SPECIFICATIONS FOR CERTAIN FLAVOURINGS

At its 44th meeting JECFA considered a new approach to the safety evaluation of flavourings. This approach incorporates a series of criteria whose use enables the evaluation of a large number of these agents in a consistent and timely manner. At the 73rd meeting of the Committee specifications of identity and purity were prepared for 177 new flavourings (JECFA No. 1898-2042, 2044-2068 and 2070-2076, see page 50).

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

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

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

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

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

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

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

4. Information on the status of the safety evaluation.

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

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

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

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

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

Revised specifications

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

New specifications

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

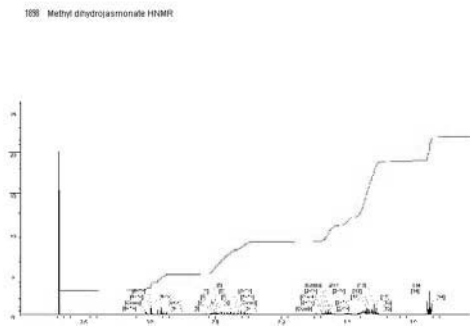
JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2064	**Benzyl levulinate**	4623	C12H14O3	Practically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

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

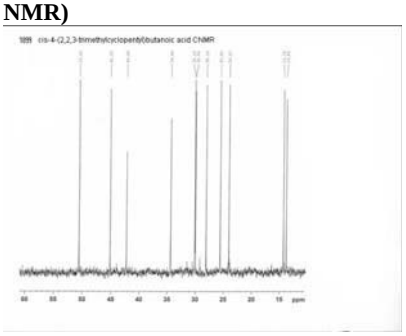
JECFA No	Name	FEMA	Chemical formula	Solubility	ID test	R. I.	Other requirements
	Chemical Name	FLAVIS	M.W.	Solubility in ethanol	Assay min %	S. G.	
Status	*Synonyms*	COE	Physical form / odour	B.P. °C	Acid Value		Information required
Session		CAS					
2073	**3-Octyl butyrate**	4402	C12H24O2	Practically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

Spectra of certain flavouring agents

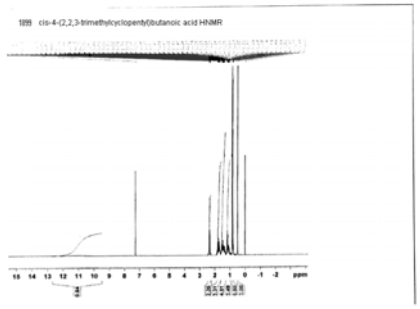
1898 Methyl dihydrojasmonate (1H-NMR)



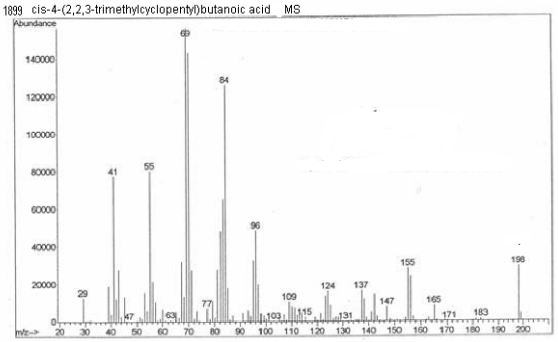
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (13C-NMR)



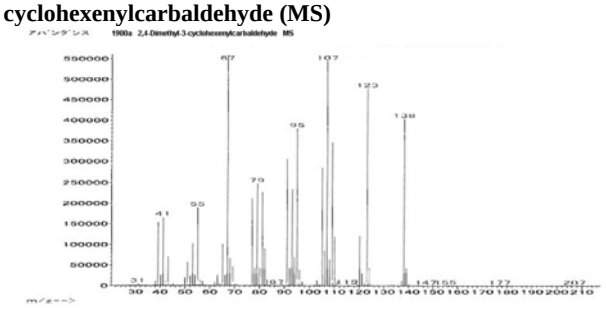
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (1H-NMR)



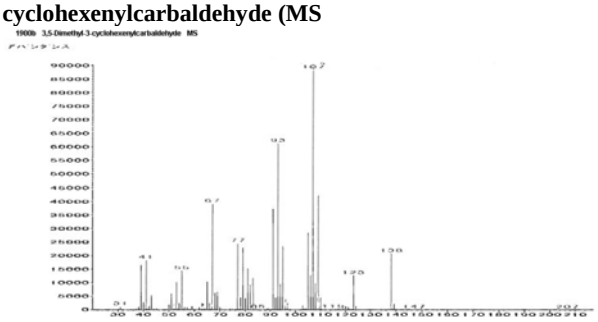
1899 cis-4-(2,2,3-Trimethylcyclopentyl)butanoic acid (MS)



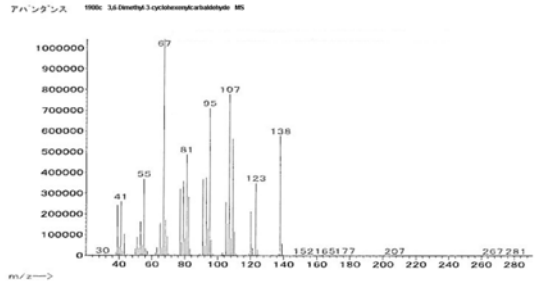
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS)



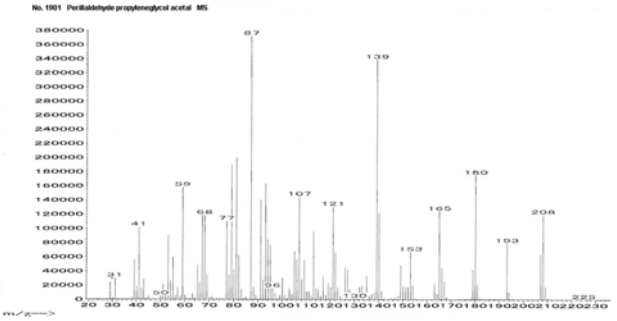
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS



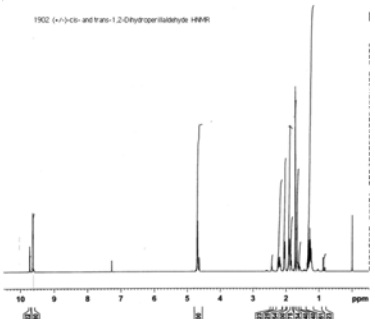
1900 Mixture of 2,4-, 3,5- and 3,6-Dimethyl-3-cyclohexenylcarbaldehyde (MS



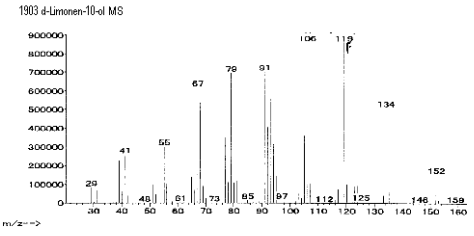
1901 Perillaldehyde propyleneglycol acetal (MS)



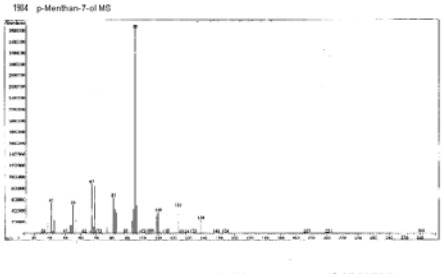
1902 (+/-)-cis- and trans-1,2-Dihydroperillaldehyde (1H-NMR)



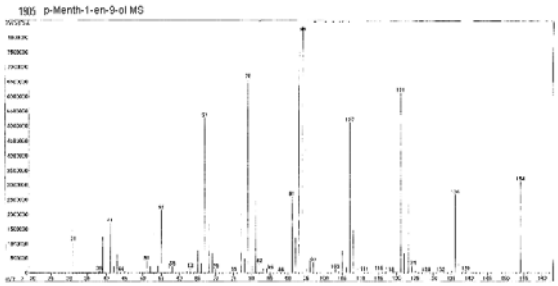
1903 d-Limonen-10-ol (MS)



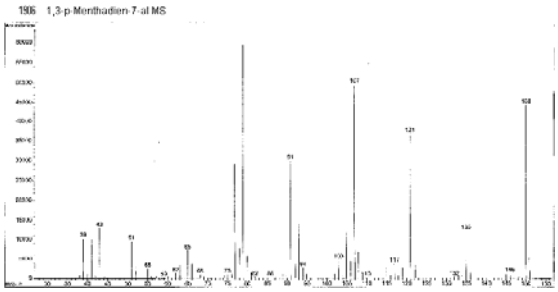
1904 p-Menthan-7-ol (MS)



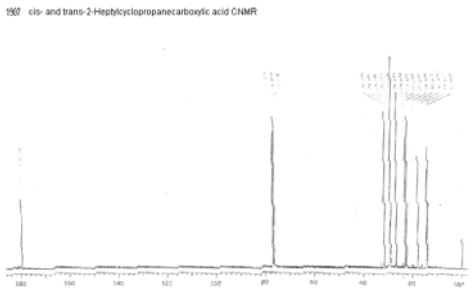
1905 p-Menth-1-en-9-ol (MS)



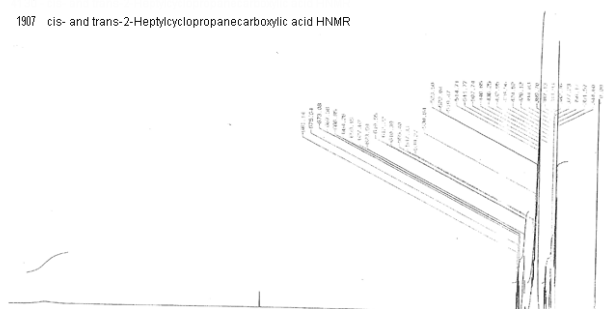
1906 1,3-p-Menthadien-7-al (MS)



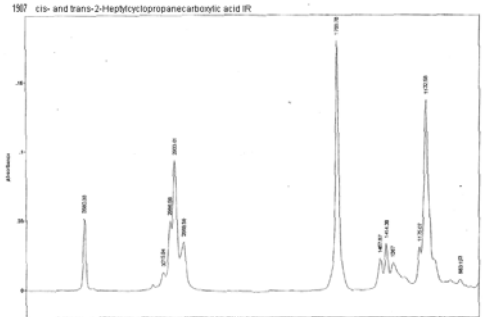
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (13C-NMR)



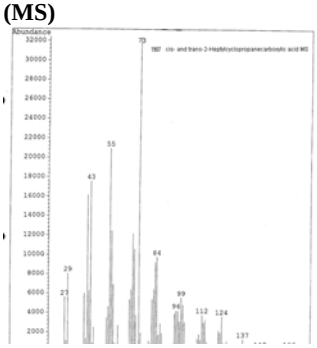
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (1H-NMR)



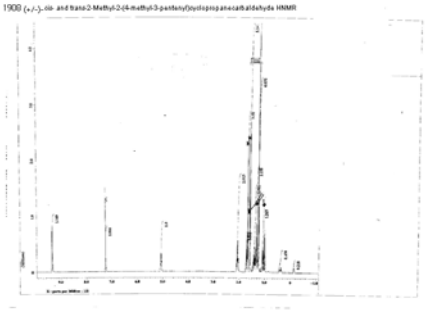
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (IR)



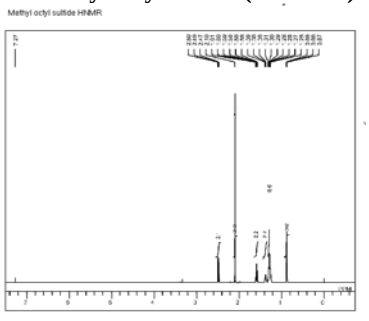
1907 cis- and trans-2-Heptylcyclopropanecarboxylic acid (MS)



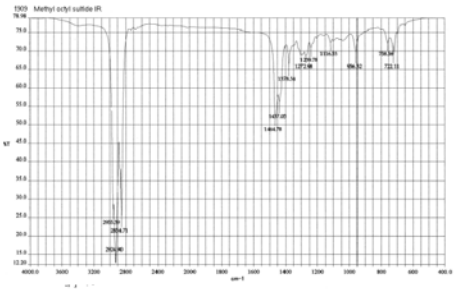
1908 (+/-)-cis- and trans-2-Methyl-2-(4-methyl-3-pentenyl)cyclopropanecarbaldehyde (1H-NMR)



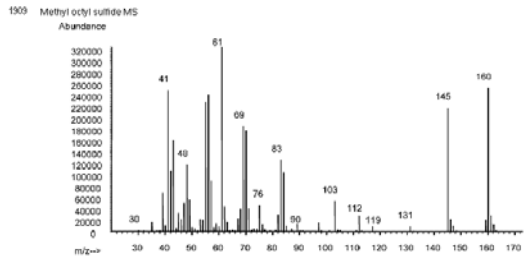
1909 Methyl octyl sulfide (1H-NMR)



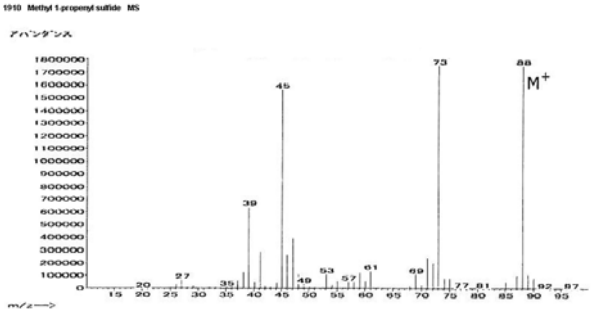
1909 Methyl octyl sulfide (IR)



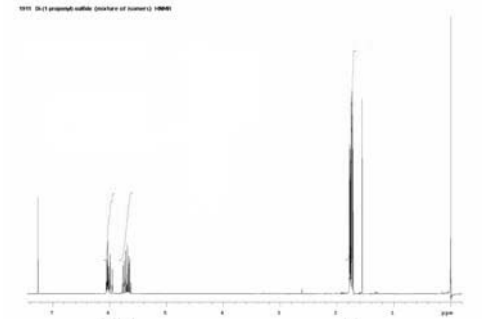
1909 Methyl octyl sulfide (MS)



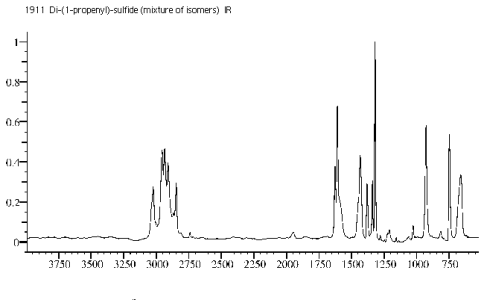
1910 Methyl 1-propenyl sulfide (MS)



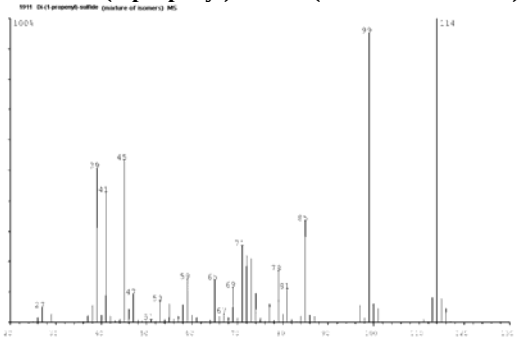
1911 Di-(1-propenyl) sulfide (mixture of isomers) (1H-NMR)



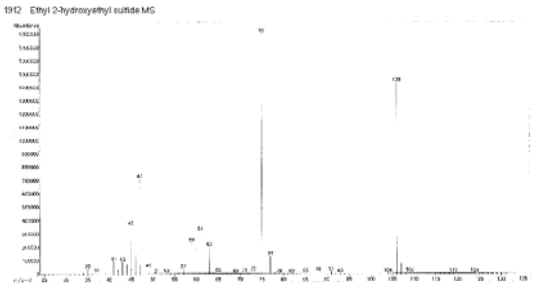
1911 Di-(1-propenyl) sulfide (mixture of isomers) (IR)



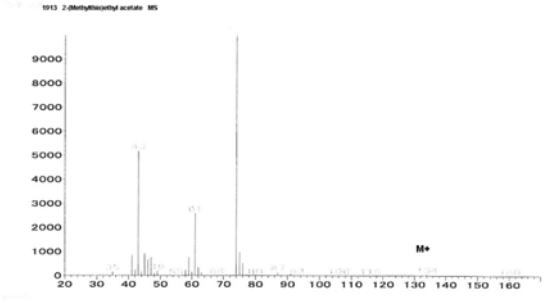
1911 Di-(1-propenyl) sulfide (mixture of isomers) (MS)



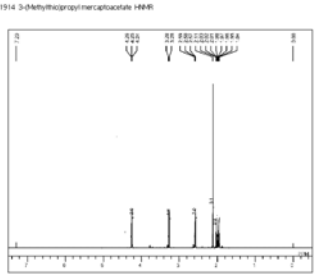
1912 Ethyl 2-hydroxyethyl sulfide (MS)



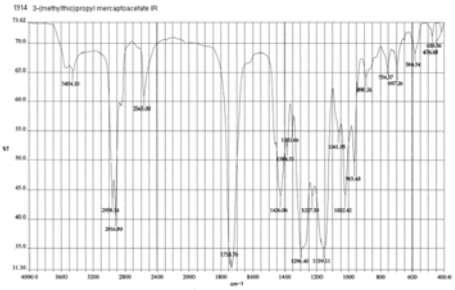
1913 2-(Methylthio)ethyl acetate (MS)



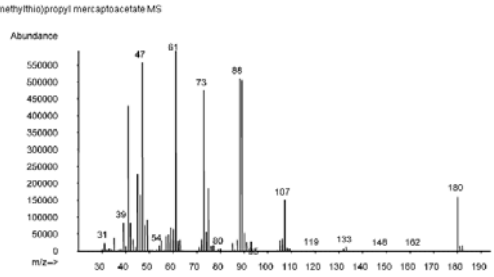
1914 3-(Methylthio)propyl mercaptoacetate (1H-NMR)



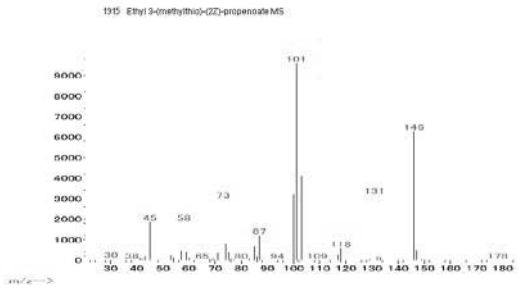
1914 3-(Methylthio)propyl mercaptoacetate (IR)



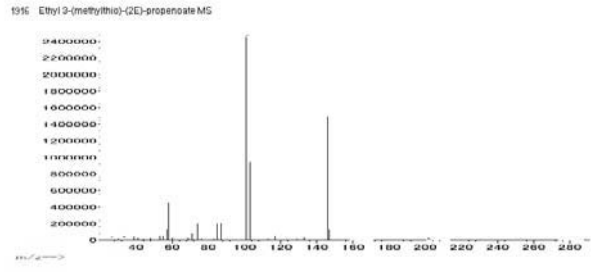
1914 3-(Methylthio)propyl mercaptoacetate (MS)



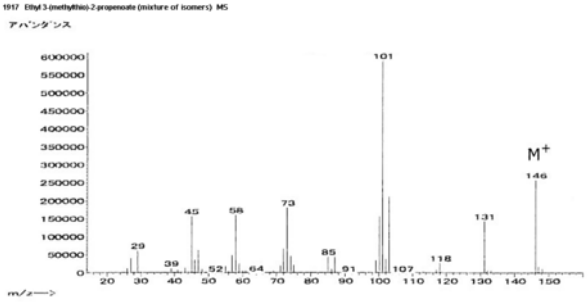
1915 Ethyl 3-(methylthio)-(2Z)-propenoate (MS)



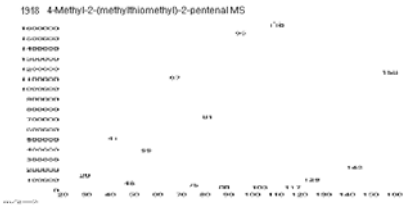
1916 Ethyl 3-(methylthio)-(2E)-propenoate (MS)



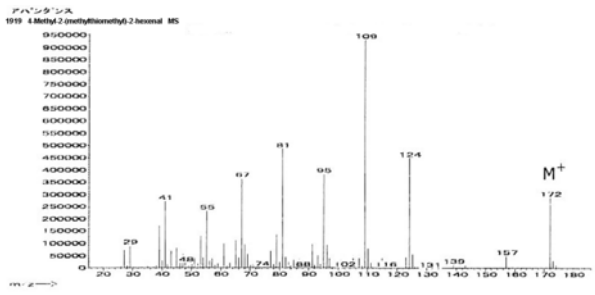
1917 Ethyl 3-(methylthio)-2-propenoate (mixture of isomers) (MS)



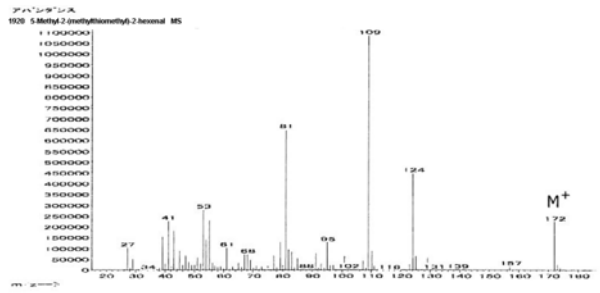
1918 4-Methyl-2-(methylthiomethyl)-2-pentenal (MS)



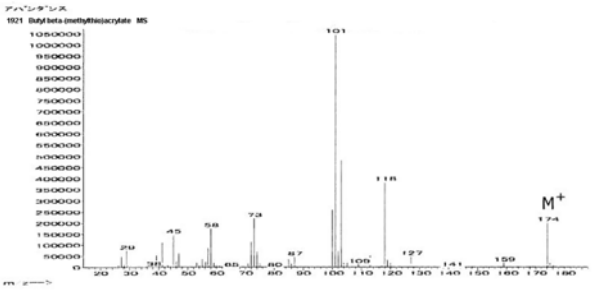
1919 4-Methyl-2-(methylthiomethyl)-2-hexenal (MS)



