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FAO JECFA Monographs 13



COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS

Joint FAO/WHO Expert Committee on Food Additives

76th meeting 2012

World Health Organization

Food and Agriculture Organization of the United Nations

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FOOD AND AGRICULTURE ORGANIZATION OF THE UNITED NATIONS
Rome, 2013

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Geneva, 5 – 14 June, 2012

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INTRODUCTION

This volume of FAO JECFA Monographs contains specifications of identity and purity prepared at the 76th meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), held in Geneva on 5 - 14 June 2012. The specifications monographs are one of the outputs of JECFA's risk assessment of food additives, and should be read in conjunction with the safety evaluation, reference to which is made in the section at the head of each specifications monograph. Further information on the meeting discussions can be found in the summary report of the meeting (see Annex 1), and in the full report which will be published in the WHO Technical Report series. Toxicological monographs of the substances considered at the meeting will be published in the WHO Food Additive Series.

Specifications monographs prepared by JECFA up to the 65th meeting, other than specifications for flavouring agents, have been published in consolidated form in the Combined Compendium of Food Additive Specifications which is the first publication in the series FAO JECFA Monographs. This publication consists of four volumes, the first three of which contain the specifications monographs on the identity and purity of the food additives and the fourth volume contains the analytical methods, test procedures and laboratory solutions required and referenced in the specifications monographs. FAO maintains an on-line searchable database of all JECFA specifications monographs from the FAO JECFA Monographs, which is available at: http://www.fao.org/ag/agn/jecfa-additives/search.html . The specifications for flavourings evaluated by JECFA, and previously published in FAO Food and Nutrition Paper 52 and subsequent Addenda, are included in a database for flavourings (flavouring agent) specifications which has been updated and modernized. All specifications for flavourings that have been evaluated by JECFA since its 44th meeting, including the 76th meeting, are available in the new format online searchable database at the JECFA website at FAO: http://www.fao.org/ag/agn/jecfa-flav/search.html. The databases have query pages and background information in English, French, Spanish, Arabic and Chinese. Information about analytical methods referred to in the specifications is available in the Combined Compendium of Food Additive Specifications (Volume 4), which can be accessed from the query pages.

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

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

Contact and Feedback

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

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SPECIFICATIONS FOR CERTAIN FOOD ADDITIVES

New and revised specifications

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

Ethyl cellulose (R)

Magnesium dihydrogen diphosphate (N)

Mineral Oil [medium viscosity] (N)

Modified Starches – Starch sodium octenylsuccinate (R)

3-Phytase from *Aspergillus niger* expressed in *Aspergillus niger*.(N).

Serine protease (chymotrypsin) from *Nocardiopsis prasina* expressed in *Bacillus licheniformis* (N)

Serine protease (trypsin) from *Fusarium oxysporum* expressed in *Fusarium venenatum*.(N)

Titanium dioxide (R)

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

The specifications for mineral oil (medium and low viscosity) were withdrawn, since the temporary ADI for low viscosity oils (Class II and III) has been withdrawn. For the remaining mineral oils of medium viscosity (Class I), which enjoy a separate ADI, new specifications were prepared.

New and revised INS numbers were assigned to food additives by the Codex Alimentarius Commission at its 34th session in 2012, (REP12/CAC, paragraphs 46-47). and corrections for the INS number for sodium potassium hexametaphosphate was corrected to read 452(vi) and the previously recommended INS 561, for potassium aluminium silicate was discontinued. The number for sodium potassium hexametaphosphate, in the corresponding JECFA food additive specifications monographs in the on-line database, will be amended, and is not reproduced in this publication.

The Commission adopted the draft amendments to the INS as proposed by the CCEXEC and recommended to the CCFA to reconsider a new INS number for “potassium aluminium silicate, based pearlescent pigments on the basis of the description of the specifications monograph prepared by the 74th JECFA.

Specifications for potassium bromate were revoked by the 35th session of the Codex Alimentarius Commission.

ETHYL CELLULOSE

Revised specification prepared at the 76th JECFA (2012), published in FAO JECFA Monographs 13 (2012) superseding specifications prepared at the 26th JECFA (1982), published in FNP 25 (1982) and FNP 52 (1992). Metals and arsenic specifications revised at the 57th JECFA (2001). A group ADI 'not specified' was established at the 35th JECFA (1989).

SYNONYMS INS No. 462

DEFINITION Ethyl ether of cellulose, prepared from wood pulp or cotton by treatment with alkali and ethylation of the alkali cellulose with ethyl chloride. The article of commerce can be specified further by viscosity. Antioxidants permitted for use in food may be added for stabilizing purposes.

Chemical names Cellulose ethyl ether, ethyl ether of cellulose

C.A.S. number 9004-57-3

Assay Not less than 44% and not more than 50% of ethoxyl groups ($-OC_2H_5$) on the dried basis (equivalent to not more than 2.6 ethoxyl groups per anhydroglucose unit).

DESCRIPTION Free-flowing, white to light tan powder

FUNCTIONAL USES Tableting aid, binder, filler, diluent of colour and other food additives

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4) Practically insoluble in water, in glycerol, and in propane-1,2-diol, but soluble in varying proportions in certain organic solvents, depending upon the ethoxyl content. Ethyl cellulose containing less than 46-48% of ethoxyl groups is freely soluble in tetrahydrofuran, methyl acetate and aromatic hydrocarbon ethanol mixtures. Ethyl cellulose containing 46-48% or more of ethoxyl groups is freely soluble in ethanol, methanol, toluene and ethyl acetate.

Film forming test Dissolve 5 g of the sample in 95 g of an 80:20 (w/w) mixture of toluene-ethanol. A clear, stable, slightly yellow solution is formed. Pour a few ml of the solution onto a glass plate, and allow the solvent to evaporate. A thick, tough continuous, clear film remains. The film is flammable.

pH (Vol. 4)	Neutral to litmus (1 in 20 suspension)

PURITY

Loss on drying (Vol. 4)	Not more than 3% (105°, 2 h)
Sulfated ash (Vol. 4)	Not more than 0.4% Test 1 g of the sample (Method I)
Lead (Vol. 4)	Not more than 2 mg/kg Determine using an AAS (Electrothermal atomization technique) appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).
METHOD OF ASSAY	Determine the ethoxyl content as directed under *Ethoxyl and Methoxyl Group Determination* (see Volume 4).

MAGNESIUM DIHYDROGEN DIPHOSPHATE

New specifications prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012). No ADI was established. A group MTDI of 70 mg/kg bw, expressed as phosphorus from all food sources, was established at the 26th JECFA (1982).

SYNONYMS Acid magnesium pyrophosphate, monomagnesium dihydrogen pyrophosphate; magnesium diphosphate, INS No. 450 (ix)

DEFINITION Magnesium dihydrogen diphosphate is the acidic magnesium salt of diphosphoric acid. It is manufactured by adding an aqueous dispersion of magnesium hydroxide slowly to phosphoric acid, until a molar ratio about 1:2 between Mg and P is reached. The temperature is held under 60° during the reaction. About 0.1% hydrogen peroxide is added to the reaction mixture and the slurry is then dried and milled.

Chemical names	Monomagnesium dihydrogen diphosphate
C.A.S. number	20768-12-1
Chemical formula	$MgH_2P_2O_7$
Formula weight	200.25
Assay	Not less than 68.0% and not more than 70.5% expressed as P_2O_5 Not less than 18.0% and not more than 20.5% expressed as MgO

DESCRIPTION White crystals or powder

FUNCTIONAL USES Acidifier, stabilizer, raising agent

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)	Slightly soluble in water, practically insoluble in ethanol
Test for magnesium (Vol. 4)	Passes test

PURITY

Loss on ignition (Vol. 4)	Not more than 12% (800°, 0.5 h)
Orthophosphate	Not more than 4% as $(PO_4)^{3-}$ See description under TESTS
Calcium (Vol. 4)	Not more than 0.4% Determine using an AAS/ICP-AES technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).
Fluoride (Vol. 4)	Not more than 20 mg/kg Method III; use an appropriate sample size and appropriate volumes of standard solution for the construction of standard curve.
Aluminium (Vol. 4)	Not more than 50 mg/kg Determine using an AAS/ICP-AES technique appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).
Arsenic (Vol. 4)	Not more than 1 mg/kg Determine using an AAS (Hydride generation technique) appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).
Cadmium (Vol. 4)	Not more than 1 mg/kg Determine using an AAS (Electrothermal atomization technique) appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).
Lead (Vol. 4)	Not more than 1 mg/kg Determine using an AAS (Electrothermal atomization technique) appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).

TESTS

PURITY TESTS

Orthophosphate

Determination of orthophosphate by Ion Chromatography with suppressed conductivity detection

Principle:
Orthophosphate in magnesium dihydrogen diphosphate is separated on an ion-exchange column with potassium hydroxide as eluent and detected using conductivity detector.

Equipment and Reagents:
Ion chromatograph with gradient pump, autosampler, anion self regenerating suppressor (ASRS) and conductivity detector, Dionex ICS 2000 or equiv.
Sodium phosphate, dibasic, Analytical grade, Aldrich or equiv.
Tetrasodium pyrophosphate decahydrate, Analytical grade, Fluka or equiv.
Potassium hydroxide, Analar grade, BDH or equiv.
Deionized water (18 MΩ.cm)

Preparation of standard and sample solutions:
Stock mixed standard solution: Accurately weigh calculated quantities to get about 25 mg of orthophosphate (PO_4^{3-}) and 30 mg of pyrophosphate ($P_2O_7^{4-}$), quantitatively transfer into a 100-ml volumetric flask and make up to volume with deionized water.

Working mixed standard solutions: Pipette 5, 10, 15, 20, 25 ml of stock mixed standard solution into a series of 50-ml volumetric flasks and make up to volume with deionized water.

Preparation of sample: Accurately weigh about 0.100 g of magnesium dihydrogen diphosphate, quantitatively transfer into a 100-ml volumetric flask, dissolve and make upto volume with deionized water.

Chromatographic conditions:
Column: Ion-exchange column, Dionex Ion Pac AS 16 (2 x 250 mm) with guard column Ion Pac AG 16 (2 x 50 mm) or equiv.
Detector: Conductivity detector
Eluent: Potassium hydroxide: 80 mM in deionized water (18 MΩ.cm)
Gradient Conditions: Eluent A: Potassium hydroxide solution (80m mM) in deionized water; Eluent B: Deionized water: Start gradient by mixing eluent A and B in proportions to get eluent concentration of about 30 mM and increase to 80 mM over a period of 13-15 min. Adjust gradient conditions to separate ortho, pyro and triphosphate by injecting 10 µl of sample solution.

Flow rate: 0.25 ml/min.

Injection volume: 10 µl

Inject 10 µl each of working mixed standard solutions and construct standard curve. Inject sample and calculate the concentration of orthophosphate from the standard curve and weight of sample taken.

METHOD OF ASSAY

Determination of phosphorous as phosphorous pentoxide (P_2O_5)

Determine phosphorous using ICP-AES technique appropriate to the specified level. Set instrument parameters as specified by the instrument manufacturer and use the analytical line for P(213.618 nm). The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4. Determine the phosphorous percentage (P%) in the sample and calculate phosphorous pentoxide using the formula:

$$P_2O_5, \%w/w = P\% \times 4.983$$

Determination of magnesium as magnesium oxide (MgO)

Determine magnesium using ICP-AES technique appropriate to the specified level. Set instrument parameters as specified by the instrument manufacturer and use the analytical line for Mg (279.078 nm). The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4. Determine the magnesium percentage (Mg%) in the sample and calculate magnesium oxide using the formula:

$$MgO, \%w/w = Mg\% \times 1.658$$

MINERAL OIL (MEDIUM VISCOSITY)

Prepared at the 76th JECFA, published in FAO JECFA Monographs 13 (2012), superseding specifications for Mineral oil (Medium and low viscosity), class I prepared at the 59th JECFA (2002), published in FNP 52 Add 10 (2002) and republished in FAO JECFA Monographs 1 (2005). An ADI of 0-10 mg/kg bw was established at the 59th JECFA for mineral oil (medium and low), class I.
At the 76th JECFA the temporary ADI and the specifications for mineral oils (Medium and low viscosity), class II and class III were withdrawn.

SYNONYMS Liquid paraffin, liquid petrolatum, food grade mineral oil, white mineral oil, INS No. 905e

DEFINITION A mixture of highly refined paraffinic and naphthenic liquid hydrocarbons with boiling point above 200°; obtained from mineral crude oils through various refining steps (eg. distillation, extraction and crystallisation) and subsequent purification by acid and/or catalytic hydrotreatment; may contain antioxidants approved for food use.

C.A.S. number 8012-95-1

DESCRIPTION Colourless, transparent, oily liquid, free from fluorescence in daylight; odourless

FUNCTIONAL USES Release agent, glazing agent

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4) Insoluble in water, sparingly soluble in ethanol, soluble in ether

Burning Burns with bright flame and with paraffin-like characteristic smell

PURITY

Viscosity, 100° 8.5-11 mm^2/s
See description under TESTS

Carbon number at 5% distillation point Not less than 25
The boiling point at the 5% distillation point is higher than: 391°.
See description under TESTS

Average molecular weight 480-500
See description under TESTS

Acidity or alkalinity To 10 ml of the sample add 20 ml of boiling water and shake

	vigorously for 1 min. Separate the aqueous layer and filter. To 10 ml of the filtrate, add 0.1 ml of phenolphthalein solution TS. The solution is colourless. Not more than 0.1 ml of 0.1N sodium hydroxide is required to change the colour to pink
Readily carbonizable substances	Place 5 ml of the sample in a glass-stoppered test tube that has previously been rinsed with chromic acid cleaning mixture. Add 5 ml of sulfuric acid TS, and heat in a boiling water bath for 10 min. After the test tube has been in the bath for 30 sec, remove it quickly, and while holding the stopper in place, give three vigorous vertical shakes over an amplitude of about 10 cm. Repeat every 30 sec. Do not keep the test tube out of the bath longer than 3 sec for each shaking period. At the end of 10 min from the time when first placed in the water bath, remove the test tube. The sample remains unchanged in colour, and the acid does not become darker than standard colour produced by mixing in a similar test tube 3 ml of ferric chloride TSC, 1.5 ml of cobaltous chloride TSC, and 0.5 ml of cupric sulfate TSC, this mixture being overlaid with 5 ml of mineral oil.
Polycyclic aromatic hydrocarbons	Transfer 25.0 ml of sample to a 125 ml separating funnel with unlubricated ground-glass parts (stopper, stopcock). Add 25 ml of hexane which has been previously shaken twice with one-fifth its volume of dimethyl sulfoxide. Mix and add 5.0 ml of dimethyl sulfoxide. Shake vigorously for 1 min and allow to stand until two clear layers are formed. Transfer the lower layer to a second separating funnel, add 2 ml of hexane and shake the mixture vigorously. Allow to stand until two clear layers are formed. Separate the lower layer and measure its absorbance between 260 nm and 420 nm, using as the compensation liquid the clear lower layer obtained by vigorously shaking 5.0 ml of dimethyl sulfoxide with 25 ml of hexane for 1 min. Prepare a reference solution in trimethylpentane counting 7.0 mg of naphthalene per litre and measure the absorbance of the solution at the maximum at 275 nm, using trimethylpentane as the compensation liquid. At no wavelength between 260 nm and 420 nm does the absorbance of the test solution exceed one-third that of the reference solution at 275 nm. Use hexane, dimethyl sulfoxide and trimethylpentane in quality specified for ultraviolet spectrometry.
Solid paraffins	Dry a suitable quantity of the substance to be examined by heating at 100° for 2 h and cool in a desiccator over concentrated sulfuric acid. Place in a glass tube with an internal diameter of about 25 mm, close the tube and immerse in a bath of iced water. After 4 h the liquid is sufficiently clear for a black line, 0.5 mm wide against a white background held vertically behind the tube, to be easily seen.
Lead (Vol. 4)	Not more than 1 mg/kg Determine using an AAS (Electrothermal atomization technique) appropriate to the specified level. The selection of sample size and method of sample preparation may be based on principles of methods

described in Volume 4 (under “General Methods, Metallic Impurities”).

TESTS

PURITY TESTS

Viscosity, 100°

ASTM D 445
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Copies of the complete ASTM standard may be purchased directly from ASTM, phone: +1 610-832-9585, fax: +1 610-832-9555
e-mail: service@astm.org
http://www.astm.org

Use a viscometer of the glass capillary type, calibrated and capable of measuring kinematic viscosity with a repeatability exceeding 0.35% only in one case in twenty. Immerse the viscometer in a liquid bath at the temperature required for the test ± 0.1° ensuring that at no time of the measurement will any portion of the sample in the viscometer be less than 20 mm below the surface of the bath liquid or less than 20 mm above the bottom of the bath. Charge the viscometer with sample in the manner dictated by the design of the instrument. Allow the sample to remain in the bath for about 30 min. Where the design of the viscometer requires it, adjust the volume of sample to the mark. Use pressure to adjust the head level of the sample to a position in the capillary arm of the instrument about 5 mm ahead of the first mark. With the sample flowing freely, measure, in seconds (±0.2 sec), the time required for the meniscus to pass from the first to the second timing mark. If the time is less than 200 s, select a viscometer with a capillary of smaller diameter and repeat the operation. Make a second measurement of the flow time. If two measurements agree within 0.2%, use the average for calculating the kinematic viscosity. If the measurements do not agree, repeat the determination after thoroughly cleaning and drying the viscometer.

Viscosity, 100° (mm^2/sec) = C x t

Where
C = calibration constant of the viscometer (mm^2/sec^2)
t = flow time (sec)

Carbon number
ASTM D 2887
See TEST for Viscosity for Copyright permission.

"Carbon number" is number of carbon atoms in a molecule. Determine the boiling point distribution of the sample by gas chromatography using the following conditions:
The system must have the following performance characteristics:
Sensitivity: 1% dodecane must be detected with a peak height of at least 10% of full scale under the conditions prescribed below.
Stability: when operated at the required sensitivity level, the baseline drift is not more than 1% of full scale per hour
Repeatability of retention times: 6 sec for each component of the calibration mixture.
Resolution (R): determined for a solution of 1% of each of hexadecane and octadecane in n-octane is not less than three and not more than eight, using the following formula:

$$R = \frac{2d}{W1 + W2}$$

where
d is distance in mm between the peak maxima of hexadecane and octadecane
W1 is the peak width in mm at the baseline of hexdecane
W2 is the peak width in mm at the baseline of octadecane
Typical conditions which may be used:
Column
length: 1.5m
outside diameter: 3.2 mm
liquid phase: SE - 30.5 %
support material: Chromosorb G, mesh 60/80
Column temperature
initial: 10°
final: 350°
rate: 6.5°/min.
Carrier
gas: helium
flow: 30 ml/min.
Detector: FID
Detector temperature: 370°
Injection temperature: 370°
Sample size: 0.3 µl
Calibration mixture: Prepare a mixture of hydrocarbons of known boiling points covering the range of the sample. At least one compound must have a boiling point lower than the initial boiling point of the sample.
Procedure:
Calibration: Cool the column to the selected starting temperature (the retention time for the initial boiling point must be at least 1 min) and inject the calibration mixture. Record the retention time of each peak maximum and the peak areas for each component. Plot the retention time of each peak versus the corresponding normal boiling point of that component in degrees Celsius to obtain a calibration curve.
Sample analysis: Using the exact conditions used in the calibration run, inject the sample. Record the area of each time segment at fixed time intervals not greater than 1% of the retention time equivalent to a boiling point of 538° obtained from the calibration curve.
Calculation: Sum the area segments to obtain the cumulative area at each time interval during the run. At the point of the chromatogram, where the baseline at the end first becomes steady, observe the cumulative area counts. Move back along the record until a cumulative area equal to 99.5% of the total at the steady point appears. Mark this point as the final boiling point. Observe the area counts at the start of the run until the point is reached, where the cumulative area count is equal to 0.5% of the total area. Mark this point as the initial boiling point of the sample. Divide the cumulative area at each interval between the initial and final boiling points by the total cumulative area and multiply by 100. This will give the cumulative percent of the sample recovered at each time interval. Tabulate the cumulative percent recovered at each interval and the retention time at the end of the interval. Using linear

interpolation, if necessary, determine the retention time associated with 5% and read the corresponding boiling temperature from the calibration curve.
The boiling point at the 5% distillation point is higher than: 391°.

Average molecular weight
ASTM D 2502
See TEST for Viscosity for Copyright permission

Determine the kinematic viscosity of the sample at 37.8° and 98.9° as described in the method for Viscosity, 100°. Read the value of H that corresponds to the measured viscosity at 37.8° by the use of table 1; linear interpolation between adjacent columns may be required. Read a viscosity-molecular weight chart for H and 98.9° viscosity (the chart is available from the American Society for Testing and Materials (ASTM). A simplified version is shown in Figure 1 for illustration purposes only. Interpolate where necessary between adjacent lines of 98.89° viscosity. After locating the point corresponding to the value of H (ordinate) and the 98.89°viscosity (superimposed lines), read the molecular weight along the abscissa.

Table 1 - Tabulation of H Function

Kinematlc viscosity, mm^2/s at 37.8°	H				
	0	0.2	0.4	0.6	0.8
2	-176	-151	-126	-104	-85
3	-67	-52	-38	-25	-13
4	-1	9	19	28	36
5	44	52	59	66	73
6	79	85	90	96	101
7	106	111	116	120	124
8	128	132	136	140	144
9	147	151	154	157	160
10	163	166	169	172	175
11	178	180	183	185	188
12	190	192	195	197	199
13	201	203	206	208	210
14	211	213	215	217	219
15	212	222	224	226	227
16	229	231	232	234	235
17	237	238	240	241	243
18	244	245	247	248	249
19	2551	252	253	255	256
20	257	258	259	261	262
21	263	264	265	266	267
22	269	270	271	272	273
23	274	275	276	277	278
24	279	280	281	281	282
25	283	284	285	286	287
26	288	289	289	290	291
27	292	293	294	294	295
28	296	297	298	298	299
29	300	301	301	302	303
30	304	304	305	306	306
31	307	308	308	309	310
32	310	311	312	312	313
33	314	314	315	315	316
34	317	317	318	319	319
35	320	320	321	322	322
38	323	323	324	325	325
37	325	326	327	327	328
38	328	329	329	330	331
39	331	332	332	333	333

	H									
	0	1	2	3	4	5	6	8	9	10
40	334	336	339	341	343	345	347	349	352	354
50	355	357	359	361	363	364	366	368	369	371
60	371	374	375	377	378	380	381	382	384	385
70	386	387	388	390	391	392	393	394	395	397

80	398	399	400	401	402	403	404	405	406	407
90	409	409	410	410	411	412	413	414	415	416
100	416	417	418	419	420	420	421	422	423	423
110	424	425	425	426	427	428	428	429	430	430
120	431	432	432	433	433	434	435	435	436	437
130	437	438	438	439	439	440	441	441	442	442
140	443	443	444	444	445	446	446	447	447	448
150	448	449	449	450	450	450	451	451	452	452
160	453	453	454	454	455	455	456	456	456	457
170	457	458	458	459	459	460	460	460	461	461
180	461	462	462	463	463	463	464	464	465	465
190	465	466	466	466	467	467	468	468	468	469
	H									
	0	10	20	30	40	50	60	10	80	90
200	469	473	476	479	482	485	487	490	492	495
300	497	499	501	503	505	507	509	511	512	514
400	515	517	518	520	521	523	524	525	527	528
500	529	530	531	533	534	535	536	537	538	539
600	540	541	542	543	544	545	546	547	547	548
700	549	550	551	551	552	553	554	554	555	556
800	557	557	558	559	559	560	561	562	562	563
900	563	564	565	565	566	566	567	567	568	569
	H									
	0	100	200	300	400	500	600	700	800	900
1000	569	574	578	583	587	591	594	597	600	603
2000	605	608	610	614	616	618	620	621	623	625
3000	625	626	628	629	631	632	633	634	636	637
4000	638	639	640	641	642	643	644	645	646	647
5000	648	649	650	651	652	652	653	654	655	656
6000	656	657	658	658	659	660	660	661	662	662
7000	663	664	664	665	665	666	666	667	667	668
8000	668	669	670	670	671	671	671	672	672	673
9000	673	674	674	675	675	676	676	677	677	677
	H									
	0	1000	2000	3000	4000	5000	6000	7000	6000	9000
10000	678	681	684	688	691	694	696	699	701	703
20000	705	707	709	711	712	715	715	717	718	719
30000	720	722	723	724	725	726	727	728	729	730
40000	731	732	732	733	734	735	736	736	737	738
50000	739	739	740	741	741	742	743	743	744	744
60000	745	746	746	747	747	748	748	749	749	750
70000	750	751	751	752	752	753	753	753	754	754
80000	755	755	756	756	756	757	757	758	758	758
90000	759	759	759	760	760	760	761	761	761	762
100000	762	762	763	763	763	764	764	764	764	765

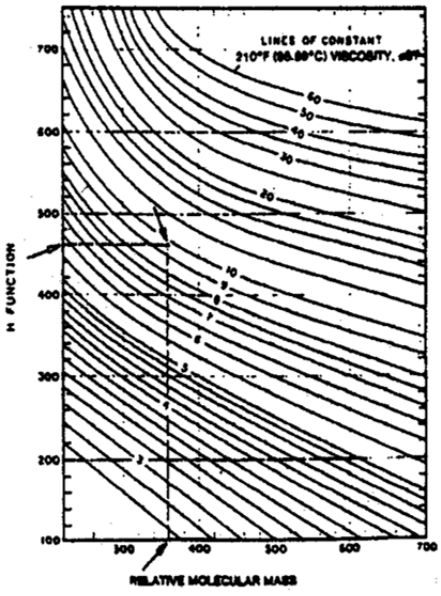


Figure 1 – Lines of constant viscosity (mm^2/s) at 98.89°

Readily carbonizable substances

Place 5g of the sample in a glass-stoppered test tube that has previously been cleaned with a chromic acid cleaning solution, rinsed with water and dried in an oven (105°, 1h). Add 5 ml of sulfuric acid TS, and place in a boiling water bath. After the test tube has been in the

bath for 30 sec, remove quickly, and while holding the stopper in place, give three vigorous vertical shakes over an amplitude of about 10 cm. Repeat every 30 sec. Do not keep the test tube out of the bath longer than 3 sec for each shaking period. At the end of 10 min from the time when first placed in the water bath, remove the test tube. The sample remains unchanged in colour, and the acid does not become darker than a very slight straw colour (Matching Fluid E , see Volume 4). No black material occurs at the interface between the two layers.

MODIFIED STARCHES

Prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012), superseding specifications prepared at the 74th JECFA (2011) and published in FAO JECFA Monographs 11 (2011). An ADI "not specified" was established at the 26th JECFA (1982) for all modified starches listed below except for acetylated oxidized starch for which an ADI "not specified" was established at the 57th JECFA (2001).

Degree of substitution of starch sodium octenyl succinate

The degree of substitution is determined by the amount of acid consumed by the sample during hydrolysis.

Procedure

Weigh accurately about 5.000 g of sample into a 150-ml beaker and wet the sample with a few ml of isopropanol. Pipette 25.0 ml of 2.5 N hydrochloric acid in isopropanol and stir the mixture with a magnetic stirrer for 30 min. Using a graduated measuring cylinder, add 100 ml of 90% isopropanol in water and stir the contents for another 10 min. Filter through a Buchner funnel and wash the filter cake with 90% isopropanol in water until the filtrate is negative for chloride (check using 0.1 N silver nitrate). Transfer the filtrate to a 600-ml beaker, rinse the flask and bring to a 300-ml volume with distilled water. Place the beaker on a boiling water bath for 10 min, while stirring the contents. While hot, titrate with 0.1 N sodium hydroxide using phenolphthalein TS as an indicator.

Calculation

$$\text{Degree of substitution} = \frac{0.162 \times A}{1 - 0.210 \times A}$$

where

A is milliequivalents of sodium hydroxide required per 1 g of starch octenyl succinate.

PHYTASE FROM *ASPERGILLUS NIGER* EXPRESSED IN *A. NIGER*

New specifications prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012). An ADI "not specified" was established at the 76th JECFA (2012).

SYNONYMS Phytase, 3-phytase

SOURCES Phytase is produced by submerged fed-batch fermentation of a non pathogenic and non toxicogenic genetically modified strain of *Aspergillus niger* which contains the phytase encoding gene derived from *Aspergillus niger*. The enzyme is secreted and then isolated from the fermentation broth by filtration to remove the biomass and concentrated by ultrafiltration. The enzyme concentrate is subjected to germ filtration and is subsequently formulated and standardized to the desired activity using food-grade compounds.

Active principles: 3-phytase

Systematic names and numbers: Myo-Inositol hexakisphosphate 3-phosphohydrolase, EC 3.1.3.8, CAS 37288-11-2

Reactions catalysed: Hydrolysis of myo-inositol hexakisphosphate (phytate) to inositol pentaphosphate (IP5), and further to give a mixture of myo-inositol di-phosphate (IP2), myo-inositol mono-phosphate (IP1) and free orthophosphate

Secondary enzyme activities: No significant levels of secondary enzyme activities

DESCRIPTION Brownish liquid or yellow to light brown powder.

FUNCTIONAL USES Enzyme preparation.
Used to degrade phytate found in plant derived foods, particularly cereal grains and legumes, in order to improve mineral bioavailability.

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

CHARACTERISTICS

IDENTIFICATION

Phytase activity: The sample shows phytase activity.
See description under TESTS.

TESTS

Phytase activity

Principle This procedure is used to determine the activity of enzymes releasing phosphate from phytate. The assay is based on enzymatic hydrolysis of sodium phytate under controlled conditions by measurement of the amount of ortho phosphate released.

The phytase activity is expressed in phytase units (FTU). One phytase unit (FTU) is defined as the amount of enzyme that liberates 1 micromole of inorganic phosphorus per minute from 0.0051 mol/l sodium phytate at 37° and pH 5.50 under the conditions of the test.

Reagents and Solutions

[NOTE- Ensure the absence of phosphate in all glassware.]

Acetate buffer pH 5.50:
Dissolve 1.76 g (1.68 ml) glacial acetic acid ($C_2H_4O_2$), 30.02 g of sodium acetate trihydrate ($C_2H_3O_2Na•3H_2O$), and 0.147 g of calcium chloride dihydrate ($CaCl_2.2H_2O$) in about 900 ml of water. Transfer the solution into a 1000-ml volumetric flask, dilute to volume with water, and mix. Adjust the pH to 5.50 ±0.05.

Substrate solution:
Dissolve 0.84 g of sodium phytate decahydrate ($C_6H_6O_{24}P_6Na_{12}•10H_2O$) in 100 ml of acetate buffer. Adjust the pH to 5.50 ±0.05 by adding 4 M acetic acid. Quantitatively transfer the mixture to a 1000 ml volumetric flask, dilute to volume with acetate buffer, and mix. Prepare fresh daily.

Nitric acid solution (27%):
While stirring, slowly add 70 ml of 65% nitric acid to 130 ml of water.

Ammonium heptamolybdate solution:
Dissolve 100 g of ammonium heptamolybdate tetrahydrate [$(NH_4)_6Mo_7O_{24}•4H_2O$] in 900 ml of water in a 1000-ml volumetric flask. Add 10 ml of 25% ammonia solution (NH_4OH – ammonium hydroxide), dilute to volume with water, and mix. This solution is stable for 4 weeks when stored at ambient temperature and shielded from light.

Ammonium vanadate solution:
Dissolve 2.35 g of ammonium monovanadate (NH_4VO_3) in 400 ml of warm (60°) water. While stirring, slowly add 20 ml of nitric acid solution (27%). Cool to ambient temperature. Quantitatively transfer the mixture to a 1000-ml volumetric flask, dilute to volume with water, and mix. This solution is stable for 4 weeks when stored at ambient temperature and shielded from light.

Colour/stop solution:
While stirring, add 25 ml of ammonium vanadate solution to 25 ml of ammonium heptamolybdate solution. Slowly add 16 ml of 65% nitric acid. Quantitatively transfer the mixture to a 100-ml volumetric flask, dilute to volume with water, and mix. Prepare fresh daily.

Potassium dihydrogen phosphate solution:
Dry a sufficient amount of >99% purity potassium dihydrogen

phosphate (KH_2PO_4) in a oven at 105° for 4 h. Cool to ambient temperature in a desiccator over dried silica gel. In two separate 1l volumetric flasks , weigh accurately 0.245 g of dried potassium dihydrogen phosphate and dilute with acetate buffer to 1 l to obtain potassium dihydrogen phosphate solutions A and B, each containing 1.80 mmol/l of potassium dihydrogen phosphate.

Phytase standard: obtained from Gist-Brocades, Delft, The Netherlands, with an assigned activity or equivalent.

Phytase standard solution:
In duplicate, accurately weigh an adequate amount of phytase standard and dissolve and dilute in acetate buffer to obtain a solution containing 0.06 ±0.01 phytase units per 2.0 ml. Quantify the activity of the phytase standard according to procedure described below.

