methanol.
Store these solutions in amber coloured bottles at 4° (the solutions are stable for 2 weeks under these conditions).

Mixed standard solution (10 mg/l):
Pipette 1 ml of each of the specific anthraquinone stock standard solutions into a 10 ml volumetric flask and dilute to volume with methanol.

Working standard solutions: To each of five 10 ml volumetric flask pipette 5, 2, 1, 0.5 and 0 ml respectively of the Mixed standard solution, pipette 1 ml of the Internal standard stock solution to each flask, mix and dilute to volume with methanol.

Sample preparation

Accurately weigh about 0.40 g of the sample into a 50 ml round-bottom flask. Add 20 ml trifluoroacetic acid and reflux at 70º for 4 hours. Cool the sample to ambient temperature and evaporate to dryness using a rotary evaporator. Add 3 ml of acetonitrile/$NaHCO_3$ (0.2%) (60:40 v/v) and sonicate for 30 min. Transfer the solution in a centrifuge tube and run it at 5000 rpm for 30 min. Filter the supernatant solution through an Extrulet column (Merck, NT1 or equivalent) previously neutralized with a pH 9.0 buffer. Pipette 900 µl of this filtered sample solution into a 2.5 ml volume vial and add 100 µl of the Internal standard stock solution and mix thoroughly.

Chromatographic conditions
Column: Hypersil C18 (250 mm x 4.6 mm ID, 5 µm) or equivalent
Mobile phase:
(A): 0.1% trifluoroacetic acid in water
(B): Acetonitrile (HPLC grade)
Injection volume: 50 µl
Run Time: 60 min
Gradient:

Min	% (A)	% (B)
0	86	14
10	86	14
15	80	20
25	80	20
55	20	80
60	0	100

Flow rate: 1 ml/min
Detector: Photodiode Array Detector. Quantification is performed at 435 nm

Standard curves
Inject 50 µl of each working standard solution and internal standard solution. Construct the standard curves by plotting the ratios of the peak areas of each of the specific anthraquinone / internal standard against the concentrations of each working standard solution (mg/l).

Procedure
Inject 50 µl of the Sample solution and the internal standard solution. Calculate the ratios of the peak areas of each specific anthraquinone / internal standard, and obtain the concentration (C) of each specific anthraquinone from the standard curves.

Calculate the percentage of each specific anthraquinone from:

$$\text{Anthraquinone (mg/kg)} = C \times 3 \times 1000 / (100 \times 0.9 \times W)$$

where
C is the concentration of specific anthraquinone (mg/l); and
W is weight of sample (g).

METHOD OF ASSAY The difference between 100 and the sum of the percent Loss on Drying, Total Ash, Acid-Insoluble Matter, Protein and Crude Fat represents the percent *Galactomannans*.

INDIGOTINE

Prepared at the 73rd JECFA (2010) and published in FAO Monographs 10 (2010), superseding specifications prepared at the 28th JECFA (1984) and published in the Combined Compendium of Food Additive Specifications, FAO JECFA Monographs 1 (2005). An ADI of 0 - 5 mg/kg bw was established at the 18th JECFA (1974).

SYNONYMS CI Food Blue 1, FD&C Blue No. 2, Indigo Carmine, CI (1975) No. 73015, INS No. 132

DEFINITION Consists essentially of a mixture of disodium 3,3' -dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate (principal component) and disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,7'-disulfonate (isomer) and subsidiary colouring matters together with sodium chloride and/or sodium sulfate as the principal uncoloured components.

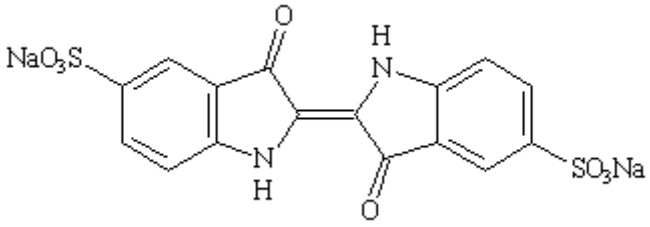
May be converted to the corresponding aluminium lake in which case only the *General Specifications for Aluminium Lakes of Colouring Matters* apply.

Chemical names Disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate (principal component)

C.A.S. number 860-22-0 (principal component)

Chemical formula $C_{16}H_8N_2Na_2O_8S_2$ (principal component)

Structural formula



Principal component

Formula weight 466.36 (principal component)

Assay Not less than 85% total colouring matters.
Not more than 18% of disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,7'-disulfonate.

DESCRIPTION Blue powder or granules

FUNCTIONAL USES Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)	Soluble in water; sparingly soluble in ethanol
Identification of colouring matters (Vol. 4)	Passes test

PURITY

Loss on drying (Vol. 4)	Not more than 15% at 135° together with chloride and sulfate calculated as sodium salts. (See Volume 4 under “SPECIFIC METHODS, Food Colours.”)
Water insoluble matter (Vol. 4)	Not more than 0.2%
Subsidiary colouring matters	Not more than 1% See description under TESTS
Organic compounds other than colouring matters (Vol. 4)	Not more than 0.5% of sum of isatin-5-sulfonic acid, 5-sulfoanthranilic acid and anthranilic acid. (See Volume 4 under “SPECIFIC METHODS, Food Colours.”) Proceed as directed under *Determination by High Performance Liquid Chromatography* using an elution gradient of 2 to 100% at 4% per min (linear) followed by elution at 100%.
Unsulfonated primary aromatic amines (Vol. 4)	Not more than 0.01% calculated as aniline (See Volume 4 under “SPECIFIC METHODS, Food Colours.”)
Ether extractable matter (Vol. 4)	Not more than 0.2% (See Volume 4 under “SPECIFIC METHODS, Food Colours, Method II.”) Use 2 g of sample for the test.
Lead (Vol. 4)	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 Volume 4 (under “General Methods, Inorganic Components, Metallic Impurities”).

TESTS

PURITY TESTS

Subsidiary colouring matters	Subsidiary colouring matters are determined by high performance liquid chromatography using the following conditions: Chromatographic system - HPLC system with a UV/VIS detector or a diode array detector, auto sampler or injector - Detector wavelength: 610 nm

- Column: C18 on silica gel (250 x 4.6 mm, 5 µm) ACE 5 C18 or equivalent
- Mobile phase: solvent A: 0.02 mol/l ammonium acetate and solvent B: acetonitrile: water (7:3 v/v)
- Gradient elution: A:B 92:8 v/v to A:B 70:30 v/v (0-15 min); to A:B 40:60 v/v (15-25 min); to A:B 92:8 v/v (25-30 min); A:B 92:8 v/v (30-35 min).
- Column temperature: 40°
- Flow rate: 1.0 ml/min
- Injection volume: 20 µl

The subsidiary colours are separated from the principal component and its isomer. The subsidiary colouring matter monosodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5 sulfonate elutes at approximately 21 min.

METHOD OF ASSAY **Total colouring matters content**

Proceed as directed under *Total Content by Titration with Titanous Chloride* in Volume 4*,* using the following (See "SPECIFIC METHODS, Food Colours"):
Weight of sample: 1.0-1.1 g
Buffer: 15 g sodium hydrogen tartrate
Weight (D) of colouring matters equivalent to
1.00 ml of 0.1 N $TiCl_3$: 23.32 mg.

Disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate,disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]- 5,7'-disulfonate (5,7' isomer) and subsidiary colouring matters by HPLC

The isomers get separated under the HPLC conditions detailed under the separation of subsidiary colouring matters, and the amounts present can be quantified using an external standard calibration.

Reagents
- Acetonitrile, HPLC grade
- Ammonium acetate, HPLC grade
- Reference standards of disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate and disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]- 5,7'-disulfonate

Standard stock solutions (1000 µg/ml): Weigh accurately 0.10 g (±0.1 mg) of each reference standard and transfer to a 100 ml volumetric flask and bring to volume with water.

Standard solutions: Prepare five solutions from the standard stock solutions in the concentration range of 1 to 20 µg/ml.

Sample solution: Weigh accurately 0.10 g (±0.1 mg) (w_2) of the sample and transfer to a 100 ml volumetric flask (v) and bring to volume with water (sample solution S_A).
Transfer 1.00 ml (v_{s1}) and 5.00 ml (v_{s5}) of the solution S_A to two 50 ml volumetric flasks (v_S), respectively, and bring to volume with water (sample solutions S_1 and S_5).

Procedure

Inject the five standard solutions for each isomer using the conditions detailed under TESTS (Subsidiary colouring matters by HPLC) and integrate peak areas at 6.5 min for the 5,5’ isomer (disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate) and 10.8 min for the 5,7’ isomer (disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]- 5,7'-disulfonate). Construct standard curve for each compound (Area vs. standard concentration, µg/ml).
Inject sample solutions S_A, S_1 and S_5. The peak area of the 5,7’ isomer for the sample solution should be in the linear range of the calibration graph, otherwise increase the volume v_{s5}. Sample solutions S_1, S_5 and S_A are to quantify disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,5'-disulfonate, disodium 3,3'-dioxo-[delta$^{2,2'}$-biindoline]-5,7'-disulfonate (5,7’ isomer) and subsidiary colouring matters, respectively.

Calculations
Calculate the concentrations (C, % (w/w)) of the two isomers and subsidiary colouring matters in the sample using the standard curves and the following formulas:

$$C_{5.5'\,\text{isomer}\,\%\,(w/w)} = \left(\frac{A_{5,5} - b_{5,5'}}{m_{5,5'}} \right) \times 10^{-6} \times \frac{v_S}{v_{s1}} \times v \times \frac{100}{w_S}$$

$$C_{5.7'\,\text{isomer}\,\%\,(w/w)} = \left(\frac{A_{5,7} - b_{5,7'}}{m_{5,7'}} \right) \times 10^{-6} \times \frac{v_S}{v_{s5}} \times v \times \frac{100}{w_S}$$

$$C_{\text{Subsidiary colouring matters}\,\%\,(w/w)} = \left(\frac{A_{sum} - b_{5,5'}}{m_{5,5'}} \right) \times 10^{-6} \times v \times \frac{100}{w_S}$$

where
$A_{5,5'}$ is the area of the peak of the 5,5’ isomer in the sample chromatogram (area units);
$A_{5,7'}$ is the area of the peak of the 5,7’ isomer in the sample chromatogram (area units);
A_{sum} is the sum of the areas of the peaks in the chromatogram (610 nm), except for the two isomers;
$b_{5,5'}$ and $b_{5,7'}$ are the linear coefficients of the calibration graphs for the 5,5’ isomer and 5,7’ isomer, respectively;
$m_{5,5'}$ and $m_{5,7'}$ are is the slope of the calibration graph (area units ml/µg) for the 5,5’ isomer and 5,7’ isomer, respectively;
w_s is the sample weight (g);
v is the volume of the sample solution s_A (ml);
v_{s1} is the volume of the sample solution s_1 (ml); and
v_{s5} is the volume of the sample solution s_5 (ml).

STEVIOL GLYCOSIDES

Prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010), superseding specifications prepared at the 69th JECFA (2008) and published in FAO JECFA Monographs 5 (2008). An ADI of 0 - 4 mg/kg bw (expressed as steviol) was established at the 69th JECFA (2008).

SYNONYMS INS no. 960

DEFINITION The product is obtained from the leaves of *Stevia rebaudiana* Bertoni. The leaves are extracted with hot water and the aqueous extract is passed through an adsorption resin to trap and concentrate the component steviol glycosides. The resin is washed with a solvent alcohol to release the glycosides and the product is recrystallized from methanol or aqueous ethanol. Ion exchange resins may be used in the purification process. The final product may be spray-dried.

Stevioside and rebaudioside A are the component glycosides of principal interest for their sweetening property. Associated glycosides include rebaudioside B, rebaudioside C, rebaudioside D, rebaudioside F, dulcoside A, rubusoside and steviolbioside which are generally present in preparations of steviol glycosides at levels lower than stevioside or rebaudioside A.

Chemical name

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

C.A.S. number

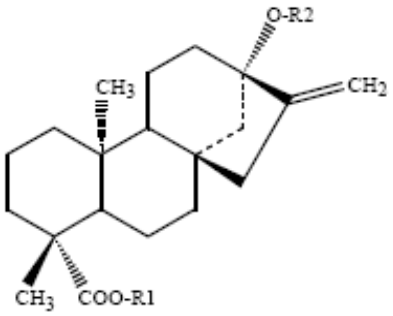
Stevioside: 57817-89-7
Rebaudioside A: 58543-16-1

Chemical formula

Stevioside: $C_{38}H_{60}O_{18}$
Rebaudioside A: $C_{44}H_{70}O_{23}$

Structural Formula

The nine named 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 B	H	*β*-Glc-*β*-Glc(2→1) | *β*-Glc(3→1)
Rebaudioside C	*β*-Glc	*β*-Glc-*α*-Rha(2→1) | *β*-Glc(3→1)
Rebaudioside D	*β*-Glc-*β*-Glc(2→1)	*β*-Glc-*β*-Glc(2→1) | *β*-Glc(3→1)
Rebaudioside F	*β*-Glc	*β*-Glc-*β*-Xyl(2→1) | *β*-Glc(3→1)
Dulcoside A	*β*-Glc	*β*-Glc-*α*-Rha(2→1)
Rubusoside	*β*-Glc	*β*-Glc
Steviolbioside	H	*β*-Glc-*β*-Glc(2→1)

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

Formula weight

Stevioside: 804.88
Rebaudioside A: 967.03

Assay

Not less than 95% of the total of the nine named steviol glycosides on the dried basis.

DESCRIPTION

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

FUNCTIONAL USES

Sweetener

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)

Freely soluble in water

Stevioside and rebaudioside A

The main peak in the chromatogram obtained by following the procedure in Method of Assay corresponds to either stevioside or

rebaudioside A.

pH (Vol. 4) — Between 4.5 and 7.0 (1 in 100 solution)

PURITY

Total ash (Vol. 4) — Not more than 1%

Loss on drying (Vol. 4) — Not more than 6% (105°, 2h)

Residual solvents (Vol. 4) — Not more than 200 mg/kg methanol and not more than 5000 mg/kg ethanol (Method I in Vol. 4, General Methods, Organic Components, Residual Solvents)

Arsenic (Vol. 4) — Not more than 1 mg/kg
Determine by the atomic absorption hydride technique (Use Method II to prepare the test (sample) solution)

Lead (Vol. 4) — Not more than 1 mg/kg
Determine using an AAS/ICP-AES 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 Vol. 4 (under “General Methods, Metallic Impurities”).

METHOD OF ASSAY — Determine the percentages of the individual steviol glycosides by HPLC (Vol. 4) under the following conditions.

Reagents
Acetonitrile: more than 95% transmittance at 210 nm.

Standards
Stevioside: more than 99.0% purity on the dried basis.
Rebaudioside A: more than 99.0% purity on the dried basis.
Mixture of nine steviol glycosides standard solution: Containing stevioside, rebaudioside A, rebaudioside B, rebaudioside C, rebaudioside D, rebaudioside F, dulcoside A, rubusoside and steviolbioside. This solution is diluted with water-acetonitrile (7:3) accordingly and is used for the confirmation of retention times. Standards are available from Wako Pure Chemical Industries, Ltd. Japan and ChromaDex, USA.

Standard solution
Accurately weigh 50 mg of stevioside and rebaudioside A standard into each of two 50-ml volumetric flasks. Dissolve and make up to volume with water-acetonitrile (7:3).

Sample solution
Accurately weigh 50-100 mg of sample into a 50-ml volumetric flask. Dissolve and make up to volume with water-acetonitrile (7:3).

Procedure
Inject 5 µl of sample solution under the following conditions.
Column: Capcell pak C_{18} MG II (Shiseido Co.Ltd) or Luna 5µ C18(2) 100A (Phenomenex) or equivalent (length: 250 mm; inner diameter:

4.6 mm, particle size: 5µm)
Mobile phase: 32:68 mixture of acetonitrile and 10 mmol/L sodium phosphate buffer (pH 2.6)
Flow rate: 1.0 ml/min
Detector: UV at 210 nm
Column temperature: 40°
Record the chromatogram for about 30 min.

Identification of the peaks and Calculation
Identify the peaks from the sample solution by comparing the retention time with the peaks from the mixture of nine steviol glycosides standard solution (see under figure). Measure the peak areas for the nine steviol glycosides from the sample solution. Measure the peak area for stevioside and rebaudioside A from their standard solutions.
Calculate the percentage of each of the eight steviol glycosides except rebaudioside A in the sample from the formula:

$$\%X = [W_S/W] \times [f_X A_X/A_S] \times 100$$

Calculate the percentage of rebaudioside A in the sample from the formula:

$$\%\textit{Rebaudioside A} = [W_R/W] \times [A_X/A_R] \times 100$$

where
X is each steviol glycoside;
W_S is the amount (mg) calculated on the dried basis of stevioside in the standard solution;
W_R is the amount (mg) calculated on the dried basis of rebaudioside A in the standard solution;
W is the amount (mg) calculated on the dried basis of sample in the sample solution;
A_S is the peak area for stevioside from the standard solution;
A_R is the peak area for rebaudioside from the standard solution;
A_X is the peak area of *X* for the sample solution; and
f_X is the ratio of the formula weight of *X* to the formula weight of stevioside: 1.00 (stevioside), 1.20 (rebaudioside A), 1.00 (rebaudioside B), 1.18 (rebaudioside C), 1.40 (rebaudioside D), 1.16 (rebaudioside F), 0.98 (dulcoside A), 0.80 (rubusoside) and 0.80 (steviolbioside).

Calculate the percentage of total steviol glycosides (sum the nine percentages).

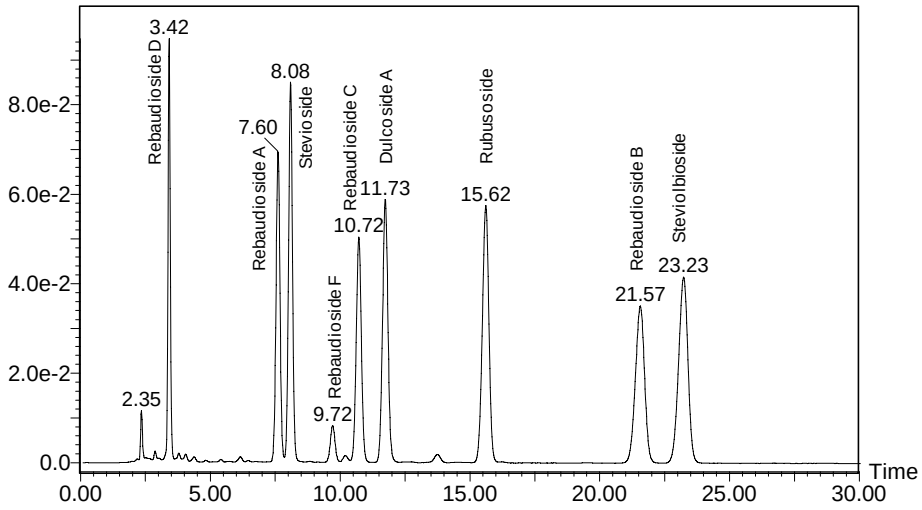


Figure. Chromatogram of mixture of nine steviol glycosides standard solution

Column: Capcell pak C_{18} MG II

Concentration: 0.5 mg/ml each except rebaudioside F (about 0.1 mg/ml)

SUCROSE ESTERS OF FATTY ACIDS

Prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010), superseding specifications prepared at the 68th JECFA (2007) and published in FAO JECFA Monographs 4 (2007). An ADI of 0 - 30 mg/kg bw for this substance together with sucroglycerides, sucrose oligoesters type I and type II and sucrose monoesters of lauric, palmitic or stearic acid was established at the 73rd JECFA (2010).

SYNONYMS Sucrose fatty acid esters, INS No. 473

DEFINITION Mono-, di- and tri-esters of sucrose with food fatty acids, prepared from sucrose and methyl and ethyl esters of food fatty acids by esterification in the presence of a catalyst or by extraction from sucroglycerides. Only the following solvents may be used for the production: dimethylformamide, dimethyl sulfoxide, ethyl acetate, isopropanol, propylene glycol, isobutanol and methyl ethyl ketone.

Assay Not less than 80% of sucrose esters

DESCRIPTION White to greyish white or pale yellow powder, stiff gel or soft solid

FUNCTIONAL USES Emulsifier

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol.4) Sparingly soluble in water, soluble in ethanol

Fatty acids Add 1 ml of ethanol to 0.1 g of the sample, dissolve by warming, add 5 ml of dilute sulfuric acid TS, heat in a waterbath for 30 min and cool. A yellowish white solid or oil is formed, which has no odour of isobutyric acid, and which dissolves when 3 ml of diethyl ether are added. Use the aqueous layer separated from the diethyl ether in the Test for sugars.

Sugars To 2 ml of the aqueous layer separated from the diethyl ether in the test for fatty acids, carefully add 1 ml of anthrone TS down the inside of a test tube; the boundary surface of the two layers turns blue or green.

PURITY

Sulfated ash (Vol.4) Not more than 2%
Test 1 g of the sample (Method I)

Acid value (Vol.4) Not more than 6

Free sucrose Not more than 5%
See description under TESTS

Dimethylformamide	Not more than 1 mg/kg See description under TESTS
Dimethyl sulfoxide	Not more than 2 mg/kg See description under TESTS
Ethyl acetate, isopropanol and propylene glycol	Not more than 350 mg/kg, singly or in combination See description under TESTS
Isobutanol	Not more than 10 mg/kg See description under TESTS
Methanol	Not more than 10 mg/kg See description under TESTS
Methyl ethyl ketone	Not more than 10 mg/kg See description under TESTS
Lead (Vol.4)	Not more than 2 mg/kg Determine using an AAS/ICP-AES 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 Volume 4 (under “General Methods, Metallic Impurities”).

TESTS

PURITY TESTS

Free sucrose

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions
Prepare a stock solution containing 5.0 mg/ml of sucrose in *N,N*-dimethylformamide. Prepare a range of standard solutions containing 0.5, 1.25 and 2.5 mg/ml of sucrose by dilutions of the stock solution with *N,N*-dimethylformamide.

Internal standard solution
Weigh accurately 0.25 g of octacosane into a 50-ml volumetric flask, add 25 ml of tetrahydrofuran to dissolve the octacosane, and add tetrahydrofuran to the mark.

Chromatography conditions
Column: 100%-Dimethylpolysiloxane (30 m x 0.32 mm i.d. with 0.25 µm film)
Carrier gas: Helium
Flow rate: 1.5 ml/min
Detector: Flame-ionization detector (FID)
Temperatures:
- injection port: 280 °
- column: Hold for 1 min at 100°, then 100-300° at 12°/min, hold for 45 min at 300°
- detector: 320 °

The retention times of free sucrose and octacosane measured under the above conditions are approx. 18.8 and 19.3 min,

respectively.

Procedure

Weigh accurately 20-50 mg of the sample into a centrifugation tube, add 1 ml internal standard solution, 1 ml *N,N*-dimethylformamide, 0.4 ml of *N,O*-bis(trimethylsilyl)acetamide (BSA) and 0.2 ml trimethylchlorosilane (TMCS). After sealing the tube, shake and let stand for 5 min at room temperature. Inject 1 μl into the chromatograph.

Standard curve

Prepare silylated standard solutions following the above procedure using 1 ml each of the standard solutions in place of the sample and *N,N*-dimethylformamide . Draw a standard curve by plotting amount of sucrose (mg) in 1 ml of the standard solution (X-axis) vs. ratio of peak area of sucrose/internal standard (Y-axis).

Measure the peak areas for sucrose and internal standard. Calculate the ratio of their peak areas, and obtain the amount of sucrose from the standard curve.

Calculate the percentage of free sucrose from:

$$\% \text{ free sucrose} = \frac{\text{amount of sucrose determined (mg)}}{\text{weight of sample (mg)}} \times 100$$

Dimethylformamide

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions

Prepare a stock solution containing 1.00 mg/ml of dimethylformamide in tetrahydrofuran. Prepare a range of standard solutions containing 0.05, 0.1 and 0.2 μg/ml of dimethylformamide by diluting the stock solution with tetrahydrofuran.

Chromatography conditions

Column: Polyethylene glycol (30 m x 0.32 mm i.d. with a 0.5 μm film)
Carrier gas: Helium
Pressure: 150 kPa (constant pressure)
Detector: Nitrogen/phosphorus detector or thermionic specific detector)
Temperatures:
- injection port: 180°
- column: Hold for 2 min at 40°, then 40-160° at 20°/min, hold for 2 min at 160°
- detector: 325°

Injection method: Splitless injection of 1.0 μl with auto-injector, followed by start of purge after 1.0 min.
The retention time of dimethylformamide measured under the above conditions is approx. 6.4 min.

Procedure
Weigh accurately 2 g of sample into a 20-ml volumetric flask, add 10 ml of tetrahydrofuran to dissolve the sample, add tetrahydrofuran to the mark, and mix the solution well. Inject 1.0 μl of the sample solution into the chromatograph.

Standard curve
Prepare daily by injecting 1.0 μl of each of the standard solutions into the chromatograph.

Calculate the concentration of dimethylformamide in mg/kg (C_{DFA}) from:

$$C_{DFA} \text{ (mg/kg)} = C \times 20 / W$$

where
C is dimethylformamide concentration determined (μg/ml); and
W is weight of sample (g).

Note: The column must be reconditioned frequently. Overnight reconditioning (flow carrier gas in the reverse direction at 180° without the connection of the detector) is required after about every 15 samples.

Dimethyl sulfoxide

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions
Prepare a 0.25 mg/ml stock solution of dimethyl sulfoxide in tetrahydrofuran. Prepare a range of solutions containing 0.1, 0.2, 0.4 and 1.0 μg/ml of dimethyl sulfoxide by dilutions of the stock solution with tetrahydrofuran.

Chromatography conditions
Column: 10% PEG 20M and 3% KOH on Chromosorb W AW DMCS 60/80 mesh (2 m x 3 mm i.d.) or equivalent. Raise the oven temperature to 180° at a rate of 10°/min and let stabilize for 24 to 48 h with 30 to 40 ml/min of nitrogen for conditioning
Carrier gas: Nitrogen
Flow rate: 30 ml/min
Detector: Flame photometric detector (using 394 nm sulfur filter)
Temperatures
- injection port: 210°
- column: 160°
The retention time of dimethyl sulfoxide measured under the above conditions is approx. 3.4 min.

Procedure
Weigh accurately 5 g of the sample into a 25-ml volumetric flask, add 10 ml of tetrahydrofuran to dissolve the sample, add tetrahydrofuran to the mark, and mix the solution well. Inject 3 μl of the sample solution into the chromatograph.

Standard curve
Prepare daily by injecting 3 μl of each of the standard solutions into

the chromatograph.

Calculate the concentration of dimethyl sulfoxide in mg/kg (C_{DMSO}) from:

$$C_{DMSO} \text{ (mg/kg)} = C \times 25 / W$$

where
C is dimethyl sulfoxide concentration determined (μg/ml); and
W is weight of sample (g).

Propylene glycol

Determine by gas chromatography (Vol. 4) under the following conditions.

Internal standard solution
Prepare a 500 μg/ml solution of ethylene glycol in tetrahydrofuran.

Standard solutions
Prepare a range of standard solutions containing 1, 5, 10, 25 and 50 μg/ml of propylene glycol with 5 μg/ml of ethylene glycol in tetrahydrofuran.

Chromatography conditions
Column: Polydimethylsiloxane (30 m x 0.32 mm i.d. with 0.25 μm film)
Carrier gas: Helium
Flow rate: 1.5 ml/min (Constant flow)
Detector: FID
Temperatures:
- injection port: 230°
- column: Hold for 3 min at 40°, then 40-250° at 20°/min, hold for 5 min at 250°
- detector: 270°
The retention times of ethylene glycol and propylene glycol derivatives under the above conditions are approx. 7.6 min and 7.8 min, respectively.

Procedure
Weigh accurately 1 g of the sample into a 10-ml volumetric flask, and add 100 μl of the internal standard solution. Dissolve and make up to the volume with tetrahydrofuran. Take 0.5 ml of the sample solution in a centrifugation tube, and add 0.25 ml of 1,1,1,3,3,3-hexamethyldisilazane (HMDS) and 0.1 ml of trimethylchlorosilane (TMCS). After sealing the tube, shake it vigorously, let stand for 30 min at room temperature, then centrifuge. Inject 1.0 μl of this centrifugal supernatant into the chromatograph.

Standard curve
Prepare following the same procedure using 0.5 ml of the standard solutions in place of the sample solution.

Calculate the concentration of propylene glycol in mg/kg (C_{PG}) from:

C_{PG} (mg/kg) = C x 10 / W

where
C is polyethylene glycol concentration determined (μg/ml); and
W is weight of sample (g).

Methanol, isopropanol, isobutanol, ethyl acetate and methyl ethyl ketone

Determined by gas chromatography (vol.4) with a head space sampler under the following conditions.

Standard solutions
Prepare standard solution A containing 4000 mg/l each of methanol, isopropanol, isobutanol, ethyl acetate and methyl ethyl ketone by weighing accurately 0.2 g of each solvent into a 50-ml volumetric flask containing approx. 20 ml of water, then adding water to volume. By dilutions of this solution, prepare solutions containing 2000 mg/l (standard solution B) and 1000 mg/l (standard solution C).

Procedure:
Weigh accurately 1 g of the sample into each of four sample vials. To one vial add 5 μl of water, to the second, third and fourth, add, respectively, standard solutions A, B and C, and seal them quickly with a septum. (The concentrations of each solvent after adding 5 μl of standard solutions A, B and C to 1 g of the sample are equal to 20, 10 and 5 mg/kg of sample, respectively). Place the sample vials in a head space sampler and analyse using the following conditions:
Column: 100% Polydimethylsiloxane (30 m x 0.53 mm i.d. with 1.5 μm film)
Carrier gas: Nitrogen
Flow rate: 3.5 ml/min
Detector: FID
Temperatures
- injection port: 110°
- column: 40°
- detector: 110°
Head space sampler:
- sample heat insulating temperature: 80°
- sample heat insulating period: 40 min
- syringe temperature: 85°
- sample gas injection: 1.0 ml

Calculation
Plot the relationship between the added amounts against the peak area for each solvent using the analytical results. The relationship should be linear. Extrapolate and determine the x-intercept (w_i), and calculate the solvent concentrations (C_i) in the sample from:

C_i (mg/kg)= w_i / W

where
w_i is x-intercept of relationship line using the standard addition method (μg); and
W is weight of sample (g).

METHOD OF ASSAY

Determine by HPLC (Vol. 4) under the following conditions.

Procedure

Accurately weigh 250 mg of the sample into a 50-ml volumetric flask. Dilute to volume with tetrahydrofuran and mix. Filter through a 0.45 μm membrane filter. Inject 80 μl of the sample solution into the pre-stabilized chromatograph.

Chromatography conditions

Column: Styrene-divinylbenzene copolymer for gel permeation chromatography (TSK-GEL G1000HXL, G2000HXL, G3000HXL, G4000HXL (each 30 cm x 7.8 mm i.d., 5 μm) in series, Tosoh Co. or equivalent)
Mobile phase: HPLC-grade degassed tetrahydrofuran
Flow rate: 0.8 ml/min
Detector: Refractive index
Temperatures:
- Column: 40°
- Detector: 40°
Record the chromatogram for about 50 min.

Typical retention times under the above conditions are described in Table 1. The reference products are available from Mitsubishi Chemical Corporation (Tokyo, Japan) or Dai-ichi Kogyo Seiyaku Co. Ltd (Kyoto, Japan) to confirm the retention time.

Table 1. Typical retention time (min) of mono-, di- and tri-esters esterified with main fatty acids

Esterified fatty acid	Mono-esters	Di-esters	Tri-esters
Lauric acid	40.0	38.2	37.0
Palmitic acid	39.3	37.2	36.0
Stearic acid	39.0	37.0	35.7
Oleic acid	39.1	37.1	35.9

Calculate the percentage of sucrose ester content in the sample from:

$$\% \text{ sucrose ester} = 100\ A/T$$

where
A is the sum of peak areas for the three main components, the mono-, di- and tri-esters; and
T is the sum of all peak areas eluting within 30 min.

SUCROSE MONOESTERS OF LAURIC, PALMITIC OR STEARIC ACID
(TENTATIVE)

New tentative specifications prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010). A group ADI of 0 - 30 mg/kg bw for this substance together with sucrose esters of fatty acids, sucroglycerides and sucrose oligoesters type I and type II was established at the 73rd JECFA (2010).

Information is required on a test method to distinguish from sucrose esters of fatty acids.

Note: The tentative specifications will be withdrawn unless the requested information is received before the end of 2011.

DEFINITION

The product consists of sucrose monoesters of individual fatty acids, namely lauric, palmitic or stearic acid. They are manufactured by a transesterification reaction of sucrose and vinyl esters of lauric, palmitic or stearic acids in dimethyl sulfoxide. Impurities are removed by a series of evaporation and solvent extraction steps. Only the following solvents may be used for the production: dimethyl sulfoxide and isobutanol.

Assay

Total content of sucrose esters: not less than 85%
Content of monoesters: not less than 90% of total sucrose esters

DESCRIPTION

White to off white powder

FUNCTIONAL USES

Emulsifier

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol.4)

Soluble in water and in ethanol

Fatty acids

Add 1 ml of ethanol to 0.1 g of the sample, dissolve by warming, add 5 ml of dilute sulfuric acid TS, heat in a waterbath for 30 min and cool. A yellowish white solid or oil is formed, which has no odour of isobutyric acid, and which dissolves when 3 ml of diethyl ether are added. Use the aqueous layer separated from the diethyl ether in the Test for sugars.

Sugars

To 2 ml of the aqueous layer separated from the diethyl ether in the test for fatty acids, carefully add 1 ml of anthrone TS down the inside of a test tube; the boundary surface of the two layers turns blue or green.

PURITY

Sulfated ash (Vol.4)

Not more than 2%
Test 1 g of the sample (Method I)

Acid value (Vol.4)	Not more than 6
Free sucrose	Not more than 5% See description under TESTS
Dimethyl sulfoxide	Not more than 2 mg/kg See description under TESTS
Isobutanol	Not more than 10 mg/kg See description under TESTS
Vinyl laurate, vinyl palmitate and vinyl stearate	Not more than 10 mg/kg See description under TESTS
Acetaldehyde	Not more than 1 mg/kg See description under TESTS
Lead (Vol.4)	Not more than 2 mg/kg Determine using an AAS/ICP-AES 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 Volume 4 (under "General Methods, Metallic Impurities").

TESTS

PURITY TESTS

Free sucrose

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions

Prepare a stock solution containing 5.0 mg/ml of sucrose in *N,N*-dimethylformamide. Prepare a range of standard solutions containing 0.5, 1.25 and 2.5 mg/ml of sucrose by dilutions of the stock solution with *N,N*-dimethylformamide.

Internal standard solution

Weigh accurately 0.25 g of octacosane into a 50-ml volumetric flask, add 25 ml of tetrahydrofuran to dissolve the octacosane, and add tetrahydrofuran to the mark.

Chromatography conditions

Column: 100%-Dimethylpolysiloxane (30 m x 0.32 mm i.d. with 0.25 µm film)
Carrier gas: Helium
Flow rate: 1.5 ml/min
Detector: Flame-ionization detector (FID)
Temperatures:
- injection port: 280 °
- column: Hold for 1 min at 100°, then 100-300° at 12°/min, hold for 45 min at 300°
- detector: 320 °

The retention times of free sucrose and octacosane measured under the above conditions are approx. 18.8 and 19.3 min, respectively.

Procedure
Weigh accurately 20-50 mg of the sample into a centrifugation tube, add 1 ml internal standard solution, 1 ml *N,N*-dimethylformamide, 0.4 ml of *N,O*-bis(trimethylsilyl)acetamide (BSA) and 0.2 ml trimethylchlorosilane (TMCS). After sealing the tube, shake and let stand for 5 min at room temperature. Inject 1 μl into the chromatograph.

Standard curve
Prepare silylated standard solutions following the above procedure using 1 ml each of the standard solutions in place of the sample and *N,N*-dimethylformamide. Draw a standard curve by plotting amount of sucrose (mg) in 1 ml of the standard solution (X-axis) vs. ratio of peak area of sucrose/internal standard (Y-axis).

Measure the peak areas for sucrose and internal standard. Calculate the ratio of their peak areas, and obtain the amount of sucrose from the standard curve.

Calculate the percentage of free sucrose from:

$$\% \text{ free sucrose} = \frac{\text{amount of sucrose determined (mg)}}{\text{weight of sample (mg)}} \times 100$$

Dimethyl sulfoxide

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions
Prepare a 0.25 mg/ml stock solution of dimethyl sulfoxide in tetrahydrofuran. Prepare a range of solutions containing 0.1, 0.2, 0.4 and 1.0 μg/ml of dimethyl sulfoxide by dilutions of the stock solution with tetrahydrofuran.

Chromatography conditions
Column: 10% PEG 20M and 3% KOH on Chromosorb W AW DMCS 60/80 mesh (2 m x 3 mm i.d.) or equivalent.
Carrier gas: Nitrogen
Flow rate: 30 ml/min
Detector: Flame photometric detector (using 394 nm sulfur filter)
Temperatures
- injection port: 210°
- column: 160°
The retention time of dimethyl sulfoxide measured under the above conditions is approx. 3.4 min.
Note: Before using the column, raise the oven temperature to 180° at a rate of 10°/min and let stabilize for 24 to 48 h with 30 to 40 ml/min of nitrogen for the column conditioning.

Procedure
Weigh accurately 5 g of the sample into a 25-ml volumetric flask, add 10 ml of tetrahydrofuran to dissolve the sample, add tetrahydrofuran to the mark, and mix the solution well. Inject 3 μl of the sample solution into the chromatograph.

Standard curve
Prepare daily by injecting 3 μl of each of the standard solutions into the chromatograph.

Calculate the concentration of dimethyl sulfoxide in mg/kg (C_{DMSO}) from:

$$C_{DMSO} \text{ (mg/kg)} = C \times 25 / W$$

where
C is dimethyl sulfoxide concentration determined (μg/ml); and
W is weight of sample (g).

Isobutanol,

Determined by gas chromatography (Vol.4) with a head space sampler under the following conditions.

Standard solutions
Prepare standard solution A containing 4000 mg/l of isobutanol by weighing accurately 0.2 g of isobutanolinto a 50-ml volumetric flask containing approx. 20 ml of water, then adding water to volume. By dilutions of this solution, prepare solutions containing 2000 mg/l (standard solution B) and 1000 mg/l (standard solution C).

Procedure
Weigh accurately 1 g of the sample into each of four sample vials. To one vial add 5 μl of water, to the second, third and fourth, add, respectively, standard solutions A, B and C, and seal them quickly with a septum. (The concentrations of each solvent after adding 5 μl of standard solutions A, B and C to 1 g of the sample are equal to 20, 10 and 5 mg/kg of isobutanol, respectively). Place the sample vials in a head space sampler and analyse using the following conditions:
Column: 100% Polydimethylsiloxane (30 m x 0.53 mm i.d. with 1.5 μm film)
Carrier gas: Nitrogen
Flow rate: 3.5 ml/min
Detector: FID
Temperatures
- injection port: 110°
- column: 40°
- detector: 110°
Head space sampler:
- sample heat insulating temperature: 80°
- sample heat insulating period: 40 min
- syringe temperature: 85°
- sample gas injection: 1.0 ml

Calculation
Plot the relationship between the added amount against the peak area for isobutanol using the analytical results. The relationship should be linear. Extrapolate and determine the x-intercept (w_i), and calculate the solvent concentrations (C_i) from:

C_i (mg/kg)= w_i / W

where
w_i is x-intercept of relationship line using the standard addition method (μg); and
W is weight of sample (g).

Vinyl laurate, vinyl palmitate and vinyl stearate

Determine by gas chromatography (Vol. 4) under the following conditions.

Standard solutions
Prepare a stock solution separately containing 100.0 μg/ml of vinyl laurate, vinyl palmitate or vinyl stearate in acetonitrile. Prepare a range of mixed standard solutions containing 0.5, 1, 2 and 5 μg/ml of vinyl laurate, vinyl palmitate and vinyl stearate in acetonitrile.

Procedure
Weigh accurately 0.5 g of the sample into a 5-ml volumetric flask. Dilute to volume with methanol and mix using Vortex until the sample dissolves. Inject 1 μl of the sample solutions into the chromatograph.

Chromatography conditions
Column: Nitroterephthalic acid modified polyethylene glycol (DB-FFAP or equivalent) (30 m x 0.32 mm i.d. with 0.5 μm film)
Carrier gas: Nitrogen
Pressure: 7.18 psi
Split ratio: 10:1
Detector: Flame-ionization detector (FID)
Temperatures:
- injection port: 230 °
- column: Hold for 4 min at 100°, then 100-230° at 45°/min, hold for 10 min at 230°
- detector: 250 °
The retention times of vinyl laurate, vinyl palmitate and vinyl stearate measured under the above conditions are approx. 9.1, 12.0 and 14.4 min, respectively.

Calculation
Calculate the content of vinyl laurate, vinyl palmitate and vinyl stearate from:

Content of vinyl laurate, vinyl palmitate and vinyl stearate (mg/kg) = C x 5 / W

where
C is concentration of vinyl laurate, vinyl palmitate and vinyl stearate determined (μg/ml); and
W is weight of sample (g).

Acetaldehyde

Principle
The volatile acetaldehyde is converted with an acidic solution of 2, 4- dinitrophenylhydrazine (DNPH) to a more stable compound, acetaldehyde-2, 4-dinitrophenylhydrazone (ADNPH) that absorbs

in the UV region. ADNPH is determined by HPLC under the following conditions.

Standard solutions
Prepare ADNPH stock solution of 40 μg/ml from ADNPH standard (Sigma) with acetonitrile. Prepare a range of solutions containing 0, 0.05, 0.1, 0.2 and 0.5 μg/ml of ADNPH by dilutions of the stock solution with acetonitrile.

Chromatography conditions
Column: NUCLEOSIL 100-5 C18 (250 mm x 4.6 mm i.d., 5 μm) or equivalent
Mobile phase: Methanol - 1.0mM LiCl solution (80:20)
Flow rate: 1.0 ml/min
Detector: UV 360 nm
Column temperatures: 40°
The retention time of ADNPH measured under the above conditions is approx. 20 min.

Procedure
Accurately weigh 0.5 g of the sample into a 5-ml volumetric flask. Add 1.5mL of methanol to dissolve the sample, add 0.5ml of DNPH reagent and make to volume with acetonitrile. Stir the mixture with a magnetic stirrer for 10min. Centrifuge and collect the liquid layer. Filter through a 0.45 μm membrane filter. Inject 20 μl of the sample solution into HPLC.

Calculation
Calculate the content of acetaldehyde from:

$$\text{Content of acetaldehyde (mg/kg)} = C \times 5 / W$$

where
C is acetaldehyde concentration determined (μg/ml); and
W is weight of sample (g).

METHOD OF ASSAY

Determine by HPLC using the following conditions:

Procedure
Accurately weigh 250 mg of the sample into a 50-ml volumetric flask. Dilute to volume with tetrahydrofuran and mix. Filter through a 0.45 μm membrane filter. Inject 80 μl of the sample into the pre-stabilized chromatograph.

Chromatography conditions
Column: Styrene-divinylbenzene copolymer for gel permeation chromatography (TSK-GEL G1000HXL, G2000HXL, G3000HXL, G4000HXL (each 30 cm x 7.8 mm i.d., 5 μm) in series, Tosoh Co. or equivalent)
Mobile phase: HPLC-grade degassed tetrahydrofuran
Flow rate: 0.8 ml/min
Detector: Refractive index
Temperatures:
- Column: 40°
- Detector: 40°

Record the chromatogram for about 50 min.

Calculate the percentage of total sucrose esters in the sample from:

$$\% \text{ sucrose esters} = 100 (A_m+A_d) / T$$

Calculate the percentage of monoesters in total sucrose esters from:

$$\% \text{ monoesters} = 100 A_m / (A_m+A_d)$$

where
A_m is the peak area of the monoesters eluting at about 39.0-40.0 min;
A_d is the peak area of the diesters eluting at about 37.0-38.2 min; and
T is the sum of all peak areas eluting within 50 min.