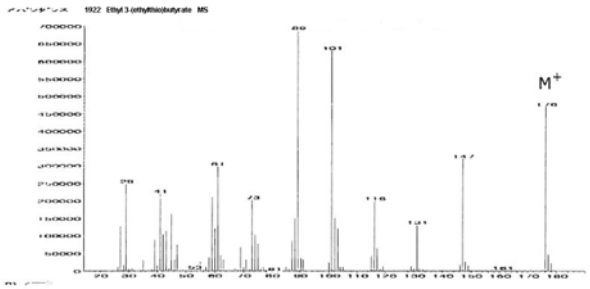
1920 5-Methyl-2-(methylthiomethyl)-2-hexenal (MS)



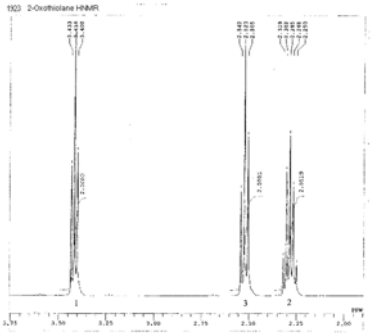
1921 Butyl beta-(methylthio)acrylate (MS)



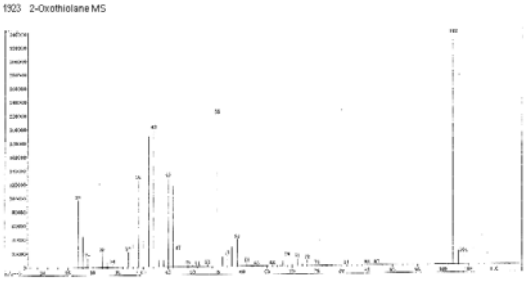
1922 Ethyl 3-(ethylthio)butyrate (MS)



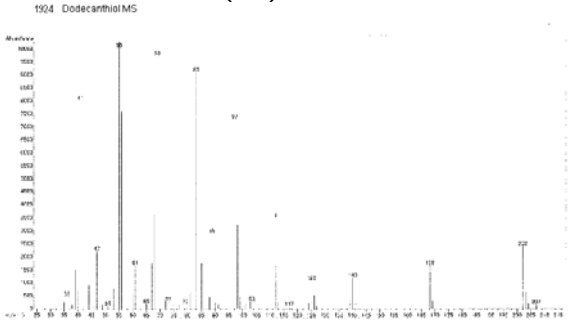
1923 2-Oxothiolane (1H-NMR)



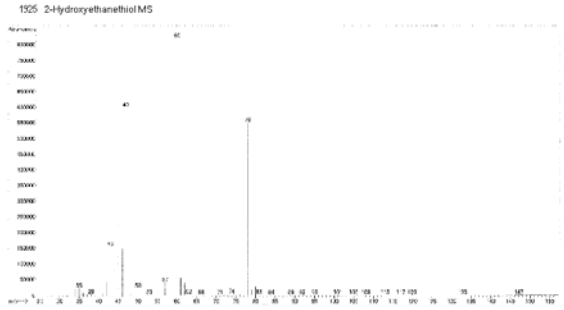
1923 2-Oxothiolane (MS)



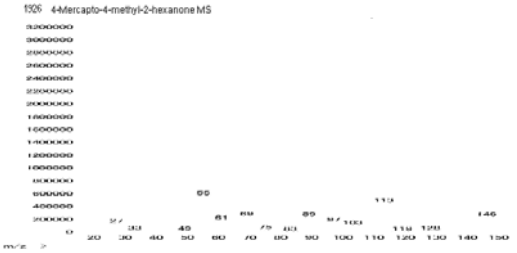
1924 Dodecanethiol (MS)



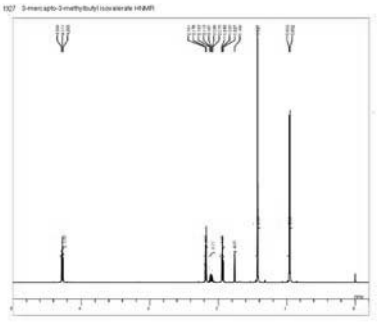
1925 2-Hydroxyethanethiol (MS)



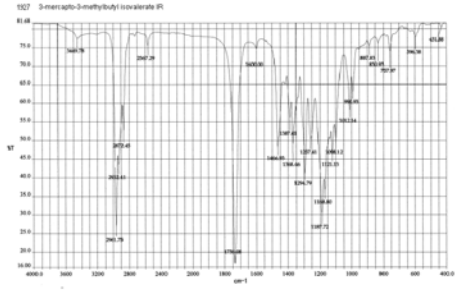
1926 4-Mercapto-4-methyl-2-hexanone (MS)



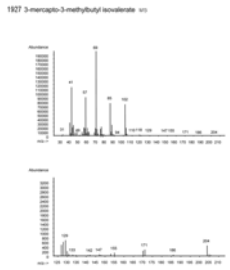
1927 3-Mercapto-3-methylbutyl isovalerate (1H-NMR)



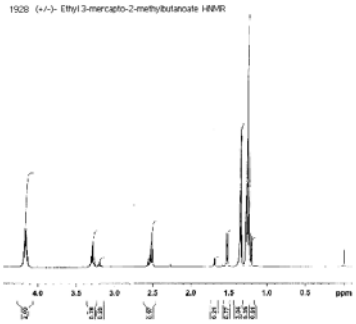
1927 3-Mercapto-3-methylbutyl isovalerate (IR)



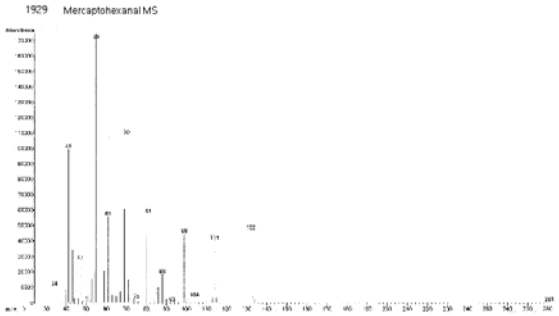
1927 3-Mercapto-3-methylbutyl isovalerate (MS)



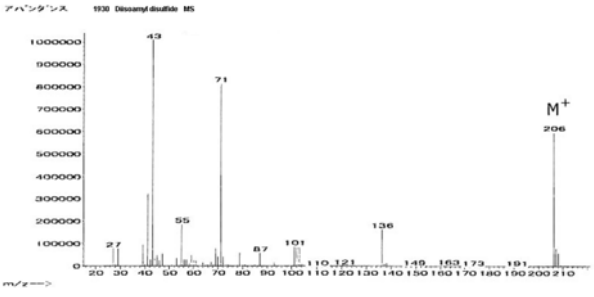
1928 (+/-)-Ethyl 3-mercapto-2-methylbutanoate (1H-NMR)



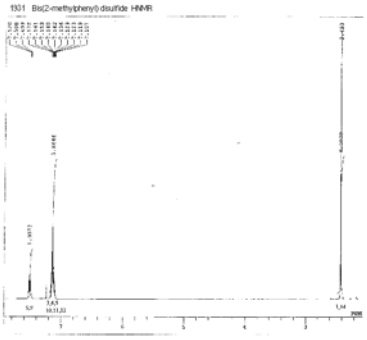
1929 3-Mercaptohexanal (MS)



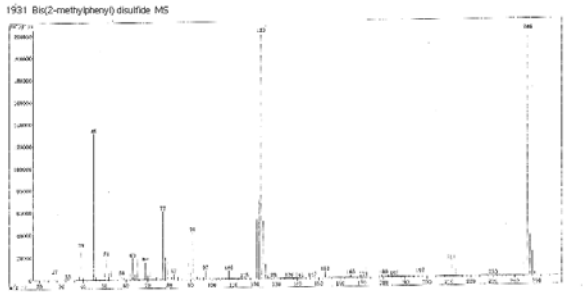
1930 Diisoamyl disulfide (MS)



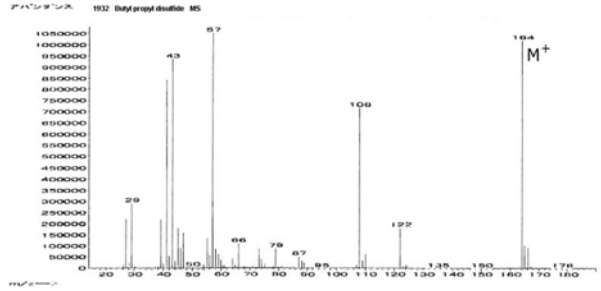
1931 Bis(2-methylphenyl) disulfide (1H-NMR)



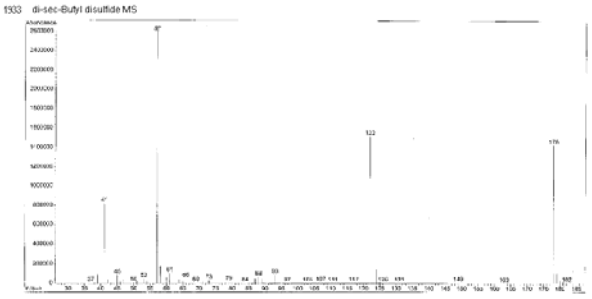
1931 Bis(2-methylphenyl) disulfide (MS)



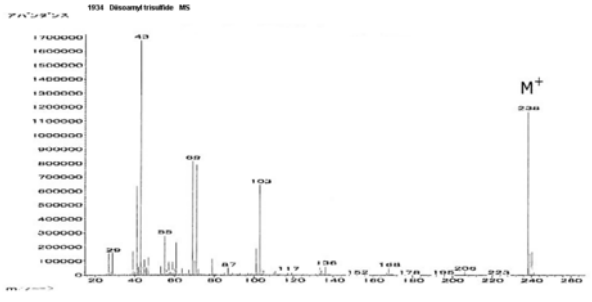
1932 Butyl propyl disulfide (MS)



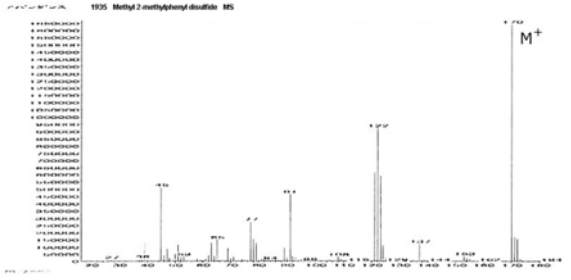
1933 di-sec-Butyl disulfide (MS)



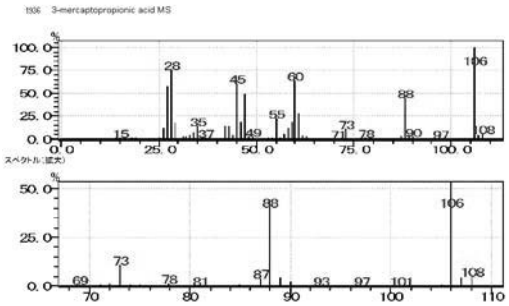
1934 Diisoamyl trisulfide (MS)



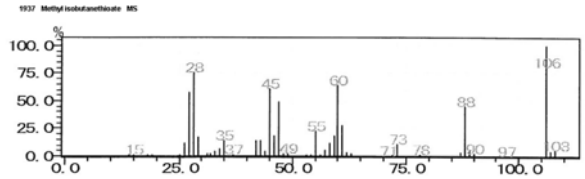
1935 Methyl 2-methylphenyl disulfide (MS)



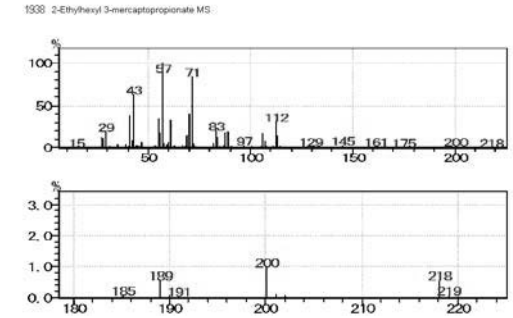
1936 3-Mercaptopropionic acid (MS)



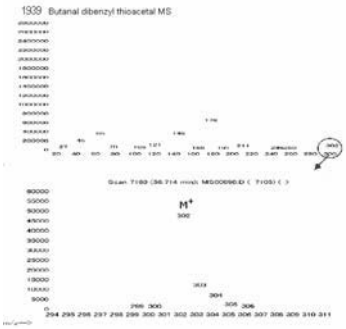
1937 Methyl isobutanethioate (MS)



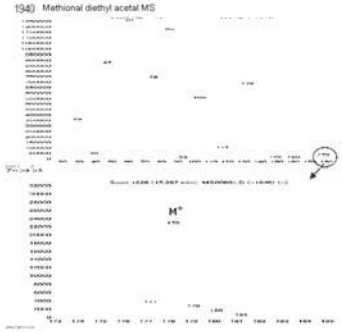
1938 2-Ethylhexyl 3-mercaptopropionate (MS)



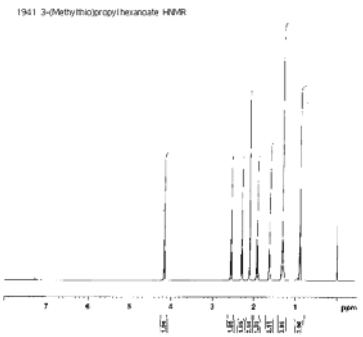
1939 Butanal dibenzyl thioacetal (MS)



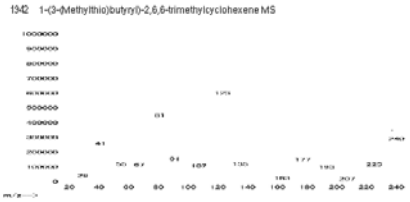
1940 Methional diethyl acetal (MS)



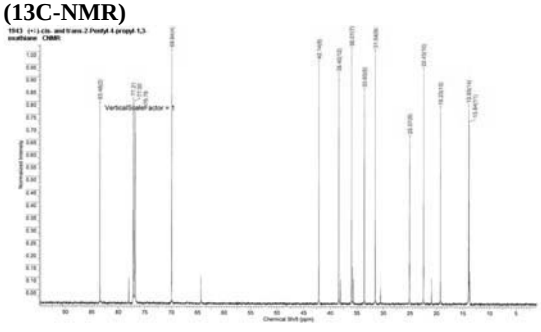
1941 3-(Methylthio)propyl hexanoate (1H-NMR)



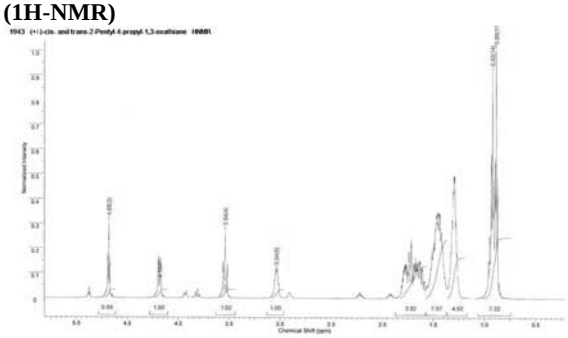
1942 1-(3-(Methylthio)-butyryl)-2,6,6-trimethylcyclohexene (MS)



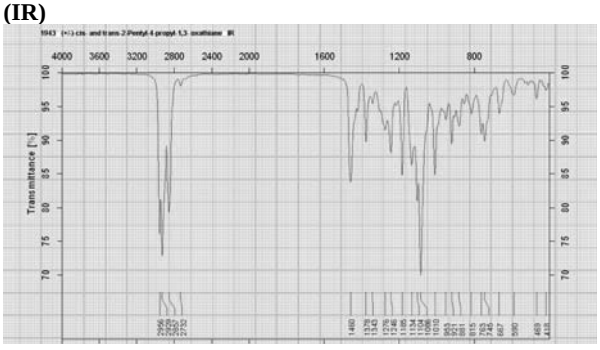
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (13C-NMR)



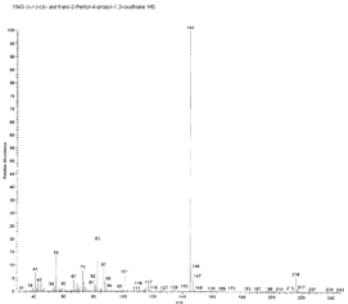
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (1H-NMR)



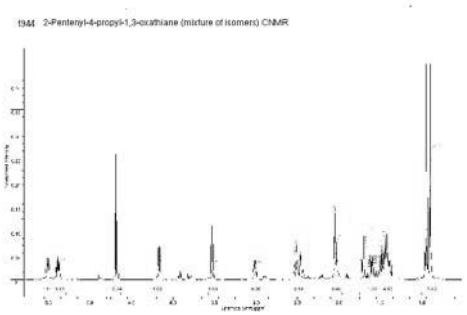
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (IR)



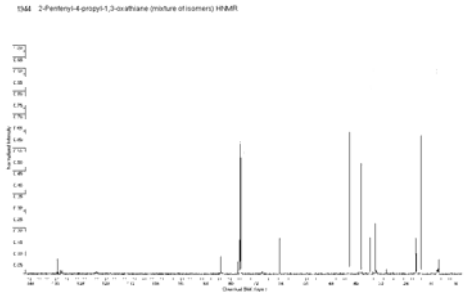
1943 (+/-)-cis- and trans-2-Pentyl-4-propyl-1,3-oxathiane (MS)



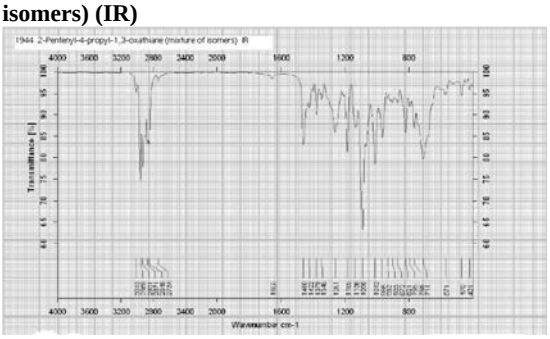
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (13C-NMR)



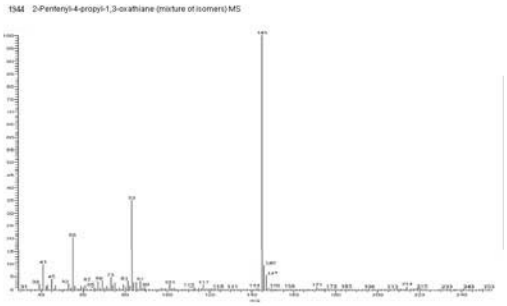
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (1H-NMR)



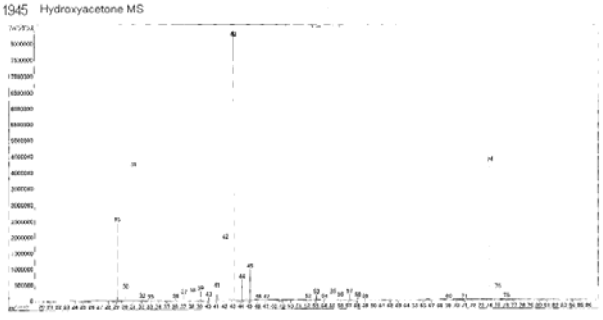
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (IR)



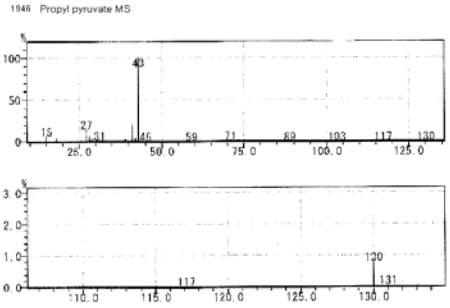
1944 2-Pentenyl-4-propyl-1,3-oxathiane (mixture of isomers) (MS)



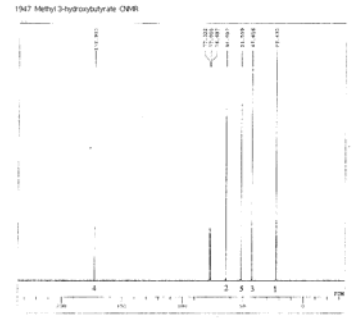
1945 Hydroxyacetone (MS)



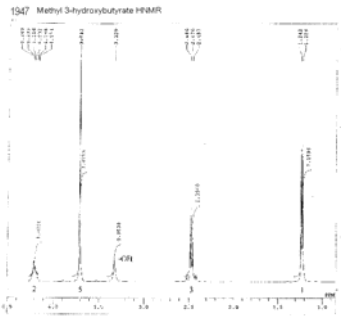
1946 Propyl pyruvate (MS)



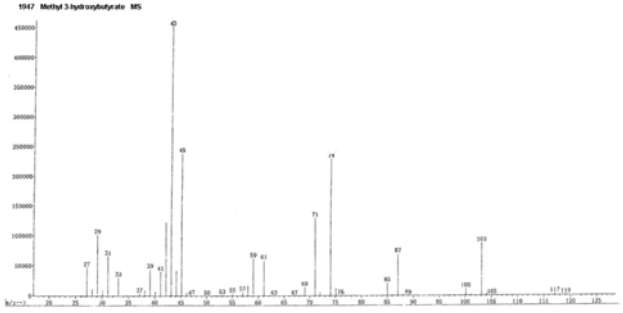
1947 Methyl 3-hydroxybutyrate (13C-NMR)



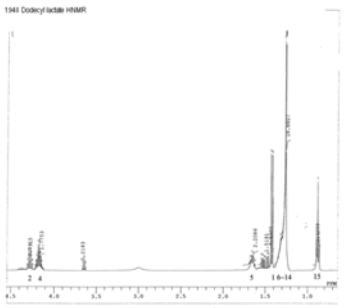
1947 Methyl 3-hydroxybutyrate (1H-NMR)



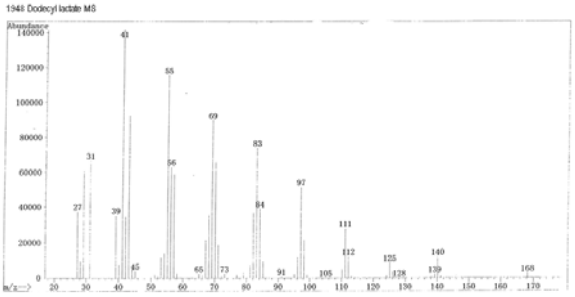
1947 Methyl 3-hydroxybutyrate (MS)



