ANALYTICAL METHODS

The following analytical methods were prepared by the Committee at the 68th meeting. This method will be made available in the on-line database for flavourings.

HPLC Method for Flavourings

3-methyl-2-oxobutanoic acid (631)
Sodium 3-methyl-2-oxobutanoate (631.1)
3-methyl-2-oxopentanoic acid (632)
Sodium 3-methyl-2-oxopentanoate (632.1)
4-methyl-2-oxopentanoic acid (633)
Sodium 4-methyl-2-oxopentanoate (633.1)
2-oxo-3-phenylpropionic acid (1478)
Sodium 2-oxo-3-phenylpropionate (1479)

Determine by HPLC using the following:

Note: All solutions should be prepared with ultra high quality (UHQ) deionized water

Apparatus:

HPLC system with a suitable pump, injector, and a data station

Column:	Stainless steel; 300 x 7.6 mm
Stationary phase:	Bio-Rad Aminex® HPX-87H or equivalent
Detector:	UV

HPLC conditions:

Column temperature:	35°
Mobile phase:	0.004 M Sulfuric acid
Flow rate:	0.6 ml/min
Injection volume:	50 µl
Detection:	210 nm
Run time:	30 min

Note: *The retention times of the compounds are as follows:*
3-methyl-2-oxobutanoic acid is 13.0 min
3-methyl-2-oxopentanoic acid is 14.8 min
4-methyl-2-oxopentanoic acid is 16.7 min
2-oxo-3-phenylpropionic acid is 24.7 min

Procedure:

Weigh about 100 mg of the sample, dissolve in a minimum amount of 0.2 M sodium hydroxide solution, and make up to 100 ml in a volumetric flask. Set up and condition the HPLC using the mobile phase. Inject the sample solution and determine the purity of the sample by the area normalization method.

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 current meeting of the Committee specifications of identity and purity were revised for 12 flavourings (page 78) and adopted for 160 new flavourings (page 80).

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; Chemical Abstract Service Registry (CAS) No; Chemical formula; Molecular weight; Physical form/odour; Solubility; Solubility in ethanol, Boiling point (B.P. - 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 (at 20º, if not otherwise stated); Specific gravity (at 25º, if not otherwise stated)

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

1. Items in normal type are additional requirements, such as further purity criteria or other tests

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

3. Substances which are listed as secondary constituents which have been taken into account in the safety evaluation of the named flavouring agent. If the commercial product contains less than 95% of the named compound, it is a requirement that the major part of the product (i.e. not less than 95%) is accounted for by the sum of the named compound and one or more of the secondary constituents.

The field named Session contains the number of the meeting at which the specifications were prepared and the status of the specification. R means "specifications revised", S means "existing specifications maintained", S,T means "existing tentative specifications maintained, (further information required)", N means "new specifications", N,T means "new tentative specifications, (further information required)", and N,C means "new specifications for a flavouring agent with a conditional safety evaluation".

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

A comprehensive index listing all names, chemical names, and synonyms is added on page 141.

REVISED SPECIFICATIONS

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.W.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
631	**3-Methyl-2-oxobutanoic acid** 3-Methyl-2-oxobutyric acid *Butanoic acid, 3-methyl-2-oxo;* *Dimethylpyruvic acid; 2-Oxoisovaleric acid*	3869 759-05-7	C5H8O3 116.1	Pale yellow liquid; fruity aroma	Soluble in water Soluble	251°	NMR MS 97%		1.436-1.446 1.115-1.120	mp = 17°	68th/R
631.1	**3-Methyl-2-oxobutanoic acid, sodium salt** Sodium 3-methyl-2-oxobutyrate *Butanoic acid, 3-methyl-2-oxo, sodium salt;* *Sodium alpha-ketoisovalerate*	3869 08.051 3715-29-5	H5H7NaO3 138.1	White powder; slight fruity aroma	Soluble in water Soluble	NA	NMR 99%		NA NA	mp = 231.7° with decomposition	68th/R
632	**3-Methyl-2-oxopentanoic acid** 3-Methyl-2-oxovaleric acid	3870 1460-34-0	C6H10O3 130.1	White crystalline powder; slight fruity aroma	Soluble in water Soluble	233°	IR 99%		NA NA	mp = 41.5°	68th/R
632.1	**3-Methyl-2-oxopentanoic acid, sodium salt** Sodium 3 methyl-2-oxovalerate *Pentanoic acid, 3-methyl-2-oxo, sodium salt;* *Valeric acid, 3-methyl-2-oxo, sodium salt*	3870 08.093 3715-31-9	C6H9NaO3 152.1	White powder; slight fruity aroma	Soluble in water Soluble	NA	NMR IR 99%		NA NA		68th/R
633	**4-Methyl-2-oxopentanoic acid** 4-Methyl-oxovaleric acid	3871 816-66-0	C6H10O3 130.1	Pale yellow liquid; fruity aroma	Soluble in water Soluble	251°	IR 99%		1.432-1.442 1.053-1.058		68th/R
633.1	**4-Methyl-2-oxopentanoic acid, sodium salt** Sodium 4-methyl-2-oxovalerate *Oxopentanoate, 4-methyl-2-oxo, sodium salt;* *Sodium 4-methyl-2-ketopentanoate;* *Sodium 4-methyl-2-oxo-pentanoate;* *Valeric acid, 4-methyl-2-oxo, sodium salt*	3871 08.052 4502-00-5	C6H9NaO3 152.1	White powder; slight fruity aroma	Soluble in water Soluble	NA	NMR 99%		NA NA		68th/R
1479	**2-Oxo-3-phenylpropionic acid, sodium salt** Benzenepropanoic acid, alpha-oxo, sodium salt	3892 114-76-1	C9H7NaO3 186.14	White crystalline powder; very faint savoury aroma	Soluble in water Soluble	NA	NMR 98%		NA NA	Decomposes without melting starting at 175°	68th/R

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.W.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1480	**Maltol** 3-Hydroxy-2-methyl-4-pyrone *2-Methylpyromeconic acid;* *Larixinic acid; INS No. 636*	2656 07.014 118-71-8	C6H6O3 126.11	White, crystalline powder; Caramel-butterscotch aroma	Sparingly soluble in water, soluble in propylene glycol Soluble	-	NMR 99% (anhydrous basis)		- -	mp = 162°	68th/R
1481	**Ethyl maltol** 2-Ethyl-3-hydroxy-4-pyrone *2-Ethyl-3-hydroxy-4H-pyran-4-one;* *2-Ethylpyromeconic acid; INS No. 637*	3487 07.047 4940-11-8	C7H8O3 140.14	White, crystalline powder; Sweet fruit-like aroma	Sparingly soluble in water, soluble in propylene glycol Soluble	-	NMR 99% (anhydrous basis)		- -	mp = 89-93°	68th/R
1482	**Maltyl isobutyrate** 2-Methyl-4H-pyran-4-one-3-yl 2-methylpropanoate *2-Methyl-4-oxo-4H-pyran-3-yl isobutyrate;* *Maltyl 2-methylpropanoate;* *2-Methyl-4-pyron-3- yl 2-methylpropanoate*	3462 09.525 65416-14-0	C10H12O4 196.20	Colourless to yellow liquid; Strawberry aroma	Insoluble in water; Soluble in propylene glycol and fixed oils Soluble	100° (0.01 mm Hg)	IR 96%	10	1.497-1.499 1.145-1.149		68th/R
1506	**3-Acetyl-2,5-dimethylfuran** 3-Acetyl-2,5-dimethylfuran *2,5-Dimethyl-3-acetylfuran*	3391 13.066 10599-70-9	C8H10O2 138.17	Clear to yellow liquid; Powerful, slightly roasted, nutty aroma	Slightly soluble in water; soluble in propylene glycol and most fixed oils Soluble	83° (11 mm Hg)	NMR 99%	1	1.488-1.490 1.037-1.039		68th/R
1559	**2,4,5-Trimethyl-delta-3-oxazoline** 2,4,5-Trimethyl-delta-3-oxazoline *2,4,5-Trimethyl-2,5-dihydrooxazole*	3525 13.039 22694-96-8	C6H11NO 113.16	Yellow orange liquid; Powerful, musty, slight green, wood, nut aroma	Soluble in water, propylene glycol; insoluble in most fixed oils Soluble	96-97°	NMR 94%		1.413-1.421 0.913-0.920	Also contains trimethyloxazole	68th/R

NEW SPECIFICATIONS

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.V.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	AV max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1616	**Methyl 4-pentenoate** Methyl 4-pentenoate *Allylacetic acid methyl ester; Methyl allylacetate*	4353 818-57-5	C6H10O2 114.14	Colourless liquid; Green fruity aroma	Insoluble in water; soluble in propylene glycol Soluble	125-127º	MS 95%		1.412-1.418 0.882-0.890		68th/N
1617	**2-Methylbut-2-en-1-ol** 2-Methylbut-2-en-1-ol	4178 02.174 4675-87-0	C5H10O 86.13	Colourless liquid; Green oily aroma	Slightly soluble Soluble	136-138º	MS 98%		1.439-1.445 0.863-0.869		68th/N
1618	**Ethyl 4-pentenoate** Ethyl 4-pentenoate *4-Ethoxycarbonylbut-1-ene*	4360 1968-40-7	C7H12O2 128.17	Colourless liquid; Green fruity aroma	Insoluble in water; soluble in propylene glycol Soluble	143-145º	MS 95%		1.410-1.420 0.893-0.903		68th/N
1619	**4-Pentenal** 4-Pentenal	4262 05.174 2100-17-6	C5H8O 84.12	Colourless liquid; Cooked brown and roasted aroma	Slightly soluble in water; soluble in pentane and diethyl ether Soluble	97-99º	NMR IR MS 97%		1.413-1.418 0.853-0.857		68th/N
1620	**3-Isopropenylpentanedioic acid** 3-Isopropenylpentanedioic acid	4352 6839-75-4	C8H12O4 172.18	Crystalline solid imparting a savoury, cooked brown or roasted flavour	Soluble in water; insoluble in non-polar organic solvents Soluble	NA	NMR IR MS 95%		NA NA	mp = 110º	68th/N
1621	**trans-3-Hexenol** 3(E)-Hexenol *(3E)-Hexenol; (E)-3-Hexen-1-ol; (E)-3-Hexenol; trans-3-Hexen-1-ol; Leaf alcohol; beta-gamma-hexenol*	4356 928-97-2	C6H12O 100.16	Colourless liquid; Grassy green aroma	Soluble in water and most fixed oils Soluble	155-157º	MS 98%		1.437-1.442 0.830-0.845		68th/N
1622	**trans-4-Hexenal** 4(E)-Hexenal *Hex-4-enal; trans-Hex-4-enal; 4-Hexenal trans; E-4-Hexenal*	4046 25166-87-4	C6H10O 98.14	Colourless liquid; Green vegetable aroma	Soluble in hexane and diethyl ether; insoluble in water Soluble	125-129º 92% (sum of cis and trans isomers)	IR MS		1.417-1.424 0.824-0.832	Contains 76% min trans-4-hexenal, 16-20% cis-4-hexenal, 2-4% 3-hexen-1-ol and 1-2% hexanal	68th/N