Procedure for quantifying the activity of the phytase standard

Using 6 individual 20-×150-mm glass test tubes add to one tube 2.00 ml of the phytase standard solution, add to 3 tubes 2.00 ml of potassium dihydrogen phosphate solution A, and to the remaining 2 tubes 2.00 ml of potassium dihydrogen phosphate solution B. Place the tubes into a 37.0±0.1° water bath, at regular time intervals and allow their contents to equilibrate for 5 min.
At time equals 5 min, in the same order and within the same time intervals as the tubes were added, add 4.0 ml of substrate solution (previously equilibrated to 37.0±0.1°), to each of the tubes. Mix the tubes, and replace in the 37.0±0.1°water bath.
At time equals 35 min, in the same order and within the same time intervals, terminate the incubation by adding 4.0 ml of colour/stop solution to each of the tubes. Mix, and cool to ambient temperature. Prepare an enzyme blank by adding 2.00 ml of phytase standard solution into one 20-×150-mm glass test tube. Prepare reagent blanks by adding 2.00 ml of water into a series of five separate 20-×150-mm glass test tubes. Add 4.0 ml of colour/stop solution to all blank tubes and mix. Next add 4.0 ml of substrate solution, and mix. Determine the absorbance of all solutions at 415 nm in a 1-cm path-length cell with a spectrophotometer, using water to zero the instrument.

Calculation of the activity of the phytase standard

Calculate the corrected absorbances (AR) for each sample preparation (absorbance of the standard phytase solution minus the corresponding absorbance of the blank) and for each potassium dihydrogen phosphate solution, Ap (absorbance of the potassium dihydrogen phosphate solution minus average absorbance of the reagent blanks). Calculate C, the phosphate concentration of each potassium dihydrogen phosphate solution:

C (mmol/2 ml) = (W ×1000 ×2)/MW.

Calculate the absorbances (D) for each potassium dihydrogen phosphate solution after correction for the amount of potassium dihydrogen phosphate weighed:
Ap/C = D (absorbance units/mmol of phosphate per 2 ml).

Calculate the average of results D, giving E (maximum allowable difference, 5%).
Calculate the activity for the phytase standard:

FTU/g = (AR ×f)/(30 ×R ×E),

where,
AR is the corrected absorbance of the phytase standard solution;
f is the total dilution factor of the standard preparation;
60 is the incubation time, in min; R equals sample weight, in g;
E is average of D factors;
W is the weight of potassium dihydrogen phosphate, in g;
MW is the molecular weight of potassium dihydrogen phosphate, 136.09 (g/mol).

Determination of phytase activity in samples

Sample preparation: Suspend or dissolve and dilute accurately weighed amounts of sample in acetate buffer so that 2.0 ml of the final solution will contain between 0.01 and 0.08 phytase units.

Preparation of phytase standard curve: Weigh, in duplicate, with an accuracy of ± 1 mg, an amount of phytase standard based on the activity which corresponds to about 20,000 phytase units in 200-ml volumetric flasks. Dissolve in and dilute to volume with acetate buffer, and mix. Use this stock solution and dilute with acetate buffer to obtain standard solutions containing approximately 0.01, 0.02, 0.04, 0.06, and 0.08 phytase units per 2.0 ml.

Add 2.00 ml of each phytase standard solution and 2.00 ml of the sample solution into separate 20-×150-mm glass test tubes. Place the tubes into a 37.0±0.1° water bath, at regular time intervals and allow their contents to equilibrate for 5 min. At time equals 5 min, in the same order as the tubes were added, add 4.0 ml of substrate solution (previously equilibrated to 37.0±0.1°) to the each of the test tubes. Mix, and replace in the 37.0±0.1°water bath. At time equals 35 min, in the same order and within the same time intervals, terminate the incubation by adding 4.0 ml of colour/stop solution to each of the tubes. Mix, and cool to ambient temperature.

Prepare enzymes blanks as described for quantifying the activity of the phytase standard. Centrifuge all test tubes for 5 min at 3000 ×g. Determine the absorbance of each solution at 415 nm in a 1-cm path-length cell with a spectrophotometer, using water to zero the instrument.

Calculation of phytase activity in samples

Calculate the corrected absorbance (sample minus blank) for each sample preparation and phytase standard solution. Plot the calculated phytase activity (FTU per 2 ml) of each phytase solution against the corresponding absorbance. From the curve, determine the phytase activity in each sample preparation (FTU per 2 ml):

Activity (FTU/g) = (FTU per 2 ml ×dilution)/sample weight

SERINE PROTEASE WITH CHYMOTRYPSIN SPECIFICITY FROM *NOCARDIOPSIS PRASINA* EXPRESSED IN *BACILLUS LICHENIFORMIS*

New specifications prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012). An ADI "not specified" was established at the 76th JECFA (2012)

SYNONYMS

Chymotrypsins A and B; α-chymar ophth; avazyme; chymar; chymotest; enzeon; quimar; quimotrase; α-chymar; α-chymotrypsin A; α-chymotrypsin

SOURCES

Produced by submerged fermentation of a genetically modified non-pathogenic and non-toxigenic strain of *Bacillus licheniformis* which contains a gene coding for serine protease with chymotrysin specificity from *Nocardiopsis prasina.* The enzyme is secreted to the broth. The cell mass and other solids are separated from the broth by vacuum drum filtration or centrifugation. Ultrafiltration and/or evaporation are applied for concentration and further purification. Residual production strain microorganisms are removed by germ filtration. The final product is formulated using food-grade stabilizing and preserving agents and is standardized to the desired activity.

Active principles	Serine protease with chymotrypsin specificity
Systematic names and numbers	EC 3.4.21.1, CAS number: 9004-07-3
Reactions catalysed	Preferential cleavage: Tyr, Trp, Phe, Leu
Secondary enzyme activities	None

DESCRIPTION

Brown liquid

FUNCTIONAL USES

Enzyme preparation.
Used in the hydrolysis of proteins like casein, whey, soy isolate, soy concentrate, wheat gluten and corn gluten in the production of partially or extensively hydrolyzed proteins of vegetable and animal origin.

GENERAL SPECIFICATIONS

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

CHARACTERISTICS

IDENTIFICATION

Serine protease activity with chymotrypsin specificity

The sample shows serine protease activity with chymotrypsin specificity.
See descriptions under TESTS

TESTS

Serine protease activity with chymotrypsin specificity

Principle:
Serine protease hydrolyses the substrate Suc-Ala-Ala-Pro-Phe-pNA. The release of p-nitroaniline (pNA) results in an increase of absorbance at 405 nm and is proportional to the enzyme activity. Enzyme activity is measured in PROT units. One PROT unit is the amount of enzyme that releases 1µmol of p-nitroaniline from 1 mM substrate (Suc-Ala-Ala-Pro-Phe-pNA) per minute at pH 9.0 and temperature 37°.

Reagents and Solutions:

0.1M Tris buffer, pH 9.0:
Weigh 12.11 g of Tris (tris(hydroxymethyl)aminomethane) and transfer it to a 1L beaker. Weigh out 8.77 g of sodium chloride and transfer to the beaker. Add 900 ml deionized water. Add 3 drops of Triton X-100 while stirring. Maintain buffer temperature between 23 and 25° prior to next step. Measure and adjust pH after all the Triton X-100 has dissolved. Adjust to pH 9.0±0.1 using 4M HCl. Transfer to a 1L volumetric flask and make up to volume with deionized water. Solution can be stored at room temperature for up to 24 h. Ensure that the buffer is stirred prior to withdrawing for testing.

Suc-Ala-Ala-Pro-Phe-pNA (Substrate) Stock Solution:
Weigh 50 mg of the Suc-Ala-Ala-Pro-Phe-pNA substrate in a small beaker. Add 1 ml of DMSO to the substrate. Mix well. Transfer solution to an appropriate container, cover with aluminum foil and store away from light. Solution can be stored at room temperature for up to 1 day.

Suc-Ala-Ala-Pro-Phe-pNA (Substrate) Working Solution:
Transfer 350 µl of Suc-Ala-Ala-Pro-Phe-pNA (Substrate) Stock Solution into a 25 ml volumetric flask. Make up to volume with 0.1M Tris Buffer, pH 9.0. Mix well, and wrap the flask immediately with foil to avoid light. Solution can be stored at room temperature in the dark, up to 6 h.
10 mM citrate buffer, pH 3.40:
Fill a 1000 ml volumetric with about 500ml deionized water. Weigh

1.56 g of citric acid monohydrate, 0.76 g tri-sodium citrate-dihydrate and 8.77 g sodium chloride and transfer to the volumetric flask. Fill the flask to about 900 ml with deionized water. Stir. Add 3 drops of Triton X-100, and continue to stir. Adjust pH to 3.40±0.03. if necessary, after the Triton X-100 has dissolved. Make up to volume with deionized water and stir. Solution is stable at room temperature for up to 3 days.

Preparation of Standards and Samples:
Preparation of stock standard: Weigh the PROT standard corresponding to 750.1 PROT (±0.7 PROT) in a 250 ml volumetric flask Dissolve and make up to volume with 10 mM citrate buffer. Stir for 15 min at room temperature. This solution can be stored at room temperature for up to 6 h.
Preparation of samples: All samples, liquid or frozen, must be brought to room temperature, and be thoroughly mixed before weighing.
Weigh a known quantity of sample within ±1 mg, transfer to an appropriate volumetric flask and make up the volume with 10 mM citrate buffer. The activity of the final dilution(s) of the sample(s) must be around 200 mPROT/ml. Dilute further with citrate buffer, if this concentration is not observed. Solutions can be stored up to 6 h at room temperature.

Procedure

Preparation of Standard Curve: Prepare a standard curve using the stock standard and 10 mM citrate buffer as shown in the table below. The solutions can be stored up to 6 h at room temperature.

Standard No.	Dilution Ratio	Example		Concentration (mPROT/ml)
		Stock Standard, µl	10 mM citrate buffer, µl	
1	50	30	1470	60.0
2	30	50	1450	100.0
3	25	60	1440	120.0
4	20	75	1425	150.0
5	15	100	1400	200.0
6	12	125	1375	250.0
7	10	150	1350	300.0

Place the Suc-Ala-Ala-Pro-Phe-pNA (Substrate) Working Solution in a water bath set to 37.0±1.0°. Set the spectrophotometer at 405 nm and the temperature of the cuvette holder at 37.0±0.5°. Pipette 2.4 ml of the working substrate solution into a cuvette. Add 600µl of each standard and sample to the cuvette. Place the cuvette in the spectrophotometer set to 37.0±0.5°. Set and start stopwatch to 1

min. Read absorbance at 20 sec intervals for 3 min.

Calculations

Calculate the average absorbance per minute for each standard via linear regression. Plot the standard curve using the average absorbance per minute calculated against activity of the standards (mPROT/ml). Read the absorbance of the sample(s) from the standard curve generated and calculate enzyme activity as shown below:

$$Activity, PROT / g = \frac{S \times V \times F}{W \times 1000}$$

Where, S is reading in mPROT/ml, from the standard curve, V is Volume of the volumetric flask used for the preparation of the sample for the standard curve in ml, F is Dilution Factor (including the 2nd dilution, if needed during sample preparation), W is weight of the sample in grams and 1000 is the Conversion Factor from mPROT to PROT.

SERINE PROTEASE WITH TRYPSIN SPECIFICITY FROM *FUSARIUM OXYSPORUM* EXPRESSED IN *FUSARIUM VENENATUM*

New specifications prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012). An ADI "not specified" was established at the 76th JECFA (2012)

SYNONYMS

α-trypsin; β-trypsin; cocoonase; parenzyme; parenzymol; tryptar; trypure; pseudotrypsin; tryptase; tripcellim; sperm receptor hydrolase

SOURCES

Produced by submerged fermentation of a genetically modified non-pathogenic and non-toxigenic strain of *Fusarium venenatum* which contains a gene coding for serine protease with trypsin specificity from *Fusarium oxysporum.* The enzyme is secreted into the broth. The cell mass and other solids are secreted into the fermentation broth, separated by vacuum drum filtration or centrifugation. Ultrafiltration and/or evaporation are applied for concentration and further purification. Residual production strain microorganisms are removed by germ filtration. The final product is formulated using food-grade stabilizing and preserving agents and is standardized to the desired activity.

Active principles	Serine protease with trypsin specificity
Systematic names and numbers	EC 3.4.21.4, CAS number: 9002-07-7
Reactions catalysed	Preferential cleavage: Arg, Lys
Secondary enzyme activities	None

DESCRIPTION

Brown liquid.

FUNCTIONAL USES

Enzyme preparation.
Used in the production of partially or extensively hydrolyzed proteins of vegetable and animal origin. These hydrolyzed proteins may be used for various applications as ingredients in food and beverages, for protein fortification or as ingredients providing functional effects such as emulsification or flavour enhancement.

GENERAL SPECIFICATIONS

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

CHARACTERISTICS

IDENTIFICATION

Serine protease activity with trypsin specificity	The sample shows serine protease activity with trypsin specificity. See descriptions under TESTS

TESTS

Serine protease activity with trypsin specificity

Principle:

Serine protease with trypsin specificity hydrolyses the substrate Ac-Arg-p-nitro-Anilide (Ac-Arg-*p*NA). The release of *p*-nitroaniline (*p*NA) results in an increase of absorbance at 405 nm and is proportional to the enzyme activity. Enzyme activity is measured in Kilo Microbial Trypsin Units (KMTU). 1 KMTU is the amount of enzyme that releases 1µmol of *p*-nitroaniline from 1mM substrate (Ac-Arg-pNA) per minute at pH 9.0 and temperature 37°.

Reagents and Solutions:

Preparation of 15% Brij 35 solution:
Bring the stock Brij 35 (30% solution) to room temperature. Pour out 1L into a 2L volumetric flask. Make up the volume with demineralized water. Stir vigorously. Store in a bottle with label up to 2 months at 4°.

Preparation of 1M Tris buffer:
Weigh and transfer 121.1g Tris (tris(hydroxymethyl)-aminomethane) into a 1L volumetric flask. Add about 800 ml of deionised water and stir on a magnetic stirrer until dissolved. Make up the volume with deionised water. This solution can be stored at room temperature for up to 1 month.

Preparation of dilution buffer (1.5 mM $CaCl_2$, 0.225 g/l Brij, 100 mM Tris, pH 8.0):

Example
Volume, 10 L: Weigh and transfer 2.20 g $CaCl_2.2H_2O$ into a 10 L volumetric flask. Add 1000 ml of 1 M Tris buffer. Add 15 ml of 15% Brij 35 solution, approximately 7000 ml of deionised water, and 275 ml of 2M hydrochloric acid. Mix until completely dissolved. Ensure that the solution temperature is between 23° to 25°. Adjust pH to 8.00±0.05. Make up the volume with deionised water. Mix thoroughly. This solution can be stored at room temperature up to 8 days. Ensure that the dilution buffer is adjusted to 23-25° prior to use by stirring.

Preparation of 5 mM Ac-Arg-*p*NA solution (Substrate Solution):

It is important to obtain a high quality substrate as well as to prepare, store and measure the substrate solution accurately. This affects the quality of analysis. Frozen substrate must be thawed completely before use, and discarded after.

Weigh and transfer quantitatively 186.0±0.2 mg Ac-Arg-*p*NA into a 100 ml volumetric flask. Make up the volume with dilution buffer. Wrap the flask immediately with aluminum foil to protect from light. Mix for 5 min (max of 10 min). Aliquot the solution into tubes of 10 ml protected from light. Solution can be stored frozen up to 28 days (no yellow colouring appears).
It is recommended to store at least 6 stock samples (at 1g aliquots) per lot for enabling bridging studies.

Preparation of Standard and Sample Solutions:

Preparation of stock standard solution:
Weigh and transfer an amount corresponding to 20.00 KMTU (±0.02 KMTU) of the serine protease with trypsin specificity standard into a 250 ml volumetric flask. Make up the volume with dilution buffer. Mix the solution for about 15 min.

Preparation of sample

Weigh between 0.5 g to 1.78 g of the serine protease with trypsin specificity sample. Ensure that samples are homogeneous. Dilute in a measuring flask with dilution buffer. NOTE: A typical dissolution volume is 250 ml of diluent buffer.

Stock sample solutions can be stored up to 8 h at room temperature. The stock sample solution is further diluted with the dilution buffer, to reach an activity of about 4.7 mKMTU/ml after final dilution. This solution can be stored at room temperature, covered, for up to 6 h.

Procedure

Prepare a standard curve using the stock standard solution as shown below:

Standard #	Dilution Ratio	Stock standard solution, µl	Dilution Buffer, µl	Concentra mKMTU/m
1	50	30	1470	1.6
2	25	60	1440	3.2
3	15	100	1400	5.3
4	12	125	1375	6.7
5	10	150	1350	8.0

Prepared Working standard solutions can be stored, covered, up to 6 h at room temperature.

Place the 5 mM Ac-Arg-*p*NA solution (substrate solution) in a water bath set to 37.0±1.0°. Set the spectrophotometer at 405 nm and the temperature of the cuvette holder at 37.0±0.5°. Pipette 2.5 ml of it into the cuvette. Add 340 ml of the working standard solution, reference standard working solution or sample to the cuvette. Place the cuvette in the spectrophotometer set to 37.0±0.5°. Set and start stopwatch to 12 sec. Read absorbance at 20 sec intervals for 3.5 min at 405 nm.

Calculations

Calculate the average absorbance per minute for each standard via linear regression. Plot the standard curve using the average absorbance per minute calculated against the activity of the standards (mKMTU/ml). Read the absorbance of the sample from the standard curve generated and calculate the enzyme activity as shown below:

$$Activity, KMTU / g = \frac{S \times V \times F}{W \times 1000}$$

where, S, is the reading in mKMTU/ml, from the standard curve, V is the volume of the measuring flask used in ml, F is the dilution factor, W is the weight of the sample in g and 1000 is the conversion factor from mKMTU to KMTU.

TITANIUM DIOXIDE

Prepared at the 76th JECFA (2012) and published in FAO JECFA Monographs 13 (2012), superseding specifications prepared at the 73rd JECFA (2010) and published in FAO JECFA Monographs 10 (2010). An ADI "not limited" was established at the 13th JECFA (1969).

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

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

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

In the chloride processes, (a) titanium-containing mineral is reacted with chlorine gas under reducing conditions to form anhydrous titanium tetrachloride, which is subsequently purified and converted to titanium dioxide either by direct thermal oxidation or by reaction with steam in the vapour phase; (b) titanium-containing mineral is reacted with concentrated hydrochloric acid to form a solution of titanium tetrachloride, which is further purified and hydrolysed to get titanium dioxide. The compound is filtered, washed and calcined.

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

C.A.S. number 13463-67-7

Chemical formula TiO_2

Formula weight 79.88

Assay Not less than 99.0% on the dried basis and on an aluminium oxide and silicon dioxide free basis.

DESCRIPTION White to slightly coloured amorphous powder

FUNCTIONAL USES Colour

CHARACTERISTICS

IDENTIFICATION

Solubility (Vol. 4)	Insoluble in water, hydrochloric acid, dilute sulfuric acid, and organic solvents. Dissolves slowly in hydrofluoric acid and hot concentrated sulfuric acid.
Colour reaction	Add 5 ml sulfuric acid to 0.5 g of the sample, heat gently until fumes of sulfuric acid appear, then cool. Cautiously dilute to about 100 ml with water and filter. To 5 ml of this clear filtrate, add a few drops of hydrogen peroxide; an orange-red colour appears immediately.

PURITY

Loss on drying (Vol. 4)	Not more than 0.5% (105°, 3 h)
Loss on ignition (Vol. 4)	Not more than 1.0% (800°) on the dried basis
Aluminium oxide and/or silicon dioxide	Not more than 2%, either singly or combined See descriptions under TESTS
Acid-soluble subst ances	Not more than 0.5%; Not more than 1.5% for products containing alumina or silica. Suspend 5 g of the sample in 100 ml 0.5 N hydrochloric acid and place on a steam bath for 30 min with occasional stirring. Filter through a Gooch crucible fitted with a glass fibre filter paper. Wash with three 10-ml portions of 0.5 N hydrochloric acid, evaporate the combined filtrate and washings to dryness, and ignite at a dull red heat to constant weight.
Water-soluble matter (Vol. 4)	Not more than 0.5% Proceed as directed under acid-soluble substances (above), using water in place of 0.5 N hydrochloric acid.
Impurities soluble in 0.5 N hydrochloric acid	Antimony: Not more than 2 mg/kg Arsenic: Not more than 1 mg/kg Cadmium: Not more than 1 mg/kg Lead: Not more than 10 mg/kg See description under TESTS
Mercury (Vol. 4)	Not more than 1 mg/kg Determine using AAS (Cold vapour generation technique). The selection of sample size and method of sample preparation may be based on principles of methods described in Volume 4 (under “General Methods, Metallic Impurities”).

TESTS

PURITY TESTS

Impurities soluble in 0.5 N hydrochloric acid

Antimony, arsenic, cadmium and lead (Vol.4)

Transfer 10.0 g of sample into a 250-ml beaker, add 50 ml of 0.5 *N* hydrochloric acid, cover with a watch glass, and heat to boiling on a hot plate. Boil gently for 15 min, pour the slurry into a 100- to 150-ml centrifuge bottle, and centrifuge for 10 to 15 min, or until undissolved material settles. Decant the supernatant through Whatman No. 4 filter paper, or equivalent, collecting the filtrate in a 100-ml volumetric flask and retaining as much as possible of the undissolved material in the centrifuge bottle. Add 10 ml of hot water to the original beaker, washing off the watch glass with the water, and pour the contents into the centrifuge bottle. Form a slurry, using a glass stirring rod, and centrifuge. Decant through the same filter paper, and collect the washings in the volumetric flask containing the initial extract. Repeat the entire washing process two more times. Finally, wash the filter paper with 10 to 15 ml of hot water. Cool the contents of the flask to room temperature, dilute to volume with water, and mix.

Determine cadmium, and lead using an AA-Electrothermal atomization technique, antimony by ICP-AES technique and arsenic using atomic absorption hydride technique.

Aluminium oxide and/or Silicon dioxide

Weigh about 0.5 g of the sample to the nearest 0.1 mg, in a platinum or nickel crucible, add 5 g potassium hydroxide and 2 g boric acid, mix and melt completely using a torch burner and allow to stand at room temperature. Place the reaction product along with crucible into 150 ml hot deionized water in a 250-ml PTFE beaker and dissolve residue by agitation. Wash the crucible with hot deionized water and remove it. Add 50 ml hydrochloric acid and transfer the contents into a 250-ml polypropylene volumetric flask. Wash the beaker three times with hot deionized water, transfer the washings to the volumetric flask and make up to volume (Solution A). Prepare the test solution by 5 times dilution of Solution A with 2% hydrochloric acid. Analyze aluminium and silica in the test solution by ICP-AES technique (Vol. 4). Set instrument parameters as specified by the instrument manufacturer. Use analytical lines for Al (396.152 nm) and Si (251.611 nm) and construct standard curve using standard solutions 0.2 – 5.0 µg/ml each. Read the concentration of Al and Si in sample solution (as µg/ml) and calculate the aluminium oxide and silicon dioxide content of the sample using the formula:

$$\%Al_2O_3 = \frac{1.889 \times C \times 250 \times 5}{W \times 10^6} \times 100$$

$$\%SiO_2 = \frac{2.139 \times C \times 250 \times 5}{W \times 10^6} \times 100$$

Where: C is concentration of Al or Si in the test solution, µg/ml
W is weight of sample, g

METHOD OF ASSAY Prepare the test solution by 1000 times dilution of Solution A (prepared in the PURITY TEST for Aluminium oxide and Silicon dioxide) with 2% hydrochloric acid, taking care that dilution factor in each dilution step shall not be more than 20. Analyze Titanium in the test solution by ICP-AES technique (Vol. 4). Set instrument parameters as specified by the instrument manufacturer. Use the analytical line for Ti (334.941 nm) and construct standard curve using Ti standard solutions: 0.5 - 1.5 µg/ml. Read the concentration in the sample solution(as µg/ml) and calculate the titanium dioxide content of the sample using the formula:

$\%TiO_2$ (on the dried basis)

$$= \frac{1.668 \times C \times 250 \times 1000}{W \times 10^6 \times (100-\%LOD-\%Al_2O_3-\%SiO_2)/100} \times 100$$

Where: C is concentration of Ti in the test solution, µg/ml
W is weight of sample, g
%LOD is % loss on drying
$\%Al_2O_3$ and $\%SiO_2$ are content (%) of Aluminium oxide and silicon oxide

ANALYTICAL METHODS

Analytical method for the determination of phosphorous as phosphorous pentoxide

The Committee at its current meeting noted that the titrimetric and gravimetric methods in the Combined Compendium of Food Additive Specifications, Volume 4 (*ref*), are not reliable for the determination of phosphorous as phosphorous pentoxide. Consequently, the Committee decided to introduce a method based on Inductively Coupled Plasma-Atomic Emission Spectrophotometry (ICP-AES) in the specifications monograph of magnesium dihydrogen diphosphate. The Committee may consider replacing corresponding methods for other diphosphate additives at a future meeting.

SPECIFICATIONS FOR CERTAIN FLAVOURING AGENTS

At the 76th meeting of the Committee prepared specifications of identity and purity of 107 new flavourings in 16 sub-categories for the following numbers: 2043, 2077 – 2123, 2125 — 2167, 2170 – 2185.

The flavouring agent 2-phenyl-2-methyl-2-hexenal (No. 2069) was submitted for evaluation in the group of aliphatic linear α,β-unsaturated aldehydes, acids and related alcohols, acetals and esters. The Committee considered that it did not belong to this group of flavouring agents and therefore was not further considered.
The safety of the submitted substance (3*R*)-4-[[(1*S*)-1-benzyl-2-methoxy-2-oxo-ethyl]amino]-3-[3-(3-hydroxy-4-methoxy-phenyl)propylamino]-4-oxo-butanoic acid hydrate (Advantame, JECFA No. 2124) in the group of amino acids and related substances was not assessed; the Committee decided that it would not be appropriate to evaluate this substance as a flavouring agent, because it is a low-calorie intense sweetener.
The safety of the two submitted substances rebaudioside C (No. 2168) and rebaudioside A (JECFA No. 2169) in the group of phenol and phenol derivatives was not assessed as the Committee decided that it would not be appropriate to evaluate these substances as flavouring agents, as they had already been evaluated as food additives (sweeteners).

Information on specifications for flavouring agents is given in the tables, 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 contain the number of the meeting at which the specifications were prepared and the status of the specification. All specifications prepared at the 76th meeting were assigned full status.

The spectra used for identification tests are provided from page 69 onwards. A list of the new flavourings evaluated in alphabetical order is added on page 87.

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2043	**2-Aminoacetophenone**	3906	C_8H_9NO	Soluble in fats, acetone; very slightly soluble in water	CNMR	1.612-1.619	
Full	1-(2-Aminophenyl)ethanone	11.008	135.17	Soluble	97	1.115-1.121	
	2-Acetylphenylamine; 2-Acetyl aniline	2041	Light yellow to dark greenish-yellow liquid; Fruity, spicy animalistic aroma	85-90 (0.5 mm Hg)			
76		551-93-9					
2077	**(2E,6E/Z,8E)-N-(2-Methylpropyl)-2,6,8-decatrienamide**	4668	$C_{14}H_{23}NO$	Insoluble in water	MS; IR	1.491-1.541	Isomers: (2E,6Z,8E) (73-76%); (2E,6E,8E)- (15-18%); (2E,6E,8Z)- (4-7%); (2Z,6Z,8E)- (1-2%); (2Z,6E,8E)- (1-2%); (2Z,6Z,8Z)- (1-2%)
Full	(1Z,2E,6Z,8E)-N-(2-Methylpropyl)deca-2,6,8-trienimidic acid		221.34	Soluble	95 (mixture of isomers)	0.9452-0.9468	
	2E,6Z,8E-Decatrienoic acid N-isobutylamide; N-Isobutyldeca-trans-2,cis-6,trans-8-trienamide; (2E,6Z,8E)-N-(2-Methylpropyl)-2,6,8-decatrienamide; Spilanthol		Clear, colourless to yellowish brown oil or semisolid; Sweet aroma with tingling sensation	140-160 (13.3 Pa)			
76		504-48-3;25394-57-4					
2078	**(2S,5R)-N-[4-(2-Amino-2-oxoethyl)phenyl]-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide**	4684	$C_{19}H_{28}N_2O_2$	Sparingly soluble in water	HNMR, IR; CNMR	NA	m.p. 186-188°
Full	(2S,5R)-N-[4-(2-amino-2-oxo-ethyl)phenyl]-2-isopropyl-5-methyl-cyclohexanecarboxamide;		316.45	Soluble	95	NA	
	4-Methyl-2-(1-[[[(2S,5R)-5-Methylethyl)cyclohexyl]carbonyl]amino]-benzeneacetamide		White crystalline solid; Cool aroma	NA			
76		1119711-29-3					

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
2079	**(1R,2S,5R)-N-(4-Methoxyphenyl)-5-methyl-2-(1-methylethyl)cyclohexanecarboxamide**	4681	$C_{18}H_{27}NO_2$	Insoluble in water; sparingly soluble in avocado oil	MS; IR; HNMR	NA	m.p. 177-178°
Full	(1R,2S,5R)-N-(4-Methoxyphenyl)-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide; (1R,2S,5R)-Methoxyphenyl)-5-methyl-2-propan-N-(4-2-ylcyclohexane-1-carboxamide		289.42 White crystals; Cool minty aroma	Sparingly soluble NA	98	NA	
76		68489-09-8					
2080	**N-Cyclopropyl-5-methyl-2-isopropylcyclohexanecarbonecarboxamide**	4693	$C_{14}H_{25}NO$	Practically insoluble to insoluble in water	CNMR	NA	m.p. 125°
Full	N-Cyclopropyl-5-methyl-2-(propan-2-yl)cyclohexanecarboximidic acid N -cyclopropyl-5-methyl-2-(1-methylethyl)-cyclohexanecarboxamide		223.35 White snowy crystals; Cool aroma	Soluble NA	95	NA	
76		73435-61-7					
2081	**N-(2-Methylcyclohexyl)-2,3,4,5,6-pentafluorobenzamide**	4678	$C_{14}H_{14}F_5NO$	Slightly soluble in water; soluble in most organic solvents	IR; HNMR, CNMR	NA	m.p. 150-152°
Full	2,3,4,5,6-Pentafluoro-N-(2-methylcyclohexyl)benzenecarboximidic acid PFMC benzamide		307.26 White solid; Sweet cooling aroma	Soluble NA	98	NA	
76		1003050-32-5					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2082	**3[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-N-propylpropanamide**	4701	$C_{15}H_{22}N_4O_4S$	0.15 mM in citric acid buffer pH 4.0; 0.16 mM in citric acid buffer pH 2.8	MS; HNMR; CNMR	NA	m.p. 229-233°
Full	(1Z)-N-{3-[(4-Imino-2,2-dioxido-3,4-dihydro-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethylpropyl}propanimidic acid		354.42	Slightly soluble	99	NA	
	3-(4-amino-1H-benzo[c][1,2,6]thiadiazin-5-yloxy)-2,2-dimethyl-N-propylpropanamide-2,2-dioxide; 3-[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-N-propyl-propanamide		Off white powder; Sweet aroma	NA			
76		1093200-92-0					
2083	**3-Pentanethiol**	4694	$C_5H_{12}S$	Very slightly soluble in water	IR, HNMR	1.444-1.448	
Full	Pentane-3-thiol		104.21	Soluble	95	0.825-0.830 (20°)	
	3-Mercapopentane		Clear to pale yellow liquid; Fruity roasted savoury aroma	112-113			
76		616-31-9					
2084	**4-Mercapto-3-methyl-2-butanol**	4698	$C_5H_{12}OS$	Soluble in water	IR, HNMR	1.470-1.474	
	3-Methyl-4-sulfanylbutan-2-ol		120.21	Soluble	95	0.968-0.980	
Full	3-Methyl-4-sulfanyl-2- butanol; 4-Thio-3-methyl-2-butanol		Clear to pale yellow liquid; Fruity meaty savoury aroma upon dilution	189-191			
76		33959-27-2					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
	Ethyl 2-Mercapto-2-methylpropionate			Very sparingly soluble	MS; IR;		
2085		4714	$C_6H_{12}O_2S$	in water	HNMR	1.424-1.464	
	Ethyl 2-methyl-2-sulfanylpropanoate		148.22	Soluble	95	1.020-1.023	
Full	Ethyl 2-mercaptopropionate		Clear to pale yellow liquid; Meaty fruity aroma upon dilution	186-187			
76		33441-50-8					
	1-(Methylthio)-3-octanone			Insoluble in water; soluble in non-polar			
2086		4707	$C_9H_{18}OS$	solvents	IR	1.461-1.463	
	1-(Methylsulfanyl)octan-3-one	12.247	174.30	Soluble	95	0.920-0.930	
Full	1-Methyl sulfanyl octan-3-one; 1-(Methylthio)octan-3-one		Clear colourless liquid;Meaty aroma with dairy undertones upon dilution	254-255			
76		61837-77-2					
	1,1-Propanedithiol			Very slightly soluble in			
2087		4670	$C_3H_8S_2$	water	IR; HNMR	1.490-1.501	
	Propane-1,1-dithiol		108.23	Soluble	95	1.014-1.016	
Full	1,1-Dimercaptopropane; 1,1-Propane dithiol		Clear colourless to light yellow liquid; Savoury sulfurous cooked onion aroma	137-138			
76		88497-17-0					
2088	**1-Methyldithio-2-propanone**	4696	$C_4H_8OS_2$	Soluble in water	IR; HNMR	1.520-1.526	SC: 2-3% 1-Mercapto-2-propanone; 2-3% 1,1'-disulfanediyldi-propan-2-one; 1-3% 1,3-dimethyltrisulfane
	1-(Methyldisulfanyl)propan-2-one		136.24	Soluble	90	1.132-1.144	
Full	Methyl 2-oxopropyl disulfide; 1-(Methyldithio)-2-propanone; 1-Methyldisulfanyl)acetone; 1-(Methyldithio)-2-propanone		Clear to pale yellow liquid; Sulfurous sweet green aroma	189-190			
76		122861-78-3					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2089	**(±) 4-Methyl-2-propyl-1,3-oxathiane**	4677	$C_8H_{16}OS$	Practically insoluble to insoluble in water	IR; HNMR	1.475-1.479	
	4-Methyl-2-propyl-1,3-oxathiane		160.28	Soluble	95	0.939-0.942 (20°)	
Full	2-Propyl-4-methyl-1,3-oxathiane		Clear colourless to yellow liquid; Sweet onion to garlic aroma	79-80 (10 mm Hg)			
76		1064678-08-5					
2090	**5-Methylfurfurylmercaptan**	4697	C_6H_8OS	Slightly soluble	HNMR, CNMR	1.523-1.529	
	(5-Methylfuran-2-yl)methanethiol	13.149	128.19	Soluble	95	1.047-1.057	
Full	5-Methyl-2-furanmethanethiol; 2-Furanmethanethiol, 5-methyl-; (5-Methylfurfuryl)mercaptan		Colorless to yellow clear liquid; Sulfurous rosted coffee aroma	177-179			
76		59303-05-8					
2091	**2-Methyl-3-furyl methylthiomethyl disulfide**	4320	$C_7H_{10}OS_3$	Sparingly soluble in water;soluble in pentane	MS; IR; HNMR; CNMR	1.614-1.619	
	2-Methyl-3-{[(methylsulfanyl)methyl]disulfanyl}furan		206.35	Soluble	95	1.258-1.262	
Full	2-Methyl-3-furyl methylthiomethyl disulfide		Colourless to light yellow liquid;	234-236			
76		333384-99-9	Brown meaty aroma at sufficient dilution				

