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 Volume 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 Volume 4 (under "General Methods, Metallic Impurities").

METHOD OF ASSAY — Determine the percentages of the individual steviol glycosides by high pressure liquid chromatography (Volume 4).

Standards
Stevioside, >99.0% purity and rebaudioside A, >97% purity (available from Wako pure Chemical Industries, Ltd. Japan).

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

Standard solutions
(a) Accurately weigh 50 mg of dried (105°, 2 h) stevioside standard into a 100-ml volumetric flask. Dissolve with mobile phase and dilute to volume with mobile phase.
(b) Repeat with previously dried rebaudioside A standard.

Sample solution
Accurately weigh 60-120 mg of dried (105°, 2 h) sample into a 100-ml volumetric flask. Dissolve with mobile phase and dilute to volume with the mobile phase.

Chromatography Conditions
Column: Supelcosil LC-NH2 or equivalent (length: 15-30 cm; inner diameter: 3.9-4.6 mm)
Mobile phase: A 80:20 mixture of acetonitrile and water (see above)
Flow rate: Adjust so that the retention time of rebaudioside A is about 21 min.

Injection volume: 5-10 µl
Detector: UV at 210 nm
Column temperature: 40°

Procedure

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

The retention times relative to rebaudioside A (1.00) are:

0.45-0.48 for stevioside 0.12-0.16 for rubusoside
0.25-0.30 for dulcoside A 0.35-0.41 for steviolbioside
0.63-0.69 for rebaudioside C 0.73-0.79 for rebaudioside B

Measure the peak areas for the seven steviol glycosides from the sample solution (the minor components might not be detected). Measure the peak area for stevioside for the standard solution.

Calculate the percentage of each of the seven steviol glycosides, *X,* in the sample from the formula:

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

where

W_S is the amount (mg) of stevioside in the standard solution
W is the amount (mg) of sample in the sample solution
A_S is the peak area for stevioside from the standard solution
A_X is the peak area of *X* for the sample solution
f_X is the ratio of the formula weight of *X* to the formula weight of stevioside: 1.00 (stevioside), 0.98 (dulcoside A), 1.20 (rebaudioside A), 1.18 (rebaudioside C), 0.80 (rubusoside), 0.80 (steviolbioside), and 1.00 (rebaudioside B).

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

SUNSET YELLOW FCF

Prepared at the 69th JECFA (2008), published in FAO JECFA Monographs 5 (2008), superseding specifications prepared at the 28th JECFA (1984), published in combined Compendium of Food Additive Specifications, FAO JECFA Monographs 1 (2005). An ADI of 0-2.5 mg/kg bw was established at the 26th JECFA (1982).

SYNONYMS CI Food Yellow 3, Orange Yellow S, CI (1975) No. 15985, INS No. 110

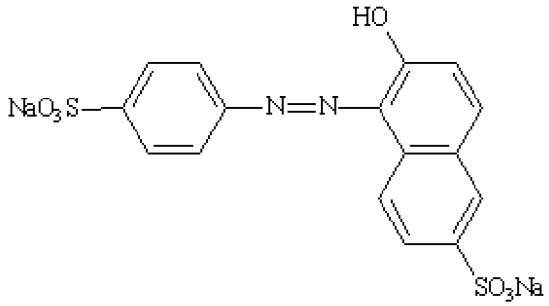
DEFINITION Sunset Yellow FCF consists principally of the disodium salt of 6-hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid and subsidiary colouring matters together with sodium chloride and/or sodium sulfate as the principal uncoloured components.
(NOTE: The colour may be converted to the corresponding aluminium lake, in which case only the *General Specifications for Aluminium Lakes of Colouring Matters* apply.)

Chemical names: Principal component:
Disodium 6-hydroxy-5-(4-sulfonatophenylazo)-2-naphthalene-sulfonate

C.A.S. number: 2783-94-0

Chemical formula: $C_{16}H_{10}N_2Na_2O_7S_2$ (Principal component)

Structural formula



(Principal component)

Formula weight: 452.38 (Principal component)

Assay: Not less than 85% total colouring matters

DESCRIPTION Orange-red powder or granules

FUNCTIONAL USES Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)	Soluble in water; sparingly soluble in ethanol
Colour test	In water, neutral or acidic solutions of Sunset Yellow FCF are yellow-orange, whereas basic solutions are red-brown. When dissolved in concentrated sulfuric acid, the additive yields an orange solution that turns yellow when diluted with water.
Colouring matters, identification (Vol. 4)	Passes test
PURITY	
Water content (Loss on drying) (Vol. 4)	Not more than 15% together with chloride and sulfate calculated as sodium salts
Water-insoluble matter (Vol. 4)	Not more than 0.2%
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 method described in Volume 4 (under “General Methods, Metallic Impurities”).
Subsidiary colouring matter content (Vol. 4)	Not more than 5% Not more than 2% shall be colours other than trisodium 2-hydroxy-1-(4-sulfonatophenylazo)naphthalene-3,6-disulfonate Use the following conditions: Chromatography solvent: 2-Butanone:acetone:water:ammonia (s.g. 0.880) (700:300:300:2) Height of ascent of solvent front: approximately 17 cm
Sudan I (1-(Phenylazo)-2-naphthalenol)	Not more than 1 mg/kg See description under TESTS
Organic compounds other than colouring matters (Vol. 4)	Not more than 0.5%, sum of the: monosodium salt of 4-aminobenzenesulfonic acid, disodium salt of 3-hydroxy-2,7-naphthalenedisulfonic acid, monosodium salt of 6-hydroxy-2-naphthalenesulfonic acid, disodium salt of 7-hydroxy-1,3-naphthalenedisulfonic acid, disodium salt of 4,4'-diazoaminobis-benzenesulfonic acid, and disodium salt of 6,6'-oxybis-2-naphthalenesulfonic acid 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
Ether-extractable matter (Vol. 4)	Not more than 0.2%

TESTS

PURITY TESTS

Sudan I (1-(Phenylazo)-2-naphthalenol)

Principle
The additive is dissolved in water and methanol and filtered solutions are analysed by Reverse-Phase Liquid Chromatography (Volume 4 under "Analytical Techniques, Chromatography"), without extraction or concentration. (Based on *J.AOAC Intl* 90, 1373-1378 (2007).)

Mobile phase
Eluant A: Ammonium acetate (LC grade), 20 mM aqueous
Eluant B: Methanol (LC grade)

Sample solution
Accurately weigh 200 mg of Sunset yellow FCF and transfer it into a 10-ml volumetric flask. Dissolve the sample in 4 ml water via swirling or sonication. Add 5 ml of methanol and swirl. Allow the solution to cool for 5 min and adjust the volume to the mark with water. Filter a part of the solution for analysis through a 13 mm syringe filter with a 0.2 µm pore size PTFE membrane by using a 5 ml polypropylene/polyethylene syringe. (NOTE: Do not substitute a PVDF filter for the PTFE filter, as a PVDF filter adsorbs Sudan I.)

Standard
Sudan I (>97%, Sigma Aldrich, or equivalent), recrystallized from absolute ethanol (5g/150 ml)

Standard stock solution
Accurately weigh a sufficient quantity of the *Standard* to prepare a solution in methanol of 0.0100 mg/ml.

Standard solutions
Transfer 0, 20, 50, 100, 150, 200, and 250 µl aliquots of the *Standard stock solution* to seven 10-ml volumetric flasks. To each flask, add 5 ml of methanol, swirl to mix, and add 4 ml of water. Dilute to volume with water, mix, and filter each solution through a PTFE membrane syringe filter (see *Sample solution*, above) into LC vials for analysis. (NOTE: These solutions nominally contain 0, 0.02, 0.05, 0.10, 0.15, 0.20, and 0.25 µg of Sudan I/ml.)

Chromatographic system
Detector: Photodiode Array (485 nm)
Columns: 150 mm x 2.1 mm id, packed with 5 µm reversed-phase C18, or equivalent, with a guard column (10 mm x 2.1 mm i.d.) – Waters Corp., or equivalent
Column temperature: 25°
Flow rate: 0.25 ml/min
Injection volume: 50 µl
Elution: 50% *Eluant A*/50% *Eluant B* for 5 min; 50 to 100% *Eluant B* in 10 min; 100% *Eluant B* for 10 min. (NOTE: The column should be requilibrated with 50% *Eluant A*/50% *Eluant B* for 10 min.)
System suitability: Inject three replicates of the *Standard solutions* with concentrations of 0.05 and 0.25 µg of Sudan I/ml. The responses for each set of three injections show relative standard deviations

of not more than 2%.

Procedure
Separately inject the seven *Standard solutions* and the *Sample solution* into the chromatograph and measure the peak areas for Sudan I. From the chromatograms for the *Standard solutions*, prepare a standard curve of the concentration of Sudan I vs the peak areas. (NOTE: The retention time for Sudan I is 19.0 min. Other peaks appearing at earlier retention times in the sample chromatograph are likely attributed to sulfonated subsidiary colours.) Determine the concentration of Sudan I in the *Sample solution* and convert it to mg/kg in the sample of Sunset Yellow FCF.

(NOTE: The limit of determination is 0.4 mg/kg.)

METHOD OF ASSAY Proceed as directed under *Colouring Matters Content by Titration with Titanous Chloride* (Volume 4, under "Food Colours, Colouring Matters"), using the following:

Weight of sample: 0.5-0.6 g
Buffer: 10 g sodium citrate
Weight (*D*) of colouring matters equivalent to 1.00 ml of 0.1 N $TiCl_3$: 11.31 mg

TRISODIUM DIPHOSPHATE

Prepared at the 69th JECFA (2008), published in FAO JECFA Monographs 5 (2008), based on the previously withdrawn tentative specifications prepared at the 61st JECFA and published in FNP 52, Add 11 (2003). A group MTDI of 70 mg/kg bw, expressed as phosphorus from all food sources, was established at the 26th JECFA (1982).

SYNONYMS Acid trisodium pyrophosphate, trisodium monohydrogen diphosphate; INS No. 450(ii)

DEFINITION Trisodium diphosphate is manufactured by calcining sodium orthophosphate having a $Na_2O:P_2O_5$ ratio of 3:2

Chemical names: Trisodium monohydrogen diphosphate

C.A.S. number: 14691-80-6 (Anhydrous)
26573-04-6 (Monohydrate)

Chemical formula: $Na_3HP_2O_7 \cdot x\ H_2O$ (x = 0 or 1)

Formula weight: 243.93 (Anhydrous)
261.95 (Monohydrate)

Assay: Not less than 57% and not more than 59% expressed as P_2O_5 on the dried basis

DESCRIPTION White powder or grains

FUNCTIONAL USES Stabilizer, leavening agent, emulsifier, nutrient

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4): Soluble in water

Sodium (Vol. 4): Passes test

Phosphate (Vol. 4): Passes test

PURITY

Loss on drying (Vol. 4): Anhydrous: Not more than 0.5 % (105°, 4 h)
Monohydrate: Not more than 1.0 % (105°, 4 h)

Loss on ignition (Vol. 4): Anhydrous: Not more than 4.5%
Monohydrate: Not more than 11.5%

Water-insoluble matter (Vol. 4): Not more than 0.2 %

Fluoride (Vol. 4): Not more than 10 mg/kg
See description under TESTS

Arsenic (Vol. 4)	Not more than 3 mg/kg Determine by the atomic absorption hydride technique. 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”).
Lead (Vol. 4)	Not more than 4 mg/kg Determine using an atomic absorption/ICP 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

Fluoride (Vol. 4)	Use Method III. The standard curve constructed in Method III may not be suitable for samples containing low fluoride levels. Therefore, it will be necessary to prepare standard solutions with concentrations other than those specified in Method III for the construction of the standard curve and to choose a sample size that will bring the fluoride concentration within the standard curve.

METHOD OF ASSAY

Using a previously dried sample, proceed as directed under *Phosphate Determination as P_2O_5, Method I,* Inorganic components (Volume 4). Each ml of 1N sodium hydroxide consumed is equivalent to 3.088 mg of P_2O_5 or 5.307 mg of trisodium monohydrogen diphosphate on the dried basis.

WITHDRAWAL OF SPECIFICATIONS FOR CERTAIN FOOD ADDITIVES

Carbohydrase from *Aspergillus niger* var.

The Committee reviewed the tentative specifications for carbohydrase from *Aspergillus niger* var. that had been prepared at its 15th meeting[1] and for which an ADI "not specified" was established at its 35th meeting[2]. The call for data for the 69th meeting requested information to revise the existing tentative specifications, stating that the specifications would be withdrawn if no information was forthcoming.

The tentative specifications for carbohydrase include α-amylase, pectinase, cellulase, gluco-amylase, and β-galactosidase (lactase). The functional uses listed in the specifications are diverse and imply that these enzymes are used in food processing as separate enzyme preparations rather than as a mixture of enzymes. Moreover, carbohydrase is not listed as a commercial enzyme by the enzyme industry associations, while all individual enzymes included in the tentative specifications are listed as commercial products.

As no information supporting the tentative specifications was received, the Committee withdrew the ADI and the tentative specifications.

Estragole

The tentative specifications for estragole used as a food additive that were prepared by the Committee at its 26th meeting[3] were withdrawn, as no other uses of estragole other than as a flavouring agent were identified.

[1] FAO Nutrition Meeting Series FAO Nutrition Meeting Series, No. 50, 1972 and republished in the Combined Compendium for Food Additive Specifications, FAO JECFA Monographs 1, 2005; WHO Technical Report Series, No. 488, 1972.
[2] WHO Technical Report Series, No. 789, 1990 and corrigenda
[3] FAO Food and Nutrition Paper No. 25, 1982, and republished in the Combined Compendium for Food Additive Specifications, FAO JECFA Monographs 1, 2005

ANALYTICAL METHODS

The following analytical methods were prepared by the Committee at the 69th meeting. This method will be made available in the on-line edition of Volume 4 of the Combined Compendium of Food Additive Specifications.

Nickel in Polyols

Note: *This method is also applicable for determination of nickel in polydextroses.*

Apparatus
Use a suitable atomic absorption spectrometer equipped with a nickel hollow cathode lamp and an air–acetylene flame to measure the absorbance of the Blank solution, the Standard solutions, and the Sample solution as directed under Procedure (below).

Sample solution
Dissolve 20.0 g of the sample in a mixture of equal volumes of dilute acetic acid TS and water and dilute to 100 ml with the same mixture of solvents. Add 2.0 ml of a 1% w/v solution of ammonium pyrrolidinedithiocarbamate and 10 ml of methyl isobutyl ketone. Mix and allow the layers to separate and use the methylisobutyl ketone layer.

Blank solution
Prepare in the same manner as the Sample solution, but omit the sample.

Standard solutions
Prepare three Standard solutions in the same manner as the Sample solution but adding 0.5 ml, 1.0 ml, and 1.5 ml, respectively, of a standard nickel solution containing 10 mg/kg Ni, in addition to the 20.0 g of the sample.

Procedure
Zero the instrument with the Blank solution. Then determine the absorbances at 232.0 nm of each of the Standard solutions and of the Sample solution at least three times each, and record the average of the steady readings for each. Between each measurement, aspirate the Blank solution, and ascertain that the reading returns to its initial blank value.

Prepare a standard curve by plotting the mean absorbances vs concentration for the Standard solutions. Extrapolate the line joining the points on the graph until it meets the concentration axis. Read the concentration of nickel in the Sample solution at the intersection of the standard curve with the concentration axis.

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 69th meeting of the Committee specifications of identity and purity were prepared for 111 new flavourings (page 91).

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); 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 (M.W.); 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 Magentic 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 69th meeting were assigned full status.

The the specifications prepared for the 6 alkoxy-substituted allylbenzenes (JECFA Nos 1787 – 1792) 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.

In addition, the specifications prepared for the group of 40 furan-substituted aliphatic hydrocarbons, alcohols, aldehydes, ketones, carboxylic acids, and related esters, sulfides, disulfides and ethers (JECFA Nos, Structural Class II: 1487, 1488, 1489, 1490, 1491, 1492, 1493, 1494, 1497, 1499, 1503, 1504, 1505, 1507, 1508, 1509, 1510, 1511, 1513, 1514, 1515, 1516, 1517, 1520, 1521, 1522, 1523, 1524, 1525, 1526; Structural Class III: 1495, 1496, 1498, 1500, 1501, 1502, 1506, 1512, 1518, 1519) by the Committee at its 65th and 68th meetings, will include include a statement that the safety evaluations for these substances had not been completed at the 69th meeting. This information is included in the on-line searchable database at the JECFA website at FAO. For further information see Annex 2.

Finally, the reevaluation of the safety of the flavouring substance 2-isopropyl-N,2,3-trimethylbutyramide (JECFA No. 1595) at the 69th meeting was not completed due to safety concerns and the specifications in the on-line searchable database at the JECFA website at FAO includes a statement to this effect. For further information see Annex 2.

The spectra used for identification tests are provided from page 108 onwards.

An index listing all the JECFA names is available on page 125.

NEW SPECIFICATIONS

No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min % A.V. max	R. I. S. G.	Other requirements/ Secondary components	Session Status
1787	**Apiole**		C12H14O4 222.24	Colourless to yellow or light green liquid; Slight parsley like aroma	Insoluble in water; soluble in ether, acetone and glacial acetic acid	294	MS 95	1.536-1.538 1.124-1.135	Safety evaluation not completed	69th Full
	4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole *1-Allyl-2,5-dimethoxy-3,4-methylenedioxybenzene*	523-80-8			Soluble					
1788	**Elemicin**		C12H16O3 208.26	Colourless to pale straw coloured viscous liquid; Spice with floral notes	Practically insoluble to insoluble in water	246	MS 95	1.529-1.534 1.058-1.070	Safety evaluation not completed	69th Full
	1,2,3-Trimethoxy-5-(2-propenyl)benzene *5-Allyl-1,2,3-trimethoxybenzene*	487-11-6			Soluble					
1789	**Estragole**	2411	C10H12O 148.21	Colourless to light yellow liquid; Anise-like aroma	Insoluble in water; soluble in alcohols	216	IR MS 95	1.519-1.524 0.960-0.968	Safety evaluation not completed	69th Full
	1-Methoxy-4(2-propenyl)-benzene *Methyl chavicol*	04.011 140-67-0			Soluble					
1790	**Methyl eugenol**	2475	C11H14O2 178.23	Colourless to pale yellow liquid; Clove-carnation aroma	Insoluble in water; soluble in most fixed oils; insoluble in glycerol and propylene glycol	249	IR MS 95	1.532-1.536 1.032-1.036	Safety evaluation not completed	69th Full
	1,2-Dimethoxy-4(2-propenyl)-benzene *1,2-Dimethoxy-4-allylbenzene*	04.012 93-15-2			Soluble					
1791	**Myristicin**		C11H12O3 192.21	Colourless oil; Warm balsamic-woody aroma	Practically insoluble to insoluble in water	250	MS 95	1.539-1.541 1.143-1.145	Safety evaluation not completed	69th Full
	4-Methoxy-6-(2-propenyl)-1,3-benzodioxole *5-Allyl-1-methoxy-2,3-(methylenedioxy)benzene*	607-91-0			Soluble					
1792	**Safrole**		C10H10O2 162.19	Colourless to slightly yellow liquid; Sasafras aroma	Practically insoluble to insoluble in water	232-234	MS 95	1.537-1.540 1.095-1.099	Safety evaluation not completed	69th Full
	5-(2-Propenyl)-1,3-benzodioxole *4-Allyl-1,2-methylenedioxylbenzene*	94-59-7			Soluble					
1793	**(Z)-2-Penten-1-ol**	4305	C5H10O 86.13	Colourless liquid; Green diffusive aroma	Slightly soluble in water; soluble in non-polar solvents	140-141	MS 95	1.427-1.433 0.844-0.850		69th Full
	2-Penten-1-ol	02.050 665 20273-24-9			Soluble					

No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min %	A.V. max	R. I. S. G.	Other requirements/ Secondary components	Session Status
1794	**(E)-2-Decen-1-ol** 2-Decen-1-ol	4304 02.137 11750 18049-18-2	C10H20O 156.27	Colourless liquid; Fatty rosy aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	116-118 (14 mm Hg)	MS 95		1.446-1.452 0.842-0.848		69th Full
1795	**(Z)-Pent-2-enyl hexanoate** (Z)-2-Pentenylhexanoic acid ester	4191 09.678 74298-89-8	C11H20O2 184.28	Colourless liquid; banana bergamot aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	240-241	MS 95		1.425-1.435 0.885-0.895		69th Full
1796	**(E)-2-Hexenyl octanoate** (E)-2-Hexenyl octanoic acid ester	4135 09.841 85554-72-9	C14H26O2 226.36	Colourless liquid; Pear aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	308-309	MS 95		1.448-1.453 0.881-0.887		69th Full
1797	**trans-2-Hexenyl 2-methylbutyrate** (2E)-2-Hexenyl 2-methylbutanoic acid ester	4274 94089-01-7	C11H20O2 184.28	Liquid; Mild fruity aroma	Insoluble in water; soluble in non-polar solvents Soluble	231-232	NMR MS 95	1.0	1.430-1.434 0.874-0.879 (20 ºC)		69th Full
1798	**Hept-trans-2-en-1-yl acetate** (2E)-2-Hepten-1-ol acetate	4125 09.385 10661 16939-73-4	C9H16O2 156.22	Colourless liquid; Fresh leaf aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	192-193	MS 95		1.428-1.434 0.889-0.895		69th Full
1799	**(E,Z)-Hept-2-en-1-yl isovalerate** 2-Heptenyl 3-methylbutanoic acid ester	4126 09.303 10664 253596-70-2	C12H22O2 198.30	Colourless liquid; Sweet green aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	262-263	NMR 95		1.443-1.449 0.868-0.873		69th Full

No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min %	A.V. max	R. I. S. G.	Other requirements/ Secondary components	Session Status
1800	**trans-2-Hexenal glyceryl acetal** (-)2-(1E)-Pentenyl-1,3-dioxan-5-ol, (+)2-(1E)-Pentenyl-1,3-dioxan-5-ol, (-)2-(1E)-Pentenyl-1,3-dioxolane-4-methanol (+)2-(1E)-1-Pentenyl-1,3-dioxolane- -4-methanol *2-(1E)-1-Pentenyl-1,3-dioxolane-4-methanol*	4273 214220-85-6/ 897630-96-5/ 897672-50-3/ 897672-51-4	C9H16O3 190.24	Liquid; Weak green and fresh aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	241-246	NMR 86 (mixture of isomers)	1.0	1.464-1.474 1.037-1.048 (20 ºC)	(+)2-(1E)-1-Pentenyl-1,3-dioxolane-4-methanol 26%; (+)2-(1E)-Pentenyl-1,3- dioxan-5-ol 22%; (-)2-(1E)-Pentenyl-1,3-dioxan-5-ol 22%; (-)2-(1E)-Pentenyl-1,3-dioxolane-4-methanol 16% SC: 3- Hexenal glyceryl acetal 8%; Hexanal glyceryl acetal 1%	69th Full
1801	**trans-2-Hexenal propylene glycol acetal** 4-Methyl-2-(1E)-1-pentenyl-1,3-dioxolane	4272 94089-21-1	C9H16O2 156.22	Liquid; Weak green and fresh aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	118-120 (20 mm Hg)	NMR 97	1.0	1.438-1.444 0.919-0.926 (20 ºC)		69th Full
1802	**cis- and trans-1-Methoxy-1-decene** 1-Decene, 1-methoxy- *1-Methoxy-1-decene*	4161 79930-37-3	C11H22O 170.29	Clear, colourless liquid; Fruity floral aroma	Soluble in non-polar solvents; insoluble in water Soluble	89-90 (9 mm Hg)	NMR IR 98 (Z-isomer isomer 40-48%; E- isomer 52-60%)		1.430-1.438 (25 ºC) 0.807-0.817		69th Full
1803	**(E)-Tetradec-2-enal** (2E)-Tetradec-2-enal	4209 05.179 51534-36-2	C14H26O 210.36	Colourless liquid; Citrus aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	88-89 (0.2 mm Hg)	MS 95		1.455-1.562 0.833-0.841		69th Full
1804	**(E)-2-Pentenoic acid** (2E)-2-Pentenoic acid	4193 08.107 10163 13991-37-2	C5H8O2 100.12	Colourless liquid; Sour caramellic aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	197-199	NMR MS 95		1.445-1.454 0.984-0.991		69th Full