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.V.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1623	**5-Hexenol** 5-Hexenol *1-Hexen-6-ol; 5-Hexene-1-ol; 6-Hydroxy-1-hexene*	4351 821-41-0	C6H12O 100.16	Colourless liquid; Green aroma	Soluble in water and most fixed oils Soluble	154-155°	NMR MS 95%		1.434-1.437 0.845-0.849		68th/N
1624	**Methyl (Z)-3-hexenoate** Methyl 3(Z)-hexenoate *Methyl cis-3-hexenoate*	4164 13894-62-7	C7H12O2 128.17	Clear, colourless liquid; Fruity, floral aroma	Soluble in fats and non-polar solvents; slightly soluble in water Soluble	85° (80 mm Hg)	NMR 95%		1.422-1.430 0.916-0.923		68th/N
1625	**cis-4-Octenol** 4(Z)-Octenol *(Z)-4-Octen-1-ol*	4354 2.244 54393-36-1	C8H16O 128.21	Clear, colourless liquid; Powerful, sweet, earthy odour with a strong herbaceous note	Insoluble in water; soluble in non-polar organic solvents Soluble	174-176°	MS 99%		1.444-1.450 0.844-0.851		68th/N
1626	**Ethyl (Z)-3-hexenoate** Ethyl 3(Z)-hexenoate *Ethyl cis-3-hexenoate*	4112 64187-83-3	C8H14O2 142.20	Clear, colourless liquid; Green, wine-like aroma	Soluble in fats and non-polar solvents; slightly soluble in water Soluble	90° (50 mm Hg)	NMR IR 96%		1.420-1.429 0.895-0.901		68th/N
1627	**3-Octenoic acid** 3-Octenoic acid *delta-3-Octenoic acid; 2-Heptene-1-carboxylic acid*	4362 1577-19-1	C8H14O2 142.20	White solid; Oily, fatty aroma	Slightly soluble in water; soluble in most organic solvents Soluble	240-242°	MS 95%		1.443-1.450 0.928-0.938 (20°)		68th/N
1628	**(Z)-3-Octenyl propionate** 3(Z)-Octenyl propionate	4189 94134-03-9	C11H20O2 184.28	Colourless to pale yellow liquid; Unique pear-like aroma with a honeydew melon nuance	Insoluble in water; soluble in most organic solvents Soluble	69-71° (1 mm Hg)	MS 95%		1.434-1.440 0.882-0.889	Also contains 2% trans isomer	68th/N
1629	**trans-4-Octenoic acid** 4(E)-Octenoic acid *4-Octenoic acid, (E)-*	4357 18776-92-6	C8H14O2 142.20	Colourless liquid; Greasy aroma	Slightly soluble in water; soluble in most organic solvents Soluble	105-106° (5 mm Hg)	MS 95%		1.436-1.440 0.924-0.930		68th/N
1630	**Methyl (Z)-5-octenoate** Methyl 5(Z)-octenoate	4165 41654-15-3	C9H16O2 156.22	Colourless liquid; Dairy, coconut aroma	Soluble in fat; slightly soluble in water Soluble	184°	NMR MS IR 95%		1.429-1.435 0.921-0.925		68th/N

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.W.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1631	**cis-5-Octenoic acid** 5(Z)-Octenoic acid *(Z)-5-Octenoic acid*	4350 41653-97-8	C8H14O2 142.20	Colourless liquid; Fatty, greasy aroma	Slightly soluble in water; soluble in most organic solvents Soluble	239-241°	MS 95%		1.444-1.450 0.955-0.971		68th/N
1632	**Ethyl 3-octenoate** Ethyl 3-octenoate *Ethyl oct-3-enoate*	4361 09.377 1117-65-3	C10H18O2 170.25	Colourless liquid; Tropical fruity aroma	Insoluble in water; soluble in most organic solvents Soluble	65-70° (1 mm Hg)	MS 95%		1.434-1.438 0.881-0.887		68th/N
1633	**cis-4-Decenol** 4(Z)-Decenol *(Z)-4-Decen-1-ol*	4349 57074-37-0	C10H20O 156.27	Colourless liquid; Waxy, fruity aroma	Soluble in diethyl ether, mineral oil, propylene glycol and most fixed oils; insoluble in glycerol and water Soluble	234-236°	MS 95%		1.449-1.455 0.844-0.850		68th/N
1634	**Isobutyl 10-undecenoate** Isobutyl 10-undecenoate	4358 5421-27-2	C15H28O2 240.39	Colourless liquid; Fatty, fruit-like aroma	Insoluble in water; soluble in most organic solvents Soluble	264-266°	NMR IR MS 98%		1.438-1.442 0.868-0.873 (20°)		68th/N
1635	**11-Dodecenoic acid** 11-Dodecenoic acid	4355 65423-25-8	C12H22O2 198.31	Colourless liquid; Fatty, citrusy aroma	Insoluble in water; soluble in most organic solvents Soluble	272-274°	MS 95%		1.447-1.457 0.890-0.897		68th/N
1636	**(Z)-4-Dodecenal** 4(Z)-Dodecenal *cis-Dodec-4-en-1-al; Tangerinal*	4036 21944-98-9	C12H22O 182.31	Colourless liquid; Fruity, citrusy aroma	Soluble in fats and non-polar solvents; insoluble in water Soluble	254°	NMR IR MS 94%		1.443-1.449 0.843-0.847	Also contains 3-4% dodecanal	68th/N
1637	**cis-9-Octadecenol** 9(Z)-Octadecenol *(Z)-9-Octadecen-1-ol; (Z)-9-Octadecenol; 9-cis-Octadecenol; cis-delta-9-Octadecenol; cis-9-Octadecen-1-ol; cis-9-Octadecenyl alcohol*	4363 143-28-2	C18H36O 268.48	Colourless to light yellow liquid; Fatty aroma with animal undertones	Insoluble in water; soluble in non-polar organic solvents Soluble	207° (13 mm Hg)	MS 85%		1.450-1.466 0.842-0.854 (20°)	Also contains 8-9% hexadecanol and 5-6% octadecanol	68th/N
1638	**cis-9-Octadecenyl acetate** 9(Z)-Octadecenyl acetate *(Z)-9-Octadecenyl acetate; cis-9- Octadecen-1-yl acetate; Oleyl acetate*	4359 693-80-1	C20H38O2 310.52	Colourless to light yellow liquid; Fatty aroma with fruity undertones	Insoluble in water; soluble in non-polar organic solvents Soluble	205-207° (13 mm Hg)	NMR MS IR 92%		1.446-1.453 0.865-0.874 (20°)	Also contains 2-3% hexadecyl acetate and 2-3% octadecyl acetate	68th/N

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.W.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1639	**Methyl 10-undecenoate** Methyl 10-undecenoate	4253 111-81-9	C12H22O2 198.31	Colourless liquid; Oily aroma	Slightly soluble in water Soluble	243-247º	MS 98%		1.436-1.442 0.885-0.891 (20º)		68th/N
1640	**(Z)-8-Tetradecenal** 8(Z)-Tetradecenal *(Z)-Tetradec-8-enal*	4066 05.208 169054-69-7	C14H26O 210.36	Clear liquid; Fruity, citrusy aroma	Soluble in water Soluble	295-299º	NMR IR MS 99%		1.446-1.450 0.833-0.845		68th/N
1641	**9-Octadecenal** 9-Octadecenal *Olealdehyde; Elialdehyde; Octadecenyl aldehyde; Oleic aldehyde*	4059 05.203 5090-41-5	C18H34O 266.47	Colourless liquid; Fatty aroma	Soluble in hexane and diethyl ether; insoluble in water Soluble	352-367º	NMR IR MS 94% (sum of cis and trans isomers)		1.448-1.458 0.837-0.845	Also contains 3-5% octadecenal	68th/N
1642	**(E)-4-Nonenal** 4(E)-Nonenal *(E)-Non-4-enal; trans-4-Nonenal*	4302 2277-16-9	C9H16O 140.23	Clear, colourless or pale yellow liquid; Fruity aroma	Sparingly soluble in water; soluble in many non-polar solvents Soluble	72-75º	NMR 93%		1.434-1.439 0.843-0.847	Also contains 1-2% 2-nonen-4-ol and 5-6% 2E,4E-nonadienal	68th/N
1643	**2,3,4-Trimethyl-3-pentanol** 2,3,4-Trimethyl-3-pentanol *Diisopropyl methyl carbinol*	3903 02.245 3054-92-0	C8H18O 130.23	Clear liquid; Fruity aroma	Soluble in heptane; insoluble in water Soluble	156-157º	NMR IR MS 97%		1.433-1.438 0.846-0.850		68th/N
1644	**(+/-)-2,4,8-Trimethyl-7-nonen-2-ol** 2,4,8-Trimethyl-7-nonen-2-ol	4212 437770-28-0	C12H24O 184.32	Clear, colourless liquid; Fruity aroma	Insoluble in water; soluble in non-polar organic solvents Soluble	60-70º (1-2 mm Hg)	NMR IR 96%		1.448-1.455 0.846-0.853		68th/N
1645	**(E)- and (Z)-2,4,8-Trimethyl-3,7-nonadien-2-ol** 2,4,8-Trimethyl-3,7-nonadien-2-ol	4211 479547-57-4	C12H22O 182.31	Clear, colourless liquid; Fruity aroma	Insoluble in water; soluble in non-polar organic solvents Soluble	70-72º (1.5 mm Hg)	NMR 96%	<1	1.463-1.471 0.858-0.864		68th/N
1646	**Nerolidol** 3,7,11-Trimethyl-1,6(cis),10-dodecatrien-3-ol *Methyl vinyl homogeranyl carbinol; 3,7-11-Trimethyl-1,6-10-dodecatrien-3-ol*	2772 02.018 7212-44-4	C15H26O 222.37	Colourless or very pale straw-coloured oily liquid; Faint woody-floral, slightly rose apple aroma	Soluble in most fixed oils and propylene glycol; slightly soluble in water; insoluble in glycerol Soluble	275-277º	NMR 97%		1.478-1.483 0.872-0.879		68th/N