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2092	**2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulfide**	4545	$C_{10}H_{14}0_2S_2$	Practically insoluble to insoluble in water	MS	1.550-1.556	Isomers: 2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulfide (29-30%); 2-Methyl-3-furyl disulfide (32-33%); 2-Methyl-3-tetra-hydrofuryl disulfide (28-29%); 2-Methyl-3-furylthiol and 2-methyl-3-tetra-hydrofuryl thiol (5-7%) Safety evaluation not complete
	2-Methyl-3-[(2-methyltetrahydrofuran-3-yl)disulfanyl]furan		230.35	Soluble	99 (sum of isomers)	1.179-1.185	
Full	2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulfide		Colourless to yellow liquid; Savoury meat-like aroma	107-122 (0.13kPa)			
76		252736-40-6					
2093	**2-Tetrahydrofurfuryl 2-mercaptopropionate**	4535	$C_8H_{14}OS$	Practically insoluble to insoluble in water	MS	1.480-1.486	
	Tetrahydrofuran-2-ylmethyl 2-sulfanylpropanoate		190.26	Soluble	96	1.132-1.138 (20°)	
Full	Tetrahydrofuran-2-yl methyl 2-sulfanylpropanoate; Tetrahydrofuran-2-yl methyl 2-sulfanyl propanoate		Colourless to yellow liquid; Meaty aroma	58-65 (0.27 kPa)			
76		99253-91-5					
2094	**Methyl 3-(furfurylthio) propionate**	4538	$C_9H_{12}O_3S$	Practically insoluble to insoluble in water	MS	1.511-1.517	
	Methyl 3-[(furan-2-ylmethyl)sulfanyl]propanoate	13.143	200.25	Soluble	98	1.167-1.173 (20°)	
Full	Methyl furfuyl mercaptopropionate		Pale yellow to amber coloured liquid; Earthy sweet aroma	113-116 (0.2 mm Hg)			
76		94278-26-9					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2095	**3-[(2-Methyl-3-furyl)thio]butanal**	4501	$C_9H_{12}O_2S$	Practically insoluble to insoluble in water	HNMR, IR, MS	1.515-1.522	
	3-[(2-Methylfuran-3-yl)sulfanyl]butanal	13.199	184.26	Soluble	97	1.101-1.121	
Full	3-(Methyl furan-3-yl)sulfanyl(2-butanal)		Yellow to light orange liquid; Meaty roasted aroma	197-198 (decomposition)	0.5		
76		915971-43-6					
2096	**1-(2-Furfurylthio)-propanone**	4676	$C_8H_{10}O_2S$	Insoluble in water; soluble in organic solvents	HNMR; IR	1.525-1.531	
	1-[(Furan-2-ylmethyl)sulfanyl]propan-2-one	13.135	170.23	Soluble	95	1.146-1.154	
Full			Colourless to yellow clear liquid;	281-282			
76		58066-86-7	Roasted coffee aroma				
2097	**2-Methyl-4,5-dihydrofuran-3-thiol**	4683	C_5H_8OS	Insoluble in water	MS, CNMR	1.497-1.534	
	2-Methyl-4,5-dihydrofuran-3-thiol	13.108	116.18	Soluble	55	1.047-1.143	SC: 35-40% 2-Methyl-3-tetrahydrofuranthiol; 5-7% 2-Methyl-3-furanthiol
Full	4,5-Dihydro-3-mercapto-2-methylfuran; 3-Furanthiol, 4,5-dihydro-2-methyl; 3-Mercapto-2-methyl-4,5-dihydrofuran		Pale yellow clear liquid; Sulfurous meaty savoury aroma upon dilution	158-160			
2098	**(±)-2-Methyltetrahydrofuran-3-thiol acetate**	4686	$C_7H_{12}O_2S$	Practically insoluble to insoluble in water	MS; IR; HNMR	1.490-1.498	
	(±)-(2-Methyltetrahydrofuran-3-yl) ethanethioate	13.182	160.23	Soluble	95	1.092-1.100 (20°)	
Full	2-Methyl tetrahydrofuran-3-thioacetate		Clear yellow liquid; Sulfurous roasted meaty aroma	246-247			
76		252736-41-7					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2099	**5-Methylfurfuryl alcohol**	4544	$C_6H_8O_2$	Soluble in water	MS	1.484-1.490	Safety evaluation not completed
	(5-Methylfuran-2-yl)methanol		112.13	Soluble	95	1.082-1.088 (20°)	
Full	Furfural propyleneglycol acetal		Colourless to pale yellow liquid; Sweet caramel like aroma	177-178			
76		3857-25-8					
2100	**Furfural propyleneglycol acetal**	4537	$C_8H_{10}O$	Practically insoluble to insoluble in water	MS	1.472-1.478	Safety evaluation not completed
	2-(Furan-2-yl)-4-methyl-1,3-dioxolane		154.16	Soluble	98	1.130-1.136 (20°)	
Full			Colourless to pale yellow clear liquid; Sweet aroma	211-213	1		
76		4359-54-0					
2101	**Furfuryl formate**	4542	$C_6H_6O_3$	Practically insoluble to insoluble in water	MS	1.463-1.469	Safety evaluation not completed
	Furan-2-ylmethyl formate		126.11	Soluble	95	1.165-1.171 (20°)	
Full	2-Furfuryl formate		Colourless to pale yellow liquid; Ethereal aroma	170-171			
76		13493-97-5					
2102	**Furfuryl decanoate**	4539	$C_{15}H_{24}O_3$	Practically insoluble to insoluble in water	HNMR	1.458-1.464	Safety evaluation not completed
	Furan-2-ylmethyl decanoate		252.35	Soluble	98	0.964-0.972 (20°)	
Full	Furfuryl caprate		Clear colourless to pale yellow liquid; Fatty caramel like aroma	298-300			
76		39252-05-6					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2103	**(E)-Ethyl 3-(2-furyl)acrylate**	4541	$C_9H_{10}O_3$	Practically insoluble to insoluble in water	MS	1.542-1.548	Safety evaluation not completed
	Ethyl (2E)-3-(furan-2-yl)prop-2-enoate		166.17	Soluble	95	1.090-1.096	
Full	Ethyl(E)-3-(2-furyl)-2-propenoate		Viscous liquid; Sweet aroma	230-233			
2104	**di-2-Furylmethane**	4540	$C_9H_8O_2$	Practically insoluble to insoluble in water	MS	1.501-1.507	Safety evaluation not completed
	2,2'-Methanediyldifuran		148.16	Soluble	95	1.097-1.103 (20°)	
Full			Colourless clear liquid; Rich roasted aroma	194-195			
76		1197-40-6					
2105	**2-Methylbenzofuran**	4543	C_9H_8O	Practically insoluble to insoluble in water	MS	1.548-1.560	Safety evaluation not completed
	2-Methyl-1-benzofuran		132.16	Soluble	95	1.052-1.057	
Full			Colourless liquid; Burnt phenolic aroma	197-198			
76		4265-25-2					
2106	**2-Pentylthiophene**	4387	$C_9H_{14}S$	Practically insoluble to insoluble in water; soluble in hexane and pentane	MS, IR, HNMR, CNMR	1.493-1.501	
	2-Pentylthiophene	15.096	154.27	Soluble	95	0.942-0.949	
Full	1-Methyl butyl thiophene; 2-Pentylthiophene; sec-Pentylthiophene	11634	Clear colourless liquid; Fruity fatty aroma with a cranberry note	202-205			
76		4861-58-9					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2107	**2-Acetyl-5-methylthiophene**	4643	C_7H_8OS	Very slightly soluble in water	MS	1.557-1.567	
	1-(5-Methylthiophen-2-yl)ethanone		140.20	Soluble	95	1.120-1.130 (20 °)	m.p. 24-28°
Full	1-(5-Methyl-thienyl)ethan-1-one; 2-Methyl-5-acetylthiophene		Colourless to pale yellow liquid to crystalline powder at lower temperatures; Roasted aroma with sweet notes	232-234			
76		13679-74-8					
2108	**2-Pentylthiazole**	4641	$C_8H_{13}NS$	Practically insoluble to insoluble in water	MS	1.493-1.499	
	2-Pentyl-1,3-thiazole		155.26	Soluble	95	0.991-0.998 (20 °)	
Full	2-Amyl thiazole		Clear colourless to yellow liquid; Roasted aroma with cocoa notes	210-211			
76		37645-62-8					
2109	**4,5-Dimethyl-2-isobutylthiazole**	4647	$C_9H_{15}NS$	Practically insoluble to insoluble in water	MS	1.490-1.498	
	4,5-Dimethyl-2-(2-methylpropyl)-1,3-thiazole	15.078	169.29	Soluble	97	0.967-0.975 (20 °)	
Full	2-Isobutyl-4,5-dimethylthiazole	11.617	Colourless to pale yellow liquid;	266-267			
76		53498-32-1	Earthy, nutty, green vegetative aroma				
2110	**3,4-Dimethylthiophene**	4645	C_6H_8S	Practically insoluble to insoluble in water	MS	1.517-1.523	
	3,4-Dimethylthiophene	15.065	112.19	Soluble	95	1.002-1.008 (20 °)	
Full		11.610	Colourless to pale yellow liquid; Savoury roasted onion aroma	144-146			
76		632-15-5					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2111	**2-Thienylmethanol**	4642	C_5H_6OS	Soluble in water	MS	1.562-1.568	
	Thiophen-2-ylmethanol		114.17	Soluble	95	1.205-1.215 (20 °)	
Full	2-Hydroxymethylthiophene; 2-Thienylcarbinol		Clear colourless to yellow liquid;	206-207			
76		636-72-6	Savoury roasted aroma with coffee notes				
2112	**1-(2-Thienyl)ethanethiol**	4646	$C_6H_8S_2$	Very slightly soluble in water	MS	1.568-1.578	
	1-(Thiophen-2-yl)ethanethiol	15.105	144.26	Soluble	95	1.141-1.151	
Full	1-Thiophen-2-ylethanethiol; 2-(1-mercaptoethyl)thiophene	11580	Colourless clear liquid; Strong mercaptan aroma	212-213			
76		94089-02-8					
2113	**5-Ethyl-2-methylthiazole**	4388	C_6H_9NS	Practically insoluble to insoluble in water	MS, HNMR, CNMR	1.501-1.511	
	4-Ethyl-2-methyl-1,3-thiazole	15.068	127.21	Soluble	95	1.026-1.036 (20 °)	
Full	5-Ethyl-2-methyl-1,3-thiazole;5-Ethyl-2-methylthiazole		Colourless liquid; Nutty chocolate aroma with fishy pyrazine notes	170-173			
76		19961-52-5					
2114	**2-Ethyl-2,5-dihydro-4-methylthiazole**	4695	$C_6H_{11}NS$	Slightly soluble in water	IR, HNMR	1.510-1.512	S.C.: 2-3% 2-Ethyl-4-methyl-4,5-dihydrothiazole-4-ol; 2-3% 3,4-Dimethylthiophene; 2-3% 2-Ethyl-4-methylthiazole
	2-Ethyl-4-methyl-2,5-dihydro-1,3-thiazole		129.22	Soluble	90	0.990-1.090 (20 °)	
Full	2-Ethyl-2,5-dihydro-4-methylthiazole; 2-Ethyl-4-methyl-3-thiazoline		Clear to pale yellow liquid; Nutty roasted vegetable aroma	188-189			
76		41803-21-8					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2115	**4-Methyl-3-thiazoline**	4644	C_4H_7NS	Practically insoluble to insoluble in water	HNMR	1.521-1.541	
	4-Methyl-2,5-dihydro-1,3-thiazole		101.17	Soluble	95	1.098-1.118 (20 °)	
Full	4-Methyl-2,5-dihydrothiazole		Colourless to yellow liquid; Garlic aroma	158-160			
76		52558-99-3					
2116	**2-Ethyl-4,6-dimethyl-dihydro-1,3,5-dithiazine**		$C_7H_{15}NS_2$	Insoluble in water; soluble in fats	IR, HNMR	1.488-1.492	S.C.:3,5-Diethyl-1,2,4-trithiolane
Full	2-Ethyl-4,6-dimethyl-1,3,5-dithiazinane		177.33	Soluble	90	0.961-0.967	(3-5%) and 2,4,6 trimethyldihydro-1,3,5-dithiazine (2-3%)
			Pale yellow liquid	105-110 (2 mm Hg)			FEMA number required
76		54717-14-5	Alliaceous aroma				
2117	**4-Amino-5,6-dimethylthieno[2,3-d]pyramidin-2(1H)-one hydrochloride**	4669	$C_8H_{10}ClN_3OS$	Soluble in 0.26 mM phosphate buffer pH 7.1; soluble in propylene glycol	MS, IR, CNMR	NA	m.p. > 260°
	4-(Amino)-5,6-dimethylthieno[2,3-d]pyrimidin-2(1H)-one hydrochloride		231.70	Soluble	99	NA	
Full			White to off-white powder	NA			
76		1033366-59-4	Sweet aroma				

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2118	**L-Isoleucine**	4675	$C_6H_{13}NO_2$	Soluble in 0.26 mM phosphate buffer pH 7.1; soluble in propylene glycol	IR	NA	m.p. > 260° (decomposition)
	(2S,3S)-2-Amino-3-methylpentanoic acid		131.17	Soluble	99	NA	
Full	(2S,3S)-α-Amino-β-methyl-n-valeric acid		White to off-white powder/odorless; Sweet aroma	NA			
76		73-32-5					
2119	**L-Threonine**	4710	$C_4H_9NO_3$	Sparingly soluble in water; soluble in buffer systems pH 5.5	IR	NA	m.p. 283-284° (decomposition)
	(2S,3R)-2-Amino-3-hydroxybutanoic acid		119.12	Practically insoluble	98	NA	
Full	2-Amino-3-hydroxybutanoic acid		White crystalline powder; Slight savoury aroma	NA			
76		72-19-5					
2120	**L-Ornithine monochlorohydrate**	4190	$C_5H_{12}N_2O_2.HCl$	Soluble in water	MS, IR, HNMR	NA	m.p.230-232° (decomposition)
	(2S)-2,5-Diaminopentanoic acid hydrochloride		168.62	Very slightly soluble	96	NA	
Full	L-Ornithine monohydrochloride		White crystalline solid or powder to syrup	NA			
76		3184-13-2	Slight savoury aroma				
2121	**L-Alanyl-L-Glutamine**	4712	$C_8H_{15}N_3O_4$	Soluble in water	IR	NA	m.p. 230-232° (decomposition)
	(2S)-5-Amino-2-[(2-aminopropanoyl)amino]-5-oxopentanoic acid		217.22	Very slightly soluble	98	NA	
Full			White crystals or crystalline powder; Weak savoury aroma	NA			
76		39537-23-0					

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
2122	**L-Methionylglycine**	4692	$C_7H_{14}N_2O_3S$	Slightly soluble in water	MS, HNMR	NA	m.p. 190-201° (decomposition)
	{[(2S)-2-Amino-4-(methylsulfanyl)butanoyl]amino}acetic acid		206.26	Practically insoluble	98	NA	
Full			White powder; Savoury meaty with cheesy notes aroma	NA			
76		14486-03-4					
2123	**Glutamyl-valyl-glycine**	4709	$C_{12}H_{21}N_3O_6$	Soluble in water	MS, HMNR	NA	m.p. 225-228° (decomposition)
	(2S)-2-Amino-5-({(2S)-1-[(carboxymethyl)amino]-3-methyl-1-oxobutan-2-yl}amino)-5-oxopentanoic acid;		303.31	Practically insoluble	99	NA	
Full	L-□-Glutamyl-L-valyl-glycine		Solid off-white powder;	NA			
76		38837-70-6	Light savoury almost yeast like aroma				
2125	**Isopropenylpyrazine**	3296	$C_7H_8N_2$	Practically insoluble to insoluble in water	MS	1.480-1.486	
	2-(Prop-1-en-2-yl)pyrazine	14.052	120.15	Soluble	95	0.964-0.968	
Full	1- (Methyl ethenyl)pyrazine; Caramel pyrazine; 2-(1-Methyl vinyl) pyrazine	11341	Colourless to pale orange liquid	NA			
76		38713-41-6	Caramel like nutty roasted aroma				
2126	**5-Ethyl-2,3-dimethylpyrazine**	4434	$C_8H_{12}N_2$	Practically insoluble to insoluble in water	HNMR, CNMR	1.494-1.502	
	5-Ethyl-2,3-dimethylpyrazine	14.170	136.19	Soluble	95	0.944-0.982 (20 °)	
Full	2,3-Dimethyl-5-ethyl pyrazine		Clear colourless or pale yellow liquid	190-191	<1.0		
76		15707-34-3	Deep roasted cocoa-like aroma				

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2127	**2-Methyl-5-vinylpyrazine**	3211	$C_7H_8N_2$	Very slightly soluble in water; soluble in acetone	MS	1.557-1.561	
	2-Ethenyl-5-methylpyrazine		120.15	Soluble	95	1.011-1.023	
Full	2-Methyl-5-vinylpyrazine	11359	Colourless to yellow liquid	65-66 (12 mm Hg)			
76		13925-08-1	Coffee like aroma				
2128	**Mixture of 2,5 and 2,7-Dimethyl-6,7-dihydro-5H-cyclopentapyrazine**	4702	$C_9H_{12}N_2$	Practically insoluble to insoluble in water	MS, IR, HNMR	1.524-1.532	2,5-isomer (60-75%); 2,7-isomer (35-40%)
	2,5-Dimethyl-6,7-dihydro-5H-cyclopenta[b]pyrazine and 2,7-Dimethyl-6,7-dihydro-5H-cyclopenta[b]pyrazine;	14.161/140.98	148.20	Soluble	95	1.020-1.030	
Full		11.310/11.309	Colourless to pale yellow liquid	230-231			
76		38917-61-2/ 38917-62-3	Roasted coffee aroma				
2129	**2-Ethoxy-3-isopropylpyrazine**	4632	$C_9H_{14}N_2O$	Slightly soluble in water	MS	1.500-1.510	
	2-Ethoxy-3-(propan-2-yl)pyrazine		166.22	Soluble	95	1.010-1.040 (20 °)	
Full	2-Ethoxy-3-(1-methylethyl)pyrazine; 2-Ethoxy3-isopropylpyrazine		Clear colourless to yellow liquid; Slightly roasted nut aroma	229-232			
76		72797-16-1					
2130	**Mixture of 3,5 and 3,6-Dimethyl-2-isobutylpyrazine**	4100	$C_{10}H_{16}N_2$	Practically insoluble to insoluble in water	HNMR	1.491-1.494	3,5-isomer (48-50%); 3,6-isomer (48-50%)
	3,5-Dimethyl-2-(2-methylpropyl)pyrazine and 3,6-Dimethyl-3-(2-methylpropyl)pyrazine		164.25	Soluble	95	0.924-0.929	
Full	2-iso Butyl-3,(5 and 6)-dimethylpyrazine; 3,5 and 3,6-Dimethyl-2-isobutyl pyrazine		Colourless transparent liquid;	73-75 (2 mm Hg)			
76		38888-81-2 and 70303-42-3	Roasted woody, meaty aroma with nutty cocoa notes				

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
2131	**2-Ethoxy-3-ethylpyrazine**	4633	$C_8H_{12}N_2O$	Practically insoluble to insoluble in water	MS	1.492-1.495	
	2-Ethoxy-3-ethylpyrazine		152.19	Soluble	95	0.981-0983 (20 °)	
Full	3-Ethyl-2-ethoxypyrazine		Clear colourless to pale yellow liquid; Raw potato like aroma	195-197			
76		35243-43-7					
2132	**2-Ethyl-3-methylthiopyrazine**	4631	$C_7H_{10}N_2S$	Practically insoluble to insoluble in water	MS	1.568-1.583	
	2-Ethyl-3-(methylsulfanyl)pyrazine		154.23	Soluble	95	1.142-1.145 (20 °)	
Full	2-(Methylthio)-3-ethylpyrazine		Clear light yellow liquid; Strong roasted meat aroma	234-236			
76		72987-62-3					
2133	**3,6-Dimethyl-2,3,3a,4,5,7a-hexahydrobenzofuran**	4315	$C_{10}H_{16}O$	Very slightly soluble in water	IR HNMR	1.478-1.481	
	3,6-Dimethyl-2,3,3a,4,5,7a-hexahydro-1-benzofuran	13.198	152.23	Soluble	96	0.966-0.970	
Full		-	Clear almost colourless liquid; Herbal dill-like aroma	207-208			
76		70786-44-6					
2134	**Ethyl linalyl ether**	4591	$C_{12}H_{22}O$	Practically insoluble to insoluble in water; soluble in DMSO	MS HNMR	1.444-1.447	
	3-Ethoxy-3,7-dimethylocta-1,6-diene	-	182.30	Sparingly soluble	98	0.829-0.832 (20º)	
Full	Linalool ethyl ether; 3- Ethoxy-3,7-dimethyl-1,6-octadiene; 3,7- Dimethyl octa-1,6-dien-3-yl ethyl ether; 3,7-Dimethylocta-1,6-dien-3-yl ethyl ether	-	Clear colourless liquid; Pleasant floral aroma	227-228			
76		72845-33-1					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2135	**Linalool oxide pyranoid**	4593	$C_{10}H_{18}O_2$	Practically insoluble to insoluble in water	MS HNMR	1.472-1.482	SC: 3-5% linalool
	6-Ethenyl-2,2,6-trimethyloxan-3-ol	-	170.25	Soluble	92	0.991-0.996 (20º)	
Full	Linalool pyran oxide; Epoxylinalool (pyranoid); 2,2,6- Trimethyl-6-vinyl tetrahydro-2H-pyran-3-ol; 2,2,6- Trimethyl-6-vinyltetrahydro-2H-pyran-3-ol; 3-Hydroxy-2,2,6-trimethyl-6-vinyl tetrahydropyran; 6- Ethenyl-2,2,6-trimethyl tetrahydro-2H-pyran-3-ol; 6-Ethenyl-2,2,6-trimethyltetrahydro-2H-pyran-3-ol; 6-Ethenyl-3,4,5,6-tetrahydro-2,2,6-trimethyl-2H-pyran-3-ol; Tetrahydro-2,2,6-trimethyl-6-vinyl-2H-pyran-3-ol	-	Colourless to pale yellow liquid; Floral aroma	223-224			
76		14049-11-7					
2136	**Isoamyl phenethyl ether**	4635	$C_{13}H_{20}O$	Soluble in water	MS	1.477-1.485	
	2-(3-Methylbutoxy)ethylbenzene	-	192.30	Soluble	98	0.897-0.913 (20º)	
Full	(2-(3-Methyl butoxy)ethyl) benzene; (2-(3-Methylbutoxy)ethyl) benzene; 1-(2-((3-Methyl butyl)oxy)ethyl) benzene; 2-(3-Methylbutoxy)ethylbenzene; 3- Methyl butyl oxyethyl benzene; Iso pentyl phenethyl ether; Green ether	-	Colourless clear liquid; Fresh green hyacinth-like aroma	109-110 (8 mm Hg)			
76		56011-02-0					
2137	**Nerolidol oxide**	4536	$C_{15}H_{26}O_2$	Practically insoluble to insoluble in water	MS	1.468-1.472	
	2-(5-Ethenyl-5-methyltetrahydrofuran-2-yl)-6-methylhept-5-en-2-ol	-	238.37	Soluble	95	0.928-0.933 (20º)	
Full	Ethenyl tetrahydro-alpha-5-dimethyl-alpha-(4-methyl-3-pentenyl)-2-furan methanol	-	Colourless liquid; Faint floral aroma	324-325 (decomposes)			Safety evaluation not completed
76		1424-83-5					

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
2138	**Methyl hexyl ether**	4291	$C_7H_{16}O$	Practically insoluble to insoluble in water	HNMR	1.393-1.402	
	1-Methoxyhexane	03.016	116.20	Soluble	95	0.765-0.775	
Full	Methyl n-hexyl ether	-	Clear colourless liquid; Pear, banana green tones upon dilution with sweet herbaceous lavender-like notes at higher concentration	126-127			
76		4747-07-3					
2139	**Myrcenyl methyl ether**	4592	$C_{11}H_{20}O$	Very slightly soluble in water; soluble in non-polar solvents	MS	1.455-1.461	
	7-Methoxy-7-methyl-3-methylidene-oct-1-ene	-	168.28	Slightly soluble	96	0.841-0.849 (20º)	
Full		-	Colourless liquid; Piney resinous aroma	208-210			
76		24202-00-4					
2140	**5-Isopropyl-2,6-diethyl-2-methyltetrahydro-2H-pyran**	4680	$C_{13}H_{26}O$	Practically insoluble to insoluble in water	MS IR HNMR	1.444-1.446	
	2,6-Diethyl-5-isopropyl-2-methyl-tetrahydropyran	13.200	198.35	Soluble	95	0.860-0.867	
Full	2,6-Diethyl-2-methyl-5-(propan-2-yl)tetrahydro-2H-pyran; 2,6- Diethyl-5-isopropyl-2-methyltetrahydropyran; 5-iso propyl-2,6-diethyl-2-methyltetrahydro-2H-pyran	-	Colourless to yellow liquid; Fresh aroma	93 (7.5 mm Hg)			
76		1120363-98-5					

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
2141	**Butyl beta-naphthyl ether**	4634	$C_{14}H_{16}O$	Insoluble in water; Soluble in non-polar organic solvents and fats	MS	NA	m.p.=31-33º
	2-Butoxynaphthalene	-	200.28	Slightly soluble	97	NA	
Full	beta-Naphthol butyl ether; Butyl 2-naphthyl ether	-	White crystalline powder; Sweet fruity floral berry aroma	NA			
76		10484-56-7					
2142	**Digeranyl ether**	4664	$C_{20}H_{34}O$	Practically insoluble to insoluble in water	MS HNMR CNMR	1.477-1.487	
	(2E)-1-[(2E)-3,7-Dimethylocta-2,6-dienoxy]-3,7-dimethylocta-2,6-diene	03.024	290.48	Soluble	95	0.867-0.876	
Full	(2E,6E)-1,1'-Oxybis(3,7- dimethyl-2,6-octadiene); (E,E)-Geranyl neryl ether; 1,1'-Oxybis(3,7- dimethyl-(2E)-octadiene)	-	Clear colourless to pale yellow liquid; Clean floral balsamic aroma	371-373 (decomposes)			
76		31147-36-1					
2143	**Ethyl alpha-ethyl-beta-methyl-beta-phenylglycidate**	4653	$C_{14}H_{18}O_3$	Sparingly soluble in water	MS	NA	m.p. = 37-42º
	Ethyl 2-ethyl-3-methyl-3-phenyloxirane-2-carboxylate	-	234.29	Soluble	95	NA	
Full	(E)-2-Ethyl-3-methyl-3-phenyl oxiranecarboxylic acid ethyl ester; alpha,beta- Epoxy-alpha-ethyl-beta-methyl hydrocinnamic acid ethyl ester; Ethyl (E)-2-ethyl-3-methyl-3-phenyl oxirane-2-carboxylate; Ethyl (E)-2-ethyl-3-methyl-3-phenyloxirane-2-carboxylate; Ethyl 2-ethyl-3-methyl-3-phenyloxirane-2-carboxylate; Ethyl trans-2-ethyl-3-methyl-3-phenyloxirane-2-carboxylate; trans-2-ethyl-3-methyl-3-phenyl oxiranecarboxylic acid ethyl ester	-	Clear colourless to pale yellow viscous liquid to solid; Sweet fruity aroma reminiscent of berries	295-297 (decomposes)			
76		19464-94-9					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2144	**Methyl beta-phenylglycidate**	4654	$C_{10}H_{10}O_3$	Practically insoluble to insoluble in water	MS HNMR	1.524-1.532	SC: 10-12% Ethyl beta-phenylglycidate
	Methyl 3-phenyloxirane-2-carboxylate	-	178.18	Soluble	85	1.161-1.172 (20º)	
Full	(±)- Methyl 2,3-epoxycinnamate; 3- Phenyl glycidic acid methyl ester; Methyl 3-phenyl oxirane-2-carboxylate; Methyl 3-phenyloxirane-2-carboxylate	-	Colourless to pale yellow clear liquid; Fresh fruity aroma	252-254			
76		37161-74-3					
2145	**d-8-p-Menthene-1,2-epoxide**	4655	$C_{10}H_{16}O$	Practically insoluble to insoluble in water	MS	1.464-1.474	Optical rotation: -69 to 72° (20°C)
	(4R)-1-Methyl-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptane	-	152.23	Soluble	95	0.926-0.936 (20º)	
Full	D-1,2-Epoxylimonene; D-Limonene 1,2-epoxide	-	Colourless to pale yellow liquid; Fresh clean citrus aroma	198			
76		1195-92-2					
2146	**l-8-p-Menthene-1,2-epoxide**	4656	$C_{10}H_{16}O$	Practically insoluble to insoluble in water	MS	1.464-1.474	Optical rotation: +73 to 78° (20°C)
	(4S)-1-Methyl-4-(prop-1-en-2-yl)-7-oxabicyclo[4.1.0]heptane	-	152.23	Soluble	95	0.926-0.936 (20º)	
Full	L-1,2-Epoxylimonene; L-Limonene 1,2-epoxide;	-	Colourless to pale yellow liquid; Cool minty aroma	197-199			
76		203719-53-3					
2147	**2,3-Epoxyoctanal**	4657	$C_8H_{14}O_2$	Practically insoluble to insoluble in water	MS HNMR	1.432-1.442	Safety evaluation not completed
	3-Pentyloxirane-2-carbaldehyde	-	142.20	Soluble	95	0.936-0.946 (20º)	
Full		-	Colourless to pale yellow liquid; Fatty aroma with citrus notes	202-204			
76		42134-50-9					