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1805	**(E)-2-Octenoic acid** (2E)-2-Octenoic acid	3957 08.114 10156 1871-67-6	C8H14O2 142.20	Colourless liquid; Buttery, butterscotch aroma	Insoluble in water; soluble in oils Soluble	139-141 (13 mm Hg)	NMR IR MS 97		1.458-1.462 0.935-0.941		69th Full
1806	**Ethyl trans-2-butenoate** 2-Butenoic acid, ethyl ester *Ethyl crotonate*	3486 10544-63-5	C6H10O2 114.14	Colourless liquid; Powerful sour caramellic-fruity aroma	Insoluble in water; soluble in oils Soluble	136-137	MS 98	2.0	1.422-1.428 0.916-0.921		69th Full
1807	**Hexyl 2-butenoate** 2-Butenoic acid, hexyl ester *Hexenyl crotonate*	3354 09.266 10688 19089-92-0	C10H18O2 170.25	Colourless liquid; Fruity aroma	Insoluble in water, propylene glycol; soluble in most fixed oils Soluble	96-98 (15 mm Hg)	NMR 95	1.0	1.428-1.442 0.880-0.905		69th Full
1808	**Ethyl trans-2-hexenoate** (2E)-2-Hexenoic acid ethyl ester	3675 09.850 631 27829-72-7	C8H14O2 142.20	Colourless liquid; Fruity, green, pulpy, pineapple, apple aroma	Slightly soluble in water; soluble in fats Soluble	110-111 (10 mm Hg)	NMR IR 95		1.429-1.434 0.895-0.90		69th Full
1809	**(E,Z)-Methyl 2-hexenoate** 2-Hexenoic acid, methyl ester *Methyl-beta-propylacrylate*	2709 2396-77-2	C7H12O2 128.17	Colourless mobile liquid; Fruity aroma	Very slightly soluble in water; soluble in oils Soluble	168-170	NMR 95		1.423-1.429 0.911-0.916		69th Full
1810	**Hexyl trans-2-hexenoate** Hexyl (E)-2-hexenoate *2-Hexenoic acid hexyl ester*	3692 09.292 33855-57-1	C12H22O2 198.31	Colourless liquid; Fruity, green, slightly fatty aroma	Slightly soluble in water; soluble in fats Soluble	121-123 (10 mm Hg)	NMR IR 92		1.439-1.445 0.880-0.890	SC: Hexyl trans-3-hexenoate (6-8%)	69th Full
1811	**Methyl trans-2-octenoate** (2E)-2-Octenoic acid methyl ester	3712 09.299 11800 7367-81-9	C9H16O2 156.23	Colourless liquid; Fruity, green aroma	Slightly soluble in water; soluble in fats Soluble	89-91 (9 mm Hg)	NMR IR MS 90		1.437-1.448 0.896-0.900	SC: Methyl trans-3-octenoate (5-6%)	69th Full

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1812	**Ethyl trans-2-octenoate** (2E)-2-Octenoic acid ethyl ester	3643 09.285 10617 7367-82-0	C10H18O2 170.24	Liquid; Green-fruity aroma	Insoluble in water; soluble in fats Soluble	93-96 (10 mm Hg)	NMR IR MS 98	1.439-1.445 0.888-0.894 (20 ºC)		69th Full
1813	**(E,Z)-Methyl 2-nonenoate** 2-Nonenoic acid, methyl ester *Neofollione*	2725 09.234 2099 111-79-5	C10H18O2 170.25	Colourless or light-yellow liquid; Green, violet aroma	Insoluble in water; soluble in non-polar solvents Soluble	114-115 (21 mm Hg)	NMR 95 1.0	1.440-1.447 0.893-0.900 (20 ºC)		69th Full
1814	**Ethyl trans-2-decenoate** (2E)-2-Decenoic acid, ethyl ester	3641 09.283 10577 7367-88-6	C12H22O2 198.31	Liquid; Fatty-waxy aroma specific to over-ripe pear	Insoluble in water; soluble in fats Soluble	133-135 (20 mm Hg)	NMR IR MS 95 1.0	1.440-1.450 0.880-0.890 (20 ºC)		69th Full
1815	**Ethyl (E)-2-methyl-2-pentenoate** 2-Methyl-(2E)-2-pentenoic acid ethyl ester	4290 1617-40-9	C8H14O2 142.20	Clear colourless liquid; Fruity aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	173-174	NMR 98	1.436-1.444 0.904-0.914		69th Full
1816	**2-Methylbutyl 3-methyl-2-butenoate** 2-Methylbutyl 3-methyl-2-butenoate *2-Methylbutyl 3-methyl-2-senecioate*	4306 97890-13-6	C10H18O2 170.25	Colourless liquid; Floral fruity aroma	Sparingly soluble in water; soluble in triacetin and propylene glycol Soluble	57-60 (3.5 mm Hg)	NMR MS 98	1.451-1.461 0.881-0.891		69th Full
1817	**(+/-) (E,Z)-5-(2,2-Dimethylcyclopropyl)-3-methyl-2-pentenal** (+/-)(E,Z)-5-(2,2-Dimethylcyclopropyl)-3-methyl-2-pentenal *Acitral*	4105 877-60-1	C11H18O 166.27	Colourless to slightly yellow liquid; Fruity aroma	Insoluble in water Soluble	234-237	NMR 90 (E-isomer 45-48% E and Z-isomer 43-45%)	1.495-1.501 0.874-0.878	SC: Citral (<10%)	69th Full

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1818	**(E,Z)-4-Methylpent-2-enoic acid**	4180	C6H10O2 114.14	Colourless liquid; Fatty fruity aroma	Slightly soluble in water	203-204	MS 98		1.442-1.453 0.950-0.960		69th
	4-Methyl-2-pentenoic acid	08.099			Soluble						Full
		10321-71-8									
1819	**(+/-)-4-Ethyloctanal**	4117	C10H20O 156.27	Clear colourless liquid; Floral-like odour	Insoluble in water; soluble in many non-polar solvents	97-99 (25 mm Hg)	NMR IR MS 95	1.0	1.427-1.434 0.834-0.842 (20º C)		69th
	(+/-)-4-Ethyloctanal	05.223									Full
		58475-04-0			Soluble						
1820	**(E)-Geranyl 2-methylbutyrate**	4122	C15H26O2 238.37	Colourless liquid; Fruity rosy aroma	Practically insoluble to insoluble in water	312-313	MS 95		1.439-1.443 0.897-0.903		69th
	(2E)-3,7-Dimethyl-2,6-octadienyl 2-methylbutanoic acid	09.382			Soluble						Full
		68705-63-5									
1821	**(E)-Geranyl valerate**	4123	C15H26O2 238.37	Colourless liquid; Fruity pineapple aroma	Practically insoluble to insoluble in water	290-291	MS 95		1.465-1.471 0.887-0.900		69th
	(2E)-3,7-Dimethyl-2,6-octadienyl pentanoic acid	09.150 468			Soluble						Full
		10402-47-8									
1822	**(E)-Geranyl tiglate**	4044	C15H24O2 236.39	Very pale yellow liquid; Floral aroma	Insoluble in water	271-272	IR MS 96	1.0	1.477-1.484 0.920-0.930		69th
	2-Methyl- (2E)-2-pentenoic acid ethyl ester *Tiglic acid, geraniol ester*	09.383 11829			Soluble				(20 ºC)		Full
		7785-33-3									
1823	**(E)-Citronellyl 2-methylbut-2-enoate**	4295	C15H26O2 238.37	Colourless liquid; Winey rosy aroma	Practically insoluble to insoluble in water	143-145 (7 mm Hg)	MS 95		1.460-1.470 0.901-0.911		69th
	2-Methyl-2-butenoic acid (2E)-3,7-dimethyl-6-octenyl ester	09.340			Soluble						Full
		24717-85-9									
1824	**(E)-Ethyl tiglate**	2460 09.495	C7H12O2 128.17	Colourless liquid; Warm-ethereal fruity aroma	Insoluble in water; soluble in oils	154-156	NMR IR 98	1.0	1.432-1.438 0.907-0.916		69th
	(2E)-2-Methyl- 2-butenoic acid ethyl ester	2185									Full
		5837-78-5			Soluble						

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1825	**(E,Z)-Geranic acid** 3,7-Dimethyl-2,6-octadienoic acid	4121 08.081 10094 459-80-3	C10H16O2 168.24	Colourless viscous liquid; Faint floral aroma	Practically insoluble to insoluble in water Soluble	149-151 (18 mm Hg)	MS 95 (E-isomer 49.4% and Z-isomer 45.6%)		1.473-1.479 0.953-0.959	m.p.= 21 ºC	69th Full
1826	**Prenyl formate** 3-Methyl-2-buten-1-ol formate	4205 09.694 68480-28-4	C6H10O2 114.14	Colourless liquid; Fruity rum-like aroma	Practically insoluble to insoluble in water Soluble	34-35 (15 mm Hg)	MS 98		1.410-1.415 0.920-0.927		69th Full
1827	**Prenyl acetate** 3-Methyl-2-buten-1-ol acetate	4202 09.692 11796 1191-16-8	C7H12O2 128.17	Colourless liquid; Natural green apple banana aroma	Practically insoluble to insoluble in water Soluble	148-149	MS 98		1.424-1.428 0.911-0.922		69th Full
1828	**Prenyl isobutyrate** 2-Methylpropanoic acid 3-methyl-2-butenyl ester	4206 09.695 76649-23-5	C9H16O2 156.22	Colourless liquid; Fruity buttery aroma	Practically insoluble to insoluble in water Soluble	77-78 (15 mmHg)	MS 99		1.427-1.434 0.887-0.896		69th Full
1829	**Prenyl caproate** Hexanoic acid 3-methyl-2-butenyl ester	4204 76649-22-4	C11H20O2 184.27	Colourless liquid; Mild green fruit aroma	Practically insoluble to insoluble in water Soluble	219-221 (25 mm Hg)	MS 96		1.434-1.440 0.880-0.888		69th Full
1830	**(+/-)-Dihydrofarnesol** 3,7,11-Trimethyl-6,10-dodecadien-1-ol *2,3-Dihydrofarnesol*	4031 51411-24-6	C15H28O 224.39	Colourless to pale yellow liquid; Floral, fruity aroma	Insoluble in water; soluble in DMSO and acetone Soluble	301-302	NMR IR 96		1.471-1.477 0.867-0.873		69th Full
1831	**(E,Z)-3,7,11-Trimethyldodeca-2,6,10-trienyl acetate** 3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol acetate *Farnesyl acetate*	4213 09.818 29548-30-9	C17H28O2 264.41	Colourless liquid; Rosy floral aroma	Practically insoluble to insoluble in water Soluble	165-166 (9 mm Hg)	MS 99 (E- isomer 64 %and Z- isomer) 35%		1.476-1.479 0.908-0.914		69th Full

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1832	**(E,Z)-Phytol** (2E,7R,11R)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol	4196 02.204 10302 150-86-7	C20H40O 296.54	Colourless to yellow viscous liquid; Faint floral aroma	Practically insoluble to insoluble in water Soluble	131-132 (0.1 mm Hg)	MS 95 (E-isomer 65%and Z-isomer 34%)		1.460-1.466 0.847-0.863		69th Full
1833	**(E,Z)-Phytyl acetate** (2E,7R,11R)-3,7,11,15-Tetramethyl-2-hexadecen-1-ol acetate	4197 09.691 10236-16-5	C22H42O2 338.57	Colourless liquid; Balsamic aroma	Practically insoluble to insoluble in water Soluble	129-131 (0.01 mm Hg)	MS 95 (E-isomer 67% and Z-isomer 32%)	1.0	1.451-1.461 0.867-0.873		69th Full
1834	**Methyl 2-methyl-2-propenoate** 2-(Methoxycarbonyl)-1-propene *Methyl 2-methacrylate*	4002 09.647 80-62-6	C5H8O2 100.13	Clear colourless liquid; Fruity aroma	Slightly soluble in water; soluble in ether and acetone Soluble	99-100	IR 99		1.411-1.417 0.934-0.938		69th Full
1835	**Isopropenyl acetate** 1-Propen-2-ol acetate	4152 09.822 108-22-5	C5H8O2 100.12	Colourless liquid; Winey ethereal aroma	Practically insoluble to insoluble in water Soluble	94-95	MS 99		1.397-1.403 0.917-0.923		69th Full
1836	**1-Octen-3-yl acetate** 1-Octen-3-ol acetate	3582 09.281 11716 2442-10-6	C10H18O2 170.25	Almost colourless liquid; Metallic, mushroom aroma	Insoluble in water, propylene glycol; soluble in most fixed oils Soluble	189-190	NMR 95	1.0	1.420-1.425 0.870-0.876		69th Full
1837	**1-Octen-3-yl butyrate** Butanoic acid, 1-ethenylhexyl ester *Butyric acid, 1-pentylallyl ester*	3612 09.282 16491-54-6	C12H22O2 198.31	Colourless liquid; Sweet, fruity, buttery, mushroom aroma	Insoluble in water; soluble in oils; slightly soluble in propylene glycol Soluble	80-81 (3.5 mm Hg)	NMR IR MS 95		1.423-1.428 0.870-0.879		69th Full

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1838	**6-Methyl-5-hepten-2-yl acetate** 6-Methyl-5-hepten-2-ol acetate	4177 19162-00-6	C10H18O2 170.25	Clear colourless liquid; Fruity aroma	Insoluble in water; soluble in non-polar solvents Soluble	183-184	NMR IR 97	1.420-1.429 0.893-0.903		69th Full
1839	**3-(Hydroxymethyl)-2-octanone** 3-(Hydroxymethyl)-2-octanone	3292 07.097 11113 59191-78-5	C9H18O2 158.24	Colourless oily liquid; Musty, herbaceous, earthy aroma	Slightly soluble in water; soluble in oils Soluble	78-84 (2 mm Hg)	NMR 90	1.416-1.422 0.874-0.878	SC: 3-Methylene-2-octanone (7%)	69th Full
1840	**(+/-) [R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one** [R-(E)]-8-Methyl-5-(1-methylethyl)-6,8-nonadien-2-one *Virginione*	4331 07.239 2278-53-7	C13H22O 194.35	Clear yellow liquid; Fruity melon-like aroma	Insoluble in water Soluble	237-238	MS 95	1.471-1.477 0.846-0.852		69th Full
1841	**(+/-)-cis- and trans-4,8-Dimethyl-3,7-nonadien-2-ol** 4,8-Dimethyl-3,7-nonadien-2-ol	4102 67845-50-5	C11H20O 168.28	Clear colourless liquid; Green tallowy aroma	Insoluble in water; soluble in most non-polar solvents Soluble	70-72 (2 mm Hg)	NMR IR 95	1.465-1.473 0.860-0.870		69th Full
1842	**(+/-)-1-Hepten-3-ol** (+/-)-1-Hepten-3-ol *Butyl vinyl carbinol*	4129 02.155 10218 4938-52-7	C7H14O 114.19	Colourless liquid; Green strong aroma at high concentration but fatty buttery aroma at low dilution	Insoluble in water; soluble in hexane and diethylether Soluble	153-154	NMR IR MS 98	1.430-1.437 0.831-0.835		69th Full
1843	**(E,Z)-4-Octen-3-one** 4-Octen-3-one	4328 14129-48-7	C8H14O 126.20	Clear colourless or pale yellow liquid; Coconut, fruity aroma	Sparingly soluble in water; soluble in many non-polar solvents Soluble	77-79 (20 mm Hg)	NMR 95	1.442-1.448 0.840-0.844		69th Full

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1844	**(E)-2-Nonen-4-one** (E)-2-Nonen-4-one	4301 27743-70-0	C9H16O 140.22	Clear colourless or pale yellow liquid; Fruity aroma	Sparingly soluble in water; soluble in non-polar solvents Soluble	89-91	NMR 95	1.443-1.449 0.855-0.859		69th Full
1845	**(E)-5-Nonen-2-one** (E)-5-Nonen-2-one	4326 27039-84-5	C9H16O 140.22	Clear colourless or pale yellow liquid; Fruit reminiscent of berries	Sparingly soluble in water; soluble in many non-polar solvents Soluble	197-198	NMR 96	1.433-1.439 0.835-0.839		69th Full
1846	**(Z)-3-Hexenyl 2-oxopropionate** 3-Oxo-propanoic acid (Z)-3-hexenyl ester	3934 09.565 10684 68133-76-6	C9H14O3 170.21	Colourless liquid; Green, spicy aroma	Insoluble in water; soluble in fats Soluble	75-77 (5 mm Hg)	NMR IR 98	1.437-1.445 0.982-0.990		69th Full
1847	**(+/-)-cis and trans-4,8-Dimethyl-3,7-nonadien-2-yl acetate** 4,8-Dimethyl-3,7-nonadien-2-ol acetate	4103 91418-25-6	C13H22O2 210.31	Clear colourless liquid; Green spicy aroma	Insoluble in water; soluble in most non-polar solvents Soluble	75-83 (2 mm Hg)	NMR IR 95	1.451-1.459 0.890-0.900		69th Full
1848	**(E)-1,5-Octadien-3-one** 1,5-Octadien-3-one	4405 07.190 65213-86-7	C8H12O 124.18	Colourless liquid; Penetrating earthy aroma	Practically insoluble to insoluble in water Soluble	168-169	MS 97	1.424-1.464 0.890-0.900		69th Full
1849	**10-Undecen-2-one** 10-Undecen-2-one	4406 36219-73-5	C11H20O 168.28	Colourless to pale yellow liquid; Citrus, fatty aroma	Practically insoluble to insoluble in water Soluble	81-82 (3 mm Hg)	MS 98	1.440-1.441 0.843-0.847		69th Full
1850	**2,4-Dimethyl-4-nonanol** 2,4-Dimethyl-4-nonanol	4407 74356-31-3	C11H24O 172.31	Colourless liquid; Fruity aroma	Very slightly soluble in water; soluble in fats Soluble	211-213	MS 84	1.439-1.447 0.821-0.827	SC:2,6,8- Trimethyl-6-hydroxy-4-nonanone (6.6%); cis-2,6,8-Trimethyl-5-nonen-4-one (6.5%); trans-2,6,8-Trimethyl-5-nonen-4-one (2.6%)	69th Full

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1851	**8-Nonen-2-one** 8-Nonen-2-one	4408 5009-32-5	C9H16O 140.22	Colourless liquid; Fruity aroma	Practically insoluble to insoluble in water Soluble	91.5-93 (26 mm Hg)	MS 99	1.436-1.437 0.853-0.855		69th Full
1852	**Menthyl valerate** 3-Methylbutanoic acid (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester	4156 09.154 472 89-47-4	C15H28O2 240.38	Colourless liquid; Sweet herbaceous aroma	Practically insoluble to insoluble in water Soluble	260-262	NMR MS 95 1.0	1.445-1.451 0.903-0.911		69th Full
1853	**2-(l-Menthoxy)ethanol** 2-[[5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-ethanol *2-(p-Menthan-3-yloxy) ethanol*	4154 38618-23-4	C12H24O2 200.36	Clear colourless viscous liquid; Minty aroma	Insoluble in water Soluble	99-100 (2 mm Hg)	NMR 99	1.457-1.467 0.920-0.940		69th Full
1854	**l-Menthyl acetoacetate** 3-Oxobutanoic acid (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester	4327 59557-05-0	C14H24O3 240.34	Clear colourless or pale yellow liquid; Minty aroma	Sparingly soluble in water; soluble in many non-polar solvents Soluble	110-115 (2.2 mm Hg)	NMR 96	1.458-1.466 0.979-0.985		69th Full
1855	**l-Menthyl (R,S)-3-hydroxybutyrate** 3-Hydroxybutanoic acid 5-methyl-2-(1-methylethyl)cyclohexyl ester	4308 108766-16-1	C14H26O3 242.35	Colourless liquid; Cool minty aroma	Slightly soluble in water; very soluble in corn oil, hexane, ether, chloroform and acetone Soluble	95-97 (0.5 mm Hg)	NMR IR 95	1.454-1.464 0.972-0.985		69th Full
1856	**l-Piperitone** (6R)-3-Methyl-6-(1-methylethyl)-2-cyclohexen-1-one	4200 07.255 2052 4573-50-6	C10H16O 152.23	Light yellowish liquid; Herbaceous minty aroma	Insoluble in water Soluble	233-235	NMR IR MS 99	1.483-1.487 0.929-0.934	NOTE: d-isomer is JECFA No. 435	69th Full
1857	**2,6,6-Trimethylcyclohex-2-ene-1,4-dione** 2,6,6-Trimethyl-2-cyclohex-2-ene-1,4-dione *keto-Isophorone*	3421 07.109 11200 1125-21-9	C9H12O2 152.20	White to colourless solid; Woody, musty sweet, aroma	Slightly soluble in water Soluble	NA	NMR IR 98	NA NA	m.p. = 23-28 ºC	69th Full

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1858	**Menthyl pyrrolidone carboxylate** 2-Isopropyl-5-methyl cyclohexyl 5-oxo-2-pyrrolidine carboxylate *D- and L-Proline*	4155 68127-22-0	C15H25NO3 267.36	Agglomerated fine white powder; Cool refreshing aroma	Slightly soluble in water Soluble	NA	NMR IR MS 98		NA NA	m.p. = 68-72 ºC	69th Full
1859	**3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one** 3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one *Freshone*	4285 06.136 831213-72-0	C13H22O3 226.30	Colourless liquid; Minty aroma	Slightly soluble in water; soluble in fats Soluble	323-325	NMR IR MS 98		1.458-1.461 1.018-1.021		69th Full
1860	**8-p-Menthene-1,2-diol** 1-Methyl-4-(1-methylethenyl)-1,2-cyclohexanediol *Limonene glycol*	4409 1946-00-5	C10H18O2 170.25	Colourless to very slightly yellow oily liquid; Cool minty aroma	Slightly soluble in water Soluble	54-57	MS 98		1.493-1.499 0.920-0.925		69th Full
1861	**d-2,8-p-Menthadien-1-ol** 1-Methyl-4-(1-methylethenyl)-2-cyclohexen-1-ol	4411 22771-44-4	C10H16O 153.23	Colourless to very slightly yellow oily liquid; Terpiniod aroma	Sparingly soluble in water Soluble	247-251	MS 95		1.484-1.494 0.936-0.946 (20 ºC)		69th Full
1862	**Dehydronootkatone** [4R-(4alpha,4a alpha,6beta)]-4,4a,5,6-Tetrahydro-4,4a-dimethyl-6-(1-methylethenyl)-2(3H)-naphthalenone *8,9-Didehydronootkatone*	4091 5090-63-1	C15H20O 216.33	Pale yellow to brown liquid; Fruity aroma with citrus undertone	Practically insoluble or insoluble in water; soluble in non-polar solvents Insoluble	129-130	NMR 95		1.559-1.569 1.009-1.019		69th Full
1863	**Isobornyl isobutyrate** 2-Methylpropanoic acid (1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester	4146 09.584 85586-67-0	C14H24O2 224.34	Colourless liquid; Earthy camphorous aroma	Practically insoluble to insoluble in water Soluble	131-133 (19 mm Hg)	MS 95		1.460-1.466 0.958-0.964		69th Full
1864	**l-Bornyl acetate** (1S,2R,4S)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol acetate	4080 09.848 5655-61-8	C12H20O2 196.29	Colourless solid; Sweet herbaceous odour	Practically insoluble to insoluble in water Soluble	224-226	NMR 95		1.456-1.462 0.981-0.987	m.p. = 29 ºC	69th Full