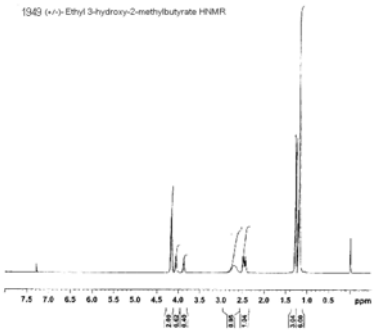
1948 Dodecyl lactate (1H-NMR)



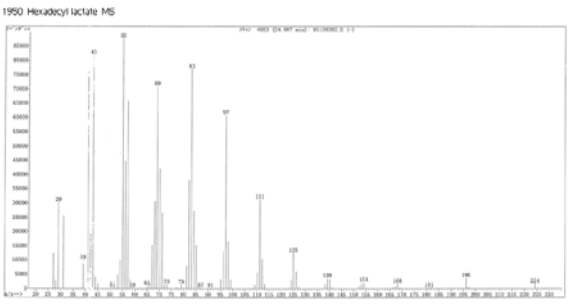
1948 Dodecyl lactate (MS)



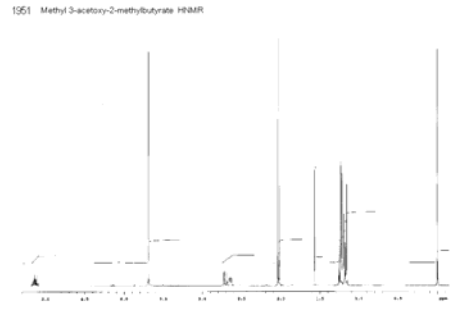
1949 (+/-)-Ethyl 3-hydroxy-2-methylbutyrate (1H-NMR)



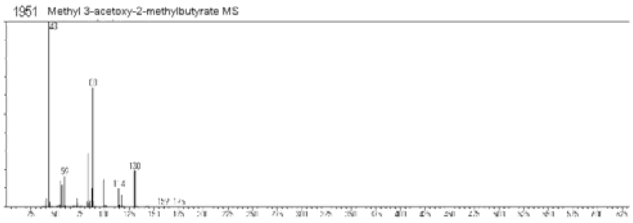
1950 Hexadecyl lactate (MS)



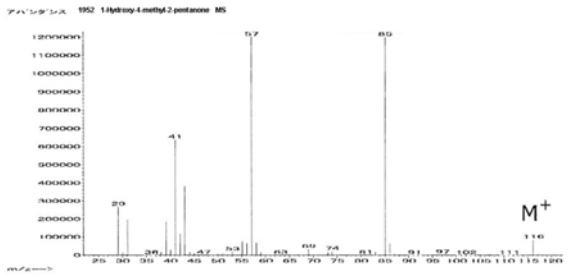
1951 Methyl 3-acetoxy-2-methylbutyrate (1H-NMR)



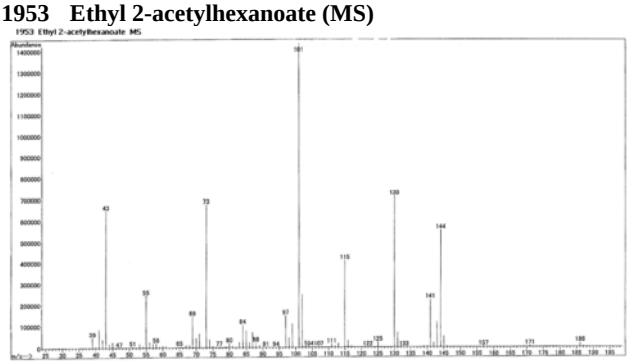
1951 Methyl 3-acetoxy-2-methylbutyrate (MS)



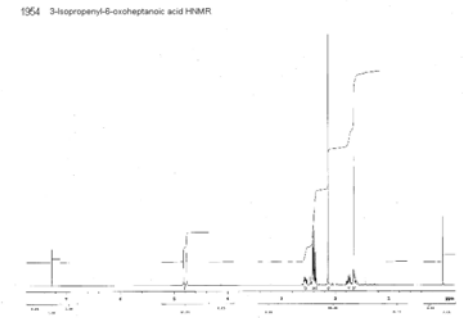
1952 1-Hydroxy-4-methyl-2-pentanone (MS)



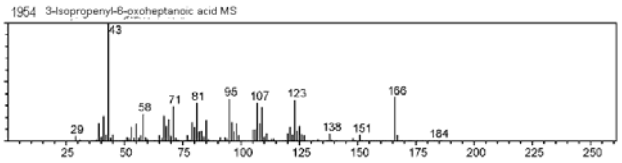
1953 Ethyl 2-acetylhexanoate (MS)



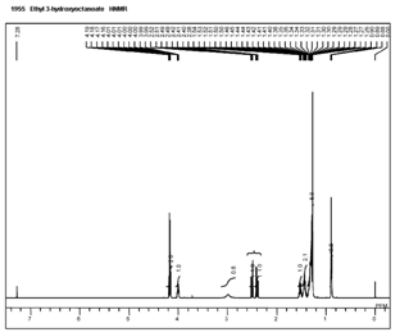
1954 3-Isopropenyl-6-oxoheptanoic acid (1H-NMR)



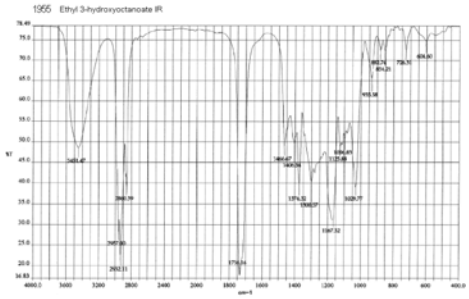
1954 3-Isopropenyl-6-oxoheptanoic acid (MS)



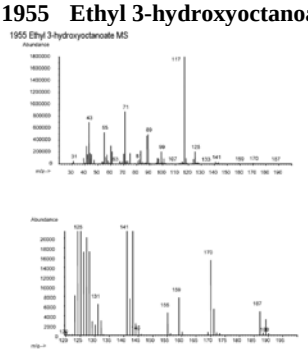
1955 Ethyl 3-hydroxyoctanoate (1H-NMR)



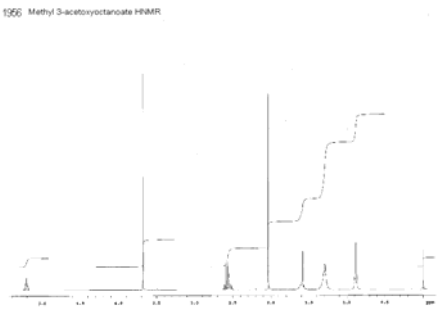
1955 Ethyl 3-hydroxyoctanoate (IR)



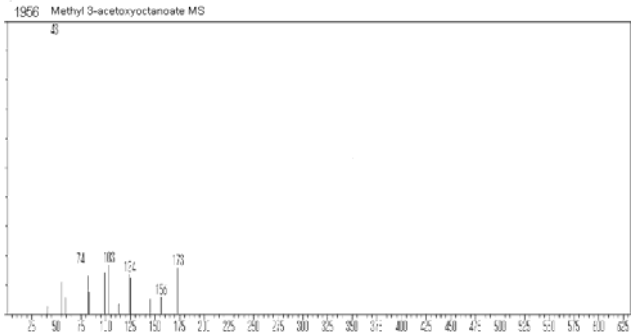
1955 Ethyl 3-hydroxyoctanoate (MS)



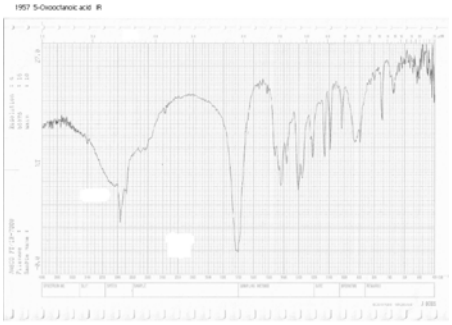
1956 Methyl 3-acetoxyoctanoate (1H-NMR)



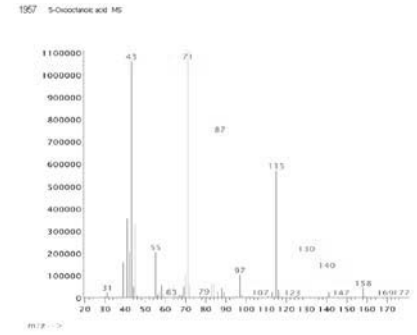
1956 Methyl 3-acetoxyoctanoate (MS)



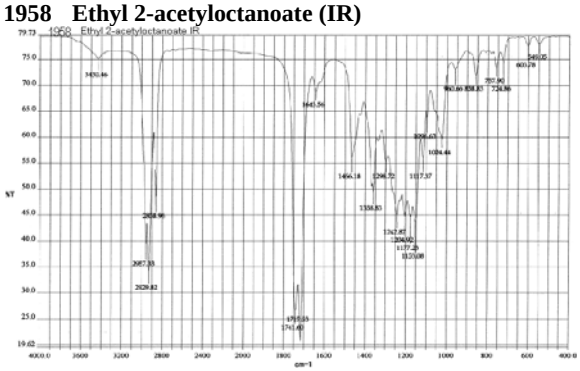
1957 5-Oxooctanoic acid (IR)



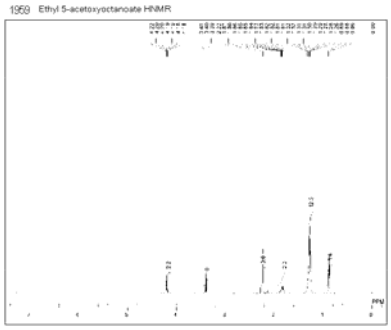
1957 5-Oxooctanoic acid (MS)



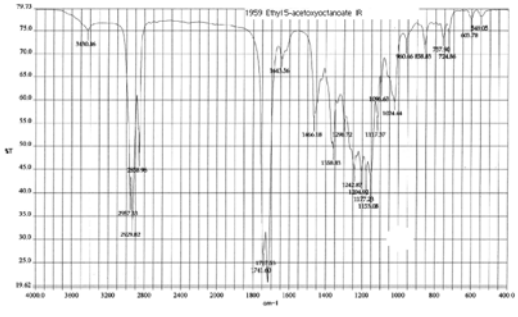
1958 Ethyl 2-acetyloctanoate (IR)



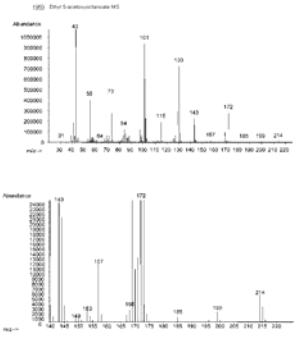
1959 Ethyl 5-acetoxyoctanoate (1H-NMR)



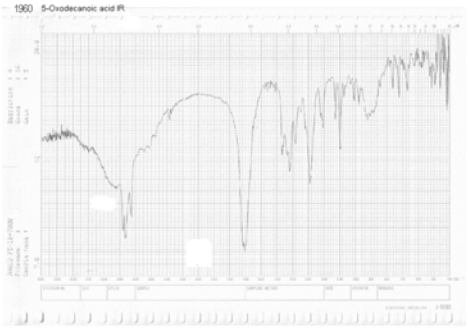
1959 Ethyl 5-acetoxyoctanoate (IR)



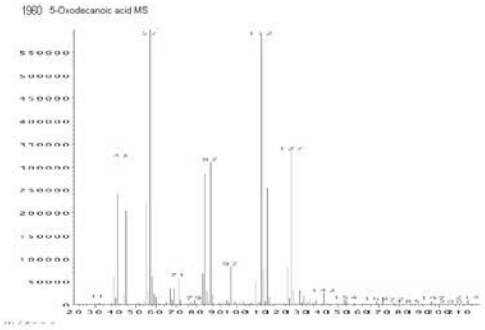
1959 Ethyl 5-acetoxyoctanoate (MS)



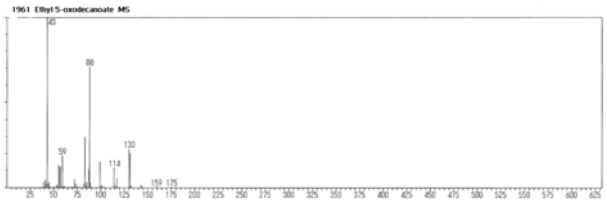
1960 5-Oxodecanoic acid (IR)



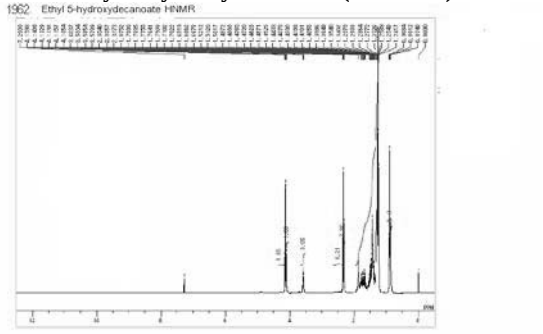
1960 5-Oxodecanoic acid (MS)



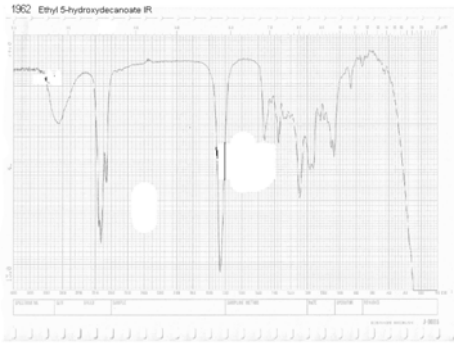
1961 Ethyl 5-oxodecanoate (MS)



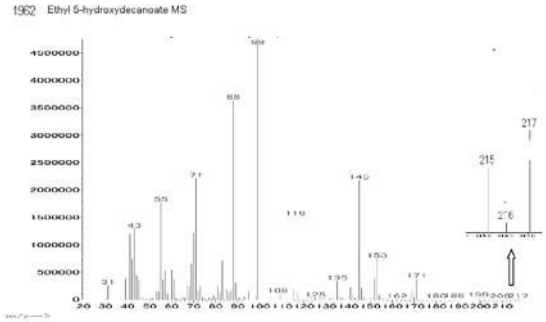
1962 Ethyl 5-hydroxydecanoate (1H-NMR)



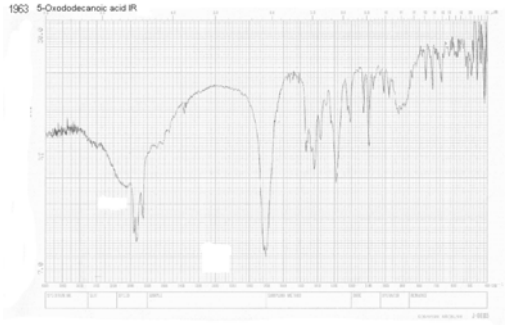
1962 Ethyl 5-hydroxydecanoate (IR)



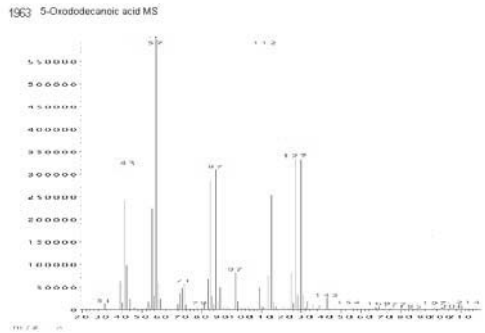
1962 Ethyl 5-hydroxydecanoate (MS)



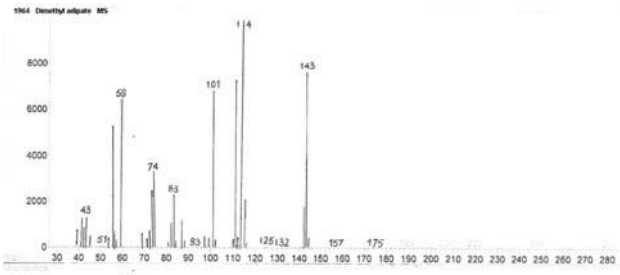
1963 5-Oxododecanoic acid (IR)



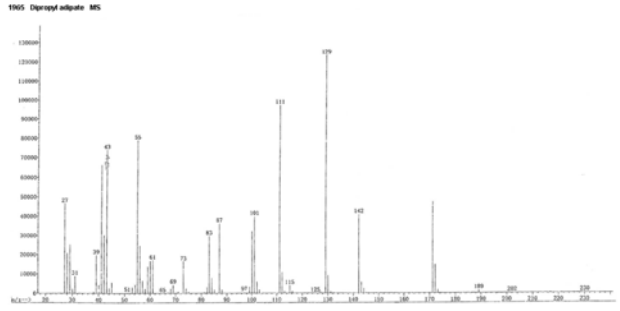
1963 5-Oxododecanoic acid (MS)



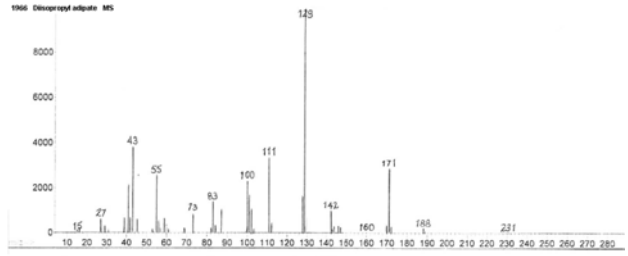
1964 Dimethyl adipate (MS)



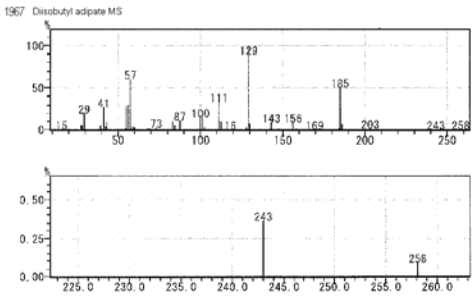
1965 Dipropyl adipate (MS)



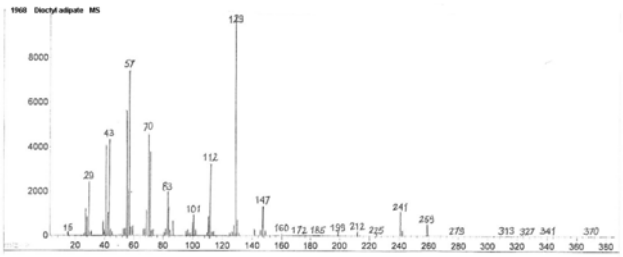
1966 Diisopropyl adipate (MS)



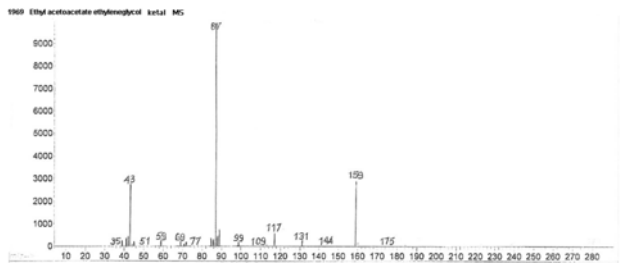
1967 Diisobutyl adipate (MS)



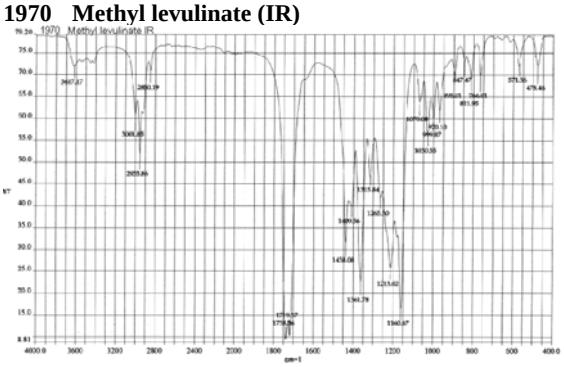
1968 Dioctyl adipate (MS)



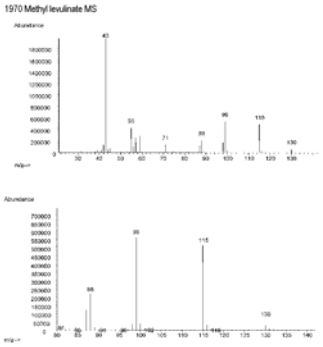
1969 Ethyl acetoacetate ethyleneglycol ketal (MS)



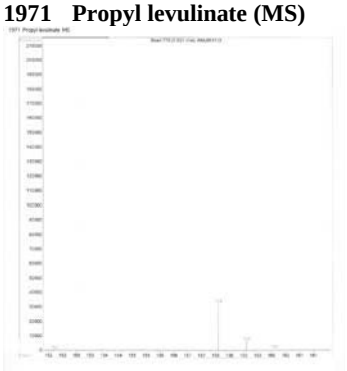
1970 Methyl levulinate (IR)



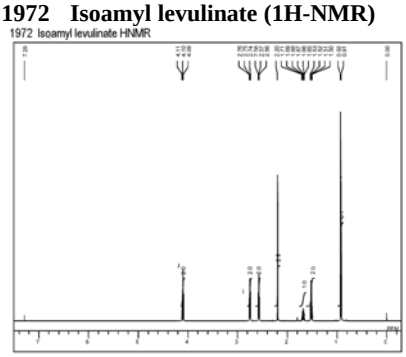
1970 Methyl levulinate (MS)



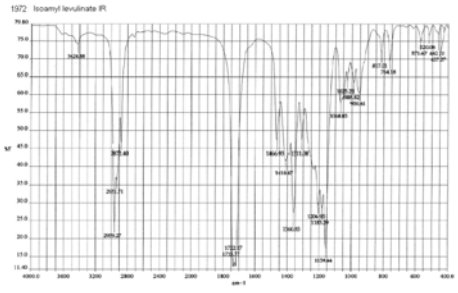
1971 Propyl levulinate (MS)



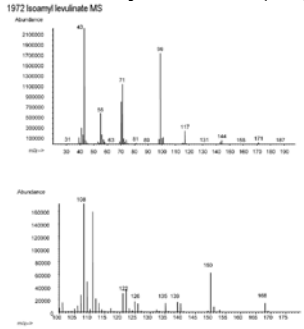
1972 Isoamyl levulinate (1H-NMR)