TITANIUM DIOXIDE

Prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010), superseding specifications prepared at the 71st JECFA (2009) and published in FAO JECFA Monographs 7 (2009). An ADI "not limited" was established at the 13th JECFA (1969).

SYNONYMS Titania; CI Pigment white 6; CI (1975) No. 77891; INS No. 171

DEFINITION

Titanium dioxide is produced by either the sulfate or the chloride process. Processing conditions determine the form (anatase or rutile structure) of the final product.

In the sulfate process, sulfuric acid is used to digest ilmenite ($FeTiO_3$) or ilmenite and titanium slag. After a series of purification steps, the isolated titanium dioxide is finally washed with water, calcined, and micronized.

In the chloride process, chlorine gas is reacted with a titanium-containing mineral under reducing conditions to form anhydrous titanium tetrachloride, which is subsequently purified and converted to titanium dioxide either by direct thermal oxidation or by reaction with steam in the vapour phase. Alternatively, concentrated hydrochloric acid can be reacted with the titanium-containing mineral to form a solution of titanium tetrachloride, which is then further purified and converted to titanium dioxide by hydrolysis. The titanium dioxide is filtered, washed, and calcined.

Commercial titanium dioxide may be coated with small amounts of alumina and/or silica to improve the technological properties of the product.

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 White to slightly coloured powder

FUNCTIONAL USES Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4) 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 fumes of sulfuric acid appear, then cool. Cautiously dilute to about 100 ml with water and filter. To 5 ml of this clear filtrate, add a few drops of hydrogen peroxide; an orange-red colour appears immediately.
PURITY	
Loss on drying (Vol. 4)	Not more than 0.5% (105°, 3 h)
Loss on ignition (Vol. 4)	Not more than 1.0% (800°) on the dried basis
Aluminium oxide and/or silicon dioxide	Not more than 2%, either singly or combined See descriptions under TESTS
Acid-soluble substances	Not more than 0.5%; Not more than 1.5% for products containing alumina or silica. Suspend 5 g of the sample in 100 ml 0.5 N hydrochloric acid and place on a 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 (Vol. 4)	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	Not more than 1 mg/kg 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 (Vol. 4)	Not more than 1 mg/kg Determine using the cold vapour atomic absorption technique. Select a sample size appropriate to the specified level

TESTS

PURITY TESTS

Impurities soluble in 0.5 N hydrochloric acid	
Antimony, arsenic, cadmium and lead (Vol.4)	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, 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 through 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 contents 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 AAS/ICP-AES technique appropriate to the specified level. Determine arsenic using atomic absorption hydride technique.

Aluminium oxide

Reagents and sample solutions

Ammonium acetate buffer solution
In a 1000-ml volumetric flask, dissolve 77 g of ammonium acetate in about 500 ml of water, add 10 ml of glacial acetic acid and dilute to volume with water.

Diammonium hydrogen phosphate solution
In a 1000-ml volumetric flask, dissolve 150 g of diammonium hydrogen phosphate in about 700 ml of water, adjust pH to 5.5 using a 1 in 2 solution of hydrochloric acid, then dilute to volume with water.

Zinc Sulfate solution (0.01 N)
Dissolve 2.9 g of zinc sulfate ($ZnSO_4 \cdot 7H_2O$) in sufficient water and make up to 1000 ml in a volumetric flask. 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 the solution 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) Add, dropwise, ammonia solution (1 in 5) until the colour is just completely changed from red to orange-yellow. Then, add 10 ml of ammonium acetate buffer solution and 10 ml of diammonium hydrogen phosphate solution. Boil the solution for 5 min, cool it quickly to room temperature in a stream of running water, add 3 drops of xylenol orange TS, and mix.

Using zinc sulfate solution as titrant, titrate the solution to the first yellow-brown or pink end-point colour that persists for 5-10 sec. (NOTE: 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)

Add 2 g of sodium fluoride, boil the mixture for 2-5 min, and cool in a stream of running water. Titrate this solution, using the zinc sulfate solution as titrant, to the same fugitive yellow-brown or pink end-point as described above.

Calculate mass (mg) of Al_2O_3 per ml of zinc sulfate solution (T) from the formula

$$T = 18.896\ W/V$$

where

W is the mass (g) of aluminium wire;
V is the ml of the zinc sulfate solution consumed in the second titration;
18.896 = (R × 1000 mg/g × 10 ml/2)/1000 ml; and
R is the ratio of the formula weight of aluminium oxide to that of elemental aluminium.

Sample Solution A

Accurately weigh 1.0 g of the sample and transfer to a 250-ml high-silica glass Erlenmeyer flask. Add 10 g of sodium bisulfate ($NaHSO_4 \cdot H_2O$). (*Note*: 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 the flask at low heat on a hot plate, and then gradually raise the temperature until full heat is reached. (*Caution:* perform this procedure in a well ventilated area) When spattering has stopped and light fumes of SO_3 appear, heat in the full flame of a Meeker burner, with the flask tilted so that the fusion of the sample and sodium bisulfate is concentrated at one end of the flask. Swirl constantly until the melt is clear (except for silica content), but guard against prolonged heating to avoid precipitation of titanium dioxide. Cool, add 25 ml sulfuric acid solution (1 in 2), and heat until the mass has dissolved and a clear solution results. Cool, and dilute to 120 ml with water. Introduce a magnetic stir bar into the flask.

Sample Solution B

Prepare 200 ml of an approximately 6.25 M solution of sodium hydroxide. Add 65 ml of this solution to Sample Solution A, while stirring with the magnetic stirrer; pour the remaining 135 ml of the alkali solution into a 500-ml volumetric flask.

Slowly, with constant stirring, add the sample mixture to the alkali solution in the 500-ml volumetric flask; 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 (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 EDTA, 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 ml]

Add, dropwise, ammonia solution (1 in 5) until the colour is just completely changed from red to orange-yellow. Then add10 ml each of ammonium acetate and diammonium hydrogen phosphate solution and boil for 5 min. Cool quickly to room temperature in a stream of running 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, discard the solution and repeat this procedure with another 100 ml of Sample Solution B, using 50 ml, rather than 25 ml, of 0.02 M disodium EDTA.

Procedure

Using the standardized zinc sulfate solution as titrant, titrate Sample Solution C to the first yellow-brown or pink end-point that persists for 5-10 sec. (*Important:* See Note under "*0.01 Zinc sulfate*"). 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 to the titration flask, boil the mixture for 2-5 min, and cool in a stream of running water. Titrate this solution, using the standardized zinc sulfate solution as titrant, 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:

$$\% Al_2O_3 = 100 \times (0.005VT)/S$$

where

V is the number of ml of 0.01 N zinc sulfate consumed in the second titration;
T is the mass of Al_2O_3 per ml of zinc sulfate solution;
S is the mass (g) of the sample taken; and
0.005 = 500 ml / (1000mg/g × 100 ml).

Silicon dioxide

Accurately weigh 1 g of the sample and transfer to a 250-ml high-silica glass Erlenmeyer flask. Add 10 g of sodium bisulfate ($NaHSO_4 \cdot H_2O$). Heat gently over a Meeker 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 cooled melt add 25 ml of sulfuric acid solution (1 in 2) and heat carefully and slowly until the melt is dissolved. Cool, and carefully add 150 ml of water by 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 filter through fine ashless filter paper, using a 60 degree gravity funnel.

Rinse 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°, and heat the partly covered crucible over a Bunsen burner. To prevent flaming of the filter paper, first heat 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° 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

Accurately weigh about 150 mg of the sample, previously dried at 105° for 3 hours, and transfer into a 500-ml conical flask. Add 5 ml of water and shake until a homogeneous, milky suspension is obtained. Add 30 ml of sulfuric acid and 12 g of ammonium sulfate, and mix. Initially heat gently, then heat strongly until a clear solution is obtained. Cool, then cautiously dilute with 120 ml of water and 40 ml of hydrochloric acid, and stir. Add 3 g of aluminium metal, and immediately insert a rubber stopper fitted with a U-shaped glass tube while immersing the other end of the U-tube into a saturated solution of sodium bicarbonate contained in a 500-ml wide-mouth bottle, and generate hydrogen. Allow to stand for a few minutes after the aluminium metal has dissolved completely to produce a transparent purple solution. Cool to below 50° in running water, and remove the rubber stopper carrying the U-tube. Add 3 ml of a saturated potassium thiocyanate solution as an indicator, and immediately titrate with 0.1 N ferric ammonium sulfate until a faint brown colour that persists for 30 seconds is obtained. Perform a blank determination and make any necessary correction. Each ml of 0.1 N ferric ammonium sulfate is equivalent to 7.990 mg of TiO_2.

WITHDRAWAL OF SPECIFICATIONS FOR CERTAIN FOOD ADDITIVES

Annatto extract (oil-processed bixin)

In the call for data for the 73rd meeting information was requested to revise the existing tentative specifications, stating that the specifications would be withdrawn if no information was forthcoming.

As no supporting information was received, the tentative specifications were withdrawn by the Committee.

SPECIFICATIONS FOR CERTAIN FLAVOURINGS

At its 44th meeting JECFA considered a new approach to the safety evaluation of flavourings. 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 73rd meeting of the Committee specifications of identity and purity were prepared for 177 new flavourings (JECFA No. 1898-2042, 2044-2068 and 2070-2076, see page 50).

In addition, the specifications for flavouring substances 4-Carvomenthenol (JECFA No. 432) and 5,6,7,8-Tetrahydroquinoxaline (JECFA No. 952) were revised (see page 49).

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

Name; Chemical name (Systematic name, normally IUPAC name); Synonyms; Flavour and Extract Manufacturers' Association of the United States (FEMA) No; FLAVIS (FL) No; Council of Europe (COE) No; Chemical Abstract Service Registry (CAS) No; Chemical formula (Formula); Molecular weight (MW); Physical form/Odour; Solubility; Solubility in ethanol, Boiling point (B.P. ºC - for information only); Identification test (ID) referring to type of test (NMR: Nuclear Magnetic Resonance spectrometry; IR: Infrared spectrometry; MS: Mass spectrometry); Assay min % (Gas chromatographic (GC) assay of flavouring agents); Acid value max; Refractive index (R.I.) (at 20º, if not otherwise stated); Specific gravity (S.G) (at 25º, if not otherwise stated).

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

1. Items that are additional requirements, such as further purity criteria or other tests

2. Items provided for information, for example the typical isomer composition of the flavouring agent. These are not considered to be requirements.

3. Substances which are listed as Secondary Constituents (SC) 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.

4. Information on the status of the safety evaluation.

The fields named Session/Status contains the number of the meeting at which the specifications were prepared and the status of the specification. All specifications prepared at the 73rd meeting were assigned full status.

The full specifications prepared for the flavouring substances with JECFA Nos 1914, 1931, 1939, 1941, 1943, 1944, 1973, 1988, 2005, 2007, 2010, 2011 and 2046, by the Committee include a statement that the safety evaluations for these substances had not been completed at the present meeting. For further information see Annex 2.

Finally, the C.A.S. number, name and synonyms for the flavouring substance cis- and trans linalool oxide (JECFA No. 1454) were corrected in the On-line edition of the JECFA flavouring specifications, as the name in the specifications, published in Food and Nutrition Paper 52. Add. 12, did not correspond to those in the JECFA report (63rd meeting) and to the substance that had been evaluated. The correct C.A.S. number for the racemic mixture of linalool oxide (furanoid form) is 60047-17-8, and the C.A.S. numbers for the cis-isomer and trans-isomer are 5989-33-3 and 34995-77-2, respectively. These specifications are not republished in this monograph (see corrigendum page 151).

The spectra used for identification tests are provided from page 103 onwards.

A list of the new flavourings evaluated in alphabetical order is added on page 137.

Revised specifications

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
439	**4-Carvomenthenol**	2248	C10H18O	Slightly soluble in water; soluble in oils	IR	1.476-1.480	
			154.25		96	0.928-0.934	
Full	p-Menth-1-en-4-ol						
		2229	Colourless to	Soluble			
73rd	*1-Methyl-4-isopropyl-1-cyclohexene-4-ol, 4-Terpinenol, Origanol, Terpineol*		pale yellow, oily liquid; Warm-peppery, mildly earthy,				
		562-74-3	musty-woody odour	212 (d-isomer)			
952	**5,6,7,8-Tetrahydroquinoxaline**	3321	C8H10N2	Sparingly soluble in water; soluble in vegetable oils,	IR	1.540-1.550	
			134.18	propylene glycol and	98	1.078-1.088	
Full	5,6,7,8-Tetrahydroquinoxaline	721		DMSO			
			Colourless to amber				
73rd	*Cyclohexapyrazine*		liquid; Cheese-like	Soluble			
		34413-35-9	odour				
				85 (3 mm Hg)			

New specifications

JECFA No / Status / Session	Name / Chemical Name / *Synonyms*	FEMA / FLAVIS / COE / CAS	Chemical formula / M.W. / Physical form / odour	Solubility / Solubility in ethanol / B.P. °C	ID test / Assay min % / Acid Value	R. I. / S. G.	Other requirements / Information required
1898	**Methyl dihydrojasmonate**	3408	C13H22O3	Soluble in oils; very slightly soluble in water	NMR	1.454-1.464	SC: 9-11% Methyl epi-dihydrojasmonate
			226.31		85	0.997-1.008 (20°)	
Full	methyl 3-oxo-2-pentylcyclopentaneacetate	09.520					
		10785	Pale straw-coloured to yellowish oily liquid; Powerful floral, jasmine-like aroma	Soluble			
73rd	*Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester, Methyl hydrojasmonate*	24851-98-7		109-112 (0.2 mm Hg)	2		
1899	**cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid**	4529	C12H22O2	Practically insoluble or insoluble in water	NMR, MS	1.461-1.467	
			198.30		97	0.955-0.961	
Full	4-((1R,3S)-2,2,3-trimethylcyclopentyl)butanoic acid						
			Colourless liquid; Sweet aroma	Very slightly soluble			
73rd		957136-80-0		140-143			
1900	**Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde**	4505	C9H14O	Practically insoluble or insoluble in water	MS	1.469-1.475	Mixture of 70-71% 2,4-Dimethyl-3-cyclohexenylcarbaldehyde; 23-24% 3,5-Dimethyl-3-cyclohexenylcarbaldehyde; and 3-5% 3,6-Dimethyl-3-cyclohexenylcarbaldehyde
			138.21		95 (sum of isomers)	0.932-0.940 (20°)	
Full	Mixture of 2,4-dimethylcyclohex-3-ene-1-carbaldehyde, 3,5-dimethylcyclohex-3-ene-1-carbaldehyde and 3,6-dimethylcyclohex-3-ene-1-carbaldehyde						
			Colourless to pale yellow liquid; with camphouraceous herbaceous aroma notes	Soluble			
73rd	*Ivy carbaldehyde, Trivertal*	27939-60-2		99-101 (30 mm Hg)	5		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1901	**Perillaldehyde propyleneglycol acetal**	4530	C13H20O2	Practically insoluble or insoluble in water	MS	1.483-1.493	SC: 3-4% Perillaldehyde; 2-3% propyleneglycol
			208.30		91	0.991-1.001 (20°)	
Full	4-methyl-2-(4-(1-methyl ethenyl)-1-cyclohexen-1-yl)-1,3-dioxolane						
			Pale yellowish oily liquid; Fatty spicy herbaceous aroma	Soluble			
73rd	*1,3-Dioxolane, 4-methyl-2-[4-(1-methylethenyl)-1-cyclohexen-1-yl]-*	121199-28-8		302-304	1		
1902	**(+/-)-cis- and trans-1,2-Dihydroperillaldehyde**	4312	C10H16O	Sparingly soluble in water; soluble in non-polar solvents	NMR	1.469-1.475	Mixture of isomers (53% cis, 27% trans);
			152.23		80	0.923-0.929	SC: 10-11% trans-4-Isopropyl-cyclohexane-1-carboxaldehyde; 4-5% cis-4-Isopropyl-cyclohexane-1-carboxaldehyde; 1-2% 4-Isopropenyl-cyclohex-1-enecarboxaldehyde
Full	Mixture of cis-4-(prop-1-en-2-yl)cyclohexanecarbaldehyde and trans-4-(prop-1-en 2-yl)cyclohexanecarbaldehyde		Clear colourless or pale yellow liquid; Spicy, herbal, fruity aroma	Soluble			
73rd	*4-Isopropenyl-cyclohexanecarboxaldehyde*	22451-50-9 / 22451-49-6		211-213; 55-58 (1 mm Hg)			
1903	**d-Limonen-10-ol**	4504	C10H16O	Practically insoluble or insoluble in water	MS	1.495-1.505	
			152.23		95	0.955-0.977 (20°)	
Full	(R)-2-(4-methylcyclohex-3-en-1-yl)prop-2-en-1-ol						
			Colourless to pale yellow liquid; Clean citrus aroma with mint undertones	Soluble			
73rd	*(+)-(R)-p-Mentha-1,8(10)-dien-9-ol*	38142-45-9		239-240			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1904	**p-Menthan-7-ol**	4507	C10H20O	Practically insoluble or insoluble in water	MS	1.466-1.471	Mixture of isomers: 70-72 % p-Menthan-7-ol
			156.27		95 (isomeric mixture)	0.912-0.920 (20°)	(unspecified stereoisomer); 28-29 % p-Menthan-7-ol
Full	(4-isopropylcyclohexyl)methanol						
			Clear colourless liquid; Fresh clean floral magnolia to grassy aroma	Soluble			(unspecified stereoisomer)
73rd	*Cyclohexanemethanol, 4-(1-methylethyl)-, Mayol (monoterpene), Muguet shiseol*	5502-75-0		215-217			
1905	**p-Menth-1-en-9-ol**	4508	C10H18O	Practically insoluble or insoluble in water	MS	1.483-1.489	Mixture of isomers: 65-67% R,R-isomer; 31-33% R,S-isomer
			154.25		96	0.936-0.946	
Full	2-(4-methyl-1-cyclohex-3-enyl)propan-1-ol			Soluble			
		18479-68-0	Clear colourless liquid; Fruity herbal aroma				
73rd	*3-Cyclohexene-1-ethanol, beta,4-dimethyl-*			115-116 (10 mm Hg)			
1906	**1,3-p-Menthadien-7-al**	4506	C10H14O	Practically insoluble or insoluble in water	MS	1.532-1.539	SC: 5-6 % Cumin aldehyde
			150.22		91	0.961-0.965 (20°)	
Full	4-isopropylcyclohexa-1,3-dienecarbaldehyde	05.133					
			Clear colourless liquid; Fatty spicy aroma	Soluble			
73rd	*1,3-Cyclohexadiene-1-carboxaldehyde, 4-(1-methylethyl)-, 1,3-Cyclohexadiene-1-carboxaldehyde, 4-isopropyl-*	1197-15-5		116-120 (9 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1907	**cis- and trans-2-Heptylcyclopropanecarboxylic acid**	4130	C11H20O2	Soluble in water and triacetin	NMR, IR, MS	1.473-1.479	Mixture of isomers: 90% cis-2 Heptylcyclopropanecarboxylic acid, 10% trans-2-Heptylcyclopropanecarboxylic acid
			184.28		95	0.990-0.995	
Full	Mixture of cis-2-heptylcyclopropanecarboxylic acid and trans-2-heptylcyclopropanecarboxylic acid		Clear liquid; Floral, spicy, herbal and citrus aroma	Soluble			
73rd	*Cyclopropanecarboxylic acid, 2-heptyl, Heptylcylopropane-1-carboxylic acid*	697290-76-9 / 697290-77-0		281-283			
1908	**(+/-)-cis- and trans-2-Methyl-2-(4-methyl-3-pentenyl)cyclopropanecarbaldehyde**	4393	C11H18O	Practically insoluble or insoluble in water	NMR	1.494- 1.531	Mixture of isomers: 90% cis,10% trans; SC: 5-10% [2-methyl-2-(4-methylpent-3- en-1-yl) cyclopropyl]methanol
			166.26		90	0.894 - 0.990	
Full	Mixture of cis-2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde and trans-2-methyl-2-(4-methylpent-3-enyl)cyclopropane-1-carbaldehyde		Colourless to slightly yellow liquid; Fruity citrus-like aroma	Freely soluble			
73rd	*Cyclopropanecarboxaldehyde, 2-methyl-2-(4-methyl-3-pentenyl)-, trans-(+/-)-*	130932-16-0 / 97231-35-1		219-236			
1909	**Methyl octyl sulfide**	4573	C9H20S	Soluble in water	NMR, IR, MS	1.445-1.465	
			160.32		95	0.840-0.860 (20°)	
Full	1-methylsulfanyloctane		Clear colourless liquid; Pungent unpleasant odour	Soluble			
73rd	*1-Methylthiooctane, 2-Thiadecane, Methyl(octyl)sulfane*	3698-95-1		217-219	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1910	**Methyl 1-propenyl sulfide**	4574	C4H8S	Practically insoluble or insoluble in water	MS	1.479-1.489	Mixture of isomers: 53% Z; 46% E
			88.17		95 (isomeric mixture)	0.887-0.893 (20°)	
Full	Mixture of (Z)-methyl(prop-1-en-1-yl)sulfane and (E)-methyl(prop-1-en-1-yl)sulfane	12.136					
		11538	Clear to pale yellow liquid; Acrid strong garlic-like aroma	Soluble			
73rd	*1-Propene, 1-(methylthio)-*	10152-77-9		102 (957 mm Hg)			
1911	**Di-(1-propenyl) sulfide (mixture of isomers)**	4386	C6H10S	Very slightly soluble in DMSO	NMR, IR, MS	1.498-1.526	Mixture of isomers: 45-46 % E,Z; 31-32% Z,Z; 18-20% E,E
			114.21		95 (isomeric mixture)	0.875-0.942	
Full	Mixture of (E)-1-[(Z)-prop-1-enyl]sulfanylprop-1-ene, (Z)-1-[(Z)-prop-1-enyl]sulfanylprop-1-ene and (E)-1-[(E)-prop-1-enyl]sulfanylprop-1-ene						
			Clear almost colourless liquid; Savoury brown aroma	Soluble			
73rd	*cis, cis-Di-1-propenyl sulfide, cis,trans-Di-1-propenyl sulfide, trans,trans-Di-1-propenyl sulfide*	37981-37-6 / 37981-36-5 / 65819-74-1		137-140			
1912	**Ethyl 2-hydroxyethyl sulfide**	4562	C4H10OS	Practically insoluble or insoluble in water	MS	1.482-1.489	
			106.19		95	1.015-1.023 (20°)	
Full	2-ethylsulfanylethanol						
			Clear colourless to yellow liquid; Powerful meat-like aroma	Soluble			
73rd	*2-(Ethylthio)-1-ethanol, 2-Ethylmercaptoethanol, 2-Hydroxyethyl ethyl sulfide, beta-Ethylthioethanol, Ethyl 2-hydroxyethyl thioether*	110-77-0		180-184			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1913	**2-(Methylthio)ethyl acetate**	4560	C5H10O2S	Practically insoluble or insoluble in water	MS	1.456-1.467	
			134.20		95	1.056-1.076	
Full	2-(methylthio)ethyl acetate	12.248		Soluble		(20°)	
73rd	*2-Acetoxyethyl methyl sulfide, Ethanol, 2-(methylthio)-, 1-acetate*	5862-47-5	Clear colourless liquid; Sweet rancid meat-like aroma	73 (15 mm Hg)			
1914	**3-(Methylthio)propyl mercaptoacetate (Safety evaluation not completed)**	4561	C6H12O2S2	Practically insoluble or insoluble in water	NMR, IR, MS	1.515-1.521	Safety evaluation not completed
			180.29		97	1.160-1.166	
Full	3-(methylthio)propyl 2-mercaptoacetate			Soluble		(20°)	
73rd	*Acetic acid, mercapto-, 3-(methylthio)propyl ester*	852997-30-9	Clear colourless to yellow liquid; Strong sweet onion-like aroma	109-111	1		
1915	**Ethyl 3-(methylthio)-(2Z)-propenoate**	4563	C6H10O2S	Practically insoluble or insoluble in water	MS	1.510-1.541	SC: 7-9% Ethyl 3-(methylthio)-trans-2-propenoate
			146.21		88	1.081-1.090	
Full	(Z)-ethyl 3-(methylthio)acrylate						
		136115-66-7	Clear colourless liquid;	Soluble			
73rd	*2-Propenoic acid, 3-(methylthio)-, ethyl ester, (2Z)-*		Acrid sweet onion-like aroma	200-202			

JECFA No / Status / Session	Name / Chemical Name / *Synonyms*	FEMA / FLAVIS / COE / CAS	Chemical formula / M.W. / Physical form / odour	Solubility / Solubility in ethanol / B.P. °C	ID test / Assay min % / Acid Value	R. I. / S. G.	Other requirements / Information required
1916	**Ethyl 3-(methylthio)-(2E)-propenoate**	4564	C6H10O2S	Practically insoluble or insoluble in water	MS	1.510-1.541	SC: 14-16% Ethyl 3-(methylthio)-cis-2-propenoate
			146.21		81	1.081-1.090	
Full	(E)-ethyl 3-(methylthio)acrylate						
73rd	*2-Propenoic acid, 3-(methylthio)-, ethyl ester, (2E)-*	136115-65-6	Clear colourless liquid; Acrid sweet onion-like aroma	Soluble 200-202			
1917	**Ethyl 3-(methylthio)-2-propenoate (mixture of isomers)**	4565	C6H10O2S	Practically insoluble or insoluble in water	MS	1.510-1.541	Mixture of isomers: 54% (Z)-Ethyl 3-(methylthio)acrylate, 46% (E)-Ethyl 3-(methylthio)acrylate
			146.21		98	1.081-1.090 (20°)	
Full	Mixture of (Z)-ethyl 3-(methylthio)acrylate and (E)-ethyl 3-(methylthio)acrylate						
73rd	*2-Propenoic acid, 3-(methylthio)-, ethyl ester*	77105-51-2	Clear colourless liquid; Acrid sweet onion-like aroma	Soluble 200-202			
1918	**4-Methyl-2-(methylthiomethyl)-2-pentenal**	4568	C8H14OS	Practically insoluble or insoluble in water	MS	1.488-1.498	
			158.26		95	0.971-0.981 (20°)	
Full	4-methyl-2-(methylthiomethyl)-2-pentenal						
73rd	*2-Methylmercaptomethyl-4-methylpent-2-enal, 2-Pentenal, 4-methyl-2-[(methylthio)methyl]-*	40878-73-7	Clear colourless to yellow liquid; Sharp pungent aroma	Soluble 69-70 (2 mm Hg)			
1919	**4-Methyl-2-(methylthiomethyl)-2-hexenal**	4566	C9H16OS	Practically insoluble or insoluble in water	MS	1.497-1.507	
			172.29		96	0.964-0.974 (20°)	
Full	4-methyl-2-(methylthiomethyl)-2-hexenal						
73rd	*2-Hexenal, 4-methyl-2-[(methylthio)methyl]-*	99910-84-6	Clear colourless to yellow liquid; Powerful onion meat to soup-like aroma	Soluble 92-102 (5 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1920	**5-Methyl-2-(methylthiomethyl)-2-hexenal**	4567	C9H16OS	Practically insoluble or insoluble in water	MS	1.494-1.504	Mixture of isomers: 50% cis, 50% trans
			172.29		95 (mixture of isomers)	0.956-0.966 (20°)	
Full	5-methyl-2-(methylthiomethyl)-2-hexenal						
			Clear colourless to yellow liquid; Strong oniony meat-like odour	Soluble			
73rd	*Methyl-2-(methylthiomethyl)-2-hexenal*	85407-25-6		96 (3 mm Hg)			
1921	**Butyl beta-(methylthio)acrylate**	4571	C8H14O2S	Practically insoluble or insoluble in water	MS	1.507-1.513	Mixture of isomers: 40% cis, 60% trans
			174.26		96 (mixture of isomers)	1.033-1.039 (20°)	
Full	butyl 3-(methylthio)acrylate			Soluble			
		77105-53-4	Clear colourless to yellow liquid; Acrid fruity aroma				
73rd				101 (2 mm Hg)			
1922	**Ethyl 3-(ethylthio)butyrate**	4572	C8H16O2S	Practically insoluble or insoluble in water	MS	1.454-1.460	
			176.28		96	0.981-0.987 (20°)	
Full	ethyl 3-(ethylthio)butanoate						
			Clear colourless liquid; Metallic fruit-like aroma	Soluble			
73rd	*Butanoic acid, 3-(ethylthio)-, ethyl ester*	90201-28-8		50-52 (2 mm Hg)			
1923	**2-Oxothiolane**	4570	C4H6OS	Practically insoluble or insoluble in water	NMR, MS	1.518-1.528	
			102.15		95	1.175-1.185 (20°)	
Full	dihydrothiophen-2(3H)-one						
			Clear colourless to yellow liquid; Burnt garlic aroma	Soluble			
73rd	*2-Oxotetrahydrothiophene, 4-Butyrothiolactone, gamma-Thiobutyrolactone, Tetrahydro-2-thiophenone, Thiacyclopentanone-2, Thiobutyrolactone, Thiolan-2-one*	1003-10-7		195-197			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1924	**Dodecanethiol**	4581	C12H26S	Practically insoluble or insoluble in water	MS	1.454-1.464	
			202.40		95	0.842-0.852 (20°)	
Full	dodecane-1-thiol						
73rd	*1-Dodecyl mercaptan, 1-Dodecylthiol, 1-Mercaptododecane, Lauryl mercaptan*	112-55-0	Clear colourless to yellow liquid; Mild skunk-like odour	Soluble 142-143 (16 mm Hg)			
1925	**2-Hydroxyethanethiol**	4582	C2H6OS	Practically insoluble or insoluble in water	MS	1.499-1.505	
			78.13		97	1.114-1.120 (20°)	
Full	2-mercaptoethanol						
73rd	*1-Hydroxy-2-mercaptoethane, 1-Mercapto-2-hydroxyethane, 2-Hydroxyethyl mercaptan, beta-Mercaptoethanol, Ethanol, 2-mercapto-*	60-24-2	Clear colourless liquid; Very unpleasant odour	Soluble 156-158			
1926	**4-Mercapto-4-methyl-2-hexanone**	4583	C7H14OS	Practically insoluble or insoluble in water	MS	1.466-1.472	
			146.25		95	0.962-0.968 (20°)	
Full	4-mercapto-4-methylhexan-2-one						
73rd	*4-Methyl-4-sulfanylhexan-2-one*	851768-52-0	Clear colourless to pale yellow liquid; Floral fruity aroma	Soluble 80-86 (22 mm Hg)			
1927	**3-Mercapto-3-methylbutyl isovalerate**	4584	C10H20O2S	Practically insoluble or insoluble in water	NMR, IR, MS	1.450-1.460	
			204.33		97	0.949-0.959 (20°)	
Full	3-mercapto-3-methylbutyl 3-methylbutanoate						
73rd	*Butanoic acid, 3-methyl-, 3-mercapto-3-methylbutyl ester*	612071-27-9	Clear colourless to yellow liquid; Fruity aroma with sulphureous undertones	Soluble 70 (11 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1928	**(+/-)-Ethyl 3-mercapto-2-methylbutanoate**	4392	C7H14O2S	Practically insoluble or insoluble in water; soluble in fats and oils	NMR	1.454-1.455	
			162.25		95	1.0047-1.0057	
Full	ethyl 3-mercapto-2-methylbutanoate						
			Clear liquid; Fruity aroma at low concentration	Soluble			
73rd		888021-82-7		40-41 (1 mm Hg)			
1929	**3-Mercaptohexanal**	4585	C6H12OS	Practically insoluble or insoluble in water	MS	1.466-1.476	
			132.22		95	0.973-0.983 (20°)	
Full	3-mercaptohexanal	12.250					
			Clear colourless liquid; Sharp penetrating onion-like aroma	Soluble			
73rd	*Hexanal, 3-mercapto-*	51755-72-7		41-42 (2 mm Hg)			
1930	**Diisoamyl disulfide**	4575	C10H22S2	Practically insoluble or insoluble in water	MS	1.481-1.491	
			206.41		96	0.912-0.922 (20°)	
Full	1,2-diisopentyldisulfane						
			Clear colourless to pale yellow liquid; Sweet oniony aroma	Soluble			
73rd	*2,9-Dimethyl-5,6-dithiadecane, Diisopentyl disulfide, Disulfide, bis(3-methylbutyl), Isoamyl disulfide*	2051-04-9		245-247			
1931	**Bis(2-methylphenyl) disulfide (Safety evaluation not completed)**	4576	C14H14S2	Practically insoluble or insoluble in water	NMR, MS	NA	Safety evaluation not completed;
			246.39		96	NA	m.p. = 36-40 ºC
Full	1,2-di-o-tolyldisulfane						
			Solid; Burnt sugar aroma	Soluble			
73rd	*2,2'-Dimethyldiphenyl disulfide, Bis(o-tolyl) disulfide, Disulfide, bis(2-methylphenyl)*	4032-80-8		NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1932	**Butyl propyl disulfide**	4577	C7H16S2	Practically insoluble or insoluble in water	MS	1.490-1.500	SC: 24-25% Dipropyl disulfide; 23-24% Dibutyl disulfide
			164.33		51	0.945-0.955 (20°)	
Full	1-butyl-2-propyldisulfane						
			Clear colourless to pale yellow liquid;	Soluble			
73rd	*1-Propyldisulfanylbutane, 4,5-Dithianonane*	72437-64-0	Sulfureous aroma	89-90 (10 mm Hg)			
1933	**di-sec-Butyl disulfide**	4578	C8H18S2	Practically insoluble or insoluble in water	MS	1.477-1.497	
			178.36		98	0.942-0.954 (20°)	
Full	1,2-di-sec-butyldisulfane						
			Clear colourless liquid; Strong sulfureous aroma	Soluble			
73rd	*1-Methylpropyl disulfide, 3,6-Dimethyl-4,5-dithiaoctane, Bis(2-butyl) disulfide, Disulfide, bis(1-methylpropyl)*	5943-30-6		218-220			
1934	**Diisoamyl trisulfide**	4580	C10H22S3	Practically insoluble or insoluble in water	MS	1.518-1.524	
			238.48		97	0.985-0.991 (20°)	
Full	1,3-diisopentyltrisulfane						
			Clear colourless to yellow liquid;	Soluble			
73rd		955371-64-9	Sulfureous garlic like aroma	89-91 (1 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1935	**Methyl 2-methylphenyl disulfide**	4579	C8H10S2	Practically insoluble or insoluble in water	MS	1.605-1.611	
			170.30		95	1.130-1.136 (20°)	
Full	1-methyl-2-(o-tolyl)disulfane						
			Clear colourless to pale yellow liquid; Strong	Soluble			
73rd	*Disulfide, methyl 2-methylphenyl, Methyl o-tolyl disulfide*	35379-09-0	sulfureous aroma	90 (3 mm Hg)			
1936	**3-Mercaptopropionic acid**	4587	C3H6O2S	Practically insoluble or insoluble in water	MS	1.490-1.496	
			106.14		98	1.220-1.226 (20°)	
Full	3-mercaptopropanoic acid						
			Clear colourless to pale yellow oily liquid;	Soluble			
73rd	*2-Mercaptoethanecarboxylic acid, 3-Thiopropanoic acid, 3-Thiopropionic acid, Propanoic acid, 3-mercapto-, Thiohydracrylic acid*	107-96-0	Roasted sulfureous aroma	110-111 (15 mmHg)			
1937	**Methyl isobutanethioate**	4586	C5H10OS	Practically insoluble or insoluble in water	MS	1.455-1.461	
			118.20		98	0.961-0.967 (20°)	
Full	S-methyl 2-methylpropanethioate						
			Clear colourless to pale yellow liquid;	Soluble			
73rd	*Propanethioic acid, 2-methyl-, S-methyl ester*	42075-42-3	Penetrating fruity aroma	70-72 (100 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1938	**2-Ethylhexyl 3-mercaptopropionate**	4588	C11H22O2S	Practically insoluble or insoluble in water	MS	1.458-1.464	
			218.36		96	0.964-0.970 (20°)	
Full	2-ethylhexyl 3-mercaptopropanoate						
			Clear colourless to pale yellow liquid; Sweet penetrating aroma	Soluble			
73rd	*3-Mercaptopropionic acid 2-ethylhexyl ester, Propanoic acid, 3-mercapto-, 2-ethylhexyl ester*	50448-95-8		283-284			
1939	**Butanal dibenzyl thioacetal (Safety evaluation not completed)**	4589	C18H22S2	Practically insoluble or insoluble in water	MS	1.585-1.591 (25°)	Safety evaluation not completed
			302.50		95		
Full	benzyl(1-(benzyloxy)butyl)sulfane					1.073-1.079	
			Clear colourless to pale yellow liquid; Pungent fruity aroma	Soluble			
73rd	*{[1-(benzylsulfanyl)butyl]sulfanyl}methylbenzene*	101780-73-8		199-201 (2 mm Hg)			
1940	**Methional diethyl acetal**	4590	C8H18O2S	Practically insoluble or insoluble in water	MS	1.447-1.453	
			178.29		96	0.952-0.958 (20°)	
Full	1,1-diethoxy-3-methylsulfanylpropane						
			Clear colourless to pale yellow liquid; Pungent cabbage aroma	Soluble			
73rd		16630-61-8		118-119 (50 mm Hg)			
1941	**3-(Methylthio)propyl hexanoate (Safety evaluation not completed)**	4436	C10H20O2S	Practically insoluble or insoluble in water	NMR	1.448- 1.468	Safety evaluation not completed
			204.33		98	0.915-0.998	
Full	3-(methylthio)propyl hexanoate						
			Clear colourless to pale yellow liquid; Sharp penetrating aroma with fruity undertones	Soluble			
73rd		906079-63-8		270-272			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1942	**1-(3-(Methylthio)-butyryl)-2,6,6-trimethylcyclohexene**	4569	C14H24OS	Practically insoluble or insoluble in water	MS	1.505-1.511	
			240.40		97	0.993-0.996 (20°)	
Full	3-(methylthio)-1-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-1-one						
			Clear colourless to yellow liquid; Strong fruit like aroma	Soluble			
73rd	*1-Butanone, 3-(methylthio)-1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-*	68697-67-6		112 (2 mm Hg)			
1943	**(+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (Safety evaluation not completed)**	4499	C12H24OS	Practically insoluble or insoluble in water	NMR, IR, MS	1.441-1.478	Safety evaluation not completed; Mixture of 85-86 % cis-2-Pentyl-4-propyl-1,3-oxathiane and 10-13% trans-2-Pentyl-4-propyl-1,3-oxathiane
			216.38		95 (mixture of isomers)	0.890-0.937	
Full	Mixture of cis-2-pentyl-4-propyl-1,3-oxathiane and trans-2-pentyl-4-propyl-1,3-oxathiane						
			Clear colourless to yellow liquid; Fruity allium aroma	Soluble			
73rd		59323-81-8		297-301			
1944	**2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (Safety evaluation not completed)**	4526	C12H22OS	Practically insoluble or insoluble in water	NMR, IR, MS	1.456-1.489	Safety evaluation not completed; 88% mixture of isomers (80% Z; 8% E); 5-8 % 2-[(2e)-Pent-2-en-1-yl]-4-propyl-1,3-oxathiane; 2-3% 2-[(1z)-Pent-1-en-1-yl]-4-propyl-1,3-oxathiane
			214.37		88	0.883-0.974	
Full	Mixture of (Z)-2-(pent-2-en-1-yl)-4-propyl-1,3-oxathiane and (E)-2-(pent-2-en-1-yl)-4-propyl-1,3-oxathiane						
			Clear colourless to yellow liquid; Sharp penetrating garlic aroma	Soluble			
73rd		1094004-39-3		295-300			