No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min % max	A.V.	R. I. S. G.	Other requirements/ Secondary components	Session Status
1865	**Thujyl alcohol** (1S,3S,4R,5R)-4-Methyl-1-(1-methylethyl)-bicyclo[3.1.0]hexan-3-ol *(-)-3-Neoisothujanol*	4079 02.207 21653-20-3	C10H18O 154.25	Colourless crystals; Minty camphorous odour	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	99-100 (12 mm Hg)	NMR 95		1.460-1.466 0.919-0.925	m.p. = 28 ºC	69th Full
1866	**Vetiverol** 1,2,3,3a,4,5,6,8a-Octahydro-4,8-dimethyl-2-(1-methylethylidene)-6-azulenol	4217 02.214 10321 89-88-3	C15H24O 220.35	Amber solid; Sweet balsamic aroma	Practically insoluble to insoluble in water Soluble	NA	NMR 95		NA NA	m.p. = 69-71 ºC	69th Full
1867	**Vetiveryl acetate** 1,2,3,3a,4,5,6,8a-Octahydro-4,8-dimethyl-2-(1-methylethylidene)-6-azulenol acetate	4218 09.821 11887 117-98-6	C17H26O2 262.39	Colourless solid; Sweet woody aroma	Practically insoluble to insoluble in water Soluble	NA	NMR 95		NA NA	m.p. = 73 ºC	69th Full
1868	**3-Pinanone** 2,6,6-Trimethylbicyclo[3.1.1]heptan-3-one *Isopinocamphone*	4198 07.171 11125 18358-53-7	C10H16O 154.24	Colourless liquid; Cedar camphor aroma	Practically insoluble to insoluble in water Soluble	69-71 (5 mm Hg)	NMR MS 95		1.472-1.478 0.963-0.969		69th Full
1869	**Isobornyl 2-methylbutyrate** 2-Methylbutanoic acid 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester	4147 09.888 94200-10-9	C15H26O2 238.37	Colourless solid; Herbaceous woody aroma	Practically insoluble to insoluble in water Soluble	NA	NMR MS 95		NA NA	m.p. = 81-84 ºC	69th Full
1870	**Verbenone** 4,6,6-Trimethylbicyclo[3.1.1]heptan-3-one *Pin-2-en-4-one*	4216 07.196 11186 80-57-9	C10H24O 150.22	Colourless liquid; Minty spicy aroma	Practically insoluble to insoluble in water; soluble in non-polar solvents Soluble	89-90 (12 mm Hg)	NMR MS 95		1.490-1.500 0.975-0.981		69th Full

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1871	**Methyl hexanoate** Methyl hexanoate	2708 09.069 319 106-70-7	C7H14O2 130.18	Colourless to pale yellow liquid; Pineapple, ethereal aroma	Insoluble in water; soluble in propylene glycol and vegetable oils Soluble	150-151	NMR 98	1.0	1.402-1.409 0.880-0.889		69th Full
1872	**Hexyl heptanoate** 1-Hexyl heptanoate	4337 1119-06-8	C13H26O2 214.32	Liquid; Herbaceous aroma	Insoluble in water; soluble in non-polar solvents Soluble	252-253	MS 98	1.0	1.426-1.430 0.860-0.865 (20 ºC)		69th Full
1873	**Hexyl nonanoate** Hexyl nonanoate	4339 6561-39-3	C15H30O2 242.40	Liquid; Fresh vegetable fruity aroma	Insoluble in water; soluble in non-polar solvents Soluble	291-292	MS 96	1.0	1.431-1.436 0.858-0.863 (20 ºC)		69th Full
1874	**Hexyl decanoate** Hexyl decanoate *Hexyl caprate*	4342 10448-26-7	C16H32O2 256.42	Liquid; Fresh green aroma	Insoluble in water; soluble in non-polar solvents Soluble	305-306	MS 98	1.0	1.432-1.438 0.857-0.863 (20 ºC)		69th Full
1875	**Heptyl heptanoate** 1-Heptyl heptanoate	4341 624-09-9	C14H28O2 228.37	Liquid; Green aroma	Insoluble in water, soluble in non-polar solvents Soluble	276-277	MS 98		1.428-1.432 0.859-0.865 (20 ºC)		69th Full
1876	**Dodecyl propionate** Dodecyl propionate	4338 6221-93-8	C15H30O2 242.40	Liquid; Slightly fruity light aroma	Insoluble in water; soluble in non-polar solvents Soluble	283-284	NMR IR MS 98	1.0	1.432-1.436 0.860-0.866 (20 ºC)		69th Full
1877	**Dodecyl butyrate** Dodecyl butyrate	4340 3724-61-6	C16H32O2 256.42	Liquid; Slightly fruity light aroma	Insoluble in water; soluble in non-polar solvents Soluble	305-306	NMR MS 98	1.0	1.433-1.438 0.857-0.862 (20 ºC)		69th Full

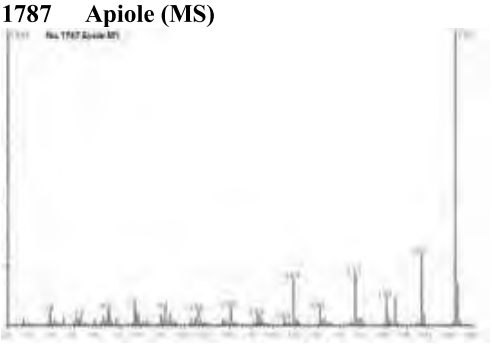
No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min % max	A.V.	R. I. S. G.	Other requirements/ Secondary components	Session Status
1878	**4-Hydroxy-3,5-dimethoxy benzaldehyde**	4049	C9H10O4 182.18	Very pale green needles; Alcoholic aroma	Insoluble in water	NA	NMR IR 98		NA NA	m.p. = 110-113 ºC	69th
	4-Hydroxy-3,5-dimethoxybenzaldehyde *Gallaldehyde 3,5-dimethyl ether*	05.153 10340 134-96-3			Soluble						Full
1879	**Vanillin 3-(l-menthoxy)propane-1,2-diol acetal**	3904	C21H32O5 364.48	Colourless powder; Minty aroma with vanilla undertones	Slightly soluble in water; soluble in fats, non-polar solvents and acetone	NA	NMR MS 94		NA NA	m.p. = 78-80 ºC	69th
	2-Methoxy-4-[4-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-1,3-dioxolan-2-yl]-phenol	02.248 180964-47-0			Soluble					SC: Vanillin (2-3%)	Full
1880	**Sodium 4-methoxybenzoyloxyacetate**	4016b	C10H9O5Na 232.17	White solid; Cooked brown and roasted aroma	Slightly soluble in water; insolube in n-octane	NA	NMR 98		NA NA	m.p. = 135 ºC	69th
	Benzoic acid, 4-methoxy-, carboxymethyl ester, sodium salt	17114-82-8			Soluble						Full
1881	**Divanillin**	4107	C16H14O6 302.28	White solid; Fruity vanilla aroma	Practically insoluble to insoluble in water; soluble in benzyl alcohol	NA	NMR 91		NA NA	m.p. = 315 ºC	69th
	6,6'-Dihydroxy-5,5'-dimethoxy-[1,1'-biphenyl]-3,3'-dicarboxaldehyde *Dehydrodivanillin*	05.221 2092-49-1			Soluble					SC: Vanillin (5-7%)	Full
1882	**Vanillin propylene glycol acetal**	3905	C11H14O4 210.23	Colourless, viscous liquid; Sweet, vanilla aroma	Insoluble in water and fat; soluble in triacetin	152-155 (1 mm Hg)	NMR 79		1.533-1.543 1.196-1.206		69th
	2-Methoxy-4-(4-methyl-1,3-dioxalan-2-yl)-phenol	06.104 68527-74-2			Soluble					SC: Vanillin (18-20%)	Full
1883	**4-Methoxybenzoyloxyacetic acid**	4016	C10H10O5 210.18	White solid; Cooked brown and roasted aroma	Slightly soluble in water; insoluble in n-octane	NA	NMR IR MS 98		NA NA	m.p. = 135 ºC	69th
	Benzoic acid, 4-methoxy-, carboxymethyl ester *Glycolic acid, p-anisate*	10414-68-3			Soluble						Full
1884	**Methyl isothiocyanate**	4426	C2H3NS 73.11	Colourless to tan liquid; Pungent, penetrating mustard-like odour	Very slightly soluble in water; freely soluble in ether	117-118	MS 96		1.495-1.499 0.938-0.942		69th
	Isothiocyanatomethane	556-61-6			Soluble						Full

No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min % max	A.V.	R. I. S. G.	Other requirements/ Secondary components	Session Status
1885	**Ethyl isothiocyanate** Isothiocyanatoethane	4420 542-85-8	C3H5NS 87.14	Colourless liquid; Sharp mustard-like aroma	Very slightly soluble in water; freely soluble in ether Soluble	130-132	MS 99		1.510-1.515 0.997-1.004		69th Full
1886	**Isobutyl isothiocyanate** 1-Isothiocyanato-2-methylpropane	4424 591-82-2	C5H9NS 115.20	Colourless to yellow liquid; Green pungent aroma	Very slightly soluble in water; freely soluble in ether Soluble	72-73 (30 mm Hg)	MS 97		1.491-1.499 0.935-0.945		69th Full
1887	**Isoamyl isothiocyanate** 1-Isothiocyanato-3-methylbutane	4423 628-03-5	C6H11NS 129.23	Colourless to yellow liquid; Sharp green irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	80-82 (12 mm Hg)	MS 98		1.493-1.499 0.939-0.945		69th Full
1888	**Isopropyl isothiocyanate** 2-Isothiocyanatopropane	4425 2253-73-8	C4H7NS 101.17	Colourless liquid; Penetrating mustard-like aroma	Very slightly soluble in water; freely soluble in ether Soluble	68-70 (67 mm Hg)	MS 95		1.489-1.497 0.947-0.955		69th Full
1889	**3-Butenyl isothiocyanate** 4-Isothiocyanato-1-butene	4418 12.283 3386-97-8	C5H7NS 113.20	Colourless liquid; Penetrating aroma	Very slightly soluble in water; freely soluble in ether Soluble	75-77 (14 mm Hg)	MS 97		1.520-1.526 0.990-0.996 (20 ºC)		69th Full
1890	**2-Butyl isothiocyanate** 2-Isothiocyanatobutane	4419 4426-79-3	C5H9NS 115.20	Colourless to yellow liquid; Sharp green slightly irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	69-70 (27 mm Hg)	MS 97		1.490-1.497 0.938-0.946		69th Full
1891	**Amyl isothiocyanate** 1-Isothiocyanatopentane	4417 629-12-9	C6H11NS 129.23	Colourless to yellow liquid; Sharp green irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	101-103 (35 mm Hg)	MS 97		1.495-1.501 0.942-0948 (20 ºC)		69th Full

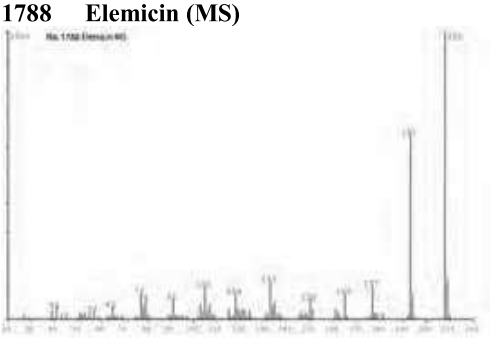
No	Name Chemical Name *Synonyms*	FEMA No FLAVIS No COE No CAS No	Formula M. W.	Physical form; odour	Solubility Solubility in ethanol	B.P. °C	ID test Assay min % A.V. max	R. I. S. G.	Other requirements/ Secondary components	Session Status
1892	**4-(Methylthio)butyl isothiocyanate** 1-Isothiocyanato-4-(methylthio)butane	4414 4430-36-8	C6H11NS2 161.29	Pale yellow liquid; Penetrating raddish-like aroma	Very slightly soluble in water; freely soluble in ether Soluble	134-136 (14 mm Hg)	MS 99	1.551-1.556 1.080-1.086 (20 ºC)		69th Full
1893	**4-Pentenyl isothiocyanate** 5-Isothiocyanato-1-pentene	4427 18060-79-2	C6H9NS 127.21	Colourless to pale yellow liquid; Strong pungent irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	57-58 (3 mm Hg)	MS 95	1.513-1.519 0.970-0.976 (20 ºC)		69th Full
1894	**5-Hexenyl isothiocyanate** 6-Isothiocyanato-1-hexene	4421 49776-81-0	C7H11NS 141.24	Colourless to pale yellow liquid; Pungent irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	74-76 (3 mm Hg)	MS 96	1.506-1.516 0.955-0.965 (20 ºC)		69th Full
1895	**Hexyl isothiocyanate** 1-Isothiocyanatohexane	4422 4404-45-9	C7H13NS 143.25	Colourless to yellow liquid; sharp green irritating aroma	Very slightly soluble in water; freely soluble in ether Soluble	72-73 (8 mm Hg)	MS 97	1.490-1.494 0.931-0.941 (20 ºC)		69th Full
1896	**5-(Methylthio)pentyl isothiocyanate** 1-Isothiocyanato-5-(methylthio)-pentane	4416 4430-42-6	C7H13NS2 175.32	Pale yellow liquid; Penetrating raddish-like aroma	Very slightly soluble in water; freely soluble in ether Soluble	131-133 (4 mm Hg)	MS 96	1.542-1.548 1.055-1.061 (20 ºC)		69th Full
1897	**6-(Methylthio)hexyl isothiocyanate** 1-Isothiocyanato-6-(methylthio)-hexane	4415 4430-39-1	C8H15NS2 189.34	Pale yellow liquid; Penetrating raddish-like aroma	Very slightly soluble in water; freely soluble in ether Soluble	128-129 (1 mm Hg)	MS 95	1.534-1.540 1.035-1.041 (20 ºC)		69th Full

Spectra of certain flavouring agents

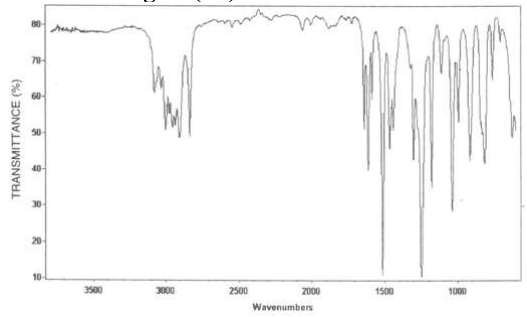
1787 Apiole (MS)



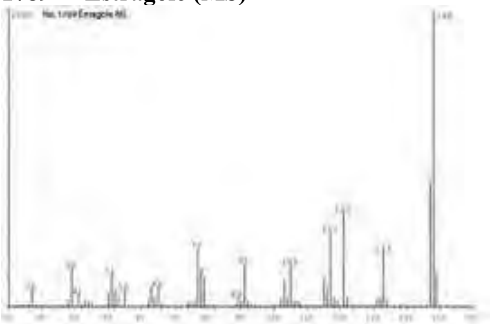
1788 Elemicin (MS)



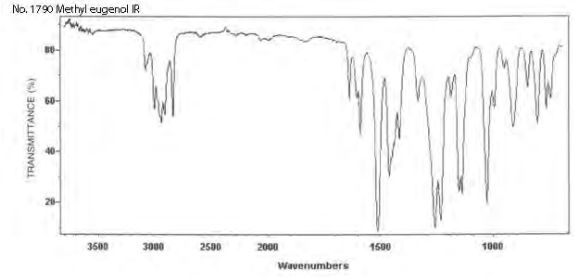
1789 Estragole (IR)



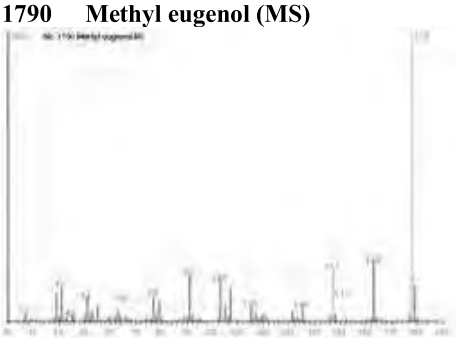
1789 Estragole (MS)



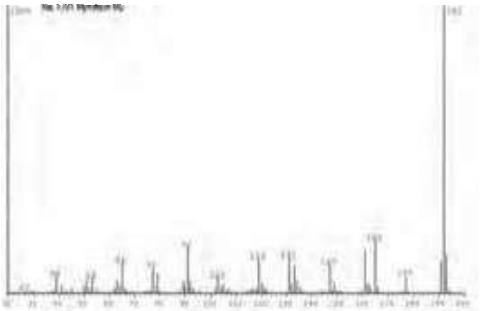
1790 Methyl eugenol (IR)



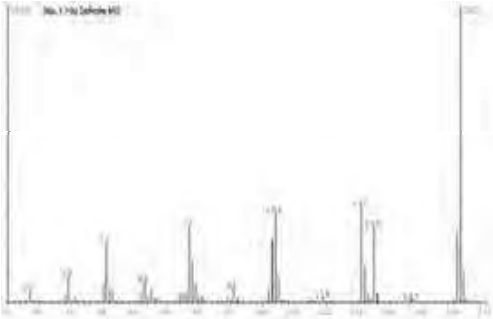
1790 Methyl eugenol (MS)



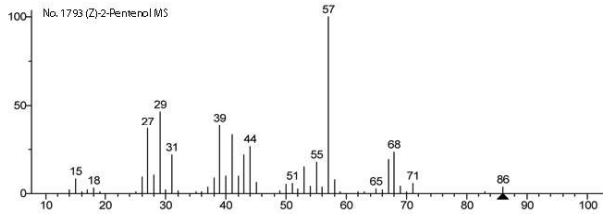
1791 Myristicin (MS)



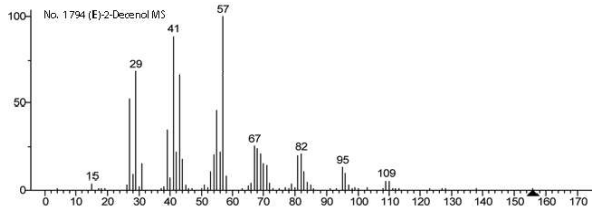
1792 Safrole (MS)



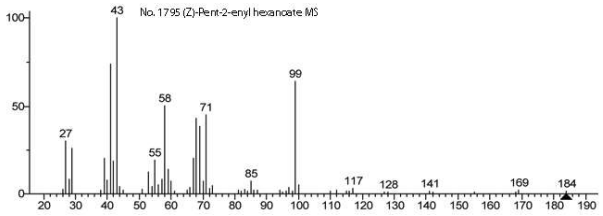
1793 (Z)-2-Penten-1-ol (MS)



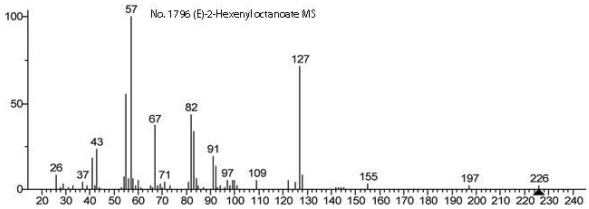
1794 (E)-2-Decen-1-ol (MS)



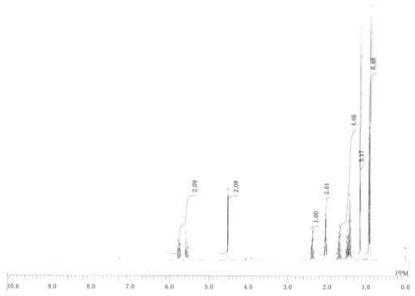
1795 (Z)-Pent-2-enyl hexanoate (MS)



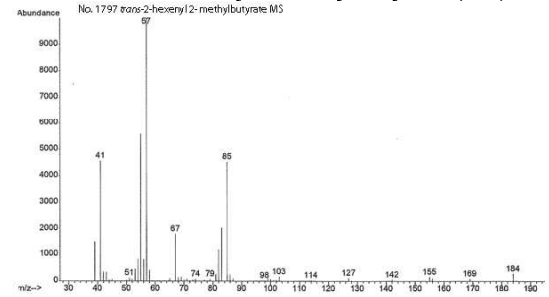
1796 (E)-2-Hexenyl octanoate (MS)



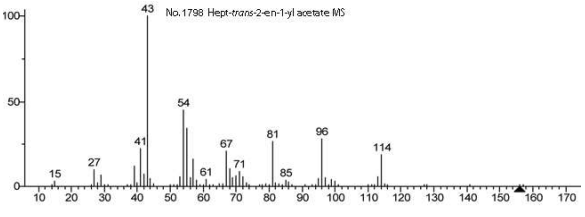
1797 trans-2-Hexenyl 2-methylbutyrate (1H-NMR)



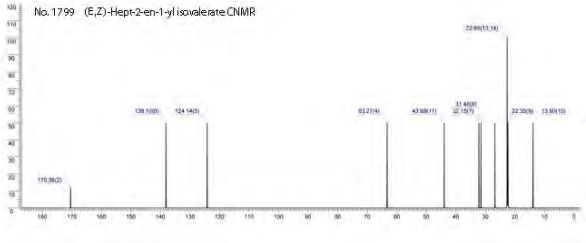
1797 trans-2-Hexenyl 2-methylbutyrate (MS)



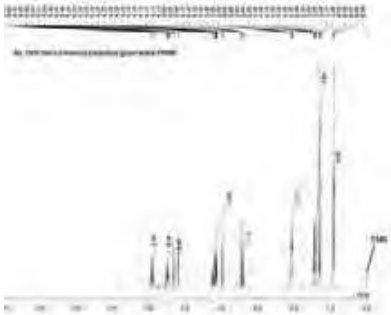
1798 Hept-trans-2-en-1-yl acetate (MS)



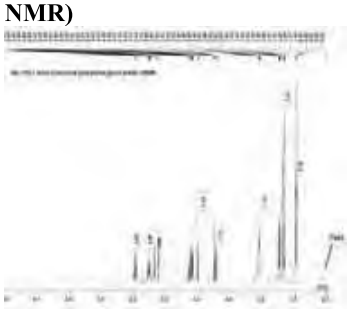
1799 (E,Z)-Hept-2-en-1-yl isovalerate (13C-NMR)