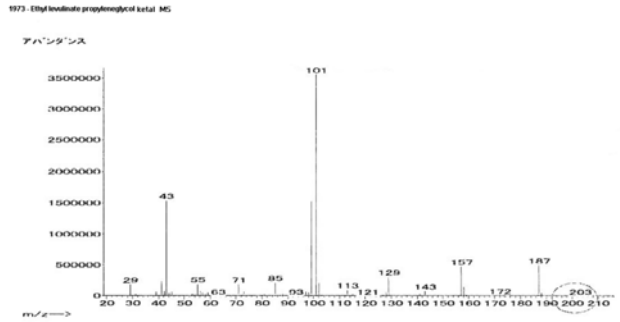
1972 Isoamyl levulinate (IR)



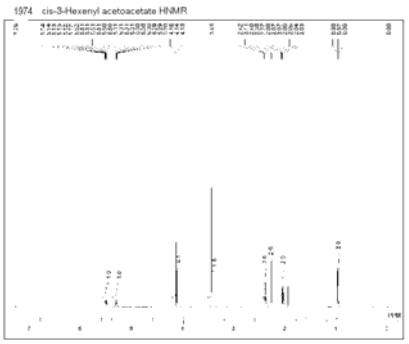
1972 Isoamyl levulinate (MS)



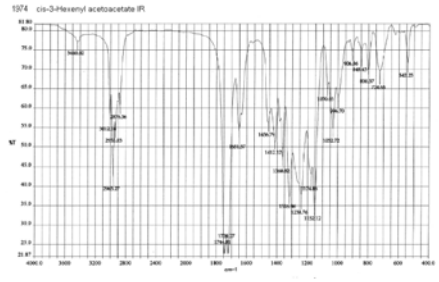
1973 Ethyl levulinate propyleneglycol ketal (MS)



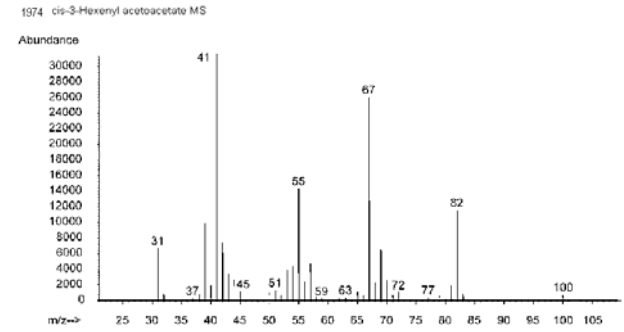
1974 cis-3-Hexenyl acetoacetate (1H-NMR)



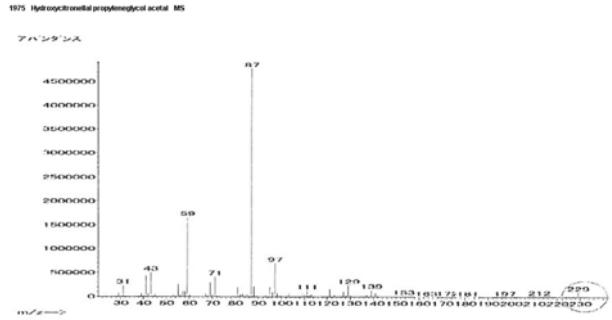
1974 cis-3-Hexenyl acetoacetate (IR)



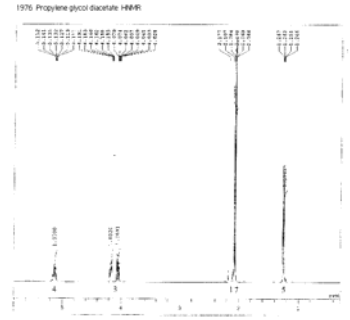
1974 cis-3-Hexenyl acetoacetate (MS)



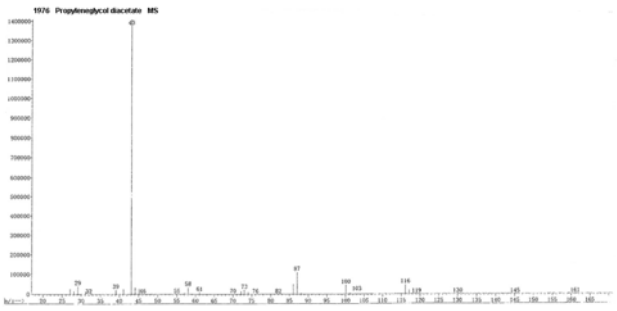
1975 Hydroxycitronellal propyleneglycol acetal (MS)



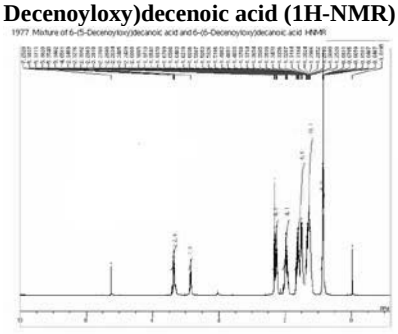
1976 Propyleneglycol diacetate (1H-NMR)



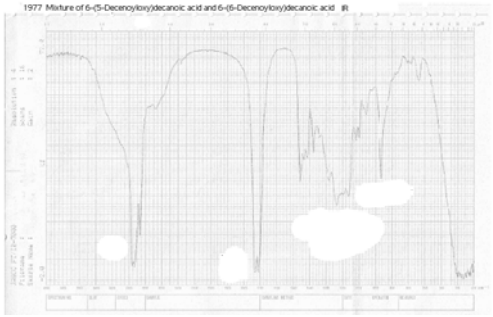
1976 Propyleneglycol diacetate (MS)



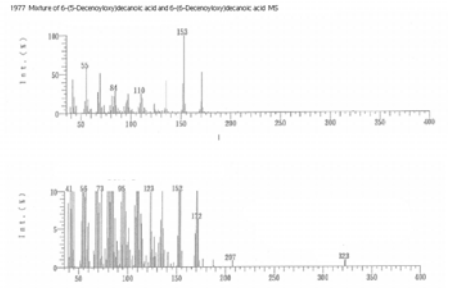
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (1H-NMR)



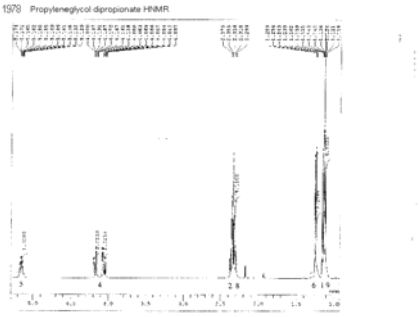
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (IR)



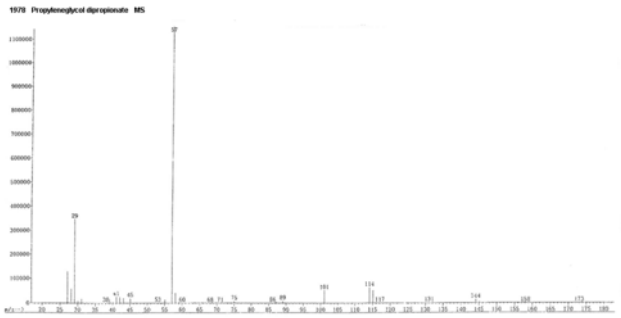
1977 Mixture of 6-(5-Decenoyloxy)decenoic acid and 6-(6-Decenoyloxy)decenoic acid (MS)



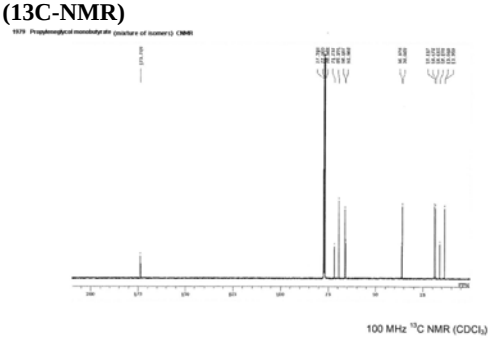
1978 Propyleneglycol dipropionate (1H-NMR)



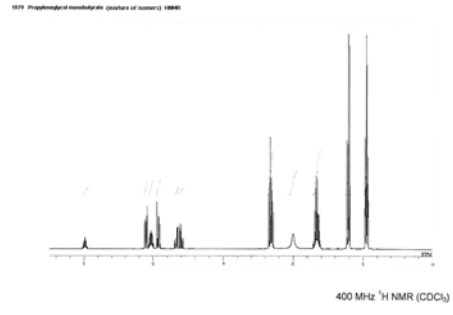
1978 Propyleneglycol dipropionate (MS)



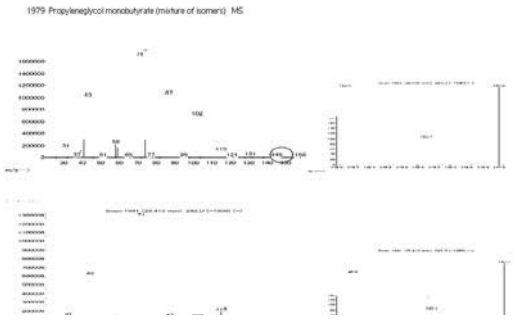
1979 Propyleneglycol monobutyrate (mixture of isomers) (13C-NMR)



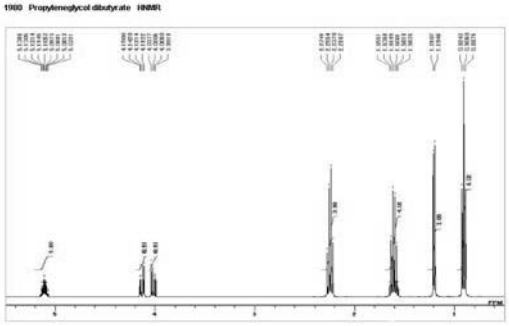
1979 Propyleneglycol monobutyrate (mixture of isomers) (1H-NMR)



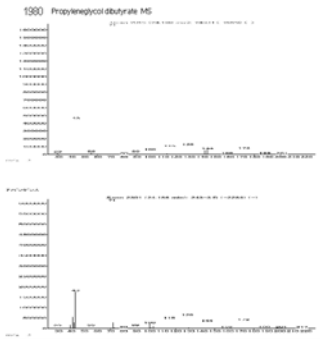
1979 Propyleneglycol monobutyrate (mixture of isomers) (MS)



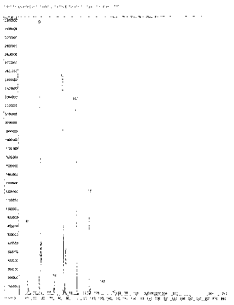
1980 Propyleneglycol dibutyrate (1H-NMR)



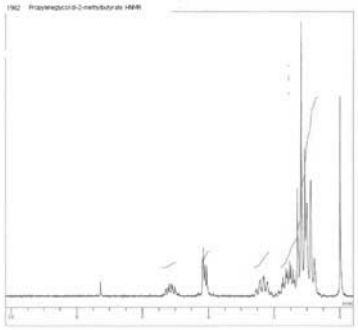
1980 Propyleneglycol dibutyrate (MS)



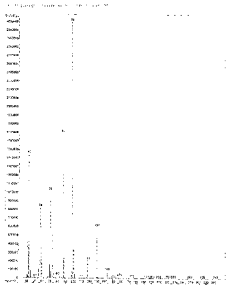
1981 Propyleneglycol mono-2-methylbutyrate (mixture of isomers) (MS)



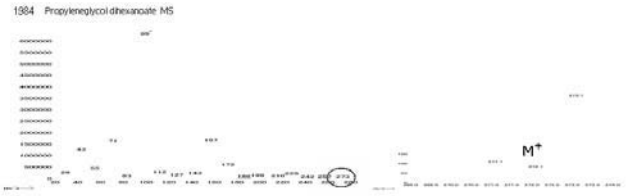
1982 Propyleneglycol di-2-methylbutyrate (1H-NMR)



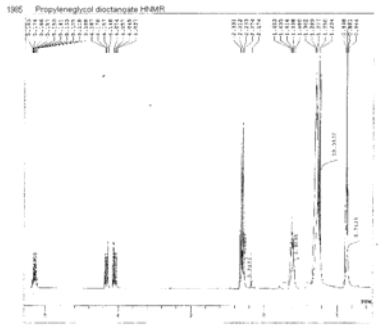
1983 Propyleneglycol monohexanoate (mixture of isomers) (MS)



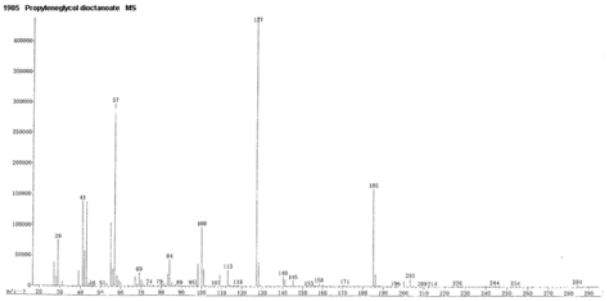
1984 Propyleneglycol dihexanoate (MS)



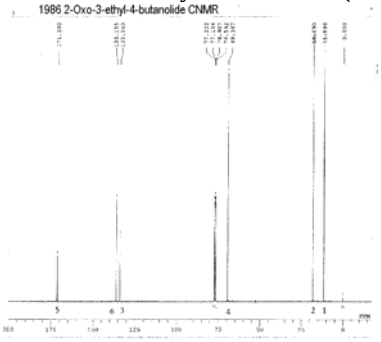
1985 Propyleneglycol dioctanoate (1H-NMR)



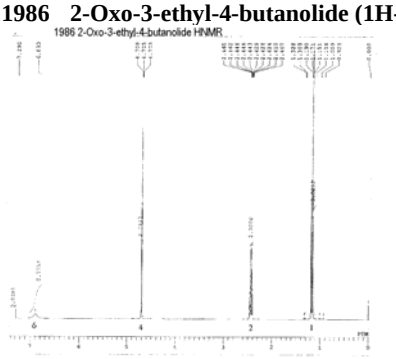
1985 Propyleneglycol dioctanoate (MS)



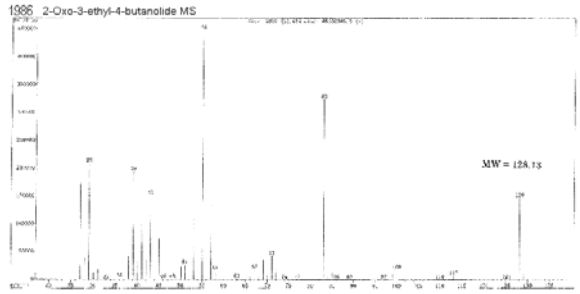
1986 2-Oxo-3-ethyl-4-butanolide (13C-NMR)



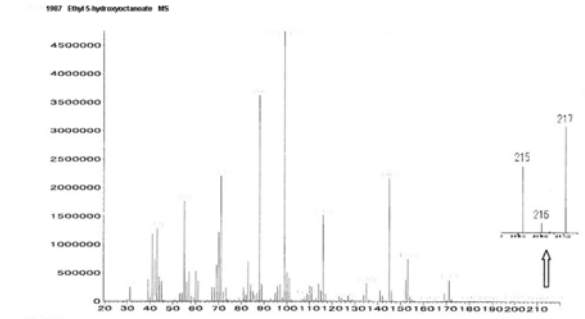
1986 2-Oxo-3-ethyl-4-butanolide (1H-NMR)



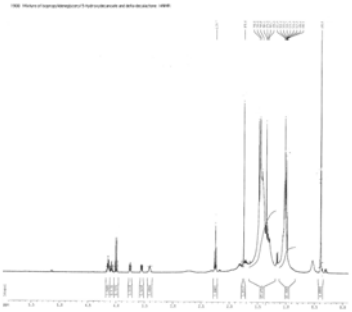
1986 2-Oxo-3-ethyl-4-butanolide (MS)



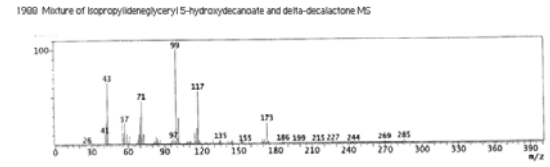
1987 Ethyl 5-hydroxyoctanoate (MS)



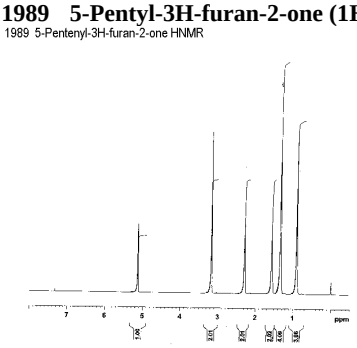
1988 Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone (1H-NMR)



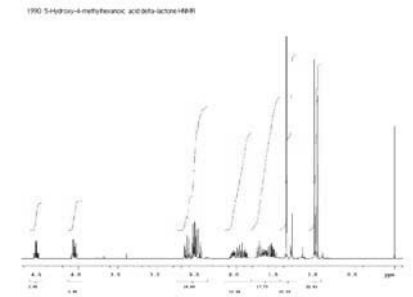
1988 Mixture of Isopropylideneglyceryl 5-hydroxydecanoate and delta-Decalactone (MS)



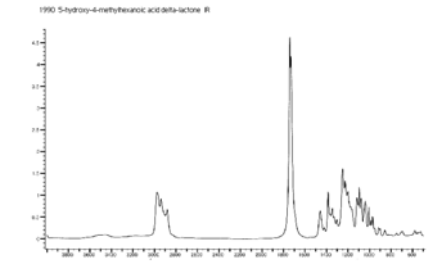
1989 5-Pentyl-3H-furan-2-one (1H-NMR)



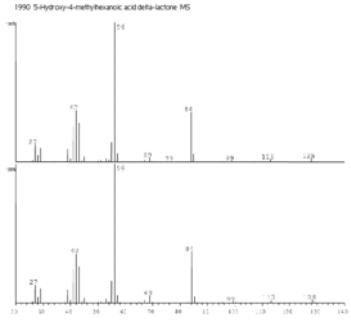
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (1H-NMR)



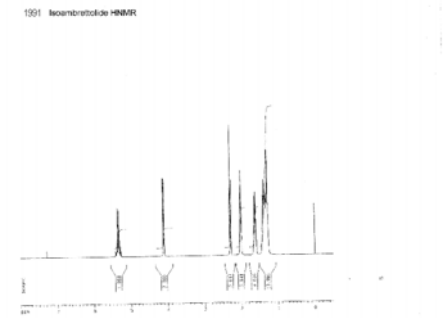
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (IR)



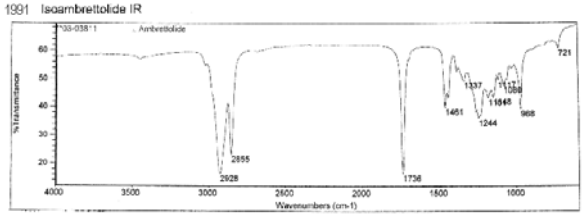
1990 5-Hydroxy-4-methylhexanoic acid delta-lactone (MS)



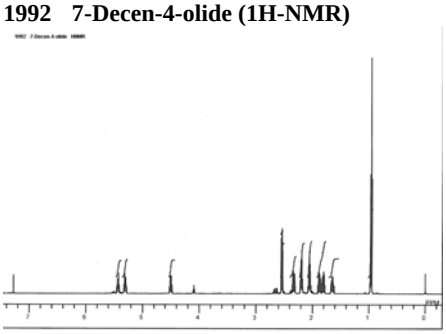
1991 Isoambrettolide (1H-NMR)



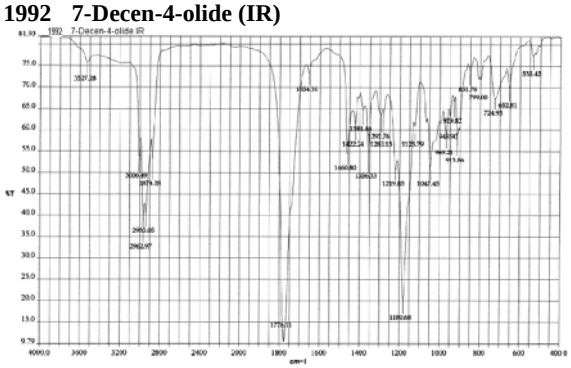
1991 Isoambrettolide (IR)



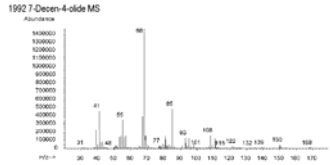
1992 7-Decen-4-olide (1H-NMR)

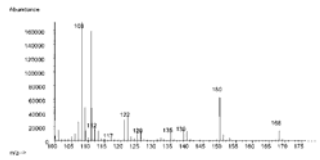


1992 7-Decen-4-olide (IR)

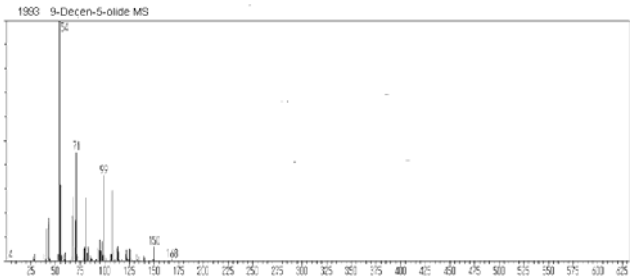


1992 7-Decen-4-olide (MS)

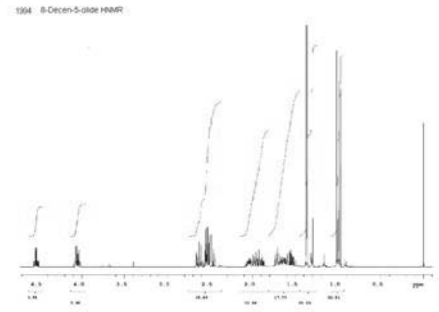




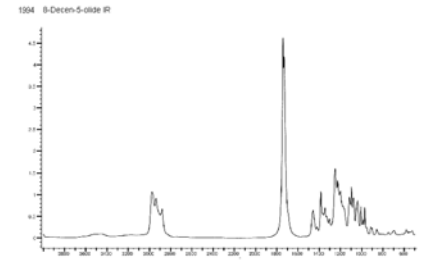
1993 9-Decen-5-olide (MS)