JECFA No / Status / Session	Name / Chemical Name / *Synonyms*	FEMA / FLAVIS / COE / CAS	Chemical formula / M.W. / Physical form / odour	Solubility / Solubility in ethanol / B.P. °C	ID test / Assay min % / Acid Value	R. I. / S. G.	Other requirements / Information required
1945	**Hydroxyacetone**	4462	C3H6O2	Soluble in water	MS	1.419-1.430	
			74.08		95	1.079-1.085	
Full	1-hydroxypropan-2-one	07.169				(20°)	
		111011	Clear colourless to	Soluble			
73rd	*2-Oxopropanol, Acetol, Acetone alcohol, Acetylcarbinol, Acetylmethanol, Hydroxymethyl methyl ketone, Hydroxypropanone*	116-09-6	yellow liquid; Pungent, sweet-caramellic, somewhat choking etheral aroma	145-146			
1946	**Propyl pyruvate**	4484	C6H10O3	Practically insoluble or insoluble in water	MS	1.406-1.414	
			130.14		98	1.012-1.020	
Full	propyl 2-oxopropanoate					(20°)	
		20279-43-0	Colourless to pale yellow liquid; Sweet	Soluble			
73rd	*Propanoic acid, 2-oxo-, propyl ester, Pyruvic acid, propyl ester*		carmelling, floral aroma	168-170			
1947	**Methyl 3-hydroxybutyrate**	4450	C5H10O3	Practically insoluble or insoluble in water	NMR, MS	1.417-1.425	
			118.13		98	1.053-1.061	
Full	methyl 3-hydroxybutanoate					(20°)	
		1487-49-6	Colourless clear liquid;	Soluble			
73rd	*3-Hydroxybutyric acid methyl ester, Butanoic acid, 3-hydroxy-, methyl ester, Butyric acid, 3-hydroxy-, methyl ester*		Mild apple like aroma	158-160	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1948	**Dodecyl lactate**	4482	C15H30O3	Practically insoluble or insoluble in water	NMR, MS	1.437-1.447	SC: 10% Dodecanol
			258.40		88	0.910-0.925 (20°)	
Full	dodecyl 2-hydroxypropanoate						
			Pale yellow clear liquid;	Soluble			
73rd	*Lactic acid, dodecyl ester, Lauryl lactate, Propanoic acid, 2-hydroxy-, dodecyl ester*	6283-92-7	Faint fatty butter-like aroma	303-304	5		
1949	**(+/-)-Ethyl 3-hydroxy-2-methylbutyrate**	4391	C7H14O3	Soluble in water, DMSO, triacetin and vegetable oils	NMR	1.405-1.447	
			146.18		95	0.953-1.053 (20°)	
Full	ethyl 3-hydroxy-2-methylbutanoate	9.361					
		10600	Clear colourless liquid; Green fruity aroma	Soluble			
73rd	*Butanoic acid, 3-hydroxy-2-methyl-, ethyl ester, Butyric acid, 3-hydroxy-2-methyl-, ethyl ester*	27372-03-8		57-58 (2.9 mm Hg)			
1950	**Hexadecyl lactate**	4483	C19H38O3	Practically insoluble or insoluble in water	MS	NA	SC: 15% Hexadecanol; m.p.= 35-44 ºC
			314.50		88	NA	
Full	hexadecyl 2-hydroxypropanoate			Soluble			
		35274-05-6	White solid; Faint fatty butter-like aroma				
73rd				NA	3		
1951	**Methyl 3-acetoxy-2-methylbutyrate**	4451	C8H14O4	Practically insoluble or insoluble in water	NMR, MS	1.413-1.423	
			174.19		95	1.034-1.044 (20°)	
Full	methyl 3-acetoxy-2-methylbutanoate	09.361					
			Colourless clear liquid; Strong sweet fruity aroma	Soluble			
73rd	*Butanoic acid, 3-(acetyloxy)-2-methyl-, methyl ester*	139564-42-4		145-152			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1952	**1-Hydroxy-4-methyl-2-pentanone**	4463	C6H12O2	Practically insoluble or insoluble in water	MS	1.427-1.433	
			116.16		95	0.952-0.958 (20°)	
Full	1-hydroxy-4-methylpentan-2-one						
		68113-55-3	Colourless clear liquid;	Soluble			
73rd	*2-Pentanone, 1-hydroxy-4-methyl-*		Strong ethereal-fruity aroma	221-222			
1953	**Ethyl 2-acetylhexanoate**	4452	C10H18O3	Practically insoluble or insoluble in water	MS	1.425-1.435	
			186.25		95	0.949-0.959 (20°)	
Full	ethyl 2-acetylhexanoate						
				Soluble			
73rd	*2-Acetylhexanoic acid ethyl ester, 3-Carbethoxy-2-heptanone, Ethyl 2-butyl-3-oxobutanoate, Ethyl 2-butylacetoacetate, Ethyl 2-butylacetylacetate*	1540-29-0	Colourless clear liquid; Fruity wine-like aroma	218-220	1		
1954	**3-Isopropenyl-6-oxoheptanoic acid**	4461	C10H16O3	Practically insoluble or insoluble in water	NMR, MS	1.440-1.480	
			184.23		98	1.009-1.039 (20°)	
Full	6-oxo-3-(prop-1-en-2-yl)heptanoic acid						
			Colourless clear liquid;	Soluble			
73rd	*Heptanoic acid, 3-(1-methylethenyl)-6-oxo-, Heptanoic acid, 3-isopropenyl-6-oxo-*	4436-82-2	Fatty floral aroma	328-330			
1955	**Ethyl 3-hydroxyoctanoate**	4453	C10H20O3	Practically insoluble or insoluble in water	NMR, IR, MS	1.430-1.438	
			188.26		98	0.947-0.955 (20°)	
Full	ethyl 3-hydroxyoctanoate	09.916					
		10603	Colourless clear liquid;	Soluble			
73rd	*Caprylic acid, beta-hydroxy-, ethyl ester, Octanoic acid, 3-hydroxy-, ethyl ester*	7367-90-0	Wine-like aroma with fruity floral notes	275-276			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1956	**Methyl 3-acetoxyoctanoate**	4454	C11H20O4	Soluble in water	NMR, MS	1.413-1.433	
			216.27		96	0.934-0.994	
Full	methyl 3-acetoxyoctanoate						
73rd	*Octanoic acid, 3-(acetyloxy)-, methyl ester*	35234-21-0	Clear colourless to yellow liquid; Sweet wine-like aroma with fruity green notes	Soluble 217-219			
1957	**5-Oxooctanoic acid**	4455	C8H14O3	Soluble in water	IR, MS	NA	m.p. = 30-34 ºC
			158.20		97	NA	
Full	5-oxooctanoic acid						
73rd	*Octanoic acid, 5-oxo-*	3637-14-7	White solid; Fruity aroma with musky undertones	Soluble NA			
1958	**Ethyl 2-acetyloctanoate**	4459	C12H22O3	Soluble in water	IR	1.430-1.440	
			214.30		95	0.934-0.940 (20°)	
Full	ethyl 2-acetyloctanoate						
73rd	*Ethyl 2-acetylcaprylate, Ethyl alpha-hexylacetoacetate, Octanoic acid, 2-acetyl-, ethyl ester*	29214-60-6	Clear colourless liquid; Fruity jasmine herbal waxy aroma	Soluble 253-254	3		
1959	**Ethyl 5-acetoxyoctanoate**	4443	C12H22O4	Soluble in water	NMR, IR, MS	1.427-1.433	
			230.30		97	0.976-0.982 (20°)	
Full	ethyl 5-acetyloxyoctanoate						
73rd	*delta-Acetoxyoctanoic acid, ethyl ester, Octanoic acid, 5-(acetyloxy)-, ethyl ester*	35234-25-4	Clear colourless to yellow liquid; Strong musky fruity aroma	Soluble 279-282	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1960	**5-Oxodecanoic acid**	4456	C10H18O3	Very slightly soluble in water	IR, MS	NA	m.p. = 53-57 ºC
			186.25		99	NA	
Full	5-oxodecanoic acid						
73rd	*Decanoic acid, 5-oxo-*	624-01-1	Clear colourless to yellow solid; Rich creamy peach-like aroma	Soluble NA			
1961	**Ethyl 5-oxodecanoate**	4457	C12H22O3	Practically insoluble or insoluble in water	MS	1.433-1.439	
			214.30		95	0.943-0.953 (20°)	
Full	ethyl 5-oxodecanoate						
73rd	*Decanoic acid, 5-oxo-, ethyl ester*	93919-00-7	Colourless clear liquid; Strong rich fruity aroma	Soluble 290-294	1		
1962	**Ethyl 5-hydroxydecanoate**	4444	C12H24O3	Very slightly soluble in water	NMR, IR, MS	1.442-1.452	SC: 40-42% delta-Decalactone
			216.32		56	0.945-0.956 (20°)	
Full	ethyl 5-hydroxydecanoate						
73rd	*5-Hydroxydecanoic acid ethyl ester, Decanoic acid, 5-hydroxy-, ethyl ester*	75587-06-3	Colourless clear liquid; Sweet fatty peach-like aroma	Soluble 280-299	10		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1963	**5-Oxododecanoic acid**	4458	C12H22O3	Very slightly soluble in water	IR, MS	NA	m.p. = 68-72 ºC
			214.30		97	NA	
Full	5-oxododecanoic acid			Soluble			
73rd	*5-Oxolauric acid, Dodecanoic acid, 5-oxo-*	3637-16-9	Waxy solid; Peaches and cream like aroma	NA			
1964	**Dimethyl adipate**	4472	C8H14O4	Very slightly soluble in water	MS	1.426-1.431	
			174.19		98	1.062-1.066 (20°)	
Full	dimethyl adipate			Soluble			
73rd	*Adipic acid, dimethyl ester, Dimethyl hexanedioate, Hexanedioic acid, dimethyl ester, Methyl adipate*	627-93-0	Clear colourless liquid; Faint alcoholic aroma	109-110 (14 mmHg)	1		
1965	**Dipropyl adipate**	4473	C12H22O4	Very slightly soluble in water	MS	1.429-1.433	
			230.30		98	0.979-0.983 (20°)	
Full	dipropyl adipate			Soluble			
73rd	*Adipic acid, dipropyl ester, Dipropyl hexanedioate, Hexanedioic acid, dipropyl ester*	106-19-4	Clear colourless liquid; Light rubbing alcohol aroma	273-274	1		
1966	**Diisopropyl adipate**	4474	C12H22O4	Practically insoluble or insoluble in water	MS	1.423-1.427	
			230.30		98	0.963-0.968 (20°)	
Full	diisopropyl adipate			Soluble			
73rd	*Adipic acid, diisopropyl ester, Hexanedioic acid, 1,6-bis(1-methylethyl) ester, Hexanedioic acid, bis(1-methylethyl) ester, Isopropyl adipate*	6938-94-9	Clear colourless liquid; Light alcoholic aroma	251-253	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1967	**Diisobutyl adipate**	4475	C14H26O4	Practically insoluble or insoluble in water	MS	1.428-1.434	
			258.35		98	0.950-0.956 (20°)	
Full	diisobutyl adipate						
73rd	*Adipic acid bis(2-methylpropyl) ester, Adipic acid, diisobutyl ester, Hexanedioic acid, bis(2-methylpropyl) ester, Isobutyl adipate*	141-04-8	Clear colourless liquid; Bland aroma	Soluble 280-281	1		
1968	**Dioctyl adipate**	4476	C22H42O4	Practically insoluble or insoluble in water	MS	1.444-1.450	
			370.57		98	0.924-0.930 (20°)	
Full	dioctyl adipate						
73rd	*Adipic acid, dioctyl ester, Hexanedioic acid, dioctyl ester, Octyl adipate*	123-79-5	Clear colourless liquid; Slight fatty aroma	Soluble 396-398	1		
1969	**Ethyl acetoacetate ethyleneglycol ketal**	4477	C8H14O4	Very slightly soluble in water	MS	1.428-1.435	
			174.19		98	1.083-1.091 (20°)	
Full	ethyl 2-(2-methyl-1,3-dioxolan-2-yl)acetate						
73rd	*1,3-Dioxolane-2-acetic acid, 2-methyl-, ethyl ester, Ethyl 3-oxobutyrate ethylene ketal, Ethyl acetoacetate 3-ethylene acetal, Fructone*	6413-10-1	Clear colourless liquid; Strong fruity apple green sweet woody aroma	Soluble 125-126	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1970	**Methyl levulinate**	4478	C6H10O3	Sparingly soluble in water	IR, MS	1.419-1.425	
			130.14		98	1.049-1.055 (20°)	
Full	methyl 4-oxopentanoate						
			Clear colourless liquid; Mild carmellic aroma	Soluble			
73rd	*4-Oxopentanoic acid methyl ester, Levulinic acid, methyl ester, Methyl 4-oxopentanoate, Methyl 4-oxovalerate, Methyl beta-acetylpropionate, Methyl levulate, Pentanoic acid, 4-oxo-, methyl ester*	624-45-3		194-196	1		
1971	**Propyl levulinate**	4480	C8H14O3	Practically insoluble or insoluble in water	MS	1.419-1.425	
			158.20		98	0.989-0.995 (20°)	
Full	propyl 4-oxopentanoate						
			Clear colourless liquid; Sweet very slight carmellic aroma	Soluble			
73rd	*Levulinic acid, propyl ester, Pentanoic acid, 4-oxo-, propyl ester*	645-67-0		220-221	1		
1972	**Isoamyl levulinate**	4481	C10H18O3	Practically insoluble or insoluble in water	NMR, IR, MS	1.427-1.433	
			186.25		98	0.957-0.963 (20°)	
Full	3-methylbutyl 4-oxopentanoate						
			Clear colourless liquid; Light ethereal carmellic aroma	Soluble			
73rd	*Isopentyl levulinate, Levulinic acid, isopentyl ester, Pentanoic acid, 4-oxo-, 3-methylbutyl ester*	71172-75-3		252-253	1		
1973	**Ethyl levulinate propyleneglycol ketal (Safety evaluation not completed)**	4479	C10H18O4	Practically insoluble or insoluble in water	MS	1.427-1.434	Safety evaluation not completed
			202.25		98	1.027-1.035 (20°)	
Full	ethyl 3-(2,4-dimethyl-1,3-dioxolan-2-yl)propanoate			Soluble			
		5413-49-0	Clear colourless liquid; Oily carmellic aroma				
73rd	*1,3-Dioxane-2-propanoic acid, 2-methyl-, ethyl ester*			240-245	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1974	**cis-3-Hexenyl acetoacetate**	4489	C10H16O3	Practically insoluble or insoluble in water	NMR, IR, MS	1.445-1.455	SC: 2-3% cis-3-Hexenol
			184.23		93	0.980-0.990	
Full	(Z)-hex-3-en-1-yl 3-oxobutanoate			Soluble		(20°)	
73rd	*Butanoic acid, 3-oxo-, (3Z)-3-hexenyl ester*	84434-20-8	Clear colourless liquid; Earthy green floral aroma	254-255			
1975	**Hydroxycitronellal propyleneglycol acetal**	4485	C13H26O3	Practically insoluble or insoluble in water	MS	1.449-1.455 (25°)	
			230.34		95	0.957-0.967 (20°)	
Full	2,6-dimethyl-7-(4-methyl-1,3-dioxolan-2-yl)heptan-2-ol			Soluble			
73rd	*1,3-Dioxolane-2-hexanol, alpha,alpha,epsilon,4-tetramethyl-*	93804-64-9	Clear colourless liquid; Delicate green to floral aroma	306-307	1		
1976	**Propyleneglycol diacetate**	4464	C7H12O4	Very slightly soluble in water	NMR, MS	1.412-1.416	
			160.17		96	1.055-1.060 (20°)	
Full	propane-1,2-diyl diacetate			Soluble			
73rd	*1,2-Diacetoxypropane, 1,2-Propanediol, diacetate, 1,2-Propylene diacetate, Methylethylene acetate, Methylethylene diacetate, Propylene acetate*	623-84-7	Colourless liquid; Very mild fruity acetic aroma	189-191	1		
1977	**Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid**	4442	C20H36O4	Practically insoluble or insoluble in water	NMR, IR, MS	1.455-1.462	Mixture: 46% 6-(5-Decenoyloxy)decenoic acid;
			340.50		96	0.936-0.948	54% 6-(6-Decenoyloxy)decenoic acid
Full	Mixture of 6-(dec-5-enoyloxy)decanoic acid and 6-(dec-6-enoyloxy)decanoic acid			Soluble		(20°)	
73rd		85392-05-8 / 85392-06-9	Clear colourless liquid; Heavy fatty fruity aroma	460-465			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1978	**Propyleneglycol dipropionate**	4465	C9H16O4	Very slightly soluble in water	NMR, MS	1.415-1.421	
			188.22		98	1.009-1.015 (20°)	
Full	propane-1,2-diyl dipropionate						
			Clear colourless liquid;	Soluble			
73rd	*1,2-Propanediol, dipropanoate, 1,2-Propanediol, dipropionate, Propionic acid, propylene ester*	10108-80-2	Mild winey-fruity aroma	228-230	1		
1979	**Propyleneglycol monobutyrate (mixture of isomers)**	4488	C7H14O3	Slightly soluble in water	NMR, MS	1.422-1.430	Mixture of isomers: 60-63% 2-Hydroxypropyl butyrate; 28-29% 1-Hydroxypropan-2-yl butyrate; 6-10% Propyleneglycol dibutyrate
			146.18		88	0.990-0.998 (20°)	
Full	Mixture of 2-hydroxypropyl butyrate and 1-hydroxypropan-2-yl butyrate						
		29592-95-8	Clear colourless liquid; Mild fruity ethereal aroma	Soluble			
73rd	*Butanoic acid, monoester with 1,2-propanediol*			227-228	1		
1980	**Propyleneglycol dibutyrate**	4466	C11H20O4	Practically insoluble or insoluble in water	NMR, MS	1.420-1.426	
			216.27		98	0.977-0.982 (20°)	
Full	propane-1,2-diyl dibutyrate						
			Clear colourless liquid;	Soluble			
73rd	*1,2-Propanediol dibutyrate, Bibutyryl 1,2-propyleneglycol, Butanoic acid, 1-methyl-1,2-ethanediyl ester, Butyric acid, propylene ester*	50980-84-2	Mild sweet fruity slightly buttery aroma	266-268	1		

JECFA No / Status / Session	Name / Chemical Name / *Synonyms*	FEMA / FLAVIS / COE / CAS	Chemical formula / M.W. / Physical form / odour	Solubility / Solubility in ethanol / B.P. °C	ID test / Assay min % / Acid Value	R. I. / S. G.	Other requirements / Information required
1981	**Propyleneglycol mono-2-methylbutyrate** (mixture of isomers)	4467	C8H16O3	Practically insoluble or insoluble in water	MS	1.422-1.432	Mixture of isomers: 60% 2-Hydroxypropyl 2-methylbutanoate; 29% 1-Hydroxypropan-2-yl 2-methylbutanoate; SC: 7-8% Di-2-methylbutyrate propyleneglycol ester
			160.21		96	0.968-0.978 (20°)	
Full	Mixture of 2-hydroxypropyl 2-methylbutanoate and 1-hydroxypropan-2-yl 2-methylbutanoate	923593-56-0 / 923593-57-1	Clear colourless liquid; Mild fruity ethereal aroma	Soluble			
73rd				238-240	1		
1982	**Propyleneglycol di-2-methylbutyrate**	4468	C13H24O4	Practically insoluble or insoluble in water	NMR	1.422-1.427	
			244.33		98	0.952-0.957 (20°)	
Full	propane-1,2-diyl bis(2-methylbutanoate)						
		155514-30-0	Clear colourless liquid; Mild fruity to slightly buttery aroma	Soluble			
73rd				291-296	1		
1983	**Propyleneglycol monohexanoate (mixture of isomers)**	4469	C9H18O3	Practically insoluble or insoluble in water	MS	1.430-1.436	Mixture of isomers: 62% 2-Hydroxypropyl hexanoate; 35% 1-Hydroxypropan-2-yl hexanoate; SC: 2% Propyleneglycol dihexanoic acid ester
			174.24		98	0.963-0.969 (20°)	
Full	Mixture of 2-hydroxypropyl hexanoate and 1-hydroxypropan-2-yl hexanoate		Clear colourless liquid; Mild fruity to green ethereal aroma	Soluble			
		39556-41-7 / 170678-49-6					
73rd	*1,2-Propanediol, 1-hexanoate, Hexanoic acid, 2-hydroxy-1-methylethyl ester*			263-265	1		
1984	**Propyleneglycol dihexanoate**	4470	C15H28O4	Practically insoluble or insoluble in water	MS	1.430-1.435	
			272.38		98	0.943-0.948 (20°)	
Full	propane-1,2-diyl dihexanoate						
		50343-36-7	Clear colourless liquid; Mild fruity to green aroma	Soluble			
73rd	*1,2-Propanediol dihexanoate, 1,2-Propylene glycol dicaproate, Hexanoic acid, 1-methyl-1,2-ethanediyl ester*			335-337	1		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1985	**Propyleneglycol dioctanoate**	4471	C19H36O4	Practically insoluble or insoluble in water	NMR, MS	1.436-1.442	
			328.49		98	0.923-0.929 (20°)	
Full	propane-1,2-diyl dioctanoate						
			Clear colourless liquid; Rich fatty fruity aroma	Soluble			
73rd	*1,2-Propanediol dioctanoate, 1,2-Propylene glycol dicaprylate, Octanoic acid, 1-methyl-1,2-ethanediyl ester, Propylene glycol dicaprylate*	7384-98-7		396-398	1		
1986	**2-Oxo-3-ethyl-4-butanolide**	4460	C6H8O3	Practically insoluble or insoluble in water	NMR, MS	NA	m.p. = 57-63 ºC
			128.13		96	NA	
Full	4-ethyldihydrofuran-2,3-dione						
			Clear colourless to pale yellow oily liquid; Faint sweet non-descript aromatic aroma	Soluble			
73rd	*2,3-Furandione, 4-ethyldihydro-*	923291-29-6		NA			
1987	**Ethyl 5-hydroxyoctanoate**	4610	C10H20O3	Practically insoluble or insoluble in water	MS	1.438-1.448	SC: 5-6% Ethanol; 17-18% 1,5-Octanolide; 21-24% 5-Hydroxydecanoic acid and Ethyl 5-hydroxyoctanoate ester
			188.26		50	0.960 - 0.970 (20°)	
Full	ethyl 5-hydroxyoctanoate						
			Colourless clear to slightly yellow liquid; Sweet fatty pinapple fruit-like aroma	Soluble			
73rd	*Octanoic acid, 5-hydroxy-, ethyl ester*	75587-05-2		252-254			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1988	**Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone (Safety evaluation not completed)**	4611	C16H30O5 302.41	Practically insoluble or insoluble in water	NMR, MS 73 (mixture)	1.449-1.459 1.006-1.026 (20°)	Safety evaluation not completed; 73% mixture (25% Isopropylideneglyceryl 5-hydroxydecanoate and 47-49% delta-Decalactone); SC: 22-24% 1,3-dioxolane-4-methanol; 1-5% 2-Propyl 5-hydroxydecanoate
Full	Mixture of (2,2-dimethyl-1,3-dioxolan-4-yl)methyl 5-hydroxydecanoate and 6-pentyltetrahydro-2H-pyran-2-one		Colourless to slightly yellow clear liquid; Sweet fatty peach-like aroma	Soluble 160-162 (10 mm Hg)			
73rd	*Decanoic acid, 5-hydroxy-, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester*	172201-58-0 / 705-86-2					
1989	**5-Pentyl-3H-furan-2-one**	4323	C9H14O2 154.21	Sparingly soluble in water; soluble in non-polar solvents	NMR 95	1.447-1.459 0.970-0.980	
Full	5-pentylfuran-2(3H)-one						
73rd	*2(3H)-Furanone, 5-pentyl-, 4-Hydroxy-3-nonenoic acid lactone, 5-(1-Pentyl)-3H-furan-2-one, 5-Amyl-3H-furan-2-one*	51352-68-2	Clear colourless or pale yellow liquid; Tropical fruit aroma with milky dairy notes	Sparingly soluble 73-74 (1.2 mm Hg)			
1990	**5-Hydroxy-4-methylhexanoic acid delta-lactone**	4141	C7H12O2 128.17	Slightly soluble in water	NMR, IR, MS 96	1.452-1.458 1.020-1.242	
Full	5,6-dimethyltetrahydro-2H-pyran-2-one						
73rd	*4-Methyl-5-hydroxyhexanoic acid lactone, 5,6-Dimethyltetrahydropyran-2-one, Hexanoic acid, 5-hydroxyl-4-methyl-, delta-lactone*	10413-18-0	Colourless to yellow liquid; Minty fruit-like aroma	Soluble 59-60 (1.9 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1991	**Isoambrettolide**	4145	C16H28O2	Soluble in non-polar solvents; insoluble in water	NMR, IR	1.477-1.482	SC: 1-3% (Z)-isomer
			252.39		95	0.949-0.957	
Full	oxacycloheptadec-10-en-2-one	10.063					
73rd	*9-Hexadecenoic acid, 16-hydroxy-, omicron-lactone, delta-9-Isoambrettolic acid, lactone*	28645-51-4	Clear colourless or pale yellow liquid; Sweet musky fruity aroma	Soluble 1.5-1.6 (0.1 mm Hg)			
1992	**7-Decen-4-olide**	4439	C10H16O2	Practically insoluble or insoluble in water	NMR, IR, MS	1.464-1.470	Mixture of isomers: 86-93% cis, 3-10 % trans
			168.23		96	0.979-0.986 (20°)	
Full	5-(hex-3-en-1-yl)dihydrofuran-2(3H)-one						
73rd	*2(3H)-Furanone, 5-(3-hexenyl)dihydro-*	67114-38-9	Almost colourless oily liquid; Powerful and very diffusive, fatty buttery, oily-nut-like aroma	Soluble 277-280			
1993	**9-Decen-5-olide**	4440	C10H16O2	Practically insoluble or insoluble in water	MS	1.434-1.454	
			168.23		97	0.915-0.973 (20°)	
Full	6-(pent-4-en-1-yl)tetrahydro-2H-pyran-2-one						
73rd	*2H-Pyran-2-one, tetrahydro-6-(4-pentenyl)-, 9-Decenoic acid, 5-hydroxy-, delta-lactone*	74585-00-5	Colourless viscous liquid; Strong sweet creamy nut-like aroma	Soluble 276-279			
1994	**8-Decen-5-olide**	4441	C10H16O2	Practically insoluble or insoluble in water	NMR, IR, MS	1.470-1.480	Mixture of isomers: 90-91% cis, 4-5% trans
			168.23		95	0.975-1.007 (20°)	
Full	6-(pent-3-en-1-yl)tetrahydro-2H-pyran-2-one	10.040					
73rd	*2H-Pyran-2-one, tetrahydro-6-(3-pentenyl)-, 8-Decenoic acid, 5-hydroxy-, delta-lactone*	32764-98-0	Clear colourless to pale yellow liquid; Oily, fruity, floral petal, jasmin, peach, apricot aroma	Soluble 300	5		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1995	**Orin lactone**	4449	C11H18O2	Practically insoluble or insoluble in water	MS	1.454-1.484	
			182.26		99	0.960-0.991 (20°)	
Full	5-methyl-5-(4-methylpent-3-en-1-yl)dihydrofuran-2(3H)-one						
		134359-15-2	Clear colourless liquid; Sweet fruity aroma reminiscent of apple	Soluble			
73rd	*(+/-)-4,8-Dimethylnon-7-en-4-olide, 2(3H)-Furanone, dihydro-5-methyl-5-(4-methyl-3- pentenyl)-*			280-282			
1996	**9-Dodecen-5-olide**	4445	C12H20O2	Practically insoluble or insoluble in water	MS	1.457-1.485	Mixture of isomers: 84-91% cis, 4-11% trans
			196.29		95	0.949-0.955 (20°)	
Full	6-(hept-4-en-1-yl)tetrahydro-2H-pyran-2-one						
		15456-68-5	Clear colourless liquid; Tenacious fatty fruity aroma	Soluble			
73rd	*9-Dodecenoic acid, 5-hydroxy-, delta-lactone*			309-311			
1997	**9-Tetradecen-5-olide**	4448	C14H24O2	Practically insoluble or insoluble in water	MS	1.445-1.472	Mixture of isomers: 91-94% cis, 3-4% trans
			224.34		97	0.921-0.952 (20°)	
Full	6-(non-4-en-1-yl)tetrahydro-2H-pyran-2-one						
		15456-70-9	Clear colourless liquid; Strong fatty fruit-like Aroma	Soluble			
73rd	*9-Tetradecenoic acid, 5-hydroxy-, delta-lactone*			343-345			
1998	**gamma-Octadecalactone**	4446	C18H34O2	Practically insoluble or insoluble in water	MS	NA	m.p. = 36-40 ºC
			282.46		95	NA	
Full	5-tetradecyldihydrofuran-2(3H)-one						
		502-26-1	Clear colourless liquid; Very weak waxy fatty aroma	Soluble			
73rd	*2(3H)-Furanone, dihydro-5-tetradecyl-, 4-Octadecanolide, gamma-Stearolactone, Octadecanoic acid, 4-hydroxy-, gamma-lactone*			NA	10		

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
1999	**delta-Octadecalactone**	4447	C18H34O2	Practically insoluble or insoluble in water	MS	NA	m.p. = 33-39 ºC
			282.46		95	NA	
Full	6-tridecyltetrahydro-2H-pyran-2-one						
		1227-51-6	Clear waxy solid; Weak fatty waxy aroma	Soluble			
73rd	*2H-Pyran-2-one, tetrahydro-6-tridecyl-, 5-Octadecanolide, delta-Stearolactone, Octadecanoic acid, 5-hydroxy-, delta-lactone*			NA	10		
2000	**4-Hydroxy-2-butenoic acid gamma-lactone**	4138	C4H4O2	Soluble in water	NMR, MS	1.466-1.472	
			84.07		97	1.183-1.187	
Full	furan-2(5H)-one	10.066					
			Colourless to pale brown yellow clear liquid; Rich winey meat-like aroma	Soluble			
73rd	*2,5-Dihydrofuranone, alpha, beta-Crotolactone, delta, alpha, beta-Butenolide*	497-23-4		52-53			
2001	**2-Nonenoic acid gamma-lactone**	4188	C9H14O2	Soluble in non-polar solvents; insoluble in water	NMR, IR, MS	1.457-1.463	
		10.054	154.21		97	0.982-0.986	
Full	5-pentylfuran-2(5H)-one						
			Colourless liquid; Minty fruit-like aroma	Soluble			
73rd	*2(5H)-Furanone, 5-pentyl-, 2-Nonenoic acid, 4-hydroxy-, gammalactone, 5-Pentyl-2-furanone*	21963-26-8		230-233			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2002	**4-Hydroxy-2,3-dimethyl-2,4-nonadienoic acid gamma-lactone**	4050	C11H16O2	Soluble in non-polar solvents; insoluble in water	NMR	1.560-1.575	SC: 1-2% 3,4-Dimethyl 5-ketobutanoic acid gamma lactone
			180.24		93	0.930-0.980 (20°)	
Full	3,4-dimethyl-5-pentylidenefuran-2(5H)-one	10.042					
		11873	Clear and colourless liquid; Spicy-herbal to mint-like aroma	Soluble			
73rd	*5-Pentylidene-3,4-dimethyl-2,5-dihydrofuran-2-one, Bovolide*	774-64-1		302-304			
2003	**Choline chloride**	4500	C5H14NOCl	Soluble in water	NMR, IR, MS	NA	m.p. > 300 ºC
			139.63		95	NA	
Full	2-hydroxy-N,N,N-trimethylethanaminium chloride						
			Colourless or white crystals also in the form of white crystalline solid	Soluble			
73rd	*2-Hydroxyethyl)trimethylammonium chloride, (beta-Hydroxyethyl)trimethylammonium chloride*	67-48-1		NA			
2004	**3-(Methylthio)propylamine**	4649	C4H11NS	Practically insoluble or insoluble in water	MS	1.489-1.495	
			105.20		98	0.958-0.964 (20°)	
Full	3-(methylthio)propan-1-amine	12.186					
			Clear slightly yellow liquid; Pungent penetrating aroma	Soluble			
73rd	*3-(Methylmercapto)propylamine, 1-Amino-3-(methylthio)propane, 3-(Methylsulfanyl)propylamine, 3-Aminopropyl methyl sulfide, S-Methylhomocysteamine*	4104-45-4		96-98 (60 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2005	**N-Ethyl-2,2-diisopropylbutanamide (Safety evaluation not completed)**	4557	C12H25NO	Practically insoluble or insoluble in water	MS	NA	Safety evaluation not completed;
			199.33		99	NA	
Full	N,2-diethyl-2-isopropyl-3-methylbutanamide						m.p. = 36-40°C
73rd	*N,2-Diethyl-2-(isopropyl)-3-methylbutyramide*	51115-70-9	White to off-white crystalline solid; Slight cooling mint aroma	Soluble NA			
2006	**Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide**	4558	C14H25NO	Insoluble in water	NMR, IR, MS	NA	m.p. = 166 ºC
			223.35		96	NA	
Full	N-(2-isopropyl-5-methylcyclohexyl)cyclopropanecarboxamide						
73rd		958660-02-1 / 958660-04-3	Pearlwhite powder; Mild savory broth-like umami aroma	Soluble NA			
2007	**(+/-)-N-Lactoyl tyramine (Safety evaluation not completed)**	4550	C11H15NO3	Very soluble in water; insoluble in pentane	NMR, IR, MS	1.570-1.576	Safety evaluation not completed;
			209.24		90	1.198-1.202	SC: 2-3% Lactic acid; 2-3% Ethyl lactate
Full	2-hydroxy-N-(4-hydroxyphenethyl)propanamide						
73rd	*2-Hydroxy-N-[2-(4-hydroxyphenyl)-ethyl]-propionamide, Lactoyl tyramine*	781674-18-8	Viscous brown liquid; Savoury cooked roasted aroma with green herbal undertones	Sparingly soluble 87-88			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2008	**N-(2-(Pyridin-2-yl)ethyl)-3-p-menthanecarboxamide**	4549	C18H28N2O	Slightly soluble in water	NMR	NA	m.p. = 83 ºC
			288.43		99	NA	
Full	2-isopropyl-5-methyl-N-(2-(pyridin-2-yl)ethyl)cyclohexanecarboxamide			Very soluble			
73rd		847565-09-7	Solid; Refreshing cool aroma	NA			
2009	**N-p-Benzeneacetonitrile** menthanecarboxamide	4496	C19H26N2O	Practically insoluble or insoluble in water	NMR, IR, MS	NA	m.p. = 145 ºC; Principal component has (1R, 3R, 4S) stereochemistry; 2-5% N-p-Benzeneacetonitrile-menthanecarboxamide, (1R, 3S, 4S), neo-isomer
			298.42		94	NA	
Full	N-(4-(cyanomethyl)phenyl)-2-isopropyl-5-methylcyclohexanecarboxamide	852379-28-3	Solid white powder; Refreshing cool aroma	Very slightly soluble			
73rd				NA			
2010	**N-(2-Hydroxyethyl)-2,3-dimethyl 2-isopropylbutanamide**	4602	C11H23NO2	Slightly soluble in water; soluble in hexanes	MS	NA	Safety evaluation not completed;
	(Safety evaluation not completed)		201.31		95	NA	m.p. = 60-65 ºC
Full	N-(2-hydroxyethyl)-2-isopropyl-2,3-dimethylbutanamide	883215-02-9	White to off-white crystalline powder;	Soluble			
73rd			Refreshing cool aroma	NA			
2011	**N-(1,1-Dimethyl-2-hydroxyethyl)-2,2-diethylbutanamide**	4603	C12H25NO2	Slightly soluble in water; soluble in hexanes	MS	NA	Safety evaluation not completed;
	(Safety evaluation not completed)		215.33		95	NA	m.p. = 50-55 ºC
Full	2,2-diethyl-N-(1-hydroxy-2-methylpropan-2-yl)butanamide			Soluble			
73rd		51115-77-6	White to off-white crystalline powder; Refreshing cool aroma	NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	**FLAVIS**	**M.W.**	**Solubility in ethanol**	**Assay min %**	**S. G.**	
Status	***Synonyms***	**COE**	**Physical form / odour**	**B.P. °C**	**Acid Value**		**Information required**
Session		**CAS**					
2012	**4-Propenylphenol**	4062	C9H10O	Soluble in non-polar solvents; insoluble in water	IR, MS	NA	Mixture of isomers: 90-91% cis, 4-5% trans
			134.18		95	NA	m.p. = 77-81 ºC
Full	4-(prop-1-en-1-yl)phenol	04.058					
		11218	Colourless solid;	Soluble			
73rd			Pungent spicy phenolic				
		539-12-8	aroma	NA			
2013	**2,4,6-Trimethylphenol**	4329	C9H12O	Sparingly soluble in water	NMR, IR, MS	NA	m.p. = 70-74 ºC
			136.19		98	NA	
Full	2,4,6-trimethylphenol						
			Pale red crystalline	Soluble			
73rd	*1-Hydroxy-2,4,6-trimethylbenzene, 2-Hydroxymesitylene, Hydroxymesitylene, Mesitol, Mesityl alcohol*	527-60-6	solid; Slight phenolic aroma	220-221 (76 mm Hg)			
2014	**Sodium 3-methoxy-4-hydroxycinnamate**	3812	C10H10O4Na	Soluble in water; insoluble in fats and oils	NMR	NA	m.p. > 300 ºC (starts to decompose ~175 °C);
			217.18		93	NA	SC: 2-5% Vanillin
Full	sodium-3-(4-hydroxy-3-methoxyphenyl)acrylate						
			Light yellow solid	Soluble			
73rd	*3-(4-Hydroxy-3-methoxyphenol)-2-propenoic acid, monosodium salt, Cinnamic acid, 4-hydroxy-3-methoxy-, monosodium salt, Ferulic acid, sodium salt*	24276-84-4	powder; Sweet clovey phenolic aroma	NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2015	**Guaiacol butyrate**	4607	C11H14O3	Practically insoluble or insoluble in water	NMR, MS	1.522-1.532	
			194.23		95	1.064-1.074	
Full	2-methoxyphenyl butyrate						
73rd	*Butanoic acid, 2-methoxyphenyl ester, Butyric acid, o-methoxyphenyl ester, Phenol, o-methoxy-, butyrate*	4112-92-9	Clear colourless to light yellow liquid; Fruity nutty aroma	Soluble 96-97 (2 mm Hg)			
2016	**Guaiacol isobutyrate**	4608	C11H14O3	Practically insoluble or insoluble in water	NMR, MS	1.517-1.527	
			194.23		95	1.056-1.065	
Full	2-methoxyphenyl isobutyrate						
73rd	*Propanoic acid, 2-methyl-, 2-methoxyphenyl ester*	723759-62-4	Clear colourless to light yellow liquid; Fruity nutty aroma	Soluble 78-80 (1 mm Hg)			
2017	**Guaiacol propionate**	4609	C10H12O3	Practically insoluble or insoluble in water	NMR, MS	1.528-1.538	
			180.20		95	1.092-1.102	
Full	2-methoxyphenyl propionate						
73rd	*Guaiacyl propionate, Phenol, o-methoxy-, propionate, Propionyl guaiacolate*	7598-60-9	Clear colourless to light yellow liquid; Fruity nutty with a hint of vanilla aroma	Soluble 117-119 (8 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2018	**4-(2-Propenyl)phenyl-beta-D-glucopyranoside**	4548	C15H20O6	Practically insoluble or insoluble in water	NMR, IR, MS	NA	m.p. = 147-149 ºC
			296.32		95	NA	
Full	(2S,3R,4S,5S,6R)-2-(4-allylphenoxy)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol			Soluble			
		64703-98-6	White powder; Sweet aroma				
73rd	*Chavicol beta-D-glucoside, p-Allylphenyl beta-D-glucopyranoside*			NA			
2019	**Phenyl butyrate**	4621	C10H12O2	Practically insoluble or insoluble in water; soluble in ether	MS	1.448-1.494	
			164.20		97	1.020-1.028 (20°)	
Full	phenyl butyrate			Soluble			
		4346-18-3	Colourless liquid; Sweet floral aroma				
73rd	*Butanoic acid, phenyl ester, Butyric acid, phenyl ester, Phenyl butanoate*			63-65 (3 mm Hg)			
2020	**Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid**	4660	C9H10O5	Sparingly soluble in water	NMR, IR, MS	NA	m.p. = 126-127 ºC
			198.17		95	NA	
Full	2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid			Sparingly soluble			
			Pale yellow powder; Sweet vanilla aroma				
73rd	*(4-Hydroxy-3-methoxyphenyl)glycolic acid, 4-Hydroxy-3-methoxymandelic acid, Vanillinmandelic acid, Vanillomandelic acid, Vanillylmandelic acid, Vanilmandelic acid*	55-10-7		NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2021	**1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one**	4665	C17H26O3	Practically insoluble or insoluble in water	NMR, IR, MS	NA	m.p. = 32-33 ºC
			278.39		95	NA	
Full	1-(4-hydroxy-3-methoxyphenyl)decan-3-one			Soluble			
73rd	*[6]-Gingerone, 3-Decanone, 1-(4-hydroxy-3-methoxyphenyl)-, Heptyl 4-hydroxy-3-methoxyphenethyl ketone, Paradol*	27113-22-0	White powder; Spicy herbal aroma	NA			
2022	**3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one**	4390	C15H14O5	Slightly soluble in water	NMR, IR, MS	NA	m.p. = 260-262 ºC
			274.27		99	NA	
Full	3-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)propan-1-one			Sparingly soluble			
73rd	*2',4',6'-Trihydroxy-3-(4- hydroxyphenyl) propiophenone, Dihydronaringenin, Naringenin dihydrochalcone, Phloretin, Phloretol*	60-82-2	Pearl white powder; Sweet aroma	NA			
2023	**Magnolol**	4559	C18H18O2	Slightly soluble in water; soluble in DMSO	MS	NA	m.p. = 101-104 ºC; SC: 3-7% Honokiol; 1-2% Eudesmol
			266.33		92	NA	
Full	5,5'-diallyl-[1,1'-biphenyl]-2,2'-diol			Sparingly soluble			
73rd	*[1,1'-Biphenyl]-2,2'-diol, 5,5'-di-2-propenyl-, 2,2'-Bichavicol, 2,2'-Biphenyldiol, 5,5'-diallyl-*	528-43-8	White powder; Bitter aroma	NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2024	**5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one**	4313	C16H14O6	Sparingly soluble in water	NMR, IR, MS	NA	m.p. = 226-227 ºC
			302.28		95	NA	
Full	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one			Soluble			
73rd	*(+/-)-5,7,3'-Trihydroxy-4'-methoxyflavanone, (+/-)-Hesperetin, 4H-1-Benzopyran-4-one, 2,3-dihydro-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-*	69097-99-0	Light yellow to light tan powder; Faint fatty vanillic aroma	NA			
2025	**Dimethylbenzyl carbinyl crotonate**	4403	C14H18O2	Practically insoluble or insoluble in water; soluble in oils	MS	1.505-1.511	
			218.29		97	0.995-1.003 (20°)	
Full	2-methyl-1-phenylpropan-2-yl but-2-enoate			Soluble			
73rd	*2-Butenoic acid, 1,1-dimethyl-2-phenylethyl ester*	93762-34-6	Colourless oily liquid; Powerful, warm, herbaceous, fruity-spicy aroma	80-82 (10 mm Hg)			
2026	**Dimethylbenzyl carbinyl hexanoate**	4404	C16H24O2	Practically insoluble or insoluble in water; soluble in oils	MS	1.479-1.486	
			248.36		96	0.952-0.959 (20°)	
Full	2-methyl-1-phenylpropan-2-yl hexanoate			Soluble			
73rd	*Hexanoic acid, 1,1-dimethyl-2-phenylethyl ester*	891781-90-1	Colourless oily liquid; Powerful, warm, herbaceous aroma	79-81 (10 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2027	**Caryophyllene alcohol**	4410	C15H26O	Practically insoluble or insoluble in water	MS	1.498-1.503	SC: 3-6% Dihydrocloven-9-ol
			222.37		92	0.983-0.989 (20°)	
Full	4,4,8-trimethyltricyclo[6.3.1.02,5]dodecan-1-ol						
		472-97-9	White crystalline solid; Warm moss-like, spicy aroma	Soluble			
73rd				287-297			
2028	**Cubebol**	4497	C15H26O	Slightly soluble in water	NMR, IR, MS	NA	m.p. = 64 -65 ºC
			222.36		95	NA	
Full	(3S,3aR,3bR,4S,7R,7aR)-4-isopropyl-3,7-dimethyloctahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-ol						
		23445-02-5	White solid crystals; Warm spicy naturally cooling mint-like aroma	Soluble			
73rd	*Cubeb camphor*			NA			
2029	**(-)-Sclareol**	4502	C20H36O2	Practically insoluble or insoluble in water	MS	NA	m.p. = 105-107 ºC
			308.50		98	NA	
Full	(1R,2R,8aS)-1-((R)-3-hydroxy-3-methylpent-4-en-1-yl)-2,5,5,8a-tetramethyldecahydronaphthalen-2-ol	02.206					
		10311	Solid; Bitter herbaceous hay-like aroma	Soluble			
73rd	*Labd-14-ene-8,13-diol, (13R)-*	515-03-7		NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2030	**(+)-Cedrol**	4503	C15H26O	Slightly soluble in water	MS	NA	m.p. = 74-77 ºC
					95	NA	
Full	(3R,3aS,6R,7R,8aS)-3,6,8,8-tetramethyloctahydro-1H-3a,7-methanoazulen-6-ol	02.120	222.37				
73rd	*8-beta, H-Cedran-8-ol*	77-53-2	Pale yellow to yellow green solid; Sweet fruity cedar-like aroma	Soluble NA			
2031	**alpha-Bisabolol**	4666	C15H26O	Practically insoluble or insoluble in water	NMR, IR, MS	1.493-1.499	SC: 1-2% beta-Bisabolol
			222.37		93	0.927-0.935	
Full	(S)-6-methyl-2-((S)-4-methylcyclohex-3-en-1-yl)hept-5-en-2-ol						
73rd	*Kamillosan, Levomenol*	23089-26-1	Clear colourless liquid; Fruity nutty aroma with hints of coconut	Soluble 151-152 (12 mmHg)			
2032	**3-Methyl-2,4-nonedione**	4057	C10H18O2	Soluble in hexane, diethylether; insoluble in water	NMR, IR, MS	1.448-1.454	
			170.25		97	0.923-0.927	
Full	3-methylnonane-2,4-dione	07.184					
73rd	*2,4-Nonanedione, 3-methyl-*	113486-29-6	Colourless to yellowish liquid; Fruity aroma with vanilla top notes	Soluble 51-53 (1 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2033	**Acetoin propyleneglycol ketal**	4532	C7H14O3	Soluble in water	MS	1.430-1.438	
			146.18		96	1.034-1.042 (20°)	
Full	1-(2,4-dimethyl-1,3-dioxolan-2-yl)ethanol						
		94089-23-3	Colourless to pale yellow viscous liquid; Fatty buttery aroma	Soluble			
73rd				75-77 (25 mm Hg)			
2034	**Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone**	3989	C7H14O2	Soluble in water	NMR, IR, MS	1.424-1.434	Mixture: 77% 3-Hydroxy-5-methyl-2-hexanone; 20% 2-Hydroxy-5-methyl-3-hexanone
			130.18		97	0.922-0.932	
Full	Mixture of 3-hydroxy-5-methylhexan-2-one and 2-hydroxy-5-methylhexan-3-one						
		163038-04-8 / 246511-74-0	Colourless liquid; Sweet, chocolate-like aroma	Soluble			
73rd				39-41 (0.06 mm Hg)			
2035	**3-Hydroxy-2-octanone**	4139	C8H16O2	Practically insoluble or insoluble in water	NMR	1.431-1.437	
			144.21		98	0.927-0.933	
Full	3-hydroxyoctan-2-one	07.238		Soluble			
			Colourless liquid;				
73rd		37160-77-3	Brown nutty aroma	90-91			
2036	**2,3-Octanedione**	4060	C8H14O2	Soluble in non-polar solvents	NMR, IR, MS	1.419-1.424	
			142.20		95	0.905-0.915	
Full	octane-2,3-dione	07.248					
		11166	Clear to yellow liquid; Fruity nutty aroma	Soluble			
73rd		585-25-1		57-59 (10 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2037	**4,5-Octanedione**	4533	C8H14O2	Practically insoluble or insoluble in water	MS	1.414-1.424	
			142.2		95	0.908-0.918 (20°)	
Full	octane-4,5-dione						
73rd	*4,5-Octadione, Bibutyryl, Di-n-butyryl, Dipropyl diketone*	5455-24-3	Yellow liquid; At high concentration powerful pungent, fatty buttery aroma; upon dilution pleasant creamy-buttery aroma	Soluble 68-70 (20 mm Hg)			
2038	**(+/-)-2-Hydroxypiperitone**	4143	C10H16O2	Slightly soluble in water	NMR, MS	NA	m.p. = 78-85 ºC
Full	2-hydroxy-6-isopropyl-3-methylcyclohex-2-enone	07.168	168.23		98	NA	
73rd	*1-Methyl-4-isopropyl-1-cyclohexen-2-ol-3-one, 1-p-Menthen-2-ol-3-one, 2-Hydroxy-p-menth-1-en-3-one, Barosma camphor, Buccocamphor, Buchu camphor*	490-03-9	Colourless to pale yellow crystals; Minty tea aroma	Soluble 231-233			
2039	**1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone**	4303	C12H18O6	Sparingly soluble in water	NMR, IR, MS	NA	m.p. = 90-91 ºC
			258.27		95	NA	
Full	1,1'-(6a-hydroxy-2,3a,5-trimethyltetrahydrofuro[2,3-d][1,3]dioxole-2,5-diyl)diethanone	18114-49-3	Yellowish solid; Roasted buttery aroma	Soluble			
73rd	*Diacetyl trimer, Furo[2,3-d]-1,3-dioxol-6a(3aH)-ol, 2,5-diacetyldihydro-2,3a,5-trimethyl-,*			NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2040	**4-Hydroxyacetophenone**	4330	C8H8O2	Practically insoluble or insoluble in water	NMR,IR	NA	m.p. = 109-112 ºC
			136.15		98	NA	
Full	1-(4-hydroxyphenyl)ethanone	07.243					
73rd		99-93-4	White to off-white crystals, chips or chunks; Slight berry to sweet balsam aroma	Soluble NA			
2041	**3-Hydroxy-4-phenylbutan-2-one**	4052	C10H12O2	Soluble in non-polar solvents; insoluble in water	NMR, MS	1.524-1.534	SC: 3-5% 4-Hydroxy-4-phenylbutan-2-one
			164.20		93	1.079-1.089 (20°)	
Full	3-hydroxy-4-phenylbutan-2-one	07.242					
73rd	*2-Butanone, 3-hydroxy-4-phenyl-*	5355-63-5	Clear, colourless liquid; Fruit and floral aroma	Soluble 97-99 (1.0 mm Hg)			
2042	**2-Methoxyacetophenone**	4163	C9H10O2	Practically insoluble or insoluble in water	NMR, IR, MS	1.536-1.542	
			150.17		99	1.088-1.092	
Full	1-(2-methoxyphenyl)ethanone	07.254					
73rd	*2-Acetylanisole, 2-Methoxyphenyl methyl ketone*	579-74-8	Light yellowish liquid; Spicy mint-like aroma	Soluble 245-248			
2044	**2-Methylacetophenone**	4316	C9H10O	Practically insoluble or insoluble in water	NMR, IR, MS	1.526-1.532	
			134.18		95	1.023-1.029	
Full	1-(o-tolyl)ethanone	07.251					
73rd	*2-Acetyltoluene, 2-Methylphenyl methyl ketone, Ethanone, 1-(2-methylphenyl)-, Methyl 2-methylphenyl ketone, Methyl o-tolyl ketone, o- Acetyltoluene*	577-16-2	Colourless to pale yellow liquid; Nutty coconut aroma	Soluble 213-215			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2045	**2-Hydroxy-5-methylacetophenone**	4594	C9H10O2	Practically insoluble or insoluble in water	MS	NA	m.p. = 45-48 °C
			150.17		97	NA	
Full	1-(2-hydroxy-5-methylphenyl)ethanone						
73rd	*2-Acetyl-4-methylphenol, Acetophenone, 2'-hydroxy-5'-methyl-, o-Acetyl-p-cresol*	1450-72-2	Colourless to pale yellow solid; Sweet heavy-floral somewhat herbaceous aroma	Soluble NA			
2046	**Dihydrogalangal acetate (Safety evaluation not completed)**	4555	C13H16O4	Practically insoluble or insoluble in water	NMR, MS	NA	Safety evaluation not completed;
			236.26		99	NA	m.p. = 41.5-43.5 ºC
Full	1-(4-acetoxyphenyl)propyl acetate			Sparingly soluble			
73rd		129319-15-9	Solid; Tingling pungent spicey aroma	NA			
2047	**2,3,3-Trimethylindan-1-one**	4556	C12H14O	Practically insoluble or insoluble in water	NMR, IR, MS	1.532-1.542	
			174.24		95	1.015-1.025	
Full	2,3,3-trimethyl-2,3-dihydro-1H-inden-1-one						
73rd	*1-Indanone, 2,3,3-trimethyl-, Saffron indenone*	54440-17-4	Colourless to clear yellow liquid; Herbal spicy saffron leather tobacco aroma	Sparingly soluble 250-252			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2048	**4-(3,4-Methylenedioxyphenyl)-2-butanone**	2701	C11H12O3	Soluble in oils; insoluble in water	NMR	NA	m.p.= 47-54 ºC
			192.21		99	NA	
Full	4-(benzo[d][1,3]dioxol-5-yl)butan-2-one	07.031					
		165	Colourless crystals or white crystalline solid; Intensely sweet, floral aroma	Soluble			
73rd	*2-Butanone, 4-(1,3-benzodioxol-5-yl)-, Heliotropyl acetone, Piperonyl acetone*	55418-52-5		NA			
2049	**2-(trans-2-Pentenyl)cyclopentanone**	4284	C10H16O	Practically insoluble or insoluble in water	IR, MS	1.465-1.472	
			152.23		98	0.890-0.915	
Full	(E)-2-(pent-2-en-1-yl)cyclopentanone						
			Colourless liquid; Jasmine, lactonic coconut creamy aroma	Slightly soluble			
73rd	*Jasminone*	51608-18-5		67-69 (0.3 mm Hg)			
2050	**2-Cyclopentylcyclopentanone**	4514	C10H16O	Practically insoluble or insoluble in water	MS	1.475-1.481	
			152.23		97	0.975-0.983 (20°)	
Full	[1,1'-bicyclopentyl]-2-one						
		4884-24-6	Clear colourless liquid; Fruity green minty aroma	Soluble			
73rd	*[Bicyclopentyl]-2-one, 2-Cyclopentylcyclopentanone, Cyclopentanone, 2-cyclopentyl-*			104-107 (2 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2051	**Cyclohexanone diethyl ketal**	4516	C10H20O2	Practically insoluble or insoluble in water	MS	1.432-1.442	
			172.26		95	0.911-0.921 (20°)	
Full	1,1-diethoxycyclohexane						
73rd	*Cyclohexanone diethyl acetal, Rhumacetal*	1670-47-9	Colourless to pale yellow clear liquid; Fruity, liquor, rum, tobacco, woody aroma	Soluble 102-103 (45 mm Hg)			
2052	**2-Cyclohexenone**	4517	C6H8O	Very slightly soluble	MS	1.485-1.491	
			96.13		98	0.988-0.998 (20°)	
Full	cyclohex-2-enone						
73rd	*Cyclohexen-3-one*	930-68-7	Pale yellow to yellow clear liquid; In dilution, roasted savoury aroma with a green undertone	Soluble 100-101 (1 mm Hg)			
2053	**3,3,5-Trimethylcyclohexyl acetate**	4512	C11H20O2	Practically insoluble or insoluble in water	NMR, MS	1.437-1.445	SC: 6-7% 3,3,5-Trimethylcyclohexanol
			184.28		90	0.913-0.924 (20°)	
Full	3,3,5-trimethylcyclohexyl acetate						
73rd	*Cyclohexanol, 3,3,5-trimethyl-, acetate, Homomenthol acetate, Homomenthyl acetate*	67859-96-5	Clear colourless liquid; Mint herbal lavandin sweet aroma	Soluble 108-110 (13 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2054	**2,6,6-Trimethyl-2-hydroxycyclohexanone**	4531	C9H16O2	Practically insoluble or insoluble in water	MS	1.466-1.472	
			156.22		95	0.988-0.994 (20°)	
Full	2-hydroxy-2,6,6-trimethylcyclohexanone						
73rd	*2,2,6-Trimethyl-6-hydroxycyclohexanone, 6-Hydroxy-2,2,6-trimethylcyclohexanone, Cyclohexanone, 2-hydroxy-2,6,6-trimethyl-*	7500-42-7	Colourless liquid; Sweet tobacco-like aroma with herbaceous undertones	Soluble 58-65 (4 mm Hg)			
2055	**Cyclotene propionate**	4511	C9H12O3	Practically insoluble or insoluble in water	MS	1.479-1.484	SC: 4-5% Cyclotene
			168.19		92	1.092-1.097 (20°)	
Full	2-methyl-5-oxocyclopent-1-en-1-yl propionate						
73rd	*2-Cyclopenten-1-one, 2-hydroxy-3-methyl-, propionate, 2-Cyclopenten-1-one, 3-methyl-2-(1-oxopropoxy)-*	87-55-8	Colourless to yellow liquid; Creamy carmellic buttery aroma	Soluble 167-169			
2056	**Cyclotene butyrate**	4648	C10H14O3	Practically insoluble or insoluble in water; soluble in fats and oils	NMR, IR, MS	1.476-1.482	
			182.22		96	1.063-1.069 (20°)	
Full	2-methyl-5-oxocyclopent-1-en-1-yl butyrate						
73rd	*Butanoic acid, 2-methyl-5-oxo-1-cyclopenten-1-yl ester, Butyric acid, 2-methyl-5-oxo-1-cyclopenten-1-yl ester*	68227-51-0	Colourless clear liquid; Fruity nutty aroma	Soluble 116-117 (2 mm Hg)			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2057	**4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers)**	4663	C13H18O 190.28	Practically insoluble or insoluble in water	NMR, IR, MS 95	1.536-1.556 0.985-1.005	Mixture of isomers: (50% E,E; 50% E,Z); SC: 5-6% 4,7,9-Megastigmatrien-3-one
Full	Mixture of (E)-4-((E)-but-2-en-1-ylidene)-3,5,5-trimethylcyclohex-2-enone and (E)-4-((Z)-but-2-en-1-ylidene)-3,5,5-trimethylcyclohex-2-enone	13215-88-8	Clear to pale yellowish liquid; Fruity floral tobacco-like aroma	Soluble 95-110 (< 1 mm Hg)			
73rd	*2-Cyclohexen-1-one, 4-(2-butenylidene)-3,5,5-trimethyl-, Megastigmatrienone*						
2058	**4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers)**	4661	C13H20O3 224.30	Practically insoluble or insoluble in water Soluble	NMR, MS 98	NA NA	Mixture of isomers: 63-68% (E), 30-35% (Z) m.p. = 98-104 ºC
Full	Mixture of (E)-4-hydroxy-4-(3-hydroxybut-1-en-1-yl)-3,5,5-trimethylcyclohex-2-enone and (Z)-4-hydroxy-4-(3-hydroxybut-1-en-1-yl)-3,5,5-trimethylcyclohex-2-enone	24427-77-8	White powder; Fruity aroma	NA			
73rd							
2059	**(-)-8,9-Dehydrotheaspirone**	4518	C13H18O2 206.28	Practically insoluble or insoluble in water	MS 95	NA NA	m.p. = 175-180 ºC
Full	(S)-2,6,10,10-tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one			Soluble			
73rd	*1-Oxaspiro[4.5]deca-2,6-dien-8-one, 2,6,10,10-tetramethyl-, (S)-*	85248-56-2	Solid; Camphoraceous woody green aroma	NA			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2060	**(+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one**	4662	C13H18O2	Practically insoluble or insoluble in water	NMR, IR, MS	NA	m.p. = 105-106 ºC
			206.28		98	NA	
Full	2,6,10,10-tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one		White powder; Woody floral aroma	Soluble			
73rd		80722-28-7		NA			
2061	**Benzyl hexanoate**	4026	C13H18O2	Practically insoluble or insoluble in water	IR, MS	1.480-1.490	
			206.28		95	0.980-0.990	
Full	benzyl hexanoate						
73rd	*Benzyl caproate, Hexanoic acid, benzyl ester, Hexanoic acid, phenylmethyl ester*	6938-45-0	Colourless to pale yellow liquid; Green apricot fruity gardenia and jasmine aroma	Soluble 270-272			
2062	**o-Anisaldehyde**	4077	C8H8O2	Soluble in water and propylene glycol	NMR, IR, MS	NA	m.p.= 34-40 ºC
			136.15		97	NA	
Full	2-methoxybenzaldehyde						
73rd	*2-Methoxybenzenecarboxaldehyde, 2-Methoxyphenylformaldehyde, o-Formylanisole, Salicylaldehyde methyl ether*	135-02-4	Light yellow solid; Sweet powdery hawthorn, vanilla, and almond aroma	Soluble NA			
2063	**Prenyl benzoate**	4203	C12H14O2	Practically insoluble or insoluble in water	MS	1.514-1.521	
			190.24		95	1.016-1.025	
Full	3-methylbut-2-en-1-yl benzoate						
73rd	*2-Buten-1-ol, 3-methyl-, benzoate*	5205-11-8	Colourless liquid; Sweet, balsamic odour with tea-like quality and natural connotations	Soluble 109-111 (2 mm Hg)			