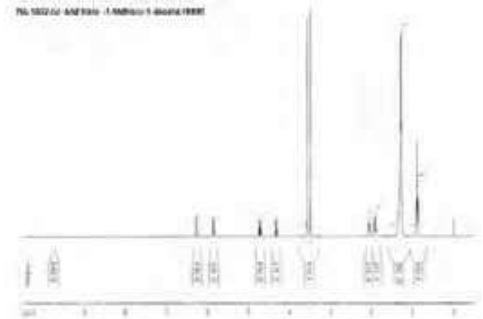
1800 trans-2-Hexenal glyceryl acetal (1H-NMR)



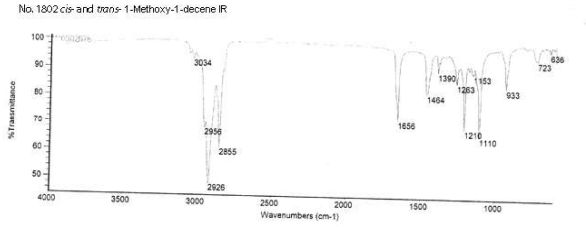
1801 trans-2-Hexenal propylene glycol acetal (1H-NMR)



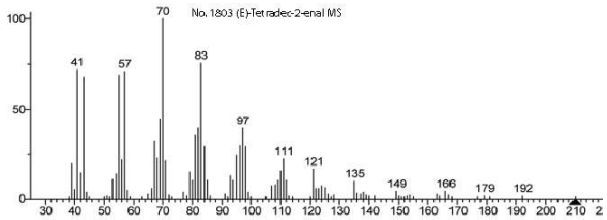
1802 cis- and trans-1-Methoxy-1-decene (1H-NMR)



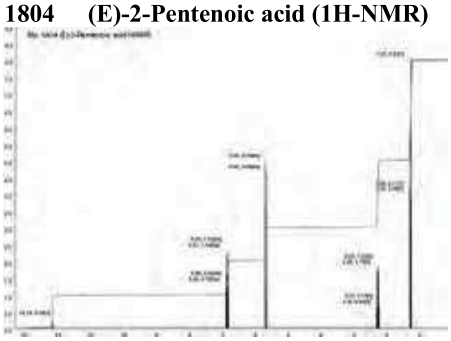
1802 cis- and trans-1-Methoxy-1-decene (IR)



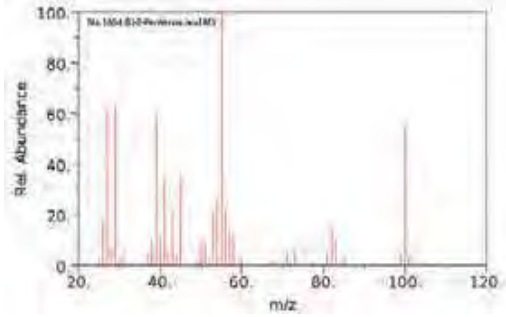
1803 (E)-Tetradec-2-enal (MS)



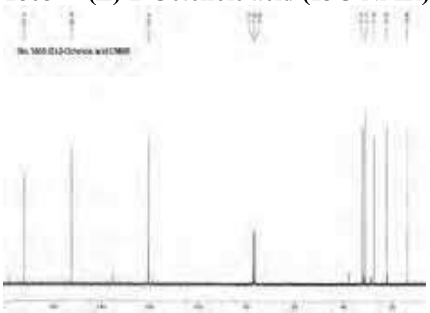
1804 (E)-2-Pentenoic acid (1H-NMR)



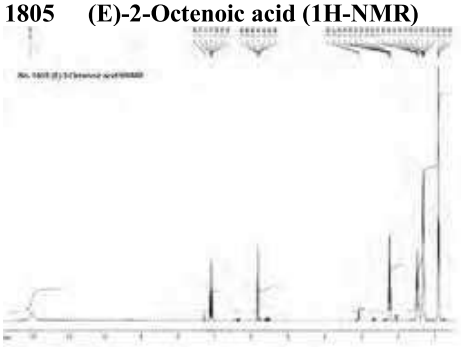
1804 (E)-2-Pentenoic acid (MS)



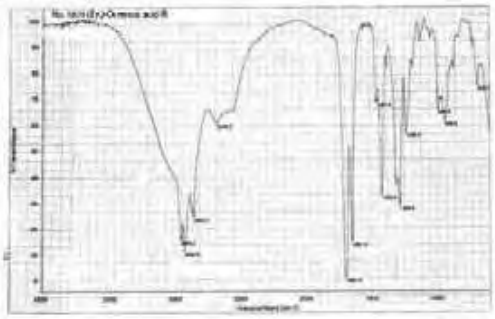
1805 (E)-2-Octenoic acid (13C-NMR)



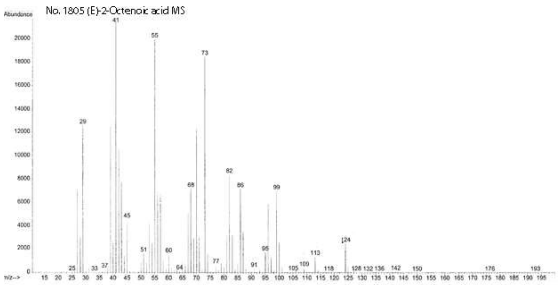
1805 (E)-2-Octenoic acid (1H-NMR)



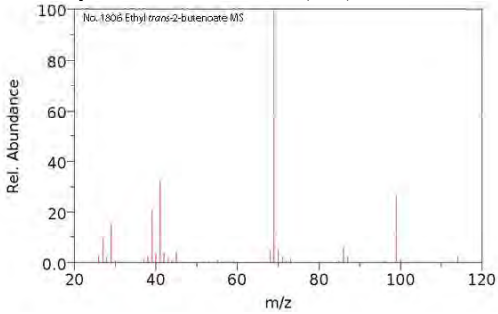
1805 (E)-2-Octenoic acid (IR)



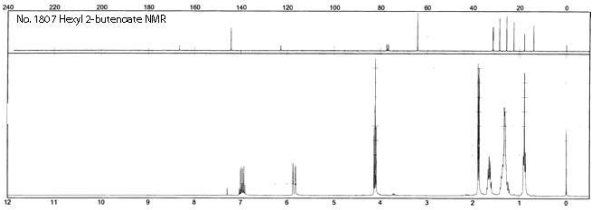
1805 (E)-2-Octenoic acid (MS)



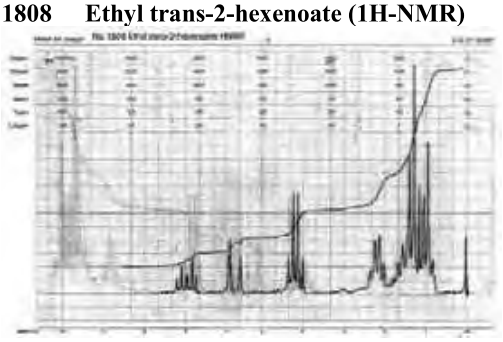
1806 Ethyl trans-2-butenoate (MS)



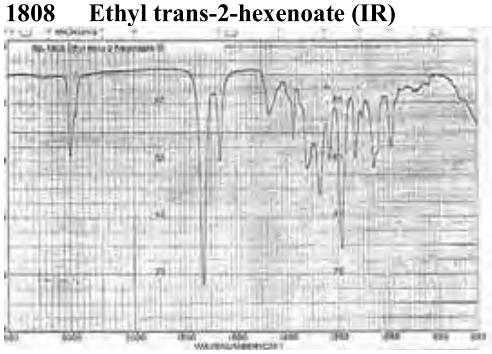
1807 Hexyl 2-butenoate (NMR)



1808 Ethyl trans-2-hexenoate (1H-NMR)



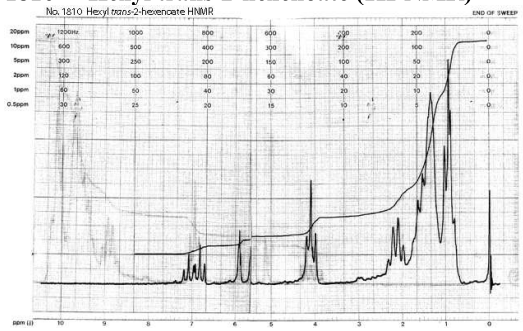
1808 Ethyl trans-2-hexenoate (IR)



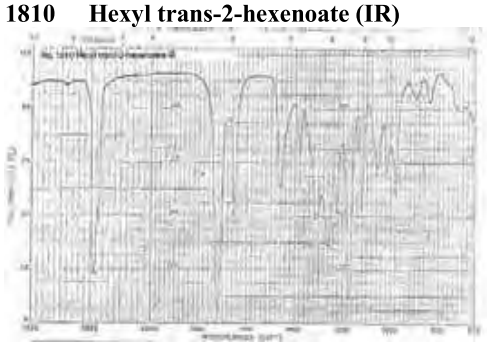
1809 (E,Z)-Methyl 2-hexenoate (1H-NMR)



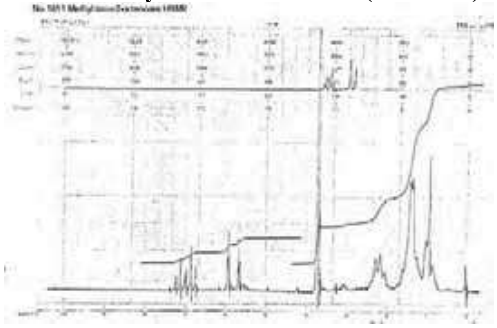
1810 Hexyl trans-2-hexenoate (1H-NMR)



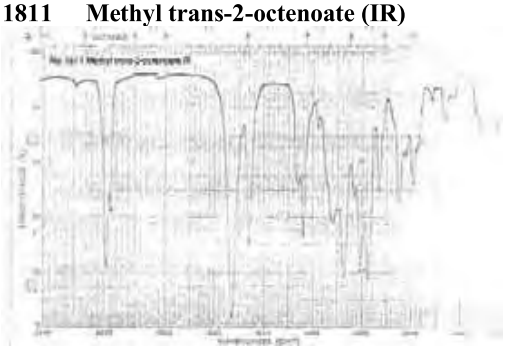
1810 Hexyl trans-2-hexenoate (IR)



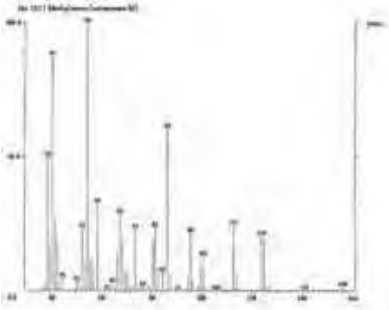
1811 Methyl trans-2-octenoate (1H-NMR)



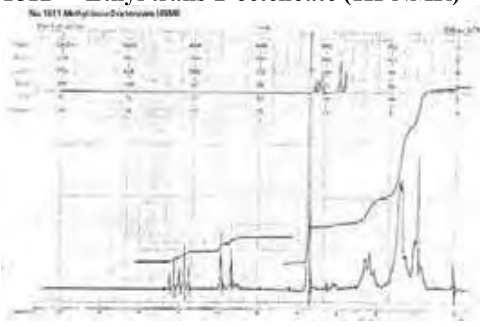
1811 Methyl trans-2-octenoate (IR)



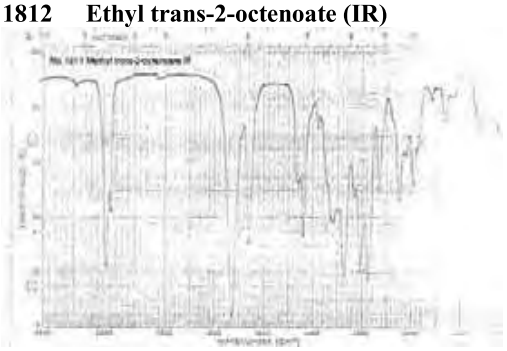
1811 Methyl trans-2-octenoate (MS)



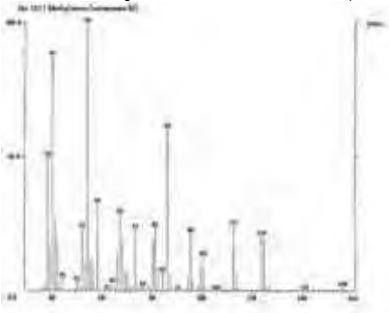
1812 Ethyl trans-2-octenoate (1H-NMR)



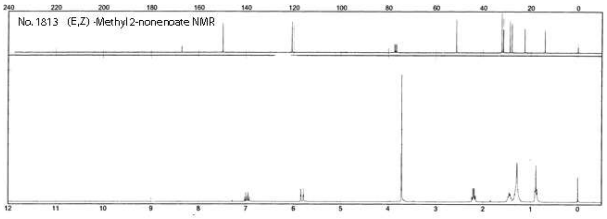
1812 Ethyl trans-2-octenoate (IR)



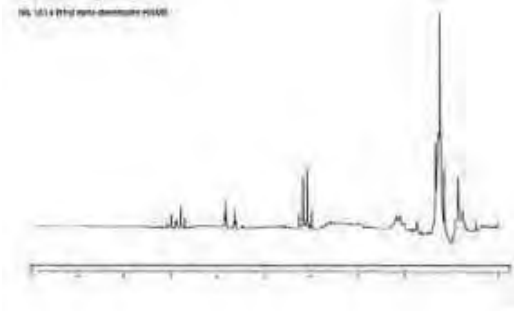
1812 Ethyl trans-2-octenoate (MS)



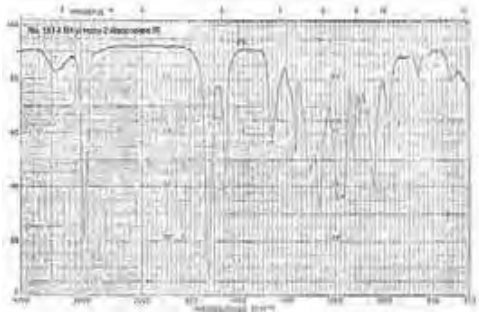
1813 (E,Z)-Methyl 2-nonenoate (NMR)



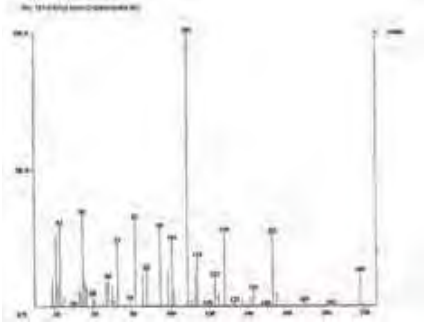
1814 Ethyl trans-2-decenoate (1H-NMR)



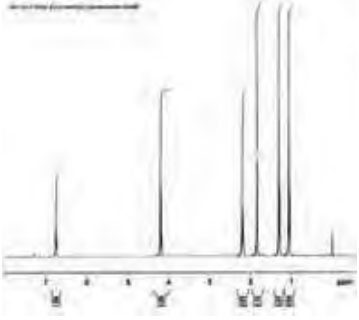
1814 Ethyl trans-2-decenoate (IR)



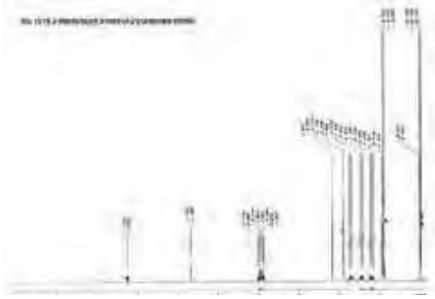
1814 Ethyl trans-2-decenoate (MS)



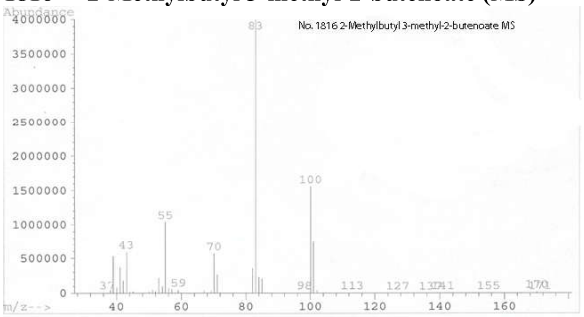
1815 Ethyl (E)-2-methyl-2-pentenoate (1H-NMR)



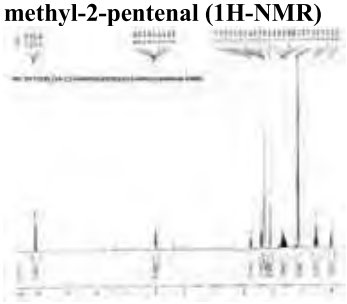
1816 2-Methylbutyl 3-methyl-2-butenoate (1H-NMR)



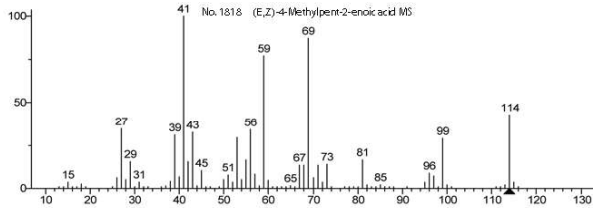
1816 2-Methylbutyl 3-methyl-2-butenoate (MS)



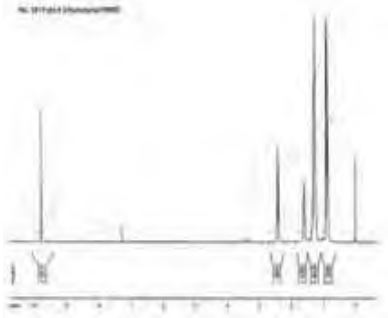
1817 (+/-) (E,Z)-5-(2,2-Dimethylcyclopropyl)-3-methyl-2-pentenal (1H-NMR)



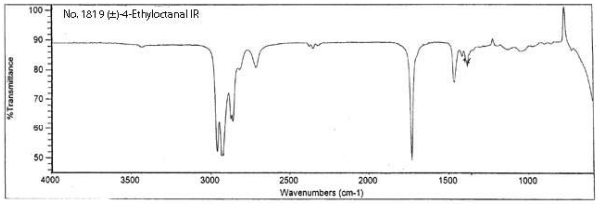
1818 (E,Z)-4-Methylpent-2-enoic acid (MS)



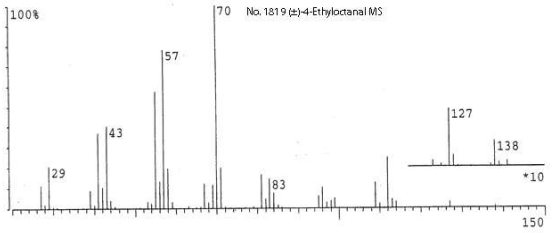
1819 (+/-)-4-Ethyloctanal (1H-NMR)



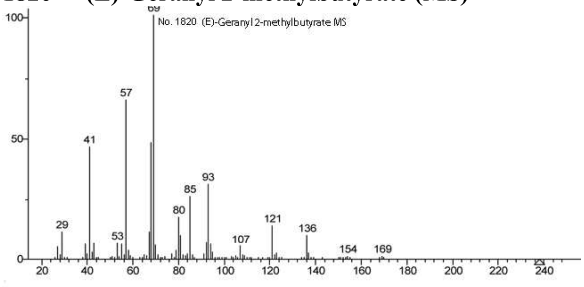
1819 (+/-)-4-Ethyloctanal (IR)



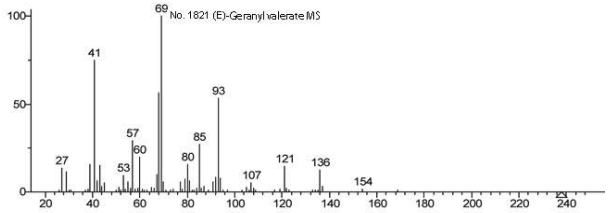
1819 (+/-)-4-Ethyloctanal (MS)



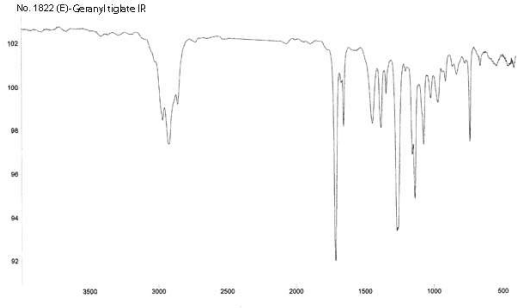
1820 (E)-Geranyl 2-methylbutyrate (MS)



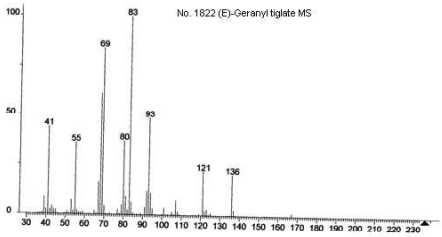
1821 (E)-Geranyl valerate (MS)



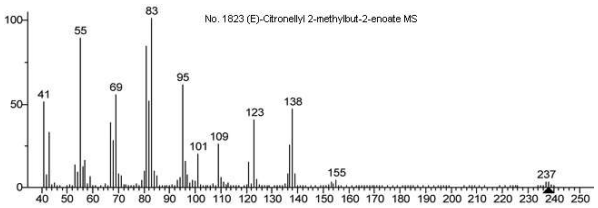
1822 (E)-Geranyl tiglate (IR)



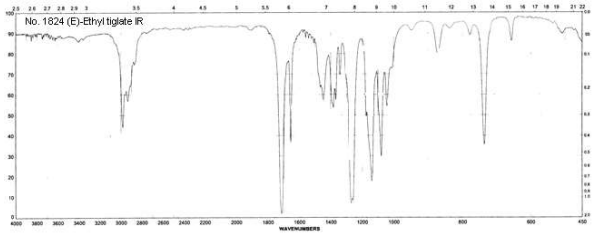
1822 (E)-Geranyl tiglate (MS)



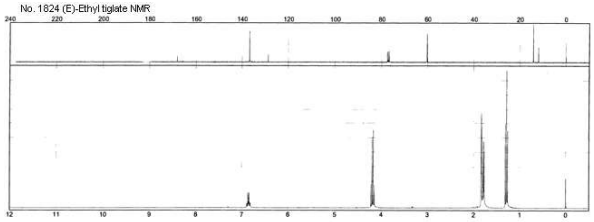
1823 (E)-Citronellyl 2-methylbut-2-enoate (MS)



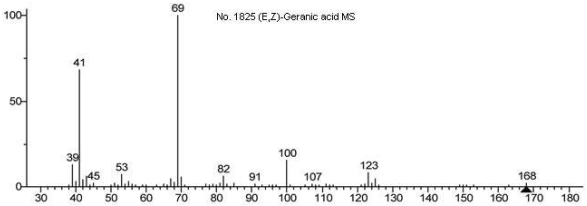
1824 (E)-Ethyl tiglate (IR)



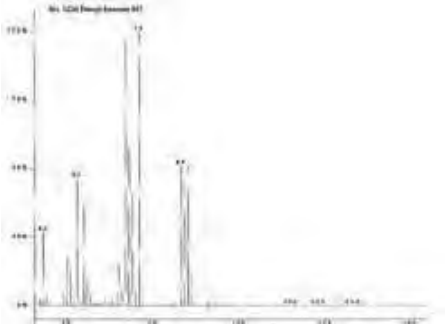
1824 (E)-Ethyl tiglate (NMR)



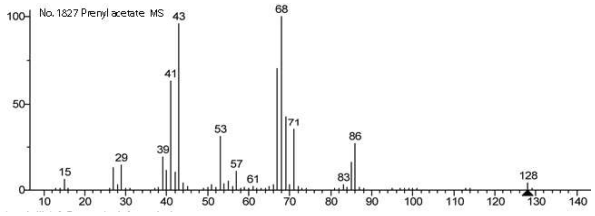
1825 (E,Z)-Geranic acid (MS)