JECFA No. Status Session	Name Chemical Name Synonyms CAS	FEMA FLAVIS COE CAS	Chemical Formula M.W Physical form; Odour CAS	Solubility Solubility in ethanol B.P. °C CAS	ID test Assay min % Acid value CAS	R.I. S.G. CAS	Other requirements Information required CAS
2148	**2,3-Epoxyheptanal**	4658	$C_7H_{12}O_2$	Practically insoluble to insoluble in water	MS HNMR	1.427-1.437	Safety evaluation not completed; SC: 2-3% trans-2-heptenal
	3-Butyloxirane-2-carbaldehyde	-	128.17	Soluble	94	0.938-0.948 (20º)	
Full		-	Colourless to pale yellow liquid; Fatty citrus aroma	60 (9 mm Hg)			
76		58936-30-4					
2149	**2,3-Epoxydecanal**	4659	$C_{10}H_{18}O_2$	Very slightly soluble in water	MS HNMR	1.436-1.446	Safety evaluation not completed; SC: 2-3% trans-2-decenal
	3-Heptyloxirane-2-carbaldehyde	-	170.25	Soluble	94	0.912-0.922 (20º)	
Full		-	Colourless to pale yellow clear liquid; Fatty citrus aroma	92-93			
76		102369-06-2					
2150	1-Ethyl-2-pyrrolecarboxaldehyde	4317	C_7H_9NO	Practically insoluble to insoluble in water	HNMR CNMR	1.541 - 1.547	Safety evaluation not completed
	1-Ethylpyrrole-2-carbaldehyde	14.169	123.15	Soluble	95	1.033 - 1.039	
Full	1-Ethyl pyrrole-2-aldehyde; 1-Ethyl pyrrole-2-carboxaldehyde; 1-Ethyl-1H-pyrrole-2-carboxaldehyde; 1-Ethyl-2-formyl pyrrole; 1- Ethyl-2-pyrrole carboxaldehyde	-	Clear colourless to yellow liquid; Burnt smokey aroma	204-206			
76		2167-14-8					

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
2151	**2,4-Dimethylpyridine**	4389	C_7H_9N	Slightly soluble in water	HNMR CNMR	1.496-1.502	
	2,4-Dimethylpyridine	14.104	107.15	Soluble	95	0.929 - 0.935 (20°)	
Full	2,4-Lutidine	-	Yellowish liquid; Smoky phenolic aroma	158-159			
76		108-47-4					
2152	**1-Methyl-1H-pyrrole-2-carboxaldehyde**	4332	C_6H_7NO	Soluble in water	MS	1.558-1.564	Safety evaluation not completed
	1-Methylpyrrole-2-carbaldehyde	14.163	109.13	Soluble	95	1.012-1.018	
Full	1-Methyl pyrrole-2-carbaldehyde; 1-Methyl pyrrole-2-carboxaldehyde; 1-Methyl-2-formyl pyrrole; 1-Methyl-2-pyrrolecarboxaldehyde; 2- formyl-1-methyl pyrrole; 2-Formyl-1-methylpyrrole	-	Clear orange to dark red liquid; Roasted nutty aroma	192-194			
76		1192-58-1					
2153	**2-Acetyl-4-isopropenylpyridine**	4636	$C_{10}H_{11}NO$	Sparingly soluble in water	MS	1.518-1.520	
	1-(4-Prop-1-en-2-ylpyridin-2-yl)ethanone	-	161.20	Soluble	95	1.006-1.008	
Tenta-tive	(4-(1-Methyl ethenyl)-2-pyridinyl) ethanone	-	Light yellow clear liquid; Grassy green aroma	270-272			Information to differentiate between JECFA Nos. 2153 and 2154
76		142896-11-5					

JECFA No. Status Session	Name Chemical Name Synonyms CAS	FEMA FLAVIS COE CAS	Chemical Formula M.W Physical form; Odour CAS	Solubility Solubility in ethanol B.P. °C CAS	ID test Assay min % Acid value CAS	R.I. S.G. CAS	Other requirements Information required CAS
2154	**4-Acetyl-2-isopropenylpyridine**	4637	$C_{10}H_{11}NO$	Practically insoluble to insoluble in water	MS HNMR	1.517-1.519	Information to differentiate between JECFA Nos. 2153 and 2154
	1-(2-Prop-1-en-2-ylpyridin-4-yl)ethanone	-	161.20	Soluble	95	1.007-1.009	
Tenta-tive	(2-(1-Methyl ethenyl)-4-pyridinyl) ethanone	-	Light yellow clear liquid; Fermented herbal green aroma	277-279			
76		142896-12-6					
2155	**2-Acetyl-4-isopropylpyridine**	4638	$C_{10}H_{13}NO$	Practically insoluble to insoluble in water	MS HNMR	1.502-1.505	
	1-(4-Propan-2-ylpyridin-2-yl)ethanone	-	163.22	Soluble	95	0.992-0.994	
Full	(4-(1-Methylethyl)-2-pyridinyl)ethanone	-	Light yellow clear liquid; Grassy green leafy aroma with violet notes	245-247			
76		142896-09-1					
2156	**2-Methoxypyridine**	4639	C_6H_7NO	Practically insoluble to insoluble in water	MS	1.501-1.507	Safety evaluation not completed
	2-Methoxypyridine	-	109.13	Soluble	96	1.044-1.050 (20°)	
Full		-	Colourless to pale yellow liquid; Green fermented tea-like aroma	142-144			
76		1628-89-3					
2157	**6-Methoxyquinoline**	4640	$C_{10}H_9NO$	Very slightly soluble in water	MS	1.622-1.625	
	6-Methoxyquinoline	-	159.18	Soluble	95	1.151-1.154 (20°)	
Full	Methyl 6-quinolyl ether	-	Colourless to pale yellow liquid; Heavy sweet aroma	294-296			
76		5263-87-6					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2158	**1-(2-Hydroxyphenyl)-3-(pyridin-4-yl)propan-1-one**	4721	$C_{14}H_{13}NO_2$	Slightly soluble in water	HNMR CNMR	NA	Safety evaluation not completed; m.p.= 77-78º
	1-(2-Hydroxyphenyl)-3-(4-pyridyl)propan-1-one	-	227.26	Soluble	98	NA	
Full		-	Light cream coloured solid; Minimal sweet aroma	NA			
76		1186004-10-3					
2159	**1-(2-Hydroxy-4-isobutoxyphenyl)-3-(pyridin-2-yl)propan-1-one**	4722	$C_{18}H_{21}NO_3$	Slightly soluble in water	MS HNMR CNMR	NA	Safety evaluation not completed; m.p.= 47- 49º
	1-(2-Hydroxy-4-isobutoxyphenyl)-3-(2-pyridyl)propan-1-one	-	299.36	Soluble	97	NA	
Full		-	Cream or off white coloured solid; Sweet savoury aroma	NA			
76		1190230-47-7					
2160	**1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridin-2-yl)propan-1-one**	4723	$C_{15}H_{15}NO_3$	Practically insoluble in phosphate buffer	MS IR HNMR CNMR	NA	Safety evaluation not completed; m.p.= 65-66°
	1-(2-Hydroxy-4-methoxyphenyl)-3-(2-pyridyl)propan-1-one	-	257.28	Soluble	98	NA	
Full		-	Solid, off-white to cream in colour; Sweet savoury aroma	NA			
76		1190229-37-8					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2161	**3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione**	4725	$C_{19}H_{19}N_5O_4$	Practically insoluble in water	IR HNMR CNMR	NA	m.p= 135-136°
	3-[1-[(3,5-Dimethylisoxazol-4-yl)methyl]pyrazol-4-yl]-1-[(3-hydroxyphenyl)methyl]imidazolidine-2,4-dione	-	381.39	Soluble	99	NA	
Full		-	White solid; Bland aroma	NA			
76		1119831-25-2					
2162	**3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-5,5-dimethylimidazolidine-2,4-dione**	4726	$C_{21}H_{23}N_5O_4$	Practically insoluble to insoluble in water; soluble in phosphate buffer, pH 7.1	HNMR CNMR	NA	m.p.= 164-165°
	3-[1-[(3,5-Dimethylisoxazol-4-yl)methyl]pyrazol-4-yl]-1-[(3-hydroxyphenyl)methyl]-5,5-dimethyl-imidazolidine-2,4-dione	-	409.44	Soluble	99	NA	
Full		-	White solid; Unremarkable aroma	NA			
76		1217341-48-4					
2163	**trans-2-Nonenyl acetate**	4552	$C_{11}H_{20}O_2$	Very slightly soluble in water	MS	1.425-1.445	
	[(E)-Non-2-enyl] acetate	-	184.28	Soluble	96	0.870-0.890	
Full	(E)- Non-2-enyl acetate; (E)- Nonen-1-ol acetate; (E)-2- Nonenyl acetate; trans-2-Nonen-1-yl acetate	-	Colorless clear liquid; Fruity waxy citrus aroma	236-237			
76		30418-89-4					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2164	**Propyl sorbate**	4614	$C_9H_{14}O_2$	Practically insoluble to insoluble in water	MS	1.488-1.491	
	Propyl (2E,4E)-hexa-2,4-dienoate	-	154.21	Soluble	95	0.919-0.924 (20º)	
Full	Propyl (2E,4E)-hexa-2,4-dienoate; Sorbic acid propyl ester; (E,E)-2,4- Hexadienoic acid propyl ester; Propyl (2E,4E)-2,4-hexadienoate; Propyl 2,4-hexadiene carboxylate; propyl 2,4-Hexadienoate; trans,trans-2,4- Hexadienoic acid propyl ester	-	Clear colourless liquid; Sweet fruity aroma	205-207			
76		10297-72-0					
2165	**cis-2-Octenol**	4615	$C_8H_{16}O$	Practically insoluble to insoluble in water	MS	1.445-1.451	
	(Z)-Oct-2-en-1-ol	**-**	**128.21**	**Soluble**	**95**	**0.847-0.853 (20º)**	
Full	(Z)-2-Octenol	-	Colourless liquid; Sweet floral aroma	195-197			
76		26001-58-1					
2166	**trans-2-Tridecenol**	4617	$C_{13}H_{26}O$	Very slightly soluble in water	MS	1.499-1.505	
	(E)-Tridec-2-en-1-ol	-	198.34	Soluble	95	0.844-0.850 (20º)	
Full	(E)-2-Tridecenol	-	Colourless clear liquid; Mild waxy aroma	278-279			
76		74962-98-4					
2167	**Ethyl 2-hexenoate (mixture of isomers)**	4613	$C_8H_{14}O_2$	Practically insoluble to insoluble in water	MS	1.430-1.440	
	Mixture of (E)-ethyl 2-hexenoate and (Z)-ethyl 2-hexenoate	-	142.20	Soluble	95	0.895-0.905 (20º)	Mixture of isomers: 64% E, 34% Z
Full		-	Clear colourless liquid; Fruity aroma	167-174			
76		1552-67-6					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2170	**3',7-Dihydroxy-4'-methoxyflavan**	4708	$C_{16}H_{16}O_4$	Practically insoluble to insoluble in water; soluble in DMSO; slightly soluble in non-polar solvents	MS IR HNMR	NA	m.p. = 163-165C
	2-(3-Hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-chromen-7-ol	-	272.30	Soluble	95	NA	
Full	3,4- Dihydro-2-(3-hydroxy-4-methoxyphenyl)-2H-1-benzopyran-7-ol	-	White solid; Sweet aroma	NA			
76		76426-35-2					
2171	**Trilobatin**	4674	$C_{21}H_{24}O_{10}$	Slightly soluble in water	HNMR CNMR	NA	m.p. = 170-171°
	1-[4-(beta-D-Glucopyranosyloxy)-2,6-dihydroxyphenyl-3-(4-hydroxyphenyl)]-1-propanone	16.112	436.41	Soluble	98	NA	
Full	Phloretin 4'O-glucoside; Prunin dihydrochalcone; 1-[4-(beta-D-Glucopyranosyloxy)-2,6-dihydroxyphenyl]-3-(4-hydroxyphenyl)-1-propanone; 4'-O-beta-D-Glucoside of phloretin; Phloretin 4'-glucoside	-	Light yellow crystalline powder; Bland sweet aroma	NA			
76		4192-90-9					
2172	**(±)-Eriodictyol**	4715	$C_{15}H_{12}O_6$	Practically insoluble to insoluble	MS IR	NA	m.p. = 209-210°
	2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydrochromen-4-one	-	288.26	Sparingly soluble	96	NA	
Full	(±)-3',4',5,7- Tetrahydroxyflavanone	-	Slightly beige solid; Bland aroma	NA			
76		4049-38-1					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2173	**3-Methylhexanal**	4261	$C_7H_{14}O$	Very slightly soluble in water; soluble in pentane and diethyl ether	CNMR	1.409-1.414	
	3-Methylhexanal	05.219	114.19	Soluble	98	0.800-0.805	
Full		-	Colourless to pale yellow clear liquid; Sweet green aroma	43			
76		19269-28-4					
2174	**6-Methylheptanal**	4498	$C_8H_{16}O$	Practically insoluble to insoluble in water	IR	1.411-1.416	
	6-Methylheptanal	05.225	128.21	Soluble	98	0.806-0.816	
Full	Isooctan-1-al	-	Clear colourless liquid; Citrusy green aroma	162-163	< 2		
76		63885-09-6					
2175	**6-Methyloctanal**	4433	$C_9H_{18}O$	Slightly soluble in water	HNMR	1.422-1.427	
	6-Methyloctanal	05.211	142.24	Soluble	96	0.810-0.813	
Full		-	Clear colourless liquid; Green aroma	182-184	< 2		
76		30689-75-9					
2176	**3,7-Dimethyloctanal**	4348	$C_{10}H_{20}O$	Practically insoluble to insoluble in water	MS	1.451-1.457 (25°)	
	3,7-Dimethyloctanal	-	156.27	Soluble	98	1.085-1.095	
Full	Tetrahydrocitral; 3,7- dimethyl octanal; 3,7-Dimethyl-1-octanal; 6,7- Dihydrocitronellal; Dihydrocitronellal; Tetrahydrogeranial	-	Clear colourless to pale yellow solution; Onion aroma with fruity undertones	270-272			
76		5988-91-0					

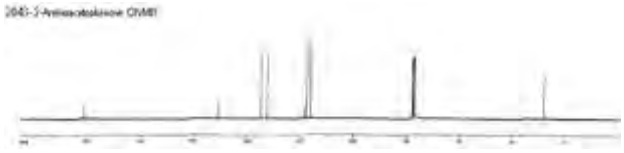
JECFA No. / Status / Session	Name / Chemical Name / Synonyms	FEMA / FLAVIS / COE / CAS	Chemical Formula / M.W / Physical form; Odour	Solubility / Solubility in ethanol / B.P. °C	ID test / Assay min % / Acid value	R.I. / S.G.	Other requirements / Information required
2177	**cis-3-Nonen-1-ol**	4412	$C_9H_{18}O$	Practically insoluble to insoluble in water	MS	1.440-1.460	
	(Z)-Non-3-en-1-ol	02.234	142.24	Soluble	95	0.841-0.849 (20°)	
Full	(3Z)- Nonenol; (Z)- Non-3-en-1-ol; (Z)-3-Nonenol; cis-3- Nonenol	10293	Clear colourless liquid; Waxy green melon aroma	65 (2 mm Hg)			
76		10340-23-5					
2178	**trans-3-Nonen-1-ol**	4605	$C_9H_{18}O$	Soluble in water	IR HNMR CNMR	1.438-1.458	
	(E)-Non-3-en-1-ol	-	142.24	Soluble	98	0.839-0.849	
Full	(3E)-3- Nonen-1-ol; (E)-3- Nonenol; trans-3- Nonenol	-	Colourless liquid; Waxy melon-cucumber aroma	210-211	0.1		
76		10339-61-4					
2179	**cis,cis-3,6-Nonadienyl acetate**	4551	$C_{11}H_{18}O_2$	Partially soluble in water	MS IR HNMR CNMR	1.444-1.455	
	[(3Z,6Z)-Nona-3,6-dienyl] acetate	-	182.26	Soluble	95	0.899-0.915	
Full	Acetic acid (Z,Z)-3,6-nonadienyl ester; (3Z,6Z)- Nonadien-1-yl acetate; (Z)-3,(Z)-6-Nonadien-1-yl acetate; (Z,Z)-3,6-Nonadienyl acetate	-	Colourless liquid; Fruity aroma	229-231	0.1		
76		83334-93-4					
2180	**trans-3-Hexenyl acetate**	4413	$C_8H_{14}O_2$	Practically insoluble to insoluble in water	HNMR	1.420-1.426	
	[(E)-Hex-3-enyl] acetate	09.928	142.20	Soluble	95	0.885-0.917 (20°)	
Full	Acetic acid trans-3-hexen-1-yl ester; (E)-Hex-3-enyl acetate; (E)-3-Hexen-1-ol acetate; Acetic acid (E)-3-hexen-1-yl ester; trans-3-Hexen-1-yl acetate	-	Clear colourless liquid; Sharp fruity green aroma reminiscent of unripe pear or banana	174-175			
76		3681-82-1					

JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2181	**cis-3-Hexenoic acid**	4493	$C_6H_{10}O_2$	Practically insoluble to insoluble in water	MS	1.437-1.443	
	(Z)-Hex-3-enoic acid	-	114.14	Soluble	95	0.962-0.968	
Full		-	Colourless to pale yellow clear liquid; Sweaty, cheesy, fruity aroma	209-210			
76		1775-43-5					
2182	**cis-3-Nonenyl acetate**	4553	$C_{11}H_{20}O_2$	Very slightly soluble	MS IR HNMR CNMR	1.428-1.438	
	[(Z)-Non-3-enyl] acetate	09.672	184.28	Soluble	97	0.879-0.890	
Full	Pear acetate; (3Z)-3- Nonenyl acetate; (Z)-Non-3-enyl acetate; (Z)-3- Nonenyl acetate	-	Colourless liquid; Green fruity aroma	225-226	0.1		
76		13049-88-2					
2183	**cis-6-Nonenyl acetate**	4554	$C_{11}H_{20}O_2$	Practically insoluble to insoluble in water; soluble in fat	MS IR HNMR CNMR	1.432-1.440	
	[(Z)-Non-6-enyl] acetate	09.673	184.28	Soluble	96	0.880-0.890	
Full	(Z)-Non-6-enyl acetate; (Z)- non-6-enyl ethanoate; (Z)-6- Nonen-1-yl acetate; (Z)-6- Nonenyl acetate; cis- Non-6-enyl acetate; cis-6- Nonen-1-yl acetate	-	Clear colourless liquid; Melon-like aroma	229-230			
76		76238-22-7					
2184	**Z-5-Octenyl acetate**	4671	$C_{10}H_{18}O_2$	Practically insoluble to insoluble in water	IR HNMR	1.419-1.448	
	(5Z)-Oct-5-en-1-yl acetate	09.950	170.25	Soluble	97	0.832-0.950	
Full	(5Z)- Octen-1-ol acetate; (Z)-5- octenyl acetate; cis-5- Octenyl acetate	-	Clear colourless liquid; Fruity banana-like aroma	225-227			
76		71978-00-2					

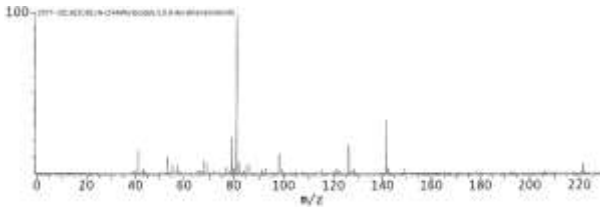
JECFA No.	Name	FEMA	Chemical Formula	Solubility	ID test	R.I.	Other requirements
Status	Chemical Name	FLAVIS	M.W	Solubility in ethanol	Assay min %	S.G.	
	Synonyms	COE	Physical form; Odour	B.P. °C	Acid value		Information required
Session		CAS					
2185	**(E)-4-Undecenal**	4672	$C_{11}H_{20}O$	Insoluble in water, Soluble in organic solvents	IR HNMR	1.422-1.459	
	(E)-Undec-4-enal	05.226	168.28	Soluble	97	0.829-0.857 (20º)	
Full	trans-Undec-4-enal	-	Clear colourless liquid; Fatty aldehydic aroma	237-238			
76		68820-35-9					

Spectra of certain flavouring agents

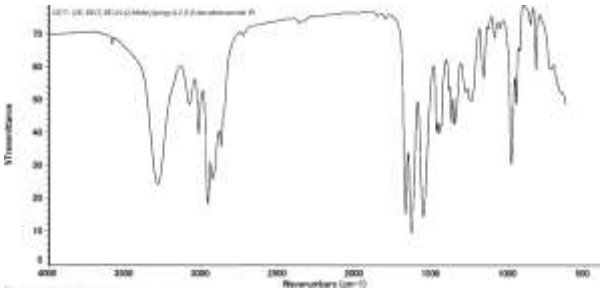
2043 2-Aminoacetophenone



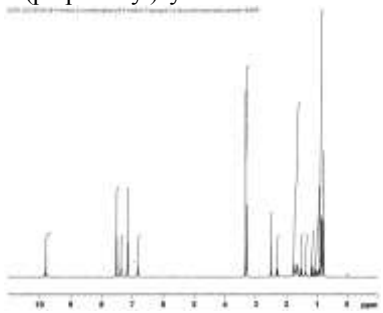
2077 (2E,6E/Z,8E)-N-(2-Methylpropyl)-2,6,8-decatrienamide (MS)



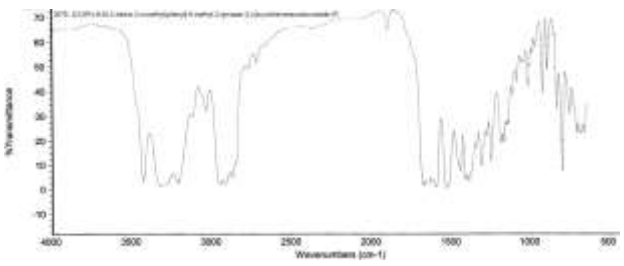
2077 (2E,6E/Z,8E)-N-(2-Methylpropyl)-2,6,8-decatrienamide (IR)



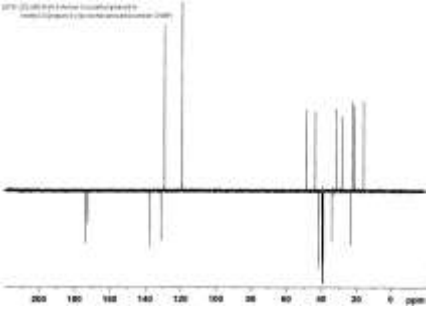
2078 (2S,5R)-N-[4-2-Amino-2-oxoethyl)phenyl]-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide (1H-NMR)



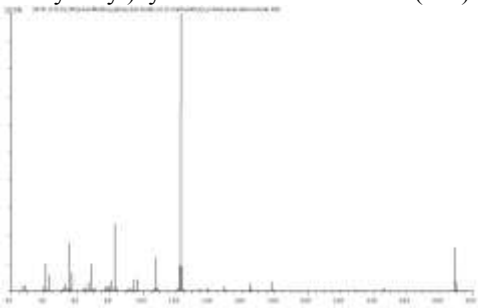
2078 (2S,5R)-N-[4-2-Amino-2-oxoethyl)phenyl]-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide (IR)



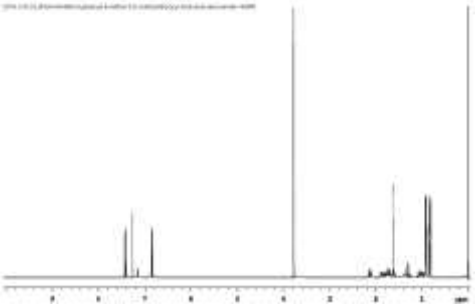
2078 (2S,5R)-N-[4-2-Amino-2-oxoethyl)phenyl]-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide (13C-NMR)



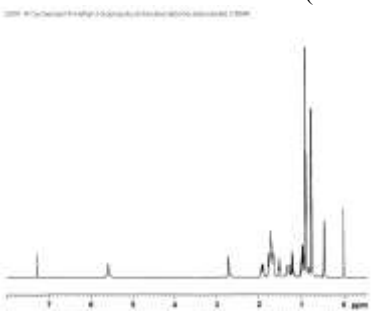
2079 (1R,2S,5R)-N-(4-Methoxyphenyl)-5-methyl-2-(1-methylethyl)cyclohexanecarboxamide (MS)



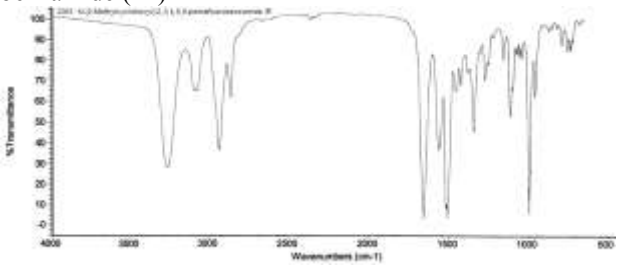
2079 (1R,2S,5R)-N-(4-Methoxyphenyl)-5-methyl-2-(1-methylethyl)cyclohexanecarboxamide (1H-NMR)



2080 N-Cyclopropyl-5-methyl-2-isopropylcyclo-hexanecarbonecarboxamide (13C-NMR)



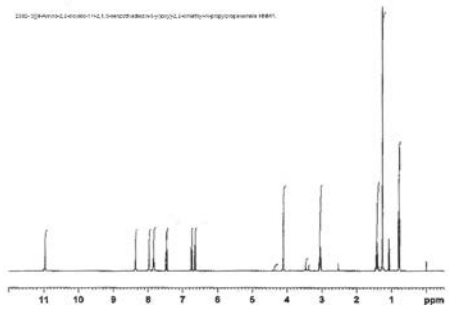
2081 N-(2-Methylcyclohexyl)-2,3,4,5,6-pentafluoro-benzamide (IR)



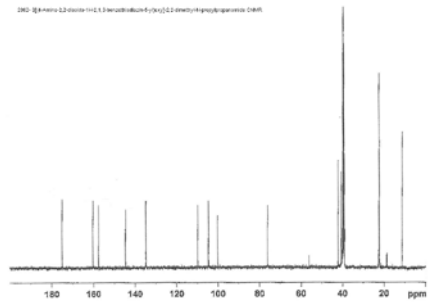
2081 N-(2-Methylcyclohexyl)-2,3,4,5,6-pentafluoro-benzamide (1H-NMR)



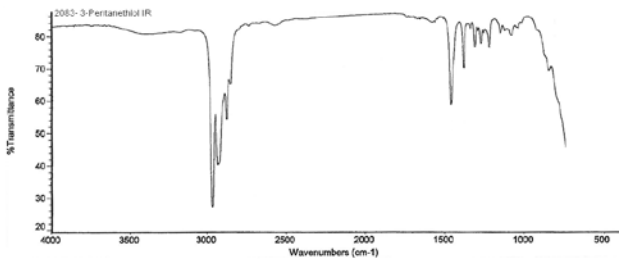
2082 3[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-N-propylpropanamide (1H-NMR)



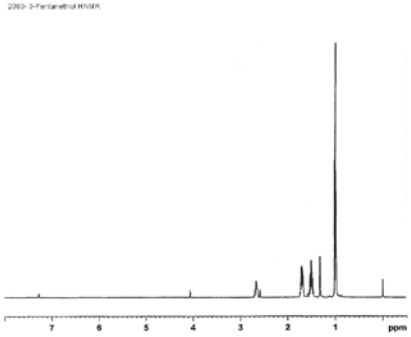
2082 3[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-N-propylpropanamide (13C-NMR)



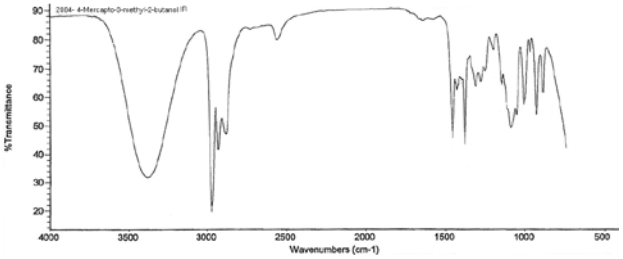
2083 3-Pentanethiol (IR)



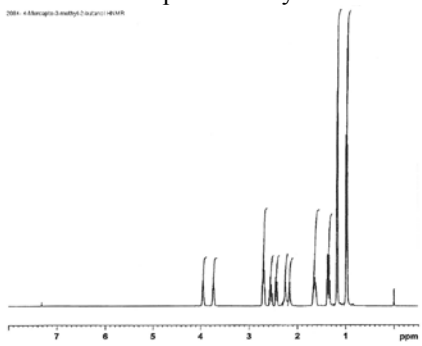
2083 3-Pentanethiol (1H-NMR)



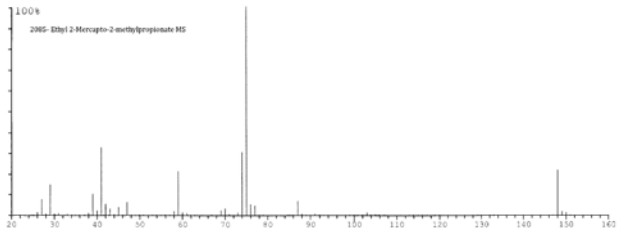
2084 4-Mercapto-3-methyl-2-butanol (IR)



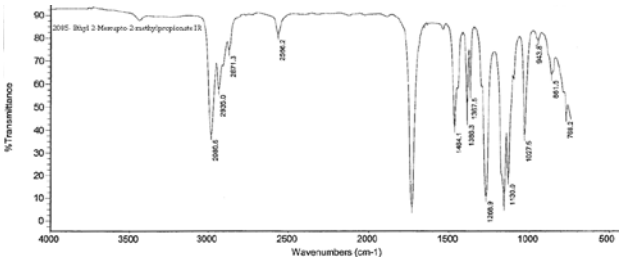
2084 4-Mercapto-3-methyl-2-butanol (1H-NMR)



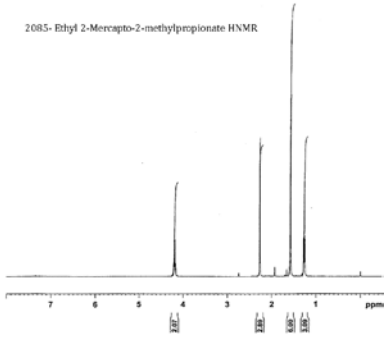
2085 Ethyl 2-Mercapto-2-methylpropionate (MS)



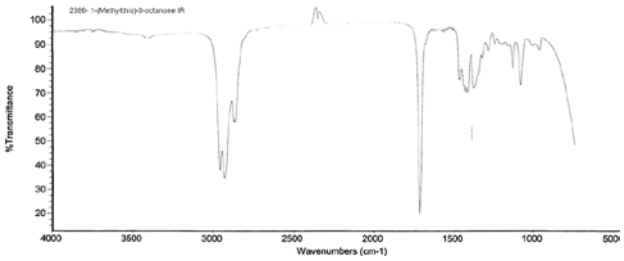
2085 Ethyl 2-Mercapto-2-methylpropionate (IR)



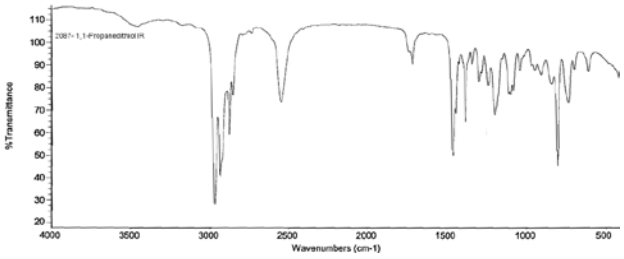
2085 Ethyl 2-Mercapto-2-methylpropionate (1H-NMR)



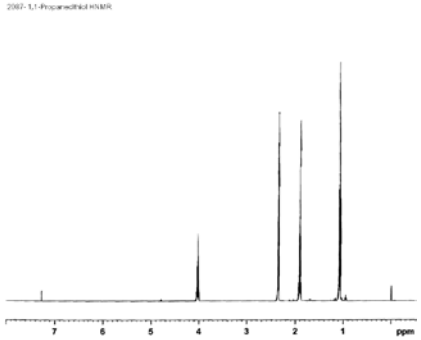
2086 1-(Methylthio)-3-octanone



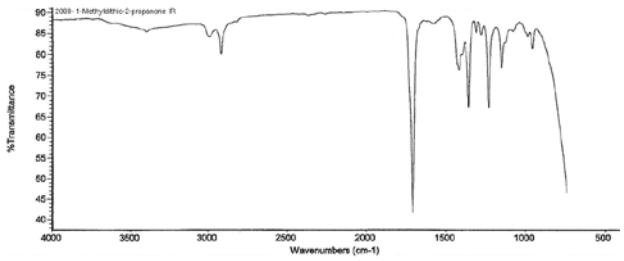
2087 1,1-Propanedithiol (IR)