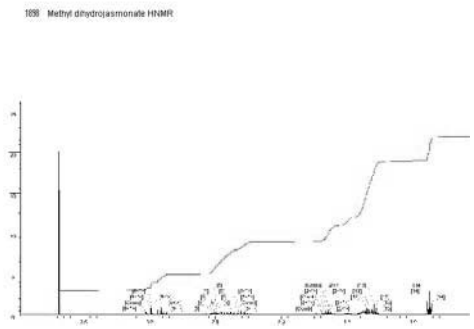
JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2064	**Benzyl levulinate**	4623	C12H14O3	Practically insoluble or insoluble in water	NMR, MS	1.503-1.509	
			206.24		95	1.095-1.101 (20°)	
Full	benzyl 4-oxopentanoate			Soluble			
73rd		6939-75-9	Viscous oil to waxy solid; Strong fruity aroma	316-318	1		
2065	**4-Methylbenzyl alcohol**	4624	C8H10O	Practically insoluble or insoluble in water	MS	NA	m.p. = 55-63 ºC
			122.16		97	NA	
Full	p-tolylmethanol			Soluble			
73rd	*(4-Methylphenyl)methanol, 4-(Hydroxymethyl)toluene, 4- Methylbenzenemethanol, p-Tolualcohol, p- Tolylcarbinol*	589-18-4	White solid; Weak floral aroma	NA	1		
2066	**Benzyl nonanoate**	4626	C16H24O2	Practically insoluble or insoluble in water	MS	1.481-1.487	
			248.36		97	0.953-0.959 (20°)	
Full	benzyl nonanoate			Soluble			
73rd	*Nonanoic acid, benzyl ester, Nonanoic acid, phenylmethyl ester*	6471-66-5	Colourless liquid; Sweet, floral aroma	126-127 (< 1 mm Hg)			
2067	**4-Methylbenzaldehyde propyleneglycol acetal**	4628	C11H14O2	Practically insoluble or insoluble in water	MS	1.507-1.515	
			178.23		95	1.041-1.051	
Full	4-methyl-2-(p-tolyl)-1,3-dioxolane			Soluble			
73rd	*1,3-Dioxolane, 4-methyl-2-(4-methylphenyl)-, 1,3-Dioxolane, 4-methyl-2-p-tolyl-*	58244-29-4	Viscous colourless liquid; Faint floral, bitter almond aroma	263-265			

JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2068	**2-Ethylhexyl benzoate**	4630	C15H22O2	Practically insoluble or insoluble in water	MS	1.487-1.497	
			234.33		95	0.963-0.973 (20°)	
Full	2-ethylhexyl benzoate						
			Colourless clear oily	Soluble			
73rd	*1-Hexanol, 2-ethyl-, benzoate, 2-Ethyl-1-hexanol benzoate, Benzoic acid, 2-ethylhexyl ester*	5444-75-7	liquid; Ethereal aroma	120-121 (3 mm Hg)			
2070	**(+/-)-Octan-3-yl formate**	4009	C9H18O2	Soluble in fats and oils; insoluble in water	NMR, IR, MS	1.413-1.417	
			158.24		98	0.865-0.875	
Full	octan-3-yl formate						
		84434-65-1	Colourless liquid; Minty,	Soluble			
73rd	*1-Ethylhex-1-yl formate, 3-Octanol, formate, Oct-3- yl formate*		spicy, herb-like aroma with fruity undertones	69-71 (7 mm Hg)			
2071	**(R)-(-)-1-Octen-3-ol**	4492	C8H16O	Insoluble in water	MS	1.435-1.441	
			128.21		98	0.832-0.838	
Full	(R)-oct-1-en-3-ol			Soluble			
		3687-48-7	Liquid; Strong genuine				
73rd			mushroom odour	173-175			
2072	**2-Pentyl 2-methylpentanoate**	4401	C11H22O2	Practically insoluble or insoluble in water; soluble in fats and oils	MS	1.410-1.146	
			186.29		99	0.847-0.853 (20°)	
Full	pentan-2-yl 2-methylpentanoate						
			Colourless to yellow	Soluble			
73rd	*Pentanoic acid, 2-methyl-, 1-methylbutyl ester*	90397-36-7	liquid; Strong penetrating pear-like aroma	76-77 (10 mm Hg)			

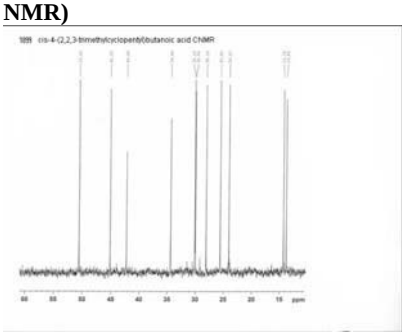
JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2073	**3-Octyl butyrate**	4402	C12H24O2	Practically insoluble or insoluble in water; soluble in fats and oils	NMR, MS	1.420-1.425	
			200.32		98	0.858-0.863 (20°)	
Full	octan-3-yl butyrate						
		20286-45-7	Colourless liquid; Green herbaceous odour	Soluble			
73rd	*Butanoic acid, 1-ethylhexyl ester, Butyric acid, 1-ethylhexyl ester*			243-245			
2074	**2-Decanone**	4271	C10H20O	Insoluble in water; soluble in fats and oils	NMR	1.421-1.431	
			156.27		96	0.821-0.831 (20°)	
Full	decan-2-one	07.150					
		11055	Liquid; Fatty peachy, aldehyde-like aroma	Insoluble			
73rd	*Methyl octyl ketone*						
		693-54-9		210-212			
2075	**6-Methyl-5-hepten-2-one propyleneglycol acetal**	4400	C11H20O2	Practically insoluble or insoluble in water; soluble in fats and oils	MS	1.439-1.446	SC: 7-9% 6-Methyl-6-hepten-2-one propyleneglycol acetal
			184.28		88	0.905-0.911 (20°)	
Full	2,4-dimethyl-2-(4-methylpent-3-en-1-yl)-1,3-dioxolane						
		68258-95-7	Colourless to slightly yellow liquid; Strong fatty, green citrus-like odour	Soluble			
73rd				107-108 (30 mm Hg)			
2076	**2-Nonanone propyleneglycol acetal**	4399	C12H24O2	Practically insoluble or insoluble in water; soluble in fats and oils	MS	1.430-1.435	
			200.32		97	0.882-0.888	
Full	2-heptyl-2,4-dimethyl-1,3-dioxolane			(20°)			
		165191-91-3	Colourless to pale yellow liquid; Fruity, floral, fatty, herbaceous odour	Soluble			
73rd				104-105 (11 mm Hg)			

Spectra of certain flavouring agents

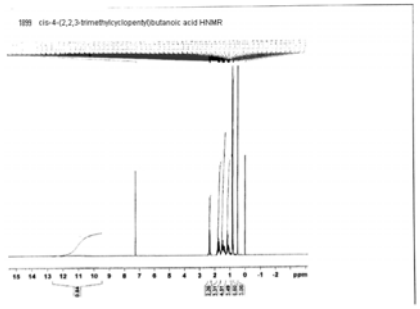
1898 Methyl dihydrojasmonate (1H-NMR)



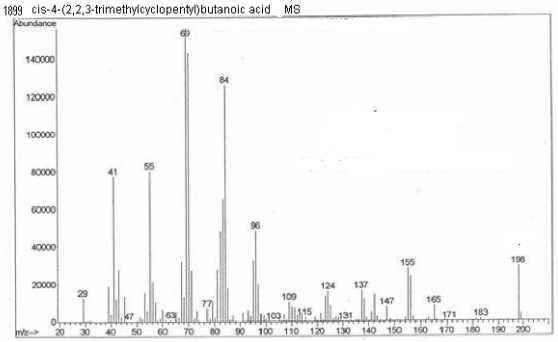
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (13C-NMR)



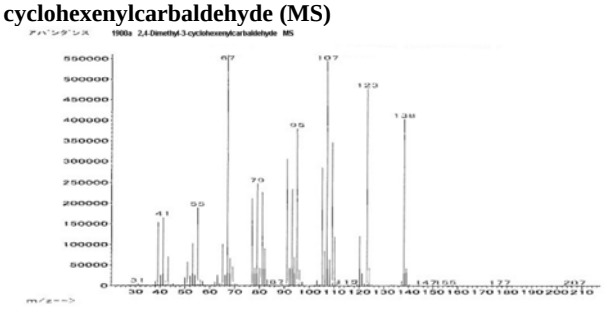
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (1H-NMR)



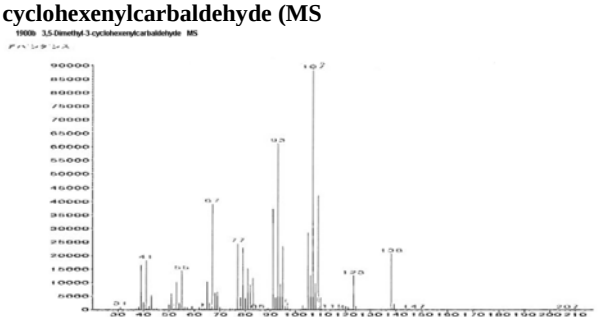
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (MS)



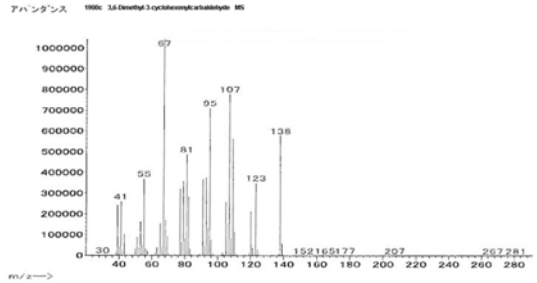
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS)



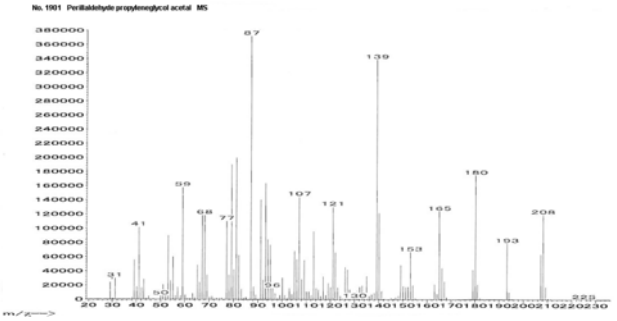
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS



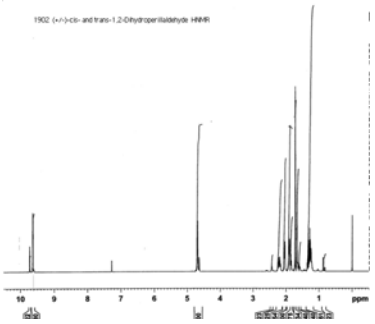
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS



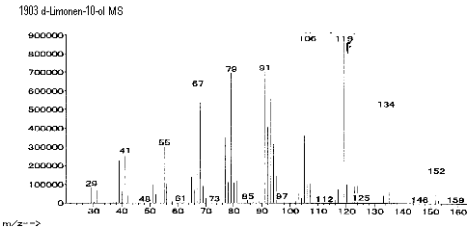
1901 Perillaldehyde propyleneglycol acetal (MS)



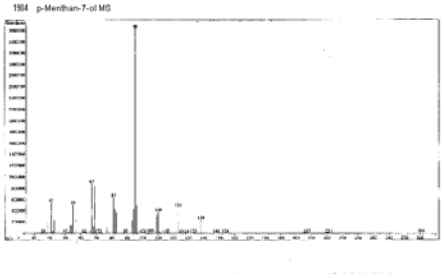
1902 (+/-)-cis- and trans-1,2-Dihydroperillaldehyde (1H-NMR)



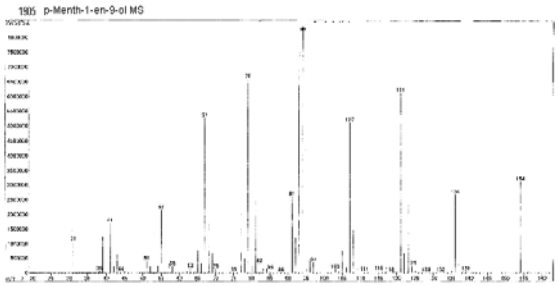
1903 d-Limonen-10-ol (MS)



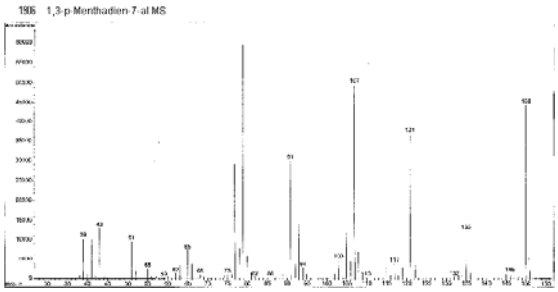
1904 p-Menthan-7-ol (MS)



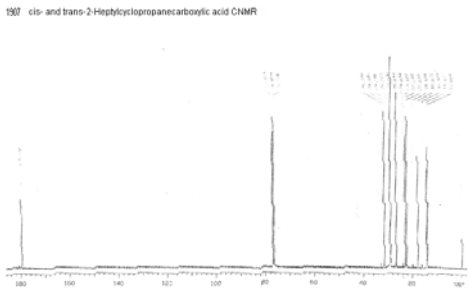
1905 p-Menth-1-en-9-ol (MS)



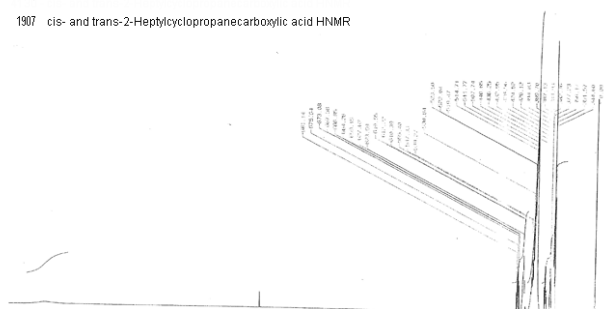
1906 1,3-p-Menthadien-7-al (MS)



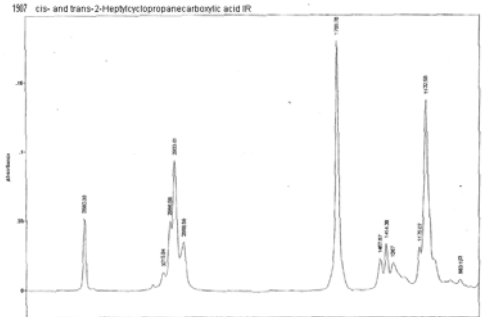
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (13C-NMR)



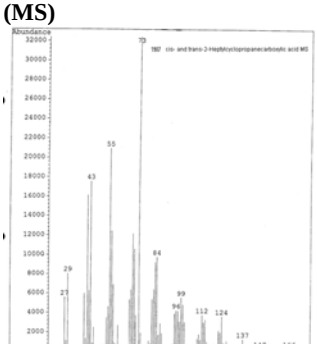
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (1H-NMR)



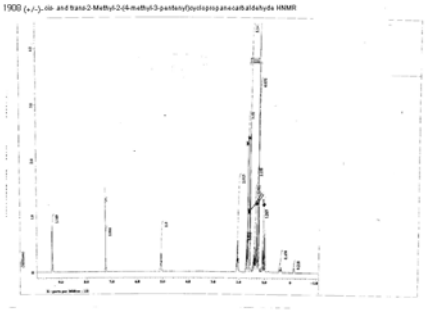
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (IR)



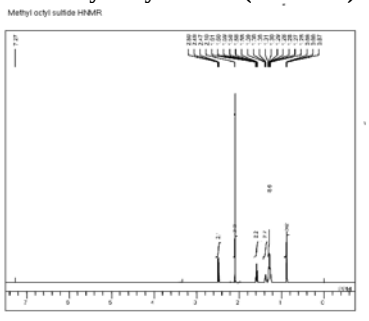
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (MS)



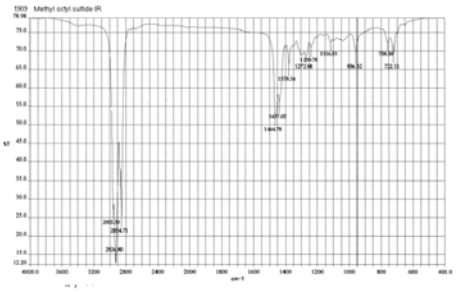
1908 (+/-)-cis- and trans-2-Methyl-2-(4-methyl-3-pentenyl)cyclopropanecarbaldehyde (1H-NMR)



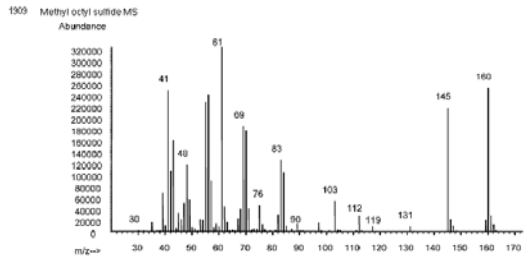
1909 Methyl octyl sulfide (1H-NMR)



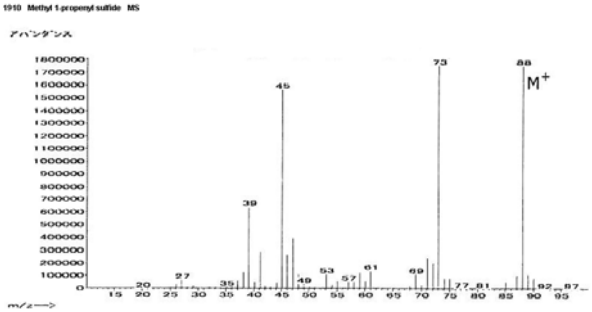
1909 Methyl octyl sulfide (IR)



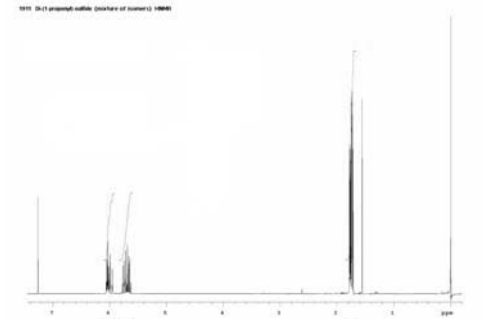
1909 Methyl octyl sulfide (MS)



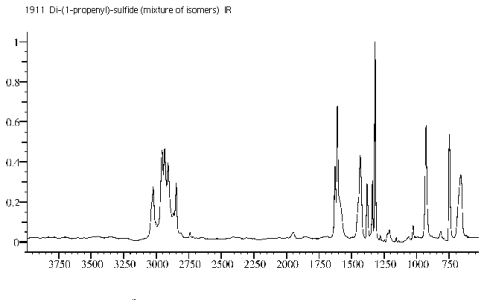
1910 Methyl 1-propenyl sulfide (MS)



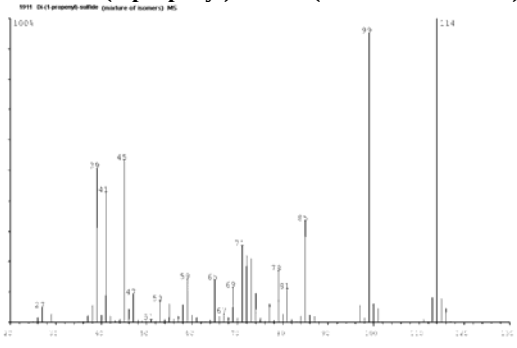
1911 Di-(1-propenyl) sulfide (mixture of isomers) (1H-NMR)



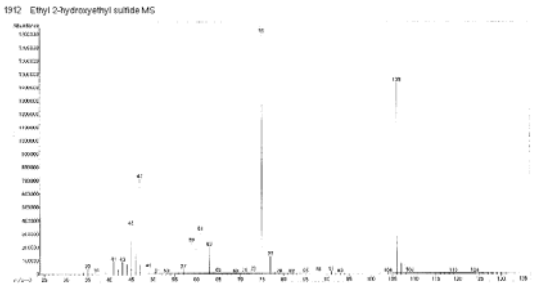
1911 Di-(1-propenyl) sulfide (mixture of isomers) (IR)



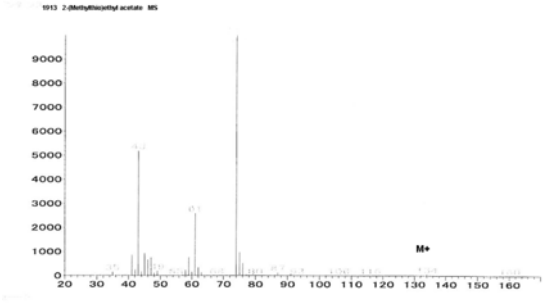
1911 Di-(1-propenyl) sulfide (mixture of isomers) (MS)



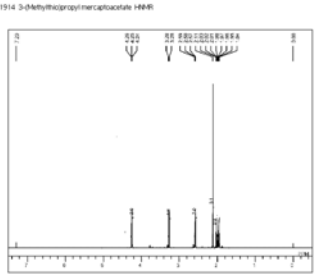
1912 Ethyl 2-hydroxyethyl sulfide (MS)



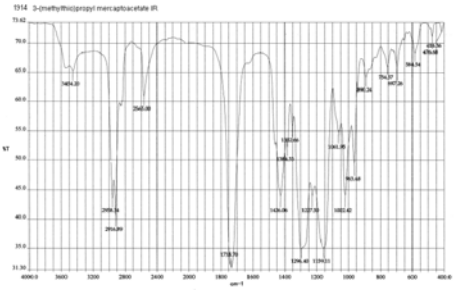
1913 2-(Methylthio)ethyl acetate (MS)



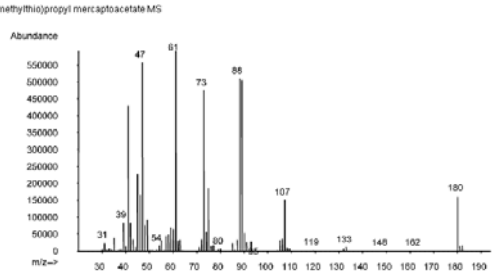
1914 3-(Methylthio)propyl mercaptoacetate (1H-NMR)



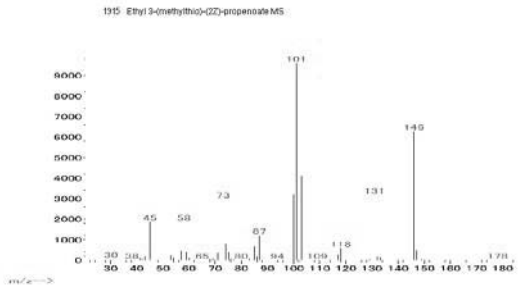
1914 3-(Methylthio)propyl mercaptoacetate (IR)



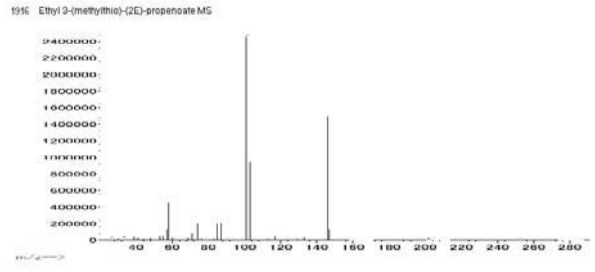
1914 3-(Methylthio)propyl mercaptoacetate (MS)



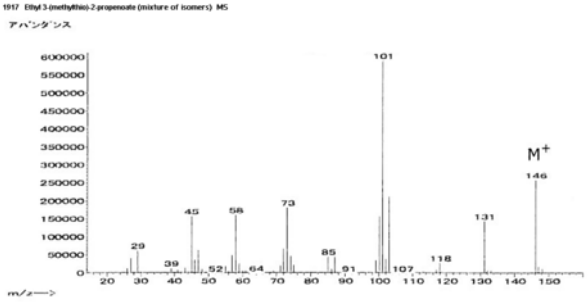
1915 Ethyl 3-(methylthio)-(2Z)-propenoate (MS)



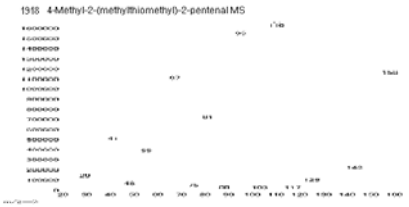
1916 Ethyl 3-(methylthio)-(2E)-propenoate (MS)



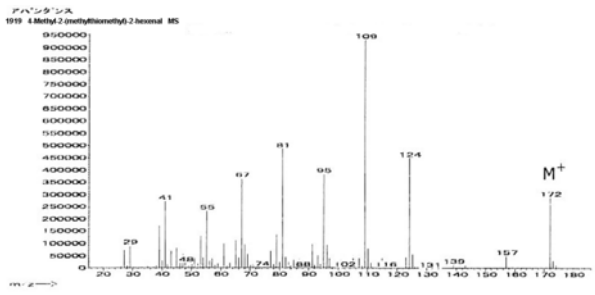
1917 Ethyl 3-(methylthio)-2-propenoate (mixture of isomers) (MS)



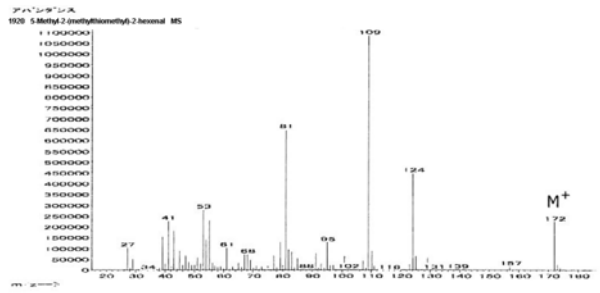
1918 4-Methyl-2-(methylthiomethyl)-2-pentenal (MS)



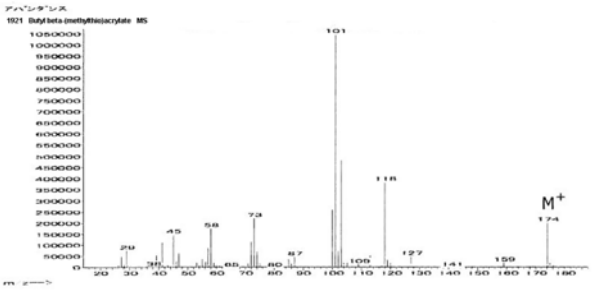
1919 4-Methyl-2-(methylthiomethyl)-2-hexenal (MS)



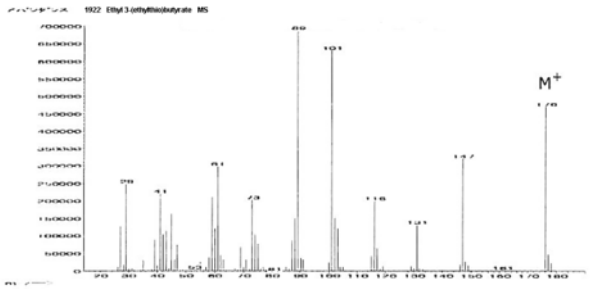
1920 5-Methyl-2-(methylthiomethyl)-2-hexenal (MS)



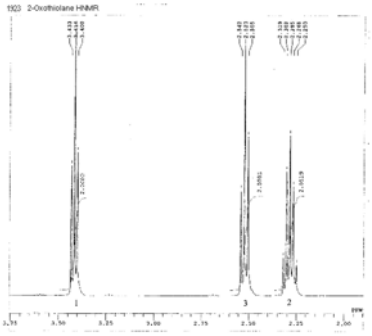
1921 Butyl beta-(methylthio)acrylate (MS)



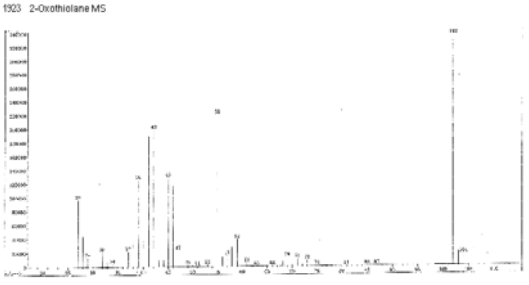
1922 Ethyl 3-(ethylthio)butyrate (MS)



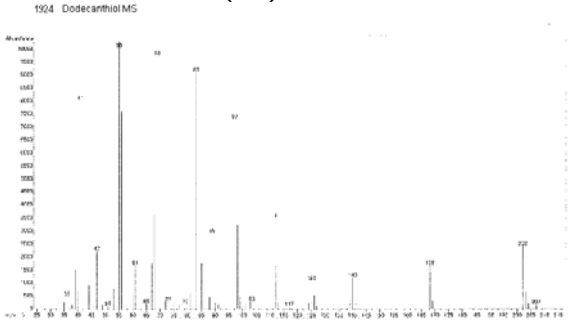
1923 2-Oxothiolane (1H-NMR)



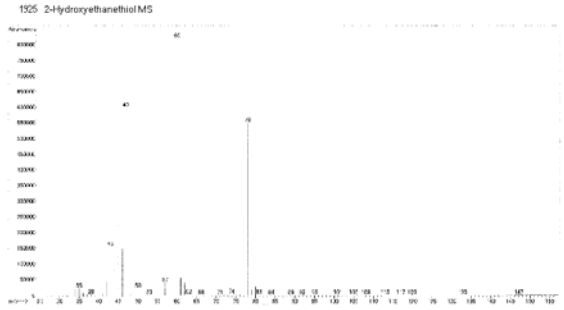
1923 2-Oxothiolane (MS)



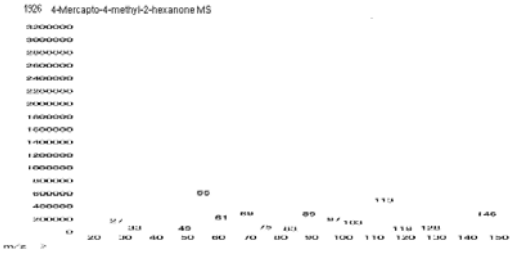
1924 Dodecanethiol (MS)



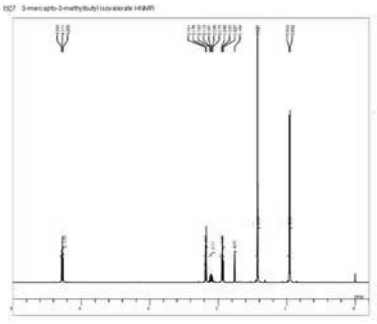
1925 2-Hydroxyethanethiol (MS)



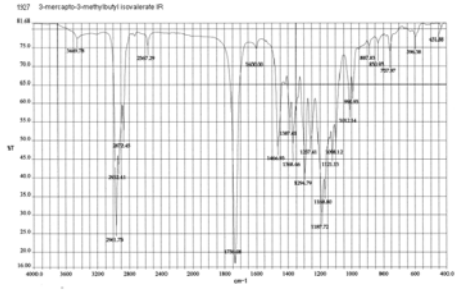
1926 4-Mercapto-4-methyl-2-hexanone (MS)



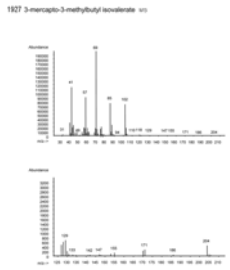
1927 3-Mercapto-3-methylbutyl isovalerate (1H-NMR)