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.V.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1647	**6-Acetoxydihydrotheaspirane** 2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-yl acetate *[2alpha,5alpha(S)]-2,6,10,10- Tetramethyl -1-oxaspiro[4.5]decan-6-yl, acetate*	3651 13.087 57893-27-3	C15H26O3 254.37	Crystalline solid; Fermented, earthy, spice-like aroma	Soluble in fats; insoluble in water Soluble	NA	NMR IR 97%		NA NA	mp = 50-53º	68th/N
1648	**6-Hydroxydihydrotheaspirane** 2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-ol *6-Hydroxy-2,6,10,10-tetramethyl-1-oxaspiro[4.5]decane*	3549 13.076 65620-50-0	C13H24O2 212.33	Colourless to yellow liquid; Camphoraceous woody green aroma	Soluble in fats; insoluble in water Soluble	211-212º	MS 98%		1.481-1.487 1.006-1.010		68th/N
1649	**1-Phenyl-3-methyl-3-pentanol** 3-Methyl-1-phenyl-3-pentanol *Phenylethyl methyl ethyl carbinol*	2883 02.037 10415-87-9	C12H18O 178.27	Colourless, slightly viscous liquid; Warm, rose-like aroma	Slightly soluble in water Soluble	253-255º	IR MS 98%		1.508-1.514 0.958-0.965 (20º)		68th/N
1650	**p-alpha,alpha-Trimethylbenzyl alcohol** 2-(4-Methylphenyl)propan-2-ol *p-Cymen-8-ol; Dimethyl p-tolyl carbinol; 2-(4-Methylphenyl)-2-propanol; 2-p-Tolyl-2-propanol*	3242 02.042 1197-01-9	C10H14O 150.22	Colourless liquid; Green, aromatic aroma	Slightly soluble in water Soluble	64º (0.6 mm Hg)	NMR 90%		1.516-1.520 0.974-0.980 (20º)	Also contains 9-11% p-isopropenyltoluene	68th/N
1651	**(+/-)-Ethyl 2-hydroxy-2-methylbutyrate** Ethyl 2-hydroxy-2-methylbutyrate	4268 77-70-3	C7H14O3 146.19	Clear, colourless liquid; Caramelised, nutty aroma	Sparingly soluble in water; soluble in most non-polar organic solvents Sparingly soluble	92º (64-68 mm Hg)	NMR 98%		1.409-1.416 0.964-0.974		68th/N
1652	**(+/-)-Ethyl 2-hydroxy-3-methylvalerate** Ethyl 2-hydroxy-3-methylpentanoate	4269 24323-38-4	C8H16O3 160.21	Clear, colourless liquid; Fruity aroma with berry notes	Sparingly soluble in water; soluble in most non-polar organic solvents Sparingly soluble	204-206º	NMR 96%		1.422-1.429 0.922-0.930		68th/N
1653	**alpha,alpha-Dimethylphenethyl alcohol** 2-Methyl-1-phenylpropan-2-ol *Benzyl dimethyl carbinol;* *2-Benzyl-2-propanol; alpha,alpha-Dimethylphenethanol; 2-Hydroxy-2-methyl-1-phenylpropane*	2393 02.035 100-86-7	C10H14O 150.22	Colourless to pale yellow viscous liquid or white crystalline solid; Warm, herbaceous, floral aroma Soluble	Soluble in mineral oil, most fixed oils and propylene glycol; insoluble in water liquid)	214-216º	NMR IR 97%		1.514-1.517 (as supercooled liquid) 0.972-0.977	mp = 23.7-24.5º	68th/N

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1654	**alpha,alpha-Dimethylphenethyl formate** 2-Methyl-1-phenyl-2-propyl formate *Benzyl dimethyl carbinyl formate;* *2-Benzyl-2-propyl formate;* *Dimethyl benzyl carbinyl formate*	2395 09.086 10058-43-2	C11H14O2 178.23	Colourless liquid; Dry, herbaceous, green, floral aroma	Soluble in mineral oil, most fixed oils and propylene glycol; insoluble in water Soluble	217-222°	NMR 93%		1.494-1.502 1.018-1.030 (20°)	Also contains 5-7% alpha,alpha-dimethylphenethyl alcohol	68th/N
1655	**alpha,alpha-Dimethylphenethyl acetate** 1,1-Dimethyl-2-phenethyl acetate *Benzyl dimethyl carbinyl acetate;* *2-Benzyl-2-propyl acetate;* *Dimethyl benzyl carbinyl acetate;* *2-Methyl-1-phenyl-2-propyl acetate*	2392 09.227 151-05-3	C12H16O2 192.26	White to colourless liquid or crystals at room temperature; Powerful floral, fruity aroma	Soluble in mineral oil, most fixed oils and propylene glycol; insoluble in water Soluble	249-251°	NMR 98%		1.490-1.495 0.995-1.002	mp = 29-30°	68th/N
1656	**alpha,alpha-Dimethylphenethyl butyrate** 1,1-Dimethyl-2-phenethyl butyrate *Benzyl dimethyl carbinol butyrate;* *2-Benzyl-2-propyl butyrate;* *Dimethyl benzyl carbinyl butyrate;* *2-Methyl-1-phenyl-2-propyl butyrate*	2394 09.232 10094-34-5	C14H20O2 220.31	Colourless liquid; Mild, herbaceous, fruity aroma	Soluble in mineral oil and most fixed oils; insoluble in water and propylene glycol Soluble	237-255°	NMR 95%		1.484-1.489 0.960-0.971		68th/N
1657	**alpha,alpha-Dimethylbenzyl isobutyrate** 1-Methyl-1-(2-phenylethyl) isobutyrate *alpha,alpha-Dimethylbenzyl 2-methyl-propanoate;* *2-Methyl-1-phenyl-2-propyl isobutyrate;* *Phenyl dimethyl carbinyl isobutyrate;* *2-Phenylpropan-2-yl isobutyrate*	2388 09.509 7774-60-9	C13H18O2 206.28	White solid; Fruity aroma	Soluble in oils; Insoluble in water Soluble	NA	NMR 95%		NA NA	mp = 71-72°	68th/N
1659	**Ethanethiol** Ethanethiol *Ethyl mercaptan*	4258 12.017 75-08-1	C2H6S 62.14	Colourless to yellow liquid; Fruity, sulfur aroma	Slightly soluble in water Soluble	35°	NMR IR 99%		1.425-1.431 0.833-0.839		68th/N
1660	**Ethane-1,1-dithiol** Ethane-1,1-dithiol	4111 69382-62-3	C2H6S2 94.20	Colourless liquid; Meaty, roasted aroma	Soluble in water Soluble	Product distils at 71-78°	NMR 1%; see 'Other requirements'		1.369-1.375 0.829-0.833	Product is a 1% solution of ethane-1,1- dithiol, purity 99% min, in ethanol	68th/N