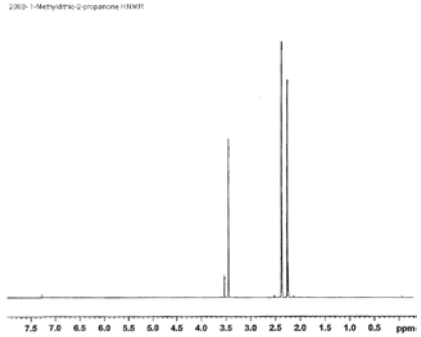
2087 1,1-Propanedithiol (1H-NMR)



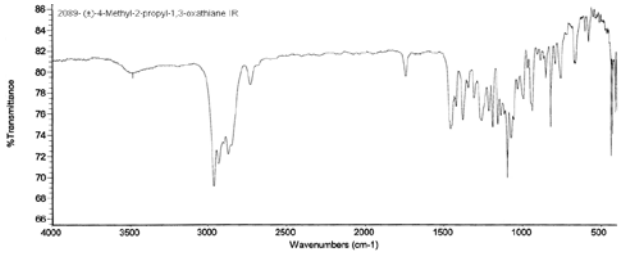
2088 1-Methyldithio-2-propanone (IR)



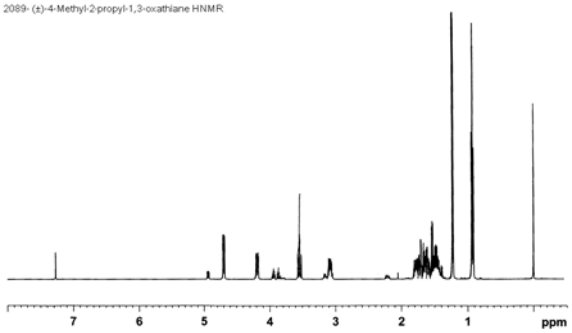
2088 1-Methyldithio-2-propanone (1H-NMR)



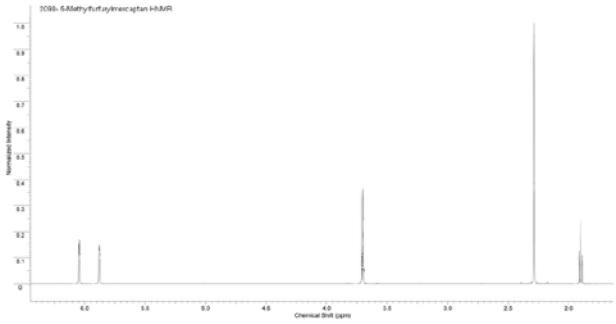
2089 (+/-)-4-Methyl-2-propyl-1,3-oxathiane (IR)



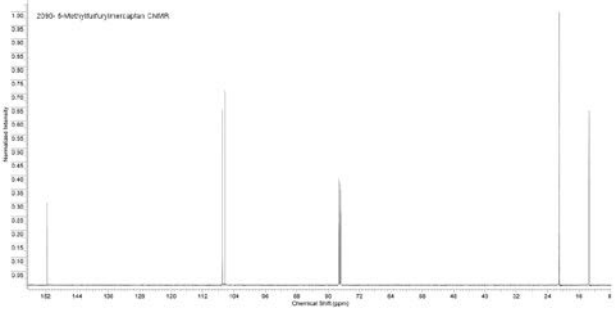
2089 (+/-)-4-Methyl-2-propyl-1,3-oxathiane (1H-NMR)



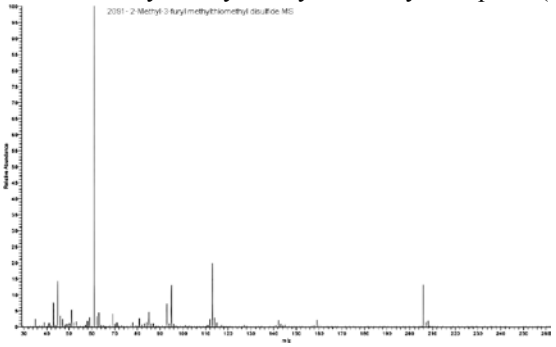
2090 5-Methylfurfurylmercaptan (1H-NMR)



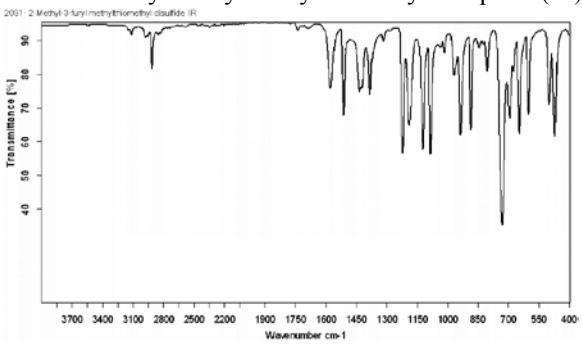
2090 5-Methylfurfurylmercaptan (13C-NMR)



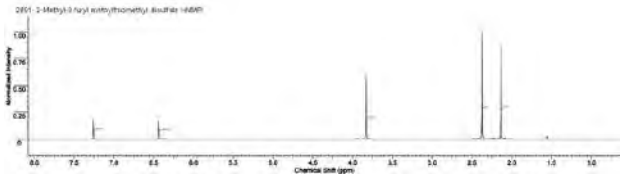
2091 2-Methyl-3-furyl methylthiomethyl disulphide (MS)



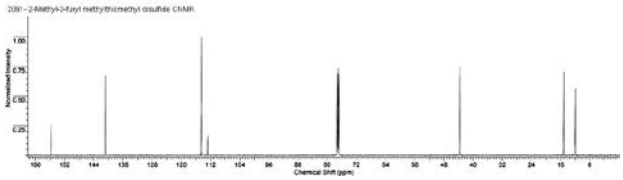
2091 2-Methyl-3-furyl methylthiomethyl disulphide (IR)



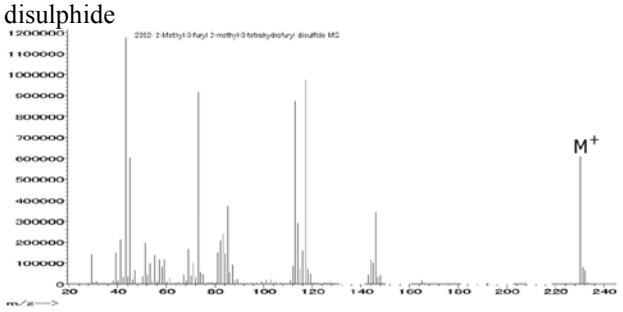
2091 2-Methyl-3-furyl methylthiomethyl disulphide (1H-NMR)



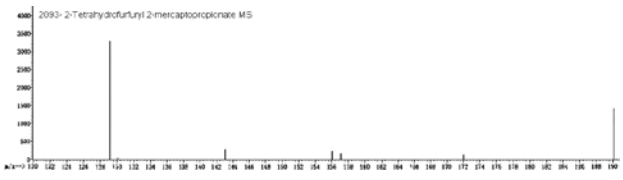
2091 2-Methyl-3-furyl methylthiomethyl disulphide (13C-HNM)



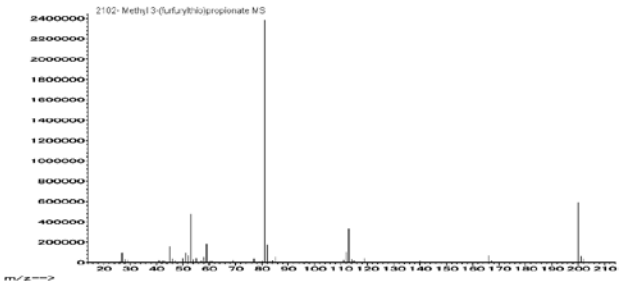
2092 2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulphide



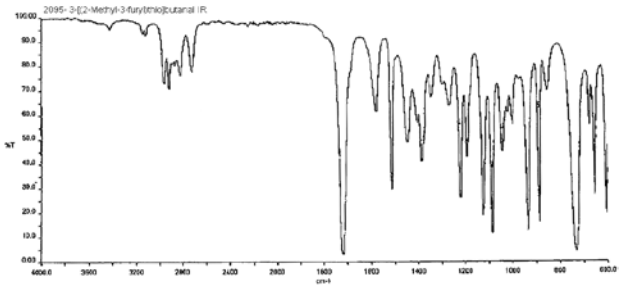
2093 2-Tetrahydrofurfuryl 2-mercaptopropionate



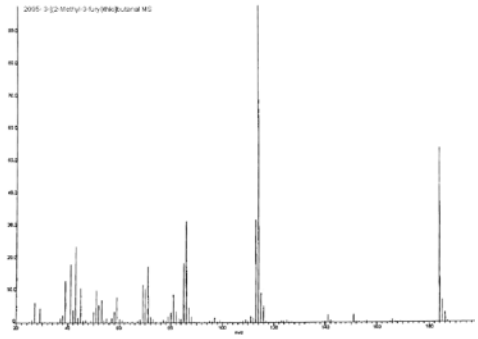
2094 Methyl 3-(furfurylthio)propionate



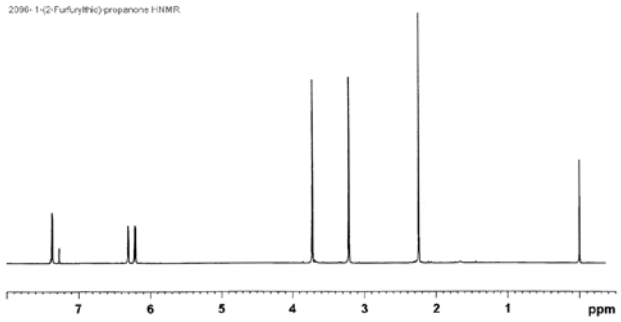
2095 3-[(2-Methyl-3-furyl)thio]butanal (IR)



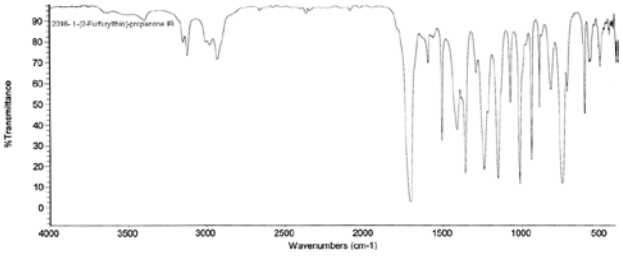
2095 3-[(2-Methyl-3-furyl)thio]butanal (MS)



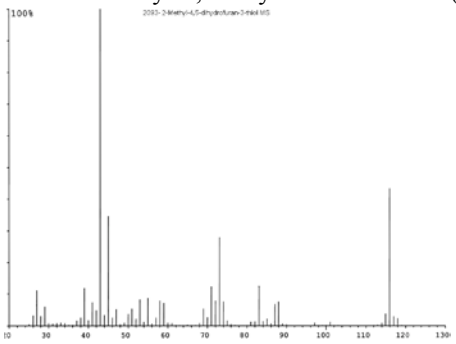
2096 1-(2-Furfurylthio)-propanone (1H-NMR)



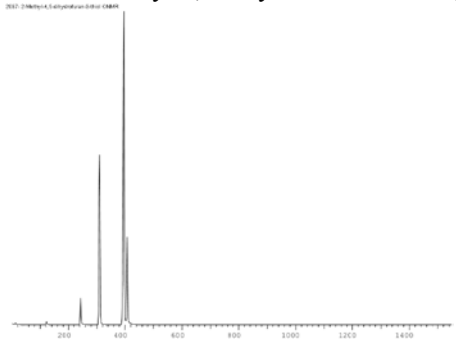
2096 1-(2-Furfurylthio)-propanone (IR)



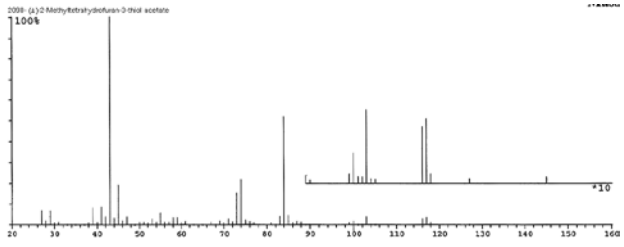
2097 2-Methyl-4,5-dihydrofuran-3-thiol (MS)



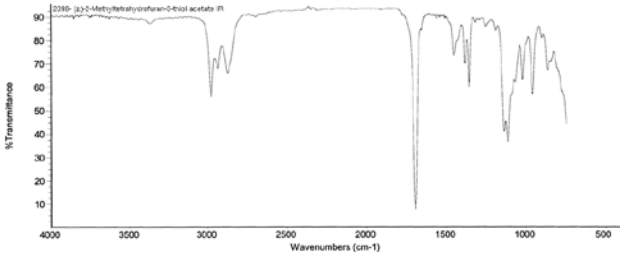
2097 2-Methyl-4,5-dihydrofuran-3-thiol (13C-NMR)



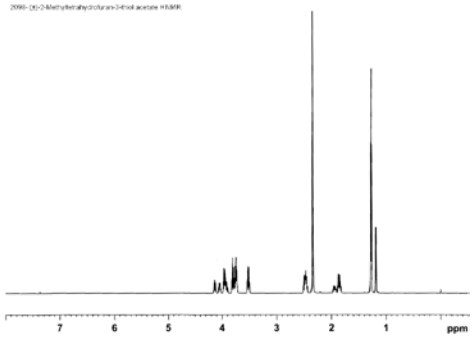
2098 (+/-)-2-Methyltetrahydrofuran-3-thiol acetate (MS)



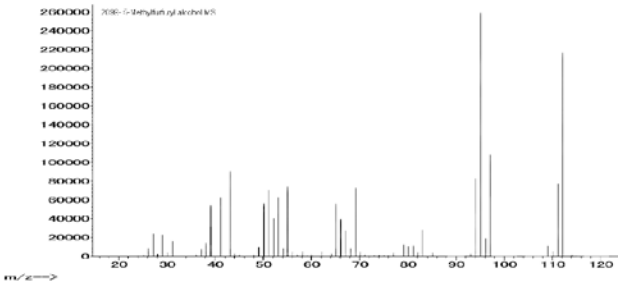
2098 (+/-)-2-Methyltetrahydrofuran-3-thiol acetate (IR)



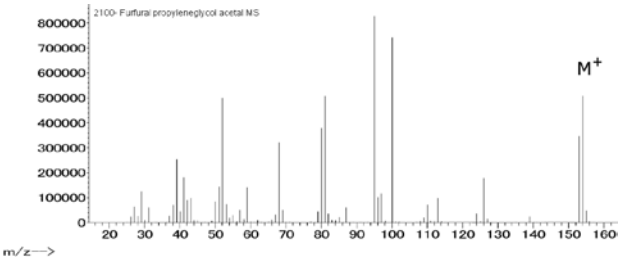
2098 (+/-)-2-Methyltetrahydrofuran-3-thiol acetate (1H-NMR)



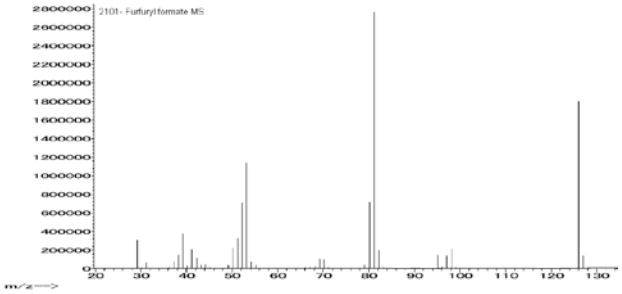
2099 5-Methylfurfuryl alcohol



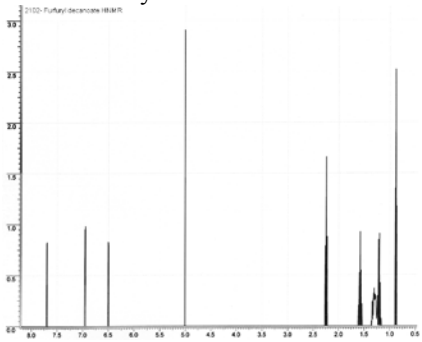
2100 Furfural propyleneglycol acetal



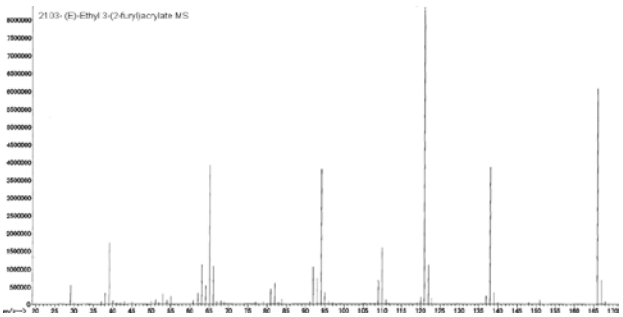
2101 Furfuryl formate



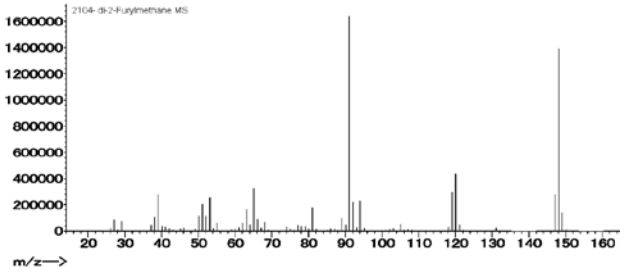
2102 Furfuryl decanoate



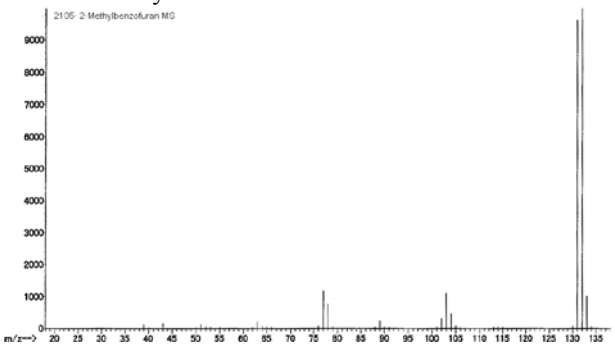
2103 (E)-Ethyl 3-(2-furyl)acrylate



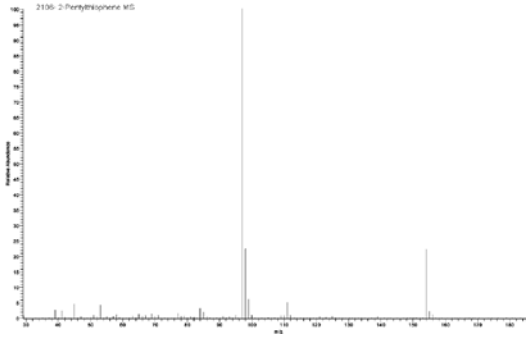
2104 di-2-Furylmethane



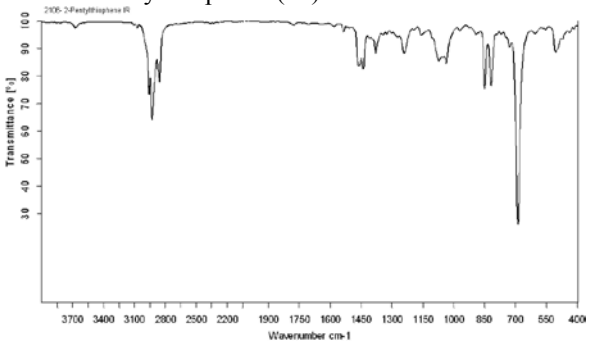
2105 2-Methylbenzofuran



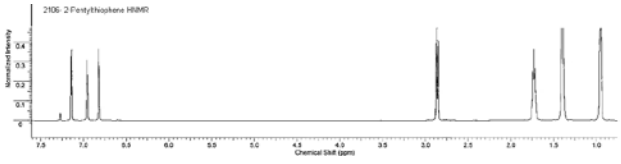
2106 2-Pentylthiophene (MS)



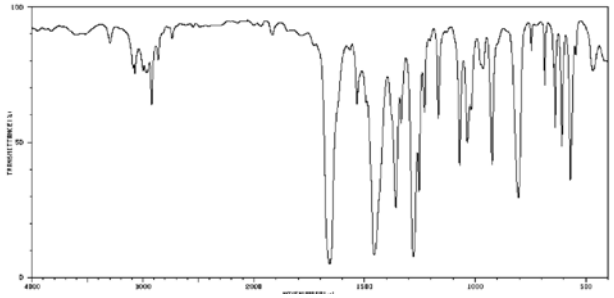
2106 2-Pentylthiophene (IR)



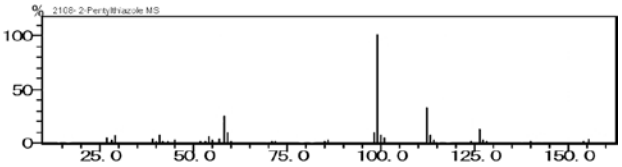
2106 2-Pentylthiophene (1H-NMR)



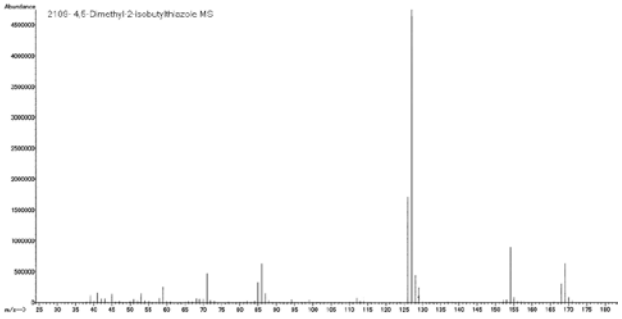
2107 2-Acetyl-5-methylthiophene



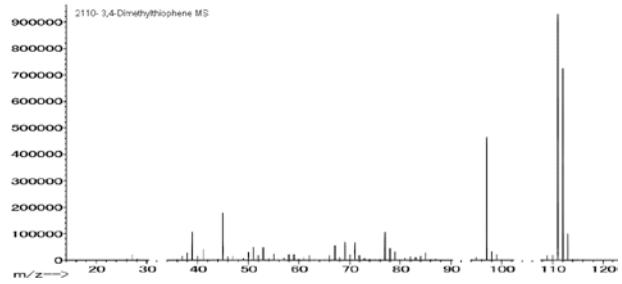
2108 2-Pentylthiazole



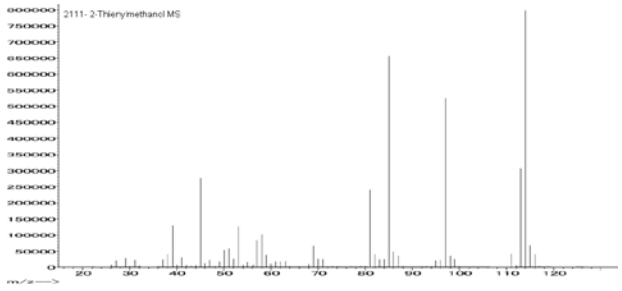
2109 4,5-Dimethyl-2-isobutylthiazole



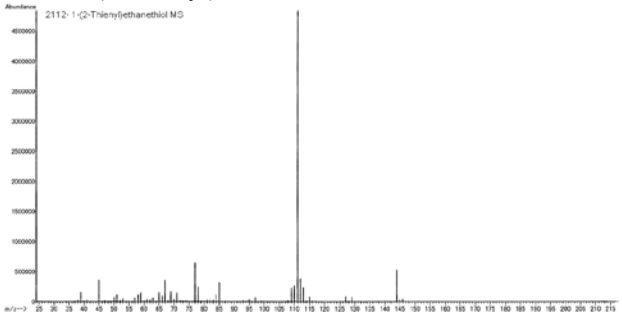
2110 3,4-Dimethylthiophene



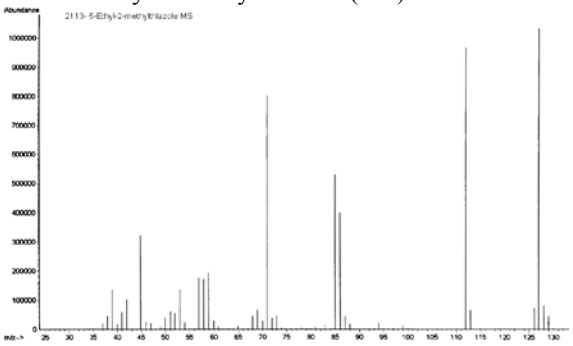
2111 2-Thienylmethanol



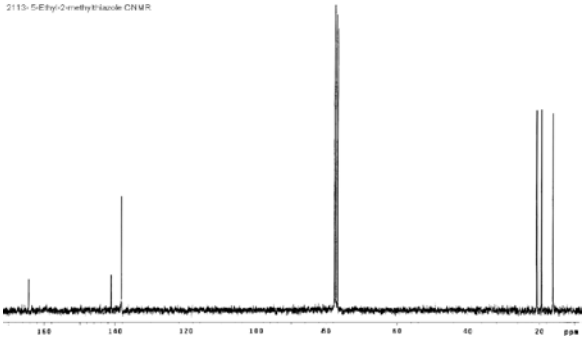
2112 1-(2-Thienyl)ethanethiol



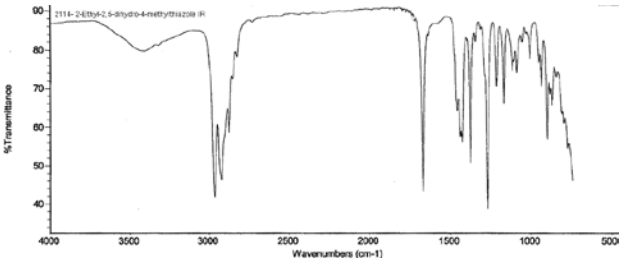
2113 5-Ethyl-2-methylthiazole (MS)



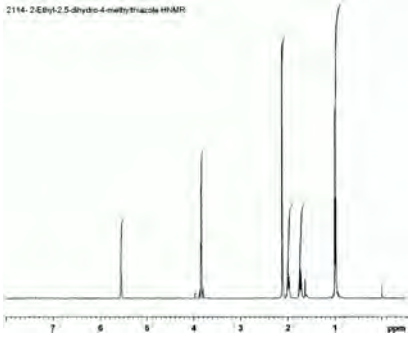
2113 5-Ethyl-2-methylthiazole (13C-NMR)



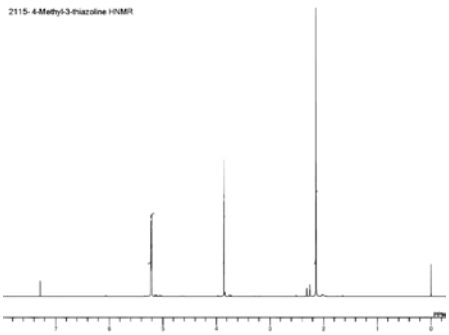
2114 2-Ethyl-2,5-dihydro-4-methylthiazole (IR)



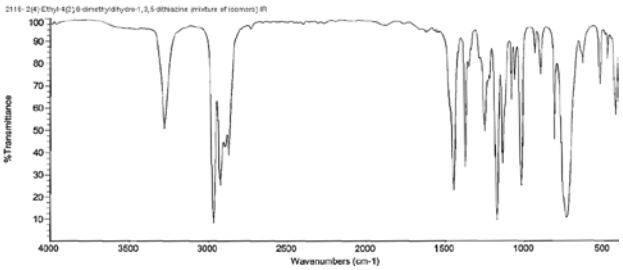
2114 2-Ethyl-2,5-dihydro-4-methylthiazole (1H-NMR)



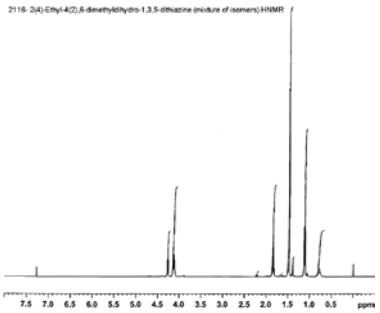
2115 4-Methyl-3-thiazoline



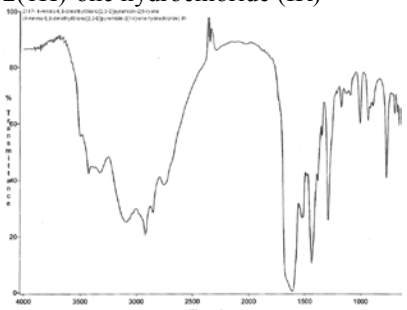
2116 2-Ethyl-4,6-dimethyl-dihydro-1,3,5-dithiazine (IR)



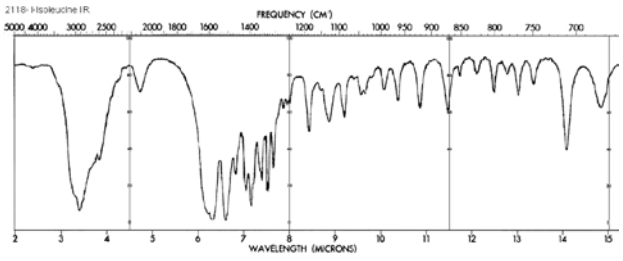
2116 2-Ethyl-4,6-dimethyl-dihydro-1,3,5-dithiazine (1H-NMR)



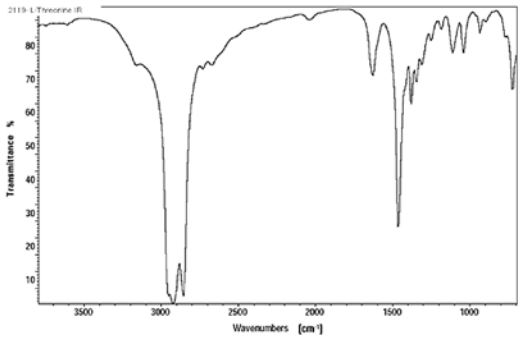
2117 4-Amino-5,6-dimethylthieno[2,3-d]pyramidin-2(1H)-one hydrochloride (IR)



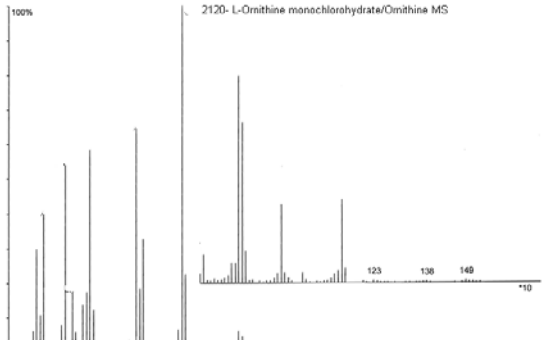
2118 L-Isoleucine



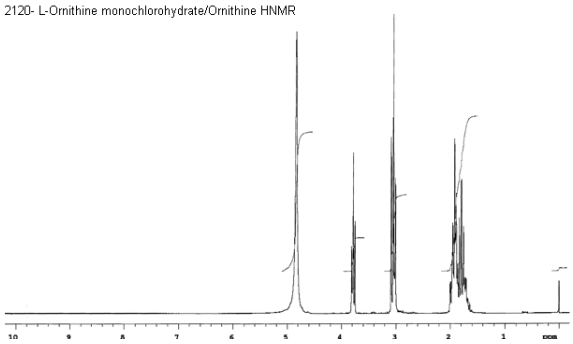
2119 L-Threonine



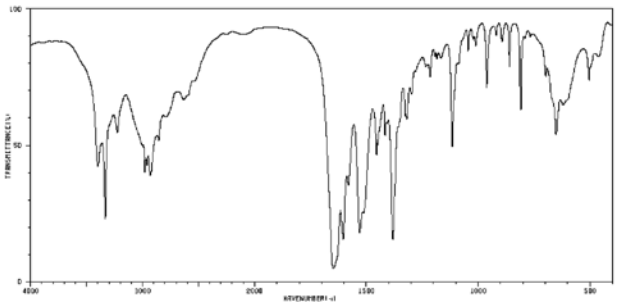
2120 L-Ornithine monochlorohydrate (MS)



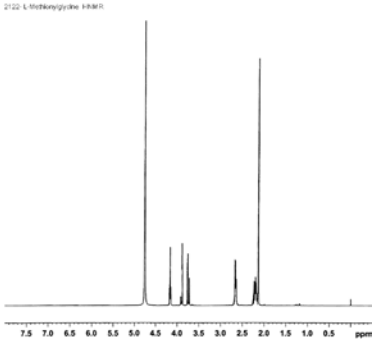
2120 L-Ornithine monochlorohydrate (1H-NMR)