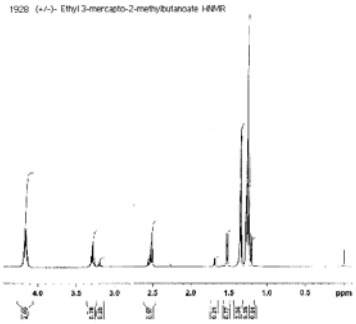
1927 3-Mercapto-3-methylbutyl isovalerate (IR)



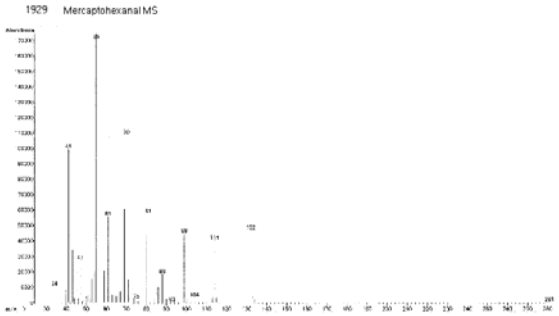
1927 3-Mercapto-3-methylbutyl isovalerate (MS)



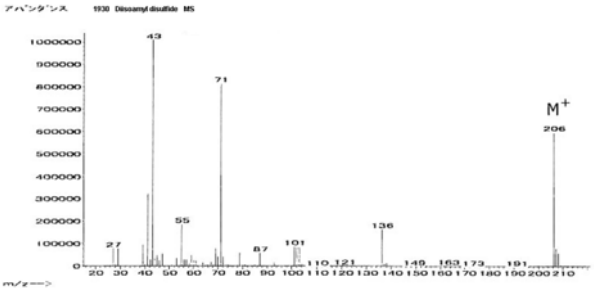
1928 (+/-)-Ethyl 3-mercapto-2-methylbutanoate (1H-NMR)



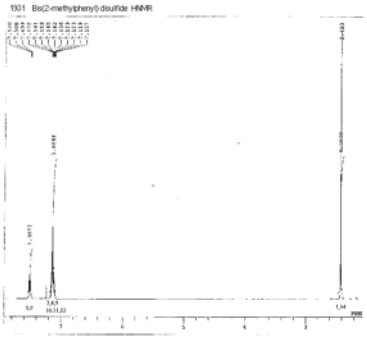
1929 3-Mercaptohexanal (MS)



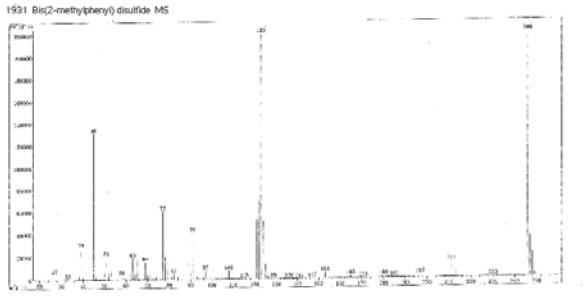
1930 Diisoamyl disulfide (MS)



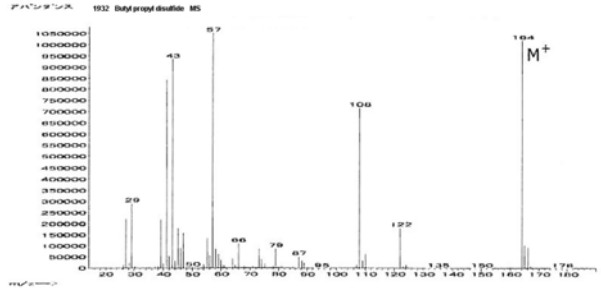
1931 Bis(2-methylphenyl) disulfide (1H-NMR)



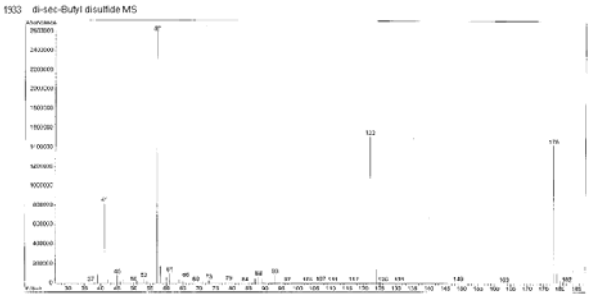
1931 Bis(2-methylphenyl) disulfide (MS)



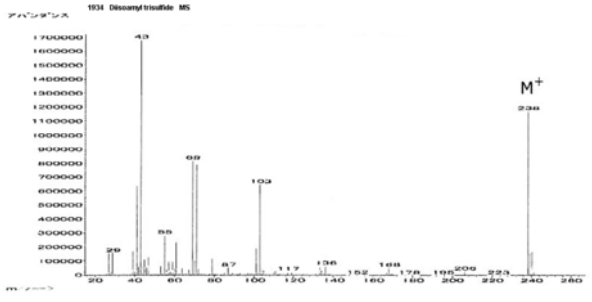
1932 Butyl propyl disulfide (MS)



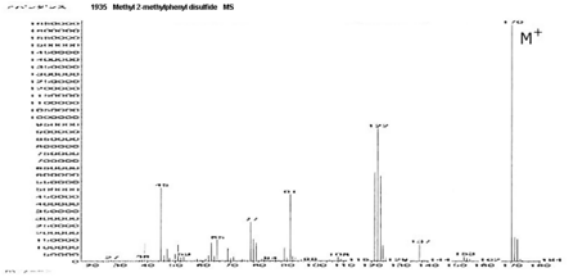
1933 di-sec-Butyl disulfide (MS)



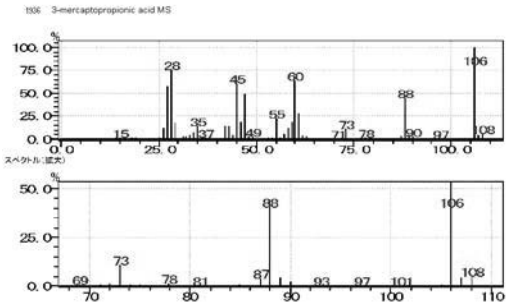
1934 Diisoamyl trisulfide (MS)



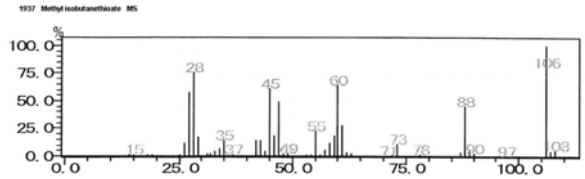
1935 Methyl 2-methylphenyl disulfide (MS)



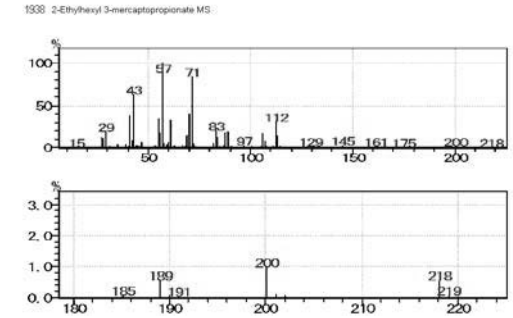
1936 3-Mercaptopropionic acid (MS)



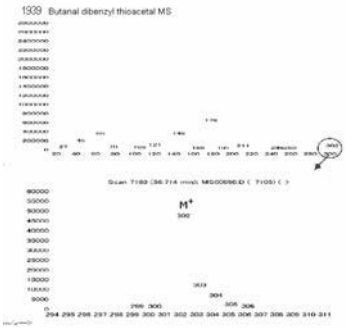
1937 Methyl isobutanethioate (MS)



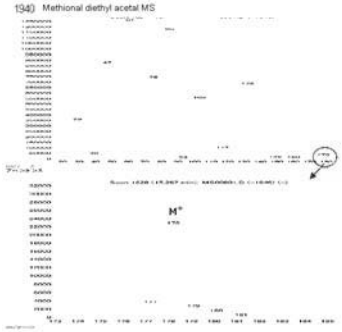
1938 2-Ethylhexyl 3-mercaptopropionate (MS)



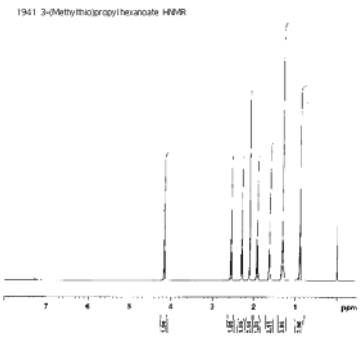
1939 Butanal dibenzyl thioacetal (MS)



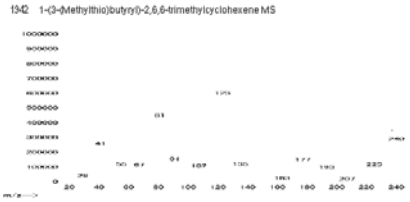
1940 Methional diethyl acetal (MS)



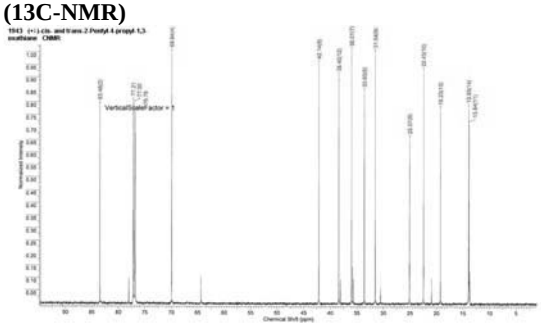
1941 3-(Methylthio)propyl hexanoate (1H-NMR)



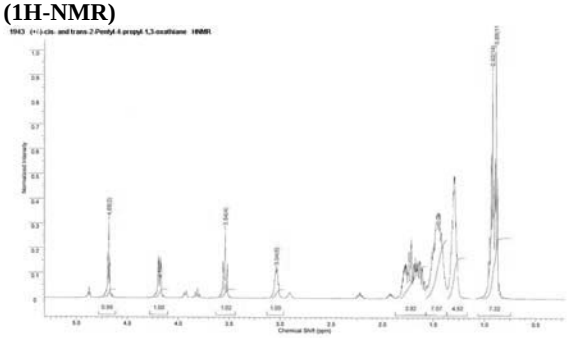
1942 1-(3-(Methylthio)-butyryl)-2,6,6-trimethylcyclohexene (MS)



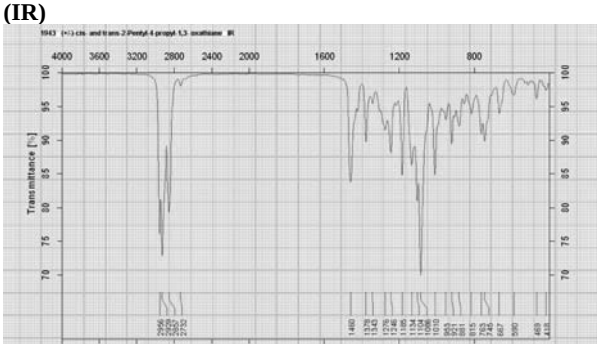
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (13C-NMR)



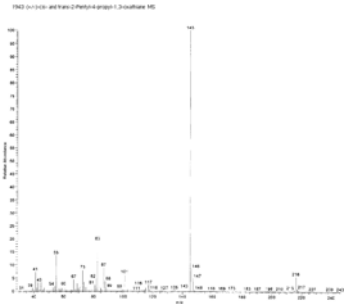
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (1H-NMR)



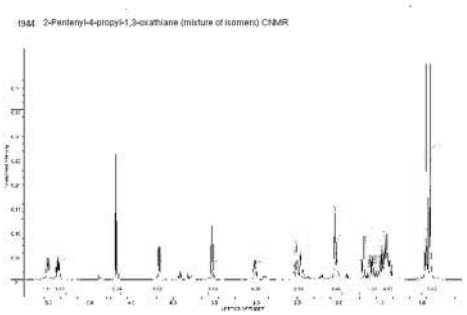
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (IR)



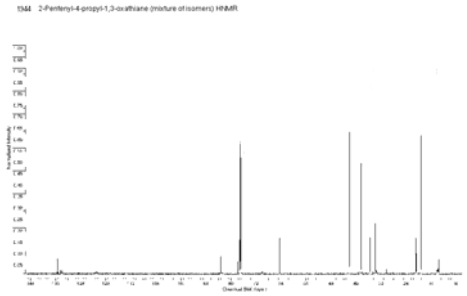
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (MS)



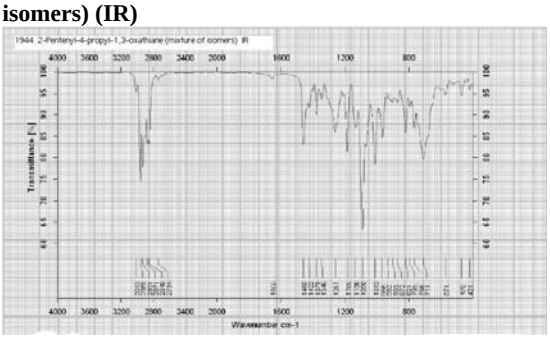
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (13C-NMR)



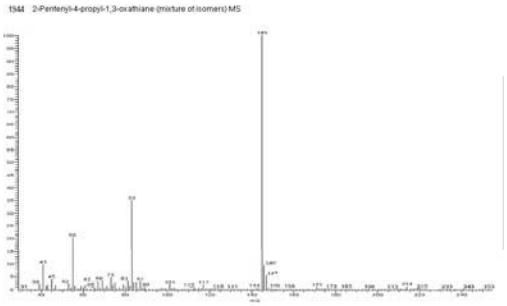
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (1H-NMR)



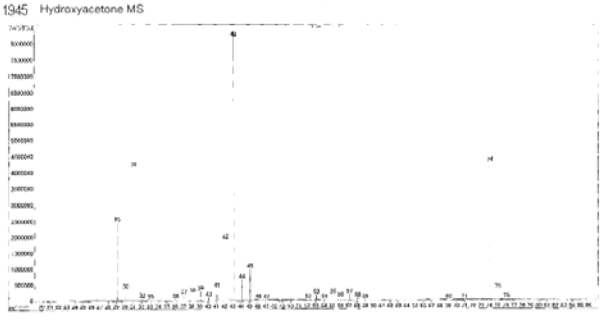
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (IR)



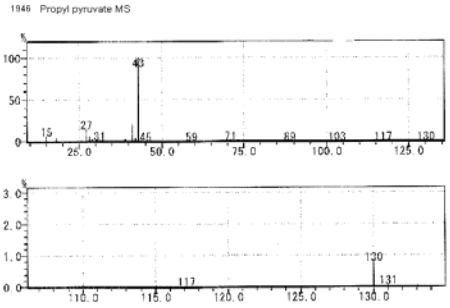
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (MS)



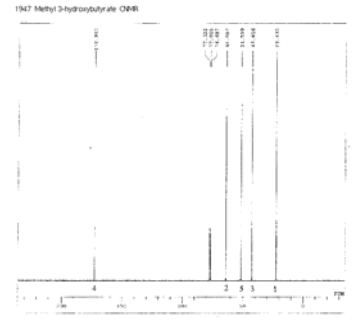
1945 Hydroxyacetone (MS)



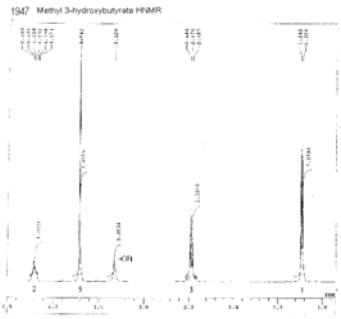
1946 Propyl pyruvate (MS)



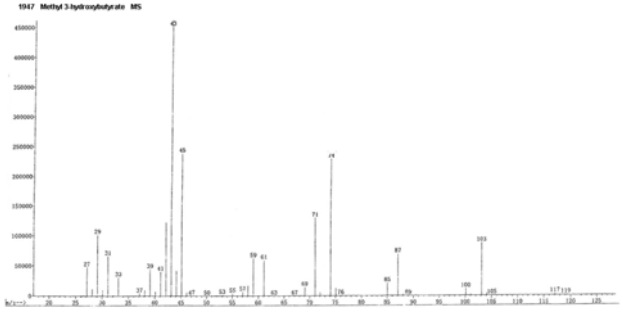
1947 Methyl 3-hydroxybutyrate (13C-NMR)



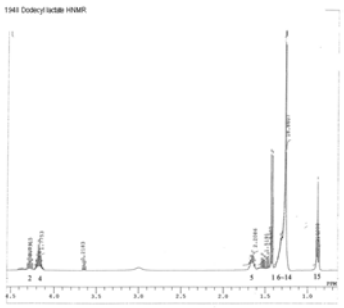
1947 Methyl 3-hydroxybutyrate (1H-NMR)



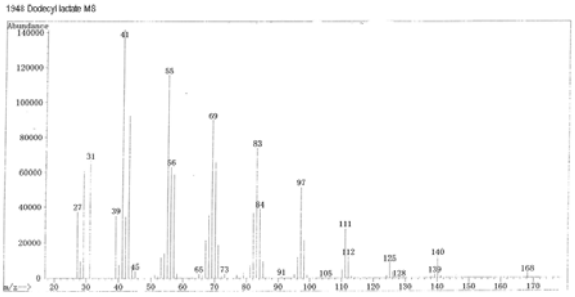
1947 Methyl 3-hydroxybutyrate (MS)



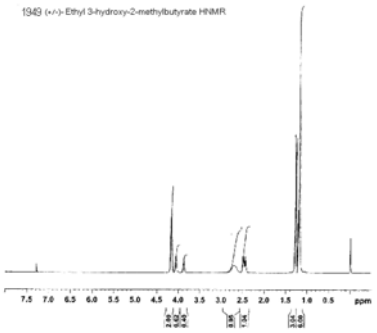
1948 Dodecyl lactate (1H-NMR)



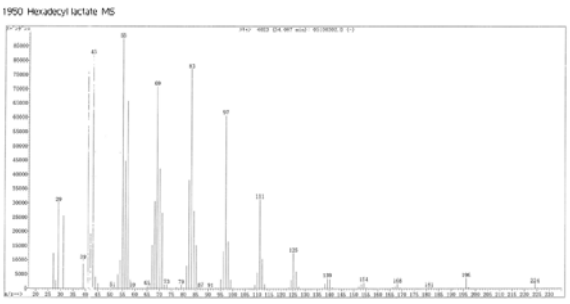
1948 Dodecyl lactate (MS)



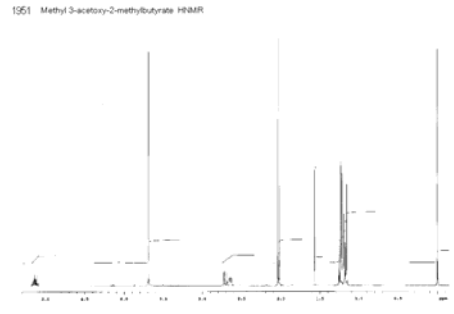
1949 (+/-)-Ethyl 3-hydroxy-2-methylbutyrate (1H-NMR)



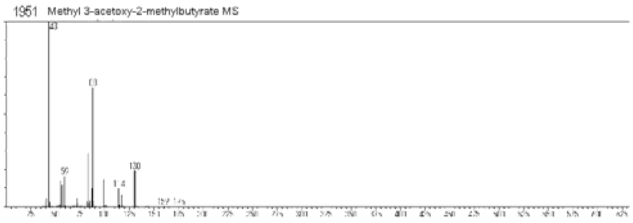
1950 Hexadecyl lactate (MS)



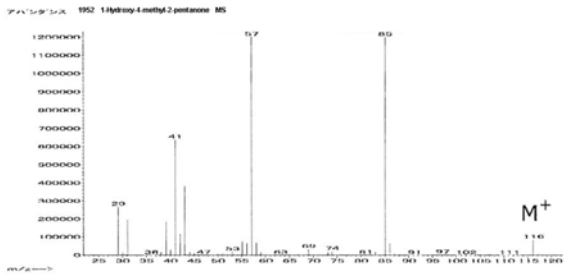
1951 Methyl 3-acetoxy-2-methylbutyrate (1H-NMR)



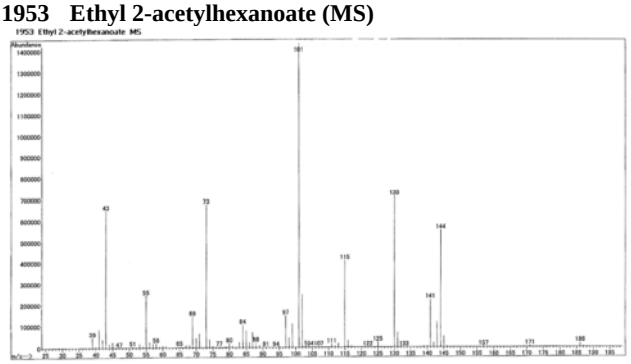
1951 Methyl 3-acetoxy-2-methylbutyrate (MS)



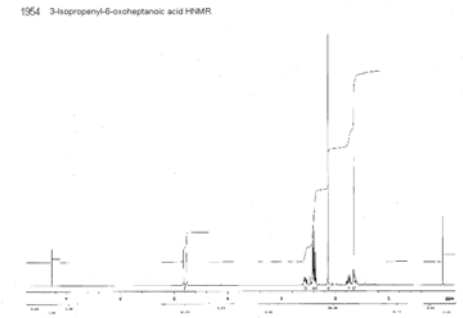
1952 1-Hydroxy-4-methyl-2-pentanone (MS)



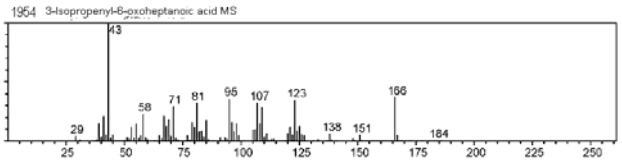
1953 Ethyl 2-acetylhexanoate (MS)



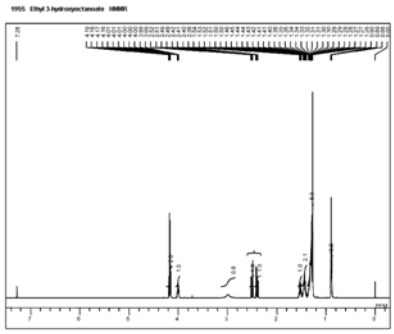
1954 3-Isopropenyl-6-oxoheptanoic acid (1H-NMR)



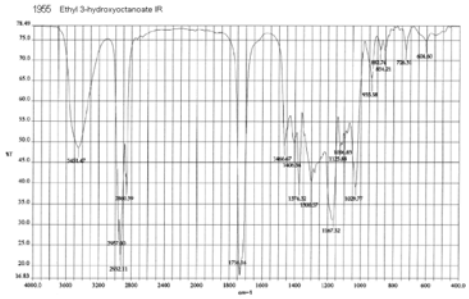
1954 3-Isopropenyl-6-oxoheptanoic acid (MS)



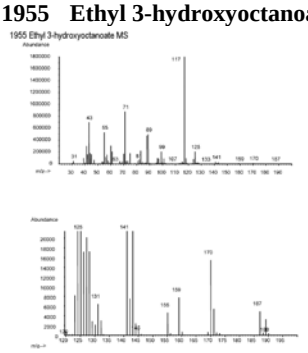
1955 Ethyl 3-hydroxyoctanoate (1H-NMR)



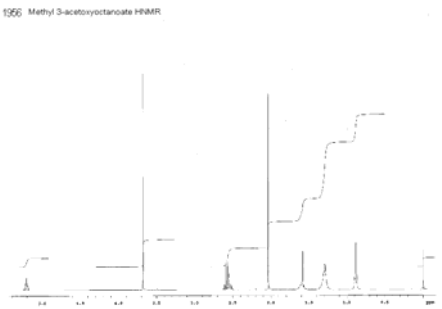
1955 Ethyl 3-hydroxyoctanoate (IR)



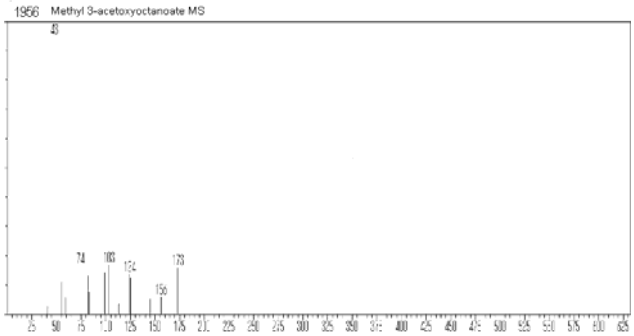
1955 Ethyl 3-hydroxyoctanoate (MS)



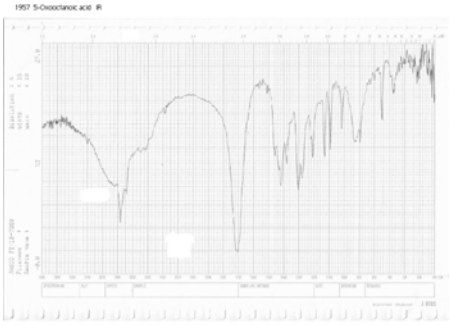
1956 Methyl 3-acetoxyoctanoate (1H-NMR)



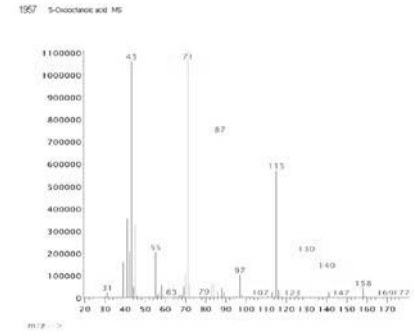
1956 Methyl 3-acetoxyoctanoate (MS)



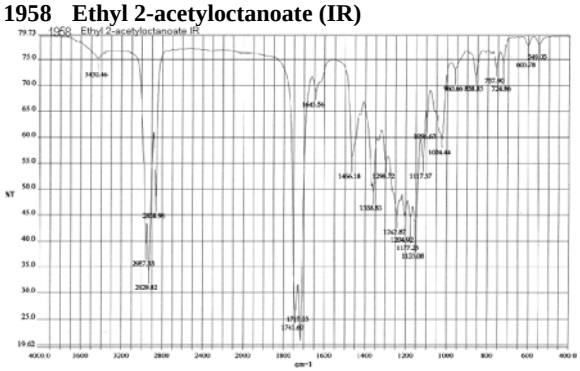
1957 5-Oxooctanoic acid (IR)



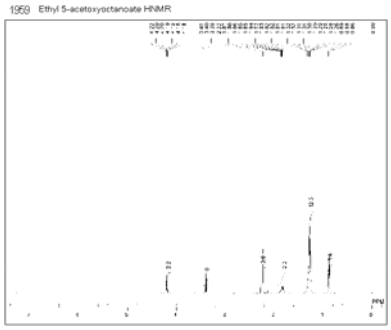
1957 5-Oxooctanoic acid (MS)



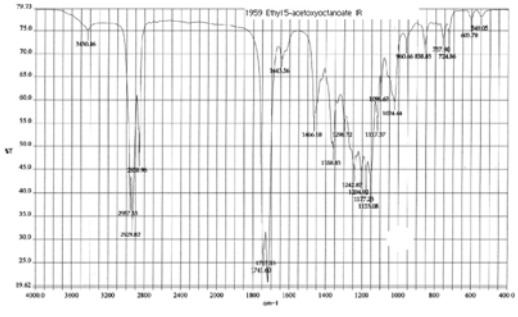
1958 Ethyl 2-acetyloctanoate (IR)



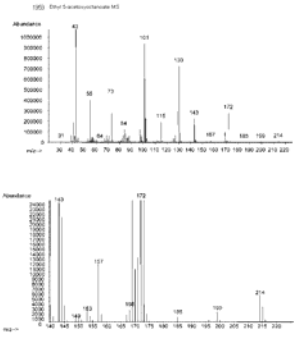
1959 Ethyl 5-acetoxyoctanoate (1H-NMR)



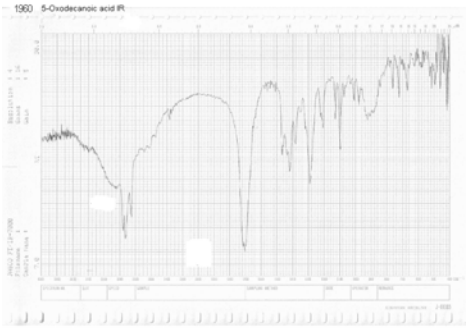
1959 Ethyl 5-acetoxyoctanoate (IR)



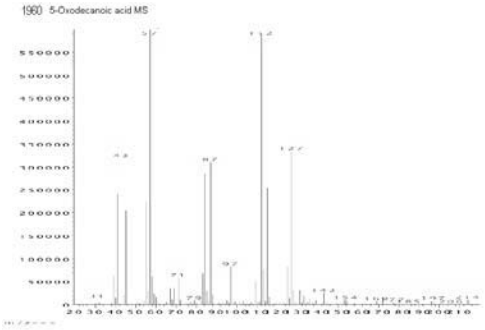
1959 Ethyl 5-acetoxyoctanoate (MS)



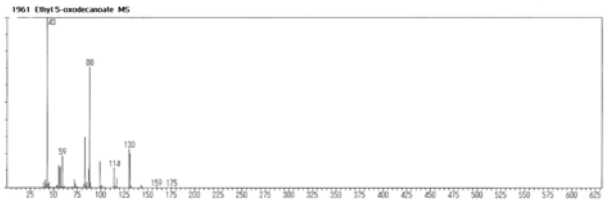
1960 5-Oxodecanoic acid (IR)



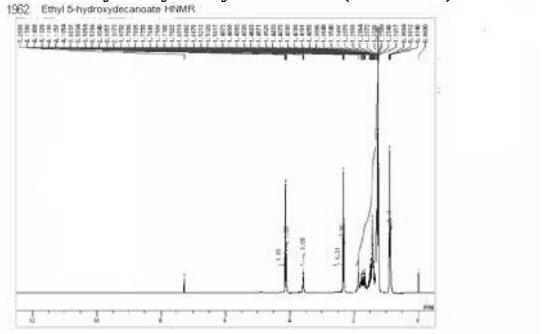
1960 5-Oxodecanoic acid (MS)



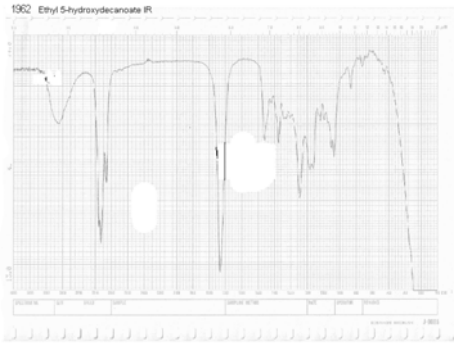
1961 Ethyl 5-oxodecanoate (MS)



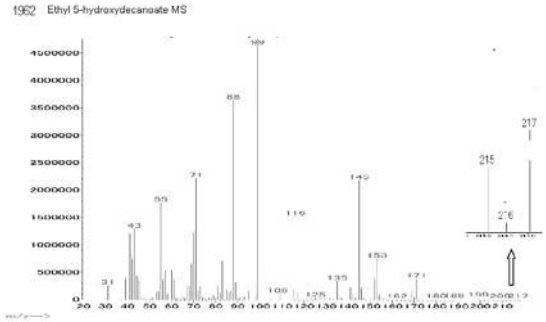
1962 Ethyl 5-hydroxydecanoate (1H-NMR)



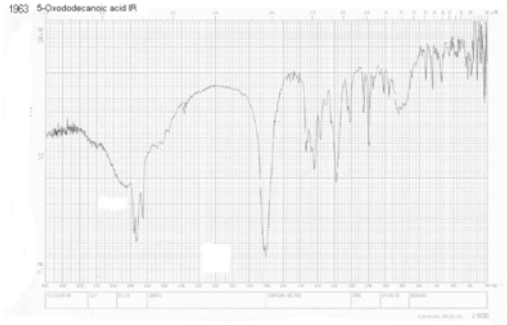
1962 Ethyl 5-hydroxydecanoate (IR)



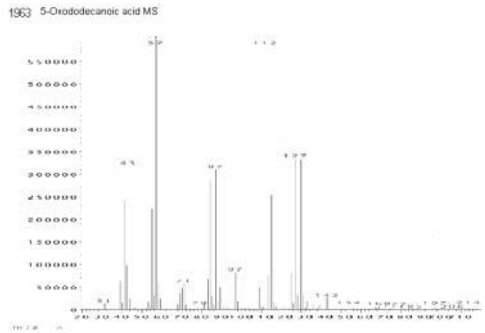
1962 Ethyl 5-hydroxydecanoate (MS)



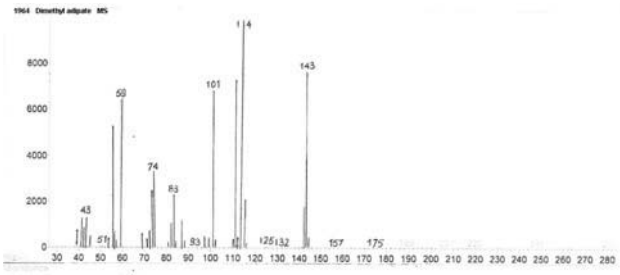
1963 5-Oxododecanoic acid (IR)



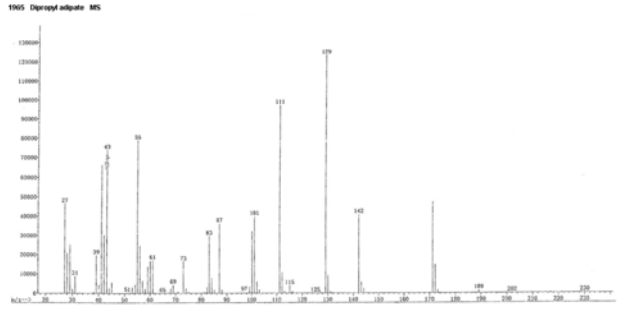
1963 5-Oxododecanoic acid (MS)



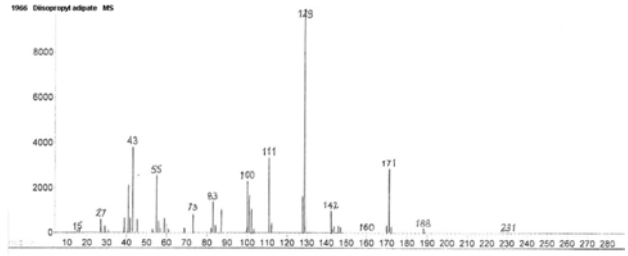
1964 Dimethyl adipate (MS)



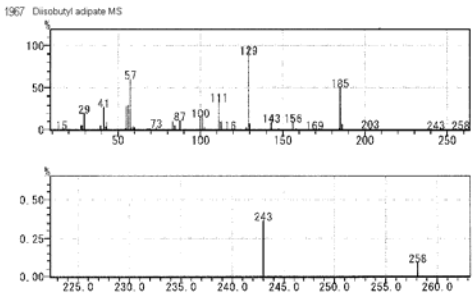
1965 Dipropyl adipate (MS)



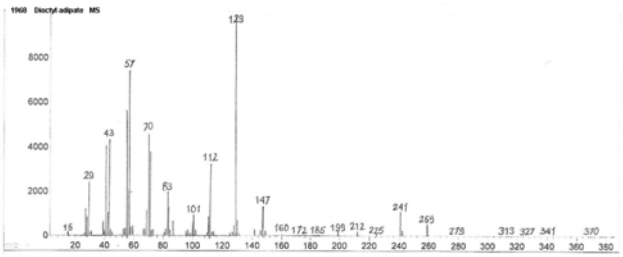
1966 Diisopropyl adipate (MS)



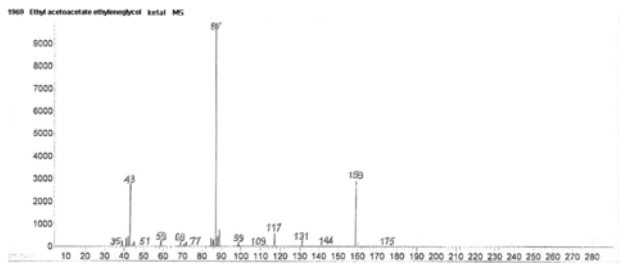
1967 Diisobutyl adipate (MS)



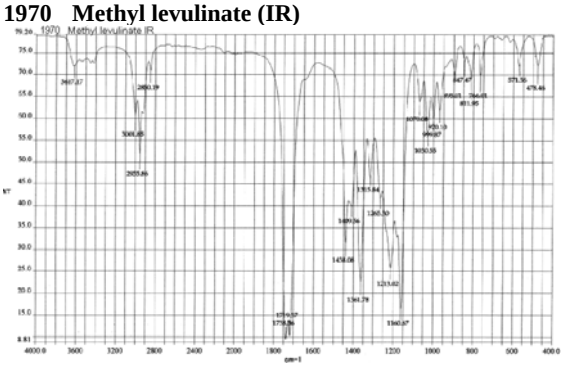
1968 Dioctyl adipate (MS)



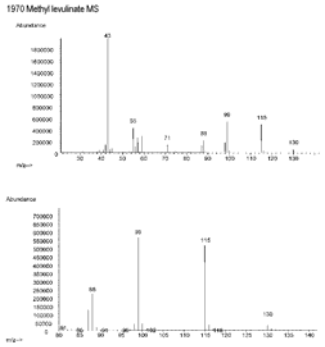
1969 Ethyl acetoacetate ethyleneglycol ketal (MS)



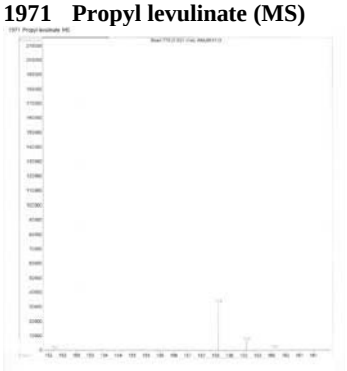
1970 Methyl levulinate (IR)



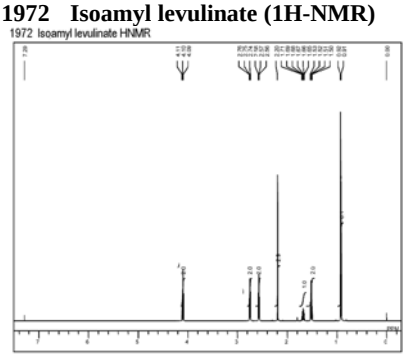
1970 Methyl levulinate (MS)



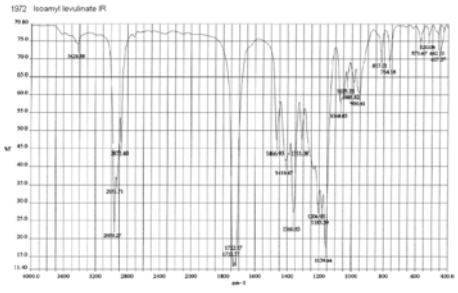
1971 Propyl levulinate (MS)



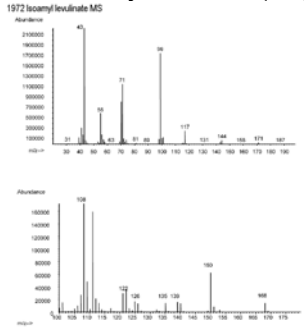
1972 Isoamyl levulinate (1H-NMR)



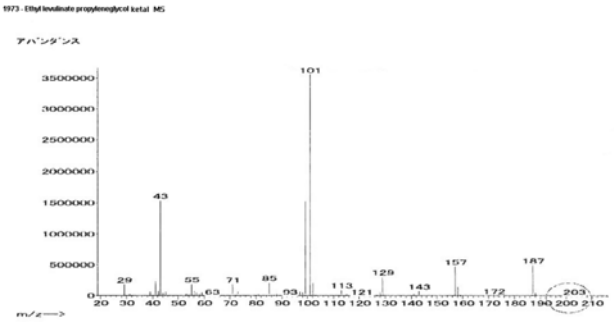
1972 Isoamyl levulinate (IR)



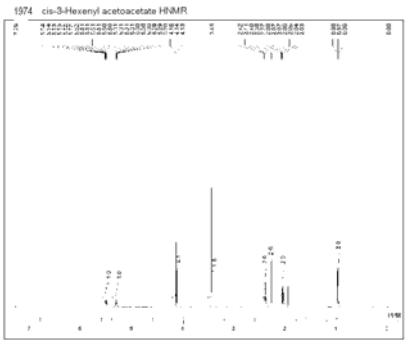
1972 Isoamyl levulinate (MS)



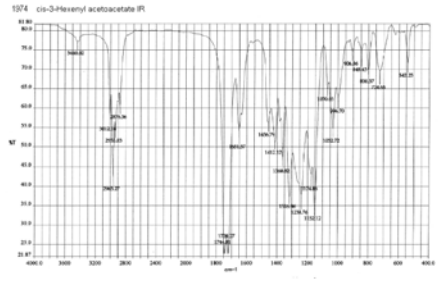
1973 Ethyl levulinate propyleneglycol ketal (MS)



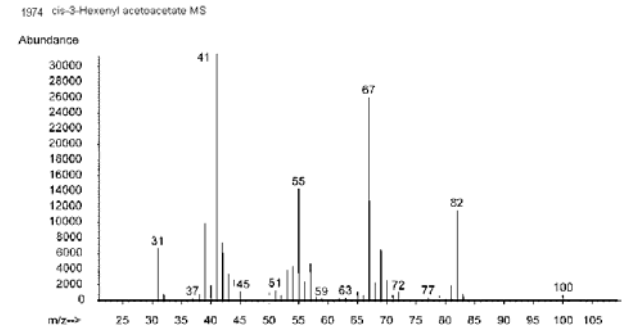
1974 cis-3-Hexenyl acetoacetate (1H-NMR)



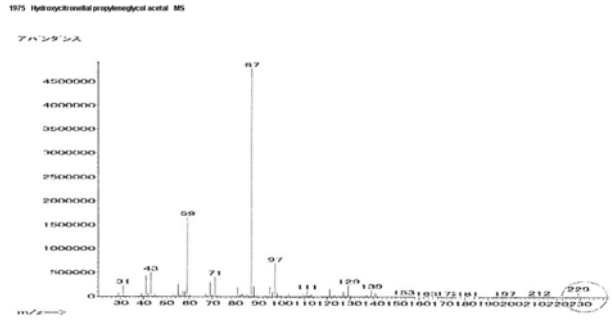
1974 cis-3-Hexenyl acetoacetate (IR)



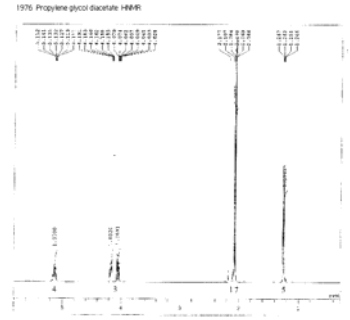
1974 cis-3-Hexenyl acetoacetate (MS)



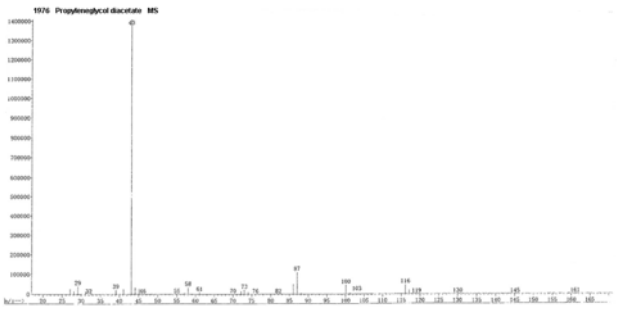
1975 Hydroxycitronellal propyleneglycol acetal (MS)



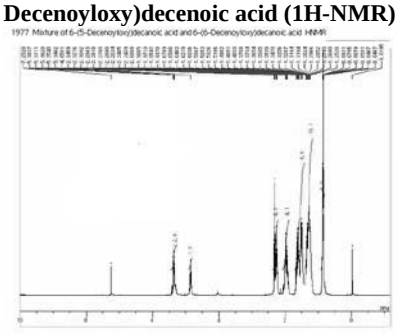
1976 Propyleneglycol diacetate (1H-NMR)