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1661	**Dimercaptomethane** Methanedithiol	4097 12.243 6725-64-0	CH4S2 80.17	Colourless liquid; Pungent odour	Soluble in water Soluble	117-119°	NMR 95%		1.578-1.584 0.827-0.831		68th/N
1662	**1-Pentanethiol** Pentane-1-thiol *Amyl mercaptan; Pentyl mercaptan; Amyl hydrosulfide; Amyl sulfhydrate*	4333 12.191 110-66-7	C5H12S 104.22	Colourless liquid; Meaty aroma	Sparingly soluble in water Soluble	124-126°	NMR MS 97%		1.441-1.450 0.831-0.844		68th/N
1663	**Heptane-1-thiol** Heptane-1-thiol *Heptyl mercaptan*	4259 12.130 1639-09-4	C7H16S 132.27	Colourless liquid; Onion aroma	Practically insoluble to insoluble in water Soluble	175-176°	NMR IR MS 98%		1.497-1.503 0.840-0.846		68th/N
1664	**2-Heptanethiol** Heptane-2-thiol *(+/-)-2-Heptanethiol*	4128 628-00-2	C7H16S 132.27	Colourless liquid; Pungent, sulfureous odour	Slightly soluble in water Soluble	98-99° (103 mm Hg)	NMR 98%		1.442-1.445 (25°) 0.839-0.844		68th/N
1665	**(+/-)-1-Phenylethylmercaptan** 1-Phenylethanethiol *1-Phenylethylthiol; 1-Phenyl ethanethiol*	4061 6263-65-6	C8H10S 138.23	Yellow oily liquid; Meat-like, pungent odour	Insoluble in water Soluble	207-208°	NMR MS 98%		1.579-1.585 1.017-1.021		68th/N
1666	**2-Mercaptoanisole** 2-Methoxybenzene-1-thiol *o-Methioxythiophenol; o-Methoxybenzenethiol; 2-Methoxythiophenol; Thioguaiacol*	4159 12.139 7217-59-6	C7H8OS 140.21	Colourless to yellowish liquid; Pungent, onion aroma	Practically insoluble or insoluble in water Soluble	225-228°	MS IR NMR 95%		1.589-1.595 1.137-1.149		68th/N
1667	**Propyl 2-mercaptopropionate** Propyl 2-mercaptopropionate	4207 19788-50-2	C6H12O2S 148.23	Colourless liquid; Cooked brown and roasted meat aroma	Sparingly soluble in water; soluble in pentane and diethyl ether Soluble	191-194°	NMR IR MS 97%		1.447-1.453 1.014-1.020		68th/N
1668	**Methionyl butyrate** 3-(Methylthio)propyl butyrate	4160 16630-60-7	C8H16O2S 176.28	Colourless liquid; Cabbage/sewer odour	Practically insoluble to insoluble in water Soluble	232°	IR 99%		1.458-1.463 0.995-1.001		68th/N
1669	**(+/-)-4-Mercapto-4-methyl-2-pentanol** 4-Mercapto-4-methyl-2-pentanol	4158 12.252 31539-84-1	C6H14OS 134.24	Clear, colourless to pale yellow liquid; Floral, fruity aroma	Soluble in water Soluble	50-51° (1 mm Hg)	NMR 98%		1.463-1.468 1.154-1.158		68th/N

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1670	**4-Mercapto-2-pentanone** 4-Mercapto-2-pentanone *4-Mercaptopentan-2-one*	4157 92585-08-5	C5H10OS 118.20	Clear, colourless liquid; Strong, pungent, meaty aroma	Soluble in ether and chloroform; insoluble in water Soluble	258-260°	MS IR NMR 1%; see 'Other requirements'		NA NA	Product is a 1% solution of 4-mercapto-2-pentanone, purity 95% min, in acetoin	68th/N
1671	**(S)-1-Methoxy-3-heptanethiol** (S)-1-Methoxy-3-heptanethiol	4162 400052-49-5	C8H18OS 162.30	Colourless liquid; Sulfureous aroma	Practically insoluble or insoluble in water Soluble	181-183°	IR NMR MS 95%		1.442-1.449 0.901-0.905		68th/N
1672	**Diisopentyl thiomalate** Di(3-methylbutyl) but-2(cis)-enebis(thioate) *Diisoamyl thiomalate;* *bis(3-Methylbutyl)mercaptosuccinate*	4096 12.108 68084-03-7	C14H26O4S 290.42	Colourless to yellow liquid; Fruity, onion odour	Practically insoluble or insoluble in water Soluble	140-150°	NMR 94%		1.453-1.459 1.006-1.013	Also contains 2-3% diisopentyl thiotartronate	68th/N
1673	**cis- and trans-Mercapto-p-menthan-3-one** 1-Mercapto-p-menthan-3-one	4300 12.259 29725-66-4	C10H18OS 186.32	Colourless to pale yellow liquid; Citrus aroma	Insoluble in water Soluble	119-123° (10 mm Hg)	NMR 89%		1.487-1.497 0.989-0.999	Also contains 8-9% piperitone and 1-2% alpha-terpineol	68th/N
1674	**Methyl 3-mercaptobutanoate** Methyl 3-mercaptobutanoate	4167 54051-19-3	C5H10O2S 134.20	Colourless liquid; Pungent, onion-like aroma	Sparingly soluble Soluble	75° (16 mm Hg)	NMR 98%		1.453-1.459 1.053-1.057		68th/N
1675	**Methylthiomethylmercaptan** (Methylthio)methanethiol	4185 12.242 29414-47-9	C2H6S2 94.20	Almost colourless liquid; Pungent, sulfureous aroma	Soluble in water Soluble	40° (20 mm Hg)	NMR 97%		1.552-1.556 1.040-1.046		68th/N
1676	**Thioacetic acid** Ethanethioic acid	4210 12.199 507-09-5	C2H4OS 76.12	Pale yellow liquid; Cooked brown and roasted meat aroma	Soluble in water, diethyl ether and acetone Soluble	88-93°	NMR IR MS 96%		1.459-1.466 1.063-1.067		68th/N
1677	**(+/-)-Isobutyl 3-methylthiobutyrate** 2-Methylpropyl 3-(methylthio)butanoate *Isobutyl 3-(methylthio)butyrate;* *2-Methylpropyl 3-(methylthio) butanoate;* *2-Methylpropyl 3-(methylthio) butyrate*	4150 12.214 127931-21-9	C9H18O2S 190.31	Colourless liquid; Pungent aroma with fruity undertones	Soluble in pentane and diethyl ether; slightly soluble in water Soluble	93-96°	IR NMR MS 97%		1.453-1.469 0.968-0.972		68th/N
1678	**S-Methyl propanethioate** S-Methyl propanethioate	4172 12.165	C4H8OS 104.17	Colourless liquid; Fruity, milk-like aroma	Insoluble in water Soluble	119-120°	MS 97%		1.458-1.464 0.990-0.996	68th/N	

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		5925-75-7									
1679	**S-Isopropyl 3-methylbut-2-enethioate** S-Isopropyl 3-methylbut-2-enethioate *S-Isopropyl thiosenecioate;* *S-isopropyl 3-methylthiocrotonate*	4260 12.134 34365-79-2	C8H14OS 158.26	Colourless to yellowish liquid; Fruity, onion aroma	Practically insoluble to insoluble in water Soluble	235-236º	NMR 95%		1.486-1.492 1.006-1.012		68th/N
1680	**S-Ethyl 2-acetylamino ethanethioate** S-Ethyl 2-acetylamino ethanethioate *N-Acetylthioglycine, S-Ethyl ester;* *N-Acetylglycin-thiolethyl ester;* *S-Ethyl 2-acetylamino ethanethiolate*	4039 4396-62-7	C6H11NO2S 161.22	Crystalline solid; Pungent meat-like odour	Soluble in diethylether; very slightly soluble in water and hexane Soluble	NA	NMR MS IR 99%	NA	NA NA	mp = 60-62º	68th/N
1681	**Allyl thiohexanoate** Allyl butanethioate *Hexanethioic acid, S-2-propenyl ester;* *2-(Allylsulfanyl)-1-heptene hydrate*	4076 12.275 156420-69-8	C9H16OS 172.29	Clear, colourless liquid; Fruity, sulphureous aroma	Soluble in heptane and triacetin; insoluble in water Soluble	195-196º	NMR MS IR 99%		1.473-1.479 0.930-0.934		68th/N
1683	**2-Methyl-1-methylthio-2-butene** 2-Methyl-1-methylthio-2-butene	4173 89534-74-7	C6H12S 116.23	Clear, colourless liquid; Cooked brown and roasted meat aroma	Very slightly soluble in water; soluble in non-polar solvents Soluble	78º	NMR MS IR 99%		1.468-1.474 0.859-0.864		68th/N
1684	**2,4,6-Trithiaheptane** 2,4,6-Trithiaheptane	4214 12.240 6540-86-9	C4H10S3 154.32	Clear, almost colourless liquid; Cooked brown roasted aroma	Soluble in triacetin Soluble	250-255º	NMR IR MS 10%; see 'Other requirements'		NA NA	Product is a 10% solution of trithiaheptane, purity 95% min, in triacetin	68th/N
1685	**(+/-)-2,8-Epithio-cis-p-menthane** 2,8-Epithio-p-menthane *4,7,7-Trimethyl-6-thiabicyclo[3.2.1]octane*	4108 12.120 68398-18-5	C10H18S 170.32	Colourless to pale yellow clear liquid; Earthy, citrus aroma with menthol-like undertones	Insoluble in water Soluble	80º (0.9 mm Hg)	MS IR 93%	2	1.513-1.521 0.997-1.001	Also contains 5-6% limonene	68th/N
1686	**3,5-Diethyl-1,2,4-trithiolane** 3,5-Diethyl-1,2,4-trithiolane isomers)	4030 15.049 54644-28-9	C6H12S3 180.36	Clear, yellow liquid; Powerful, sulfureous aroma	Soluble in heptane and triacetin; insoluble in water Soluble	70-72º (1 mm Hg)	NMR 95% (sum of cis and trans		1.558-1.570 1.147-1.160		68th/N