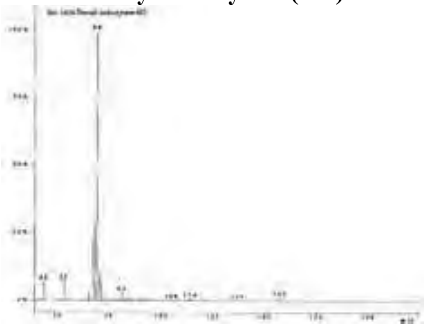
1826 Prenyl formate (MS)



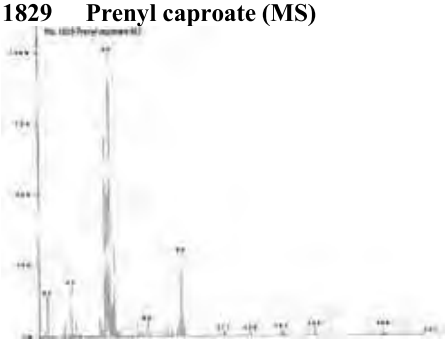
1827 Prenyl acetate (MS)



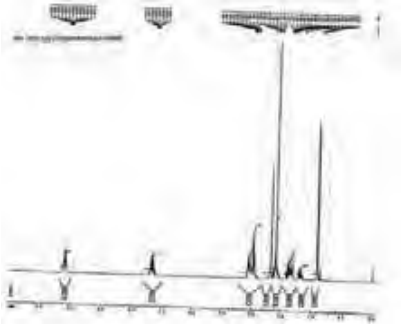
1828 Prenyl isobutyrate (MS)



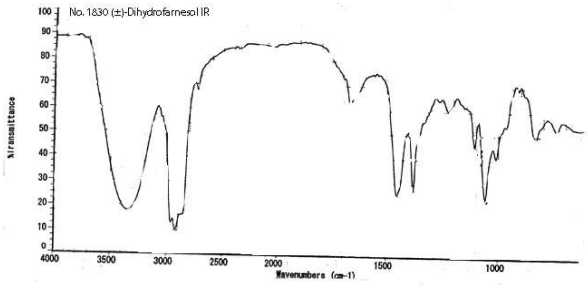
1829 Prenyl caproate (MS)



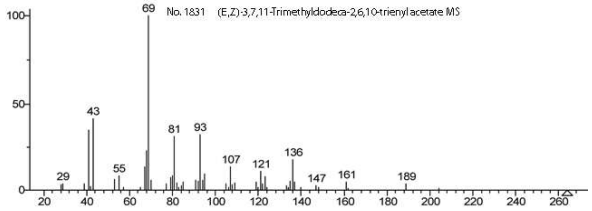
1830 (+/-)-Dihydrofarnesol (1H-NMR)



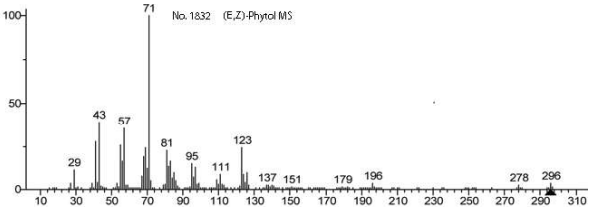
1830 (+/-)-Dihydrofarnesol (IR)



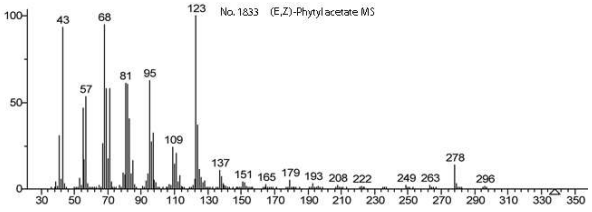
1831 (E,Z)-3,7,11-Trimethyldodeca-2,6,10-trienyl acetate (MS)



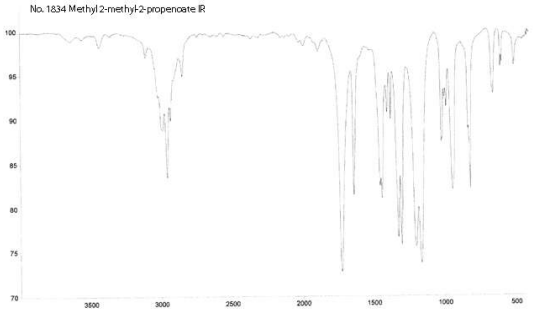
1832 (E,Z)-Phytol (MS)



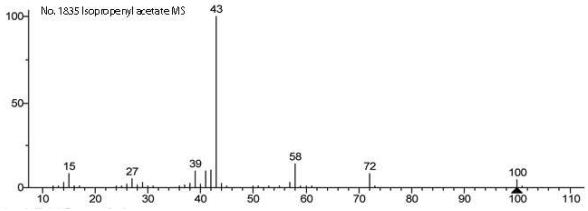
1833 (E,Z)-Phytyl acetate (MS)



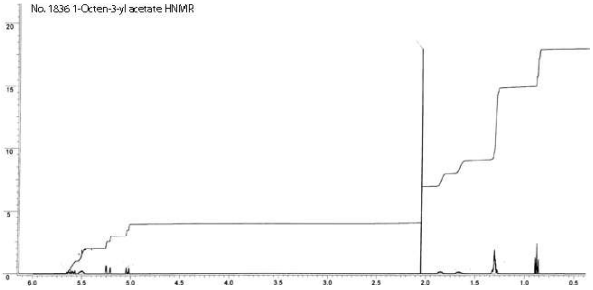
1834 Methyl 2-methyl-2-propenoate (IR)



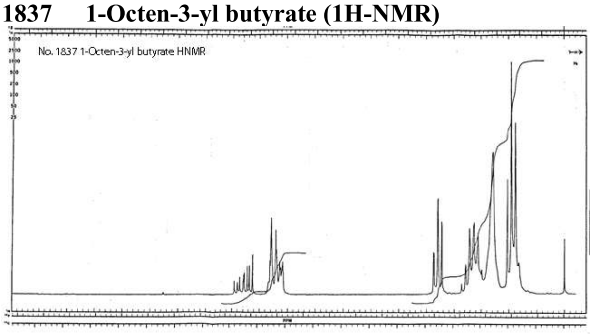
1835 Isopropenyl acetate (MS)



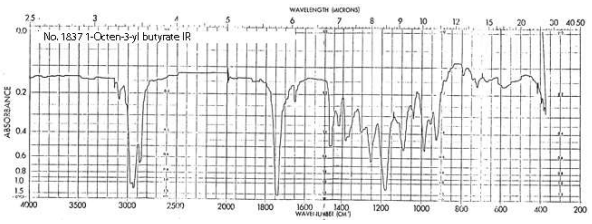
1836 1-Octen-3-yl acetate (1H-NMR)



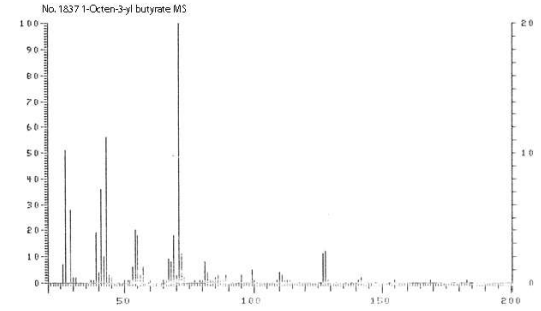
1837 1-Octen-3-yl butyrate (1H-NMR)



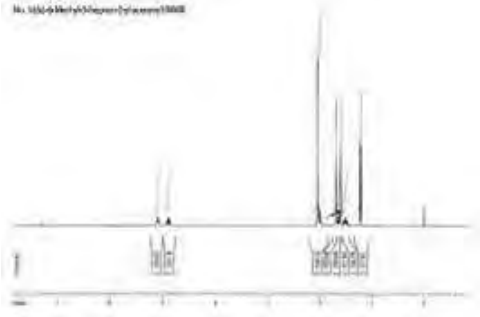
1837 1-Octen-3-yl butyrate (IR)



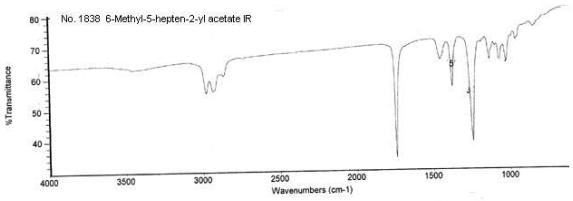
1837 1-Octen-3-yl butyrate (MS)



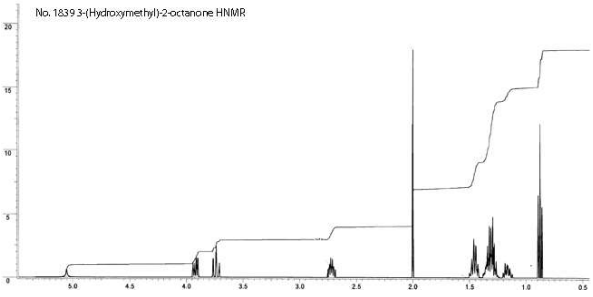
1838 6-Methyl-5-hepten-2-yl acetate (1H-NMR)



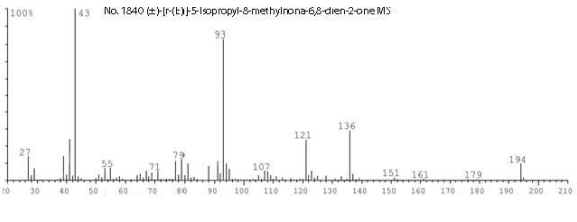
1838 6-Methyl-5-hepten-2-yl acetate (IR)



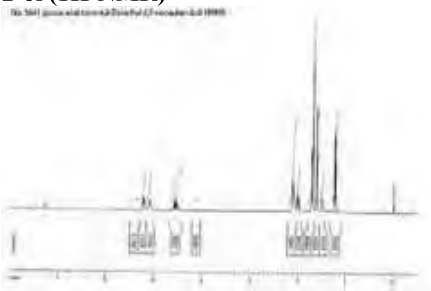
1839 3-(Hydroxymethyl)-2-octanone (1H-NMR)



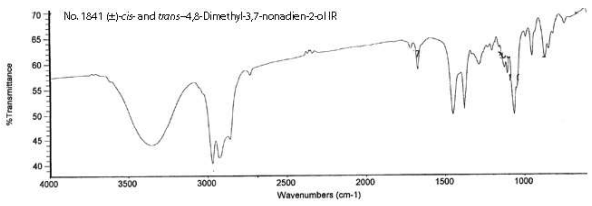
1840 (+/-) [R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one (MS)



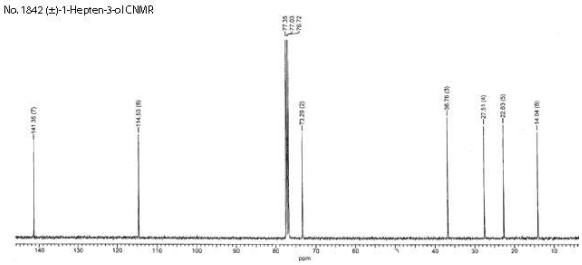
1841 (+/-)-cis- and trans-4,8-Dimethyl-3,7-nonadien-2-ol (1H-NMR)



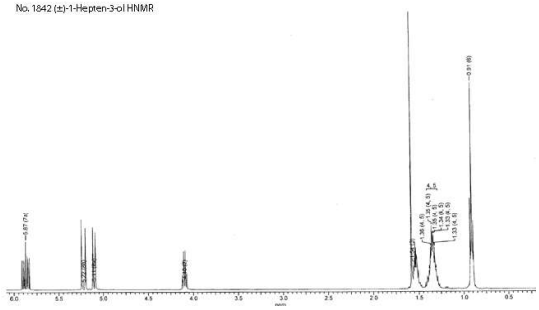
1841 (+/-)-cis- and trans-4,8-Dimethyl-3,7-nonadien-2-ol (IR)



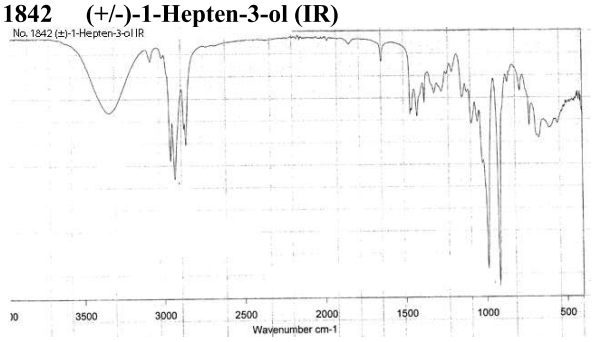
1842 (+/-)-1-Hepten-3-ol (13C-NMR)



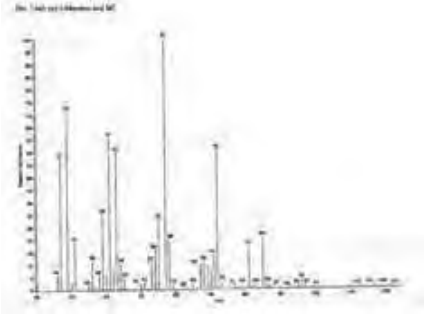
1842 (+/-)-1-Hepten-3-ol (1H-NMR)



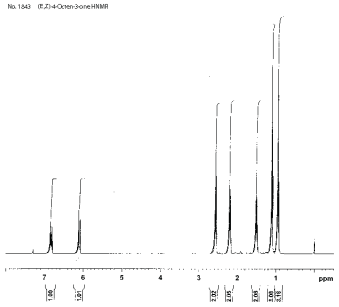
1842 (+/-)-1-Hepten-3-ol (IR)



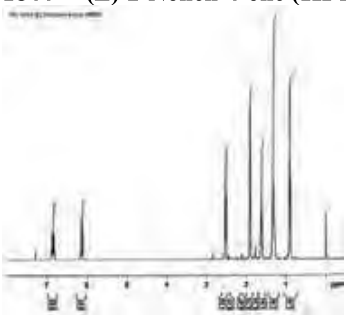
1842 (+/-)-1-Hepten-3-ol (MS)



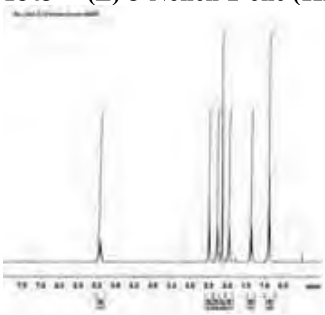
1843 (E,Z)-4-Octen-3-one (1H-NMR)



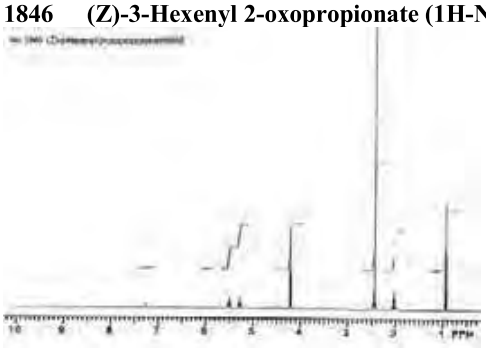
1844 (E)-2-Nonen-4-one (1H-NMR)



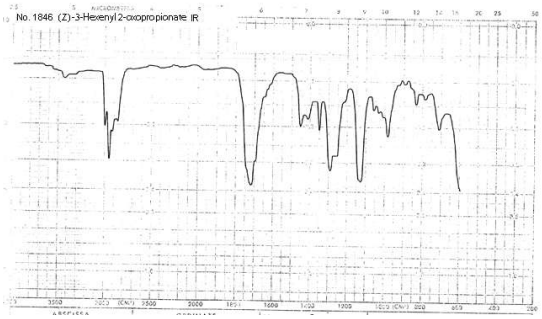
1845 (E)-5-Nonen-2-one (1H-NMR)



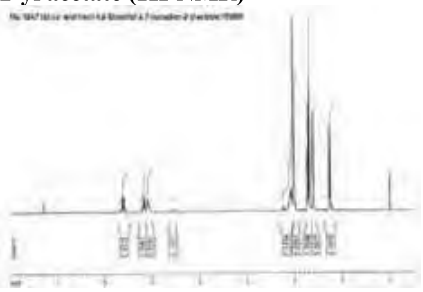
1846 (Z)-3-Hexenyl 2-oxopropionate (1H-NMR)



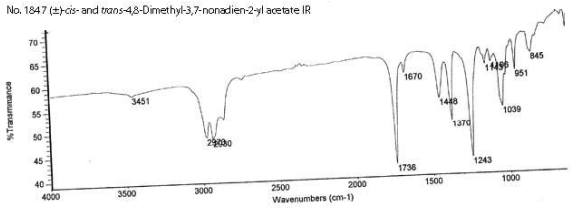
1846 (Z)-3-Hexenyl 2-oxopropionate (IR)



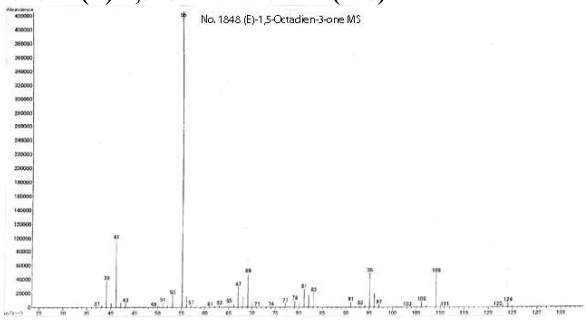
1847 (+/-)-cis and trans-4,8-Dimethyl-3,7-nonadien-2-yl acetate (1H-NMR)



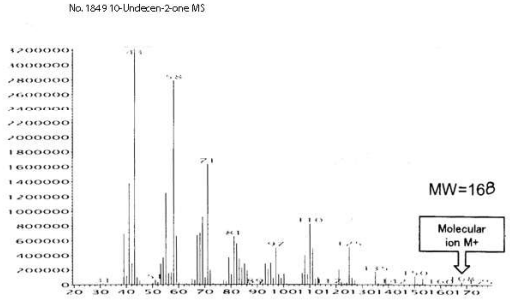
1847 (+/-)-cis and trans-4,8-Dimethyl-3,7-nonadien-2-yl acetate (IR)



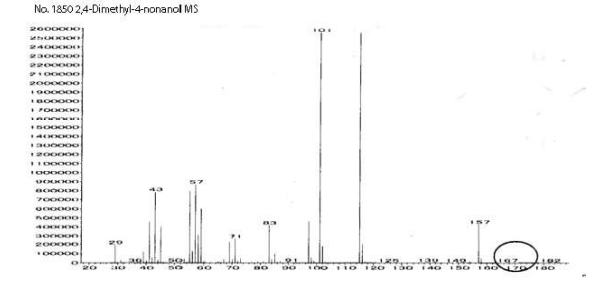
1848 (E)-1,5-Octadien-3-one (MS)



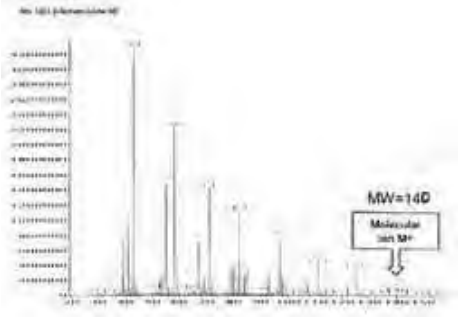
1849 10-Undecen-2-one (MS)



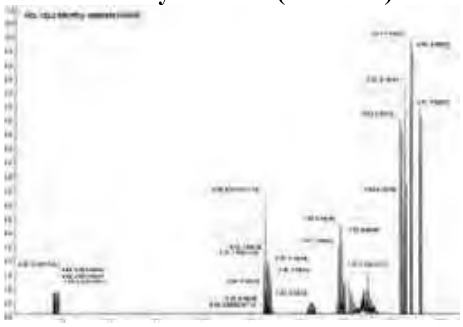
1850 2,4-Dimethyl-4-nonanol (MS)



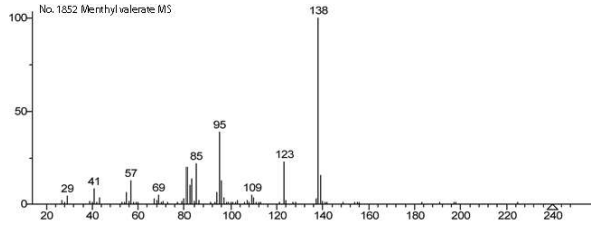
1851 8-Nonen-2-one (MS)



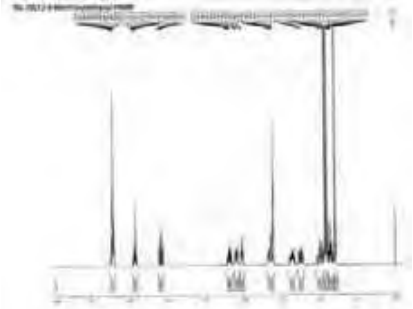
1852 Menthyl valerate (1H-NMR)



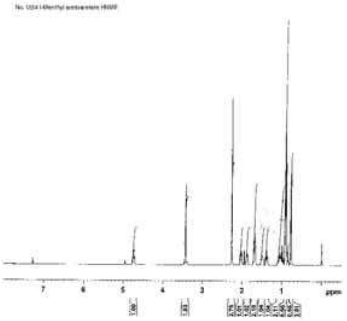
1852 Menthyl valerate (MS)



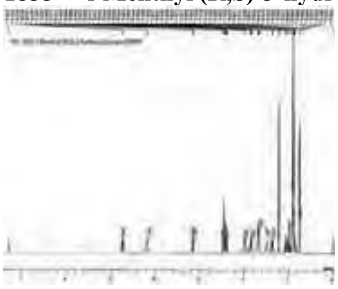
1853 2-(l-Menthoxy)ethanol (1H-NMR)



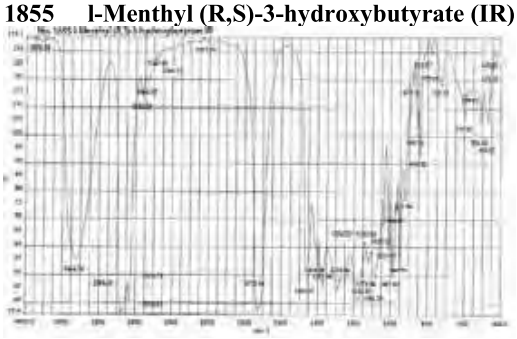
1854 l-Menthyl acetoacetate (1H-NMR)



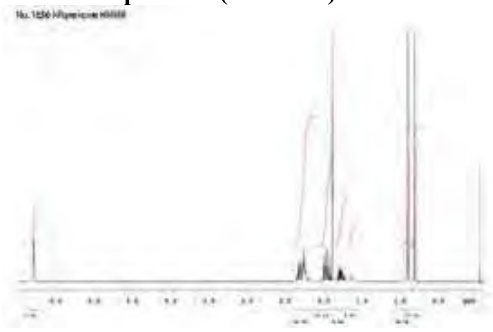
1855 l-Menthyl (R,S)-3-hydroxybutyrate (1H-NMR)