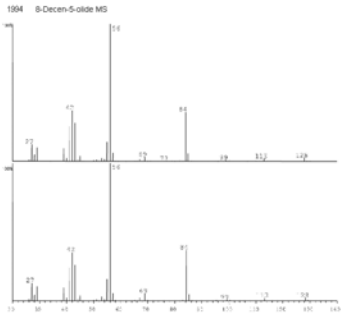
1994 8-Decen-5-olide (1H-NMR)



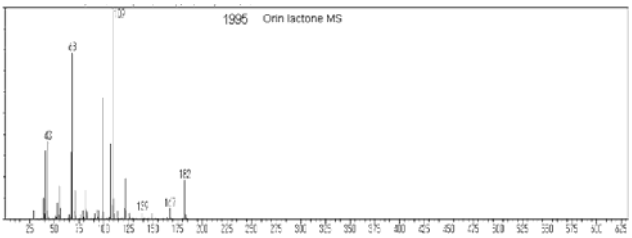
1994 8-Decen-5-olide (IR)



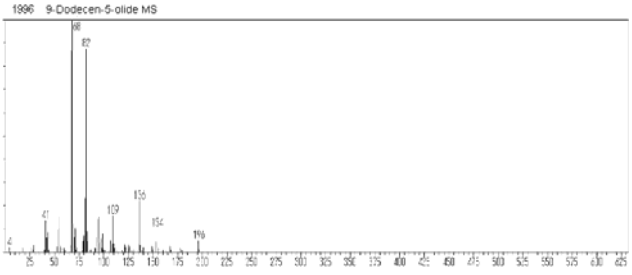
1994 8-Decen-5-olide (MS)



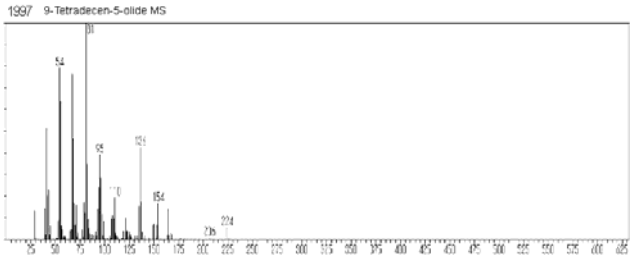
1995 Orin lactone (MS)



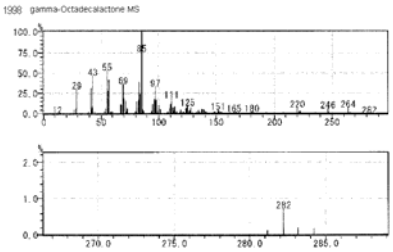
1996 9-Dodecen-5-olide (MS)



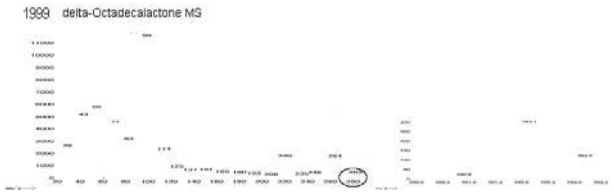
1997 9-Tetradecen-5-olide (MS)



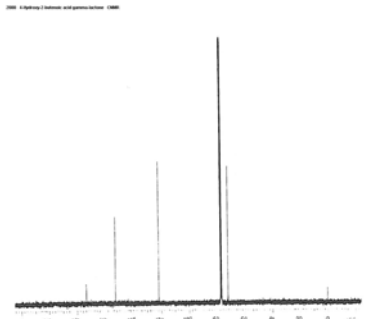
1998 gamma-Octadecalactone (MS)



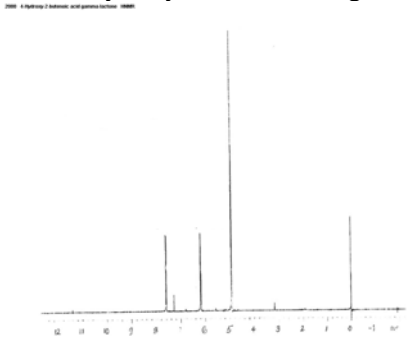
1999 delta-Octadecalactone (MS)



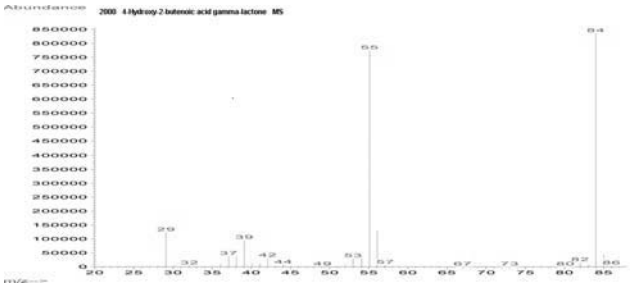
2000 4-Hydroxy-2-butenoic acid gamma-lactone (13C-NMR)



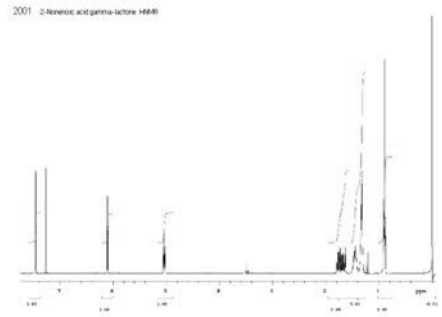
2000 4-Hydroxy-2-butenoic acid gamma-lactone (1H-NMR)



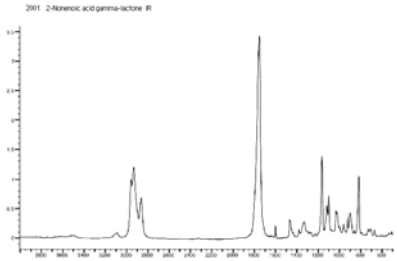
2000 4-Hydroxy-2-butenoic acid gamma-lactone (MS)



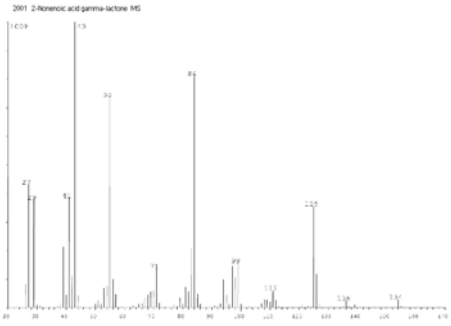
2001 2-Nonenoic acid gamma-lactone (1H-NMR)



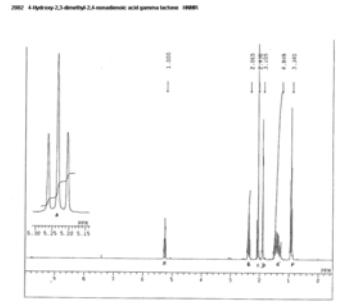
2001 2-Nonenoic acid gamma-lactone (IR)



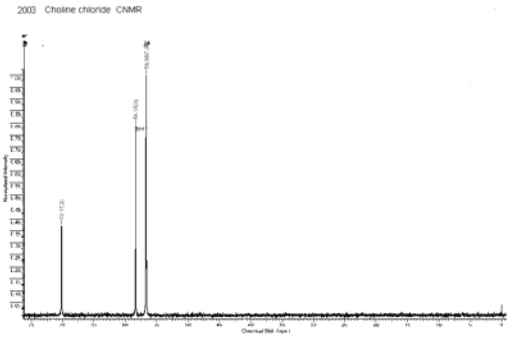
2001 2-Nonenoic acid gamma-lactone (MS)



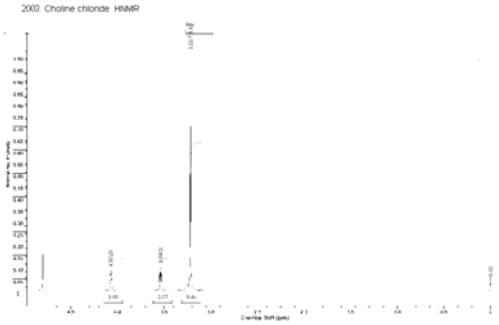
2002 4-Hydroxy-2,3-dimethyl-2,4-nonadienoic acid gamma-lactone (1H-NMR)



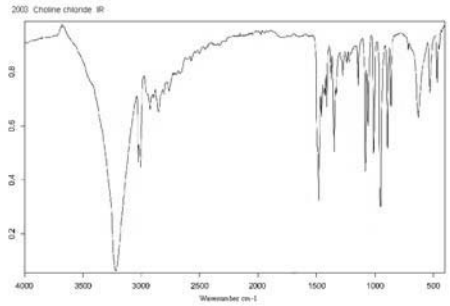
2003 Choline chloride (13C-NMR)



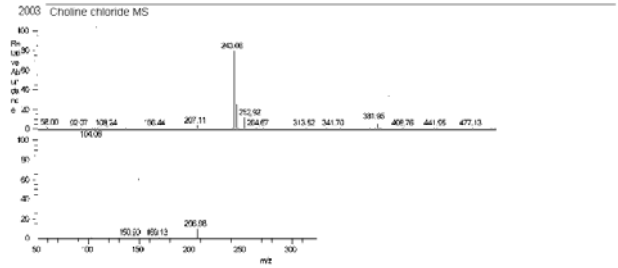
2003 Choline chloride (1H-NMR)



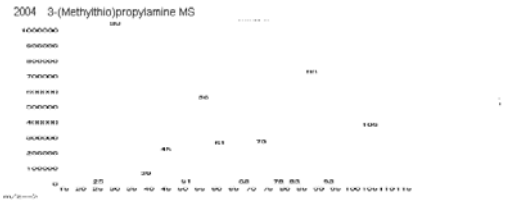
2003 Choline chloride (IR)



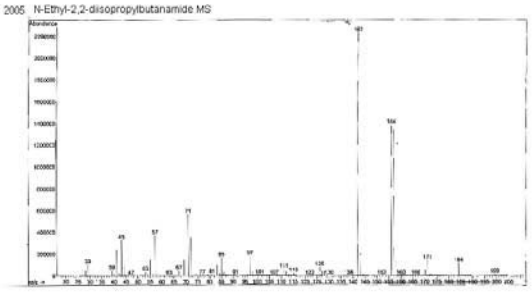
2003 Choline chloride (MS)



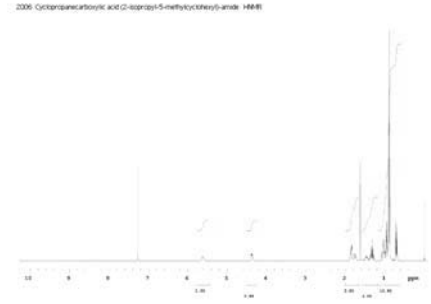
2004 3-(Methylthio)propylamine (MS)



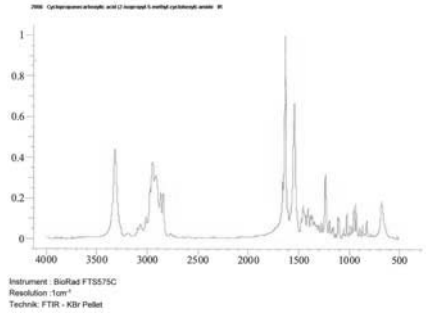
2005 N-Ethyl-2,2-diisopropylbutanamide (MS)



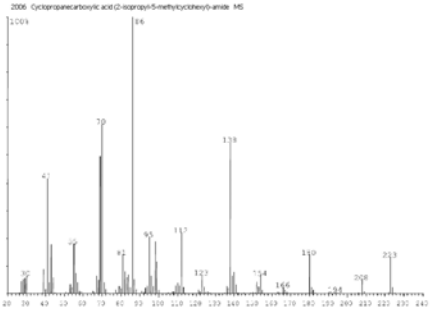
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (1H-NMR)



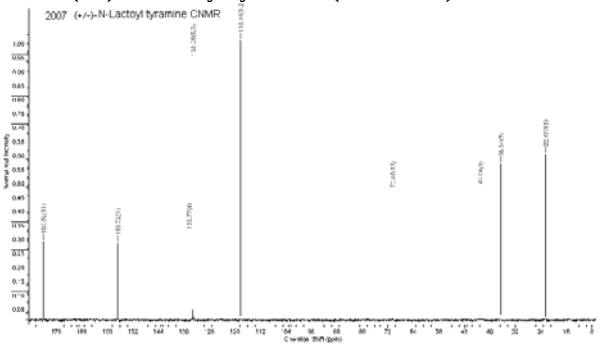
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (IR)



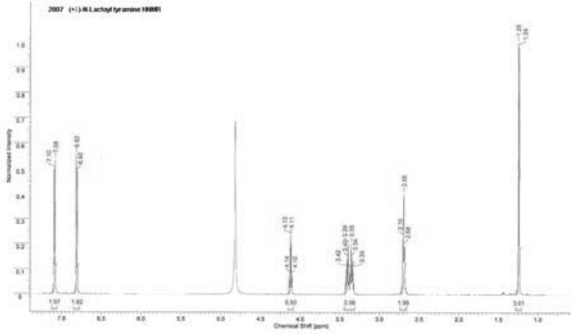
2006 Cyclopropanecarboxylic acid (2-isopropyl-5-methyl-cyclohexyl)-amide (MS)



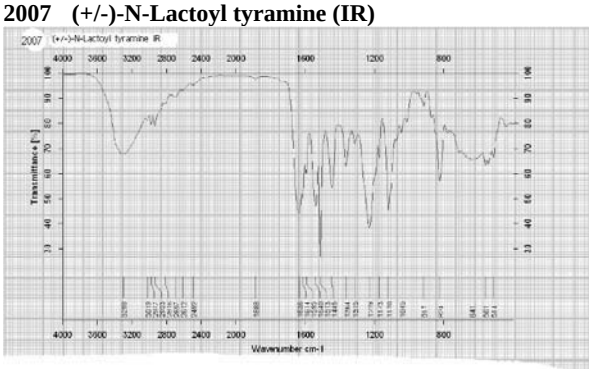
2007 (+/-)-N-Lactoyl tyramine (13C-NMR)



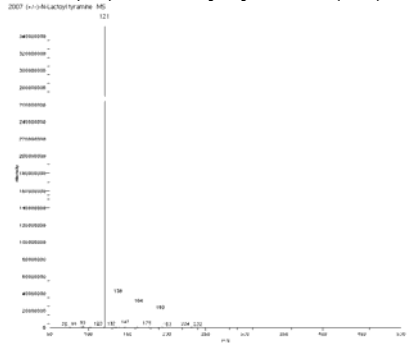
2007 (+/-)-N-Lactoyl tyramine (1H-NMR)



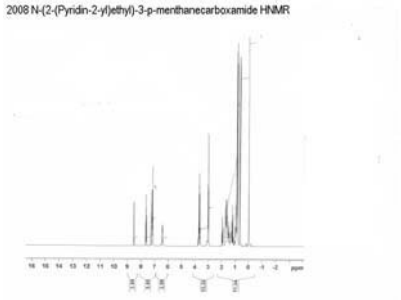
2007 (+/-)-N-Lactoyl tyramine (IR)



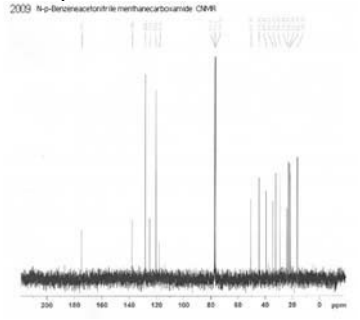
2007 (+/-)-N-Lactoyl tyramine (MS)



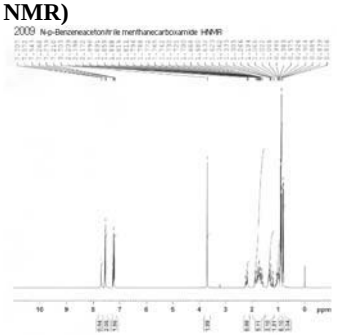
2008 N-(2-(Pyridin-2-yl)ethyl)-3-p-menthanecarboxamide (1H-NMR)



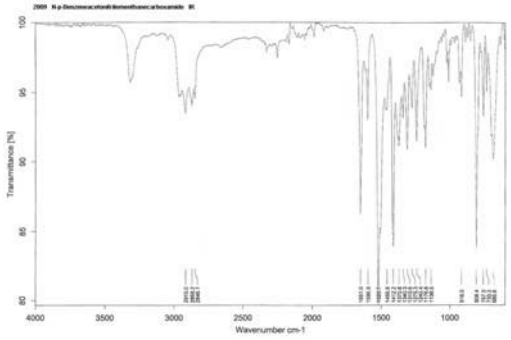
2009 N-p-Benzeneacetonitrile menthanecarboxamide (13C-NMR)



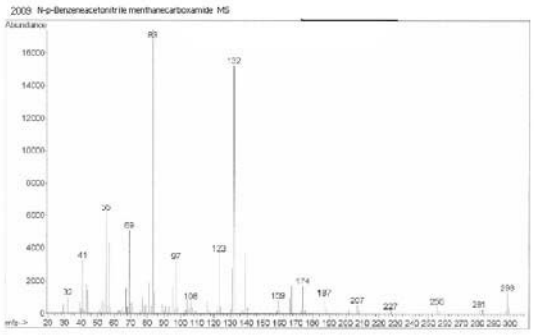
2009 N-p-Benzeneacetonitrile menthanecarboxamide (1H-NMR)



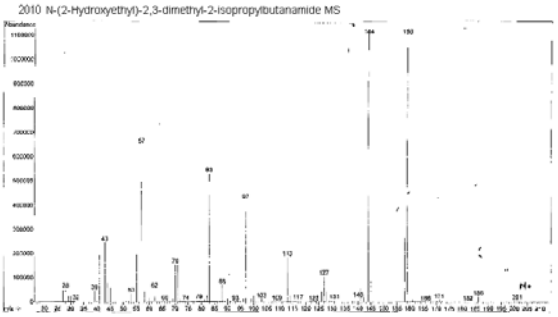
2009 N-p-Benzeneacetonitrile menthanecarboxamide (IR)



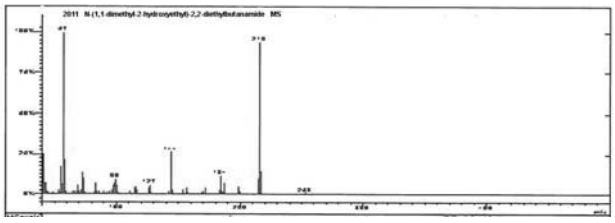
2009 N-p-Benzeneacetonitrile menthanecarboxamide (MS)



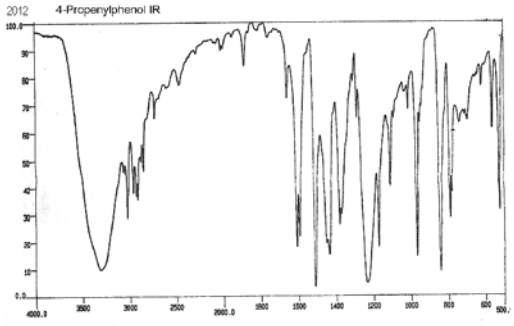
2010 N-(2-Hydroxyethyl)-2,3-dimethyl 2-isopropylbutanamide (MS)



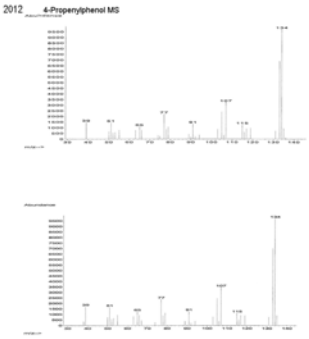
2011 N-(1,1-Dimethyl-2-hydroxyethyl)-2,2-diethylbutanamide (MS)



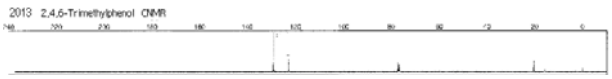
2012 4-Propenylphenol (IR)



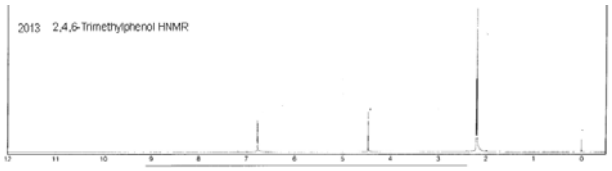
2012 4-Propenylphenol (MS)



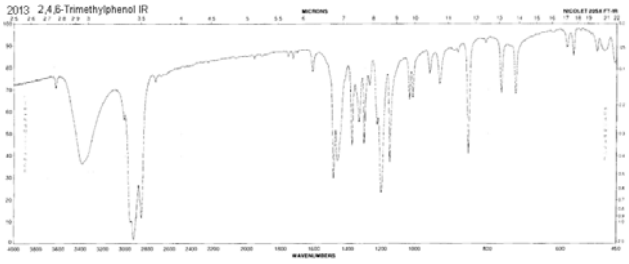
2013 2,4,6-Trimethylphenol (13C-NMR)



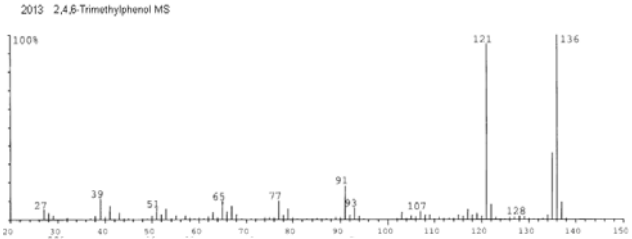
2013 2,4,6-Trimethylphenol (1H-NMR)



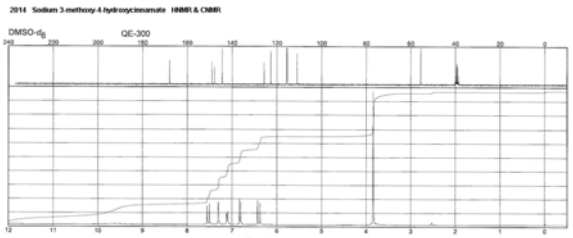
2013 2,4,6-Trimethylphenol (IR)



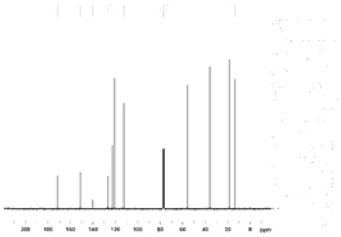
2013 2,4,6-Trimethylphenol (MS)