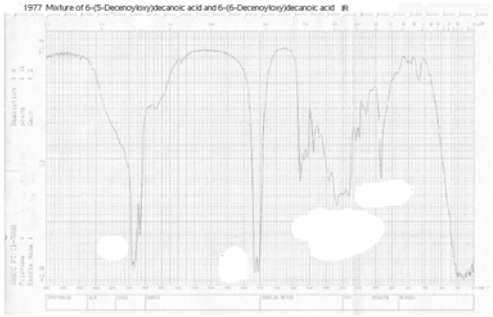
1976 Propyleneglycol diacetate (MS)



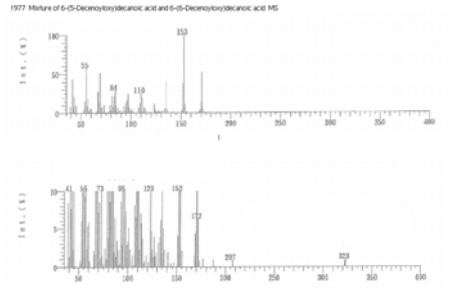
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (1H-NMR)



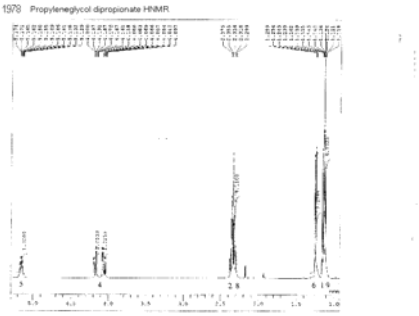
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (IR)



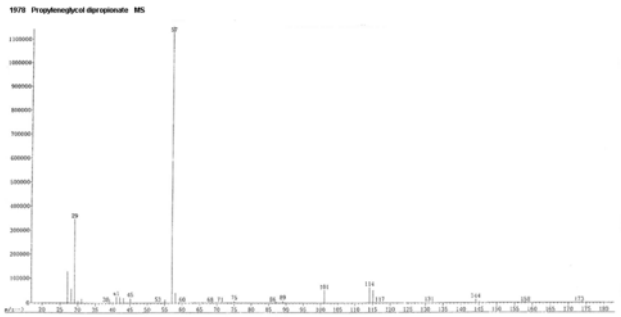
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (MS)



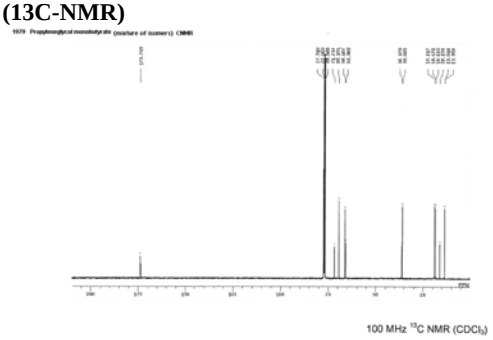
1978 Propyleneglycol dipropionate (1H-NMR)



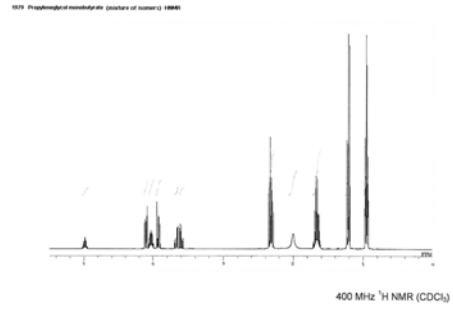
1978 Propyleneglycol dipropionate (MS)



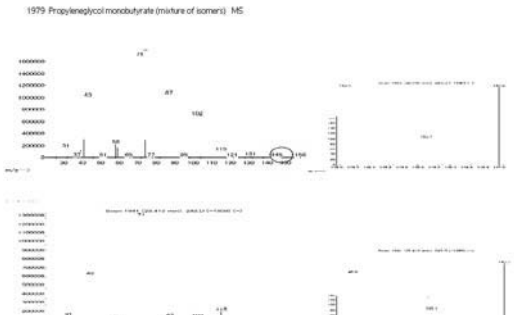
1979 Propyleneglycol monobutyrate (mixture of isomers) (13C-NMR)



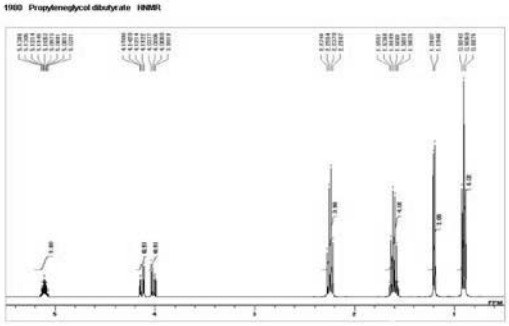
1979 Propyleneglycol monobutyrate (mixture of isomers) (1H-NMR)



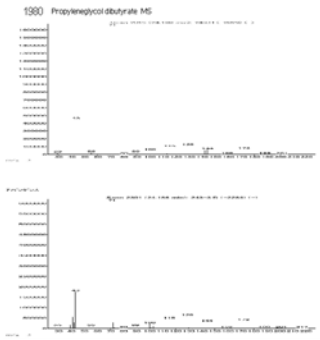
1979 Propyleneglycol monobutyrate (mixture of isomers) (MS)



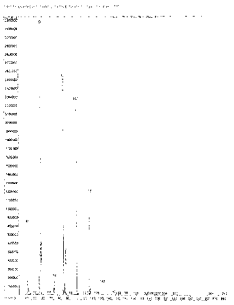
1980 Propyleneglycol dibutyrate (1H-NMR)



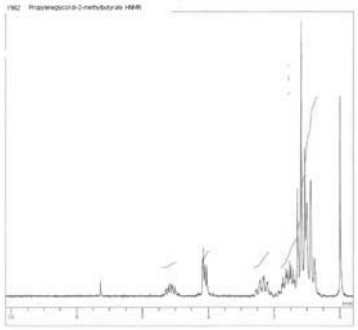
1980 Propyleneglycol dibutyrate (MS)



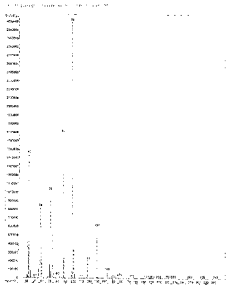
1981 Propyleneglycol mono-2-methylbutyrate (mixture of isomers) (MS)



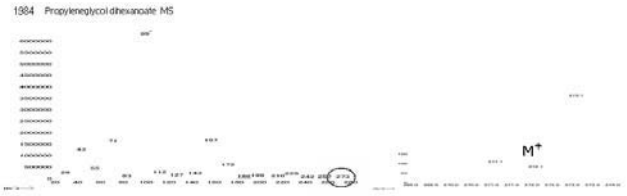
1982 Propyleneglycol di-2-methylbutyrate (1H-NMR)



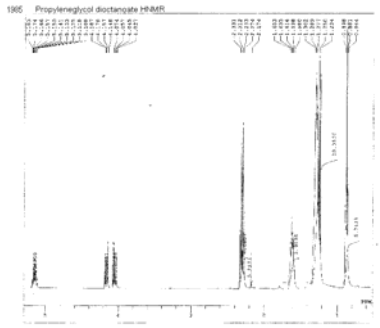
1983 Propyleneglycol monohexanoate (mixture of isomers) (MS)



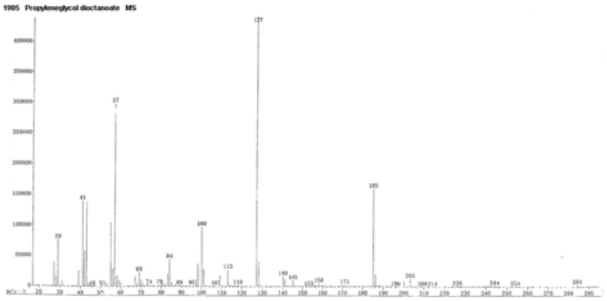
1984 Propyleneglycol dihexanoate (MS)



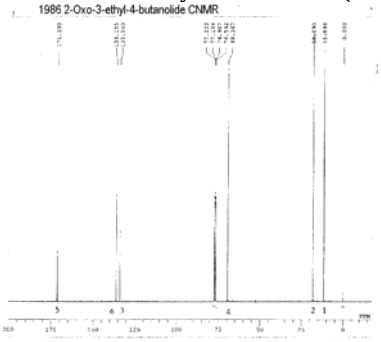
1985 Propyleneglycol dioctanoate (1H-NMR)



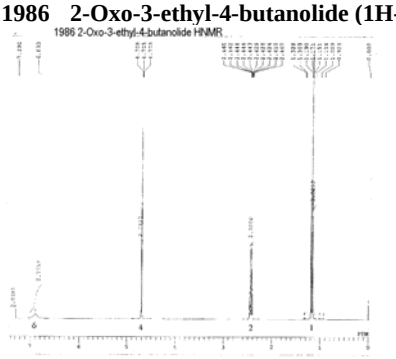
1985 Propyleneglycol dioctanoate (MS)



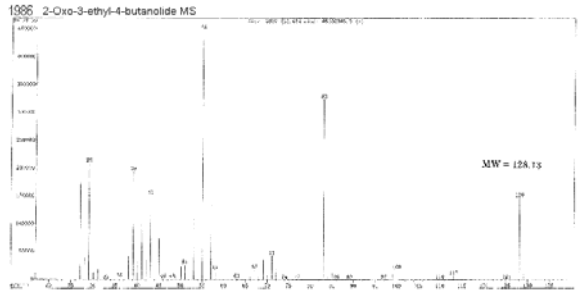
1986 2-Oxo-3-ethyl-4-butanolide (13C-NMR)



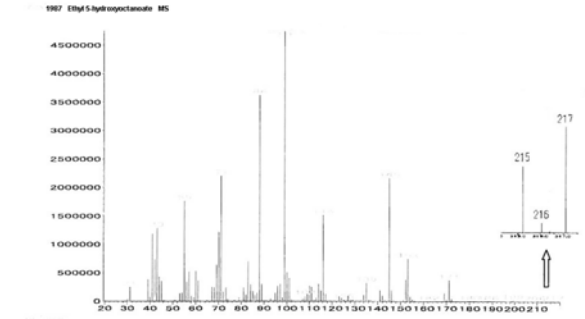
1986 2-Oxo-3-ethyl-4-butanolide (1H-NMR)



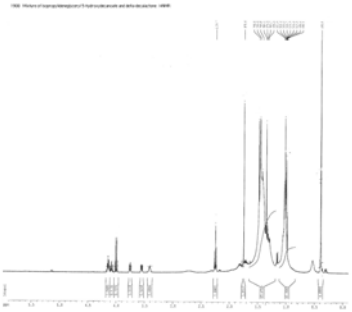
1986 2-Oxo-3-ethyl-4-butanolide (MS)



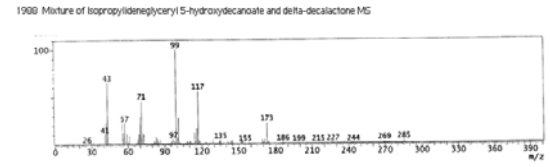
1987 Ethyl 5-hydroxyoctanoate (MS)



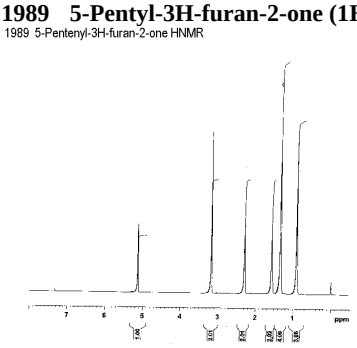
1988 Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone (1H-NMR)



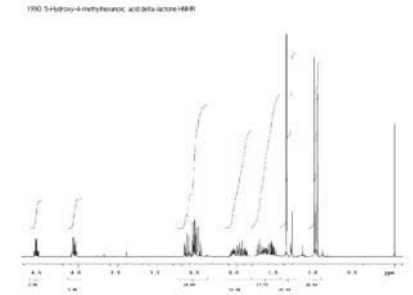
1988 Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone (MS)



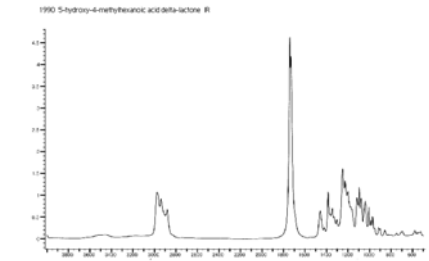
1989 5-Pentyl-3H-furan-2-one (1H-NMR)



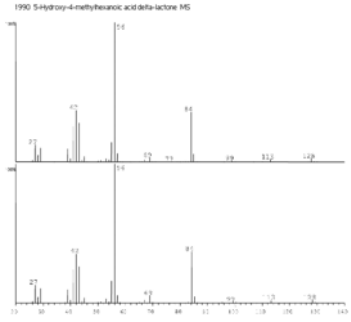
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (1H-NMR)



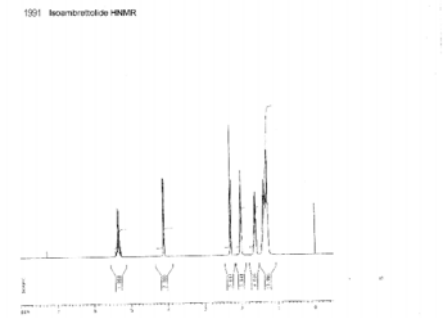
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (IR)



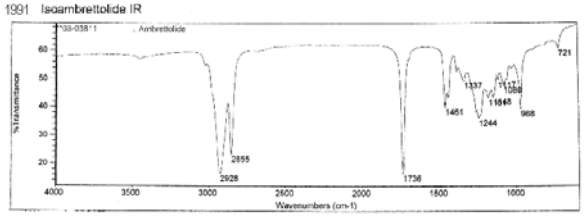
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (MS)



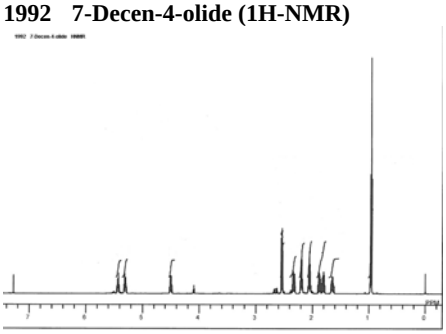
1991 Isoambrettolide (1H-NMR)



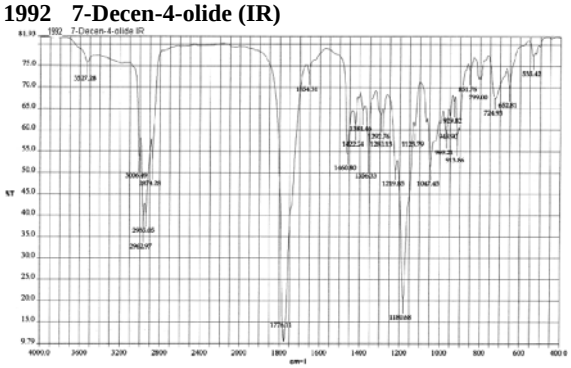
1991 Isoambrettolide (IR)



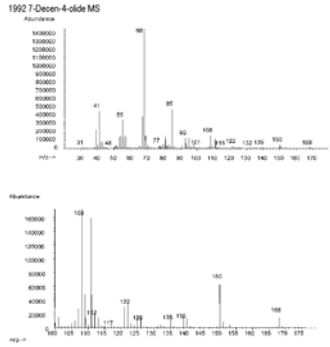
1992 7-Decen-4-olide (1H-NMR)



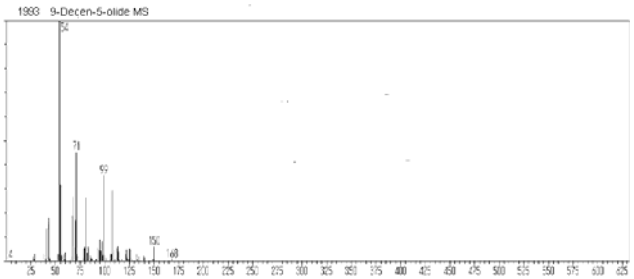
1992 7-Decen-4-olide (IR)



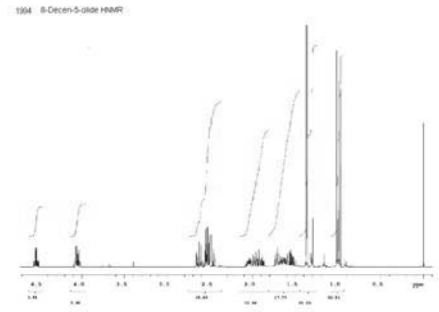
1992 7-Decen-4-olide (MS)



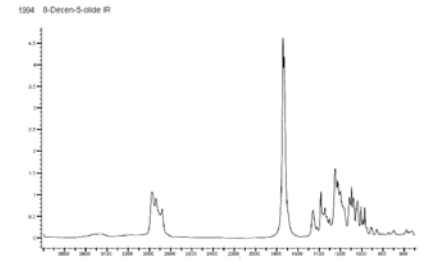
1993 9-Decen-5-olide (MS)



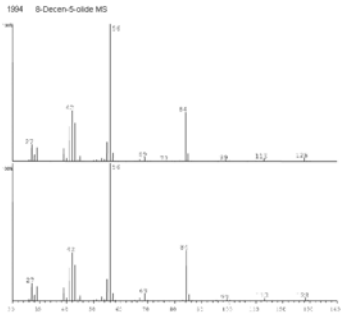
1994 8-Decen-5-olide (1H-NMR)



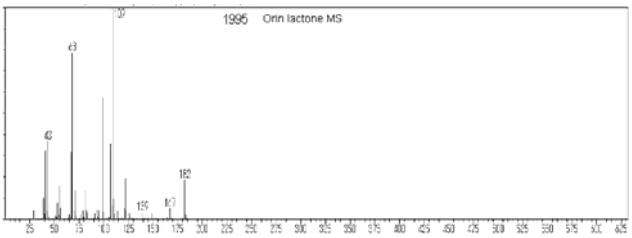
1994 8-Decen-5-olide (IR)



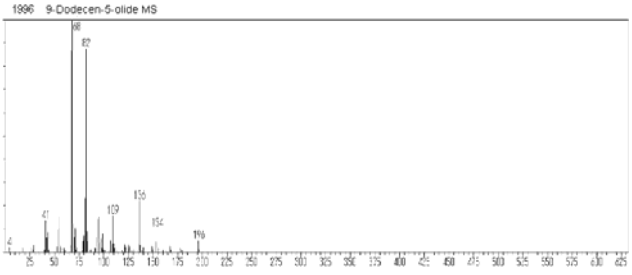
1994 8-Decen-5-olide (MS)



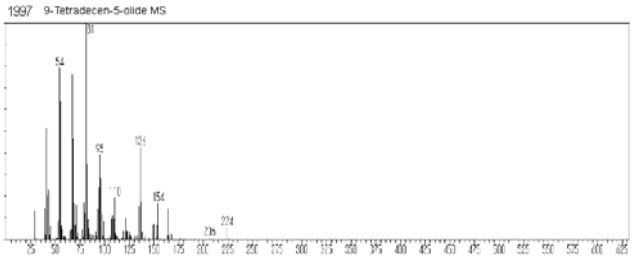
1995 Orin lactone (MS)



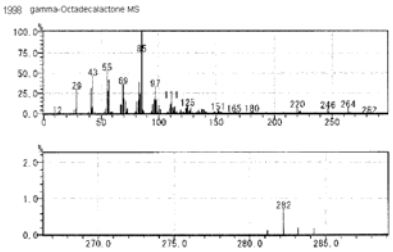
1996 9-Dodecen-5-olide (MS)



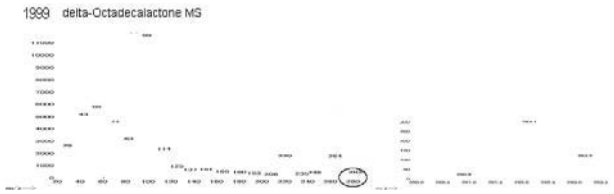
1997 9-Tetradecen-5-olide (MS)



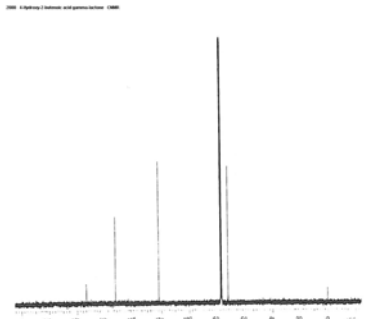
1998 gamma-Octadecalactone (MS)



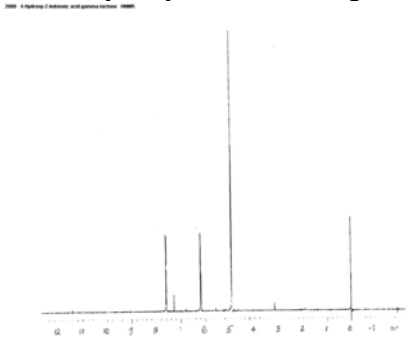
1999 delta-Octadecalactone (MS)



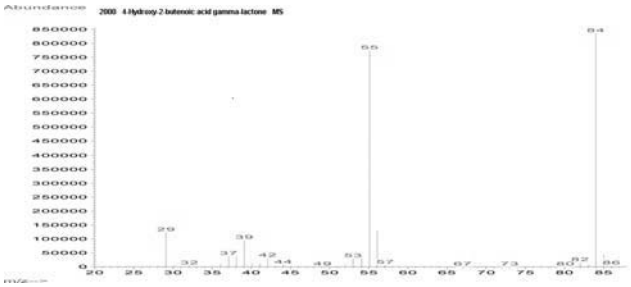
2000 4-Hydroxy-2-butenoic acid gamma-lactone (13C-NMR)



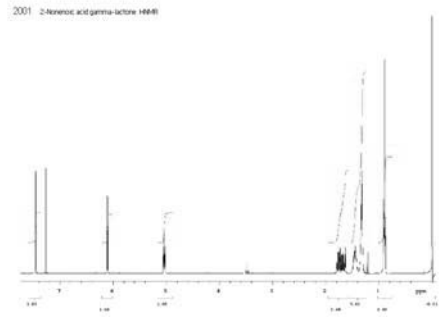
2000 4-Hydroxy-2-butenoic acid gamma-lactone (1H-NMR)



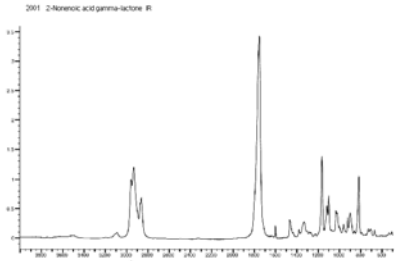
2000 4-Hydroxy-2-butenoic acid gamma-lactone (MS)



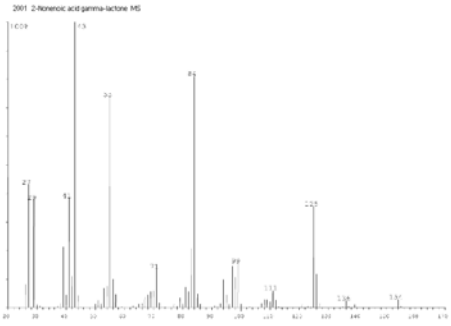
2001 2-Nonenoic acid gamma-lactone (1H-NMR)



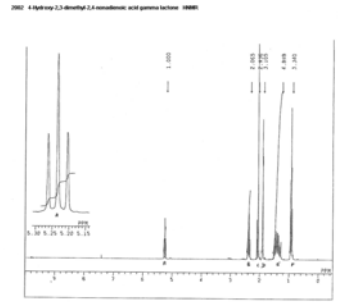
2001 2-Nonenoic acid gamma-lactone (IR)



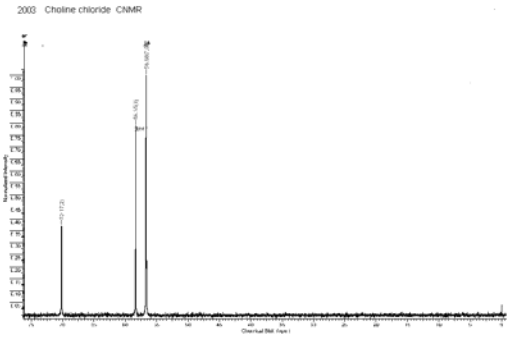
2001 2-Nonenoic acid gamma-lactone (MS)



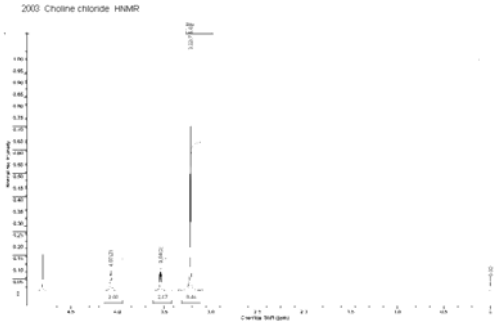
2002 4-Hydroxy-2,3-dimethyl-2,4-nonadienoic acid gamma-lactone (1H-NMR)



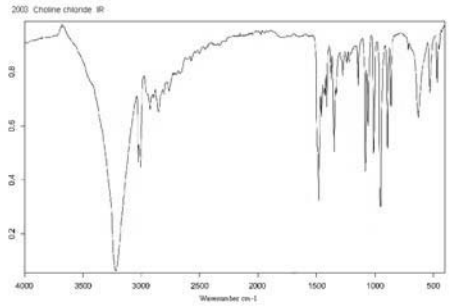
2003 Choline chloride (13C-NMR)



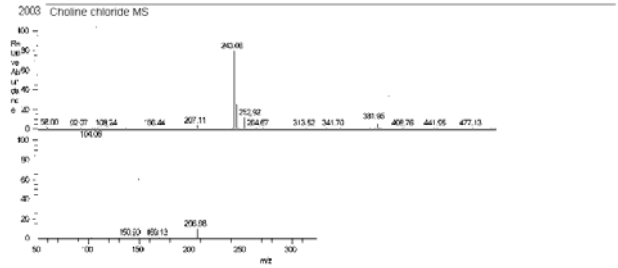
2003 Choline chloride (1H-NMR)



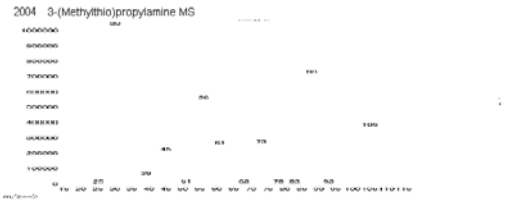
2003 Choline chloride (IR)



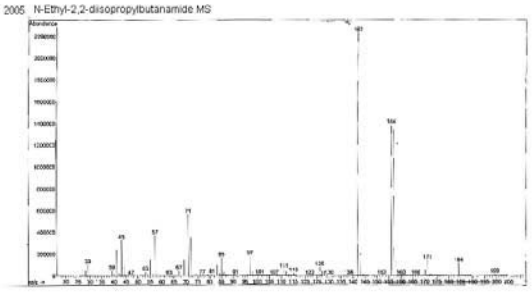
2003 Choline chloride (MS)



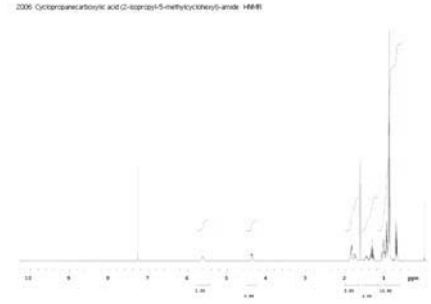
2004 3-(Methylthio)propylamine (MS)



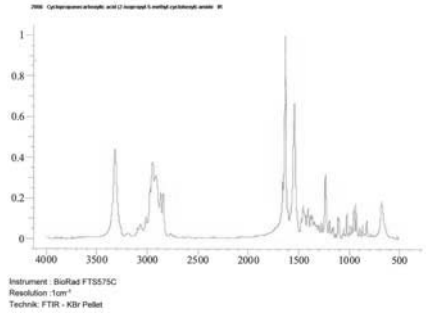
2005 N-Ethyl-2,2-diisopropylbutanamide (MS)



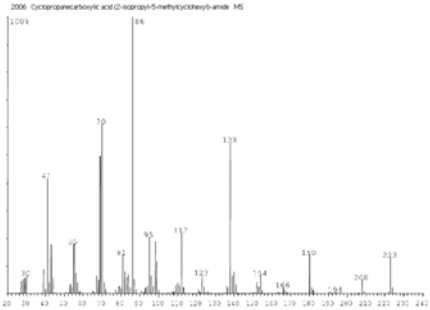
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (1H-NMR)



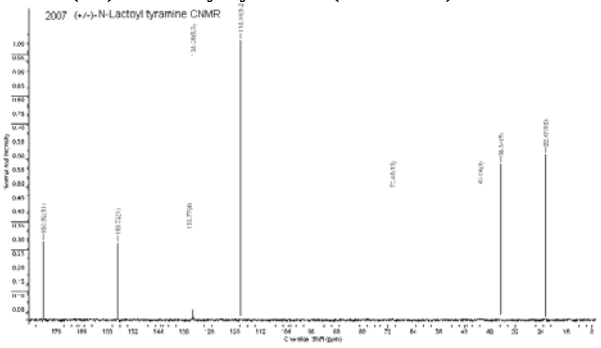
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (IR)



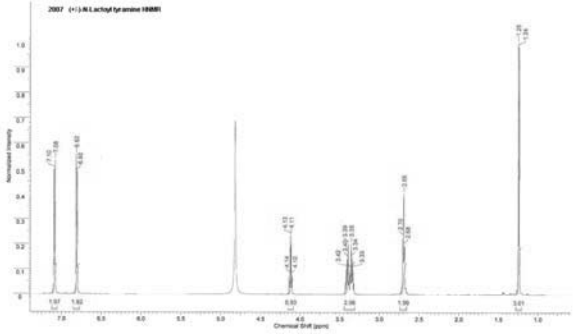
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (MS)



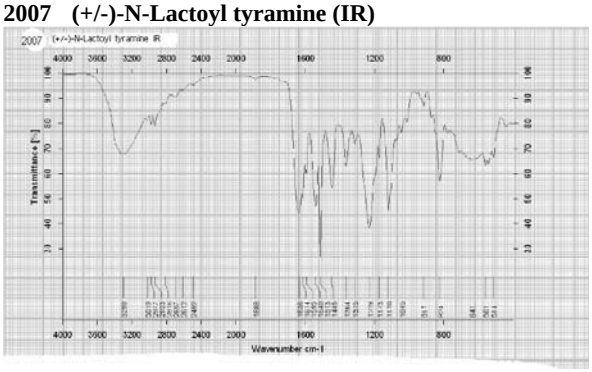
2007 (+/-)-N-Lactoyl tyramine (13C-NMR)



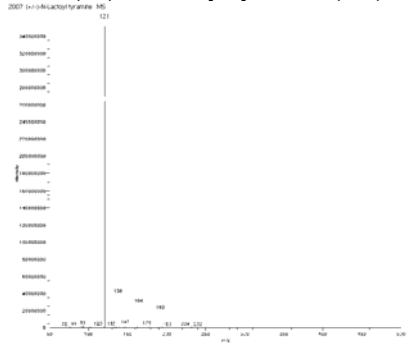
2007 (+/-)-N-Lactoyl tyramine (1H-NMR)



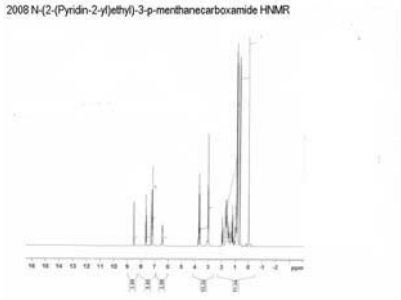
2007 (+/-)-N-Lactoyl tyramine (IR)



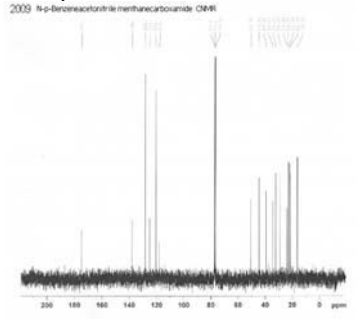
2007 (+/-)-N-Lactoyl tyramine (MS)



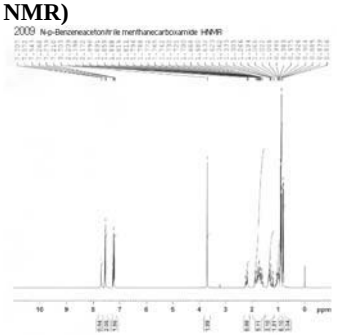
2008 N-(2-(Pyridin-2-yl)ethyl)-3-p-menthanecarboxamide (1H-NMR)



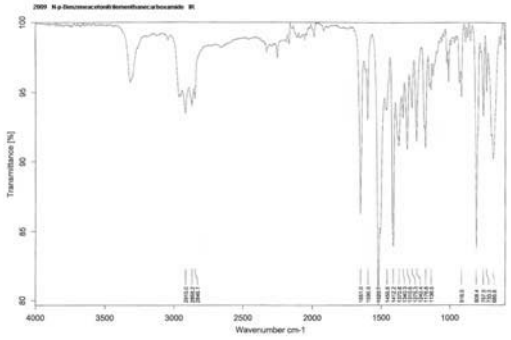
2009 N-p-Benzeneacetonitrile menthanecarboxamide (13C-NMR)



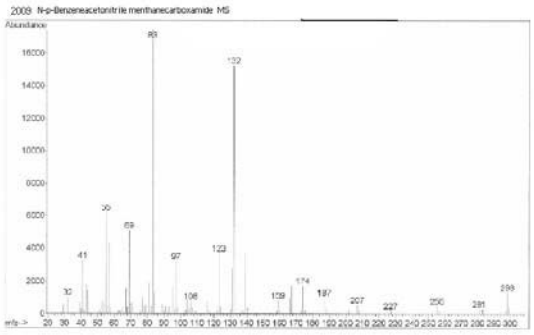
2009 N-p-Benzeneacetonitrile menthanecarboxamide (1H-NMR)



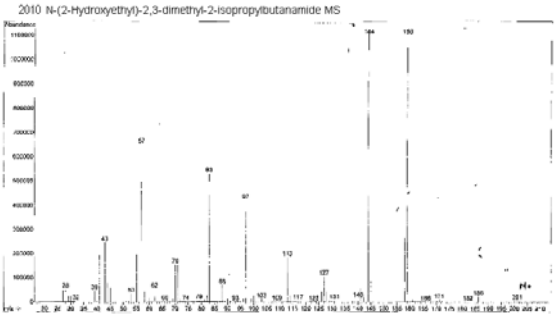
2009 N-p-Benzeneacetonitrile menthanecarboxamide (IR)



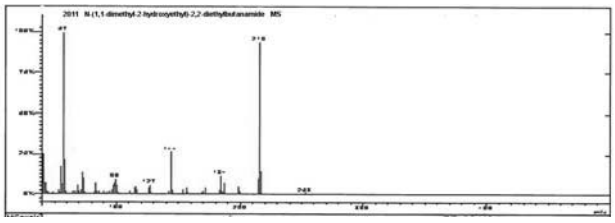
2009 N-p-Benzeneacetonitrile menthanecarboxamide (MS)



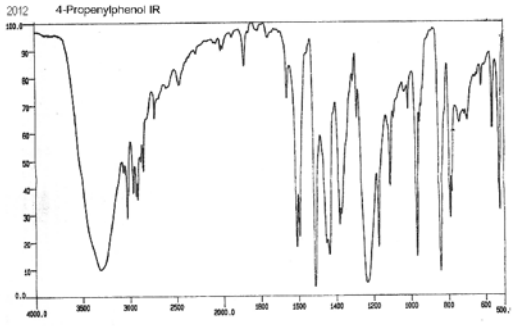
2010 N-(2-Hydroxyethyl)-2,3-dimethyl 2-isopropylbutanamide (MS)



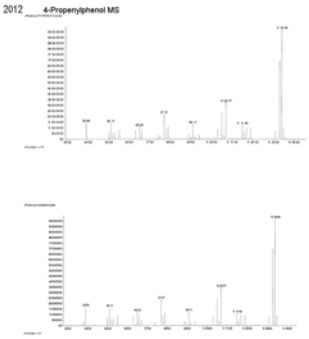
2011 N-(1,1-Dimethyl-2-hydroxyethyl)-2,2-diethylbutanamide (MS)



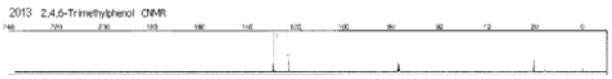
2012 4-Propenylphenol (IR)



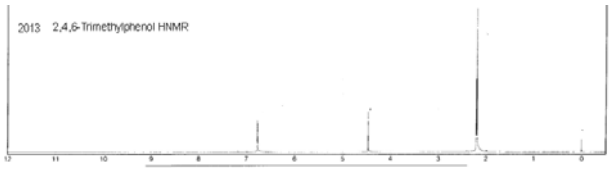
2012 4-Propenylphenol (MS)



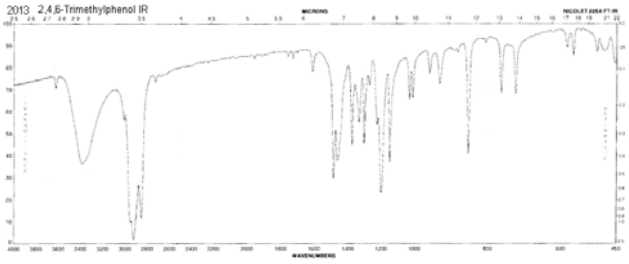
2013 2,4,6-Trimethylphenol (13C-NMR)



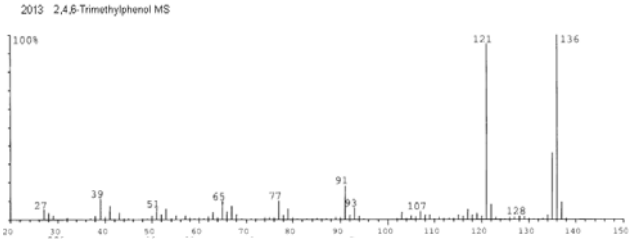
2013 2,4,6-Trimethylphenol (1H-NMR)



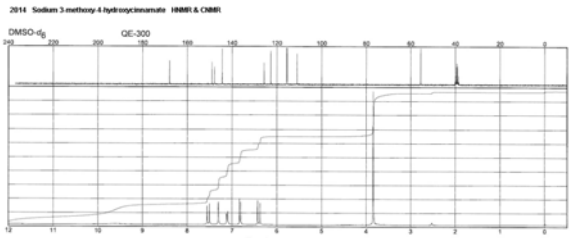
2013 2,4,6-Trimethylphenol (IR)



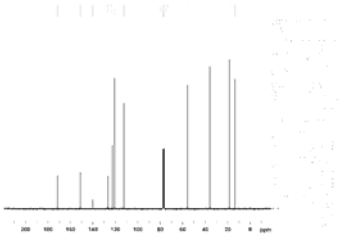
2013 2,4,6-Trimethylphenol (MS)



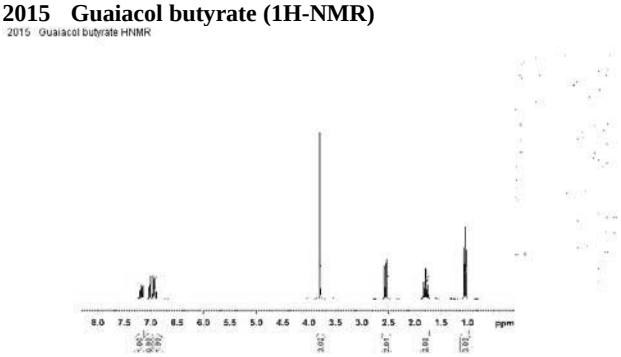
2014 Sodium 3-methoxy-4-hydroxycinnamate (13C-NMR and 1H-NMR)



2015 Guaiacol butyrate (13C-NMR)



2015 Guaiacol butyrate (1H-NMR)



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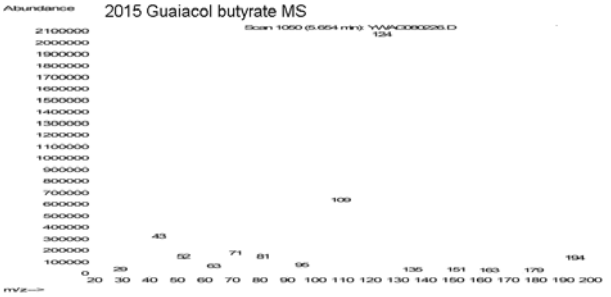
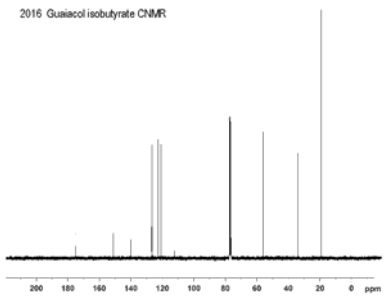
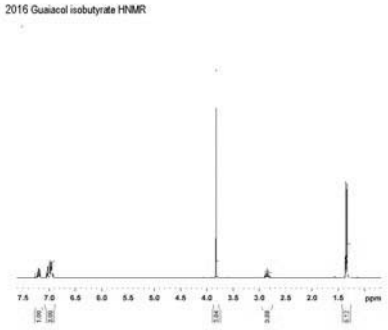


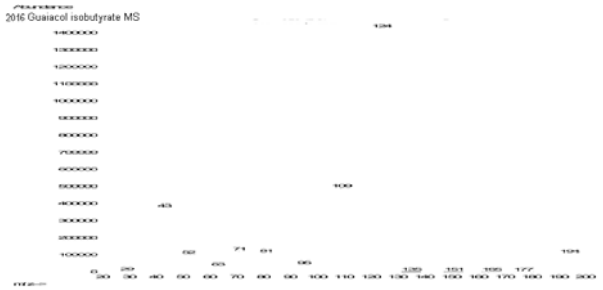
2016 Guaiacol isobutyrate (13C-NMR)



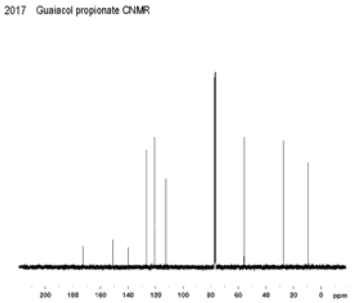
2016 Guaiacol isobutyrate (1H-NMR)



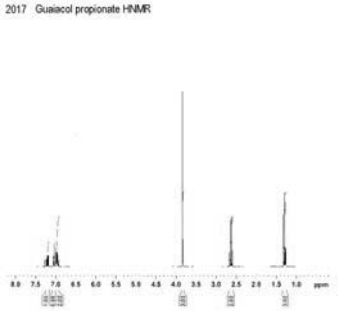
2016 Guaiacol isobutyrate (MS)



2017 Guaiacol propionate (13C-NMR)

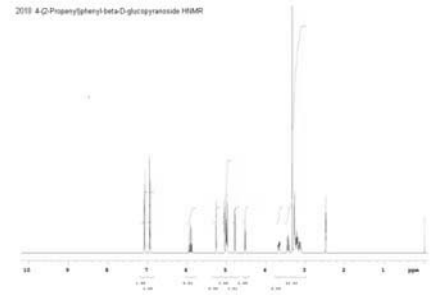


2017 Guaiacol propionate (1H-NMR)

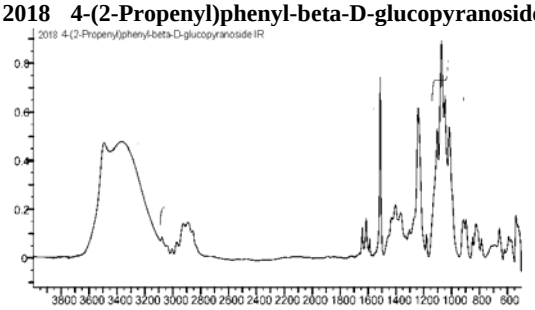


2017 Guaiacol propionate (MS)

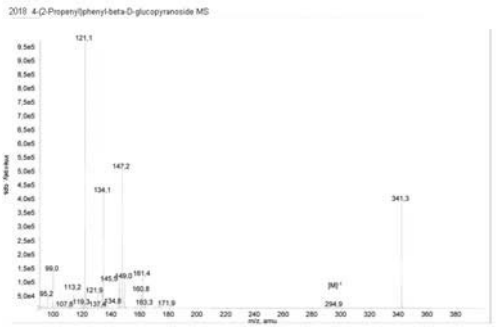
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (1H-NMR)