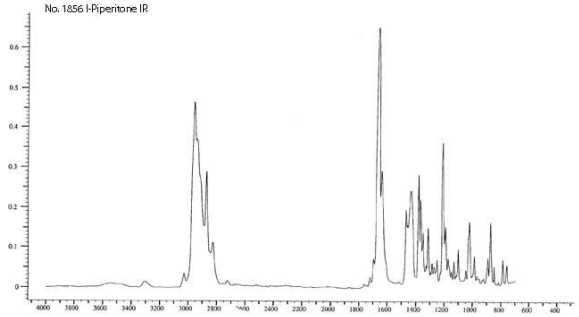
1855 l-Menthyl (R,S)-3-hydroxybutyrate (IR)



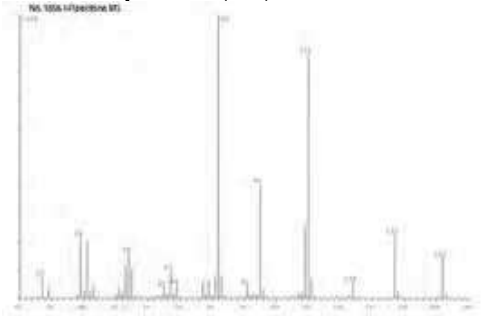
1856 l-Piperitone (1H-NMR)



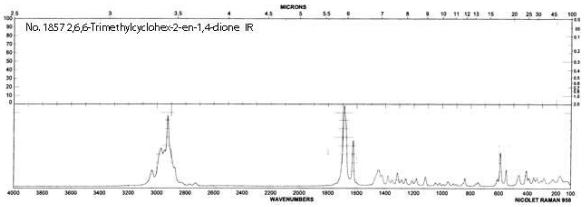
1856 l-Piperitone (IR)



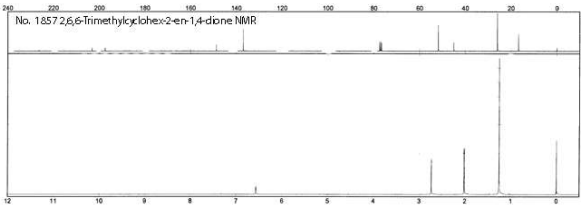
1856 l-Piperitone (MS)



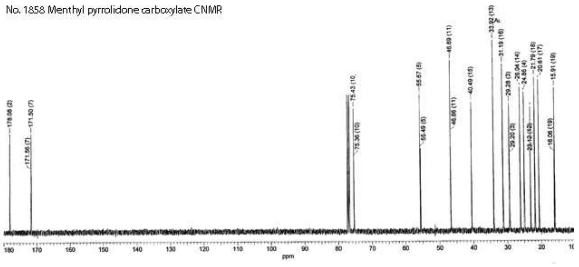
1857 2,6,6-Trimethylcyclohex-2-ene-1,4-dione (IR)



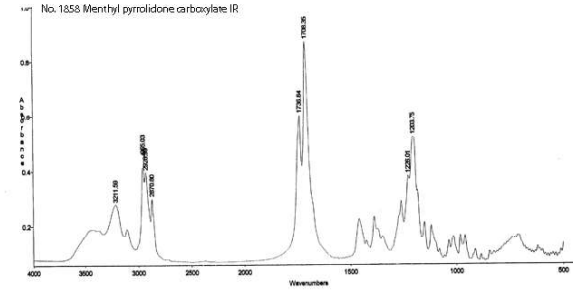
1857 2,6,6-Trimethylcyclohex-2-ene-1,4-dione (NMR)



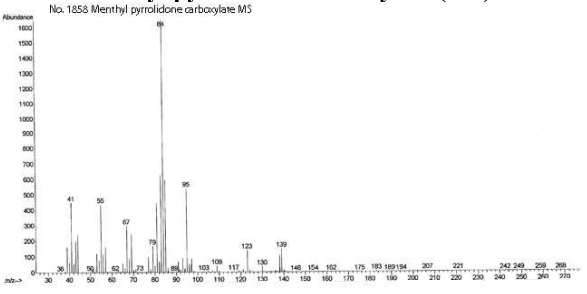
1858 Menthyl pyrrolidone carboxylate (13C-NMR)



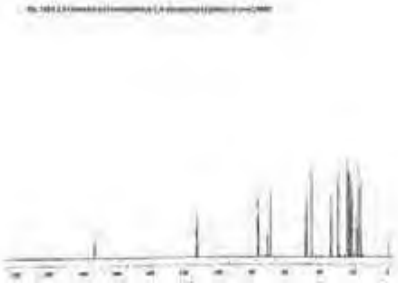
1858 Menthyl pyrrolidone carboxylate (IR)



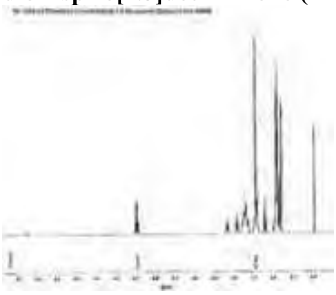
1858 Menthyl pyrrolidone carboxylate (MS)



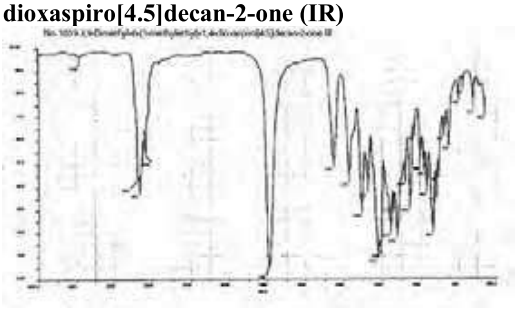
1859 3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one (13C-NMR)



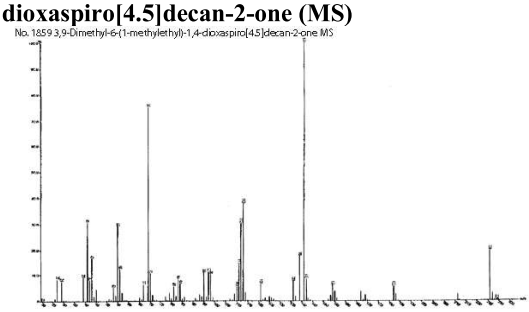
1859 3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one (1H-NMR)



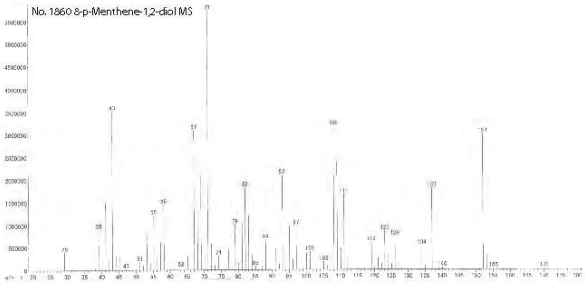
1859 3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one (IR)



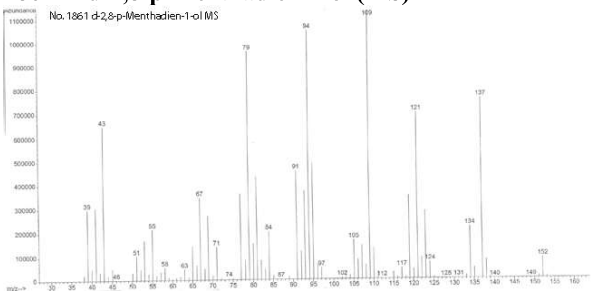
1859 3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one (MS)



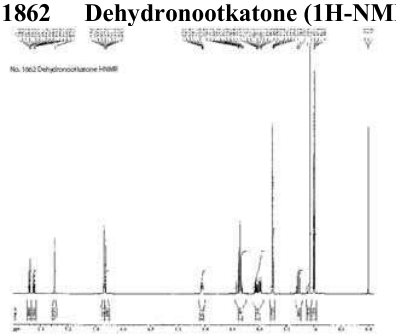
1860 8-p-Menthene-1,2-diol (MS)



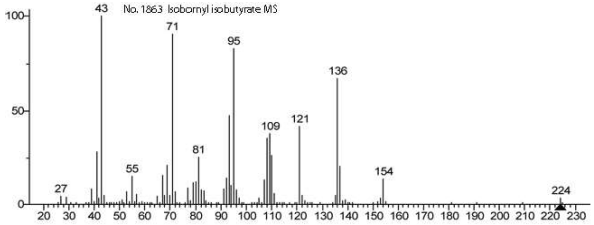
1861 d-2,8-p-Menthadien-1-ol (MS)



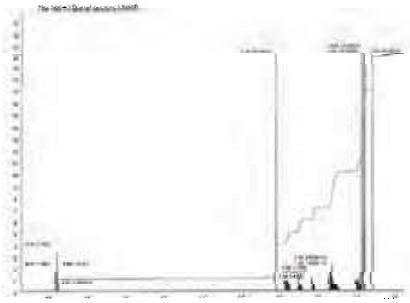
1862 Dehydronootkatone (1H-NMR)



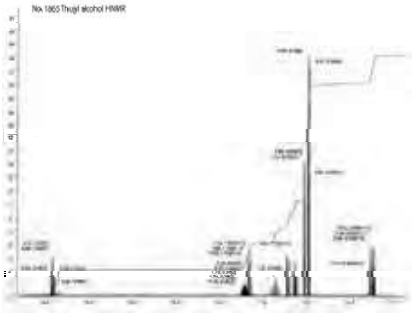
1863 Isobornyl isobutyrate (MS)



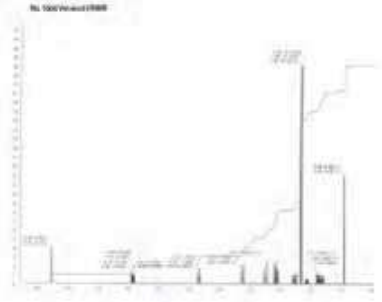
1864 l-Bornyl acetate (1H-NMR)



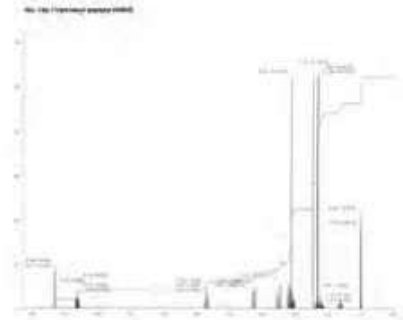
1865 Thujyl alcohol (1H-NMR)



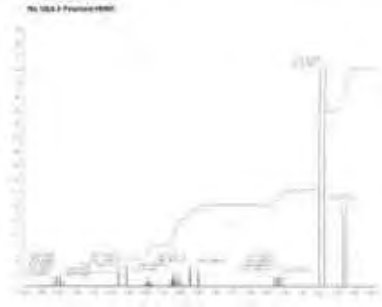
1866 Vetiverol (1H-NMR)



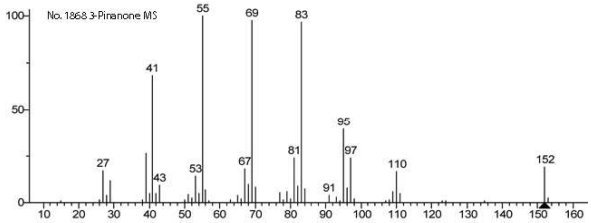
1867 Vetiveryl acetate (1H-NMR)



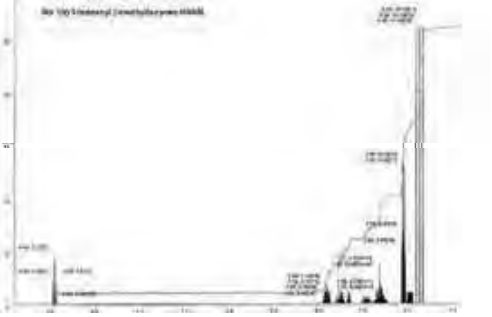
1868 3-Pinanone (1H-NMR)



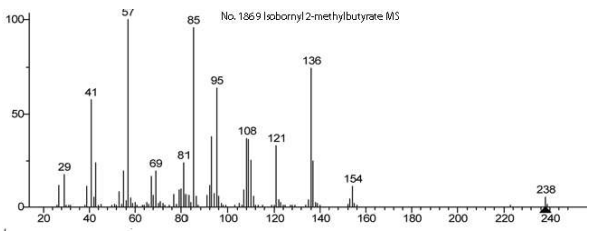
1868 3-Pinanone (MS)



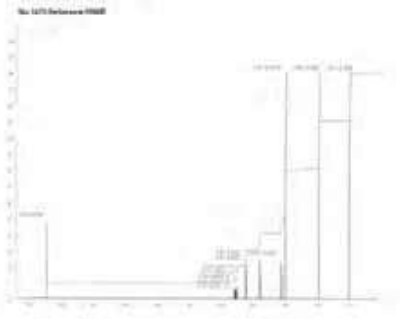
1869 Isobornyl 2-methylbutyrate (1H-NMR)



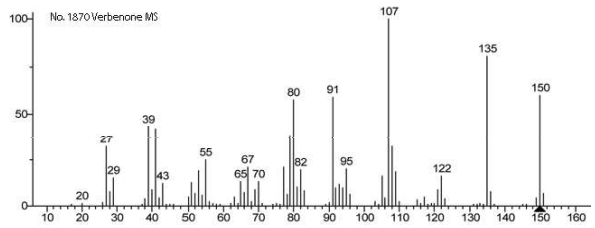
1869 Isobornyl 2-methylbutyrate (MS)



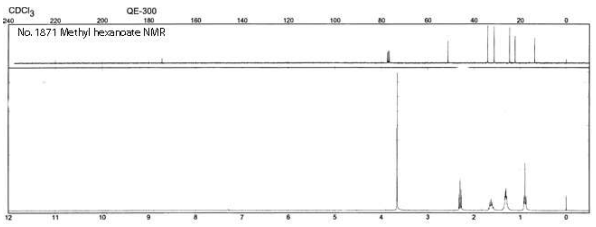
1870 Verbenone (1H-NMR)



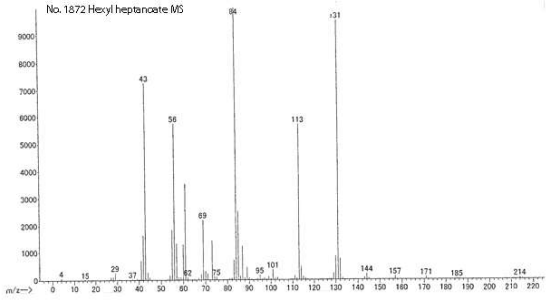
1870 Verbenone (MS)



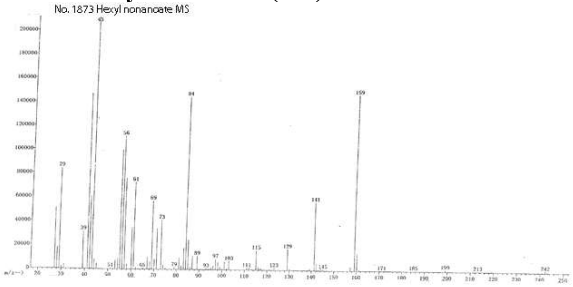
1871 Methyl hexanoate (NMR)



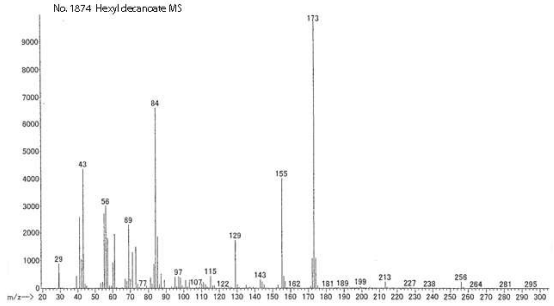
1872 Hexyl heptanoate (MS)



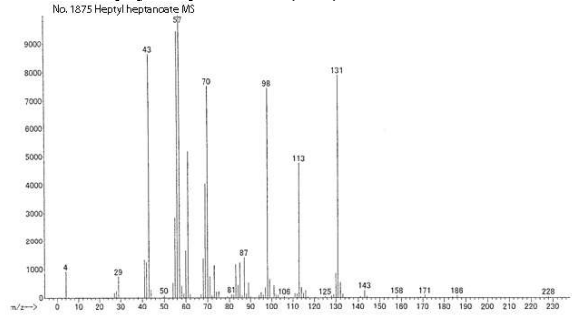
1873 Hexyl nonanoate (MS)



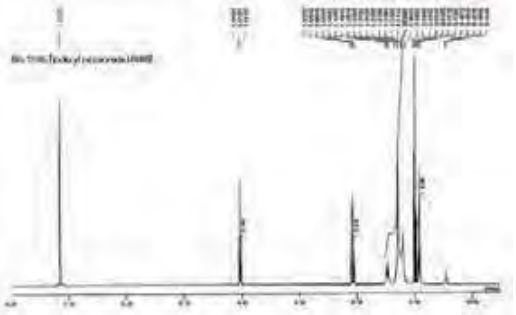
1874 Hexyl decanoate (MS)



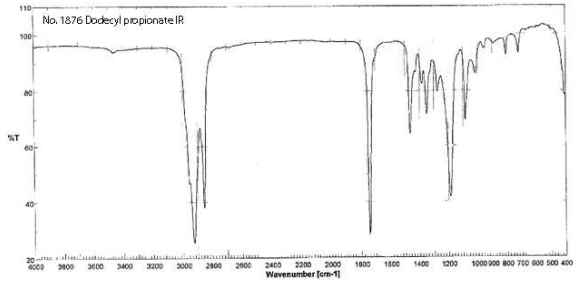
1875 Heptyl heptanoate (MS)



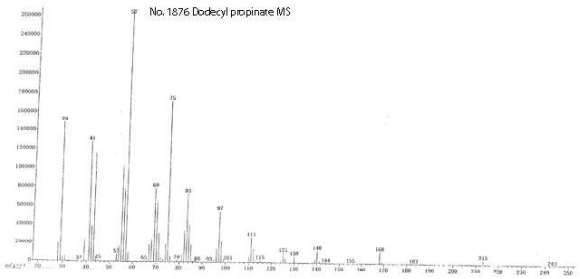
1876 Dodecyl propionate (1H-NMR)



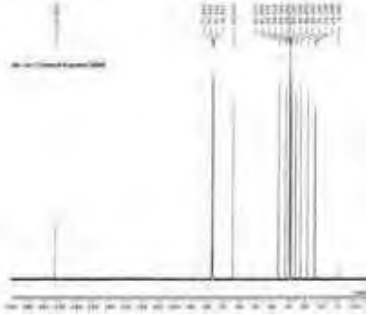
1876 Dodecyl propionate (IR)



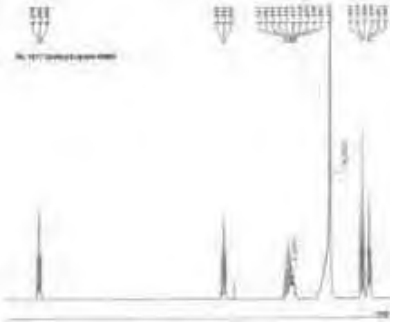
1876 Dodecyl propionate (MS)



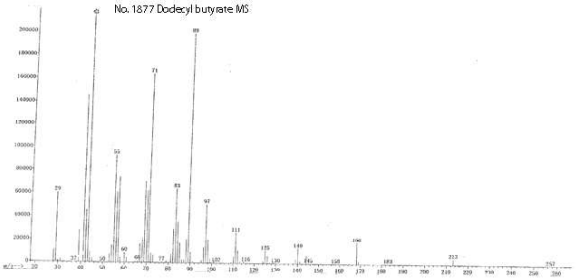
1877 Dodecyl butyrate (13C-NMR)



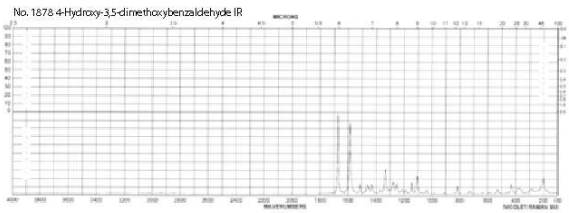
1877 Dodecyl butyrate (1H-NMR)



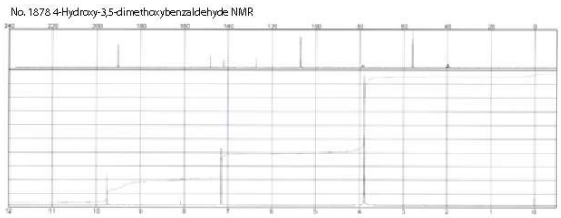
1877 Dodecyl butyrate (MS)



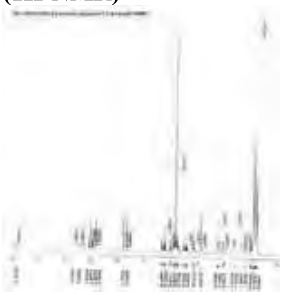
1878 4-Hydroxy-3,5-dimethoxy benzaldehyde (IR)



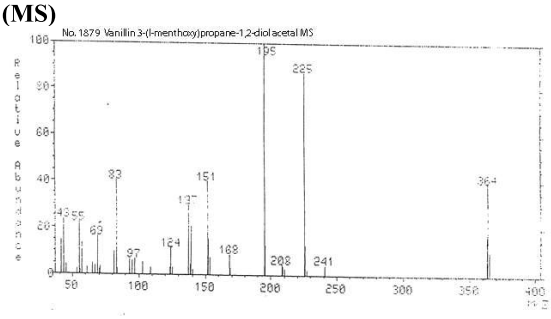
1878 4-Hydroxy-3,5-dimethoxy benzaldehyde (NMR)



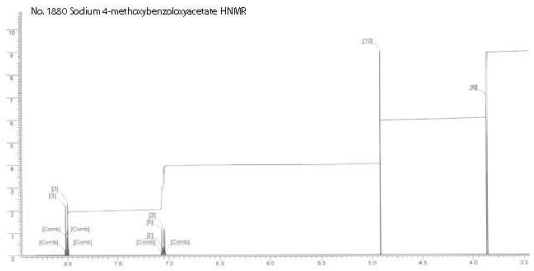
1879 Vanillin 3-(l-menthoxy)propane-1,2-diol acetal (1H-NMR)



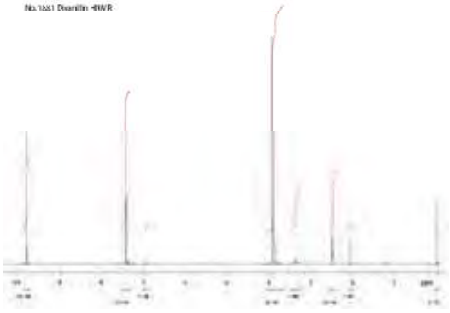
1879 Vanillin 3-(l-menthoxy)propane-1,2-diol acetal (MS)



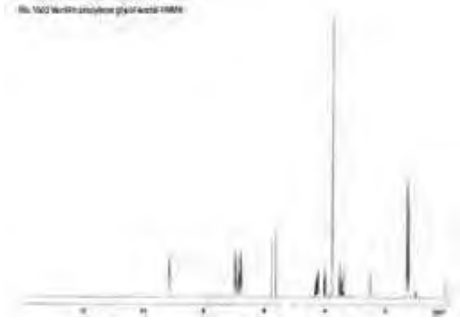
1880 Sodium 4-methoxybenzoyloxyacetate (1H-NMR)