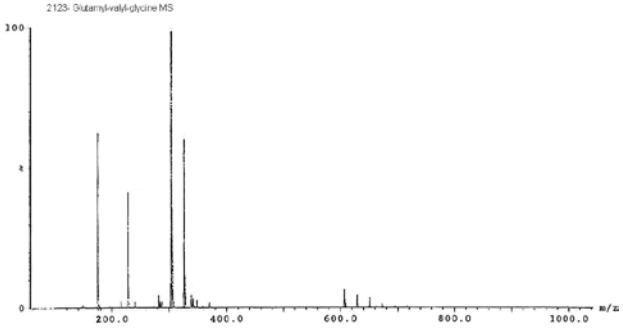
2121 L-Alanyl-L-Glutamine



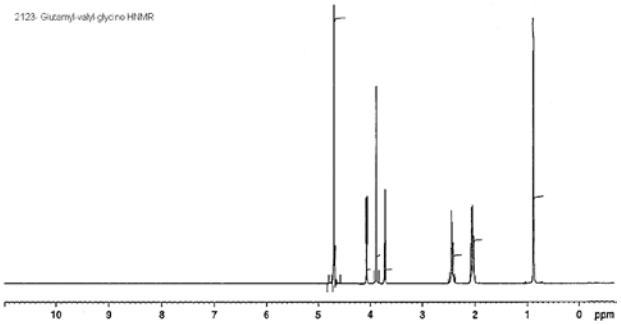
2122 L-Methionylglycine (1H-NMR)



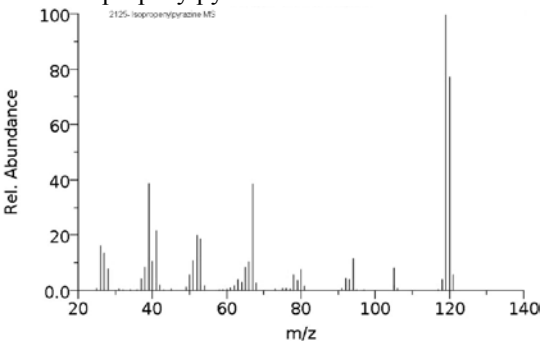
2123 Glutamyl-valyl-glycine (MS)



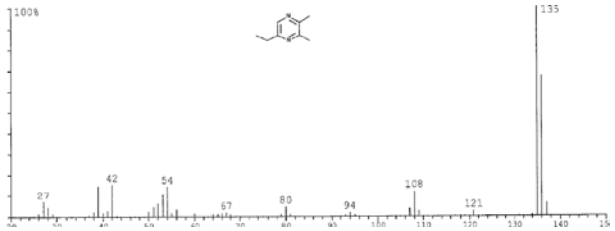
2123 Glutamyl-valyl-glycine (1H-NMR)



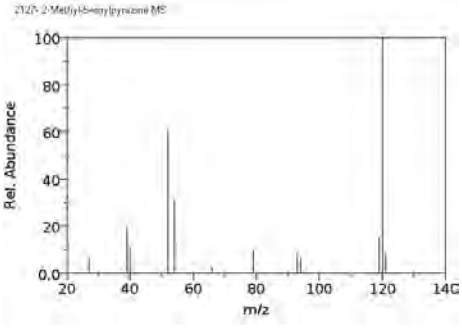
2125 Isopropenylpyrazine



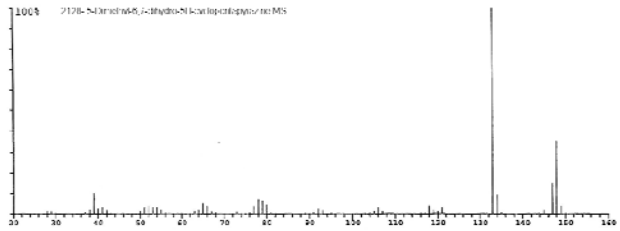
2126 5-Ethyl-2,3-dimethylpyrazine



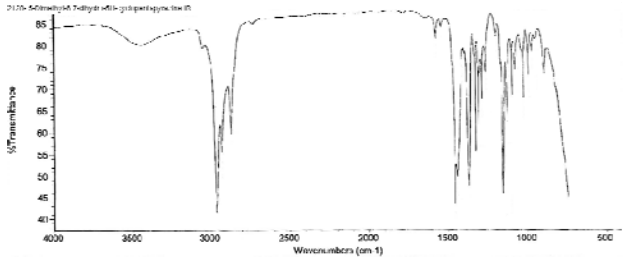
2127 2-Methyl-5-vinylpyrazine



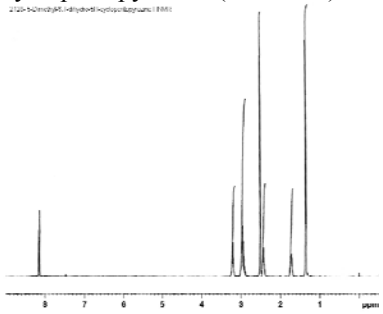
2128 Mixture of 2,5 and 2,7-Dimethyl-6,7-dihydro-5H-cyclopentapyrazine (MS)



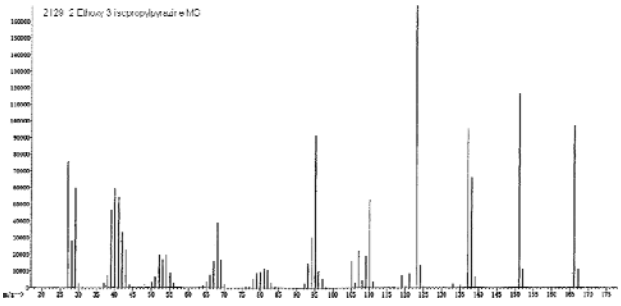
2128 Mixture of 2,5 and 2,7-Dimethyl-6,7-dihydro-5H-cyclopentapyrazine (IR)



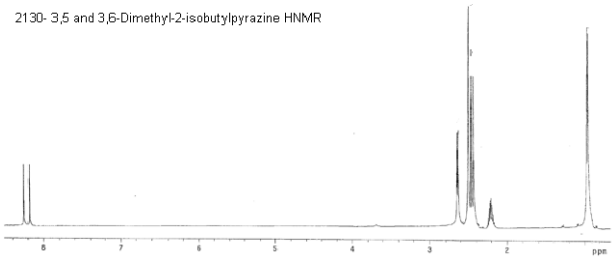
2128 Mixture of 2,5 and 2,7-Dimethyl-6,7-dihydro-5H-cyclopentapyrazine (1H-NMR)



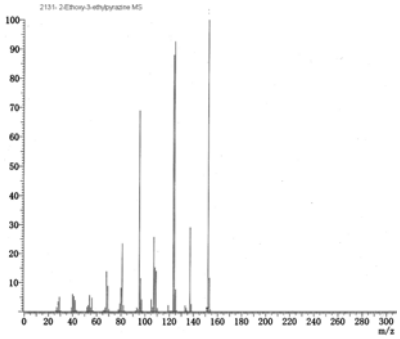
2129 2-Ethoxy-3-isopropylpyrazine



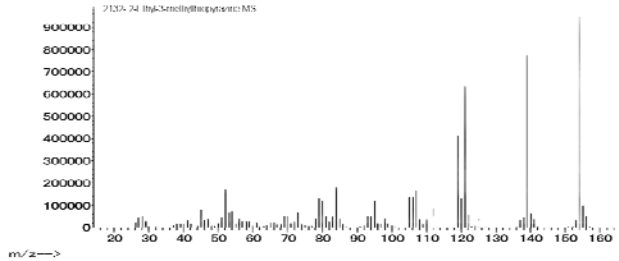
2130 Mixture of 3,5- and 3,6-Dimethyl-2-isobutylpyrazine



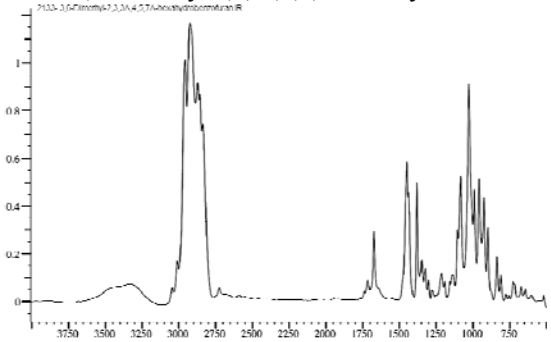
2131 2-Ethoxy-3-ethylpyrazine



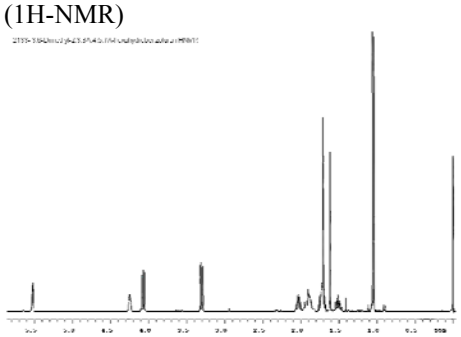
2132 2-Ethyl-3-methylthiopyrazine



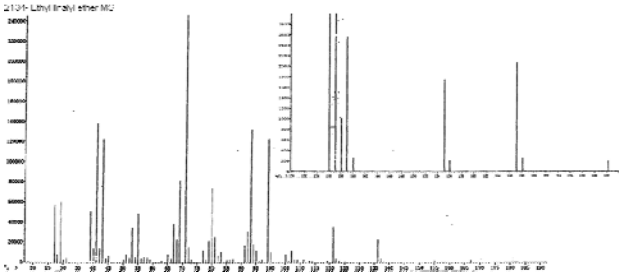
2133 3,6-Dimethyl-2,3,3a,4,5,7a-hexahydrobenzofuran (IR)



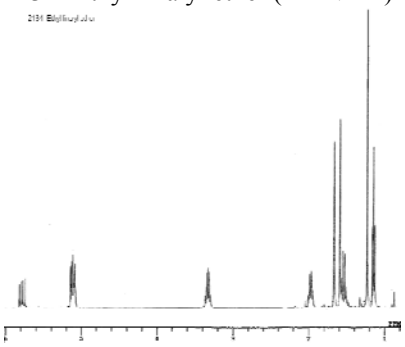
2133 3,6-Dimethyl-2,3,3a,4,5,7a-hexahydrobenzofuran (1H-NMR)



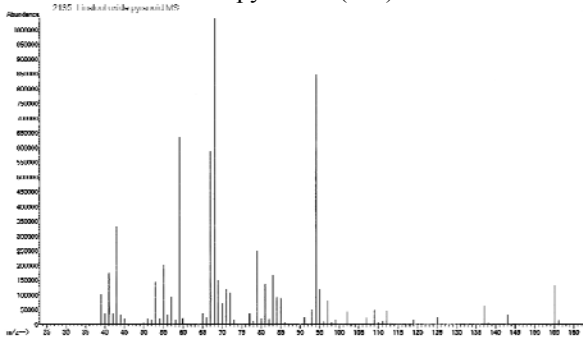
2134 Ethyl linalyl ether (MS)



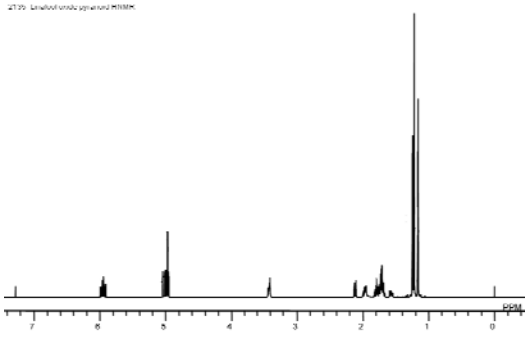
2134 Ethyl linalyl ether (1H-NMR)



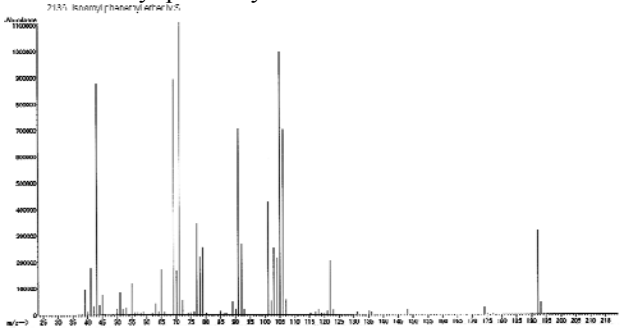
2135 Linalool oxide pyranoid (MS)



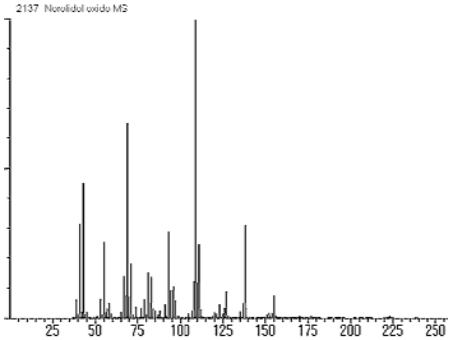
2135 Linalool oxide pyranoid (1H-NMR)



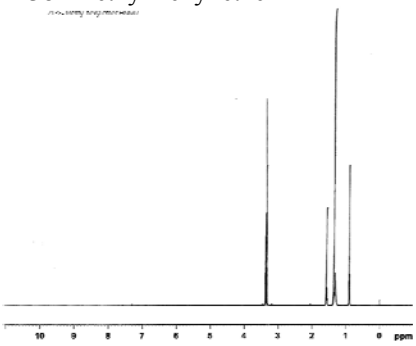
2136 Isoamyl phenethyl ether



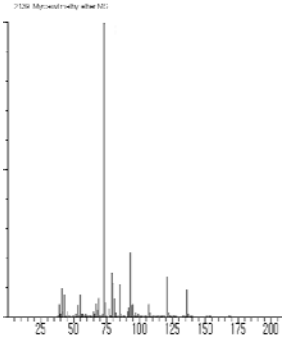
2137 Nerolidol oxide



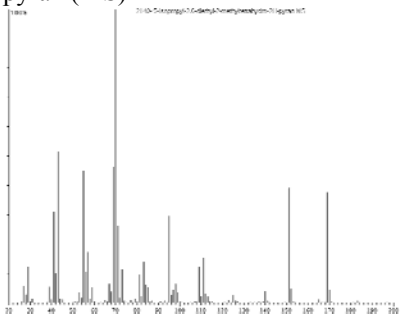
2138 Methyl hexyl ether



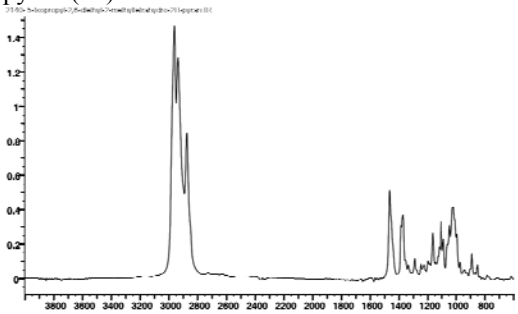
2139 Myrcenyl methyl ether



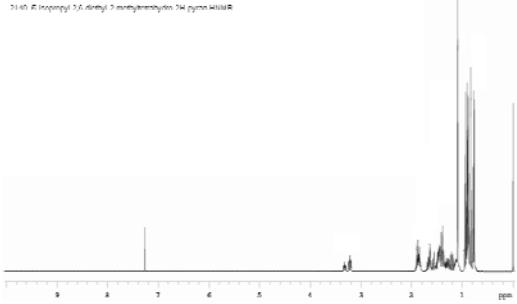
2140 5-Isopropyl-2,6-diethyl-2-methyltetrahydro-2H-pyran (MS)



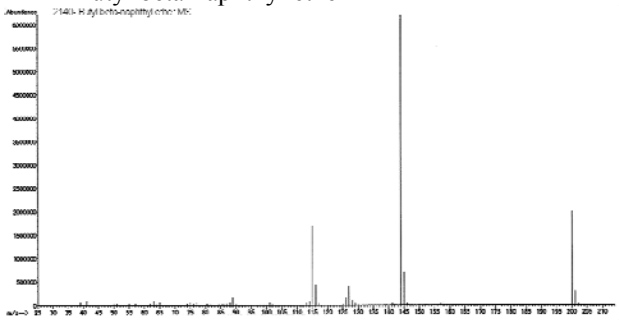
2140 5-Isopropyl-2,6-diethyl-2-methyltetrahydro-2H-pyran (IR)



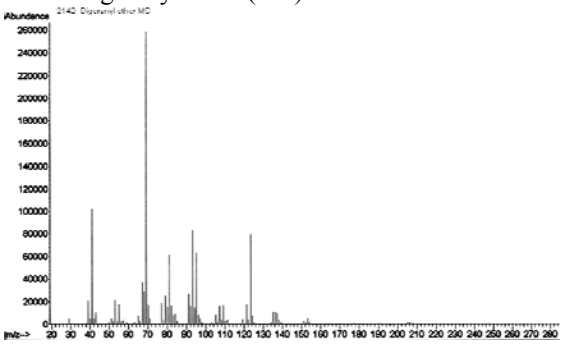
2140 5-Isopropyl-2,6-diethyl-2-methyltetrahydro-2H-pyran (1H-NMR)^



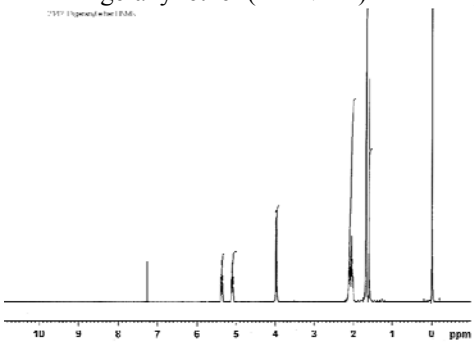
2141 Butyl beta-naphthyl ether



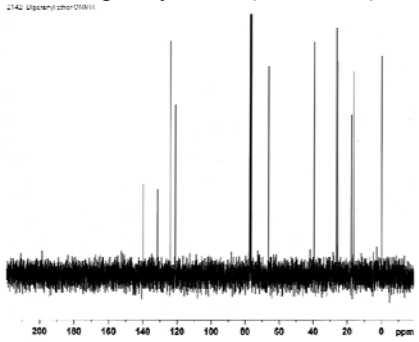
2142 Digeranyl ether (MS)



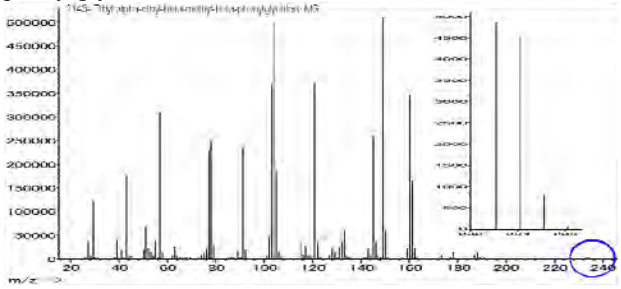
2142 Digeranyl ether (1H-NMR)



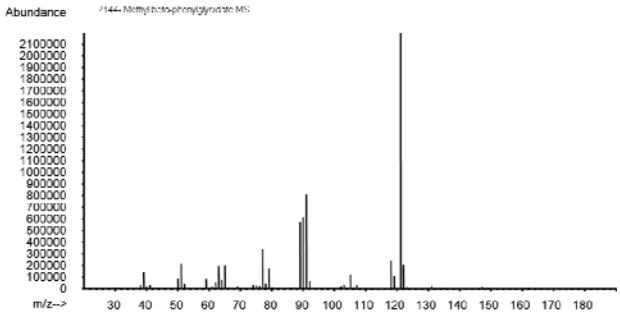
2142 Digeranyl ether (13C-NMR)



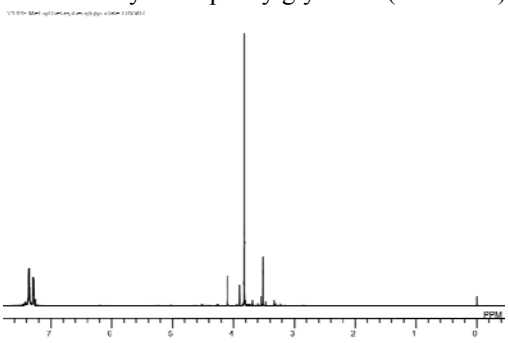
2143 Ethyl alpha-ethyl-beta-methyl-beta-phenylglycidate



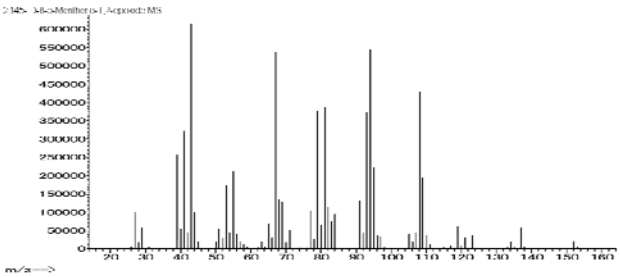
2144 Methyl beta-phenylglycidate (MS)



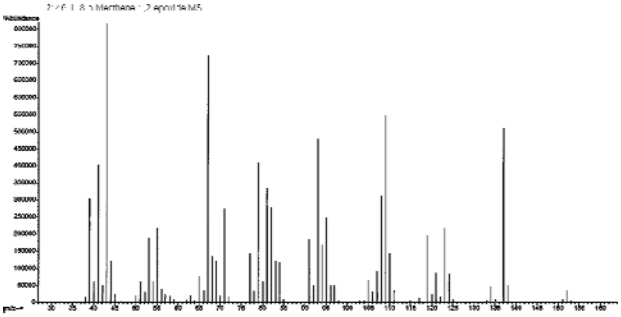
2144 Methyl beta-phenylglycidate (1H-NMR)



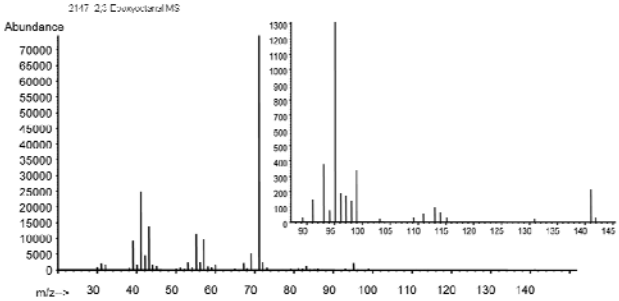
2145 d-8-p-Menthene-1,2-epoxide



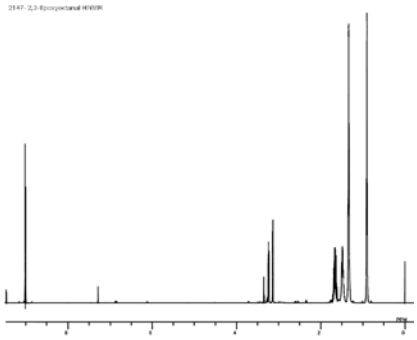
2146 l-8-p-Menthene-1,2-epoxide



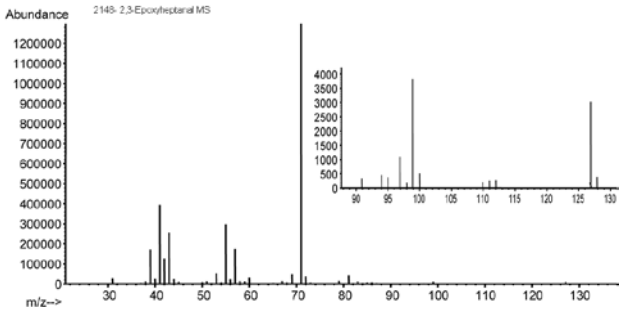
2147 2,3-Epoxyoctanal (MS)



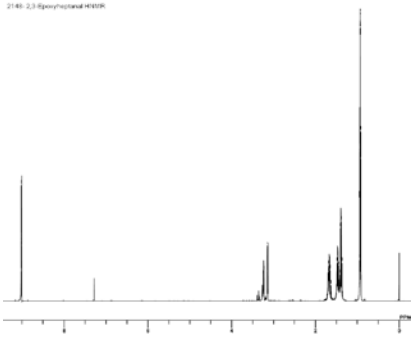
2147 2,3-Epoxyoctanal (1H-NMR)



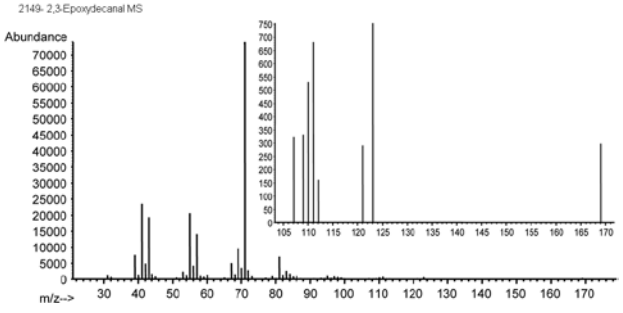
2148 2,3-Epoxyheptanal (MS)



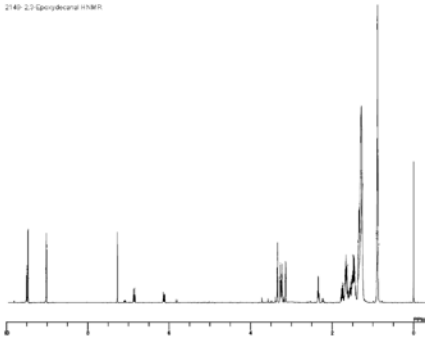
2148 2,3-Epoxyheptanal (1H-NMR)



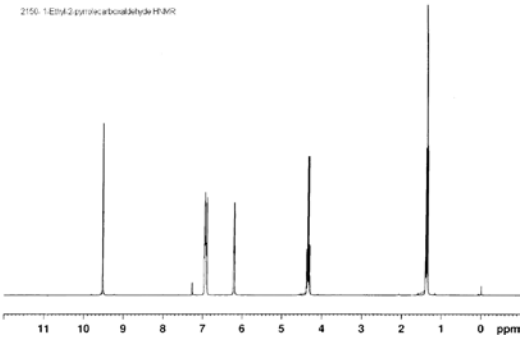
2149 2,3-Epoxydecanal (MS)



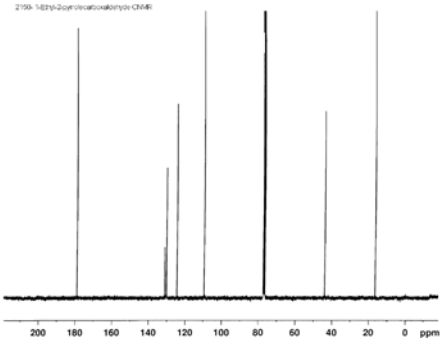
2149 2,3-Epoxydecanal (1H-NMR)



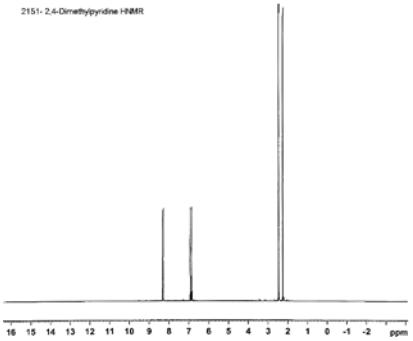
2150 1-Ethyl-2-pyrrolecarboxaldehyde (1H-NMR)



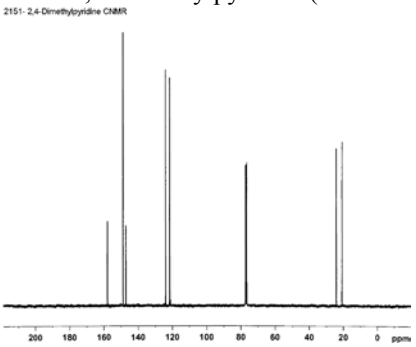
2150 1-Ethyl-2-pyrrolecarboxaldehyde (13C-NMR)



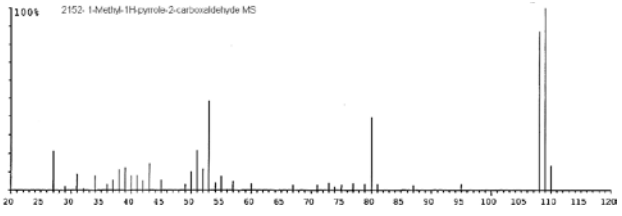
2151 2,4-Dimethylpyridine (1H-NMR)



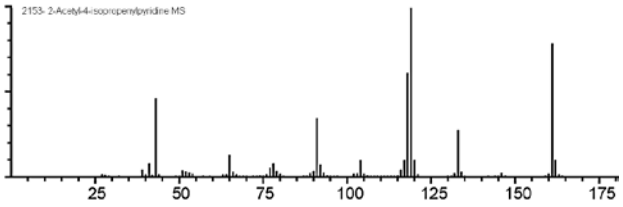
2151 2,4-Dimethylpyridine (13C-NMR)



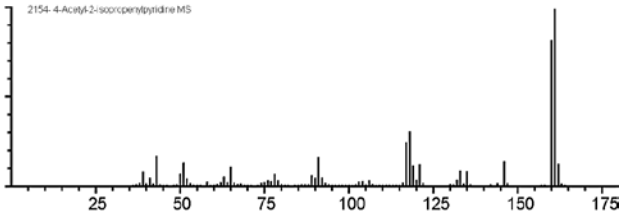
2152 1-Methyl-1H-pyrrole-2-carboxaldehyde



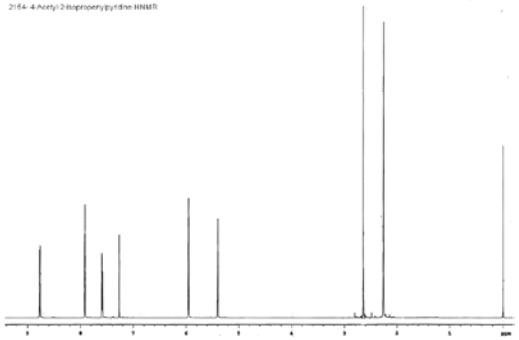
2153 2-Acetyl-4-isopropenylpyridine (MS)



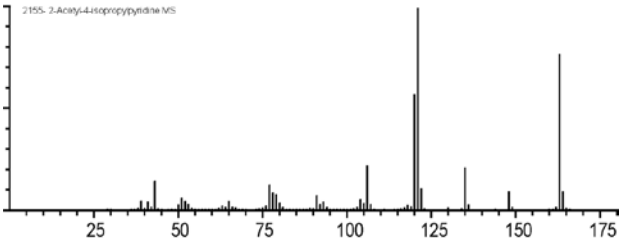
2154 4-Acetyl-2-isopropenylpyridine (MS)



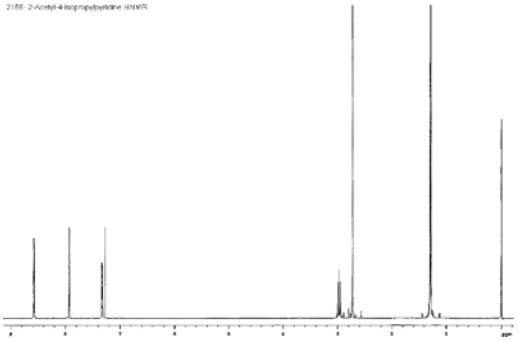
2154 4-Acetyl-2-isopropenylpyridine (1H-NMR)



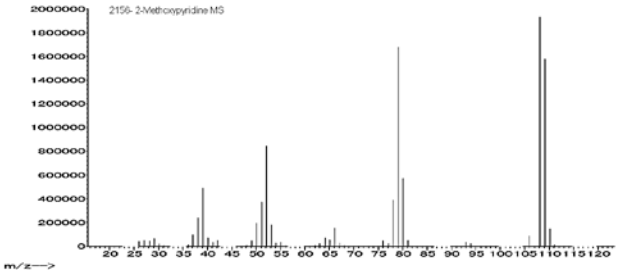
2155 2-Acetyl-4-isopropylpyridine (MS)



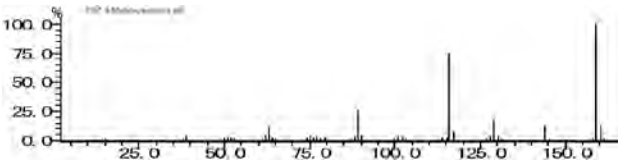
2155 2-Acetyl-4-isopropylpyridine (1H-NMR)



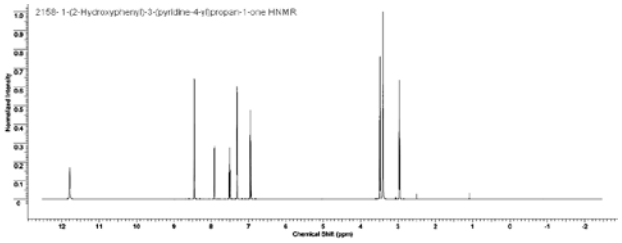
2156 2-Methoxypyridine



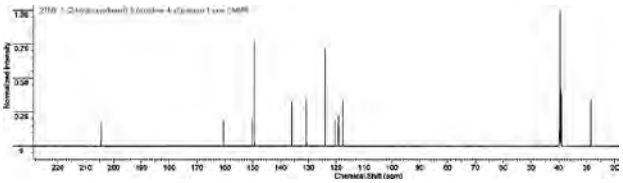
2157 6-Methoxyquinoline



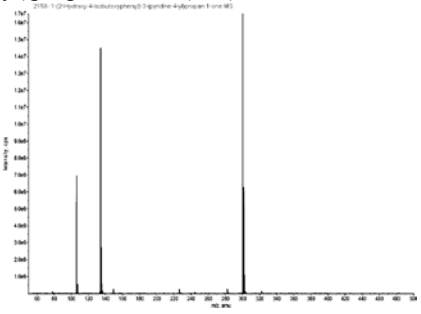
2158 1-(2-Hydroxyphenyl)-3-(pyridin-4-yl)propan-1-one (1H-NMR)