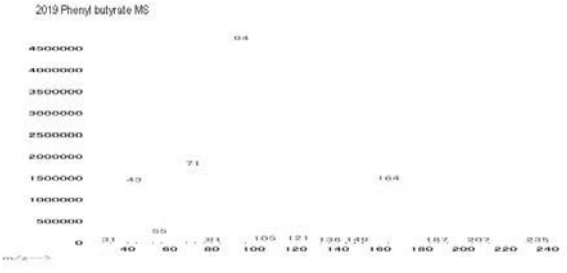
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (IR)



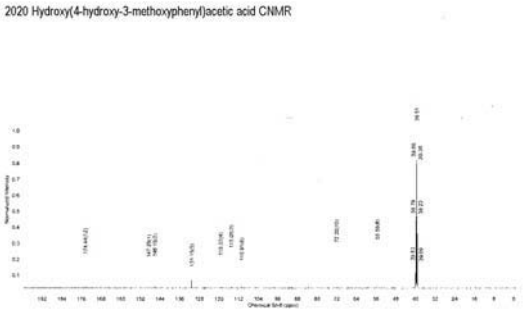
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (MS)



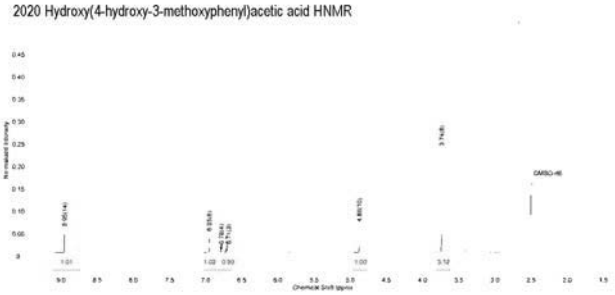
2019 Phenyl butyrate (MS)



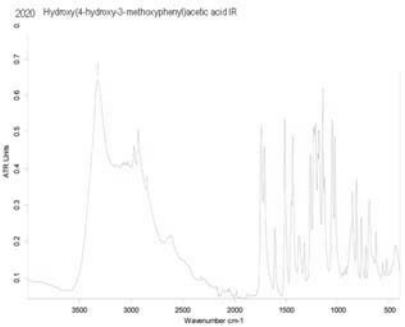
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (13C-NMR)



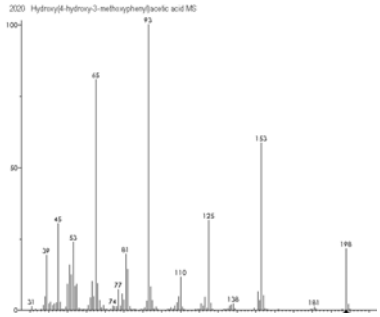
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (1H-NMR)



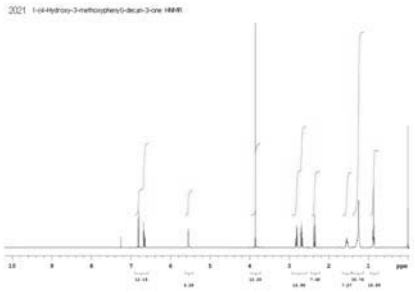
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (IR)



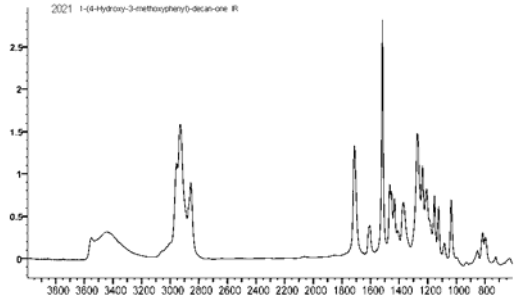
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (MS)



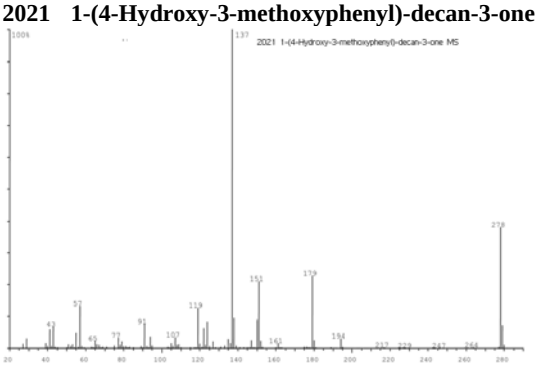
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (1H-NMR)



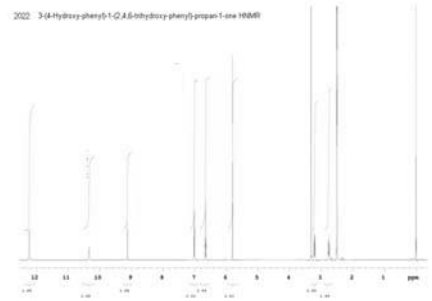
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (IR)



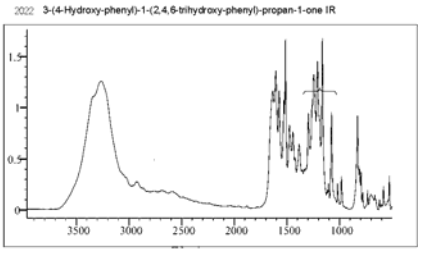
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (MS)



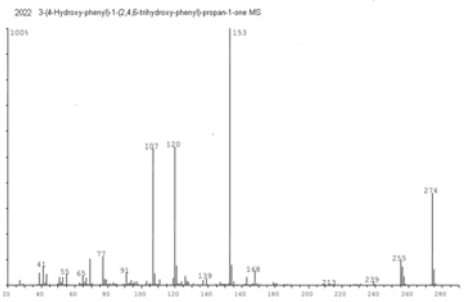
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (1H-NMR)



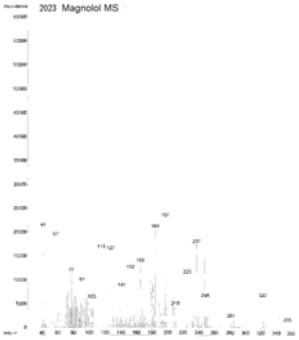
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (IR)



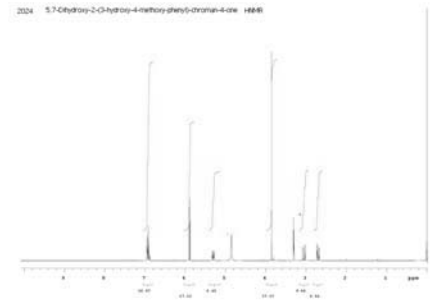
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (MS)



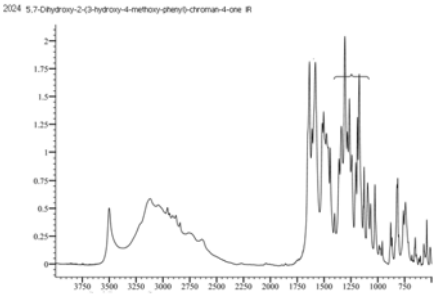
2023 Magnolol (MS)



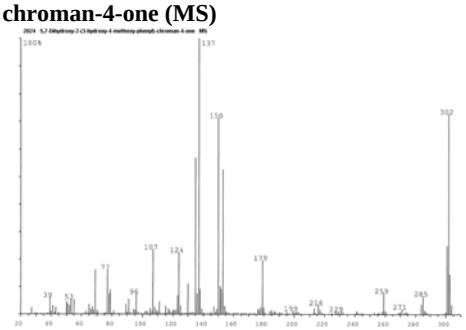
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (1H-NMR)



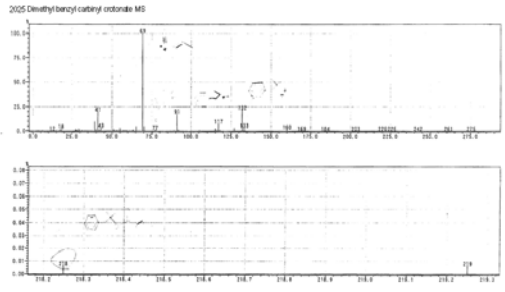
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (IR)



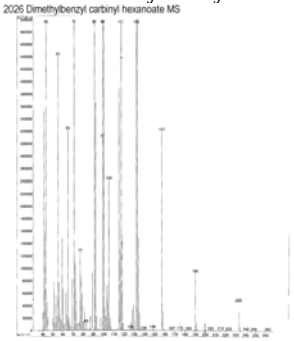
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (MS)



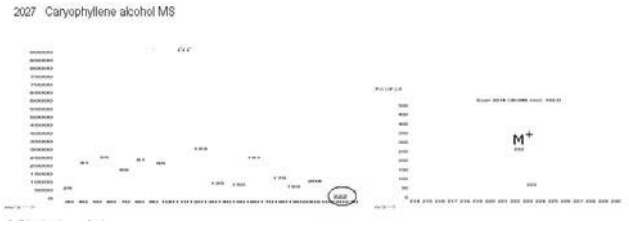
2025 Dimethylbenzyl carbinyl crotonate (MS)



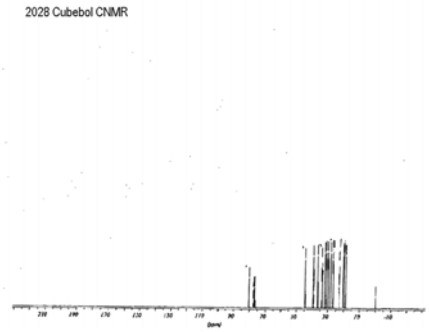
2026 Dimethylbenzyl carbinyl hexanoate (MS)



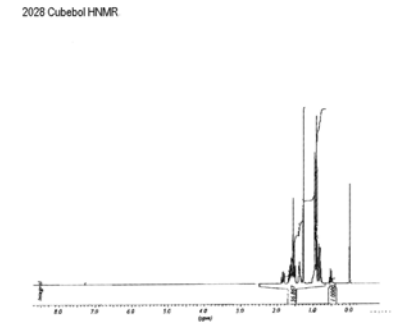
2027 Caryophyllene alcohol (MS)



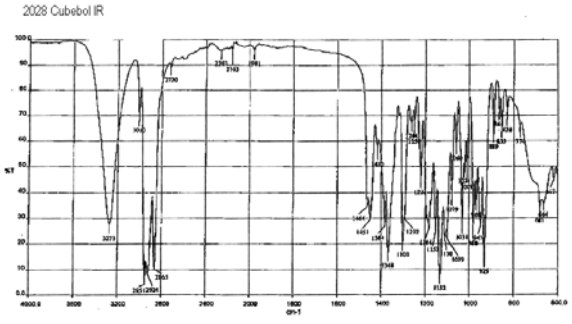
2028 Cubebol (13C-NMR)



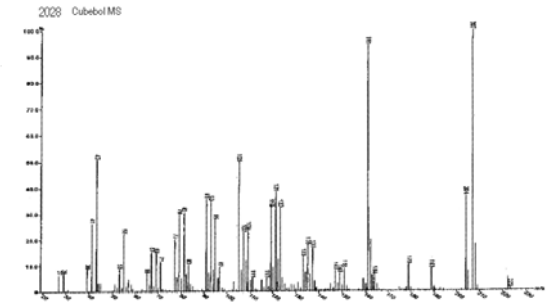
2028 Cubebol (1H-NMR)



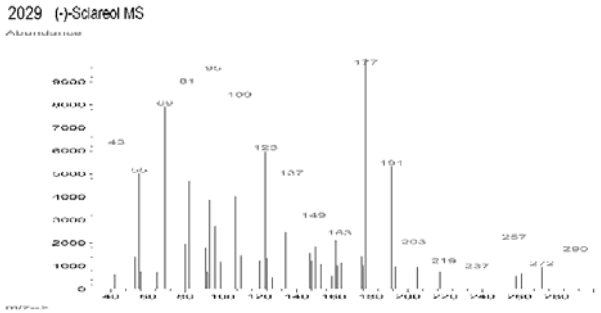
2028 Cubebol (IR)



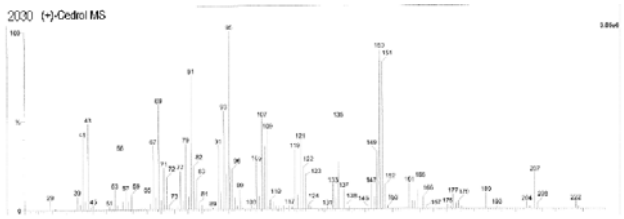
2028 Cubebol (MS)



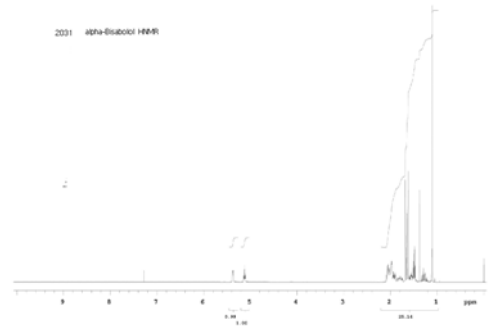
2029 (-)-Sclareol (MS)



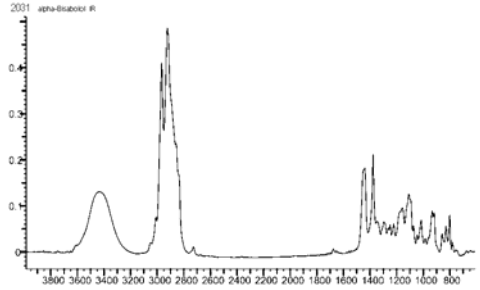
2030 (+)-Cedrol (MS)



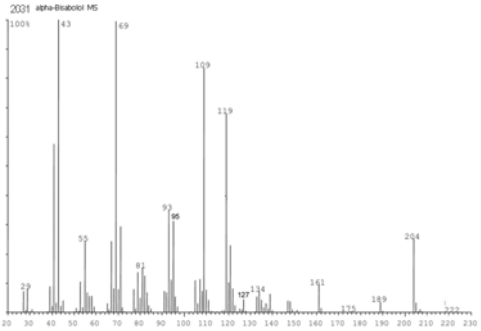
2031 alpha-Bisabolol (1H-NMR)



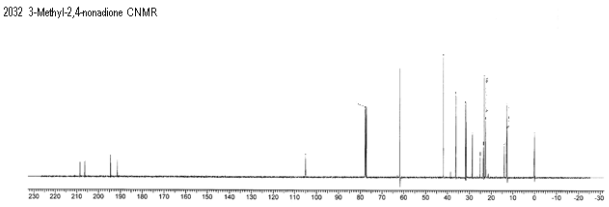
2031 alpha-Bisabolol (IR)



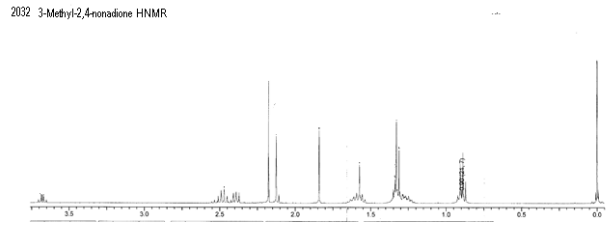
2031 alpha-Bisabolol (MS)



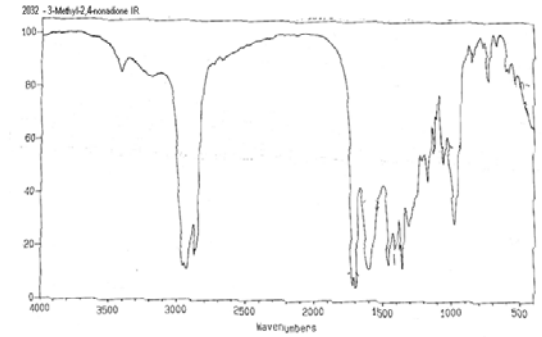
2032 3-Methyl-2,4-nonedione (13C-NMR)



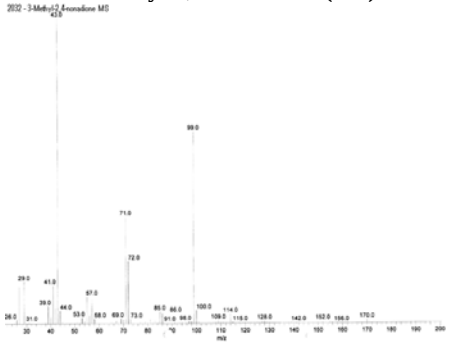
2032 3-Methyl-2,4-nonedione (1H-NMR)



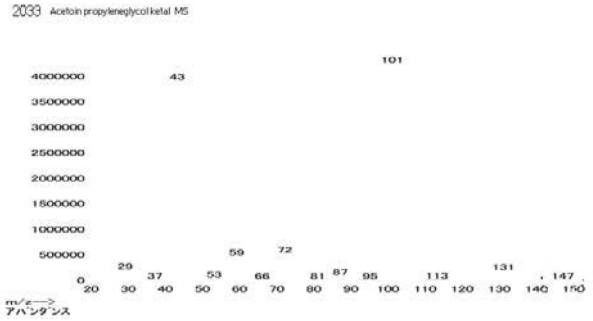
2032 3-Methyl-2,4-nonedione (IR)



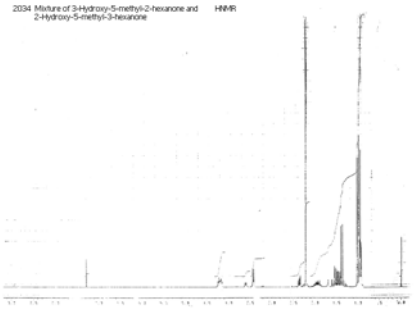
2032 3-Methyl-2,4-nonedione (MS)



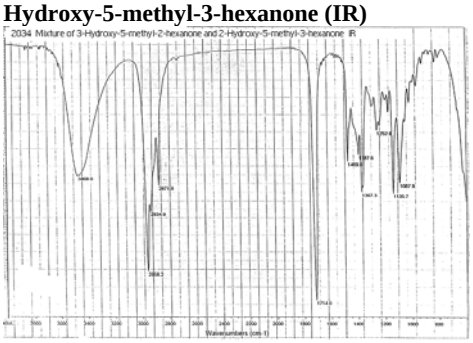
2033 Acetoin propyleneglycol ketal (MS)



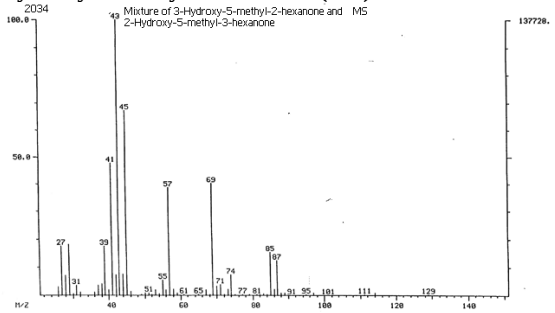
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (1H-NMR)



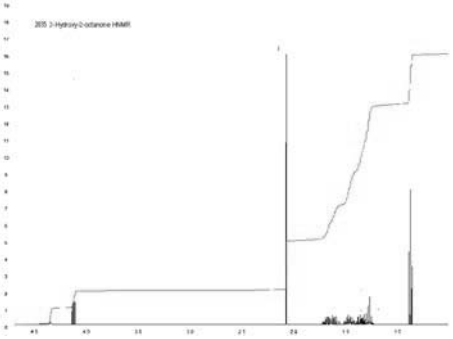
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (IR)



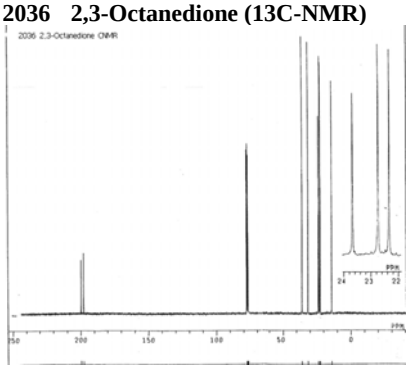
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (MS)



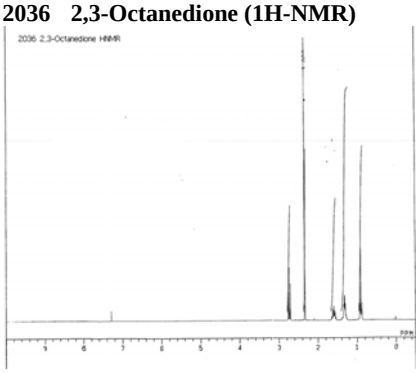
2035 3-Hydroxy-2-octanone (1H-NMR)



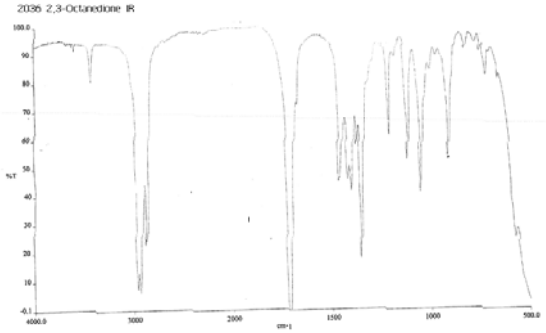
2036 2,3-Octanedione (13C-NMR)



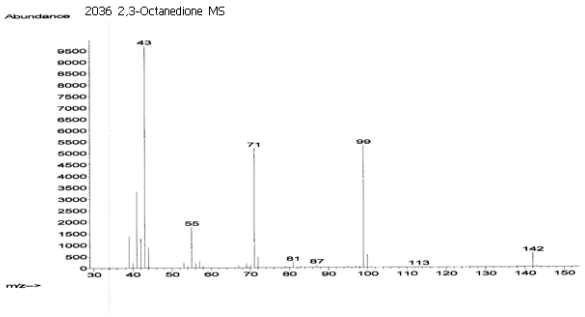
2036 2,3-Octanedione (1H-NMR)



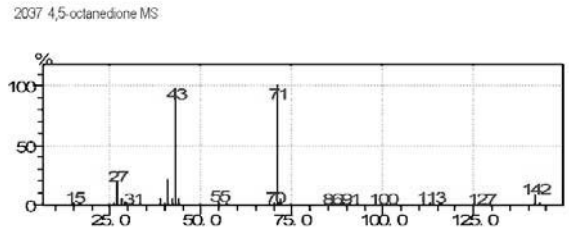
2036 2,3-Octanedione (IR)



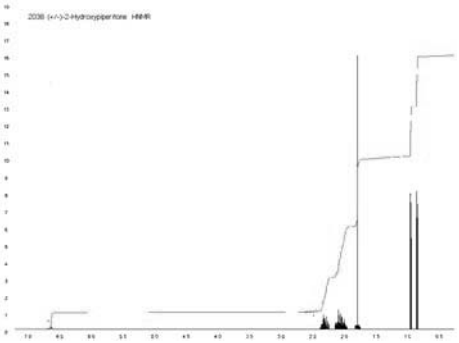
2036 2,3-Octanedione (MS)



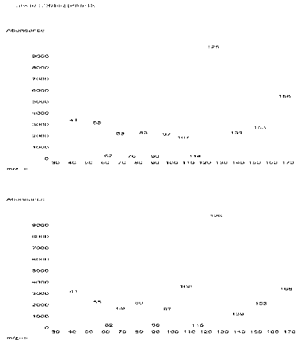
2037 4,5-Octanedione (MS)



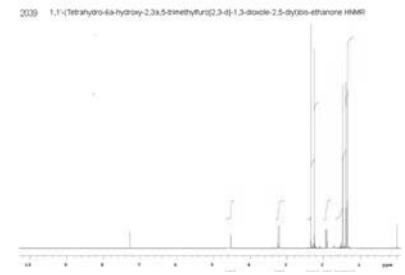
2038 (+/-)-2-Hydroxypiperitone (1H-NMR)



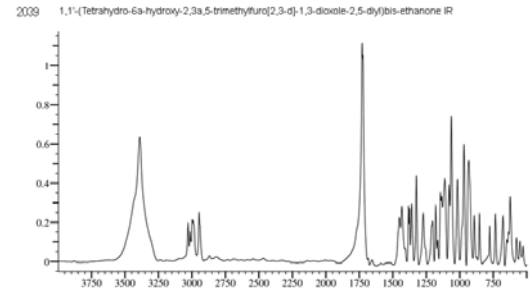
2038 (+/-)-2-Hydroxypiperitone (MS)



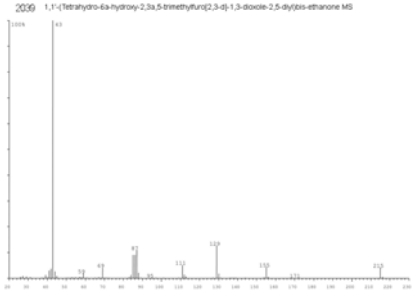
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (1H-NMR)



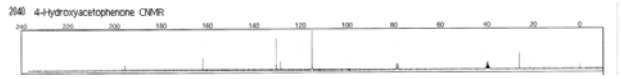
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (IR)



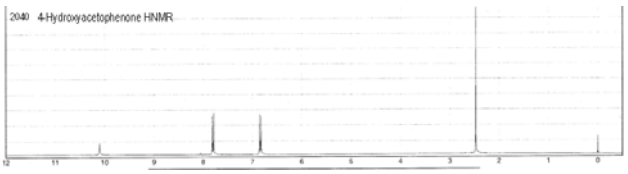
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (MS)



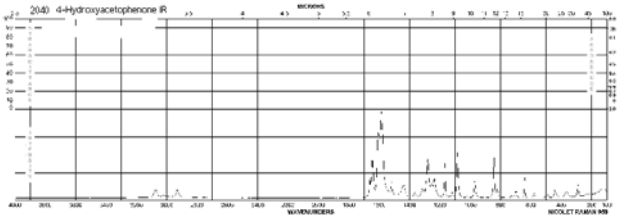
2040 4-Hydroxyacetophenone (13C-NMR)



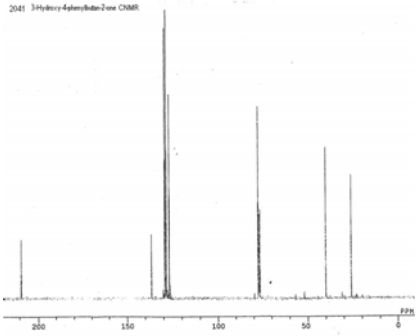
2040 4-Hydroxyacetophenone (1H-NMR)



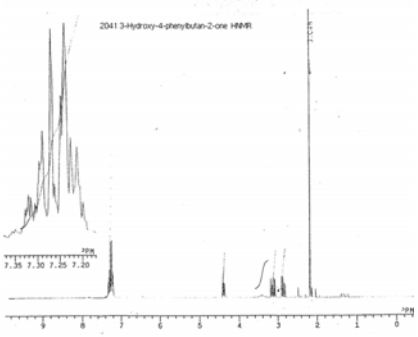
2040 4-Hydroxyacetophenone (IR)



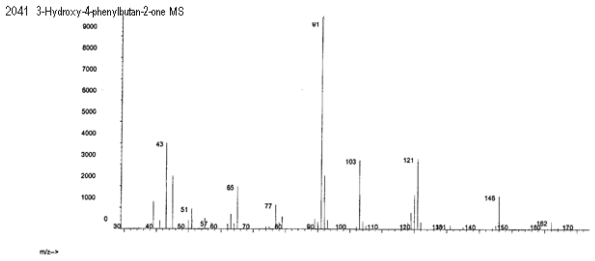
2041 3-Hydroxy-4-phenylbutan-2-one (13C-NMR)



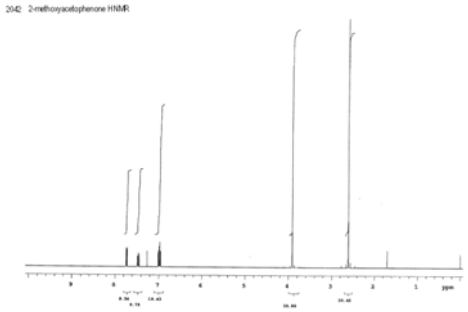
2041 3-Hydroxy-4-phenylbutan-2-one (1H-NMR)



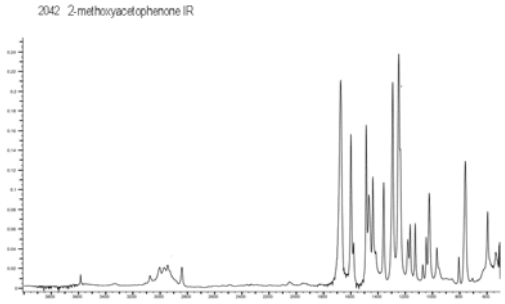
2041 3-Hydroxy-4-phenylbutan-2-one (MS)



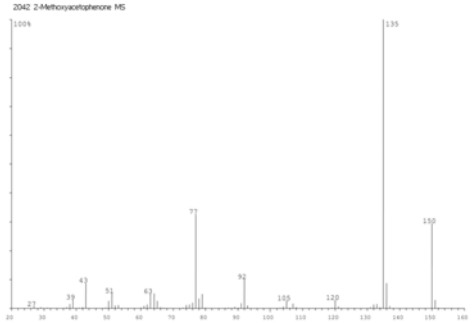
2042 2-Methoxyacetophenone (1H-NMR)



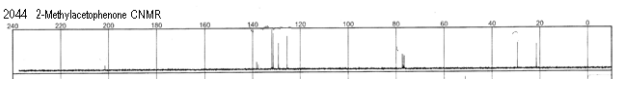
2042 2-Methoxyacetophenone (IR)



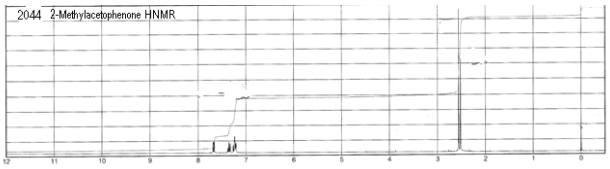
2042 2-Methoxyacetophenone (MS)



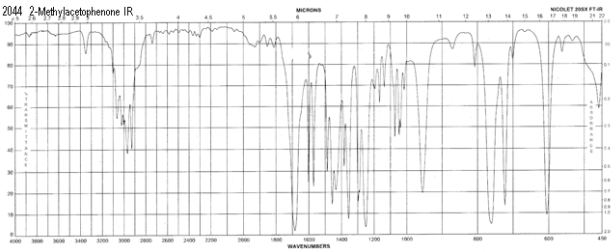
2044 2-Methylacetophenone (13C-NMR)



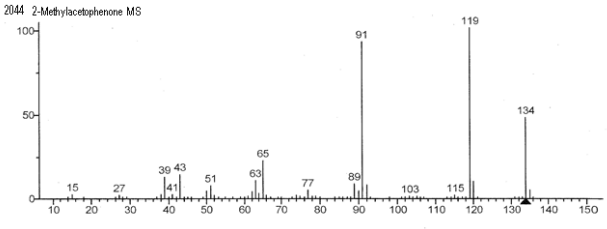
2044 2-Methylacetophenone (1H-NMR)



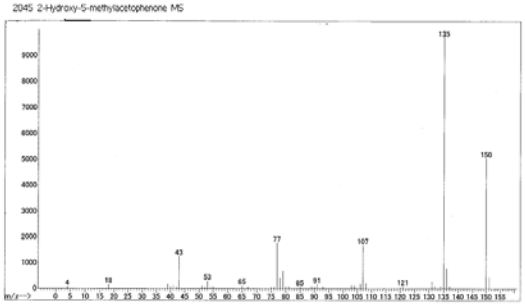
2044 2-Methylacetophenone (IR)



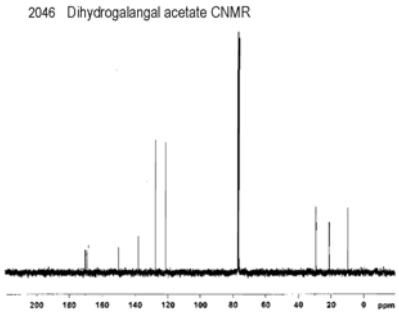
2044 2-Methylacetophenone (MS)



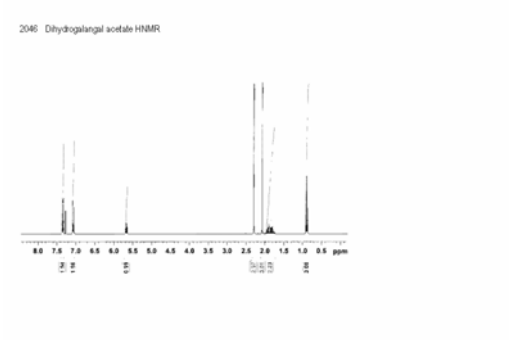
2045 2-Hydroxy-5-methylacetophenone (MS)



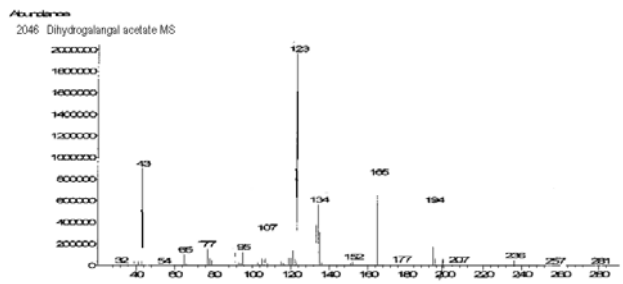
2046 Dihydrogalangal acetate (13C-NMR)



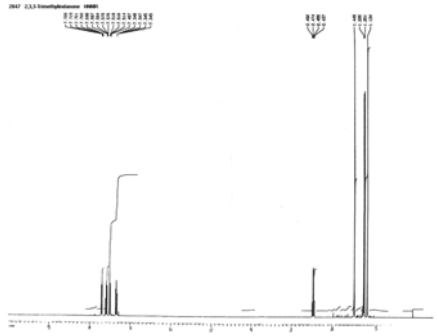
2046 Dihydrogalangal acetate (1H-NMR)



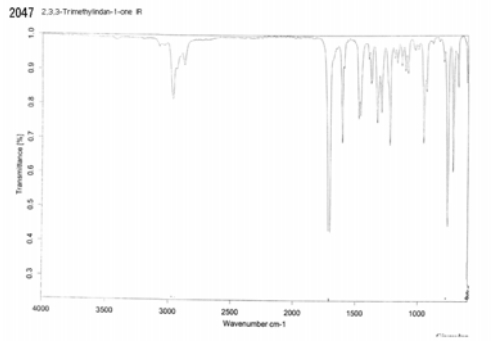
2046 Dihydrogalangal acetate (MS)



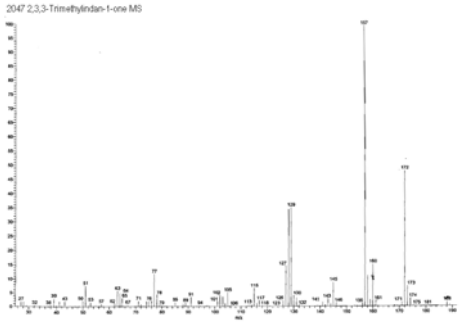
2047 2,3,3-Trimethylindan-1-one (1H-NMR)



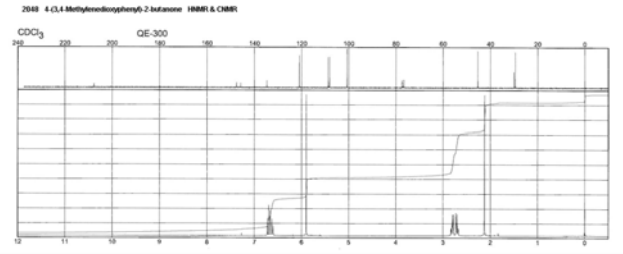
2047 2,3,3-Trimethylindan-1-one (IR)



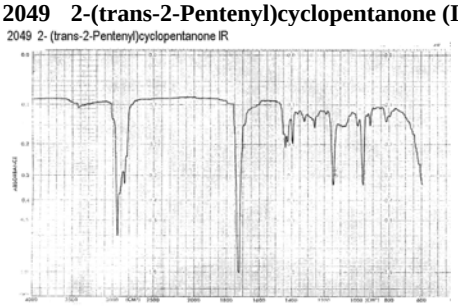
2047 2,3,3-Trimethylindan-1-one (MS)



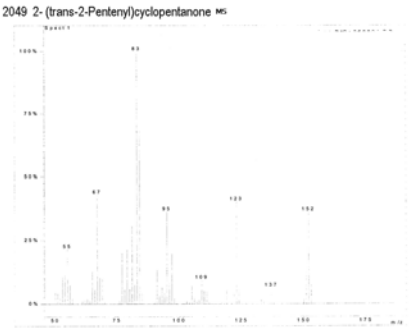
2048 4-(3,4-Methylenedioxyphenyl)-2-butanone (NMR)



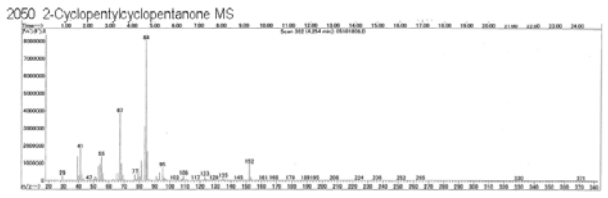
2049 2-(trans-2-Pentenyl)cyclopentanone (IR)



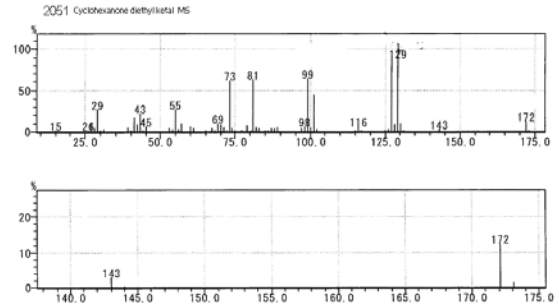
2049 2-(trans-2-Pentenyl)cyclopentanone (MS)



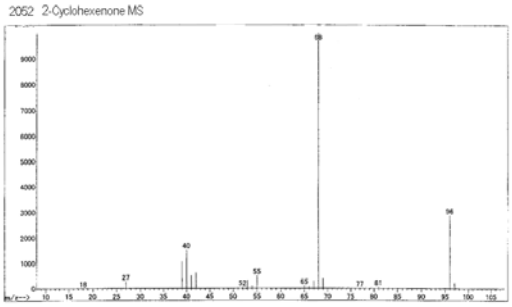
2050 2-Cyclopentylcyclopentanone (MS)



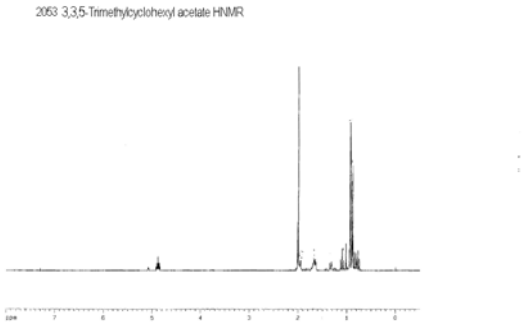
2051 Cyclohexanone diethyl ketal (MS)



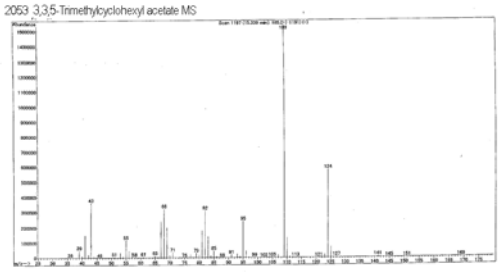
2052 2-Cyclohexenone (MS)



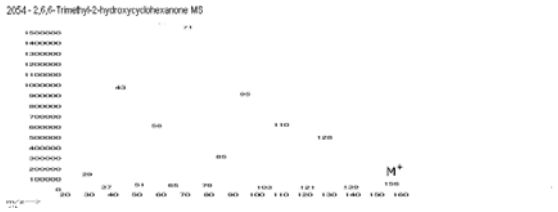
2053 3,3,5-Trimethylcyclohexyl acetate (1H-NMR)



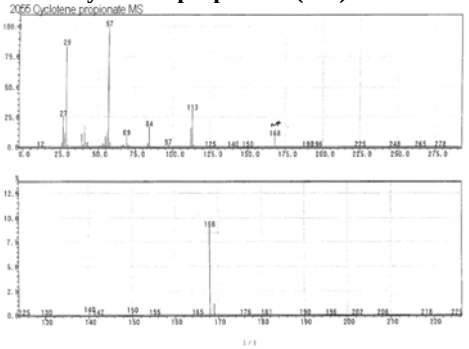
2053 3,3,5-Trimethylcyclohexyl acetate (MS)



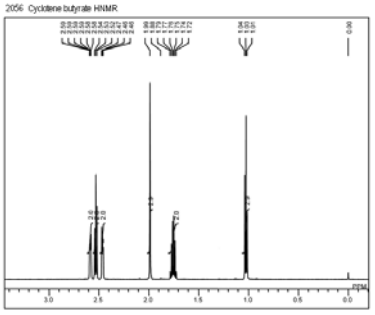
2054 2,6,6-Trimethyl-2-hydroxycyclohexanone (MS)



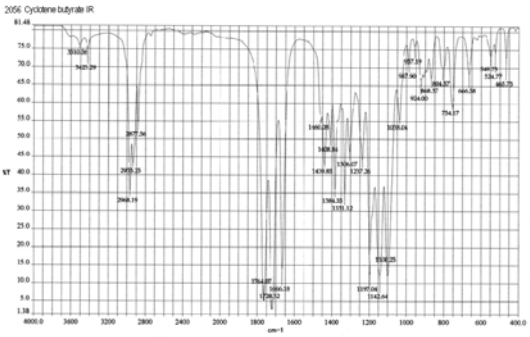
2055 Cyclotene propionate (MS)



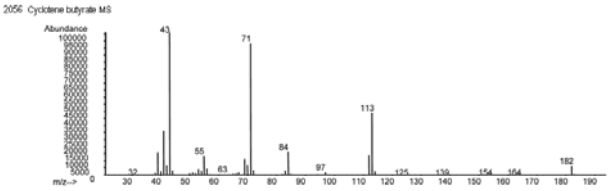
2056 Cyclotene butyrate (1H-NMR)



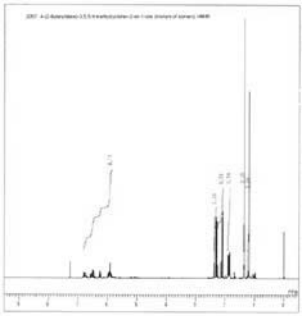
2056 Cyclotene butyrate (IR)



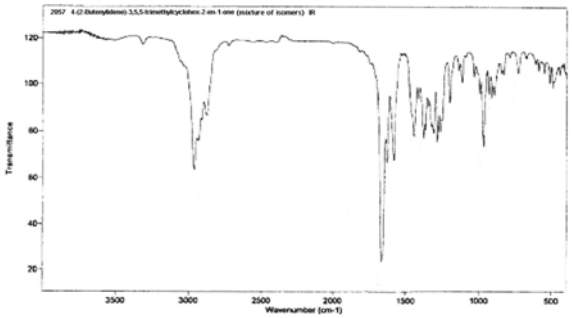
2056 Cyclotene butyrate



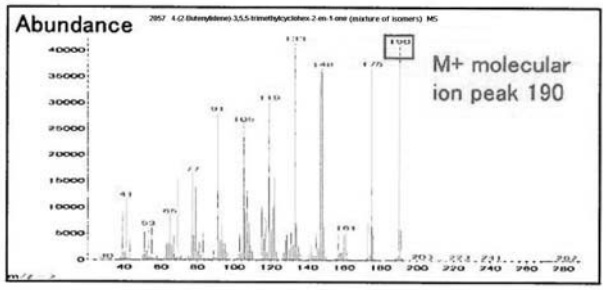
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (1H-NMR)