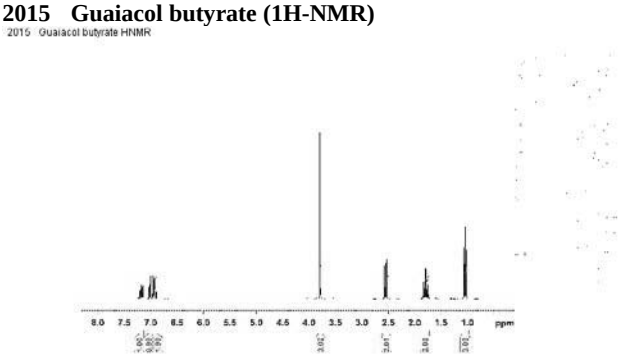
2014 Sodium 3-methoxy-4-hydroxycinnamate (13C-NMR and 1H-NMR)



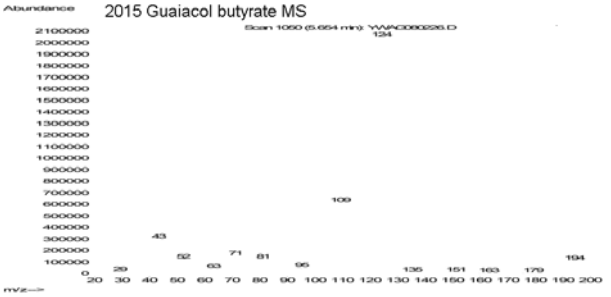
2015 Guaiacol butyrate (13C-NMR)



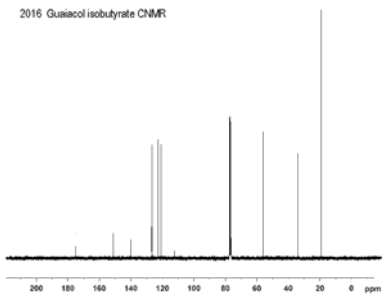
2015 Guaiacol butyrate (1H-NMR)



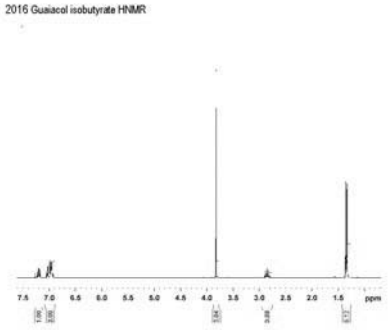
2015 Guaiacol butyrate (MS)



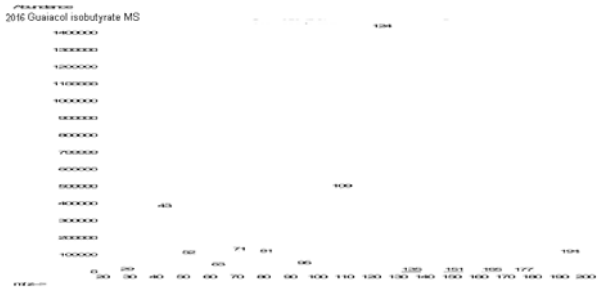
2016 Guaiacol isobutyrate (13C-NMR)



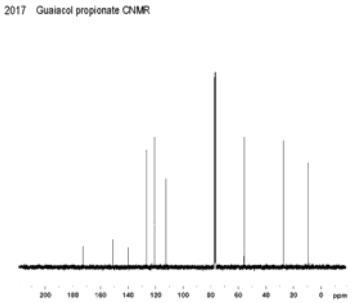
2016 Guaiacol isobutyrate (1H-NMR)



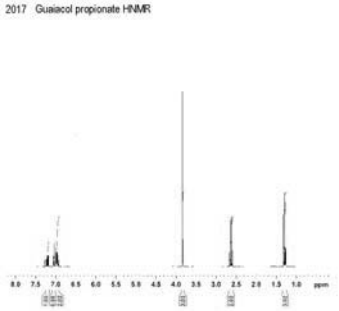
2016 Guaiacol isobutyrate (MS)



2017 Guaiacol propionate (13C-NMR)

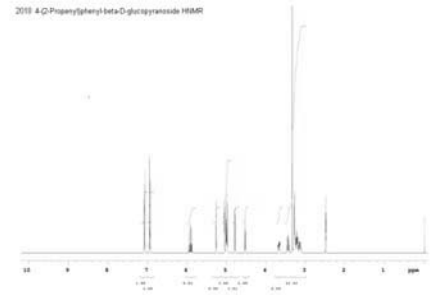


2017 Guaiacol propionate (1H-NMR)

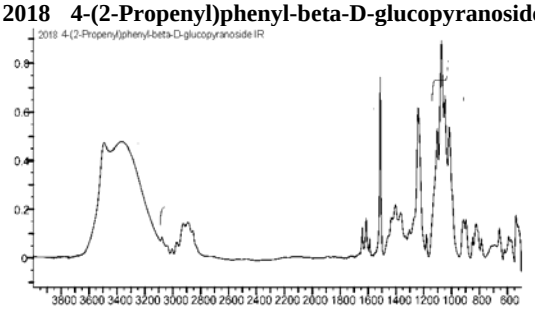


2017 Guaiacol propionate (MS)

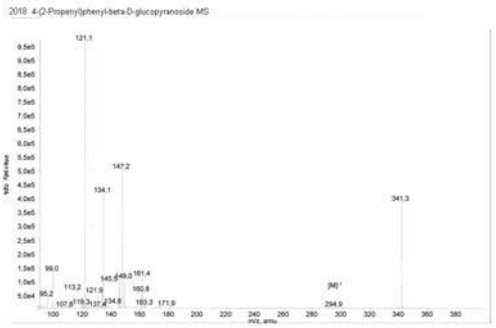
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (1H-NMR)



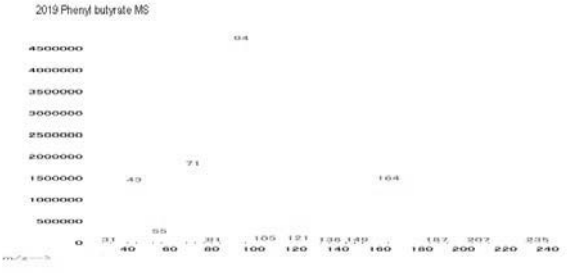
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (IR)



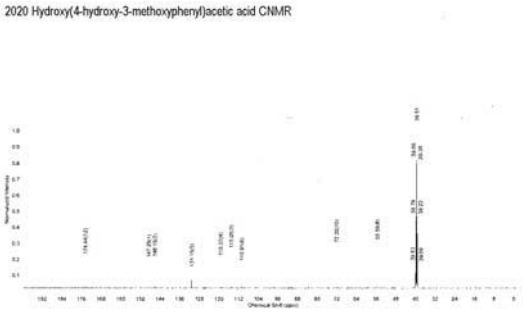
2018 4-(2-Propenyl)phenyl-beta-D-glucopyranoside (MS)



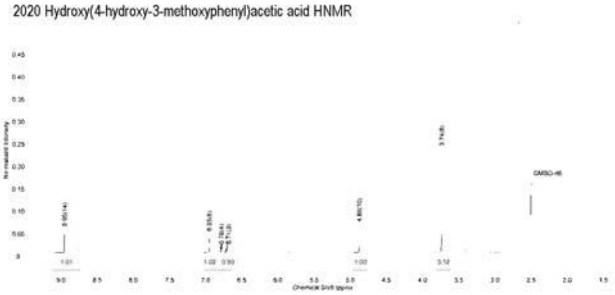
2019 Phenyl butyrate (MS)



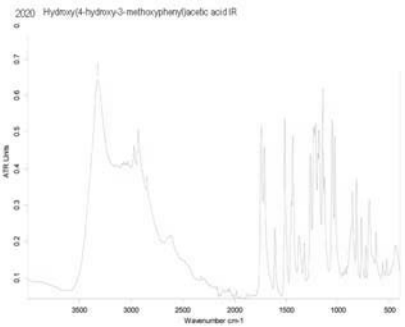
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (13C-NMR)



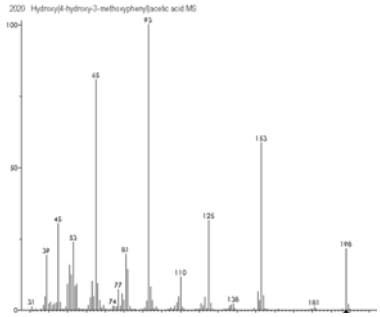
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (1H-NMR)



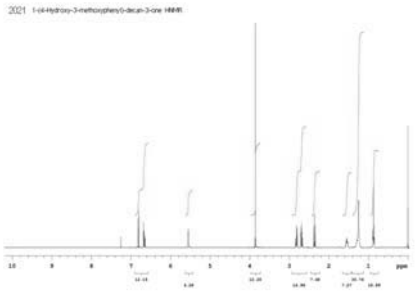
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (IR)



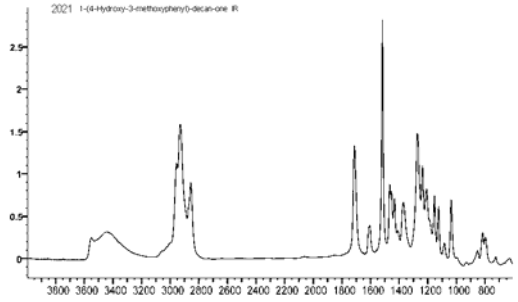
2020 Hydroxy(4-hydroxy-3-methoxyphenyl)acetic acid (MS)



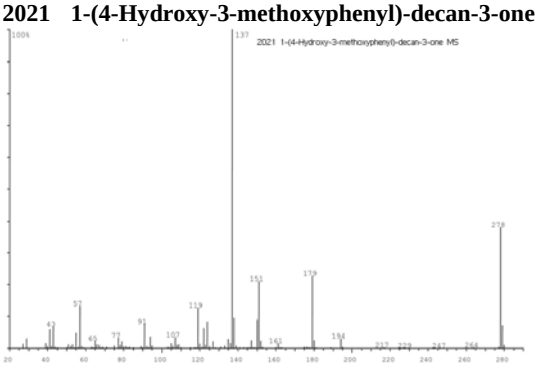
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (1H-NMR)



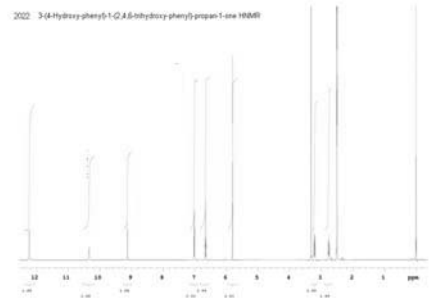
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (IR)



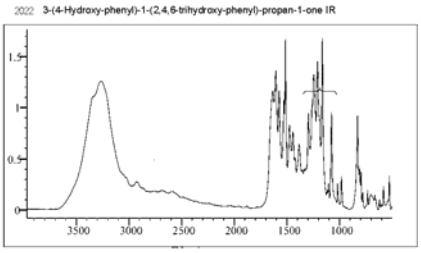
2021 1-(4-Hydroxy-3-methoxyphenyl)-decan-3-one (MS)



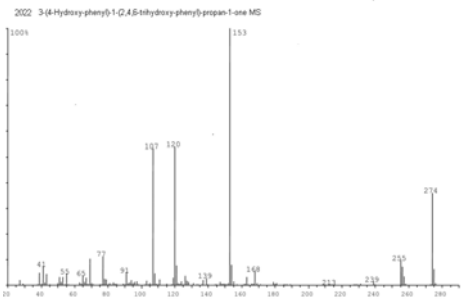
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (1H-NMR)



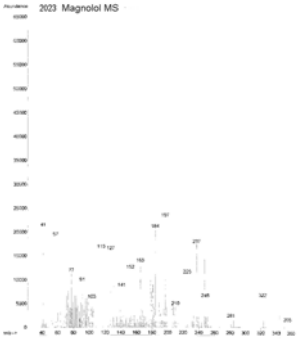
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (IR)



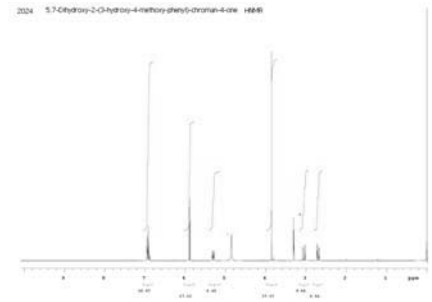
2022 3-(4-Hydroxy-phenyl)-1-(2,4,6-trihydroxy-phenyl)-propan-1-one (MS)



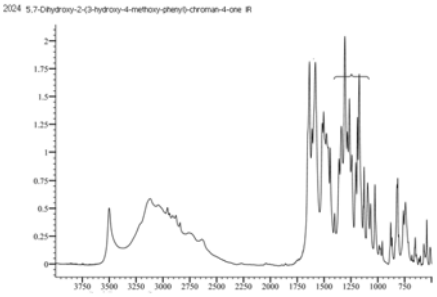
2023 Magnolol (MS)



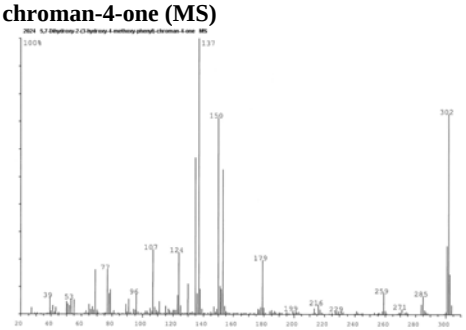
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (1H-NMR)



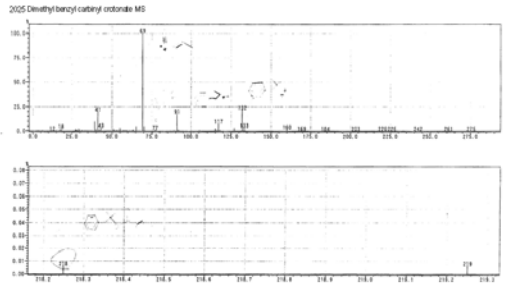
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (IR)



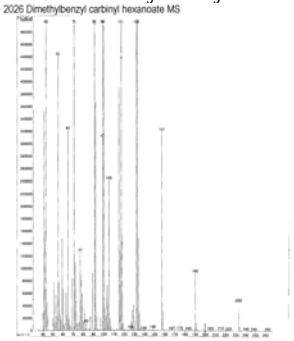
2024 5,7-Dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-chroman-4-one (MS)



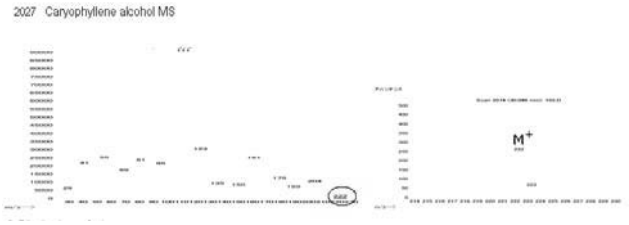
2025 Dimethylbenzyl carbinyl crotonate (MS)



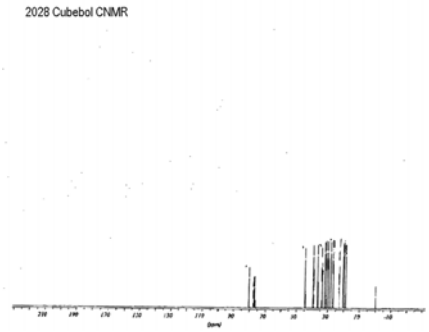
2026 Dimethylbenzyl carbinyl hexanoate (MS)



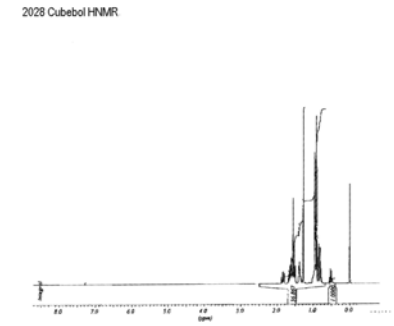
2027 Caryophyllene alcohol (MS)



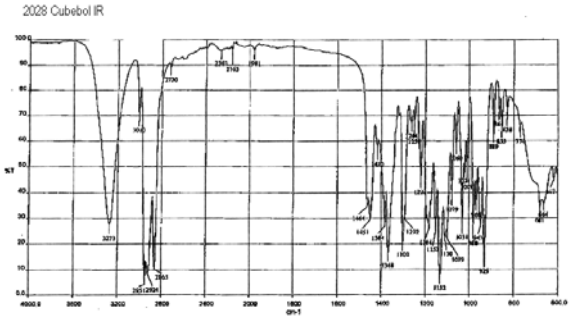
2028 Cubebol (13C-NMR)



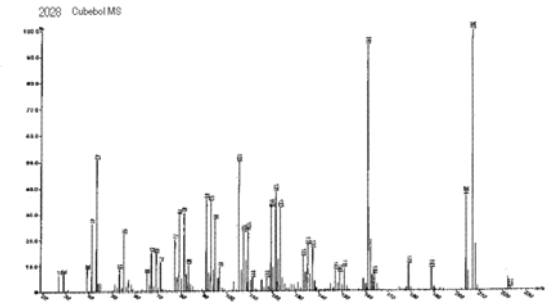
2028 Cubebol (1H-NMR)



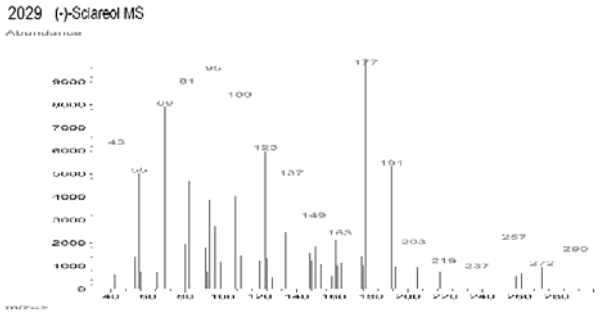
2028 Cubebol (IR)



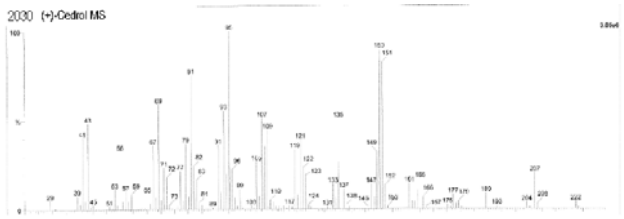
2028 Cubebol (MS)



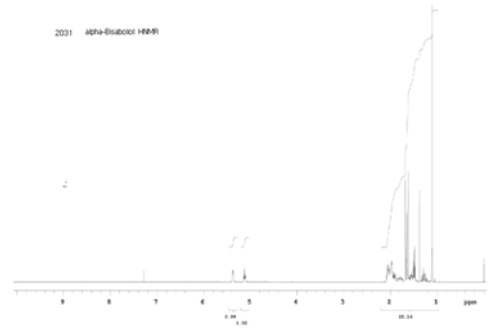
2029 (-)-Sclareol (MS)



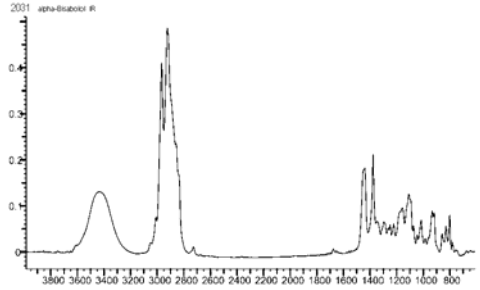
2030 (+)-Cedrol (MS)



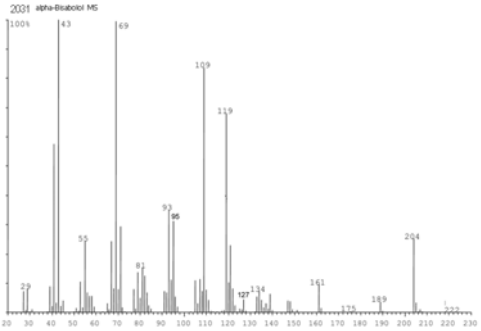
2031 alpha-Bisabolol (1H-NMR)



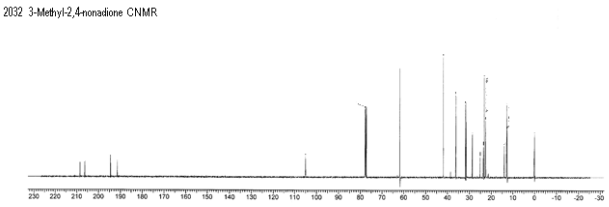
2031 alpha-Bisabolol (IR)



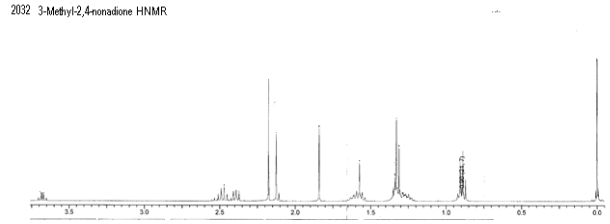
2031 alpha-Bisabolol (MS)



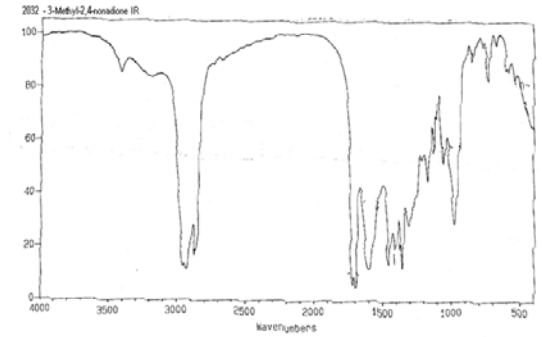
2032 3-Methyl-2,4-nonedione (13C-NMR)



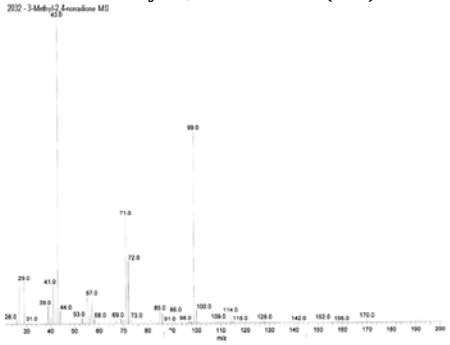
2032 3-Methyl-2,4-nonedione (1H-NMR)