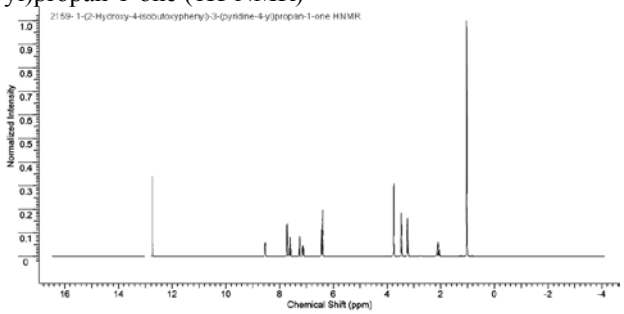
2158 1-(2-Hydroxyphenyl)-3-(pyridin-4-yl)propan-1-one (13C-HNMR)



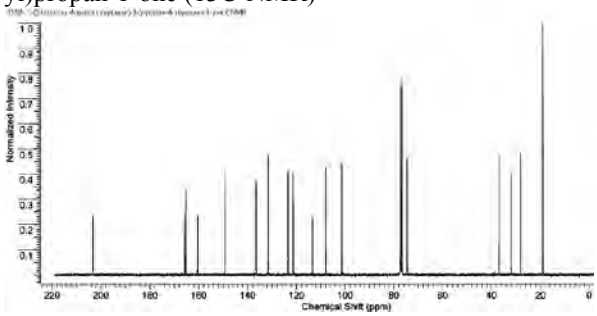
2159 1-(2-Hydroxy-4-isobutoxyphenyl)-3-(pyridin-2-yl)propan-1-one (MS)



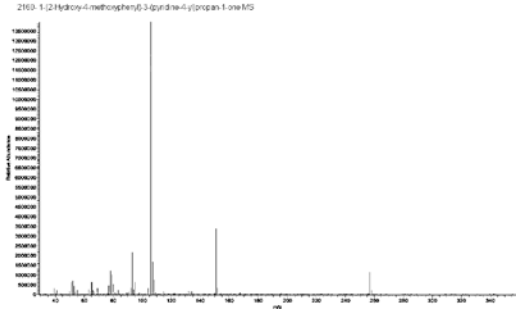
2159 1-(2-Hydroxy-4-isobutoxyphenyl)-3-(pyridin-2-yl)propan-1-one (1H-NMR)



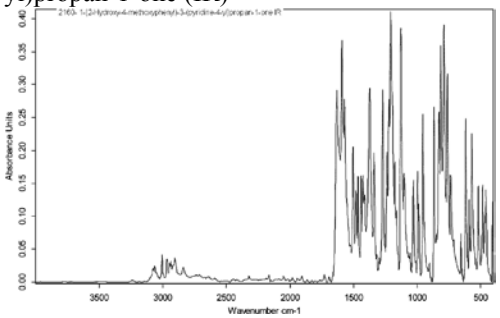
2159 1-(2-Hydroxy-4-isobutoxyphenyl)-3-(pyridin-2-yl)propan-1-one (13C-NMR)



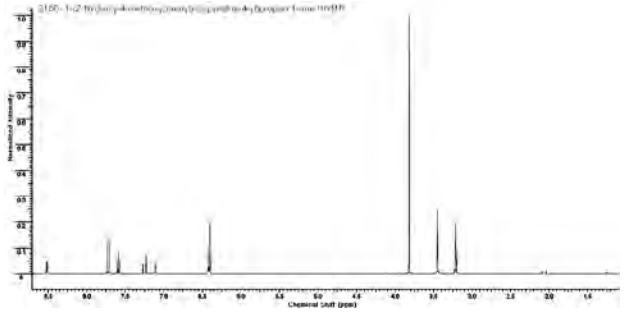
2160 1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridin-2-yl)propan-1-one (MS)



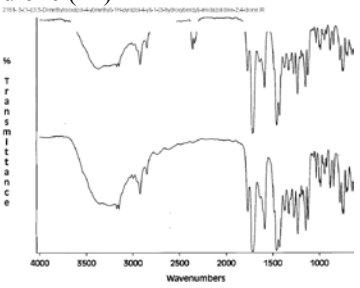
2160 1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridin-2-yl)propan-1-one (IR)



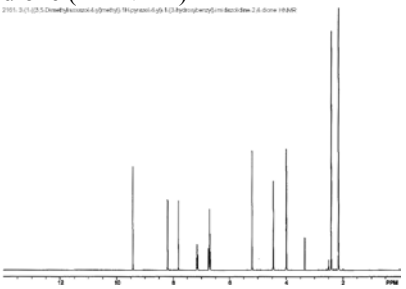
2160 1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridin-2-yl)propan-1-one (1H-NMR)



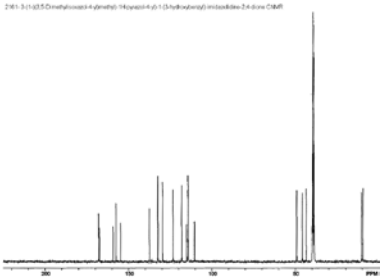
2161 3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione (IR)



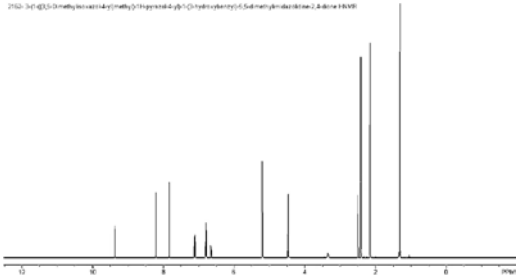
2161 3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione (1H-NMR)



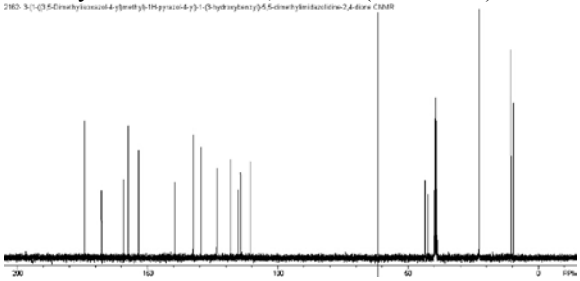
2161 3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione (13C-NMR)



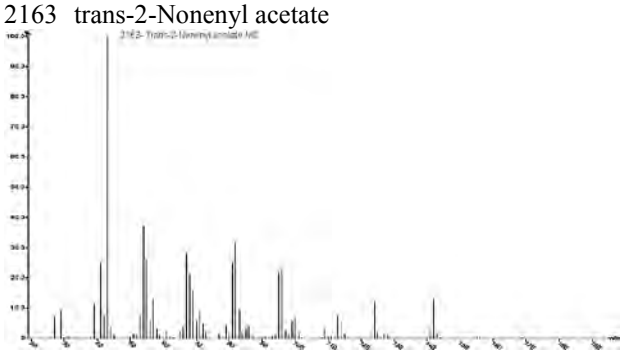
2162 3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-5,5-dimethylimidazolidine-2,4-dione (1H-NMR)



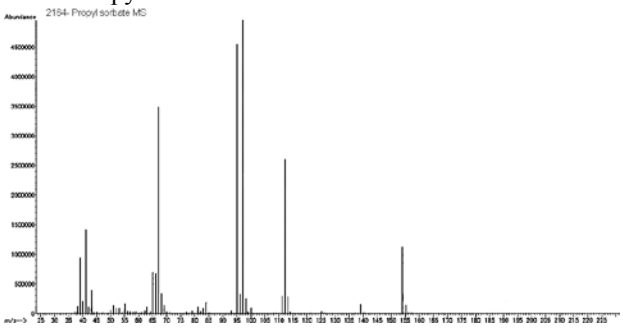
2162 3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-5,5-dimethylimidazolidine-2,4-dione (13C-NMR)



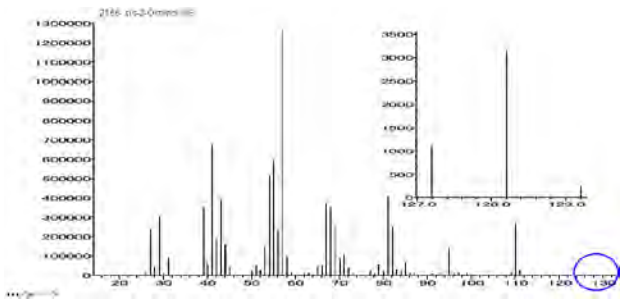
2163 trans-2-Nonenyl acetate



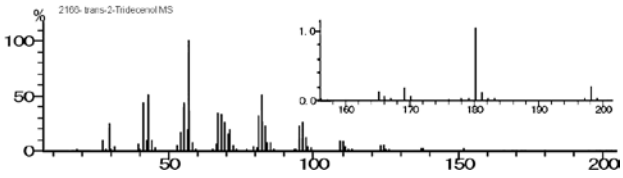
2164 Propyl sorbate



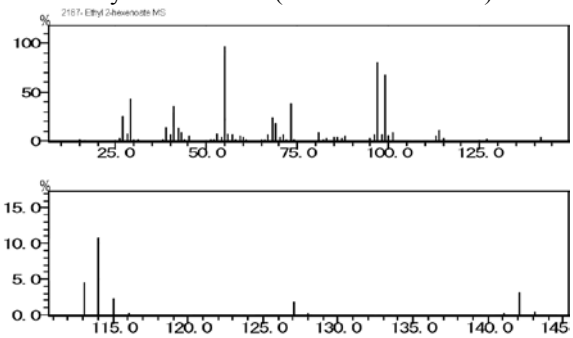
2165 cis-2-Octenol



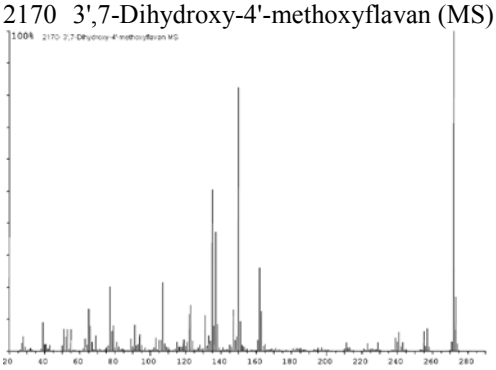
2166 trans-2-Tridecenol



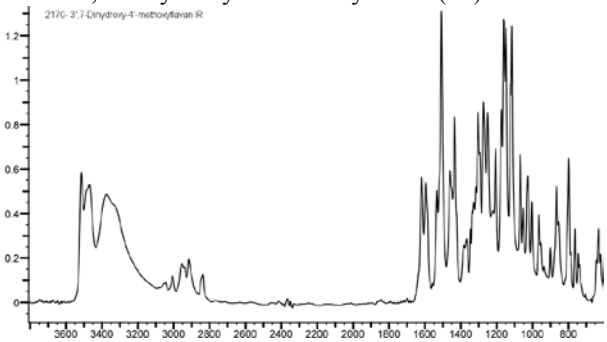
2167 Ethyl 2-hexenoate (mixture of isomers)



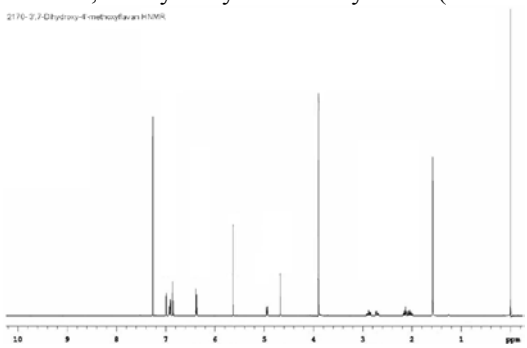
2170 3',7-Dihydroxy-4'-methoxyflavan (MS)



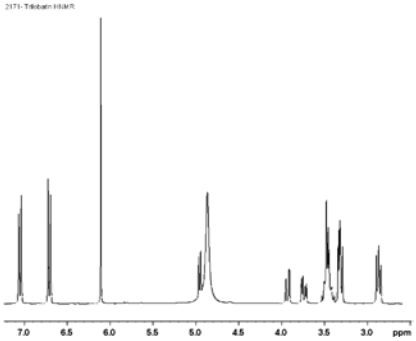
2170 3',7-Dihydroxy-4'-methoxyflavan (IR)



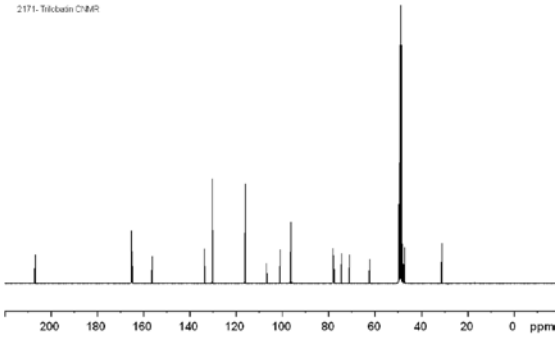
2170 3',7-Dihydroxy-4'-methoxyflavan (1H-NMR)



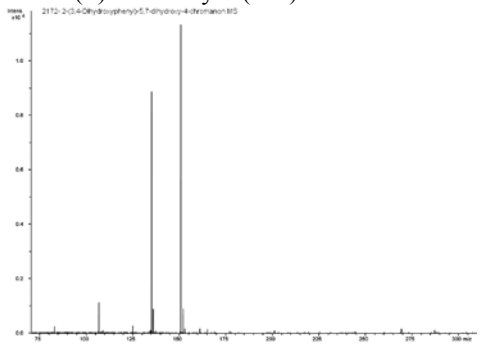
2171 Trilobatin (1H-NMR)



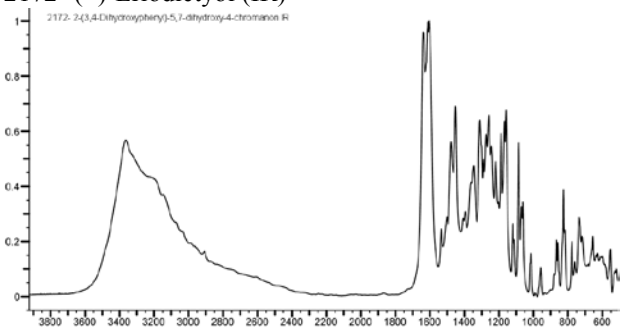
2171 Trilobatin (13C-NMR)



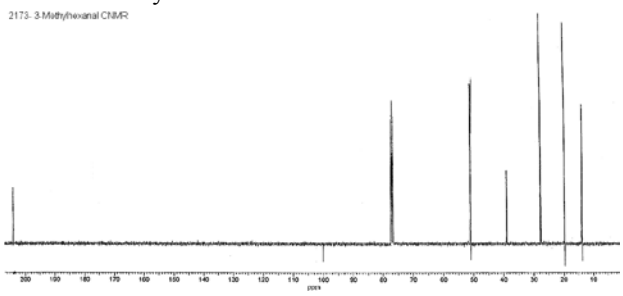
2172 (±)-Eriodictyol (MS)



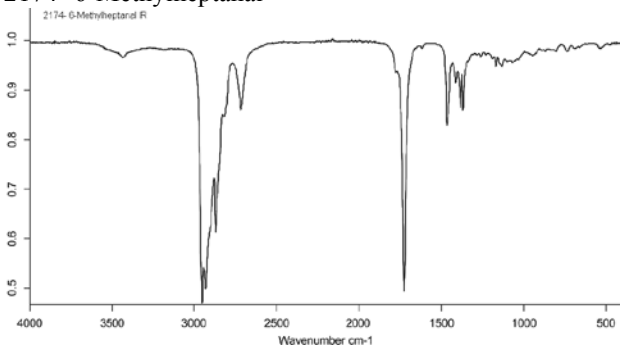
2172 (±)-Eriodictyol (IR)



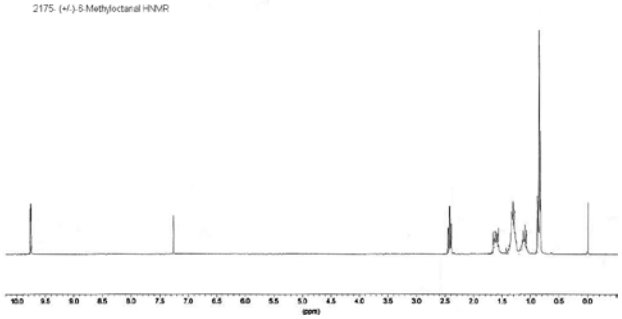
2173 3-Methylhexanal



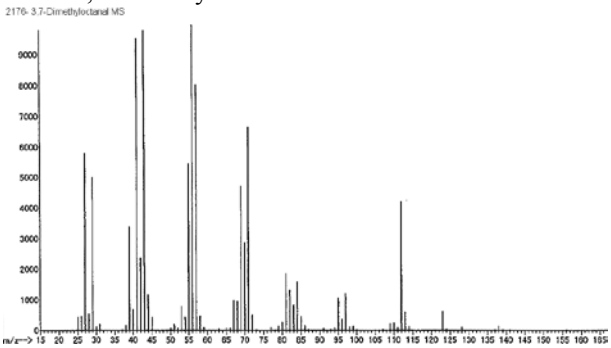
2174 6-Methylheptanal



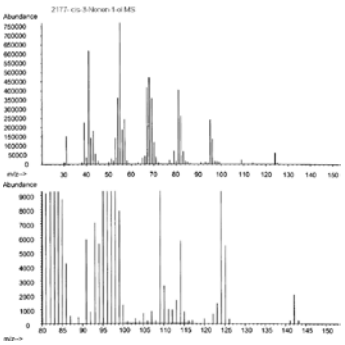
2175 6-Methyloctanal



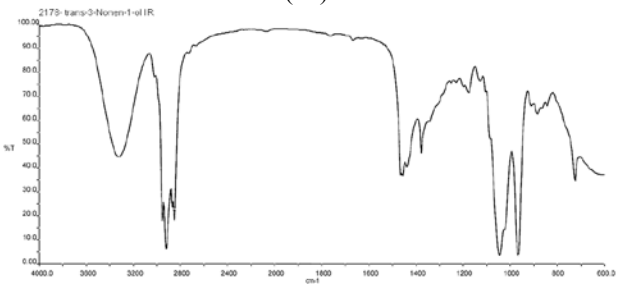
2176 3,7-Dimethyloctanal



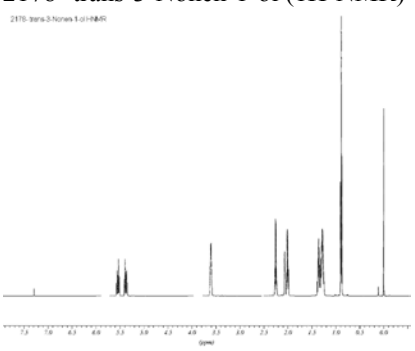
2177 cis-3-Nonen-1-ol



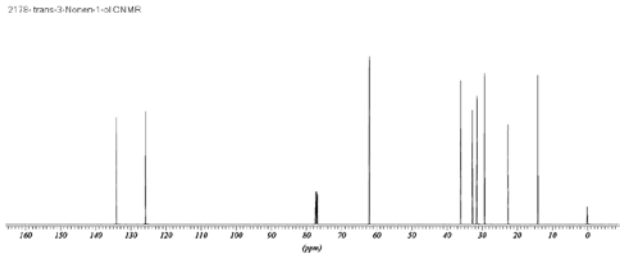
2178 trans-3-Nonen-1-ol (IR)



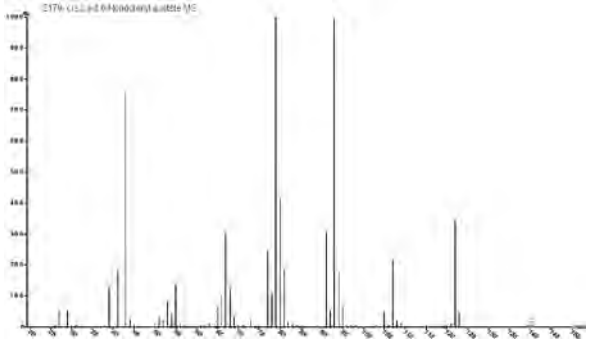
2178 trans-3-Nonen-1-ol (1H-NMR)



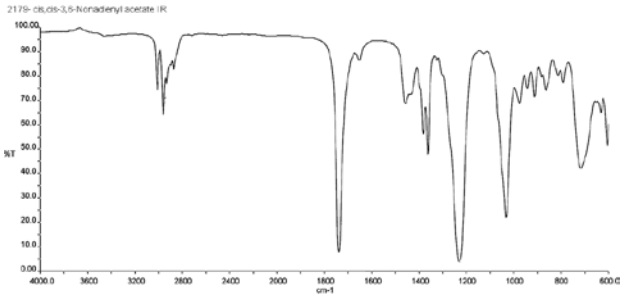
2178 trans-3-Nonen-1-ol (13C-NMR)



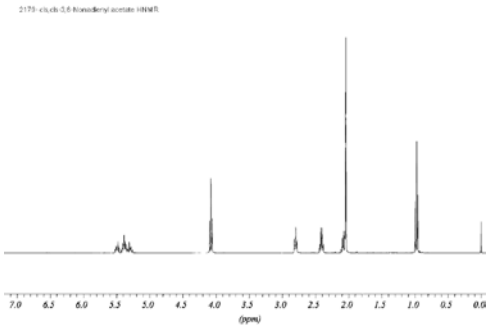
2179 cis,cis-3,6-Nonadienyl acetate (MS)



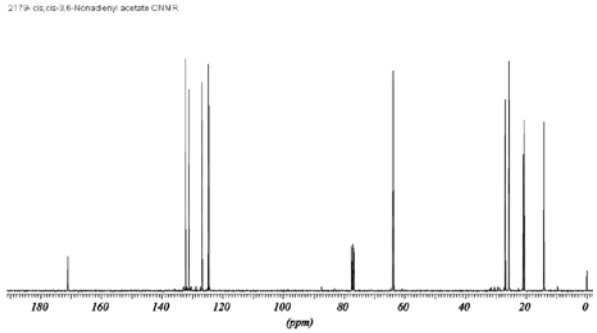
2179 cis,cis-3,6-Nonadienyl acetate (IR)



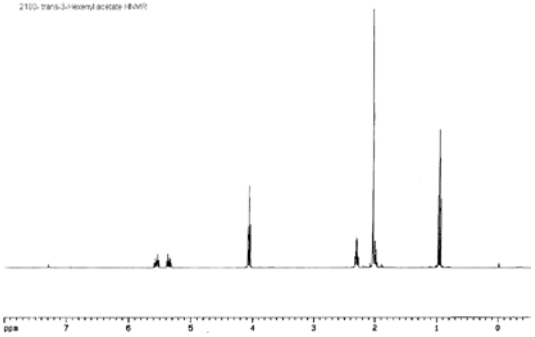
2179 cis,cis-3,6-Nonadienyl acetate (1H-NMR)



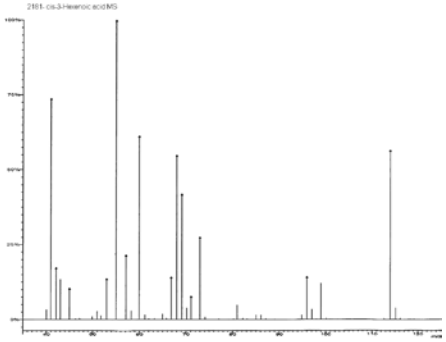
2179 cis,cis-3,6-Nonadienyl acetate (13C-NMR)



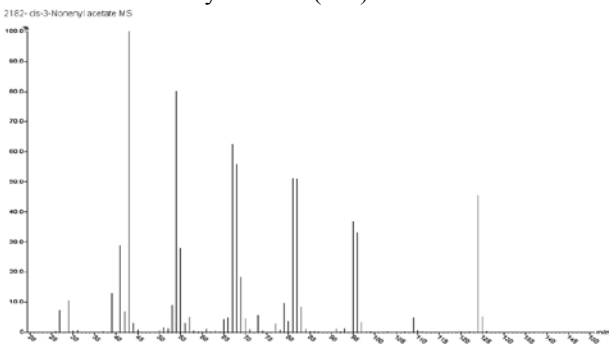
2180 trans-3-Hexenyl acetate



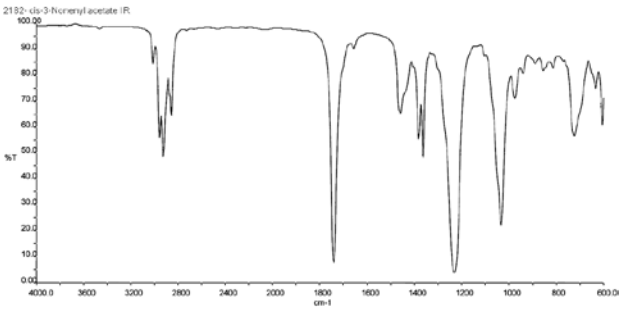
2181 cis-3-Hexenoic acid



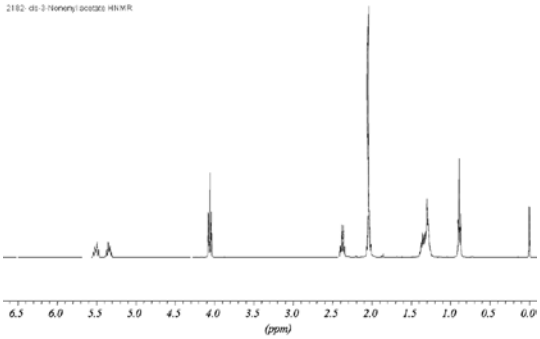
2182 cis-3-Nonenyl acetate (MS)



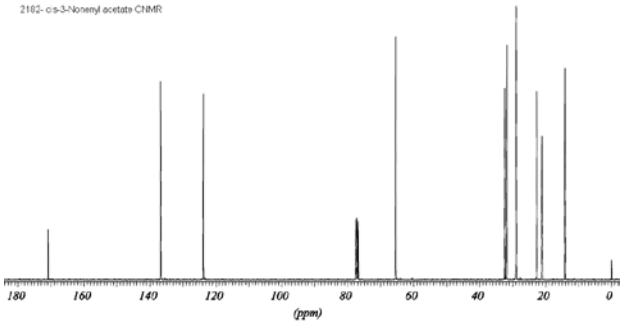
2182 cis-3-Nonenyl acetate (IR)



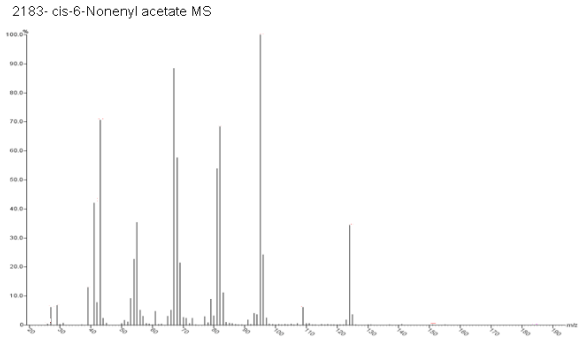
2182 cis-3-Nonenyl acetate (1H-NMR)



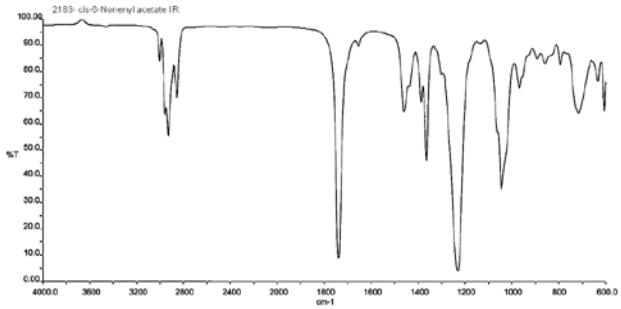
2182 cis-3-Nonenyl acetate (13C-NMR)



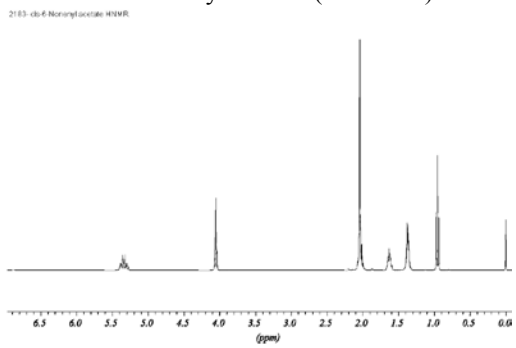
2183 cis-6-Nonenyl acetate (MS)



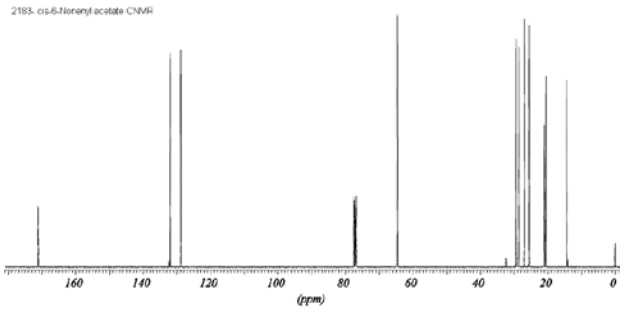
2183 cis-6-Nonenyl acetate (IR)



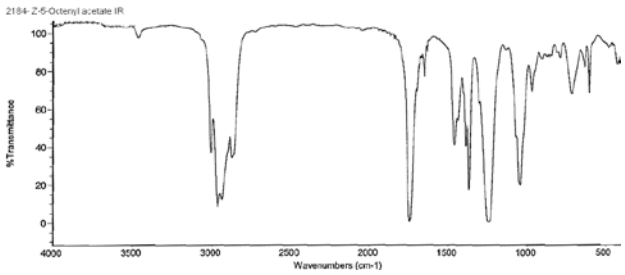
2183 cis-6-Nonenyl acetate (1H-NMR)



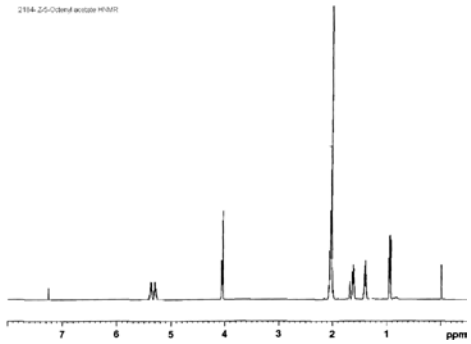
2183 cis-6-Nonenyl acetate (13C-NMR)



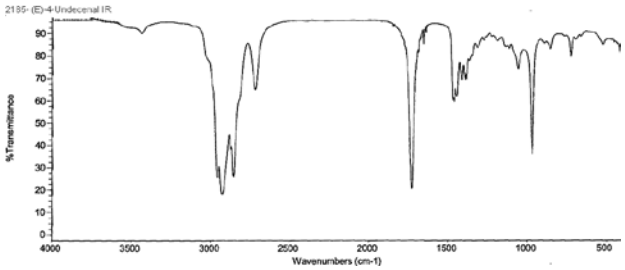
2184 (Z)-5-Octenyl acetate (IR)



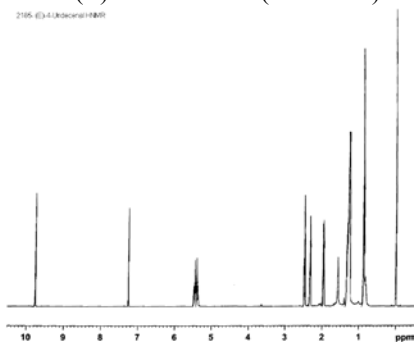
2184 (Z)-5-Octenyl acetate (1H-NMR)



2185 (E)-4-Undecenal (IR)



2185 (E)-4-Undecenal (1H-NMR)