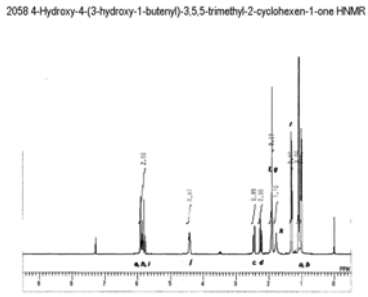
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (IR)



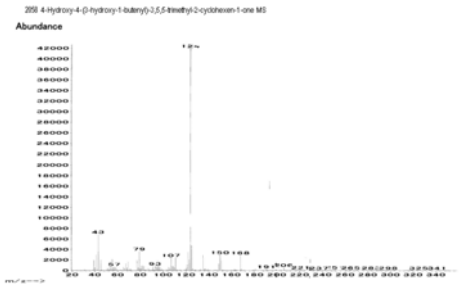
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (MS)



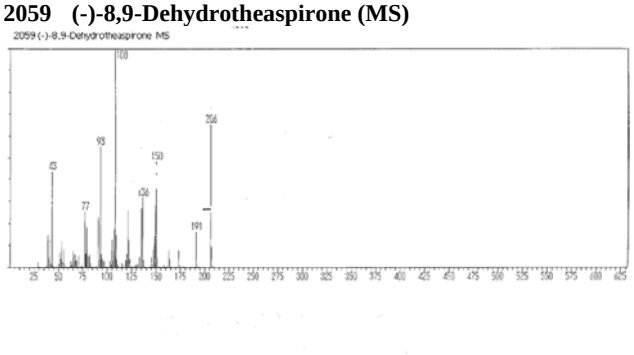
2058 4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers) (1H-NMR)



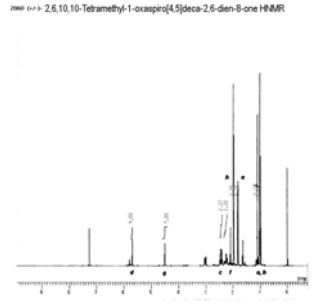
2058 4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers) (MS)



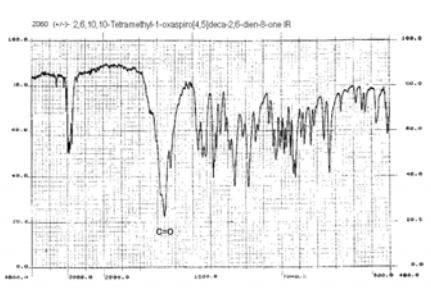
2059 (-)-8,9-Dehydrotheaspirone (MS)



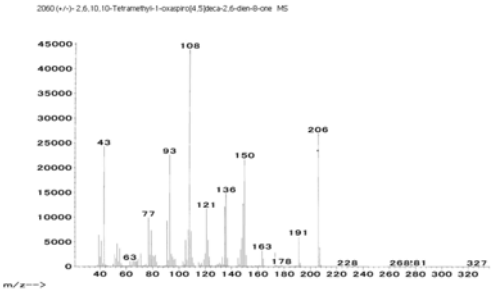
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (1H-NMR)



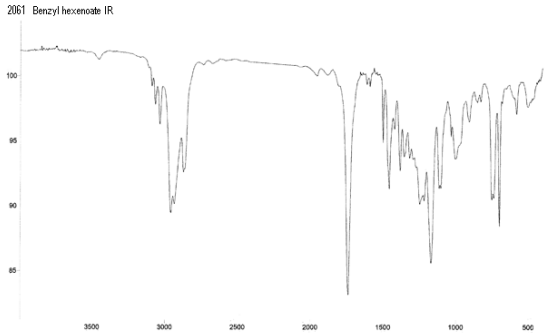
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (IR)



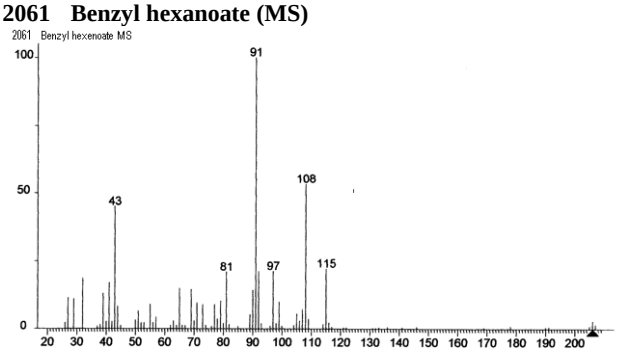
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (MS)



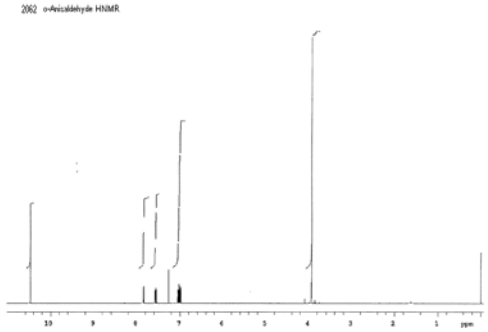
2061 Benzyl hexanoate (IR)



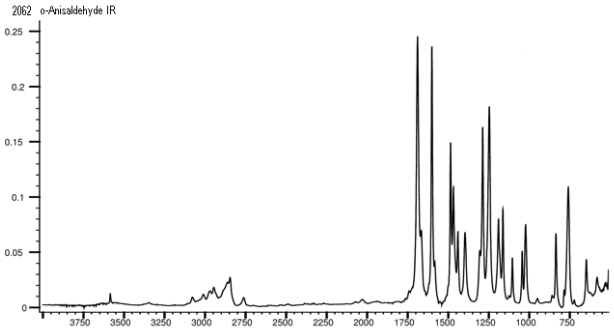
2061 Benzyl hexanoate (MS)



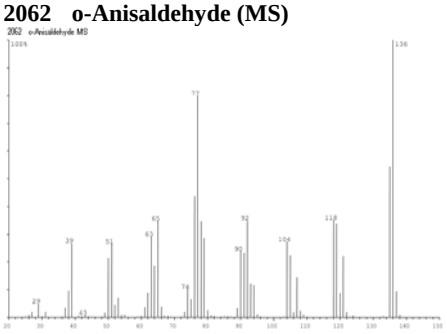
2062 o-Anisaldehyde (1H-NMR)



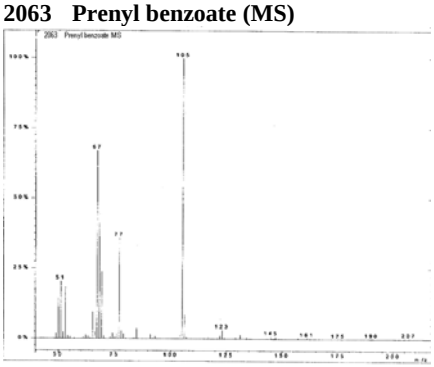
2062 o-Anisaldehyde (IR)



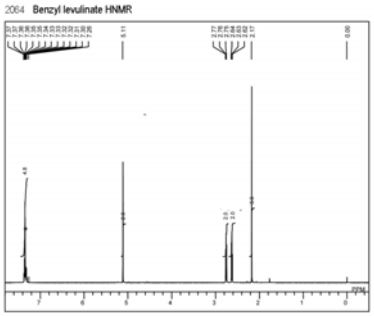
2062 o-Anisaldehyde (MS)



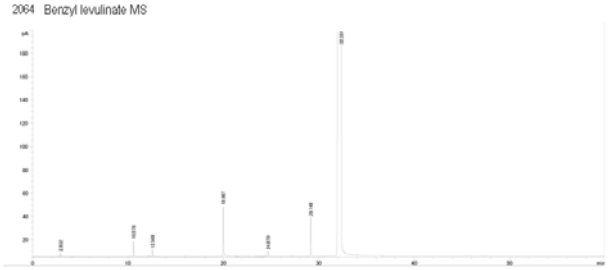
2063 Prenyl benzoate (MS)



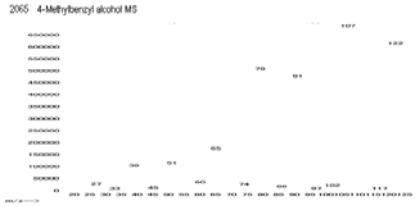
2064 Benzyl levulinate (1H-NMR)



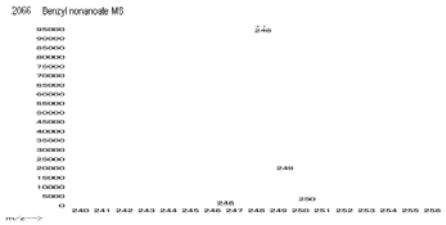
2064 Benzyl levulinate (MS)



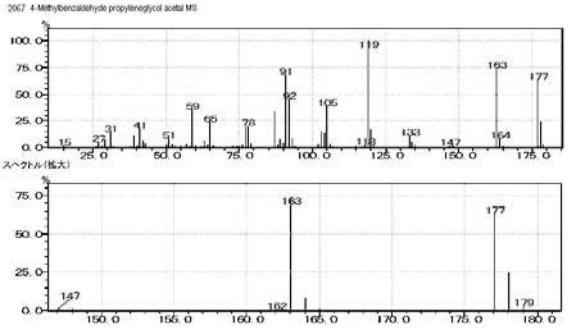
2065 4-Methylbenzyl alcohol (MS)



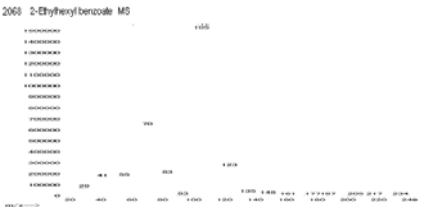
2066 Benzyl nonanoate (MS)



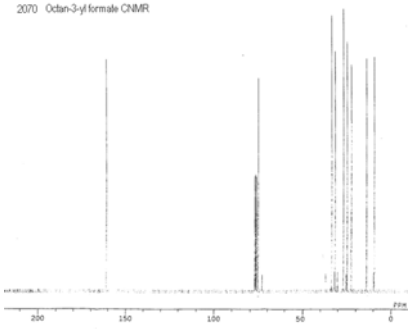
2067 4-Methylbenzaldehyde propyleneglycol acetal (MS)



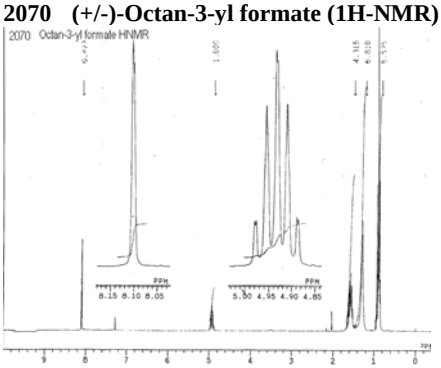
2068 2-Ethylhexyl benzoate (MS)



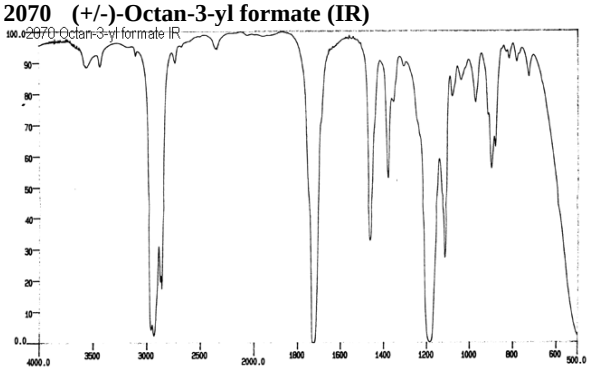
2070 (+/-)-Octan-3-yl formate (13C-NMR)



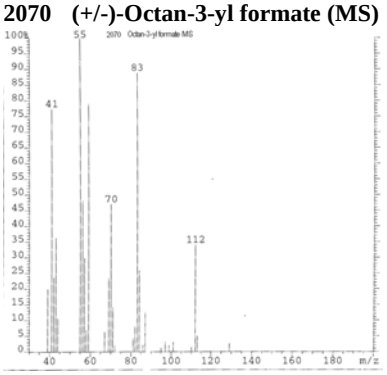
2070 (+/-)-Octan-3-yl formate (1H-NMR)



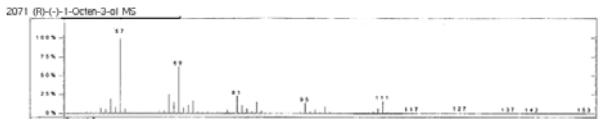
2070 (+/-)-Octan-3-yl formate (IR)



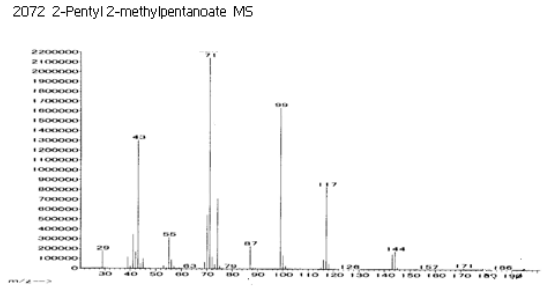
2070 (+/-)-Octan-3-yl formate (MS)



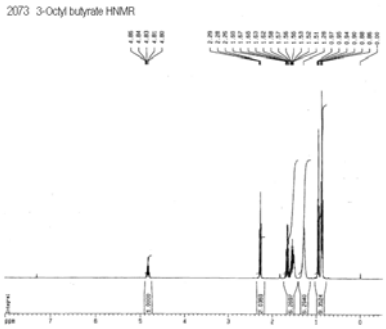
2071 (R)-(-)-1-Octen-3-ol (MS)



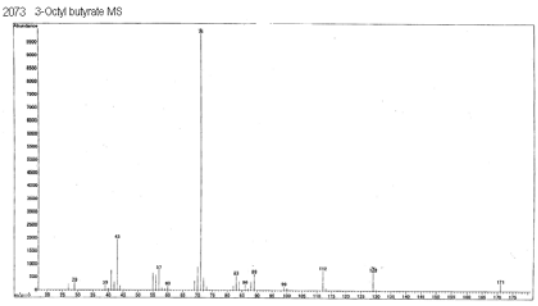
2072 2-Pentyl 2-methylpentanoate (MS)



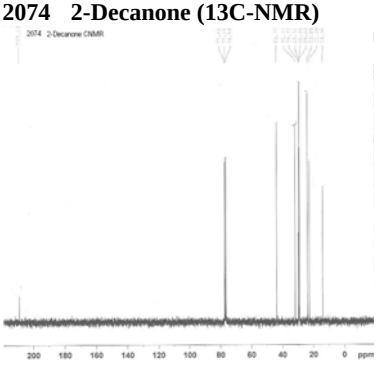
2073 3-Octyl butyrate (1H-NMR)



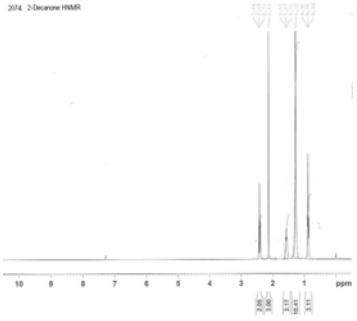
2073 3-Octyl butyrate (MS)



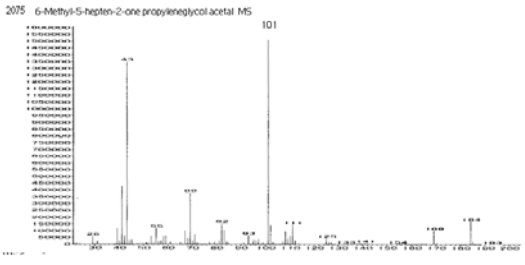
2074 2-Decanone (13C-NMR)



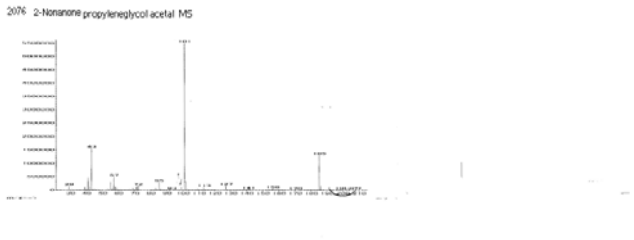
2074 2-Decanone (1H-NMR)



2075 6-Methyl-5-hepten-2-one propyleneglycol acetal (MS)



2076 2-Nonanone propyleneglycol acetal (MS)



List of new flavourings evaluated in alphabetical order

Acetoin propyleneglycol ketal	2033
o-Anisaldehyde	2062
N-p-Benzeneacetonitrile menthanecarboxamide	2009
Benzyl hexanoate	2061
Benzyl levulinate	2064
Benzyl nonanoate	2066
alpha-Bisabolol	2031
Bis(2-methylphenyl) disulfide	1931
Butanal dibenzyl thioacetal	1939
4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers)	2057
Butyl beta-(methylthio)acrylate	1921
di-sec-Butyl disulfide	1933
Butyl propyl disulfide	1932
Caryophyllene alcohol	2027
(+)-Cedrol	2030
Choline chloride	2003
Cubebol	2028
Cyclohexanone diethyl ketal	2051
2-Cyclohexenone	2052
2-Cyclopentylcyclopentanone	2050
Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide	2006
Cyclotene butyrate	2056
Cyclotene propionate	2055
2-Decanone	2074
7-Decen-4-olide	1992
9-Decen-5-olide	1993
8-Decen-5-olide	1994
Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid	1977
Dihydrogalangal acetate	2046
(+/-)-cis- and trans-1,2-Dihydroperillaldehyde	1902
5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one	2024
(-)-8,9-Dehydrotheaspirone	2059
Diisoamyl disulfide	1930
Diisoamyl trisulfide	1934
Diisobutyl adipate	1967
Diisopropyl adipate	1966
Dimethyl adipate	1964
Dimethylbenzyl carbinyl crotonate	2025
Dimethylbenzyl carbinyl hexanoate	2026
Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde	1900
N-(1,1-Dimethyl-2-hydroxyethyl)-2,2-diethylbutanamide	2011
Dioctyl adipate	1968
Di-(1-propenyl) sulfide (mixture of isomers)	1911
Dipropyl adipate	1965
Dodecanethiol	1924
9-Dodecen-5-olide	1996
Dodecyl lactate	1948
Ethyl 2-acetylhexanoate	1953
Ethyl 2-acetyloctanoate	1958
Ethyl acetoacetate ethyleneglycol ketal	1969
Ethyl 5-acetoxyoctanoate	1959
N-Ethyl-2,2-diisopropylbutanamide	2005

Ethyl 3-(ethylthio)butyrate	1922
2-Ethylhexyl benzoate	2068
2-Ethylhexyl 3-mercaptopropionate	1938
Ethyl 5-hydroxydecanoate	1962
Ethyl 2-hydroxyethyl sulfide	1912
(+/-)-Ethyl 3-hydroxy-2-methylbutyrate	1949
Ethyl 3-hydroxyoctanoate	1955
Ethyl 5-hydroxyoctanoate	1987
Ethyl levulinate propyleneglycol ketal	1973
Ethyl 3-(methylthio)-2-propenoate (mixture of isomers)	1917
Ethyl 3-(methylthio)-(2E)-propenoate	1916
Ethyl 3-(methylthio)-(2Z)-propenoate	1915
(+/-)-Ethyl 3-mercapto-2-methylbutanoate	1928
Ethyl 5-oxodecanoate	1961
Guaiacol butyrate	2015
Guaiacol isobutyrate	2016
Guaiacol propionate	2017
cis- and trans-2-Heptylcyclopropanecarboxylic acid	1907
Hexadecyl lactate	1950
cis-3-Hexenyl acetoacetate	1974
Hydroxyacetone	1945
4-Hydroxyacetophenone	2040
4-Hydroxy-2-butenoic acid gamma-lactone	2000
Hydroxycitronellal propyleneglycol acetal	1975
4-Hydroxy-2,3-dimethyl-2,4-nonadienoic acid gamma-lactone	2002
2-Hydroxyethanethiol	1925
N-(2-Hydroxyethyl)-2,3-dimethyl 2-isopropylbutanamide	2010
4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers)	2058
Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid	2020
1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one	2021
2-Hydroxy-5-methylacetophenone	2045
5-Hydroxy-4-methylhexanoic acid delta-lactone	1990
Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone	2034
1-Hydroxy-4-methyl-2-pentanone	1952
3-Hydroxy-2-octanone	2035
3-Hydroxy-4-phenylbutan-2-one	2041
3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one	2022
(+/-)-2-Hydroxypiperitone	2038
Isoamyl levulinate	1972
Isoambrettolide	1991
3-Isopropenyl-6-oxoheptanoic acid	1954
Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone	1988
d-Limonen-10-ol	1903
Magnolol	2023
1,3-p-Menthadien-7-al	1906
p-Menth-1-en-9-ol	1905
p-Menthan-7-ol	1904
3-Mercapto-3-methylbutyl isovalerate	1927
3-Mercaptohexanal	1929
3-Mercaptopropionic acid	1936
4-Mercapto-4-methyl-2-hexanone	1926
Methional diethyl acetal	1940
2-Methoxyacetophenone	2042
2-Methylacetophenone	2044

Methyl 3-acetoxy-2-methylbutyrate	1951
Methyl 3-acetoxyoctanoate	1956
4-Methylbenzaldehyde propyleneglycol acetal	2067
4-Methylbenzyl alcohol	2065
Methyl dihydrojasmonate	1898
4-(3,4-Methylenedioxyphenyl)-2-butanone	2048
6-Methyl-5-hepten-2-one propyleneglycol acetal	2075
Methyl 3-hydroxybutyrate	1947
Methyl isobutanethioate	1937
Methyl levulinate	1970
(+/-)-cis- and trans-2-Methyl-2-(4-methyl-3-pentenyl)cyclopropanecarbaldehyde	1908
Methyl 2-methylphenyl disulfide	1935
4-Methyl-2-(methylthiomethyl)-2-hexenal	1919
4-Methyl-2-(methylthiomethyl)-2-pentenal	1918
5-Methyl-2-(methylthiomethyl)-2-hexenal	1920
3-Methyl-2,4-nonedione	2032
Methyl octyl sulfide	1909
Methyl 1-propenyl sulfide	1910
1-(3-(Methylthio)-butyryl)-2,6,6-trimethylcyclohexene	1942
2-(Methylthio)ethyl acetate	1913
3-(Methylthio)propyl hexanoate	1941
3-(Methylthio)propyl mercaptoacetate	1914
3-(Methylthio)propylamine	2004
2-Nonanone propyleneglycol acetal	2076
2-Nonenoic acid gamma-lactone	2001
gamma-Octadecalactone	1998
delta-Octadecalactone	1999
(+/-)-Octan-3-yl formate	2070
(R)-(-)-1-Octen-3-ol	2071
3-Octyl butyrate	2073
2,3-Octanedione	2036
4,5-Octanedione	2037
Orin lactone	1995
5-Oxodecanoic acid	1960
5-Oxododecanoic acid	1963
2-Oxo-3-ethyl-4-butanolide	1986
5-Oxooctanoic acid	1957
2-Oxothiolane	1923
2-(trans-2-Pentenyl)cyclopentanone	2049
2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers)	1944
2-Pentyl 2-methylpentanoate	2072
5-Pentyl-3H-furan-2-one	1989
(+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane	1943
Perillaldehyde propyleneglycol acetal	1901
Phenyl butyrate	2019
Prenyl benzoate	2063
4-Propenylphenol	2012
4-(2-Propenyl)phenyl-beta-D-glucopyranoside	2018
Propyl levulinate	1971
Propyl pyruvate	1946
Propyleneglycol diacetate	1976
Propyleneglycol dibutyrate	1980
Propyleneglycol dihexanoate	1984
Propyleneglycol di-2-methylbutyrate	1982
Propyleneglycol dioctanoate	1985
Propyleneglycol dipropionate	1978

Propyleneglycol monobutyrate (mixture of isomers)	1979
Propyleneglycol monohexanoate (mixture of isomers)	1983
Propyleneglycol mono-2-methylbutyrate (mixture of isomers)	1981
N-(2-(Pyridin-2-yl)ethyl)-3-p-menthanecarboxamide	2008
(-)-Sclareol	2029
Sodium 3-methoxy-4-hydroxycinnamate	2014
9-Tetradecen-5-olide	1997
1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone	2039
(+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one	2060
cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid	1899
3,3,5-Trimethylcyclohexyl acetate	2053
2,6,6-Trimethyl-2-hydroxycyclohexanone	2054
2,3,3-Trimethylindan-1-one	2047
2,4,6-Trimethylphenol	2013

ANNEX 1: SUMMARY OF RECOMMENDATIONS FROM THE 69TH JECFA

Toxicological recommendations and information on specifications

Food additives considered for specifications only

Food additive	Specifications[a]
Activated carbon	R
Annatto extract (oil-processed bixin)	W
Cassia gum	R
Indigotine	R
Steviol glycosides	R
Sucrose esters of fatty acids	R
Sucrose monoesters of lauric, palmitic or stearic acid	N, T
Titanium dioxide	R

[a] N, new specifications; R, existing specifications revised; T, tentative specifications; W, existing specifications withdrawn.

Flavouring agents evaluated by the Procedure for the Safety Evaluation of Flavouring Agents[1]

A. Alicyclic primary alcohols, aldehydes, acids and related esters

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid	1899	N	No safety concern
(2,4)-, (3,5)- and (3,6)-Dimethyl-3-cyclohexenylcarbaldehyde	1900	N	No safety concern
(±)-*cis*- and *trans*-1,2-Dihydroperillaldehyde	1902	N	No safety concern
d-Limonen-10-ol	1903	N	No safety concern
p-Menthan-7-ol	1904	N	No safety concern
p-Menth-1-en-9-ol	1905	N	No safety concern
1,3-*p*-Menthadien-7-al	1906	N	No safety concern
Structural class II			
Methyl dihydrojasmonate	1898	N	No safety concern
cis- and *trans*-2-Heptylcyclopropanecarboxylic acid	1907	N	No safety concern
(±)-*cis*- and *trans*-2-Methyl-2-(4-methyl-3-pentenyl)cyclopropanecarbaldehyde	1908	N	No safety concern

[1] The flavouring agent 2-aminoacetophenone (No. 2043) was on the agenda to be evaluated in the group of aromatic substituted secondary alcohols, ketones and related esters. Although the compound fulfils some of the structural requirements for this group, the main toxicologically relevant structural feature is the amino group; hence, the compound was not evaluated and should be evaluated in the future in the group of aliphatic and aromatic amines and amides. The flavouring agent (±)-2-phenyl-4-methyl-2-hexenal (No. 2069) was on the agenda to be evaluated in the group of benzyl derivatives. However, as this compound did not meet the structural requirements for this group, the compound was not evaluated at this meeting.

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III		N	
Perillaldehyde propyleneglycol acetal	1901	N	No safety concern

[a] N, new specifications.

B. Simple aliphatic and aromatic sulfides and thiols

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Subgroup i: Simple sulfides			
Structural class I			
Methyl octyl sulfide	1909	N	No safety concern
Methyl 1-propenyl sulfide	1910	N	No safety concern
Di-(1-propenyl)-sulfide (mixture of isomers)	1911	N	No safety concern
Structural class III			
Butanal dibenzyl thioacetal	1939	N	**Additional data required to complete evaluation**
Subgroup ii: Acyclic sulfides with oxidized side-chains			
Structural class I			
Ethyl 2-hydroxyethyl sulfide	1912	N	No safety concern
2-(Methylthio)ethyl acetate	1913	N	No safety concern
Ethyl 3-(methylthio)-(2*Z*)-propenoate	1915	N	No safety concern
Ethyl 3-(methylthio)-(2*E*)-propenoate	1916	N	No safety concern
Ethyl 3-(methylthio)-2-propenoate (mixture of isomers)	1917	N	No safety concern
4-Methyl-2-(methylthiomethyl)-2-pentenal	1918	N	No safety concern
4-Methyl-2-(methylthiomethyl)-2-hexenal	1919	N	No safety concern
5-Methyl-2-(methylthiomethyl)-2-hexenal	1920	N	No safety concern
Butyl β-(methylthio)acrylate	1921	N	No safety concern
Ethyl 3-(ethylthio)butyrate	1922	N	No safety concern
Methional diethyl acetal	1940	N	No safety concern
3-(Methylthio)propyl hexanoate	1941	N	**Additional data required to complete evaluation**
Structural class III			
1-(3-(Methylthio)-butyryl)-2,6,6-trimethylcyclohexene	1942	N	No safety concern
Subgroup iii: Cyclic sulfides			
Structural class II			
2-Oxothiolane	1923	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III			
(±)-*cis*- and *trans*-2-Pentyl-4-propyl-1,3-oxathiane	1943	N	**Additional data required to complete evaluation**
2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers)	1944	N	**Additional data required to complete evaluation**
Subgroup iv: Simple thiols			
Structural class I			
Dodecanethiol	1924	N	No safety concern
Subgroup v: Thiols with oxidized side-chains			
Structural class I			
2-Hydroxyethanethiol	1925	N	No safety concern
4-Mercapto-4-methyl-2-hexanone	1926	N	No safety concern
3-Mercapto-3-methylbutyl isovalerate	1927	N	No safety concern
(±)-Ethyl 3-mercapto-2-methylbutanoate	1928	N	No safety concern
3-Mercaptohexanal	1929	N	No safety concern
3-Mercaptopropionic acid	1936	N	No safety concern
2-Ethylhexyl 3-mercaptopropionate	1938	N	No safety concern
Structural class III			
3-(Methylthio)propyl mercaptoacetate	1914	N	**Additional data required to complete evaluation**
Subgroup vii: Simple disulfides			
Structural class I			
Diisoamyl disulfide	1930	N	No safety concern
Butyl propyl disulfide	1932	N	No safety concern
di-*sec*-Butyl disulfide	1933	N	No safety concern
Structural class III			
Bis(2-methylphenyl) disulfide	1931	N	**Additional data required to complete evaluation**
Methyl 2-methylphenyl disulfide	1935	N	No safety concern
Subgroup ix: Trisulfides			
Structural class I			
Diisoamyl trisulfide	1934	N	No safety concern
Subgroup xi: Thioesters			
Structural class I			
Methyl isobutanethioate	1937	N	No safety concern

[a] N, new specifications.

C. Aliphatic primary alcohols, aldehydes, carboxylic acids, acetals and esters containing additional oxygenated functional groups

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
Hydroxyacetone	1945	N	No safety concern
Propyl pyruvate	1946	N	No safety concern
Methyl 3-hydroxybutyrate	1947	N	No safety concern
Dodecyl lactate	1948	N	No safety concern
(±)-Ethyl 3-hydroxy-2-methylbutyrate	1949	N	No safety concern
Hexadecyl lactate	1950	N	No safety concern
Methyl 3-acetoxy-2-methylbutyrate	1951	N	No safety concern
1-Hydroxy-4-methyl-2-pentanone	1952	N	No safety concern
Ethyl 2-acetylhexanoate	1953	N	No safety concern
3-Isopropenyl-6-oxoheptanoic acid	1954	N	No safety concern
Ethyl 3-hydroxyoctanoate	1955	N	No safety concern
Methyl 3-acetoxyoctanoate	1956	N	No safety concern
5-Oxooctanoic acid	1957	N	No safety concern
Ethyl 2-acetyloctanoate	1958	N	No safety concern
Ethyl 5-acetoxyoctanoate	1959	N	No safety concern
5-Oxodecanoic acid	1960	N	No safety concern
Ethyl 5-oxodecanoate	1961	N	No safety concern
Ethyl 5-hydroxydecanoate	1962	N	No safety concern
5-Oxododecanoic acid	1963	N	No safety concern
Dimethyl adipate	1964	N	No safety concern
Dipropyl adipate	1965	N	No safety concern
Diisopropyl adipate	1966	N	No safety concern
Diisobutyl adipate	1967	N	No safety concern
Dioctyl adipate	1968	N	No safety concern
Methyl levulinate	1970	N	No safety concern
Propyl levulinate	1971	N	No safety concern
Isoamyl levulinate	1972	N	No safety concern
cis-3-Hexenyl acetoacetate	1974	N	No safety concern
Propyleneglycol diacetate	1976	N	No safety concern
Mixture of 6-(5-decenoyloxy)decanoic acid and 6-(6-decenoyloxy)decanoic acid	1977	N	No safety concern
Propyleneglycol dipropionate	1978	N	No safety concern
Propyleneglycol monobutyrate (mixture of isomers)	1979	N	No safety concern
Propyleneglycol dibutyrate	1980	N	No safety concern
Propyleneglycol mono-2-methylbutyrate (mixture of isomers)	1981	N	No safety concern
Propyleneglycol di-2-methylbutyrate	1982	N	No safety concern
Propyleneglycol monohexanoate (mixture of isomers)	1983	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Propyleneglycol dihexanoate	1984	N	No safety concern
Propyleneglycol dioctanoate	1985	N	No safety concern
2-Oxo-3-ethyl-4-butanolide	1986	N	No safety concern
Ethyl 5-hydroxyoctanoate	1987	N	No safety concern
Structural class III			
Ethyl acetoacetate ethyleneglycol ketal	1969	N	No safety concern
Ethyl levulinate propyleneglycol ketal	1973	N	**Additional data required to complete evaluation**
Hydroxycitronellal propyleneglycol acetal	1975	N	No safety concern
Mixture of isopropylideneglyceryl 5-hydroxyoctanoate and δ-decalactone	1988	N	**Additional data required to complete evaluation**

[a] N, new specifications.

D. Aliphatic lactones

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
5-Pentyl-3H-furan-2-one	1989	N	No safety concern
5-Hydroxy-4-methylhexanoic acid δ-lactone	1990	N	No safety concern
Isoambrettolide	1991	N	No safety concern
7-Decen-4-olide	1992	N	No safety concern
9-Decen-5-olide	1993	N	No safety concern
8-Decen-5-olide	1994	N	No safety concern
Orin lactone	1995	N	No safety concern
9-Dodecen-5-olide	1996	N	No safety concern
9-Tetradecen-5-olide	1997	N	No safety concern
γ-Octadecalactone	1998	N	No safety concern
δ-Octadecalactone	1999	N	No safety concern
Structural class III			
4-Hydroxy-2-butenoic acid γ-lactone	2000	N	No safety concern
2-Nonenoic acid γ-lactone	2001	N	No safety concern
4-Hydroxy-2,3-dimethyl-2,4-nonadienoic acid γ-lactone	2002	N	No safety concern

[a] N, new specifications.

E. Aliphatic and aromatic amines and amides

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
Choline chloride	2003	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
3-(Methylthio)propylamine	2004	N	No safety concern
Structural class III			
N-Ethyl-2,2-diisopropylbutanamide	2005	N	**Additional data required to complete evaluation**
Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide	2006	N	No safety concern
(±)-*N*-Lactoyl tyramine	2007	N	**Additional data required to complete evaluation**
N-(2-(Pyridin-2-yl)ethyl)-3-*p*-menthanecarboxamide	2008	N	No safety concern
N-*p*-Benzeneacetonitrile menthanecarboxamide	2009	N	No safety concern
N-(2-Hydroxyethyl)-2,3-dimethyl-2-isopropylbutanamide	2010	N	**Additional data required to complete evaluation**
N-(1,1-Dimethyl-2-hydroxyethyl)-2,2-diethylbutanamide	2011	N	**Additional data required to complete evaluation**

[a] N, new specifications.

F. Phenol and phenol derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
4-Propenylphenol	2012	N	No safety concern
2,4,6-Trimethylphenol	2013	N	No safety concern
Sodium 3-methoxy-4-hydroxycinnamate	2014	N	No safety concern
Guaicol butyrate	2015	N	No safety concern
Guaicol isobutyrate	2016	N	No safety concern
Guaicol propionate	2017	N	No safety concern
4-(2-Propenyl)phenyl-β-D-glucopyranoside	2018	N	No safety concern
Phenyl butyrate	2019	N	No safety concern
Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid	2020	N	No safety concern
Structural class II			
1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one	2021	N	No safety concern
Structural class III			
3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one	2022	N	No safety concern
Magnolol	2023	N	No safety concern
5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one	2024	N	No safety concern

[a] N, new specifications.

G. Aliphatic acyclic and alicyclic terpenoid tertiary alcohols and structurally related substances

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
Dimethylbenzyl carbinyl crotonate	2025	N	No safety concern
Dimethylbenzyl carbinyl hexanoate	2026	N	No safety concern
Caryophyllene alcohol	2027	N	No safety concern
Cubebol	2028	N	No safety concern
(−)-Sclareol	2029	N	No safety concern
(+)-Cedrol	2030	N	No safety concern
α-Bisabolol	2031	N	No safety concern

[a] N, new specifications.

H. Aliphatic acyclic and alicyclic α-diketones and related α-hydroxyketones

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
3-Methyl-2,4-nonedione	2032	N	No safety concern
Mixture of 3-hydroxy-5-methyl-2-hexanone and 2-hydroxy-5-methyl-3-hexanone	2034	N	No safety concern
3-Hydroxy-2-octanone	2035	N	No safety concern
2,3-Octanedione	2036	N	No safety concern
4,5-Octanedione	2037	N	No safety concern
(±)-2-Hydroxypiperitone	2038	N	No safety concern
Structural class III			
Acetoin propyleneglycol ketal	2033	N	No safety concern
1,1′-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone	2039	N	No safety concern

[a] N, new specifications.

I. Aromatic substituted secondary alcohols, ketones and related esters

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
4-Hydroxyacetophenone	2040	N	No safety concern
3-Hydroxy-4-phenylbutan-2-one	2041	N	No safety concern
2-Methoxyacetophenone	2042	N	No safety concern
2-Methylacetophenone	2044	N	No safety concern
2-Hydroxy-5-methylacetophenone	2045	N	No safety concern
Dihydrogalangal acetate	2046	N	**Additional data required to complete evaluation**
2,3,3-Trimethylindan-1-one	2047	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III			
4-(3,4-Methylenedioxyphenyl)-2-butanone	2048	N	No safety concern

[a] N, new specifications.

J. Alicyclic ketones, secondary alcohols and related esters

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
Cyclohexanone diethyl ketal	2051	N	No safety concern
3,3,5-Trimethylcyclohexyl acetate	2053	N	No safety concern
Structural class II			
2-(*trans*-2-Pentenyl)cyclopentanone	2049	N	No safety concern
2-Cyclopentylcyclopentanone	2050	N	No safety concern
2-Cyclohexenone	2052	N	No safety concern
2,6,6-Trimethyl-2-hydroxycyclohexanone	2054	N	No safety concern
Cyclotene propionate	2055	N	No safety concern
Cyclotene butyrate	2056	N	No safety concern
4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers)	2057	N	No safety concern
4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one	2058	N	No safety concern
Structural class III			
(−)-8,9-Dehydrotheaspirone	2059	N	No safety concern
(±)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one	2060	N	No safety concern

[a] N, new specifications.

K. Benzyl derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
Benzyl hexanoate	2061	N	No safety concern
o-Anisaldehyde	2062	N	No safety concern
Prenyl benzoate	2063	N	No safety concern
Benzyl levulinate	2064	N	No safety concern
4-Methylbenzyl alcohol	2065	N	No safety concern
Benzyl nonanoate	2066	N	No safety concern
Structural class II			
2-Ethylhexyl benzoate	2068	N	No safety concern
Structural class III			
4-Methylbenzaldehyde propyleneglycol acetal	2067	N	No safety concern

[a] N, new specifications.

L. Aliphatic secondary alcohols, ketones and related esters and acetals

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
(±)-Octan-3-yl formate	2070	N	No safety concern
2-Pentyl 2-methylpentanoate	2072	N	No safety concern
3-Octyl butyrate	2073	N	No safety concern
Structural class II			
(*R*)-(−)-1-Octen-3-ol	2071	N	No safety concern
2-Decanone	2074	N	No safety concern
Structural class III			
6-Methyl-5-hepten-2-one propylene glycol acetal	2075	N	No safety concern
2-Nonanone propylene glycol acetal	2076	N	No safety concern

[a] N, new specifications.

Flavouring agents considered for specifications only

No.	Flavouring agent	Specifications[a]
439	4-Carvomenthenol	R
952	5,6,7,8-Tetrahydroquinoxaline	R

[a] R, revised specifications.

ANNEX 2: RECOMMENDATIONS AND FURTHER INFORMATION REQUIRED

Further information required or desired

β-apo-8′-carotenal, β-apo-8′-carotenoic acid ethyl ester and β-carotene (synthetic)
The revision of the specifications monographs of β-apo-8′-carotenal, β-apo-8′-carotenoic acid ethyl ester and β-carotene (synthetic) was deferred to a future meeting, pending submission of the data necessary for revision of purity tests for carotenoids and subsidiary colouring matter.

Sucrose monoesters of lauric, palmitic or stearic acid
A test method capable of distinguishing sucrose monoesters of lauric, palmitic or stearic acid from sucrose esters of fatty acids is needed. The tentative specifications for sucrose monoesters of lauric, palmitic or stearic acid will be withdrawn if the requested data are not received by the end of 2011.

Additional data required to complete the evaluation according to the Procedure for the Safety Evaluation of Flavouring Agents
Additional data are required to complete the toxicological evaluations of 13 flavouring agents (Nos 1914, 1931, 1939, 1941, 1943, 1944, 1973, 1988, 2005, 2007, 2010, 2011 and 2046).

HPLC methods for subsidiary dyes and isomers in food colours
The Committee noted the need for high-performance liquid chromatographic (HPLC) methods for the separation and quantification of subsidiary dyes and isomers in food colours to replace the paper chromatographic method in Volume 4 of the Combined Compendium of Food Additive Specifications (FAO, JECFA Monographs 1, 2006). To this end, producers of food colours, industries and organizations are encouraged to notify the FAO JECFA Secretariat of the availability of appropriate methods.

CORRIGENDA

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS
FAO FOOD AND NUTRITION PAPER 52, Addendum 12, ROME, 2004.

Page 93, Flavouring agent JECFA No. 1454: The name is corrected to **cis- and trans- Linalool oxide**, to correspond to the information in the report from the 63rd meeting of JECFA (WHO Technical Report Series No. 928, 2005, p. 108) and which was the substance that was evaluated. The Chemical Abstract Services (C.A.S.) number is corrected to 60047-17-8, and the C.A.S. numbers of the cis- and trans-form of linalool oxide are also given, 5989-33-3 and 34995-77-2, respectively. The synonyms are modified to read: Linalool oxide (furanoid form) and 2-Methyl-5-(1-hydroxy-1-methylethyl)-2-vinyltetrahydrofuran.

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS
FAO JECFA MONOGRAPHS 7, ROME, 2009.

Page 47, In the revised specifications for Modified starches, the heading of Table 1 had been omitted in this revision and is reinserted above the subheadings Modification, Process limitations and End-product specifications.

FAO TECHNICAL PAPERS

FAO JECFA MONOGRAPHS

1 Combined compendium of food additive specifications – JECFA specifications monographs from the 1st to the 65th meeting. (E)
Vol. 1 Food additives A – D
Vol. 2 Food additives E – O
Vol. 3 Food additives P – Z
Vol. 4 Analytical methods, test procedures and laboratory solutions

2 Residue evaluation of certain veterinary drugs - Joint FAO/WHO Expert Committee on Food Additives 66th meeting 2006 (E)

3 Compendium of food additive specifications - Joint FAO/WHO Expert Committee on Food Additives 67th meeting 2006 (E)

4 Compendium of food additive specifications - Joint FAO/WHO Expert Committee on Food Additives 68th meeting 2007 (E)

5 Compendium of food additive specifications - Joint FAO/WHO Expert Committee on Food Additives 69th meeting 2008 (E)

6 Residue evaluation of certain veterinary drugs - Joint FAO/WHO Expert Committee on Food Additives 70th meeting 2008 (E)

7 Compendium of food additive specifications - Joint FAO/WHO Expert Committee on Food Additives 71st meeting 2006 (E)

8 Safety evaluation of certain contaminants in food - Joint FAO/WHO Expert Committee on Food Additives 72nd meeting 2010 (E)
Joint FAO/WHO publication WHO Food Additives Series No. 63/ FAO JECFA Monographs 8, in preparation.

9 Residue evaluation of certain vweterinary drugs RESIDUE EVALUATION
Joint FAO/WHO Expert Committee on Food Additives Meeting 2010 – Evaluation of data on ractopamine residues in pig tissues (E)

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