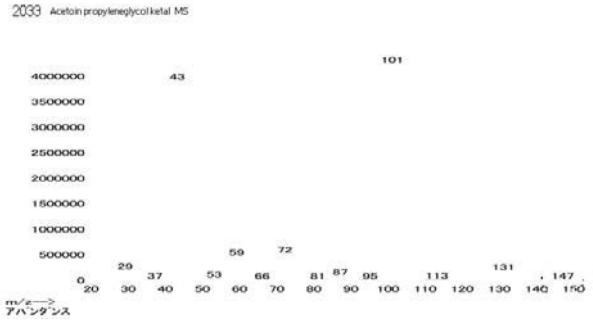
2032 3-Methyl-2,4-nonedione (IR)



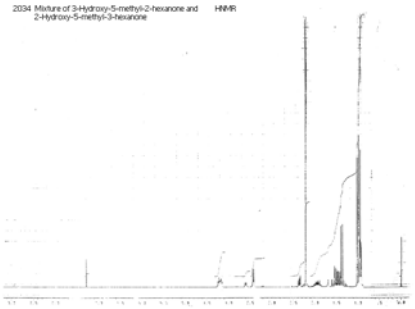
2032 3-Methyl-2,4-nonedione (MS)



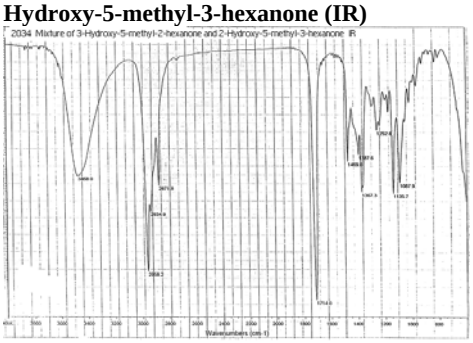
2033 Acetoin propyleneglycol ketal (MS)



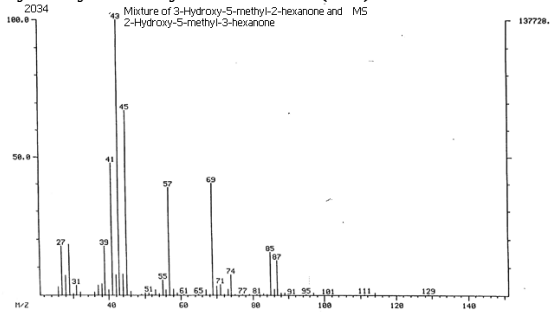
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (1H-NMR)



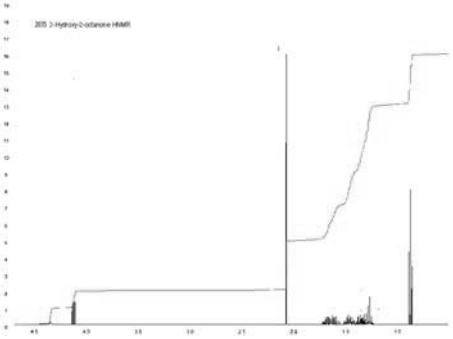
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (IR)



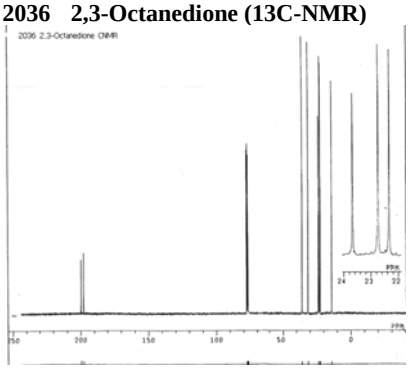
2034 Mixture of 3-Hydroxy-5-methyl-2-hexanone and 2-Hydroxy-5-methyl-3-hexanone (MS)



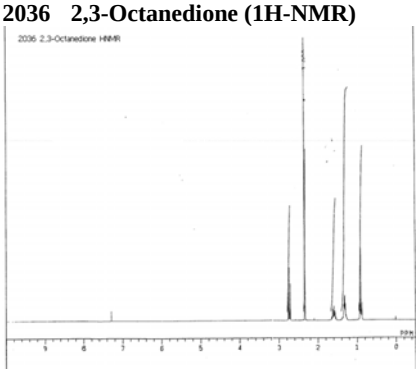
2035 3-Hydroxy-2-octanone (1H-NMR)



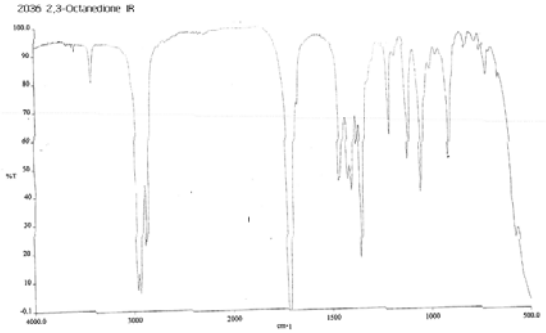
2036 2,3-Octanedione (13C-NMR)



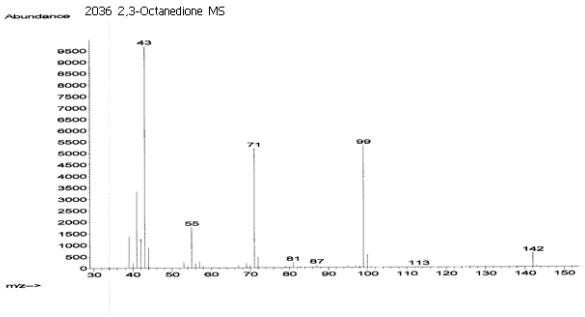
2036 2,3-Octanedione (1H-NMR)



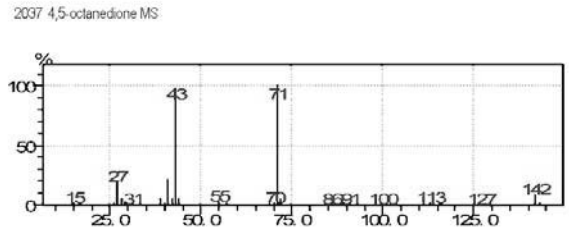
2036 2,3-Octanedione (IR)



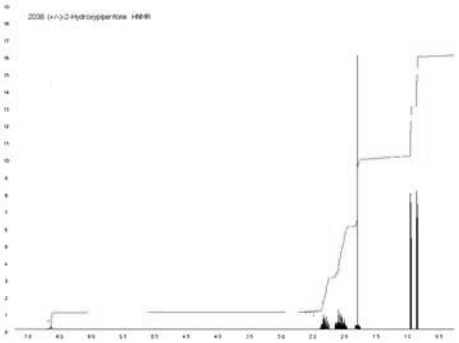
2036 2,3-Octanedione (MS)



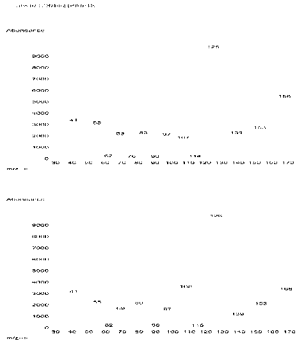
2037 4,5-Octanedione (MS)



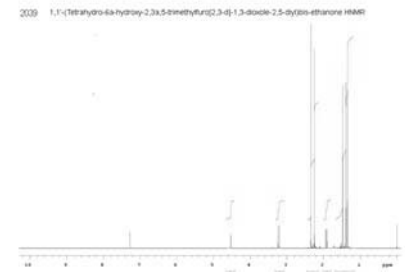
2038 (+/-)-2-Hydroxypiperitone (1H-NMR)



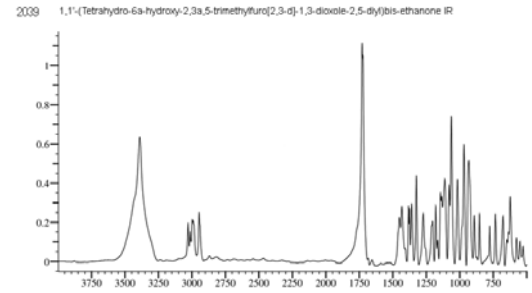
2038 (+/-)-2-Hydroxypiperitone (MS)



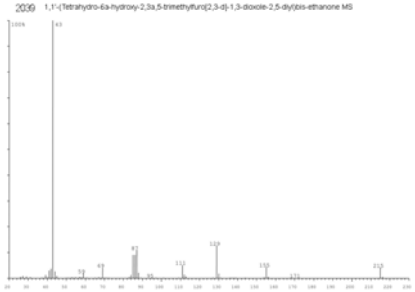
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (1H-NMR)



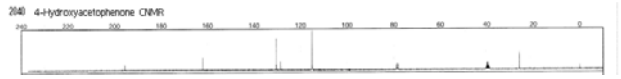
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (IR)



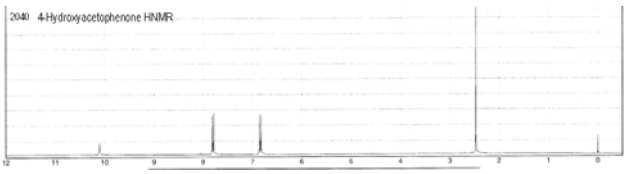
2039 1,1'-(Tetrahydro-6a-hydroxy-2,3a,5-trimethylfuro[2,3-d]-1,3-dioxole-2,5-diyl)bis-ethanone (MS)



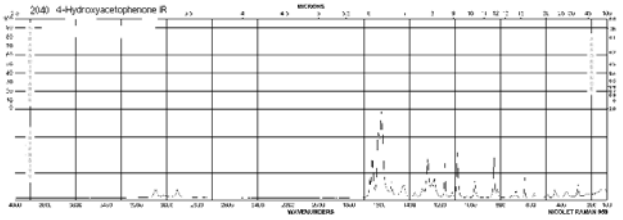
2040 4-Hydroxyacetophenone (13C-NMR)



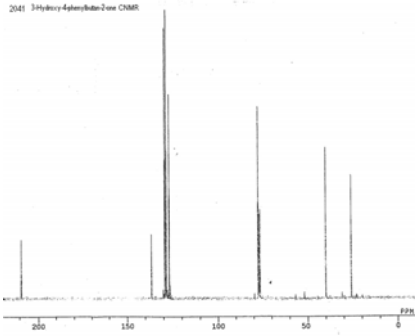
2040 4-Hydroxyacetophenone (1H-NMR)



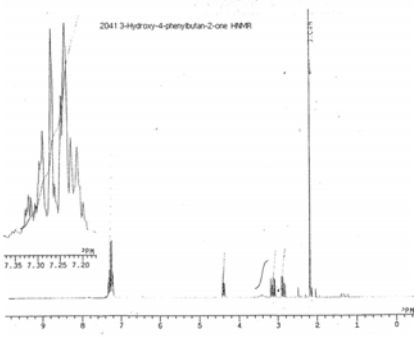
2040 4-Hydroxyacetophenone (IR)



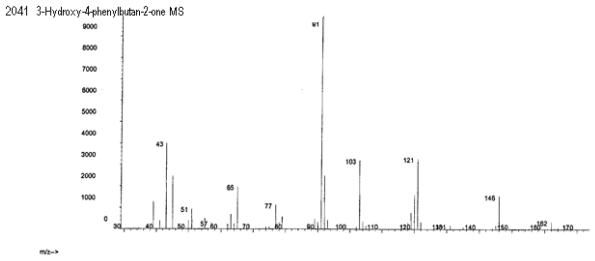
2041 3-Hydroxy-4-phenylbutan-2-one (13C-NMR)



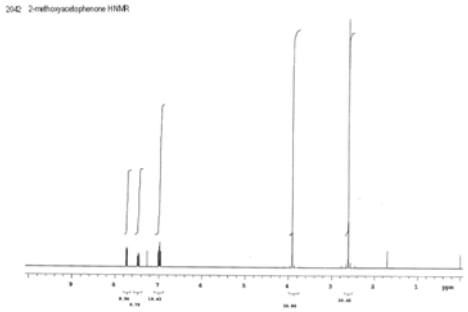
2041 3-Hydroxy-4-phenylbutan-2-one (1H-NMR)



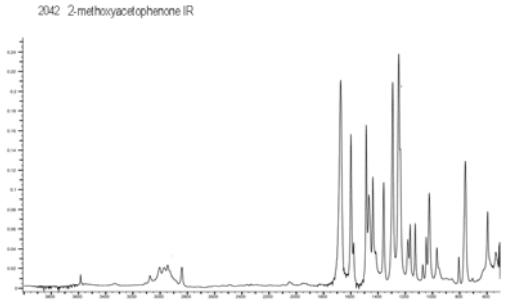
2041 3-Hydroxy-4-phenylbutan-2-one (MS)



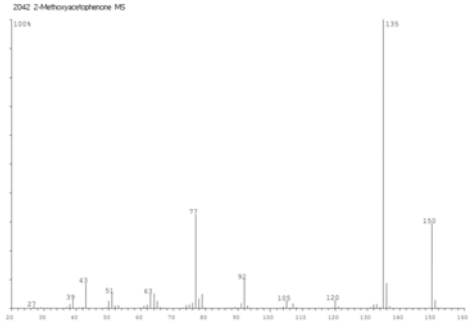
2042 2-Methoxyacetophenone (1H-NMR)



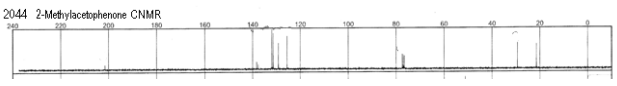
2042 2-Methoxyacetophenone (IR)



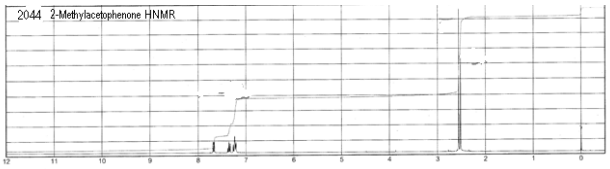
2042 2-Methoxyacetophenone (MS)



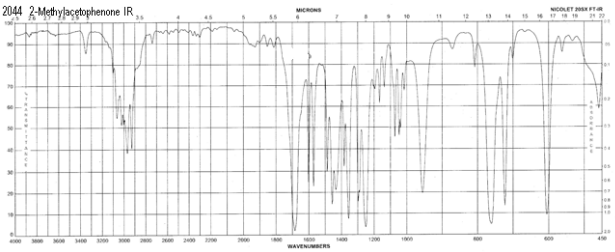
2044 2-Methylacetophenone (13C-NMR)



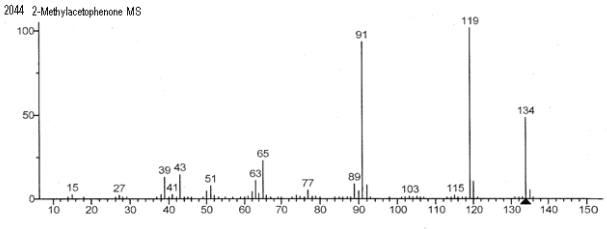
2044 2-Methylacetophenone (1H-NMR)



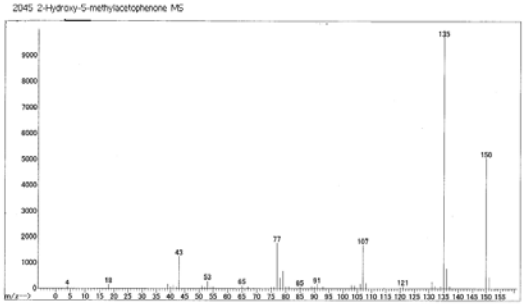
2044 2-Methylacetophenone (IR)



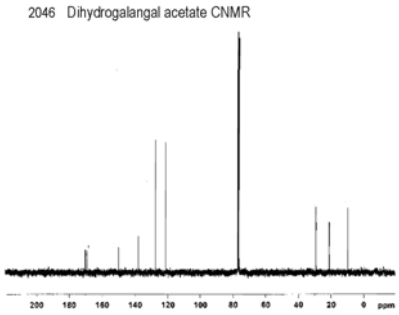
2044 2-Methylacetophenone (MS)



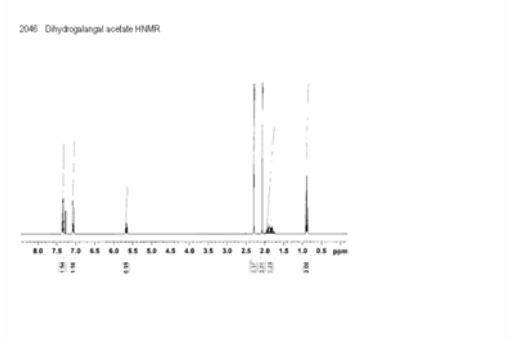
2045 2-Hydroxy-5-methylacetophenone (MS)



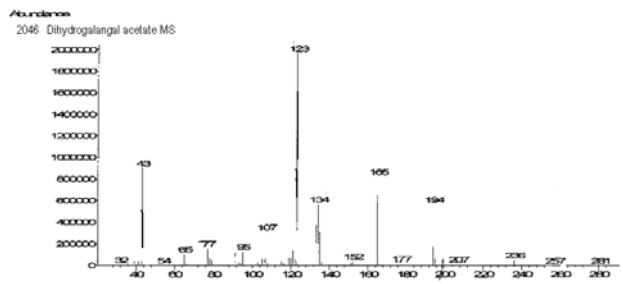
2046 Dihydrogalangal acetate (13C-NMR)



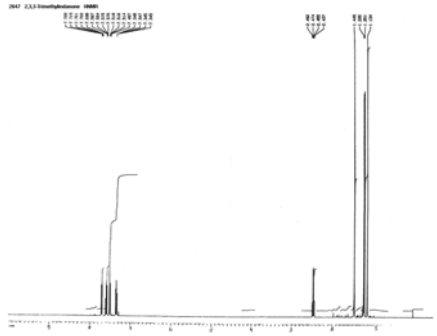
2046 Dihydrogalangal acetate (1H-NMR)



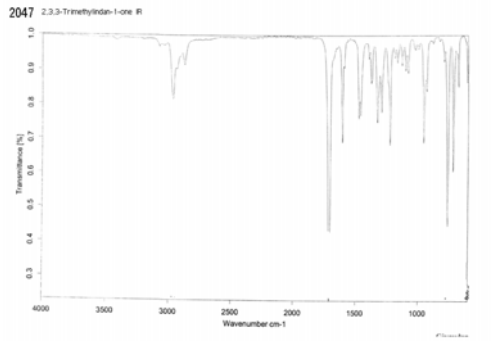
2046 Dihydrogalangal acetate (MS)



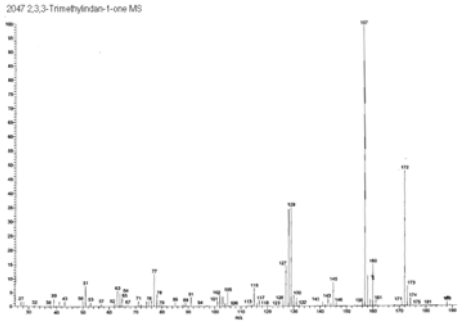
2047 2,3,3-Trimethylindan-1-one (1H-NMR)



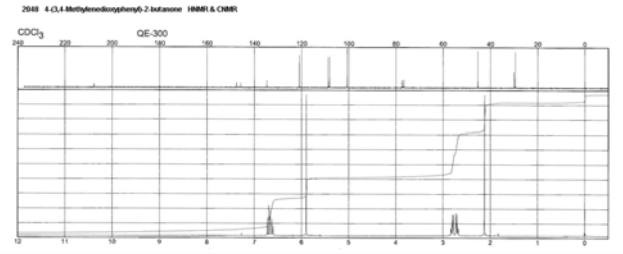
2047 2,3,3-Trimethylindan-1-one (IR)



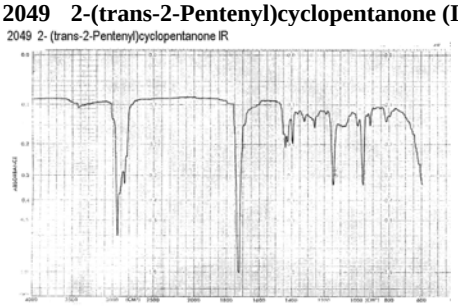
2047 2,3,3-Trimethylindan-1-one (MS)



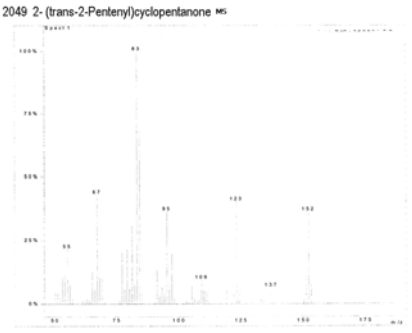
2048 4-(3,4-Methylenedioxyphenyl)-2-butanone (NMR)



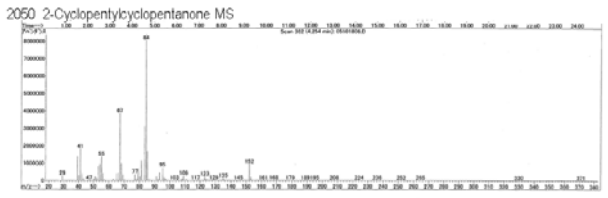
2049 2-(trans-2-Pentenyl)cyclopentanone (IR)



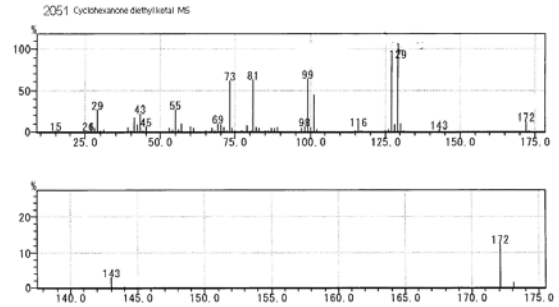
2049 2-(trans-2-Pentenyl)cyclopentanone (MS)



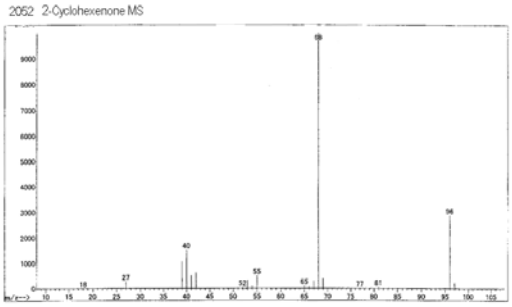
2050 2-Cyclopentylcyclopentanone (MS)