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1687	**3,6-Diethyl-1,2,4,5-tetrathiane, mixture with 3,5-diethyl-1,2,4-trithiolane** Mixture of 3,6-Diethyl-1,2,4,5-tetrathiane and 3,5-Diethyl-1,2,4-trithiolane	4094 12.274 54717-12-3/ 54644-28-9	C6H12S4/ C6H12S3 212.43/180.36	Clear, colourless liquid; Cooked brown and roasted aroma	Insoluble in water Soluble	64-70º (1 mm Hg)	NMR 1%; see 'Other requirements'		NA NA	Product is a 1% solution of a mixture of the named components, purity 95% min, in vegetable oil	68th/N
1688	**3-(Methylthio)-2-butanone** 3-(Methylthio)-2-butanone	4181 53475-15-3	C5H10OS 118.20	Colourless to yellow liquid; Pungent odour	Sparingly soluble Soluble	50-54º (20 mm Hg)	NMR IR 97%		1.469-1.471 0.975-0.979		68th/N
1689	**4-(Methylthio)-2-pentanone** 4-(Methylthio)-2-pentanone	4182 143764-28-7	C6H12OS 132.23	Almost colourless liquid; Pungent odour	Slightly soluble Soluble	181-183º	NMR MS 98%		1.4680-1.4720 0.973-0.979		68th/N
1690	**Methyl 3-(methylthio)butanoate** Methyl 3-(methylthio)butanoate *3-(Methylthio) butyric acid methyl ester;* *3-Methylsulfanyl-butyric acid methyl ester*	4166 207983-28-6	C6H12O2S 148.23	Colourless liquid; Sweet, cooked aroma	Insoluble in water Soluble	87º (58 mm Hg)	NMR 98%		1.468-1.474 1.029-1.033		68th/N
1691	**Methyl (methylthio)acetate** Methyl (methylthio)acetate *Methyl 2-(methylthio)acetate;* *(Methylthio)acetic acid methyl ester*	4003 12.146 16630-66-3	C4H8O2S 120.17	Clear, colourless liquid; Fruity, pungent aroma	Soluble in non-polar solvents; insoluble in water Soluble	144-145º	NMR IR MS 98%		1.464-1.466 1.105-1.115 (20º)		68th/N
1692	**(+/-)-3-(Methylthio)heptanal** 3-(Methylthio)heptanal	4183 12.273 51755-70-5	C8H16OS 160.28	Clear, colourless liquid; Cooked brown and roasted aroma	Insoluble in water; soluble in heptane and triacetin Soluble	95-96º	NMR IR MS 92%		1.469-1.475 0.943-0.947	Also contains 5-7% 2-(E)-heptenal	68th/N
1693	**Ethyl methyl disulfide** Ethyl methyl disulfide *Methyldisulfanyl-ethane;* *2,3-Dithiapentane*	4040 12.153 20333-39-5	C3H8S2 108.23	Clear, colourless or pale yellow liquid; Sulfureous aroma	Soluble in non-polar solvents; Insoluble in water Soluble	136-138º	NMR MS IR 80%		1.410-1.418 1.017-1.027 (20º)	Also contains 7-8% diethyl disulfide and 8-10% dimethyl disulfide	68th/N
1694	**Ethyl propyl disulfide** Ethyl propyl disulfide *1-Ethyldisulfanyl-propane;* *3,4-Dithiaheptane*	4041 12.126 30453-31-7	C5H12S2 136.28	Clear, colourless or pale yellow liquid; Sulfureous aroma	Soluble in non-polar solvents; insoluble in water Soluble	179-181º	NMR MS IR 95%		1.483-1.493 0.943-0.953		68th/N

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1695	**Ethyl propyl trisulfide** Ethyl propyl trisulfide *3,4,5-Trithianonane*	4042 12.256 31499-70-4	C5H12S3 168.35	Clear, pale yellow liquid; Spicy, herb-like aroma	Soluble in non-polar solvents; insoluble in water Soluble	234-237°	NMR MS IR 98% (sum of three components)		1.544-1.559 1.071-1.083 (20°)	Contains 48-50% ethyl propyl trisulfide, 20-30% diethyl trisulfide and 20-30% dipropyl trisulfide	68th/N
1696	**Methyl isopentyl disulfide** Methyl 3-methylbutyl disulfide	4168 72437-56-0	C6H14S2 150.31	Colourless to yellow liquid; Brown, roasted aroma	Sparingly soluble in water Soluble	183-185°	NMR 92%		1.516-1.522 0.943-0.948	Also contains 3-5% crotonic acid	68th/N
1697	**Amyl methyl disulfide** Pentyl methyl disulfide *1-Methyldisulfanyl-pentane;* *2,3-Dithiaoctane*	4025 12.253 72437-68-4	C6H14S2 150.31	Clear, pale yellow liquid; Sulfureous aroma	Soluble in non-polar solvents; insoluble in water Soluble	198-202°	NMR MS IR 97%		1.485-1.495 0.943-0.953 (20°)		68th/N
1698	**Butyl ethyl disulfide** Butyl ethyl disulfide *1-Ethyldisulfanyl-butane;* *3,4-Dithiaoctane*	4027 12.254 63986-03-8	C6H14S2 150.31	Clear, colourless or pale yellow liquid; Sulfureous aroma	Soluble in non-polar solvents; insoluble in water Soluble	198-202°	NMR MS IR 90%		1.492-1.502 0.954-0.964 (20°)	Also contains 2-3% diethyl disulfide and 5-6% dibutyl disulfide	68th/N
1699	**Diethyl disulfide** Diethyl disulfide *3,4-Dithiahexane;* *Ethyl disulfide*	4093 12.012 110-81-6	C4H10S2 122.26	Colourless to yellowish liquid; Onion/cabbage odour	Practically insoluble to insoluble in water Soluble	151-152°	MS IR 99%		1.502-1.508 0.990-0.996		68th/N
1700	**Allyl propyl disulfide** Allyl propyl disulfide *4,5-Dithia-1-octene; Propyl allyl disulfide*	4073 12.021 2179-59-1	C6H12S2 148.29	Colourless to yellowish liquid; Fruity, garlic odour	Practically insoluble to insoluble in water Soluble	66° (10 mm Hg)	NMR 93%		1.497-1.517 0.999-1.005	Also contains 1-2% allyl propyl sulfide and 1-2% dipropylsulfide	68th/N
1701	**Diethyl trisulfide** Diethyl trisulfide *3,4,5-Trithiaheptane*	4029 12.114 3600-24-6	C4H10S3 154.32	Clear, colourless or pale yellow liquid; Powerful sulfureous aroma	Soluble in non-polar solvents; insoluble in water Soluble	216-218°	NMR MS 95%		1.556-1.560 1.121-1.231 (20°)		68th/N
1702	**Propyl propane thiosulfonate** Propyl propane thiosulfonate	4263 1113-13-9	C6H14O2S2 182.31	Colourless to yellow liquid; Cooked brown roasted aroma	Sparingly soluble in water; moderately soluble in pentane; soluble in toluene Moderately soluble	113° (1-2 mm Hg)	NMR MS IR 95%		1.481-1.488 1.119-1.123		68th/N

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1703	**(+/-)-3-(Ethylthio)butanol** 3-(Ethylthio)butanol	4282 117013-33-9	C6H14OS 134.24	Pale yellow to colourless liquid; Cooked brown roasted nutty aroma	Insoluble in water; slightly soluble in heptane and triacetin Slightly soluble	79-81° (1 mm Hg)	NMR IR MS 96%		1.468-1.476 0.941-0.947		68th/N
1704	**Hexyl 3-mercaptobutanoate** Hexyl 3-mercaptobutanoate *3-Mercaptobutanoic acid hexyl ester;* *Hexyl 3-mercaptobutyrate*	4136 796857-79-9	C10H20O2S 204.33	Almost colourless liquid; Fruit/spice/herb aroma	Sparingly soluble in water; soluble in triacetin and propylene glycol Soluble	82° (2 mm Hg)	NMR 98%		1.462-1.463 0.949-0.954		68th/N
1705	**(+/-)-3-Mercapto-1-butyl acetate** 3-Mercapto-1-butyl acetate *3-Mercaptobutyl acetate;* *3-Thiobutyl acetate*	4325 89534-38-3	C6H12O2S 148.23	Clear, colourless liquid; Fruit aroma	Slightly soluble in water; soluble in many non-polar solvents Soluble	77° (10 mm Hg)	NMR 95%		1.458-1.459 1.025-1.029		68th/N
1706	**3-Mercapto-3-methyl-1-butyl acetate** 3-Mercapto-3-methylbutyl acetate *3-Methyl-3-sulfanylbutyl acetate*	4324 50746-09-3	C7H14O2S 162.25	Clear, colourless liquid; Fruit aroma	Slightly soluble in water; soluble in many non-polar solvents Soluble	69° (6 mm Hg)	NMR 95%		1.455-1.456 1.003-1.007		68th/N
1707	**2,5-Dithiahexane** 2,5-Dithiahexane *1,2-bis(Methylthio)ethane;* *1,2-bis(Methylmercapto)ethane*	4298 6628-18-8	C4H10S2 122.26	Clear, colourless or pale yellow liquid; Dairy aroma with sulfureous note	Insoluble in water; soluble in non-polar solvents Soluble	178-179°	NMR 99%		1.526-1.533 1.039-1.049		68th/N
1708	**3-Mercaptoheptyl acetate** 3-Mercaptoheptyl acetate	4289 548774-80-7	C9H18O2S 190.31	Colourless liquid; Sulfury, fruity aroma	Soluble in water and in fats Soluble	242°	NMR MS IR 99%		1.457-1.463 0.980-0.984		68th/N
1709	**bis(1-Mercaptopropyl)sulfide** bis(1-Mercaptopropyl)sulfide	4297 53897-60-2	C6H14S3 182.38	Liquid; Sulphury odour	Slightly soluble in water; soluble in many non-polar solvents Soluble	225-226° (76 mm Hg)	NMR IR 92% (sum of two components) See 'Other requirements'		1.545-1.551 1.080-1.084	Contains 56% min bis(1-mercaptopropyl)sulfide, 36% min 3,5-diethyl-1,2,4-trithiolane; contains approx. 5% dipropylsulfide	68th/N

