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meeting requested information to revise the existing tentative specifications, stating that the specifications would be withdrawn if no information was forthcoming.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specifications for estragole used as a food additive that were prepared by the Committee at its 26th meeting[3] were withdrawn, as no other uses of estragole other than as a flavouring agent were identified.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** 4,7-Dimethoxy-5-(2-propenyl)-1,3-benzodioxole *1-Allyl-2,5-dimethoxy-3,4-methylenedioxybenzene*	 523-80-8	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 Soluble	294	MS 95	1.536-1.538 1.124-1.135	Safety evaluation not completed	69th Full
1788	**Elemicin** 1,2,3-Trimethoxy-5-(2-propenyl)benzene *5-Allyl-1,2,3-trimethoxybenzene*	 487-11-6	C12H16O3 208.26	Colourless to pale straw coloured viscous liquid; Spice with floral notes	Practically insoluble to insoluble in water Soluble	246	MS 95	1.529-1.534 1.058-1.070	Safety evaluation not completed	69th Full
1789	**Estragole** 1-Methoxy-4(2-propenyl)-benzene *Methyl chavicol*	2411 04.011 140-67-0	C10H12O 148.21	Colourless to light yellow liquid; Anise-like aroma	Insoluble in water; soluble in alcohols Soluble	216	IR MS 95	1.519-1.524 0.960-0.968	Safety evaluation not completed	69th Full
1790	**Methyl eugenol** 1,2-Dimethoxy-4(2-propenyl)-benzene *1,2-Dimethoxy-4-allylbenzene*	2475 04.012 93-15-2	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 Soluble	249	IR MS 95	1.532-1.536 1.032-1.036	Safety evaluation not completed	69th Full
1791	**Myristicin** 4-Methoxy-6-(2-propenyl)-1,3-benzodioxole *5-Allyl-1-methoxy-2,3-(methylenedioxy)benzene*	 607-91-0	C11H12O3 192.21	Colourless oil; Warm balsamic-woody aroma	Practically insoluble to insoluble in water Soluble	250	MS 95	1.539-1.541 1.143-1.145	Safety evaluation not completed	69th Full
1792	**Safrole** 5-(2-Propenyl)-1,3-benzodioxole *4-Allyl-1,2-methylenedioxylbenzene*	 94-59-7	C10H10O2 162.19	Colourless to slightly yellow liquid; Sasafras aroma	Practically insoluble to insoluble in water Soluble	232-234	MS 95	1.537-1.540 1.095-1.099	Safety evaluation not completed	69th Full
1793	**(Z)-2-Penten-1-ol** 2-Penten-1-ol	4305 02.050 665 20273-24-9	C5H10O 86.13	Colourless liquid; Green diffusive aroma	Slightly soluble in water; soluble in non-polar solvents Soluble	140-141	MS 95	1.427-1.433 0.844-0.850		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
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 °C)	(+)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 °C)		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 °C) 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

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
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

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
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

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
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						

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
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

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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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		69th Full

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1878	**4-Hydroxy-3,5-dimethoxy benzaldehyde** 4-Hydroxy-3,5-dimethoxybenzaldehyde *Gallaldehyde 3,5-dimethyl ether*	4049 05.153 10340 134-96-3	C9H10O4 182.18	Very pale green needles; Alcoholic aroma	Insoluble in water Soluble	NA	NMR IR 98	NA NA	m.p. = 110-113 ºC	69th Full
1879	**Vanillin 3-(l-menthoxy)propane-1,2-diol acetal** 2-Methoxy-4-[4-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-1,3-dioxolan-2-yl]-phenol	3904 02.248 180964-47-0	C21H32O5 364.48	Colourless powder; Minty aroma with vanilla undertones	Slightly soluble in water; soluble in fats, non-polar solvents and acetone Soluble	NA	NMR MS 94	NA NA	m.p. = 78-80 ºC SC: Vanillin (2-3%)	69th Full
1880	**Sodium 4-methoxybenzoyloxyacetate** Benzoic acid, 4-methoxy-, carboxymethyl ester, sodium salt	4016b 17114-82-8	C10H9O5Na 232.17	White solid; Cooked brown and roasted aroma	Slightly soluble in water; insolube in n-octane Soluble	NA	NMR 98	NA NA	m.p. = 135 ºC	69th Full
1881	**Divanillin** 6,6'-Dihydroxy-5,5'-dimethoxy-[1,1'-biphenyl]-3,3'-dicarboxaldehyde *Dehydrodivanillin*	4107 05.221 2092-49-1	C16H14O6 302.28	White solid; Fruity vanilla aroma	Practically insoluble to insoluble in water; soluble in benzyl alcohol Soluble	NA	NMR 91	NA NA	m.p. = 315 ºC SC: Vanillin (5-7%)	69th Full
1882	**Vanillin propylene glycol acetal** 2-Methoxy-4-(4-methyl-1,3-dioxalan-2-yl)-phenol	3905 06.104 68527-74-2	C11H14O4 210.23	Colourless, viscous liquid; Sweet, vanilla aroma	Insoluble in water and fat; soluble in triacetin Soluble	152-155 (1 mm Hg)	NMR 79	1.533-1.543 1.196-1.206	SC: Vanillin (18-20%)	69th Full
1883	**4-Methoxybenzoyloxyacetic acid** Benzoic acid, 4-methoxy-, carboxymethyl ester *Glycolic acid, p-anisate*	4016 10414-68-3	C10H10O5 210.18	White solid; Cooked brown and roasted aroma	Slightly soluble in water; insoluble in n-octane Soluble	NA	NMR IR MS 98	NA NA	m.p. = 135 ºC	69th Full
1884	**Methyl isothiocyanate** Isothiocyanatomethane	4426 556-61-6	C2H3NS 73.11	Colourless to tan liquid; Pungent, penetrating mustard-like odour	Very slightly soluble in water; freely soluble in ether Soluble	117-118	MS 96	1.495-1.499 0.938-0.942		69th Full

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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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		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 °C)		69th Full