List of new flavourings evaluated in alphabetical order

4-Acetyl-2-isopropenylpyridine	2154
2-Acetyl-4-isopropenylpyridine	2153
2-Acetyl-4-isopropylpyridine	2155
2-Acetyl-5-methylthiophene	2107
L-Alanyl-L-glutamine	2121
3[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-*N*-propylpropanamide	2082
(2*S*,5*R*)-*N*-[4-(2-Amino-2-oxoethyl)phenyl]-5- methyl-2-(propan-2-yl)cyclohexanecarboxamide	2078
4-Amino-5,6-dimethylthieno[2,3-d]pyrimidin-2(1H)-one hydrochloride	2117
2-Aminoacetophenone	2043
Butil β-naphthyl ether	2141
N-Cyclopropyl-5-methyl-2-isopropylcyclohexanecarboxamide	2080
Di-2-furylmethane	2104
Digeranyl ether	2142
3',7-Dihydroxy-4-methoxyflavan	2170
3,6-Dimethyl-2,3,3a,4,5,7ahexahydrobenzofuran	2133
3,5- and 3,6-Dimethyl-2-isobutylpyrazine	2130
4,5-Dimethyl-2-isobutylthiazole	2109
A ixture of 2,5-dimethyl-6,7-dihydro-5Hcyclopentapyrazine'and 2,7-dimethyl-6,7- dihydro-5H-cyclopentapyrazine	2128
3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1Hpyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione	2161
3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1Hpyrazol-4-yl)-1-(3-hydroxybenzyl)-5,5-dimethylimidazolidine-2,4-dione	2162
3,7-Dimethyloctanal	2176
2,4-Dimethylpyridine	2151
3,4-Dimethylthiophene	2110
2,3-Epoxydecanal	2149
2,3-Epoxyheptanal	2148
2,3-Epoxyoctanal	2147
(±)-Eriodictyol	2172
2-Ethoxy-3-ethylpyrazine 2	2131
2-Ethoxy-3-isopropylpyrazine	2065
Ethyl 2-mercapto-2-methylpropionate	2085
(*E*)-Ethyl 3-(2-furyl)acrylate	2103
Ethyl linalyl ether	2134
Ethyl α-ethyl- β-methyl- β-phenylglycidate	2143
5-Ethyl-2,3-dimethylpyrazine	2126
2-Ethyl-2,5-dihydro-4-methylthiazole	2114

5-Ethyl-2-methylthiazole	2113
1-Ethyl-2-pyrrolecarboxaldehyde	2150
-Ethyl-3-methylthiopyrazine	2132
2-Ethyl-4,6-dimethyldihydro-1,3,5-dithiazine	2116
Ethyl 2-hexenoate (mixture of isomers)	2167
Furfural propyleneglycol acetal	2100
Furfuryl decanoate	2102
Furfuryl formate	2101
1-(2-Furfurylthio)-propanone	2096
Glutamyl-valyl-glycine	2123
cis-3-Hexenoic acid	2181
trans-3-Hexenyl acetate	2180
1-(2-Hydroxy-4-isobutoxyphenyl)-3- (pyridine-2-yl)propan-1-one N	2159
1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridine-2-yl)propan-1-one	2160
1-(2-Hydroxyphenyl)-3-(pyridine-4-yl)propan-1-one	2158
Isoamyl phenethyl ether	2136
L-Isoleucine	2118
Isopropenylpyrazine	2125
5-Isopropyl-2,6-diethyl-2- methyltetrahydro-2H-pyran	2140
Linalool oxide pyranoid	2135
d-8-*p*-Menthene-1,2-epoxide	2145
l-8-*p*-Menthene-1,2-epoxide	2146
4-Mercapto-3-methyl-2-butanol	2084
L-Methionylglycine	2122
(1*R*,2*S*,5*R*)-*N*-(4-Methoxyphenyl)-5-methyl-2-(1- methylethyl)cyclohexanecarboxamide	2079
2-Methoxypyridine	2156
6-Methoxyquinoline	2157
Methyl 3-(furfurylthio)propionate	2094
Methyl hexyl ether	2138
Methyl β-phenylglycidate	2144
1-Methyl-1H-pyrrole-2-carboxaldehyde	2152
4-Methyl-2-propyl-1,3-oxathiane	2089
2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulfide	2092
2-Methyl-3-furyl methylthiomethyl disulfide	2091
3-[(2-Methyl-3-furyl)thio]butanal	2095
4-Methyl-3-thiazoline	2115
2-Methyl-4,5-dihydrofuran-3-thiol	2097
2-Methyl-5-vinylpyrazine	2127
2-Methylbenzofuran	2105
N-(2-Methylcyclohexyl)-2,3,4,5,6-Pentafluorobenzamide	2081

1-Methyldithio-2-propanone	2088
5-Methylfurfuryl alcohol	2099
5-Methylfurfuryl mercaptan	2090
6-Methylheptanal	2174
3-Methylhexanal	2173
6-Methyloctanal	2175
(2*E*,6*E*/*Z*,8*E*)-*N*-(2-Methylpropyl)-2,6,8-decatrienamide	2077
2-Methyltetrahydrofuran-3-thiol acetate	2098
1-(Methylthio)-3-octanone	2086
Myrcenyl methyl ether	2139
Nerolidol oxide	2137
cis,*cis*-3,6-Nonadienyl acetate	2179
cis-3-Nonen-1-ol	2177
trans-3-Nonen-1-ol	2178
cis-3-Nonenyl acetate	2182
cis-6-Nonenyl acetate	2183
trans-2-Nonenyl acetate	2163
cis-2-Octenol	2165
(*Z*)-5-Octenyl acetate	2184
L-Ornithine (as the monochlorohydrate)	2120
3-Pentanethiol	2083
2-Pentylthiazole	2108
2-Pentylthiophene	2106
1,1-Propanedithiol	2087
N Propyl sorbate	2164
2-Tetrahydrofurfuryl 2-mercaptopropionate	2093
1-(2-Thienyl)ethanethiol	2112
2-Thienylmethanol	2111
L-Threonine	2119
trans-2-Tridecenol	2166
Trilobatin	2171
(*E*)-4-Undecenal	2185

ANNEX 1. SUMMARY OF RECOMMENDATIONS FROM THE 76th JECFA

Toxicological information and information on specifications

Food additives considered for specifications only

Food additive	Specifications[a]
Ethyl cellulose	R Mineral oil
(medium viscosity)	N[b] Modified
starches	R Titanium
dioxide	R

[a] N, new specifications; R, existing specifications revised.
[b] The existing specifications for mineral oil (medium and low viscosity) were withdrawn (see below).

Food additives evaluated toxicologically and assessed for dietary exposure

Food additive	Specifications[a]	Acceptable or tolerable daily intakes and other toxicological recommendations
Magnesium dihydrogen diphosphate	N	Although an acceptable daily intake (ADI) "not specified"[b] has been established for a number of magnesium salts used as food additives, the estimated chronic dietary exposures to magnesium (960 mg/day for a 60 kg adult at the 95th percentile) from the proposed uses of magnesium dihydrogen diphosphate are up to twice the background exposures from food previously noted by the Committee (180–480 mg/day) and in the region of the minimum laxative effective dose of approximately 1000 mg of magnesium when taken as a single dose. The estimates of dietary exposure to phosphorus from the proposed uses of magnesium dihydrogen diphosphate were in the region of, or slightly exceeded, the maximum tolerable daily intake (MTDI) of 70 mg/kg body weight (bw) for phosphate salts, expressed as phosphorus, from this source alone. Thus, the MTDI is further exceeded when other sources of phosphate in the diet are taken into account. **The Committee therefore concluded that the proposed use levels and food categories result in an estimated dietary exposure to magnesium dihydrogen diphosphate that is of potential concern.** **The Committee emphasized that in evaluating individual phosphate-containing food additives, there is a need for assessment of total dietary exposure to phosphorus.** **The Committee recommended that total dietary exposure to magnesium from food additives and other sources in the diet should be assessed.** The information submitted to the Committee and in the scientific literature did not indicate that the MTDI of 70 mg/kg bw for phosphate salts, expressed as phosphorus, is insufficiently health protective. On the contrary, because the basis for its derivation might not be relevant to humans, it could be overly conservative. Therefore, **the Committee recommended that the toxicological basis of the MTDI for phosphate salts expressed as phosphorus be reviewed.**

Food additive	Specifications[a]	Acceptable or tolerable daily intakes and other toxicological recommendations
Mineral oil (medium and low viscosity) classes II and III	W	**The Committee concluded that the newly submitted data did not adequately address its previous requests for information** on the relevance to humans of the response of F344 and Sprague-Dawley rats to mineral oil (medium and low viscosity) classes II and III. The studies were conducted with a single administration, and it was not possible to predict the concentration in the target organ (liver) at steady state, or the potential for accumulation, in humans. Information requested at the forty-fourth meeting on compositional factors of mineral oils that influence absorption and toxicity had not been provided for materials meeting the criteria of mineral oil (medium and low viscosity) classes II and III. The Committee noted that hydrocarbon deposits with carbon numbers consistent with mineral oils, including those of classes II and III, and associated lesions have been reported in human tissues, demonstrating the potential relevance to humans of the effects in the F344 rat. Because all blood levels were below the limit of detection in the single-dose human toxicokinetic study, it was not possible to reach conclusions on the rate of elimination of mineral oils in humans or on the concentration in the liver at steady state following prolonged exposure. Therefore, the new data did not provide information that would allow an ADI to be established based on internal exposure. Similarly, it was not possible to establish an ADI based on external dose in the absence of information on the relative accumulation potential of classes II and III mineral oils in humans compared with rats. The Committee noted that the temporary group ADI for mineral oil (medium and low viscosity) classes II and III had been established in 1995 and extended on a number of occasions. As data supporting the establishment of a full ADI had not been made available, **the previously established temporary group ADI was withdrawn.**
3-Phytase from *Aspergillus niger* expressed in *Aspergillus niger*	N	Comparing the conservative exposure estimate with the no-observed-adverse-effect level (NOAEL) from the 13-week study of oral toxicity in rats, the margin of exposure is approximately 250. **The Committee allocated an ADI "not specified"[b] for 3-phytase enzyme preparation from *A. niger* expressed in *A. niger* used in the applications specified and in accordance with good manufacturing practice.**
Serine protease (chymotrypsin) from *Nocardiopsis prasina* expressed in *Bacillus licheniformis*	N	Comparing the exposure estimate with the NOAEL from the 13-week study of oral toxicity in rats, the margin of exposure is approximately 350. **The Committee allocated an ADI "not specified"[b] for serine protease (chymotrypsin) enzyme preparation from *N. prasina* expressed in the production strain *B. licheniformis*, used in the applications specified and in accordance with good manufacturing practice.**

Food additive	Specifications[a]	Acceptable or tolerable daily intakes and other toxicological recommendations
Serine protease (trypsin) from *Fusarium oxysporum* expressed in *Fusarium venenatum*	N	Comparing the dietary exposure estimate with the NOAEL from the 13-week study of oral toxicity in rats, the margin of exposure is approximately 1200. **The Committee allocated an ADI "not specified"[b] for serine protease (trypsin) enzyme preparation from *F. oxysporum* expressed in the production strain *F. venenatum*, used in the applications specified and in accordance with good manufacturing practice.**

[a] N, new specifications; W, existing specifications withdrawn.

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

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

A. Aliphatic and aromatic amines and amides

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
2-Aminoacetophenone	2043	N	No safety concern
Structural class III			
(2*E*,6*E*/*Z*,8*E*)-*N*-(2-Methylpropyl)-2,6,8-decatrienamide	2077	N	No safety concern
(2*S*,5*R*)-*N*-[4-(2-Amino-2-oxoethyl)phenyl]-5-methyl-2-(propan-2-yl)cyclohexanecarboxamide	2078	N	No safety concern
(1*R*,2*S*,5*R*)-*N*-(4-Methoxyphenyl)-5-methyl-2-(1-methylethyl)cyclohexanecarboxamide	2079	N	No safety concern
N-Cyclopropyl-5-methyl-2-isopropylcyclohexanecarboxamide	2080	N	No safety concern

[1] The flavouring agent **2-phenyl-2-methyl-2-hexenal (No. 2069)** was submitted for evaluation in the group of aliphatic linear α,β-unsaturated aldehydes, acids and related alcohols, acetals and esters; the Committee considered that it did not belong to this group of flavouring agents, and therefore it was not further considered. The safety of the submitted substance **(3*R*)-4-[[(1*S*)-1-benzyl-2-methoxy-2-oxo-ethyl]amino]-3-[3-(3-hydroxy-4-methoxy-phenyl)propylamino]-4-oxo-butanoic acid hydrate (Advantame, No. 2124)** in the group of amino acids and related substances was not assessed; the Committee decided that it would not be appropriate to evaluate this substance as a flavouring agent, because it is a low-calorie intense sweetener. The safety of the two submitted substances **rebaudioside C (No. 2168)** and **rebaudioside A (No. 2169)** in the group of phenol and phenol derivatives was not assessed; the Committee decided that it would not be appropriate to evaluate these substances as flavouring agents, as they had already been evaluated as food additives (sweeteners).

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
N-(2-Methylcyclohexyl)-2,3,4,5,6-pentafluorobenzamide	2081	N	No safety concern
3[(4-Amino-2,2-dioxido-1H-2,1,3-benzothiadiazin-5-yl)oxy]-2,2-dimethyl-*N*-propylpropanamide	2082	N	No safety concern

[a] N, new specifications.

B. Aliphatic and aromatic ethers

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
3,6-Dimethyl-2,3,3a,4,5,7a-hexahydrobenzofuran	2133	N	No safety concern
Ethyl linalyl ether	2134	N	No safety concern
Linalool oxide pyranoid	2135	N	No safety concern
Nerolidol oxide	2137	N	**Additional data required to complete evaluation**
Methyl hexyl ether	2138	N	No safety concern
Myrcenyl methyl ether	2139	N	No safety concern
Digeranyl ether	2142	N	No safety concern
Structural class III			
Isoamyl phenethyl ether	2136	N	No safety concern
5-Isopropyl-2,6-diethyl-2-methyltetrahydro-2H-pyran	2140	N	No safety concern
Butyl β-naphthyl ether	2141	N	No safety concern

[a] N, new specifications.

C. Aliphatic hydrocarbons, alcohols, aldehydes, ketones, carboxylic acids and related esters, sulfides, disulfides and ethers containing furan substitution

The Committee concluded that the Procedure could not be applied to this group because of unresolved toxicological concerns. Studies that could assist in the safety evaluation include investigations of the influence of the nature and position of furan ring substitutions on metabolism and covalent binding to macromolecules, demonstration of the ring opening and reactivity of the resulting products. Depending on the findings, additional genotoxicity or other studies might be needed.

Flavouring agent	No.	Specifications[a]
2-Pentylfuran	1491	M
2-Heptylfuran	1492	M
2-Decylfuran	1493	M
3-Methyl-2-(3-methylbut-2-enyl)-furan	1494	M
3-(2-Furyl)acrolein	1497	M
3-(5-Methyl-2-furyl)prop-2-enal	1499	M
2-Furyl methyl ketone	1503	M
2-Acetyl-5-methylfuran	1504	M

Flavouring agent	No.	Specifications[a]
2-Acetyl-3,5-dimethylfuran	1505	M
2-Butyrylfuran	1507	M
(2-Furyl)-2-propanone	1508	M
2-Pentanoylfuran	1509	M
1-(2-Furyl)butan-3-one	1510	M
4-(2-Furyl)-3-buten-2-one	1511	M
Ethyl 3-(2-furyl)propanoate	1513	M
Isobutyl 3-(2-furan)propionate	1514	M
Isoamyl 3-(2-furan)propionate	1515	M
Isoamyl 4-(2-furan)butyrate	1516	M
Phenethyl 2-furoate	1517	M
Furfuryl methyl ether	1520	M
Ethyl furfuryl ether	1521	M
Difurfuryl ether	1522	M
2,5-Dimethyl-3-furanthiol acetate	1523	M
Furfuryl 2-methyl-3-furyl disulfide	1524	M
3-[(2-Methyl-3-furyl)thio]-2-butanone	1525	M
O-Ethyl S-(2-furylmethyl)thiocarbonate	1526	M
2,3-Dimethylbenzofuran	1495	M
2,4-Difurfurylfuran	1496	M
2-Methyl-3(2-furyl)acrolein	1498	M
3-(5-Methyl-2-furyl)-butanal	1500	M
2-Furfurylidene-butyraldehyde	1501	M
2-Phenyl-3-(2-furyl)prop-2-enal	1502	M
3-Acetyl-2,5-dimethylfuran	1506	M
Pentyl 2-furyl ketone	1512	M
Propyl 2-furanacrylate	1518	M
2,5-Dimethyl-3-oxo-(2H)-fur-4-yl butyrate	1519	M
(*E*)-Ethyl 3-(2-furyl)acrylate	2103	N
Di-2-furylmethane	2104	N
2-Methylbenzofuran	2105	N

[a] M, specifications maintained; N, new specifications.

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

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
trans-2-Nonenyl acetate	2163	N	No safety concern
Propyl sorbate	2164	N	No safety concern
cis-2-Octenol	2165	N	No safety concern
trans-2-Tridecenol	2166	N	No safety concern
Ethyl 2-hexenoate (mixture of isomers)	2167	N	No safety concern

[a] N, new specifications.

E. Amino acids and related substances

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
L-Ornithine (as the monochlorohydrate)	2120	N	No safety concern
L-Alanyl-L-glutamine	2121	N	No safety concern
L-Methionylglycine	2122	N	No safety concern
Glutamyl-valyl-glycine	2123	N	No safety concern

[a] N, new specifications.

The Committee considered that the use of the Procedure for the Safety Evaluation of Flavouring Agents was inappropriate for two members of this group—namely, L-isoleucine (No. 2118) and L-threonine (No. 2119). In view of the fact that these substances are macronutrients and normal components of protein, the Committee concluded that the use of these substances as flavouring agents would not raise any safety concerns at current estimated dietary exposures.

Flavouring agent	No.	Specifications[a]
L-Isoleucine	2118	N
L-Threonine	2119	N

[a] N, new specifications.

F. Epoxides

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III			
Ethyl α-ethyl-β-methyl-β-phenylglycidate	2143	N	No safety concern
Methyl β-phenylglycidate	2144	N	No safety concern
d-8-*p*-Menthene-1,2-epoxide	2145	N	No safety concern
l-8-*p*-Menthene-1,2-epoxide	2146	N	No safety concern
2,3-Epoxyoctanal	2147	N	**Additional data required to complete evaluation**
2,3-Epoxyheptanal	2148	N	**Additional data required to complete evaluation**
2,3-Epoxydecanal	2149	N	**Additional data required to complete evaluation**

[a] N, new specifications.

G. Furfuryl alcohol and related substances

New in vitro and in vivo studies raise concerns regarding the potential genotoxicity of furfuryl alcohol and derivatives that can be metabolized to furfuryl alcohol (e.g. furfuryl esters). The Committee concluded that this group of flavouring agents could not be evaluated according to the Procedure because of the unresolved concerns regarding genotoxicity. In addition, the group ADI previously established by the Committee will need to be reconsidered at a future meeting.

Flavouring agent	No.	Specifications[a]
5-Methylfurfuryl alcohol	2099	N
Furfural propyleneglycol acetal	2100	N
Furfuryl formate	2101	N
Furfuryl decanoate	2102	N

[a] N, new specifications.

H. Linear and branched-chain aliphatic, unsaturated, unconjugated alcohols, aldehydes, acids and related esters

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
cis-3-Nonen-1-ol	2177	N	No safety concern
trans-3-Nonen-1-ol	2178	N	No safety concern
cis,*cis*-3,6-Nonadienyl acetate	2179	N	No safety concern
trans-3-Hexenyl acetate	2180	N	No safety concern
cis-3-Hexenoic acid	2181	N	No safety concern
cis-3-Nonenyl acetate	2182	N	No safety concern
cis-6-Nonenyl acetate	2183	N	No safety concern
(*Z*)-5-Octenyl acetate	2184	N	No safety concern
(*E*)-4-Undecenal	2185	N	No safety concern

[a] N, new specifications.

I. Miscellaneous nitrogen-containing compounds

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-imidazolidine-2,4-dione	2161	N	No safety concern
3-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-pyrazol-4-yl)-1-(3-hydroxybenzyl)-5,5-dimethylimidazolidine-2,4-dione	2162	N	No safety concern

[a] N, new specifications.

J. Phenol and phenol derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III			
3′,7-Dihydroxy-4′-methoxyflavan	2170	N	No safety concern
Trilobatin	2171	N	No safety concern
(±)-Eriodictyol	2172	N	No safety concern

[a] N, new specifications.

K. Pyrazine derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
Isopropenylpyrazine	2125	N	No safety concern
5-Ethyl-2,3-dimethylpyrazine	2126	N	No safety concern
2-Methyl-5-vinylpyrazine	2127	N	No safety concern
A mixture of 2,5-dimethyl-6,7-dihydro-5H-cyclopentapyrazine and 2,7-dimethyl-6,7-dihydro-5H-cyclopentapyrazine	2128	N	No safety concern
2-Ethoxy-3-isopropylpyrazine	2065	N	No safety concern
Structural class III			
3,5- and 3,6-Dimethyl-2-isobutylpyrazine	2130	N	No safety concern
2-Ethoxy-3-ethylpyrazine	2131	N	No safety concern
2-Ethyl-3-methylthiopyrazine	2132	N	No safety concern

[a] N, new specifications.

L. Pyridine, pyrrole and quinoline and related N-heterocyclic derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
1-Ethyl-2-pyrrolecarboxaldehyde	2150	N	**Additional data required to complete evaluation**
2,4-Dimethylpyridine	2151	N	No safety concern (temporary)[b]
1-Methyl-1H-pyrrole-2-carboxaldehyde	2152	N	**Additional data required to complete evaluation**
Structural class III			
2-Acetyl-4-isopropenylpyridine	2153	T	No safety concern
4-Acetyl-2-isopropenylpyridine	2154	T	No safety concern
2-Acetyl-4-isopropylpyridine	2155	N	No safety concern
2-Methoxypyridine	2156	N	**Additional data required to complete evaluation**
6-Methoxyquinoline	2157	N	No safety concern
1-(2-Hydroxyphenyl)-3-(pyridine-4-yl)propan-1-one	2158	N	**Additional data required to complete evaluation**
1-(2-Hydroxy-4-isobutoxyphenyl)-3-(pyridine-2-yl)propan-1-one	2159	N	**Additional data required to complete evaluation**
1-(2-Hydroxy-4-methoxyphenyl)-3-(pyridine-2-yl)propan-1-one	2160	N	**Additional data required to complete evaluation**

[a] N, new specifications; T, tentative specifications.
[b] The evaluation for No. 2151 is temporary pending receipt of additional toxicological data.

M. Saturated aliphatic acyclic branched-chain primary alcohols, aldehydes and acids

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class I			
3-Methylhexanal	2173	N	No safety concern
6-Methylheptanal	2174	N	No safety concern
6-Methyloctanal	2175	N	No safety concern
3,7-Dimethyloctanal	2176	N	No safety concern

[a] N, new specifications.

N. Simple aliphatic and aromatic sulfides and thiols

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Subgroup ii: Acyclic sulfides with oxidized side-chains			
Structural class I			
1-(Methylthio)-3-octanone	2086	N	No safety concern
Subgroup iii: Cyclic sulfides			
Structural class III			
4-Methyl-2-propyl-1,3-oxathiane	2089	N	No safety concern
Subgroup iv: Simple thiols			
Structural class I			
3-Pentanethiol	2083	N	No safety concern
Subgroup v: Thiols with oxidized side-chains			
Structural class I			
4-Mercapto-3-methyl-2-butanol	2084	N	No safety concern
Ethyl 2-mercapto-2-methylpropionate	2085	N	No safety concern
Subgroup vi: Dithiols			
Structural class III			
1,1-Propanedithiol	2087	N	No safety concern
Subgroup viii: Disulfides with oxidized side-chains			
Structural class III			
1-Methyldithio-2-propanone	2088	N	No safety concern

[a] N, new specifications.

O. Sulfur-containing heterocyclic compounds

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class II			
2-Pentylthiophene	2106	N	No safety concern
2-Acetyl-5-methylthiophene	2107	N	No safety concern

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
2-Pentylthiazole	2108	N	No safety concern
4,5-Dimethyl-2-isobutylthiazole	2109	N	No safety concern
Structural class III			
3,4-Dimethylthiophene	2110	N	No safety concern
2-Thienylmethanol	2111	N	No safety concern
1-(2-Thienyl)ethanethiol	2112	N	No safety concern
5-Ethyl-2-methylthiazole	2113	N	No safety concern
2-Ethyl-2,5-dihydro-4-methylthiazole	2114	N	No safety concern
4-Methyl-3-thiazoline	2115	N	No safety concern
2-Ethyl-4,6-dimethyldihydro-1,3,5-dithiazine	2116	N	No safety concern
4-Amino-5,6-dimethylthieno[2,3-d]pyrimidin-2(1H)-one hydrochloride	2117	N	No safety concern

[a] N, new specifications.

P. Sulfur-substituted furan derivatives

Flavouring agent	No.	Specifications[a]	Conclusion based on current estimated dietary exposure
Structural class III			
5-Methylfurfuryl mercaptan	2090	N	No safety concern
2-Methyl-3-furyl methylthiomethyl disulfide	2091	N	No safety concern
2-Methyl-3-furyl 2-methyl-3-tetrahydrofuryl disulfide	2092	N	No safety concern

2-Tetrahydrofurfuryl 2-mercaptopropionate	2093	N	**Additional data required to complete evaluation**
Methyl 3-(furfurylthio)propionate	2094	N	No safety concern
3-[(2-Methyl-3-furyl)thio]butanal	2095	N	No safety concern
1-(2-Furfurylthio)-propanone	2096	N	No safety concern
2-Methyl-4,5-dihydrofuran-3-thiol	2097	N	No safety concern
2-Methyltetrahydrofuran-3-thiol acetate	2098	N	No safety concern

[a] N, new specifications.

General considerations

Statement on the inclusion of secondary additives in a specifications monograph

Some food additives may require the addition of one or more secondary additives to ensure their stability and effective use in foods. Examples may include, but are not limited to, the use of antioxidants or preservatives to promote the stability of a primary additive or anti- caking agents, diluents or emulsifiers to ensure its technological function. In cases where the Committee has considered the use of a secondary additive or class of additives with a particular technological purpose to be appropriate, a short statement allowing for the addition of secondary additives will be included in the definition section of the specifications monograph.

Accordingly, any secondary additive must have been determined to be safe for use in food by the Committee. They should be of food-grade quality and used at the minimum level required to achieve the intended technological function.

Analytical method for the determination of phosphorus as phosphorus pentoxide

The Committee at its current meeting noted that the titrimetric and gravimetric methods in the *Combined Compendium of Food Additive Specifications*, Volume 4 (FAO JECFA Monographs 1, 2006), are not reliable for the determination of phosphorus as phosphorus pentoxide. The Committee may consider replacing corresponding methods for other diphosphate additives at a future meeting.

Food additives containing aluminium and/or silicon

The Committee, while reviewing the specifications of food additives containing aluminium and silicon, considered it relevant to update the test methods for the determination of aluminium oxide and silicon dioxide. Some of the test methods for certain of these food additives use potentially corrosive or hazardous reagents that are not always permitted in current laboratory practices because of safety concerns. The Committee also noted that the specifications for some additives were rather old or tentative and that it requires additional information to revise the specifications. Consequently, the Committee recommends placing these additives on the agenda for re-evaluation.

Test methods for modified starches

In addition to revising the specific test for degree of substitution of starch sodium octenylsuccinate (INS No. 1450) in the specifications monograph of modified starches, the Committee considered that it would be necessary to align the description of the test to be consistent with the end product specifications at a future meeting. In addition, the Committee considered that it would also be necessary to revise the specifications for all the modified starches, including test methods.

Improvements to the submission of specifications data for flavouring agents

The Committee at its current meeting made recommendations to improve the quality of data submitted for flavouring agents. These include submission of raw data (e.g. spectra, molecular structure, composition of isomers, physical and chemical properties, and method for determination of minimum assay) used to establish the specifications for each flavouring agent at submission. In addition, tabulated summary data (e.g. spreadsheet) for all the flavouring agents should be provided. It is strongly recommended that for each flavouring agent, the following spectra, with detailed experimental conditions, be provided: nuclear magnetic resonance spectrometry, Fourier-transform infrared spectroscopy and mass spectrometry. Spectra should be of such quality that they can be used for identification purposes. Data provided should be consistent with the product in commerce. The data should be provided

in a timely manner that permits the Committee to perform a thorough review. All data should receive a thorough quality control review by the sponsor before submission to the Committee.

Improvements to the presentation of specifications data for flavouring agents

The Committee recommends that the chemical structures for the flavouring agents be included as part of the specifications presented online. In addition, an annotation of the method used to determine the minimum assay value of the flavouring agent should be included. The Committee also noted that it would be more useful to separate the current specification for "Physical Form/Odour" into two separate entries. It was also recommended that a separate entry for melting point be included in the specifications for flavouring agents.

Evaluation of flavour modifiers

A number of the flavouring agents submitted to the present meeting (Nos 2077, 2080–2082, 2119, 2121, 2123, 2158–2162 and 2170–2172) modify the flavour of other dietary components. At the present meeting, the Committee has adopted the term *flavour modifier* for all agents that alter or mask the flavours of flavouring agents or other dietary components.

The Committee noted that the chemical structures of some flavour modifiers (e.g. Nos 2081, 2082, 2161, 2162 and 2170–2172) have characteristics that have not been found in previously evaluated flavouring agents. The flavour modifiers evaluated at the present meeting had low estimated dietary exposures and could be evaluated using the Procedure for the Safety Evaluation of Flavouring Agents. The Committee agreed that flavour modifiers would be identified in evaluations of flavouring agents. The Committee emphasized that the safety evaluations undertaken on flavouring agents and flavour modifiers relate to the use levels submitted to the Committee for evaluation.

ANNEX 2. RECOMMENDATIONS AND FURTHER INFORMATION REQUIRED

Food additives containing aluminium and/or silicon

The Committee, while reviewing the specifications of food additives containing aluminium and silicon, considered it relevant to update the test methods for the determination of aluminium oxide and silicon dioxide. Some of the test methods for the food additives listed below contained potentially corrosive or hazardous reagents that are not always permitted in the current laboratory practices because of safety considerations. The Committee also noted that the specifications of some additives were rather old or tentative and requires additional information to revise the specifications. Consequently, the Committee recommends placing these additives on the agenda for reevaluation.

Food Additive	Specifications	Remarks on current assay
Calcium aluminium silicate (INS 556)	28th, 1984	Assay by gravimetry, includes hydrofluoric acid and perchloric acid
Aluminium silicate (INS 559)	57th, 2001	No assay
Calcium silicate (INS 552)	17th, 1973	No assay
Silicon dioxide (INS 551)	17th, 1973	Assay by gravimetry and includes hydrofluoric acid
Sodium aluminosilicate (INS 554)	17th, 1973	No assay, identification test includes hydrofluoric acid
Potassium aluminium silicate (INS 555)	74th, 2011	Tentative specifications. Assay method is based on alkali fusion followed by ICP-AES determination.
Potassium aluminium silicate – based pearlescent pigments	74th, 2011	Tentative specifications. Assay method is based on alkali fusion followed by ICP-AES determination.

Test method for modified starches

In addition to revising the specific test for degree of substitution of Starch sodium octenylsuccinate (INS No. 1450) in the specifications monograph of modified starches, the Committee considered that it would be necessary to align the description of the test to be consistent with the end product specifications at a future meeting. In addition, the Committee considered it would also be necessary to revise the specifications for all the modified starches, including test methods.

FAO TECHNICAL PAPERS

FAO JECFA MONOGRAPHS

Note: JECFA Monographs are available in English only.

1. Combined compendium of food additive specifications – JECFA specifications monographs from the 1st to the 65th meeting. Vol. 1: Food additives A – D; Vol. 2: Food additives E – O; Vol. 3: Food additives P – Z; Vol. 4: Analytical methods, test procedures and laboratory solutions.
2. Residue evaluation of certain veterinary drugs – Joint FAO/WHO Expert Committee on Food Additives, 66th meeting 2006
3. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives, 67th meeting 2006
4. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives – 68th meeting 2007
5. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives, 69th meeting 2008
6. Residue evaluation of certain veterinary drugs – Joint FAO/WHO Expert Committee on Food Additives. 70th meeting 2008
7. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives, 71st meeting 2009
8. Safety evaluation of certain contaminants in food – Joint FAO/WHO Expert Committee on Food Additives, 72nd meeting 2010. Joint FAO/WHO publication: WHO Food Additives Series No. 63/FAO JECFA Monographs 8
9. Residue evaluation of certain veterinary drugs – Joint FAO/WHO Expert Committee on Food Additives, Meeting 2010 – Evaluation of data on ractopamine residues in pig tissues
10. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives, 73rd meeting 2010
11. Compendium of food additive specifications – Joint FAO/WHO Expert Committee on Food Additives, 74th meeting 2011
12. Residue evaluation of certain veterinary drugs – Joint FAO/WHO Expert Committee on Food Additives, 75th meeting 2011

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COMPENDIUM OF FOOD ADDITIVE SPECIFICATIONS

Joint FAO/WHO Expert Committee on Food Additives

76th Meeting 2012

This document contains food additive specification monographs, analytical methods, flavouring agent specifications and other information prepared at the seventy-sixth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA), which was held in Geneva, Switzerland from 5 – 14 June 2012. The specification monographs provide information on the identity and purity of food additives used directly in foods or in food production. The main three objectives of these specifications are to identify the food additive that has been subjected to testing for safety, to ensure that the additives are of the quality required for use in food or in processing and to reflect and encourage good manufacturing practice. This publication and other documents produced by JECFA contain information that is useful to all those who work with or are interested in food additives, including flavouring agents, and their safe use in food.

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