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1710	**S-Allyl-L-cysteine** S-Allyl-L-cysteine *(2R)-2-Amino-3-(prop-2-en-1-ylsulfanyl) propanoic acid;* *(2R)-3-(Allylthio)-2-aminopropanoic acid;* *(R)-Allylthio-2-aminopropionic acid;* *S-Allylcysteine; (+)-S-Allylcysteine;* *S-2-Propenylcysteine*	4322 21593-77-1	C6H11NO2S 161.22	White powder; Cooked roasted brown aroma	Sparingly soluble in water Slightly soluble	NA	NMR MS IR 95%		NA NA	mp = 214-216º	68th/N
1711	**2,4-Dimethyl-1,3-dioxolane** 2,4-Dimethyl-1,3-dioxolane *Acetaldehyde cyclic propylene acetal;* *Propylene acetal*	4099 3390-12-3	C5H10O2 102.13	Colourless liquid; Dairy aroma with fruity overtones	Slightly soluble in water Soluble	100-101º	NMR 95%	1	1.390-1.401 0.921-0.928		68th/N
1712	**2-Hexyl-4,5-dimethyl-1,3-dioxolane** 2-Hexyl-4,5-dimethyl-1,3-dioxolane *Heptanal 2,3-butandiol acetal*	4048 06.089 6454-22-4	C11H22O2 186.29	Clear, colourless liquid; Dairy aroma with fruity overtones	Soluble in non-polar solvents Soluble	101º (9 mm Hg)	NMR MS IR 96%	1	1.425-1.430 0.876-0.886		68th/N
1715	**cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate** Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	4294 06.087 6290-17-1	C9H16O4 188.22	Colourless liquid; Soft, fruity notes	Insoluble in water Soluble	85º	IR 95%	1	1.422-1.432 1.048-1.054		68th/N
1716	**Dihydroxyacetone dimer** 2,5-Dihydroxy-1,4-dioxane-2,5-dimethanol	4033 62147-49-3	C6H12O6 180.16	Hygroscopic, crystalline, white to off-white powder; Sweet, cooling, aroma	Slightly soluble in water Soluble	NA	NMR MS 97%	NA	NA NA	mp = 75-80º	68th/N
1717	**1-Hydroxy-2-butanone** 1-Hydroxybutan-2-one *2-Oxo-1-butanol; Propionyl carbinol;* *Ethyl hydroxymethyl ketone; 1-Butanol-2-one*	3173 07.090 5077-67-8	C4H8O2 88.11	Colourless liquid; Fruity aroma	Insoluble in water; soluble in diethyl ether Soluble	152-154º	MS 90%		1.417-1.423 1.017-1.022 (20º)	Also contains 5-10% acetoin	68th/N
1718	**Ethyl 3-acetoxy-2-methylbutyrate** Ethyl 3-acetoxy-2-methylbutyrate *3-Acetoxy-2-methyl butyric acid ethyl ester*	4038 09.919 139564-43-5	C9H16O4 188.22	Clear, colourless liquid; Fruity aroma	Soluble in non-polar solvents; insoluble in water Soluble	205-206º	NMR MS IR 95%		1.417-1.420 1.003-1.013		68th/N

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1719	**Methyl 5-acetoxyhexanoate** Methyl 5-acetoxyhexanoate *5-Acetoxyhexanoic acid methyl ester*	4055 09.632 35234-22-1	C9H16O4 188.22	Clear, colourless liquid; Fruity aroma	Soluble in non-polar solvents; insoluble in water Soluble	194-196°	NMR MS IR 97%		1.519-1.529 1.017-1.027		68th/N
1726	**(+/-)-1-Acetoxy-1-ethoxyethane** 1-Acetoxy-1-ethoxyethane *Ethoxyethyl acetate*	4069 1608-72-6	C6H12O3 132.16	Clear, colourless liquid; Refreshing, fruity aroma	Soluble in water Soluble	136-138°	MS NMR 95%		1.386-1.392 0.947-0.951		68th/N
1727	**Acetaldehyde hexyl isoamyl acetal** 1-Hexyloxy-1-(3-methylbutyl)oxypropane	4365 06.114 233665-90-2	C13H28O2 216.36	Colourless liquid; Sweet, fruity aroma	Insoluble in water; soluble in organic solvents Soluble	240-241°	MS 97% (sum of three components)		1.418-1.423 0.833-0.838	Contains acetaldehyde hexyl isoamyl acetal (51-53%), acetaldehyde dihexyl acetal (26-28%) and acetaldehyde diisoamyl acetal (17-19%)	68th/N
1728	**1,1-Dimethoxy-trans-2-hexene** 1,1-Dimethoxyhex-2(E)-ene *trans-2-Hexenal dimethyl acetal*	4098 06.072 18318-83-7	C8H16O2 144.21	Colourless liquid; Green fruity aroma	Practically insoluble to insoluble in water Soluble	158°	NMR 95%		1.420-1.424 0.867-0.871		68th/N
1729	**Acetaldehyde diisoamyl acetal** 1,1-Di(3-methylbutoxy)ethane *3-Methyl-1-[1-(3-methyl-butoxy)-ethoxy]-butane;* *1,1-Di-isopentyloxyethane*	4024 06.055 13002-09-0	C12H26O2 202.34	Clear, colourless liquid; Strong, sweet, fruity aroma	Soluble in non-polar solvents; insoluble in water Soluble	70° (2.5 mm Hg)	NMR MS IR 95%	1	1.410-1.420 0.822-0.832		68th/N
1730	**Isovaleraldehyde diethyl acetal** 1,1-Diethoxy-3-methylbutane *1,1-Diethoxyisopentane;* *3-Methylbutanal diethyl acetal*	4371 06.059 3842-03-3	C9H20O2 160.26	Clear, colourless liquid; Fruity, fatty aroma	Insoluble in water; soluble in organic solvents Soluble	159-162°	NMR MS IR 95%		1.395-1.403 0.825-0.832		68th/N
1731	**Valeraldehyde dibutyl acetal** 1,1-Dibutoxypentane	4375 13112-65-7	C13H28O2 216.36	Clear, colourless liquid; Sweet, nutty aroma	Insoluble in water; soluble in organic solvents Soluble	251-252°	MS 97%		1.417-1.423 0.833-0.839		68th/N
1732	**Isovaleraldehyde propyleneglycol acetal** 2-Isobutyl-4-methyl-1,3-dioxolane *4-Methyl-2-(2-methylpropyl)-1,3-dioxolane*	4286 18433-93-7	C8H16O2 144.21	Clear, colourless liquid; Fruity, slightly fatty aroma	Insoluble in water; soluble in organic solvents Soluble	164-165°	NMR MS IR 95%	1	1.412-1.420 0.895-0.902		68th/N

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1733	**Isovaleraldehyde glyceryl acetal** 4-Hydroxymethyl-2-(2-methylpropyl)-1,3-dioxolane and 5-Hydroxy-2-(2-methylpropyl)-1,3-dioxane	4380 54355-74-7	C8H16O3 160.21	Clear, colourless liquid; Fruity, fatty aroma	Insoluble in water; soluble in organic solvents Soluble	238-239°	NMR MS IR 98% (sum of two components)	1	1.443-1.450 1.024-1.031	Contains 67-69% 4-Hydroxymethyl-2-(2-methylpropyl)-1,3-dioxolane and 28-30% 5-Hydroxy-2-(2-methylpropyl) -1,3- dioxane	68th/N
1734	**Valeraldehyde propyleneglycol acetal** 2-Butyl-4-methyl-1,3-dioxolane	4372 74094-60-3	C8H16O2 144.21	Clear, colourless liquid; Nutty, fatty aroma	Insoluble in water; soluble in organic solvents Soluble	176-177°	MS 98%	1	1.415-1.420 0.900-0.906		68th/N
1735	**Hexanal hexyl isoamyl acetal** 1-Hexyloxy-1-(3-methylbutyl)oxyhexane	4369 896447-13-5	C17H36O2 272.47	Clear, colourless liquid; Sweet, green aroma	Insoluble in water; soluble in organic solvents Soluble	305-306°	NMR MS IR 97% (sum of three components)	1	1.427-1.432 0.835-0.840	Contains hexanal hexyl isoamyl acetal (50-52%), hexanal dihexyl acetal (25-27%) and hexanal diisoamyl acetal (20-22%)	68th/N
1736	**Hexanal octane-1,3-diol acetal** 2,4-Dipentyl-1,3-dioxane	4377 202188-46-3	C14H28O2 228.38	Clear, colourless liquid; Fatty, green aroma	Insoluble in water; soluble in organic solvents Soluble	287-288°	MS 96%	1	1.425-1.432 0.869-0.875		68th/N
1737	**Hexanal butane-2,3-diol acetal** 4,5-Dimethyl-2-pentyl-1,3-dioxolane	4384 155639-75-1	C10H20O2 172.27	Clear, colourless liquid; Sweet, fatty, green aroma	Insoluble in water; soluble in organic solvents Soluble	211-213°	MS 98%	1	1.430-1.437 0.845-0.851		68th/N
1738	**Hexanal dihexyl acetal** 1,1-bis(Hexyloxy)hexane	4370 33673-65-3	C18H38O2 286.50	Clear, colourless liquid; Mild, green, grassy aroma	Insoluble in water; soluble in organic solvents Soluble	326-327°	NMR MS 95%	1	1.431-1.436 0.838-0.844		68th/N
1739	**Heptanal propyleneglycol acetal** 2-Hexyl-4-methyl-1,3-dioxolane *Heptanal, cyclic propylene acetal*	4368 4351-10-4	C10H20O2 172.27	Clear, colourless liquid; Green, fatty aroma	Insoluble in water; soluble in organic solvents Soluble	217-218°	MS 98%	1	1.425-1.430 0.889-0.895		68th/N
1740	**2,6-Dimethyl-5-heptenal propyleneglycol acetal** 2-(1,5-Dimethyl-4-hexenyl)-4-methyl-1,3-dioxolane	4382 74094-63-6	C12H22O2 198.31	Clear, colourless liquid; Strong, green, citrusy aroma	Insoluble in water; soluble in organic solvents Soluble	243-244°	MS 97%	1	1.447-1.453 0.910-0.916		68th/N