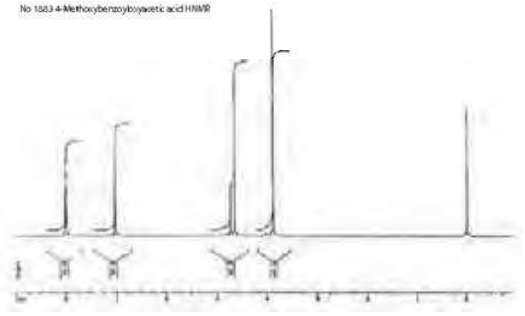
1881 Divanillin (1H-NMR)



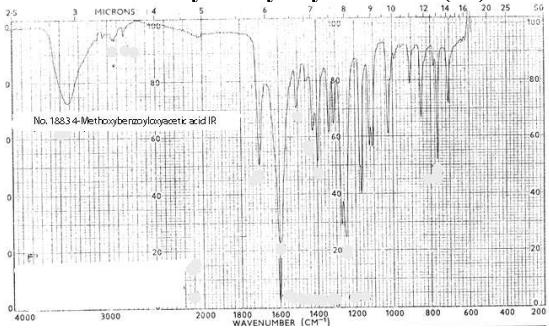
1882 Vanillin propylene glycol acetal (1H-NMR)



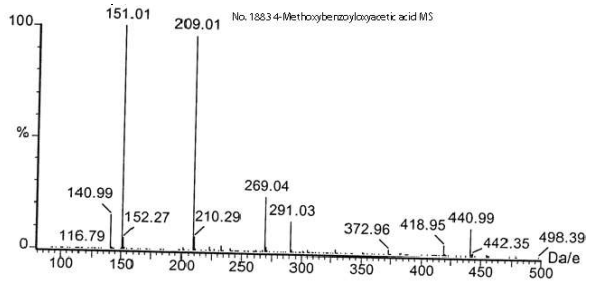
1883 4-Methoxybenzoyloxyacetic acid (1H-NMR)



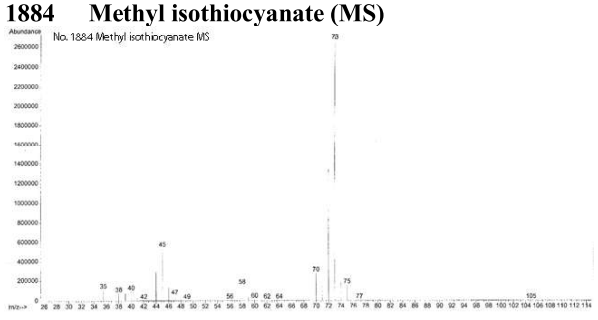
1883 4-Methoxybenzoyloxyacetic acid (IR)



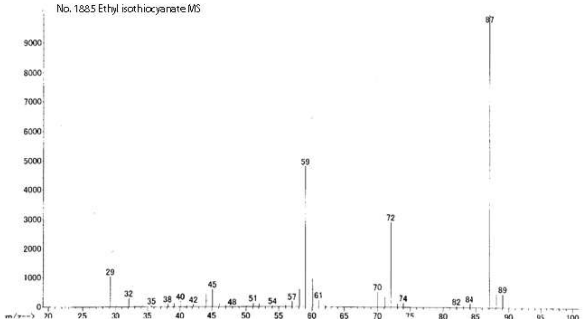
1883 4-Methoxybenzoyloxyacetic acid (MS)



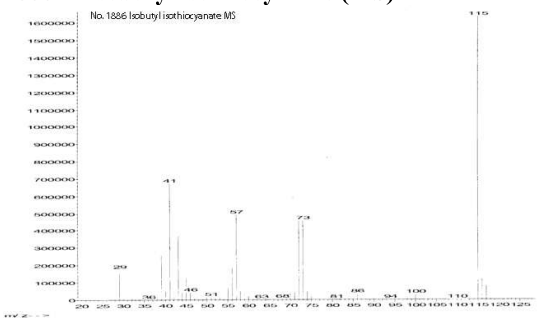
1884 Methyl isothiocyanate (MS)



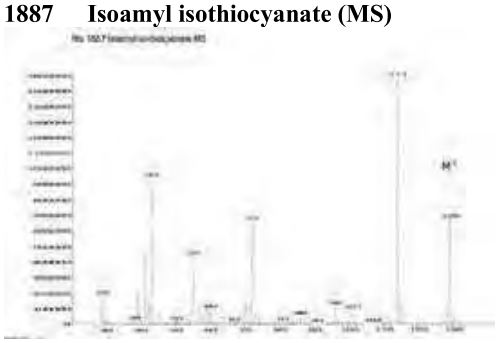
1885 Ethyl isothiocyanate (MS)



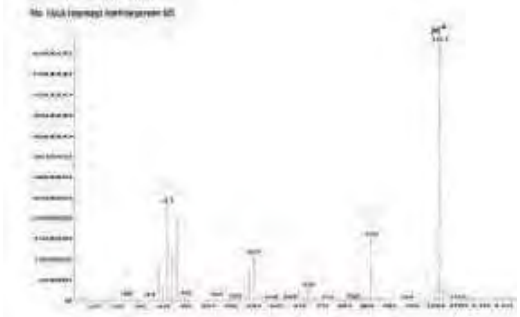
1886 Isobutyl isothiocyanate (MS)



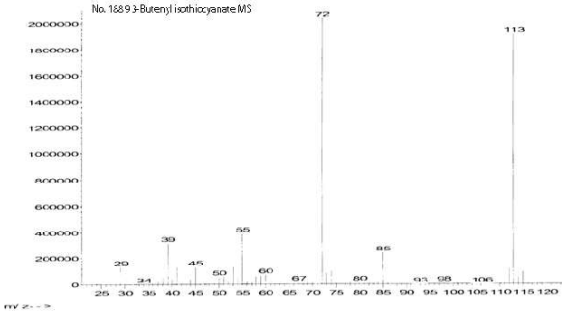
1887 Isoamyl isothiocyanate (MS)



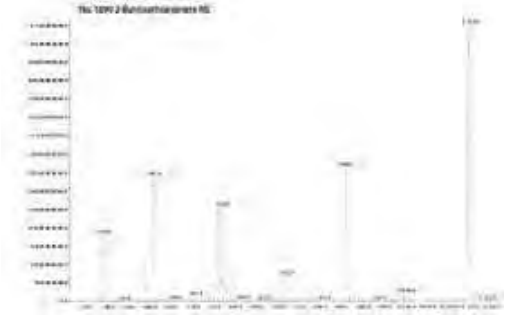
1888 Isopropyl isothiocyanate (MS)



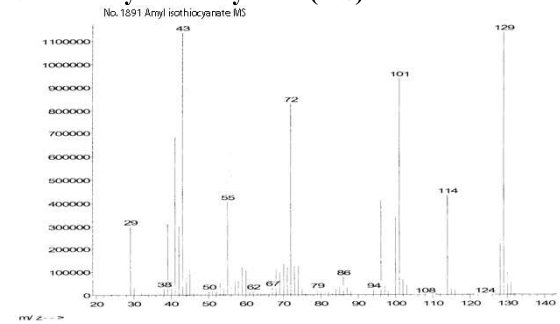
1889 3-Butenyl isothiocyanate (MS)



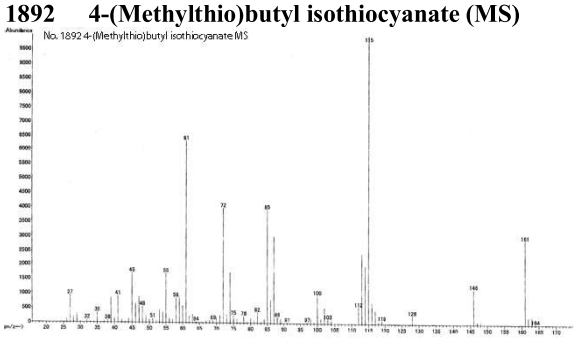
1890 2-Butyl isothiocyanate (MS)



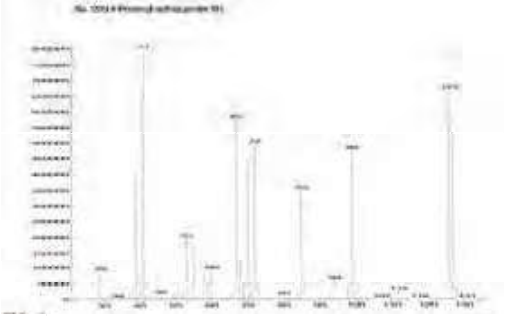
1891 Amyl isothiocyanate (MS)



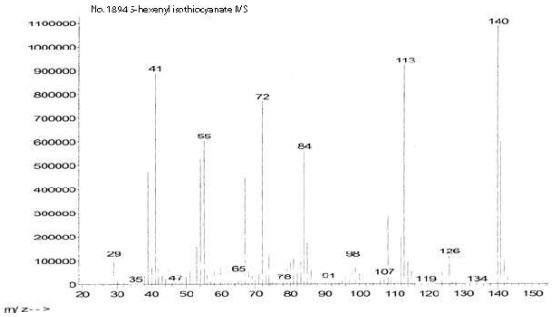
1892 4-(Methylthio)butyl isothiocyanate (MS)



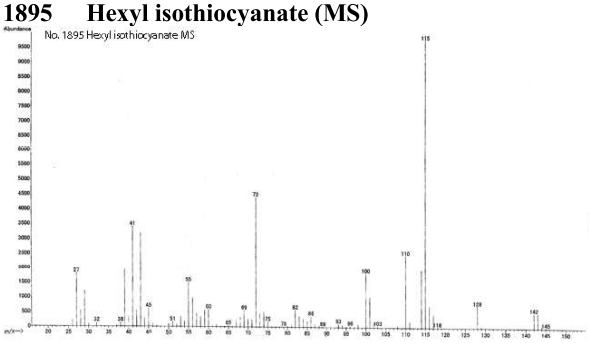
1893 4-Pentenyl isothiocyanate (MS)



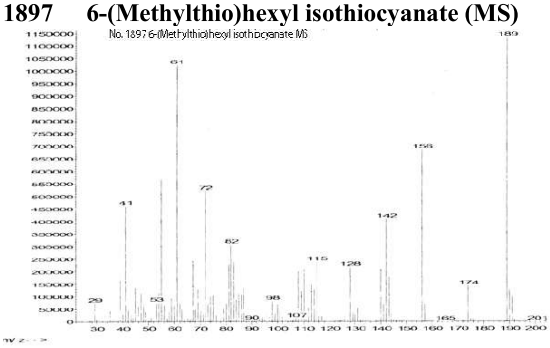
1894 5-Hexenyl isothiocyanate (MS)



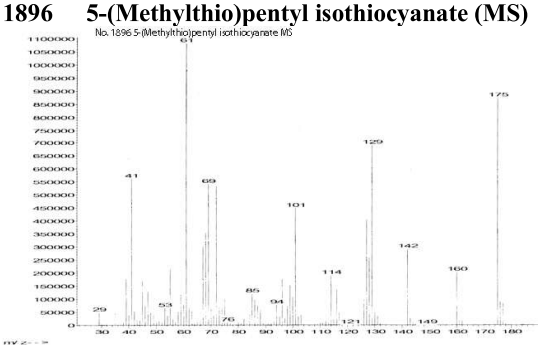
1895 Hexyl isothiocyanate (MS)



1897 6-(Methylthio)hexyl isothiocyanate (MS)



1896 5-(Methylthio)pentyl isothiocyanate (MS)



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ANNEX 1: SUMMARY OF RECOMMENDATIONS FROM THE 69TH JECFA

Toxicological recommendations and information on specifications

1. Food additives and ingredients evaluated toxicologically or assessed for dietary exposure

Food additive	Specifications[a]	Acceptable daily intake (ADI) and other toxicological recommendations
Asparaginase from *Aspergillus niger* expressed in *A. niger*	N	**ADI "not specified"[b]** when used in the applications specified and in accordance with good manufacturing practice.
Ethyl lauroyl arginate	N	**ADI of 0–4 mg/kg bw for Ethyl-N$^{\alpha}$-lauroyl-L-arginate HCl** based on a NOAEL of 442 mg/kg bw per day in two reproductive toxicity studies and a safety factor of 100. The Committee noted that some of the estimates of high exposure (greater than 95th percentile) exceeded the ADI, but recognized that these estimates were highly conservative and that actual intakes were likely to be within the ADI.
Calcium lignosulfonate (40-65) The suffix (40-65) reflects the weight-average molecular weight range (40 000–65 000) to distinguish it from other calcium lignosulfonates in commerce	N	**ADI of 0–20 mg/kg bw** based on a NOEL of 2000 mg/kg bw per day from a 90-day toxicity study and a safety factor of 100. The maximum potential dietary exposure to calcium lignosulfonate (40–65) was low and not expected to exceed 7 mg/kg bw per day from use as a carrier of fat-soluble vitamins and carotenoids in food and supplements.
Paprika extract Since the source material and the manufacturing process differ for paprika preparations used as a spice and as a food colour, the name "paprika extract" was adopted for use as a food colour, leaving the term "paprika oleoresin" for use as a spice.	N,T	The Committee did **not allocate an ADI**. Concern was expressed as to whether the material tested in the 90-day and long-term studies was representative of all commercial production of paprika extract used as food colour. The fact that the material tested contained less than 0.01% capsaicin and the fact that the Committee did not receive adequate data to establish a limit for capsaicin in the specifications for paprika extract added to this concern. New tentative specifications were prepared, pending receipt of additional information on paprika extract used as food colour, including concentrations of capsaicin (to differentiate from materials used as flavours) and additional information about the composition of batches of extract produced by a variety of manufacturers.
Phospholipase C expressed in *Pichia pastoris*	N	**ADI "not specified"[b]** when used in the applications specified and in accordance with good manufacturing practice.

Food additive	Specifications[a]	Acceptable daily intake (ADI) and other toxicological recommendations
Phytosterols, phytostanols and their esters	N	**Group ADI of 0–40 mg/kg bw for phytosterols, phytostanols and their esters, expressed as the sum of phytosterols and phytostanols in their free form**, based on an overall NOAEL of 4200 mg/kg bw per day to which a safety factor of 100 was applied. The overall NOAEL was identified using the combined evidence from several studies of short-term (90 day) toxicity. The Committee considered the margin between this overall NOAEL and the lowest LOAEL from the 90 day toxicity studies of 9000 mg/kg bw per day as adequate for this overall NOAEL to be used as the basis for establishing an ADI. This conclusion is supported by the results of the available studies of reproductive toxicity, Based on available data the Committee concluded that dietary exposure to phytosterols and -stanols would typically be within the ADI.
Polydimethylsiloxane (PDMS)	R	**Temporary ADI of 0–0.8 mg/kg bw for PDMS,** based on the previous ADI and **applying an additional safety factor of 2.** The previously established ADI of 0–1.5 mg/kg bw was withdrawn. Results of studies to elucidate the mechanism and relevance of ocular toxicity observed in the submitted toxicology studies, as well as data on actual use levels in foods should be provided before the end of 2010. The temporary ADI applies to PDMS that meets the revised specifications prepared.
Steviol glycosides	R	**ADI of 0–4 mg/kg bw expressed as steviol**, based on a NOEL of 970 mg/kg bw per day from a long-term experimental study with stevioside (383 mg/kg bw per day expressed as steviol) and a safety factor of 100. The results of the new studies presented to the Committee showed no adverse effects of steviol glycosides when taken at doses of about 4 mg/kg bw per day, expressed as steviol, for up to 16 weeks by individuals with type 2 diabetes mellitus and individuals with normal or low-normal blood pressure for 4 weeks. Some estimates of high-percentile dietary exposure to steviol glycosides exceeded the ADI, particularly when assuming complete replacement of caloric sweeteners with steviol glycosides. The Committee recognized that these estimates were highly conservative and that actual intakes were likely to be within the ADI.
Sulfites Dietary exposure assessment		The main contributors to total dietary exposure to sulfites differ between countries owing to differing patterns of use of sulfites in foods and of consumption of foods to which sulfites may be added. Thus dried fruit, sausages and nonalcoholic beverages were the main contributors of sulfites in some countries, while in other countries these foods are generally produced without the use of sulfites. In countries where wine is regularly consumed, it was one of the main contributors to dietary exposure in adults. Dietary exposure in high regular consumers of wine (97.5th percentile) was shown to exceed the ADI for sulfites (0-0.7 mg/kg bw) based either on MLs in Codex GSFA, on MLs in national legislation or on the average concentration determined analytically (about 100 mg/l).

		In children and teenagers, a significant contribution to mean exposure to sulfites could come from fruit juices and soft drinks (including cordial), sausages, various forms of processed potatoes, dried fruit and nuts. Other significant contributions to dietary exposure in the adult population come from dried fruit, sausages and beer. The Committee provided recommendation on further relevant actions to be considered by countries and the Codex Alimentarius Commission (see Annex 2).

[a] N: new specifications prepared; R: existing specifications revised; S: existing specifications maintained; T: tentative specifications.

[b] ADI 'not specified' is used to refer to a food substance of very low toxicity which, on the basis of the available data (chemical, biochemical, toxicological and other) and the total dietary intake of the substance arising from its use at the levels necessary to achieve the desired effects and from its acceptable background levels in food, does not, in the opinion of the Committee, represent a hazard to health. For that reason, and for the reasons stated in the individual evaluations, the establishment of an ADI expressed in numerical form is not deemed necessary. An additive meeting this criterion must be used within the bounds of good manufacturing practice, i.e. it should be technologically efficacious and should be used at the lowest level necessary to achieve this effect, it should not conceal food of inferior quality or adulterated food, and it should not create a nutritional imbalance.

2. Food additives, including flavouring agents, considered for specifications only

Food Additive	Specifications[a]
Canthaxanthin	R
Carob bean gum and carob bean gum (clarified)	R
Chlorophyllin, copper complexes sodium and potassium salts	R
Carbohydrase from *Aspergillus niger var.*	W
Estragole	W
Fast Green FCF	R
Guar gum and guar gum (clarified)	R
Iron oxides	R
Isomalt	R
Monomagnesium phosphate	N
Patent Blue V	R
Sunset Yellow FCF	R
Trisodium diphosphate	N

[a] N: New specifications prepared; R: Existing specifications revised; T: tentative specifications; W: Existing specifications withdrawn.

3. Flavouring agents

3.1. Flavourings evaluated by the Procedure for the Safety Evaluation of Flavouring Agents

3.1.1 Aliphatic, linear α,β-unsaturated aldehydes, acids and related alcohols, acetals and esters

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural Class I			
(Z)-2-Penten-1-ol	1793	N	No safety concern
(E)-2-Decen-1-ol	1794	N	No safety concern
(Z)-Pent-2-enyl hexanoate	1795	N	No safety concern
(E)-2-Hexenyl octanoate	1796	N	No safety concern
trans-2-Hexenyl 2-methylbutyrate	1797	N	No safety concern
Hept-trans-2-en-1-yl acetate	1798	N	No safety concern
(E,Z)-Hept-2-en-1-yl isovalerate	1799	N	No safety concern
trans-2-Hexenal glyceryl acetal	1800	N	No safety concern
trans-2-Hexenal propylene glycol acetal	1801	N	No safety concern
cis- and trans-1-Methoxy-1-decene	1802	N	No safety concern
(E)-Tetradec-2-enal	1803	N	No safety concern
(E)-2-Pentenoic acid	1804	N	No safety concern
(E)-2-Octenoic acid	1805	N	No safety concern
Ethyl trans-2-butenoate	1806	N	No safety concern
Hexyl 2-butenoate	1807	N	No safety concern
Ethyl trans-2-hexenoate	1808	N	No safety concern
(E,Z)-Methyl 2-hexenoate	1809	N	No safety concern
Hexyl trans-2-hexenoate	1810	N	No safety concern
Methyl trans-2-octenoate	1811	N	No safety concern
Ethyl trans-2-octenoate	1812	N	No safety concern
(E,Z)-Methyl 2-nonenoate	1813	N	No safety concern
Ethyl trans-2-decenoate	1814	N	No safety concern

[a]N: new specifications prepared

3.1.2 Aliphatic branched-chain saturated and unsaturated alcohols, aldehydes, acids, and related esters

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural class I			
Ethyl (E)-2-methyl-2-pentenoate	1815	N	No safety concern
2-Methylbutyl 3-methyl-2-butenoate	1816	N	No safety concern
(+/-)(E,Z)-5-(2,2-Dimethylcyclopropyl)-3-methyl-2-pentenal	1817	N	No safety concern
(E,Z)-4-Methylpent-2-enoic acid	1818	N	No safety concern
(+/-)-4-Ethyloctanal	1819	N	No safety concern
(E)-Geranyl 2-methylbutyrate	1820	N	No safety concern
(E)-Geranyl valerate	1821	N	No safety concern
(E)-Geranyl tiglate	1822	N	No safety concern
(E)-Citronellyl 2-methylbut-2-enoate	1823	N	No safety concern
(E)-Ethyl tiglate	1824	N	No safety concern
(E,Z)-Geranic acid	1825	N	No safety concern
Prenyl formate	1826	N	No safety concern
Prenyl acetate	1827	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Prenyl isobutyrate	1828	N	No safety concern
Prenyl caproate	1829	N	No safety concern
(+/-)-Dihydrofarnesol	1830	N	No safety concern
(E,Z)-3,7,11-Trimethyldodeca-2,6,10-trienyl acetate	1831	N	No safety concern
(E,Z)-Phytol	1832	N	No safety concern
(E,Z)-Phytyl acetate	1833	N	No safety concern
Structural class II			
Methyl 2-methyl-2-propenoate	1834	N	No safety concern

[a]N: new specifications prepared

3.1.3 Aliphatic secondary alcohols, ketones and related esters

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural class I			
Isopropenyl acetate	1835	N	No safety concern
1-Octen-3-yl acetate	1836	N	No safety concern
1-Octen-3-yl butyrate	1837	N	No safety concern
6-Methyl-5-hepten-2-yl acetate	1838	N	No safety concern
3-(Hydroxymethyl)-2-octanone	1839	N	No safety concern
(+/-)-[R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one	1840	N	No safety concern
(+/-)-cis- and trans-4,8-Dimethyl-3,7-nonadien-2-ol	1841	N	No safety concern
2,4-Dimethyl-4-nonanol	1850	N	No safety concern
Structural class II			
(+/-)-1-Hepten-3-ol	1842	N	No safety concern
(E, Z)-4-Octen-3-one	1843	N	No safety concern
(E)-2-Nonen-4-one	1844	N	No safety concern
(E)-5-Nonen-2-one	1845	N	No safety concern
(Z)-3-Hexenyl 2-oxopropionate	1846	N	No safety concern
(+/-)-cis- and trans-4,8-Dimethyl-3,7-nonadien-2-yl acetate	1847	N	No safety concern
(E)-1,5-Octadien-3-one	1848	N	No safety concern
10-Undecen-2-one	1849	N	No safety concern
8-Nonen-2-one	1851	N	No safety concern

[a]N: new specifications prepared.

3.1.4 Substances structurally related to menthol

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural Class I			
Menthyl valerate	1852	N	No safety concern
2-(l-Menthoxy)ethanol	1853	N	No safety concern
l-Menthyl acetoacetate	1854	N	No safety concern
l-Menthyl (R,S)-3-hydroxybutyrate	1855	N	No safety concern
8-p-Menthene-1,2-diol	1860	N	No safety concern
Structural Class II			
l-Piperitone	1856	N	No safety concern
2,6,6-Trimethylcyclohex-2-ene-1,4-dione	1857	N	No safety concern
Menthyl pyrrolidone carboxylate	1858	N	No safety concern
3,9-Dimethyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decan-2-one	1859	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
d-2,8-p-Menthadien-1-ol	1861	N	No safety concern

[a]N: new specifications prepared.