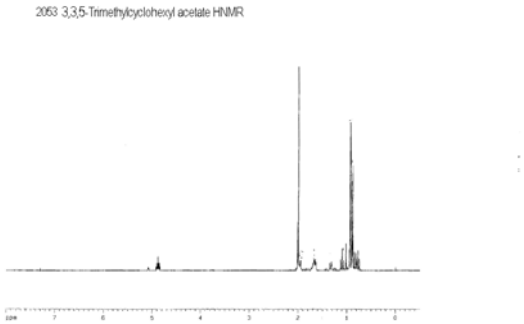
2051 Cyclohexanone diethyl ketal (MS)



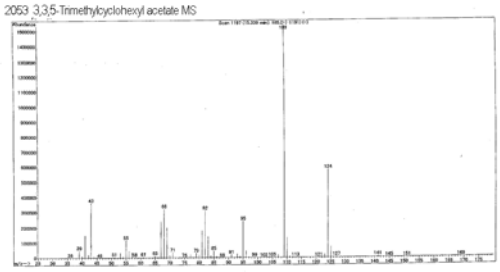
2052 2-Cyclohexenone (MS)



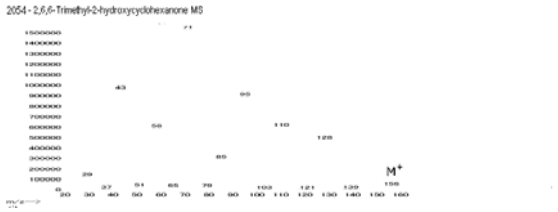
2053 3,3,5-Trimethylcyclohexyl acetate (1H-NMR)



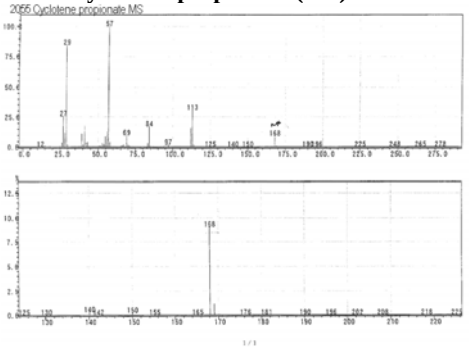
2053 3,3,5-Trimethylcyclohexyl acetate (MS)



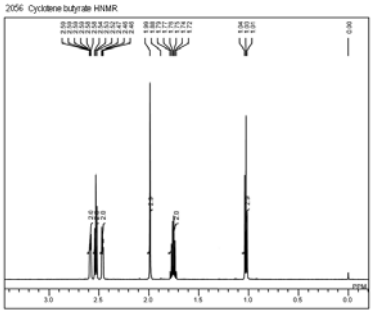
2054 2,6,6-Trimethyl-2-hydroxycyclohexanone (MS)



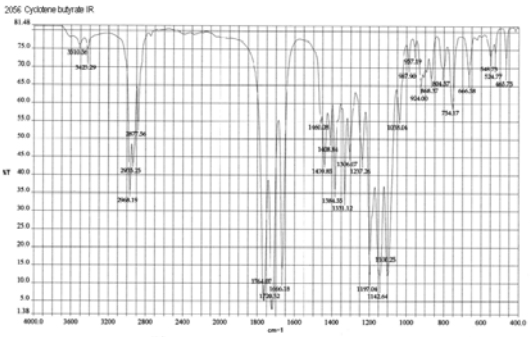
2055 Cyclotene propionate (MS)



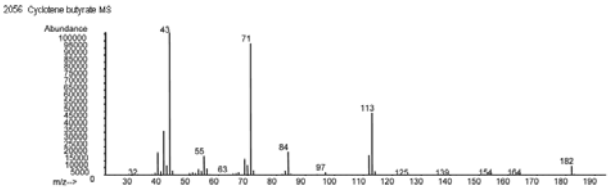
2056 Cyclotene butyrate (1H-NMR)



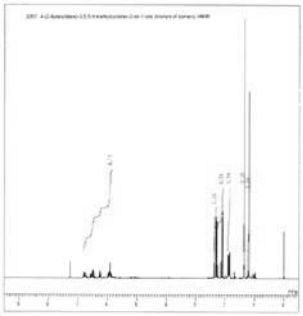
2056 Cyclotene butyrate (IR)



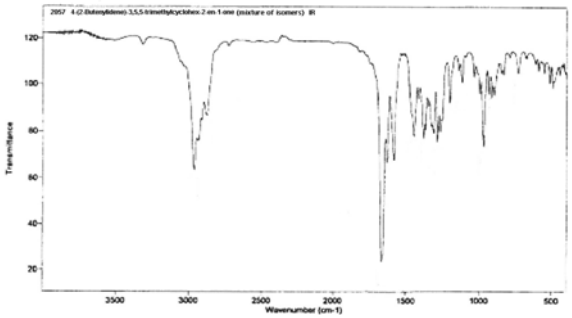
2056 Cyclotene butyrate



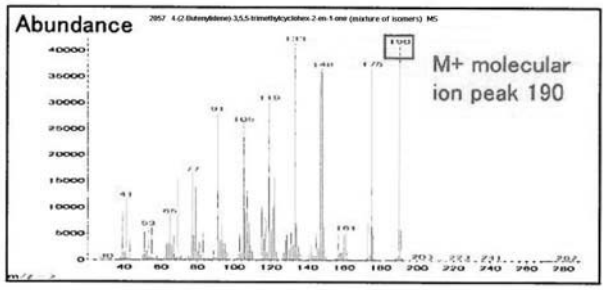
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (1H-NMR)



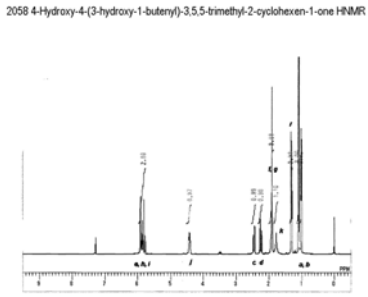
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (IR)



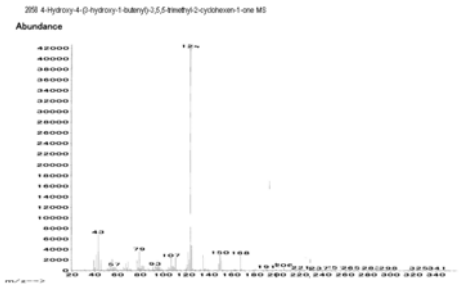
2057 4-(2-Butenylidene)-3,5,5-trimethylcyclohex-2-en-1-one (mixture of isomers) (MS)



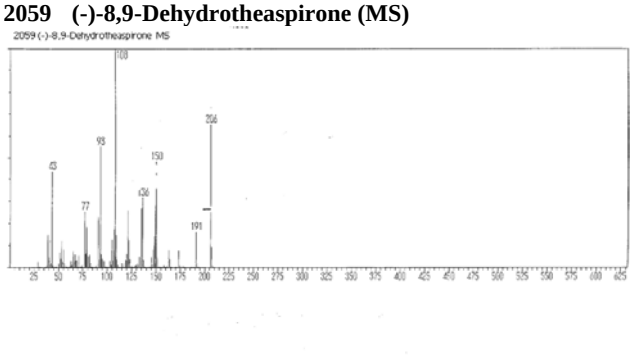
2058 4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers) (1H-NMR)



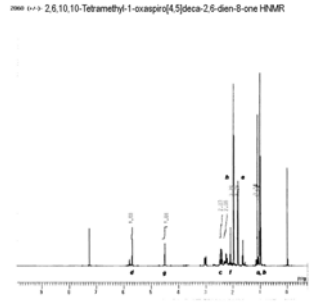
2058 4-Hydroxy-4-(3-hydroxy-1-butenyl)-3,5,5-trimethyl-2-cyclohexen-1-one (mixture of isomers) (MS)



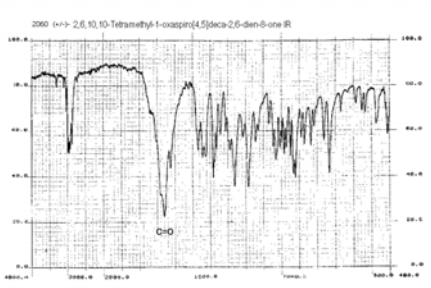
2059 (-)-8,9-Dehydrotheaspirone (MS)



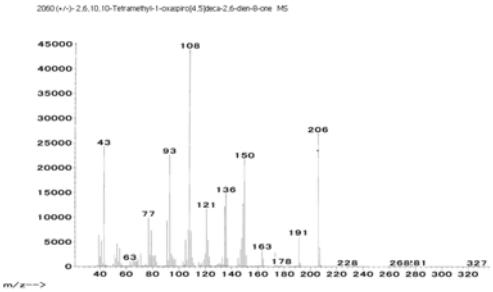
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (1H-NMR)



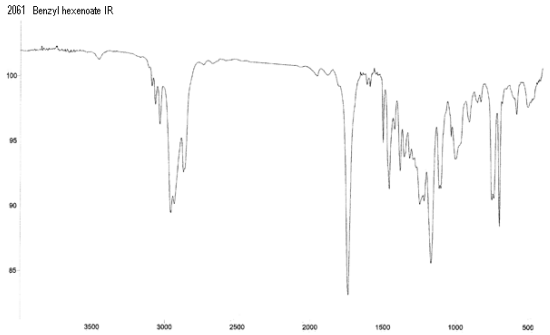
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (IR)



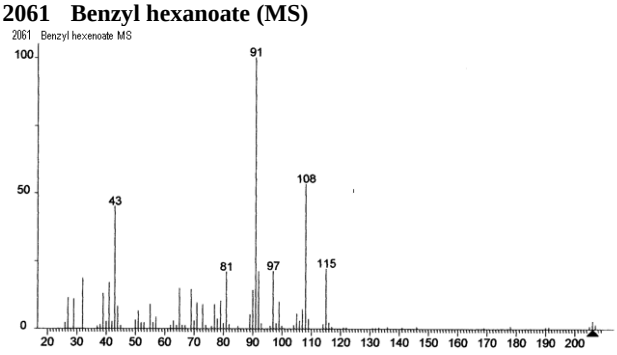
2060 (+/-)-2,6,10,10-Tetramethyl-1-oxaspiro[4.5]deca-2,6-dien-8-one (MS)



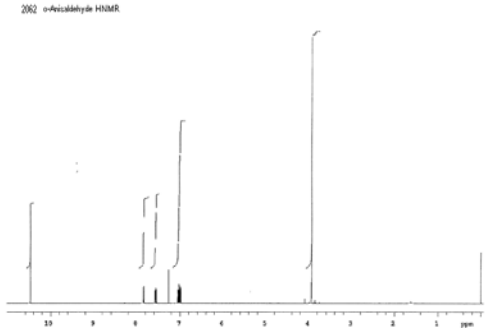
2061 Benzyl hexanoate (IR)



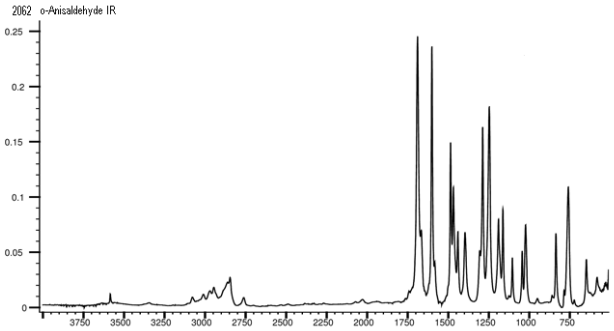
2061 Benzyl hexanoate (MS)



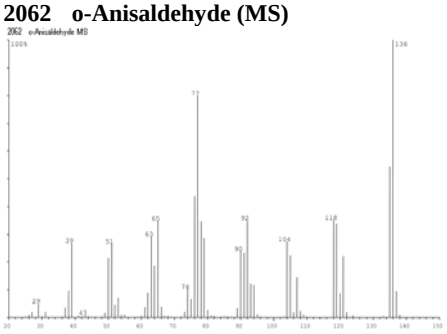
2062 o-Anisaldehyde (1H-NMR)



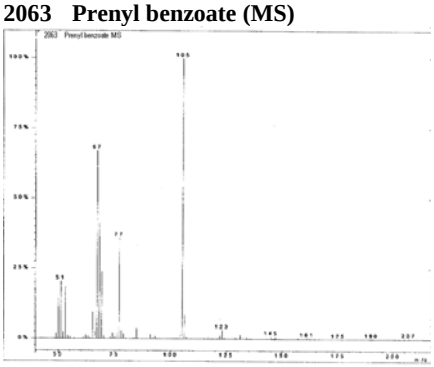
2062 o-Anisaldehyde (IR)



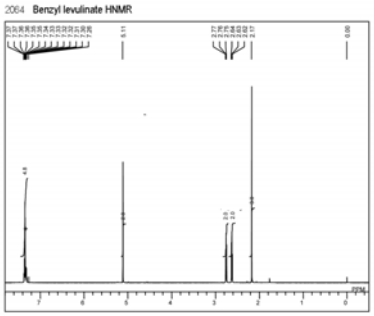
2062 o-Anisaldehyde (MS)



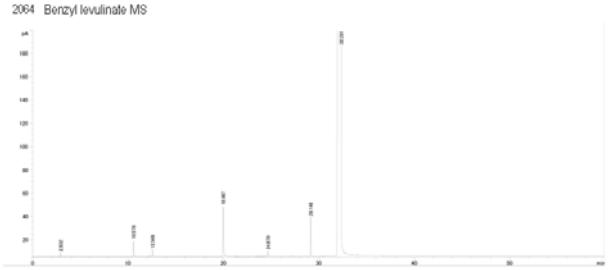
2063 Prenyl benzoate (MS)



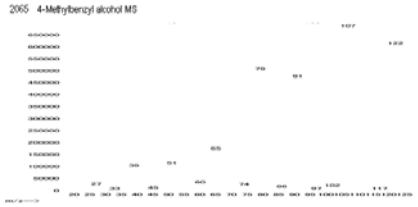
2064 Benzyl levulinate (1H-NMR)



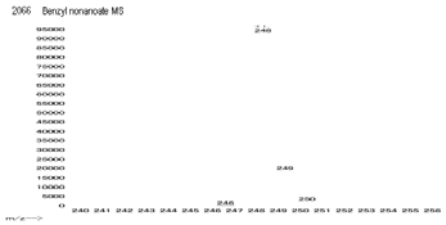
2064 Benzyl levulinate (MS)



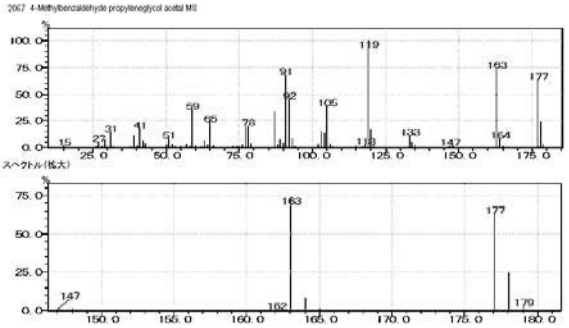
2065 4-Methylbenzyl alcohol (MS)



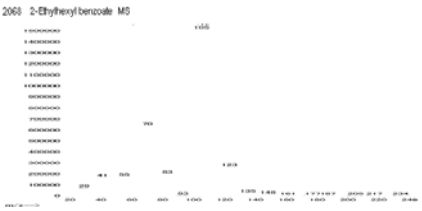
2066 Benzyl nonanoate (MS)



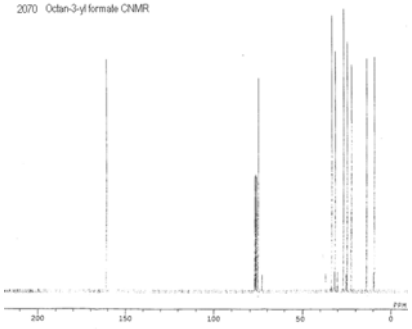
2067 4-Methylbenzaldehyde propyleneglycol acetal (MS)



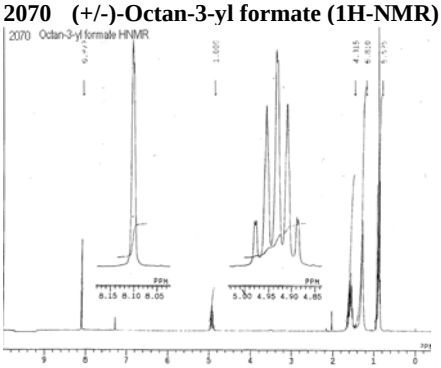
2068 2-Ethylhexyl benzoate (MS)



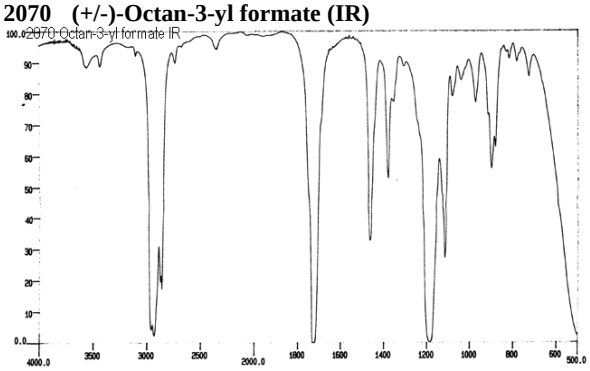
2070 (+/-)-Octan-3-yl formate (13C-NMR)



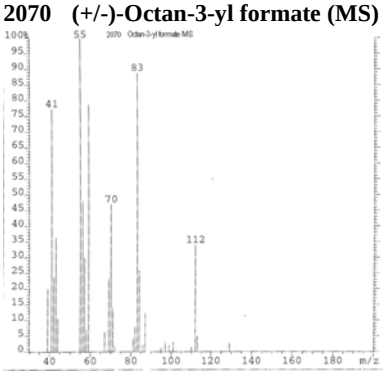
2070 (+/-)-Octan-3-yl formate (1H-NMR)



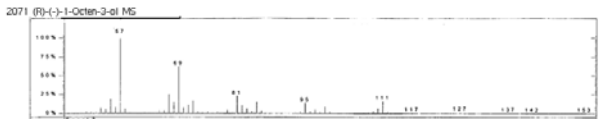
2070 (+/-)-Octan-3-yl formate (IR)



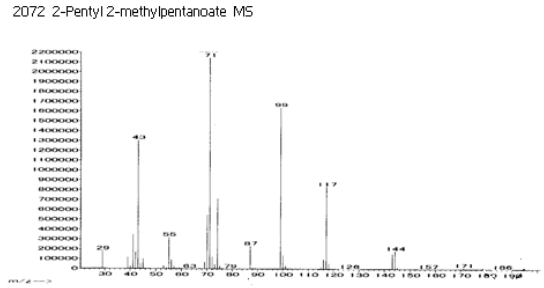
2070 (+/-)-Octan-3-yl formate (MS)



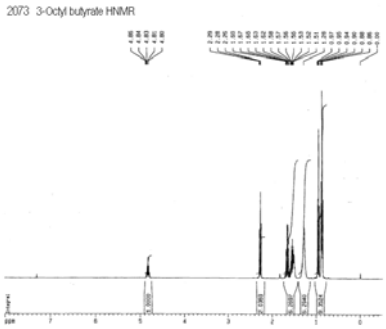
2071 (R)-(-)-1-Octen-3-ol (MS)



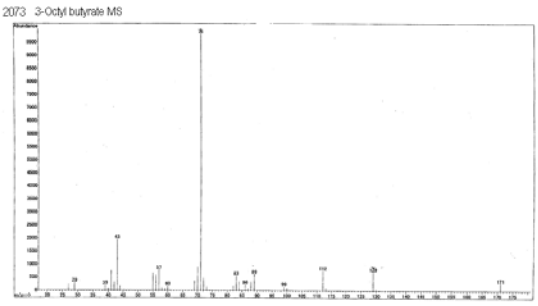
2072 2-Pentyl 2-methylpentanoate (MS)



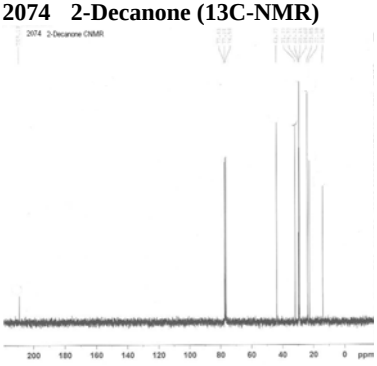
2073 3-Octyl butyrate (1H-NMR)



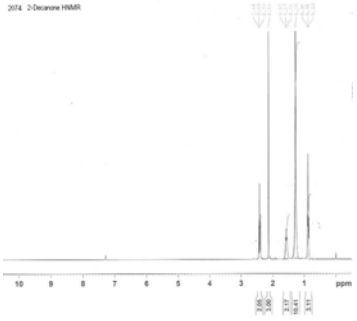
2073 3-Octyl butyrate (MS)



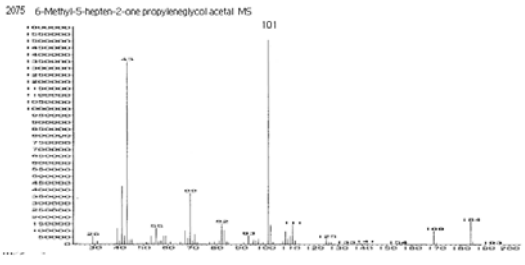
2074 2-Decanone (13C-NMR)



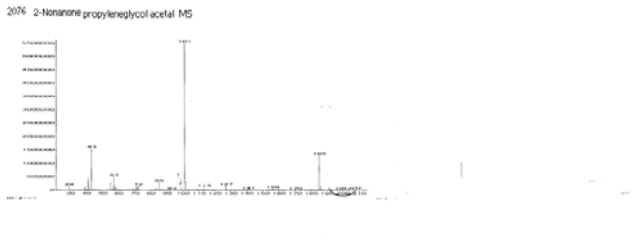
2074 2-Decanone (1H-NMR)



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



2076 2-Nonanone propyleneglycol acetal (MS)



List of new flavourings evaluated in alphabetical order

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

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

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