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1741	**Octanal propyleneglycol acetal** 2-Heptyl-4-methyl-1,3-dioxolane	4383 74094-61-4	C11H22O2 186.29	Clear, colourless liquid; Green, woody aroma	Insoluble in water; soluble in organic solvents Soluble	236-237°	NMR MS IR 97%	1	1.427-1.434 0.886-0.893		68th/N
1742	**Nonanal dimethyl acetal** 1,1-Dimethoxynonane *Pelargonaldehyde dimethyl acetal;* *Pelargonic aldehyde dimethyl acetal*	4367 18824-63-0	C11H24O2 188.31	Clear, colourless liquid; Fresh, fruity aroma	Insoluble in water; soluble in organic solvents Soluble	214-215°	MS 98%	1	1.418-1.424 0.847-0.853		68th/N
1743	**Nonanal propyleneglycol acetal** 4-Methyl-2-octyl-1,3-dioxolane *2-Octyl-4-methyl-1,3-dioxolane*	4373 68391-39-9	C12H24O2 200.32	Clear, colourless liquid; Fruity aroma	Insoluble in water; soluble in organic solvents Soluble	253-254°	NMR MS IR 98%	1	1.430-1.436 0.884-0.889		68th/N
1744	**Decanal propyleneglycol acetal** 4-Methyl-2-nonyl-1,3-dioxolane *2-Nonyl-4-methyl-1,3-dioxolane*	4364 5421-12-5	C13H26O2 214.35	Clear, colourless liquid; Green, floral aroma	Insoluble in water; soluble in organic solvents Soluble	270-271°	NMR MS IR 98%	1	1.433-1.439 0.881-0.887		68th/N
1745	**Undecanal propyleneglycol acetal** 2-Decyl-4-methyl-1,3-dioxolane	4374 74094-62-5	C14H28O2 228.38	Clear, colourless liquid; Sweet, fatty, floral aroma	Insoluble in water; soluble in organic solvents Soluble	286-287°	MS 95%	1	1.435-1.441 0.879-0.885		68th/N
1746	**Dodecanal dimethyl acetal** 1,1-Dimethoxydodecane *1,1'-bis(Methoxy)dodecane;* *Dodecanaldimethyl acetal;* *Lauryl aldehyde dimethyl acetal*	4366 14620-52-1	C14H30O2 230.39	Clear, colourless liquid; Fatty, citrus-like aroma	Insoluble in water; soluble in organic solvents Soluble	268-269°	MS 98%	1	1.428-1.434 0.847-0.853		68th/N
1747	**Acetaldehyde di-cis-3-hexenyl acetal** 1,1-bis[3(Z)-Hexenyloxy]propane	4381 63449-64-9	C14H26O2 226.36	Clear, colourless liquid; Strong, green, herbaceous aroma	Insoluble in water; soluble in organic solvents Soluble	278-279°	NMR MS 96%	1	1.442-1.448 0.864-0.870		68th/N
1748	**Isobutanal propyleneglycol acetal** 2-Isopropyl-4-methyl-1,3-dioxolane *4-Methyl-2-(1-methylethyl)-1,3-dioxolane*	4287 67879-60-1	C7H14O2 130.19	Clear, colourless liquid; Penetrating, winey aroma	Insoluble in water; soluble in organic solvents Soluble	142-143°	NMR MS IR 96%	1	1.407-1.412 0.903-0.909		68th/N
1749	**Acetaldehyde 1,3-octanediol acetal** 2-Methyl-4-pentyl-1,3-dioxane	4376 202188-43-0	C10H20O2 172.27	Clear, colourless liquid; Green, ethereal aroma	Insoluble in water; soluble in organic solvents Soluble	219-220°	MS 96%	1	1.429-1.433 0.900-0.906		68th/N

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1750	**1-(3-Hydroxy-5-methyl-2-thienyl)ethanone** 1-(3-Hydroxy-5-methyl-2-thienyl)ethanone	4142 15.127 133860-42-1	C7H8O2S 156.21	White, cream-coloured solid; Meaty, cooked, brown or roasted aroma	Slightly soluble in water Soluble	NA	NMR 98%		NA NA	mp = 73-75º	68th/N
1751	**2-(5-Methyl-4-thiazolyl)ethyl formate** 2-(5-Methyl-4-thiazolyl)ethyl formate	4275 90731-56-9	C7H9NO2S 171.22	Colourless to yellow liquid; Nutty, brown, roasted aroma	Soluble in non-polar solvents; slightly soluble in water Soluble	155-156º	NMR MS 95%	2	1.518-1.524 1.215-1.221		68th/N
1752	**2-(4-Methyl-5-thiazolyl)ethyl propionate** 2-(4-Methyl-5-thiazolyl)ethyl propionate	4276 324742-96-3	C9H13NO2S 199.27	Colourless to yellow liquid; Roasted, nutty aroma	Soluble in non-polar solvents; insoluble in water Soluble	99-105º (1 mm Hg)	NMR 98%	1	1.502-1.506 1.136-1.140		68th/N
1753	**2-(4-Methyl-5-thiazolyl)ethyl butanoate** 2-(4-Methyl-5-thiazolyl)ethyl butanoate	4277 94159-31-6	C10H15NO2S 213.30	Colourless to yellow liquid; Roasted, nutty aroma	Soluble in non-polar solvents; insoluble in water Soluble	101-107º (1 mm Hg)	NMR 98%	1	1.496-1.510 1.106-1.112		68th/N
1754	**2-(4-Methyl-5-thiazolyl)ethyl isobutyrate** 2-(4-Methyl-5-thiazolyl)ethyl isobutyrate	4278 324742-95-2	C10H15NO2S 213.30	Colourless to yellow liquid; Roasted nutty aroma	Soluble in non-polar solvents; slightly soluble in water Soluble	100-104º (2 mm Hg)	NMR 98%	1	1.494-1.500 1.102-1.108		68th/N
1755	**2-(4-Methyl-5-thiazolyl)ethyl hexanoate** 2-(4-Methyl-5-thiazolyl)ethyl hexanoate	4279 94159-32-7	C12H19NO2S 241.35	Colourless to yellow liquid; Roasted, nutty aroma	Soluble in non-polar solvents; Slightly soluble in water Soluble	143-145º (2 mm Hg)	NMR 98%	1	1.492-1.497 1.065-1.071		68th/N
1756	**2-(4-Methyl-5-thiazolyl)ethyl octanoate** 2-(4-Methyl-5-thiazolyl)ethyl octanoate	4280 163266-17-9	C14H23NO2S 269.41	Colourless to yellow liquid; Roasted, nutty aroma	Soluble in non-polar solvents; insoluble in water Soluble	154-156º (2 mm Hg)	NMR 98%	1	1.498-1.494 1.036-1.042		68th/N

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1757	**2-(4-Methyl-5-thiazolyl)ethyl decanoate** 2-(4-Methyl-5-thiazolyl)ethyl decanoate	4281 101426-31-7	C16H27NO2S 297.46	Colourless to yellow liquid; Roasted, nutty aroma	Soluble in non-polar solvents; insoluble in water Soluble	177-179° (1.5 mm Hg)	NMR 95%	1	1.486-1.492 1.012-1.018		68th/N
1758	**2,5-Dimethylthiazole** 2,5-Dimethylthiazole	4035 15.063 4175-66-0	C5H7NS 113.18	Yellow liquid; Cooked, brown and roasted nutty aroma	Soluble in non-polar solvents; slightly soluble in water Soluble	148-150°	NMR MS IR 95%		1.523-1.527 1.114-1.124 (20°)		68th/N
1759	**2-Acetyl-2-thiazoline** 2-Acetyl-2-thiazoline *Acetyl thiazoline-2;* *2-Acetyl-4,5-dihydrothiazole*	3817 15.010 29926-41-8	C5H7NOS 129.18	Brown solid; Green, onion, herbal, grassy aroma	Insoluble in water and heptane Soluble	NA	NMR MS IR 98%		NA NA	mp = 26-28°	68th/N
1760	**2-Propionyl-2-thiazoline** 2-Propionyl-2-thiazoline *1-(4,5-Dihydro-1,3-thiazol-2-yl)-1-propanone*	4064 15.128 29926-42-9	C6H9NOS 143.21	Colourless to light yllow liquid; Meaty, nutty, cooked, brown roasted aroma	Soluble in heptane; insoluble in water Soluble	237-241°	NMR MS IR 99%		1.514-1.517 1.230-1.245		68th/N
1761	**cis- and trans-5-Ethyl-4-methyl-2-(2-methylpropyl)-thiazoline** 5-Ethyl-4-methyl-2-(2-methylpropyl)-thiazoline *5-Ethyl-2,5-dihydro-4-methyl-2-(2-methylpropyl)-thiazole; 2-Isobutyl-4-methyl-5-ethylthiazoline*	4319 83418-53-5	C10H19NS 185.33	Yellow liquid; Meaty, nutty, cooked, brown roasted aroma	Soluble in water Soluble	252-253°	NMR MS 96%		1.483-1.489 0.942-0.947		68th/N
1762	**cis- and trans-5-Ethyl-4-methyl-2-(1-methylpropyl)-thiazoline** 5-Ethyl-4-methyl-2-(1-methylpropyl)-thiazoline *5-Ethyl-2,5-dihydro-4-methyl-2-(1-methylpropyl)-thiazole*	4318 83418-54-6	C10H19NS 185.33	Yellow liquid; Meaty, nutty, cooked, brown roasted aroma	Soluble in water Soluble	253°	NMR MS 97%		1.487-1.493 0.950-0.956		68th/N