3.1.5 Monocyclic and bicyclic secondary alcohols, ketones and related esters

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural Class I			
Dehydronootkatone	1862	N	No safety concern
Isobornyl isobutyrate	1863	N	No safety concern
l-Bornyl acetate	1864	N	No safety concern
Thujyl alcohol	1865	N	No safety concern
Structural class II			
Vetiverol	1866	N	No safety concern
Vetiveryl acetate	1867	N	No safety concern
3-Pinanone	1868	N	No safety concern
Isobornyl 2-methylbutyrate	1869	N	No safety concern
Verbenone	1870	N	No safety concern

[a]N: new specifications prepared.

3.1.6 Aliphatic acyclic primary alcohols with aliphatic linear saturated carboxylic acids

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural class I			
Methyl hexanoate	1871	N	No safety concern
Hexyl heptanoate	1872	N	No safety concern
Hexyl nonanoate	1873	N	No safety concern
Hexyl decanoate	1874	N	No safety concern
Heptyl heptanoate	1875	N	No safety concern
Dodecyl propionate	1876	N	No safety concern
Dodecyl butyrate	1877	N	No safety concern

[a]N: new specifications prepared.

3.1.7 Hydroxy- and alkoxy- substituted benzyl derivatives

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural class I			
4-Hydroxy-3,5-dimethoxy benzaldehyde	1878	N	No safety concern
Vanillin 3-(l-menthoxy)propane-1,2-diol acetal	1879	N	No safety concern
Sodium 4-methoxybenzoyloxyacetate	1880	N	No safety concern
Vanillin propylene glycol acetal	1882	N	No safety concern
4-Methoxybenzoyloxyacetic acid	1883	N	No safety concern
Structural class III			
Divanillin	1881	N	No safety concern

[a]N: new specifications prepared.

3.1.8 Miscellaneous nitrogen-containing substances

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Structural class II			
Methyl isothiocyanate	1884	N	No safety concern
Ethyl isothiocyanate	1885	N	No safety concern
Isobutyl isothiocyanate	1886	N	No safety concern
Isoamyl isothiocyanate	1887	N	No safety concern
Isopropyl isothiocyanate	1888	N	No safety concern
3-Butenyl isothiocyanate	1889	N	No safety concern
2-Butyl isothiocyanate	1890	N	No safety concern
4-(Methylthio)butyl isothiocyanate	1892	N	No safety concern
4-Pentenyl isothiocyanate	1893	N	No safety concern
5-Hexenyl isothiocyanate	1894	N	No safety concern
5-(Methylthio)pentyl isothiocyanate	1896	N	No safety concern
6-(Methylthio)hexyl isothiocyanate	1897	N	No safety concern
Structural class III			
Amyl isothiocyanate	1891	N	No safety concern
Hexyl isothiocyanate	1895	N	No safety concern

[a]N: new specifications prepared.

3.1.9 Furan-substituted aliphatic hydrocarbons, alcohols, aldehydes, ketones, carboxylic acids and related esters, sulfides, disulfides and ethers

The Committee concluded that the Procedure could not be applied to this group, because of the unresolved toxicological concerns. Studies that would assist in the safety evaluation include investigations of the influence of the nature and position of ring substitution on metabolism and on covalent binding to macromolecules. Depending on the findings, additional studies might include assays related to the mutagenic and carcinogenic potential of representative members of this group.

Flavouring agent	JECFA No.	Specifications[a]
Structural Class II		
2-Methylfuran	1487	S
2,5-Dimethylfuran	1488	S
2-Ethylfuran	1489	S
2-Butylfuran	1490	S
2-Pentylfuran	1491	S
2-Heptylfuran	1492	S
2-Decylfuran	1493	S
3-Methyl-2-(3-methylbut-2-enyl)-furan	1494	S
3-(2-Furyl)acrolein	1497	S
3-(5-Methyl-2-furyl)prop-2-enal	1499	S
2-Furyl methyl ketone	1503	S
2-Acetyl-5-methylfuran	1504	S
2-Acetyl-3,5-dimethylfuran	1505	S
2-Butyrylfuran	1507	S
(2-Furyl)-2-propanone	1508	S
2-Pentanoylfuran	1509	S
1-(2-Furyl)butan-3-one	1510	S
4-(2-Furyl)-3-buten-2-one	1511	S
Ethyl 3-(2-furyl)propanoate	1513	S
Isobutyl 3-(2-furan)propionate	1514	S
Isoamyl 3-(2-furan)propionate	1515	S

Flavouring agent	JECFA No.	Specifications[a]
Isoamyl 4-(2-furan)butyrate	1516	S
Phenethyl 2-furoate	1517	S
Furfuryl methyl ether	1520	S
Ethyl furfuryl ether	1521	S
Difurfuryl ether	1522	S
2,5-Dimethyl-3-furanthiol acetate	1523	S
Furfuryl 2-methyl-3-furyl disulfide	1524	S
3-[(2-Methyl-3-furyl)thio]-2-butanone	1525	S
O-Ethyl S-(2-furylmethyl)thiocarbonate	1526	S
Structural Class III		
2,3-Dimethylbenzofuran	1495	S
2,4-Difurfurylfuran	1496	S
2-Methyl-3(2-furyl)acrolein	1498	S
3-(5-Methyl-2-furyl)-butanal	1500	S
2-Furfurylidene-butyraldehyde	1501	S
2-Phenyl-3-(2-furyl)prop-2-enal	1502	S
3-Acetyl-2,5-dimethylfuran	1506	S
Pentyl 2-furyl ketone	1512	S
Propyl 2-furanacrylate	1518	S
2,5-Dimethyl-3-oxo-(2H)-fur-4-yl butyrate	1519	S

[a]S: Specifications maintained. The specifications monographs will include a statement that the safety evaluation has not been completed.

3.1.10 Alkoxy-substituted allylbenzenes present in foods, essential oils, and used as flavouring agents

The Committee concluded that the data reviewed on the six alkoxy-substituted allylbenzenes provide evidence of toxicity and carcinogenicity to rodents given high doses for several of these substances. A mechanistic understanding of these effects and their implications for human risk have yet to be fully explored, and will have a significant impact on the assessment of health risks from alkoxy-substituted allylbenzenes at the concentrations at which they occur in food.

Flavouring agent	No.	Specifications[a]
Apiole	1787	N
Elemicin	1788	N
Estragole	1789	N
Methyl eugenol	1790	N
Myristicin	1791	N
Safrole	1792	N

[a]N: new specifications prepared. The specifications monographs will include a statement that the safety evaluation has not been completed.

3.2 Re-evaluation of safety of certain flavourings

At the fifty-ninth, sixty-first, sixty-third and sixty-fifth meetings of the Committee, only “anticipated” annual volumes of productions were provided for some flavouring agents and used in the MSDI calculation. These volumes were used for expedience in completing a safety evaluation, but the conclusions of the Committee were made conditional pending the submission of actual poundage data.

Actual production volumes were subsequently submitted for all 143 requested flavouring agents and were evaluated by the Committee. The two flavouring substances requiring a re-evaluation were No. 1414, l-monomenthyl glutarate and No. 1595, 2-isopropyl-N,2,3-trimethylbutyramide.

The Committee concluded that the Procedure could not be applied to 2-isopropyl-*N*,2,3-trimethylbutyramide, because of evidence of clastogenicity in the presence, but not in the absence, of metabolic activation.

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
Ethyl cyclohexanecarboxylate	963	S	No safety concern
10-Hydroxymethylene-2-pinene	986	S	No safety concern
2,5-Dimethyl-3-furanthiol	1063	S	No safety concern
Propyl 2-methyl-3-furyl disulfide	1065	S	No safety concern
Bis(2-methyl-3-furyl) disulfide	1066	S	No safety concern
Bis(2,5-dimethyl-3-furyl) disulfide	1067	S	No safety concern
Bis(2-methyl-3-furyl) tetrasulfide	1068	S	No safety concern
2,5-Dimethyl-3-furan thioisovalerate	1070	S	No safety concern
Furfuryl isopropyl sulfide	1077	S	No safety concern
2-Methyl-3,5- or 6-(furfurylthio)pyrazine	1082	S	No safety concern
3-[(2-Methyl-3-furyl)thio]-4-heptanone	1085	S	No safety concern
2,6-Dimethyl-3-[(2-methyl-3-furyl)thio]-4-heptanone	1086	S	No safety concern
4-[(2-Methyl-3-furyl)thio]-5-nonanone	1087	S	No safety concern
2-Methyl-3-thioacetoxy-4,5-dihydrofuran	1089	S	No safety concern
4-Hydroxy-4-methyl-5-hexenoic acid gamma-lactone	1157	S	No safety concern
(+/-) 3-Methyl-gamma-decalactone	1158	S	No safety concern
4-Hydroxy-4-methyl-7-cis-decenoic acid gamma-lactone	1159	S	No safety concern
Tuberose lactone	1160	S	No safety concern
Dihydromintlactone	1161	S	No safety concern
Mintlactone	1162	S	No safety concern
Dehydromenthofurolactone	1163	S	No safety concern
(+/-)-(2,6,6-Trimethyl-2-hydroxycyclohexylidene) acetic acid gamma-lactone	1164	S	No safety concern
2-(4-Methyl-2-hydroxyphenyl)propionic acid gamma-lactone	1167	S	No safety concern
2,4-Hexadien-1-ol	1174	S	No safety concern
(E,E)-2,4-Hexadienoic acid	1176	S	No safety concern
(E,E)-2,4-Octadien-1-ol	1180	S	No safety concern
2,4-Nonadien-1-ol	1183	S	No safety concern
(E,Z)-2,6-Nonadien-1-ol acetate	1188	S	No safety concern
(E,E)-2,4-Decadien-1-ol	1189	S	No safety concern
Methyl (E)-2-(Z)-4-decadienoate	1191	S	No safety concern
Ethyl 2,4,7-decatrienoate	1193	S	No safety concern
(+/-) 2-Methyl-1-butanol	1199	S	No safety concern
2-Methyl-2-octenal	1217	S	No safety concern
4-Ethyloctanoic acid	1218	S	No safety concern
8-Ocimenyl acetate	1226	S	No safety concern
3,7,11-Trimethyl-2,6,10-dodecatrienal	1228	S	No safety concern
12-Methyltridecanal	1229	S	No safety concern
1-Ethoxy-3-methyl-2-butene	1232	S	No safety concern
2,2,6-Trimethyl-6-vinyltetrahydropyran	1236	S	No safety concern
Cycloionone	1239	S	No safety concern
2,4-Dimethylanisole	1245	S	No safety concern
1,2-Dimethoxybenzene	1248	S	No safety concern
4-Propenyl-2,6-dimethoxyphenol	1265	S	No safety concern
erythro and threo-Mercapto-2-methylbutan-1-ol	1289	S	No safety concern
(±)2-Mercapto-2-methylpentan-1-ol	1290	S	No safety concern
3-Mercapto-2-methylpentanal	1292	S	No safety concern
4-Mercapto-4-methyl-2-pentanone	1293	S	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
spiro[2,4-Dithia-1-methyl-8-oxabicyclo(3.3.0)octane-3,3'-(1'-oxa-2'-methyl)-cyclopentane]	1296	S	No safety concern
2,3,5-Trithiahexane	1299	S	No safety concern
Diisopropyl trisulfide	1300	S	No safety concern
2-(2-Methylpropyl)pyridine	1311	S	No safety concern
2-Propionylpyrrole	1319	S	No safety concern
2-Propylpyridine	1322	S	No safety concern
4-Methylbiphenyl	1334	S	No safety concern
delta-3-Carene	1342	S	No safety concern
Farnesene (alpha and beta)	1343	S	No safety concern
1-Methyl-1,3-cyclohexadiene	1344	S	No safety concern
trans-2-Octen-1-yl acetate	1367	S	No safety concern
trans-2-Octen-1-yl butanoate	1368	S	No safety concern
cis-2-Nonen-1-ol	1369	S	No safety concern
(E)-2-Octen-1-ol	1370	S	No safety concern
(E)-2-Butenoic acid	1371	S	No safety concern
(E)-2-Decenoic acid	1372	S	No safety concern
(E)-2-Heptenoic acid	1373	S	No safety concern
(Z)-2-Hexen-1-ol	1374	S	No safety concern
trans-2-Hexenyl butyrate	1375	S	No safety concern
(E)-2-Hexenyl formate	1376	S	No safety concern
trans-2-Hexenyl isovalerate	1377	S	No safety concern
trans-2-Hexenyl propionate	1378	S	No safety concern
trans-2-Hexenyl pentanoate	1379	S	No safety concern
(E)-2-Nonenoic acid	1380	S	No safety concern
(E)-2-Hexenyl hexanoate	1381	S	No safety concern
(Z)-3- & (E)-2-Hexenyl propionate	1382	S	No safety concern
2-Undecen-1-ol	1384	S	No safety concern
Dihydronootkatone	1407	S	No safety concern
beta-Ionyl acetate	1409	S	No safety concern
alpha-Isomethylionyl acetate	1410	S	No safety concern
3-(l-Menthoxy)-2-methylpropane-1,2-diol	1411	S	No safety concern
Bornyl butyrate	1412	S	No safety concern
d,l-Menthol-(±)-propylene glycol carbonate	1413	S	No safety concern
l-Monomenthyl glutarate	1414	S	No safety concern
l-Menthyl methyl ether	1415	S	No safety concern
p-Menthane-3,8-diol	1416	S	No safety concern
Taurine	1435	S	No safety concern
L-Arginine	1438	S	No safety concern
L-Lysine	1439	S	No safety concern
Tetrahydrofurfuryl cinnamate	1447	S	No safety concern
(±)-2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propionaldehyde	1457	S	No safety concern
Ethyl 2-ethyl-3-phenylpropanoate	1475	S	No safety concern
2-Oxo-3-phenylpropionic acid and	1478	S	No safety concern
Sodium 2-Oxo-3-phenylpropionate	1479	S	No safety concern
2-Methyl-3-(1-oxopropoxy)-4H-pyran-4-one	1483	S	No safety concern
4-Allylphenol	1527	S	No safety concern
2-Methoxy-6-(2-propenyl)phenol	1528	S	No safety concern
Eugenyl isovalerate	1532	S	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusions based on current estimated intake
cis-3-Hexenyl anthranilate	1538	S	No safety concern
Citronellyl anthranilate	1539	S	No safety concern
Ethyl N-methylanthranilate	1546	S	No safety concern
Ethyl N-ethylanthranilate	1547	S	No safety concern
Isobutyl N-methylanthranilate	1548	S	No safety concern
Methyl N-formylanthranilate	1549	S	No safety concern
Methyl N-acetylanthranilate	1550	S	No safety concern
Methyl N,N-dimethylanthranilate	1551	S	No safety concern
N-Benzoylanthranilic acid	1552	S	No safety concern
Trimethyloxazole	1553	S	No safety concern
2,5-Dimethyl-4-ethyloxazole	1554	S	No safety concern
2-Ethyl-4,5-dimethyloxazole	1555	S	No safety concern
2-Isobutyl-4,5-dimethyloxazole	1556	S	No safety concern
2-Methyl-4,5-benzo-oxazole	1557	S	No safety concern
2,4-Dimethyl-3-oxazoline	1558	S	No safety concern
Butyl isothiocyanate	1561	S	No safety concern
Benzyl isothiocyanate	1562	S	No safety concern
Phenethyl isothiocyanate	1563	S	No safety concern
4,5-Dimethyl-2-propyloxazole	1569	S	No safety concern
4,5-Epoxy-(E)-2-decenal	1570	S	No safety concern
beta-Ionone epoxide	1571	S	No safety concern
Epoxyoxophorone	1573	S	No safety concern
Ethylamine	1579	S	No safety concern
Propylamine	1580	S	No safety concern
Isopropylamine	1581	S	No safety concern
Isobutylamine	1583	S	No safety concern
sec-Butylamine	1584	S	No safety concern
Pentylamine	1585	S	No safety concern
2-Methylbutylamine	1586	S	No safety concern
Hexylamine	1588	S	No safety concern
2-(4-Hydroxyphenyl)ethylamine	1590	S	No safety concern
1-Amino-2-propanol	1591	S	No safety concern
Butyramide	1593	S	No safety concern
1,6-Hexalactam	1594	S	No safety concern
2-Isopropyl-N,2,3-trimethylbutyramidee	1595	S	**Further information is needed**
N-Ethyl (E)-2,(Z)-6-nonadienamide	1596	S	No safety concern
N-Cyclopropyl (E)-2,(Z)-6-nonadienamide	1597	S	No safety concern
N-Isobutyl (E,E)-2,4-decadienamide	1598	S	No safety concern
(±)-N,N-Dimethyl menthyl succinamide	1602	S	No safety concern
1-Pyrroline	1603	S	No safety concern
2-Acetyl-1-pyrroline	1604	S	No safety concern
2-Propionylpyrroline	1605	S	No safety concern
Isopentylidene isopentylamine	1606	S	No safety concern
2-Methylpiperidine	1608	S	No safety concern
Triethylamine	1611	S	No safety concern
Tripropylamine	1612	S	No safety concern
N,N-Dimethylphenethylamine	1613	S	No safety concern
Trimethylamine oxide	1614	S	No safety concern
Piperazine	1615	S	No safety concern

ANNEX 2: RECOMMENDATIONS AND FURTHER INFORMATION REQUIRED

Paprika extract

Data on the composition and capsaicin content of batches of paprika extract for use as a colour produced by a variety of manufacturers. Information as to whether the material used in the toxicological tests submitted was representative of all the products in commerce. If not, additional toxicological data on representative material would be needed for the evaluation of paprika extract for use as a colour.

The Committee recommended that the specifications for paprika oleoresin be revised at a future meeting in order to allow the differentiation of paprika extract used as a colour from paprika oleoresin used as a flavour.

Polydimethylsiloxane

Results of studies to elucidate the mechanism and relevance of the ocular toxicity observed in the experimental studies and data on actual use levels in foods should be provided before the end of 2010.

Sulfites – dietary exposure assessment and maximum levels (MLs) in foods

Countries that have not yet done so could consider collecting data on the current use of sulfites in food and beverages available on their markets and investigating whether dietary exposure in some subpopulations exceeds the ADI. On the basis of this investigation, individual countries and the food industry could consider the possibility of taking one or more of the following measures to reduce dietary exposure to sulfites so that the ADI is not exceeded in the population:

(1) align national legislation with Codex MLs where these are lower;
(2) take action to effectively enforce national MLs;
(3) encourage research on alternative methods of preservation, particularly on applications in which the use of sulfites is responsible for a significant contribution;
(4) take action so that the use of sulfites is reduced in foods where safe alternative solutions are available.

Codex Alimentarius Commission codes of practices for certain groups of food commodities, such as fruit juice, dried fruit and processed meat, could be amended to include suggestions to help countries and the food industry in the implementation of a reduction of the use of sulfites in food.

Furan-substituted aliphatic hydrocarbons, alcohols, aldehydes, ketones, carboxylic acids and related esters, sulfides, disulfides and ethers (JECFA Nos, Structural Class II: 1487, 1488, 1489, 1490, 1491, 1492, 1493, 1494, 1497, 1499, 1503, 1504, 1505, 1507, 1508, 1509, 1510, 1511, 1513, 1514, 1515, 1516, 1517, 1520, 1521, 1522, 1523, 1524, 1525, 1526; Structural Class III: 1495, 1496, 1498, 1500, 1501, 1502, 1506, 1512, 1518, 1519)

The Committee concluded that the Procedure could not be applied to this group of flavouring agents, because of the unresolved toxicological concerns. Studies that would assist in the safety evaluation include investigations of the influence of the nature and position of ring substitution on metabolism and on covalent binding to macromolecules. Depending on the findings, additional studies might include assays related to the mutagenic and carcinogenic potential of representative members of this group of flavours.

Alkoxy-substituted allylbenzenes present in foods, essential oils, and used as flavouring agents (Apiole JECFA No. 1787, Elemicin No. 1788, Estragole No. 1789, Methyl eugenol No. 1790, Myristicin No 1791, Safrole No 1792)

There is evidence of toxicity and carcinogenicity to rodents given high doses for several of these substances. A mechanistic understanding of these effects and their implications for human risk have yet to be fully explored, and will have a significant impact on the assessment of health risks from alkoxy-

substituted allylbenzenes at the concentrations at which they occur in food. Further research is needed to assess the potential risk to human health from low-level dietary exposure to alkoxy-substituted allylbenzenes present in foods and essential oils and used as flavouring agents.

2-isopropyl-N,2,3-trimethylbutyramide (JECFA No. 1595)

The Committee concluded that the Procedure could not be applied to 2-isopropyl-N,2,3-trimethylbutyramide, because of because of evidence of clastogenicity in the presence, but not in the absence, of metabolic activation. Information that would assist in resolving the concerns would include data on the potential of this compound to form reactive metabolites and on whether clastogenicity is also expressed in vivo, as well as additional information on the effects found in the kidney (tubular nephrosis, tubular dilatation with granular casts and hyaline droplet formation) at relatively low doses.

CORRIGENDA

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS
FAO FOOD AND NUTRITION PAPER 52, Addendum 9, ROME, 2001.

Page 129, Flavouring agent **2-Ethyl-6-methyl pyrazine** (JECFA No. 769): The entry on Assay minium % is corrected to exclude the presence of the 2,3-isomer as follows: 95 (sum of 2,5- and 2,6-isomers).

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS
FAO FOOD AND NUTRITION PAPER 52, Addendum 11, ROME, 2003.

Page 120, the name of flavouring agent with JECFA No. 1290 is corrected to **(+/-)2-Mercapto-2-methylpentan-1-ol**.

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

Page 89, Flavouring agent **DL-(3-Amino-3-carboxypropyl)dimethylsulfonium chloride** (JECFA No. 1427: the Chemical Abstract Services number is corrected to 3493-12-7, to reflect the DL-form of the substance, and the missing letter l in sulfonium is added.

COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS
FAO FOOD AND NUTRITION PAPER 52, Addendum 13, ROME, 2005.

Page 59, Flavouring agent **2,5-Dimethyl-3-oxo-(2H)-fur-4-yl butyrate** (JECFA No. 1519): the entry on Secondary Components is modified to indicate the concentration ranges as follows: SC: 1-3% 4-Hydroxy-2,5-dimethyl-3(2H)-furanone and 1-3% Butyric acid

Page 59, Flavouring agent **Furfuryl 2-methyl-3-furyl disulfide** (JECFA No. 1524): the entry on Secondary Components is modified to indicate the concentration range as follows: SC: 6-7% Di-(2-methyl-3-furyl) disulfide.

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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 2006 (E)

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COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS

Joint FAO/WHO Expert Committee on Food Additives

69th meeting 2008

This document contains food additive specifications monographs, analytical methods and other information, prepared at the sixty-ninth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), which was held in Rome, Italy, from 17 to 26 June 2008. The specifications monographs provide information on the identity and purity of food additives used directly in foods or in food production. The main three objectives of these specifications are to identify the food additive that has been subjected to testing for safety, to ensure that the additive is of the quality required for use in food or in processing, and to reflect and encourage good manufacturing practice. This publication and other documents produced by JECFA contain information that is useful to all those who work with or are interested in food additives and their safe use in food.