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1763	**Pyrrolidino-[1,2e]-4H-2,4-dimethyl-1,3,5-dithiazine** 2,4-Dimethyl-1-aza-3,5-dithiabicyclo[4.3.0]nonane *2,4-Dimethyltetrahydropyrrolo[2,1-d][1,3,5]-dithiazine;* *2,4-Dimethyl(4H)pyrrolidino[1,2e]-1,3,5-dithiazine*	4321 116505-60-3	C8H15NS2 189.35	Crystalline solid; Meaty, cooked, brown roasted aroma	Practically insoluble or insoluble in water; soluble in pentane and diethyl ether Soluble	NA	NMR MS IR 96%		NA NA	mp > 50º	68th/N
1764	**2-Hexylthiophene** 2-Hexylthiophene	4137 15.076 18794-77-9	C10H16S 168.30	Colourless to pale yellow liquid; Meat-like aroma	Soluble in most organic solvents; Insoluble in water Soluble	229-230º	MS 99%		1.492-1.498 0.930-0.938 (20º)		68th/N
1765	**3-(Methylthio)methylthiophene** 3-(Methylthio)methylthiophene	4184 15.126 61675-72-7	C6H8S2 144.26	Clear, colourless liquid; Cooked, brown and roasted dairy aroma	Soluble in most organic solvents; insoluble in water Soluble	210-211º	NMR IR MS 97%		1.580-1.585 1.522-1.525		68th/N
1766	**5-Acetyl-2,3-dihydro-1,4-thiazine** 5-Acetyl-2,3-dihydro-1,4-thiazine	4296 143.21 164524-93-0	C6H9NOS	Brown crystals; Nutty, cooked, brown and roasted aroma	Insoluble in water; soluble in methylene chloride Slightly soluble	NA	NMR 99%		NA NA	mp = 120-125º	68th/N
1767	**N-Heptan-4-yl)benzo[d][1,3] dioxole-5-carboxamide** N-(1-Propylbutyl)-1,3-benzodioxole-5-carboxamide	4232 745047-51-2	C15H21NO3 263.34	Off-white powder; Savoury, meat-like aroma	Soluble in non-polar organic solvents; insoluble in water Sparingly soluble	NA	NMR IR MS 99%		NA NA	mp = 116-117º	68th/N
1768	**N1-(2,4-Dimethoxybenzyl)-N2-(2-(pyridin-2-yl)ethyl)oxalamide** N-[(2,4-Dimethoxyphenyl)methyl]-N'-[2-(pyridinyl)ethyl]ethanediamide	4233 745047-53-4	C18H21N3O4 343.38	Off-white powder; Savoury, meat-like aroma	Soluble in non-polar organic solvents; insoluble in water Sparingly soluble	NA	NMR IR MS 99%		NA NA	mp = 123-124º	68th/N
1769	**N1-(2-Methoxy-4-methylbenzyl)-N2-(2-(5- methylpyridin-2-yl)ethyl) oxalamide** N-[(2-Methoxy-4-methylphenyl)methyl]-N'-[2-(5-methyl-2-pyridinyl)ethyl] ethanediamide	4234 745047-94-3	C19H23N3 O3 341.41	Off-white powder; Savoury, meat-like aroma	Soluble in non-polar organic solvents; insoluble in water Sparingly soluble	NA	NMR IR MS 99%		NA NA	mp = 132-133º	68th/N

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1770	**N1-(2-Methoxy-4-methylbenzyl)-N2-(2-(pyridin-2-yl)ethyl)oxalamide** N-[(2-Methoxy-4-methylphenyl)methyl]-N'-[2-(pyridinyl)ethyl]ethanediamide	4231 745047-97-6	C18H21N3O3 327.38	Off-white powder; Savoury, meat-like aroma	Soluble in non-polar organic solvents; insoluble in water Sparingly soluble	NA	NMR IR 99%		NA NA	mp = 128-129º	68th/N
1771	**4-Aminobutyric acid** 4-Aminobutyric acid	4288 17.055 56-12-2	C4H9NO2 103.12	White, powdery solid; Savoury, meat-like aroma	Slightly soluble in water; soluble in many non-polar solvents Insoluble	NA	NMR MS IR 99%		NA NA	mp = 200-202º	68th/N
1772	**N-Gluconyl ethanolamine** N-(2-Hydroxyethyl)galactonamide	4254 686298-93-1	C8H17NO7 239.23	White, crystalline powder; Cooked brown and roasted aroma	Very soluble in water; insoluble in pentane Slightly soluble	NA	NMR MS IR 99%		NA NA	mp = 99-100º	68th/N
1773	**N-Gluconyl ethanolamine phosphate** N-[2-(Phosphonooxy)ethyl]galactonamide	4255 791807-20-0	C8H18NO10P 319.21	White, crystalline powder; Cooked brown and roasted aroma	Very soluble in water; insoluble in pentane Slightly soluble	NA	NMR MS 95%		NA NA	mp = 138-139º	68th/N
1774	**N-Lactoyl ethanolamine** 2-Hydroxy-N-(2-hydroxyethyl)propanamide	4256 5422-34-4	C5H11NO3 133.15	Viscous, brownish liquid; Cooked brown roasted aroma	Very soluble in water; insoluble in pentane and diethyl ether Slightly soluble	372-380º	NMR IR MS 90%		1.475-1.481 1.182-1.186	Also contains 6-8% 2-aminoethanol lactate	68th/N
1775	**N-Lactoyl ethanolamine phosphate** 2-Hydroxy-N-[2-(phosphonooxy)ethyl]propanamide	4257 782498-03-7	C5H12NO6P 213.13	Viscous, oily liquid; Cooked brown and roasted aroma	Very soluble in water; insoluble in pentane Slightly soluble	387-400º	NMR IR MS 90%		1.498-1.514 1.517-1.524	Also contains 6-10% ammonium formate	68th/N
1776	**N-[(Ethoxycarbonyl)methyl)-p-menthane-3-carboxamide** N-[(Ethoxycarbonyl)methyl)-p-menthane-3-carboxamide *[1R-(1alpha,2beta,5alpha)]-N-[5-Methyl-2-(1-methylethyl)cyclohexyl]carbonyl glycine ethyl ester*	4309 68489-14-5	C15H27NO3 269.38	White crystals or powder; Cool menthol aroma	Practically insoluble or insoluble in water; slightly soluble in heptane; very slightly soluble in propylene glycol and ethyl acetate Soluble	151º (2 mm Hg)	NMR IR MS 99%		NA NA	mp = 80-82º	68th/N

No	Name Chemical name *Synonyms*	FEMA No Flavis No CAS No	Formula M.W.	Physical form; Odour	Solubility Solubility in ethanol	B.P.	ID test Assay min	A.V. max	R.I. S.G.	Other requirements/ SC (secondary constituents)	Session
1777	**N-[2-(3,4-Dimethoxyphenyl)ethyl]-3,4-dimethoxycinnamic acid amide** N-[2-(3,4-Dimethoxyphenyl)ethyl]-3,4-dimethoxycinnamic acid amide *2-Propenamide, 3-(3,4- dimethoxyphenyl)-N-[2-(3,4-dimethoxyphenyl)ethyl]-; Rubenamin*	4310 16.090 69444-90-2	C21H25NO5 371.43	Solid; Savoury, meat-like aroma	Insoluble in water; soluble in non-polar solvents Insoluble	NA	NMR IR MS 99%		NA NA	mp = 128°	68th/N
1779	**N-3,7-Dimethyl-2,6-octadienyl cyclopropylcarboxamide** N-[(2E)-3,7-Dimethyl-2,6-octadienyl]-cyclopropanecarboxamide	4267 744251-93-2	C14H23NO 221.34	Colourless to pale yellow solid; Cooked brown and roasted meaty aroma	Sparingly soluble in water; very soluble in non-polar organic solvents Sparingly soluble	NA	IR NMR 98%		NA NA	mp = 53-57°	68th/N
1780	**2,4-Hexadienyl acetate** Hexa-2,4-dienyl acetate *Sorbyl acetate*	4132 09.573 1516-17-2	C8H12O2 140.18	Colourless liquid; Powerful, sweet, pineapple aroma	Practically insoluble or insoluble in water Soluble	100° (20 mm Hg)	NMR 98%		1.470-1.476 0.928-0.932		68th/N
1781	**2,4-Hexadienyl propionate** Hexa-2,4-dienyl propionate *Sorbyl propionate*	4131 16491-25-1	C9H14O2 154.21	Colourless liquid; Sweet, fruity, pineapple, wine-like aroma	Practically insoluble or insoluble in water Soluble	75° (15 mm Hg)	NMR 98%		1.453-1.459 0.918-0.922		68th/N
1782	**2,4-Hexadienyl isobutyrate** Hexa-2,4-dienyl isobutyrate *Sorbyl isobutyrate*	4134 16491-24-0	C10H16O2 168.24	Light yellow liquid; Sweet, pineapple aroma with cinnamon undertones	Practically insoluble or insoluble in water Soluble	80° (15 mm Hg)	NMR 98%		1.464-1.470 0.902-0.906		68th/N
1783	**2,4-Hexadienyl butyrate** Hexa-2,4-dienyl butyrate *Sorbyl butyrate*	4133 16930-93-1	C10H16O2 168.24	Light yellow liquid; Fruity, wine-like aroma with cheesy undertones	Practically insoluble or insoluble in water Soluble	80° (15 mm Hg)	NMR 98%		1.467-1.473 0.908-0.912		68th/N
1784	**2,4-Heptadien-1-ol** Hepta-2,4-dien-1-ol	4127 02.153 33467-79-7	C7H12O 112.17	Colourless liquid; Green, fruity aroma	Slightly soluble Soluble	80° (14 mm Hg)	MS 95%		1.487-1.493 0.877-0.881		68th/N
1785	**Nona-2,4,6-trienal** Nona-2,4,6-trienal	4187 05.173 57018-53-8	C9H12O 136.19	Colourless liquid; Green, cucumber aroma	Practically insoluble or insoluble in water Soluble	193-194°	MS 95%		1.550-1.556 0.867-0.873		68th/N
1786	**2,4,7-Decatrienal** Deca-2,4,7-trienal	4089 05.141 51325-37-2	C10H14O 150.22	Orange liquid; Green, citrusy aroma	Practically insoluble or insoluble in water Soluble	232-234°	IR 98% (sum of three isomers)		1.538-1.544 0.900-0.904		68th/N