Electronic Supplementary Material (ESI) for Analyst.
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Supporting Information

Improved molecular level identification of organic compounds using multidimensional chromatographic separation, dual ionization energies and high resolution mass spectrometry

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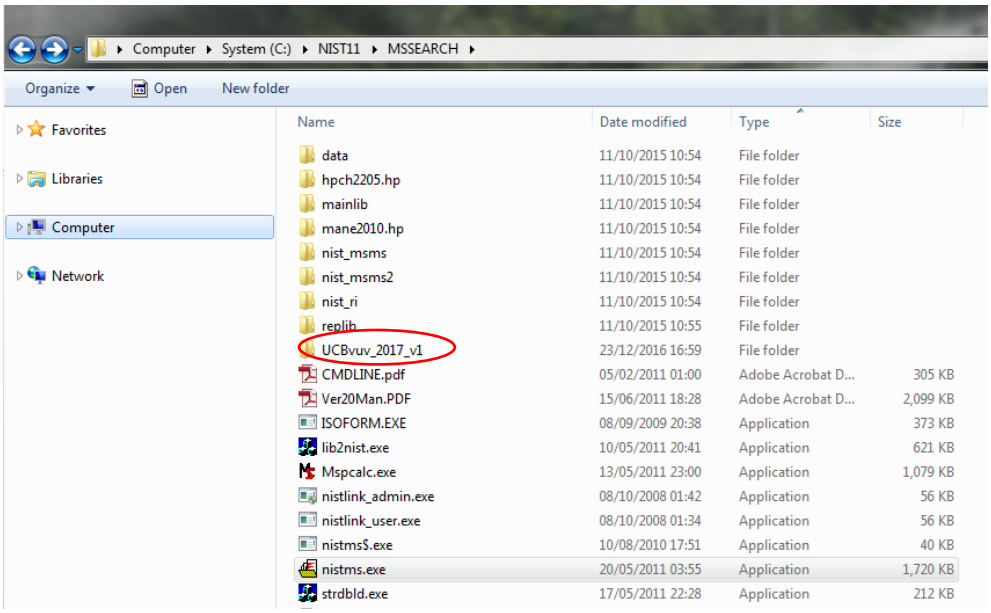
Generated EI MS library (UCBvuv_2017_v1)

A searchable EI mass spectral library specifically generated with atmospherically relevant compounds of interest from this work in a format compatible with the NIST MSSEARCH program is available to download from:
https://nature.berkeley.edu/ahg/MSLibrary/UCB_VUV_Lib_v1.

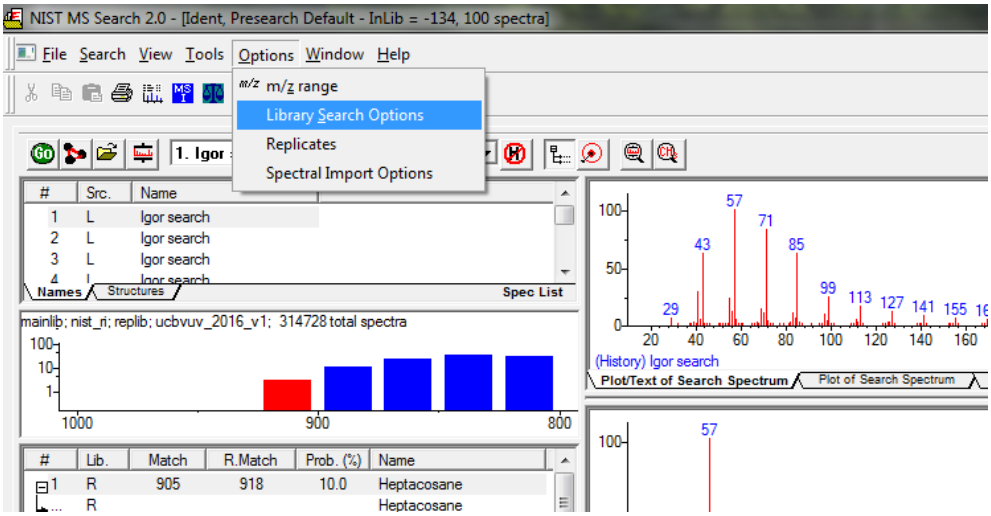
Instructions on how to use the EI MS library generated from this work (UCBvuv_2017_v1)

Here we include a step by step guide on how to use the EI MS library generated in this work using the NISTMS programme (UCBvuv_2017_v1).

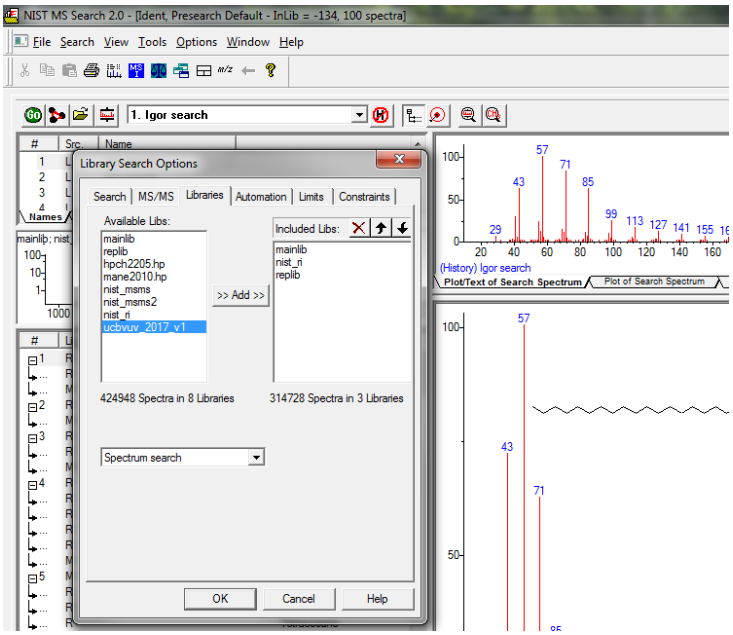
1. Copy the UCBvuv_2017_v1 into the NIST\MSSEARCH folder on the C:\ drive. This is the folder that contains the nistms.exe programme.



2. Open the nistms.exe programme and select the Options\Library Search Options.



3. Select the Libraries tab and you will see the UCBvuv_2017_v1 library as one of the available libraries.



4. Add the UCBvuv_2017_v1 library to the included library list and click OK.

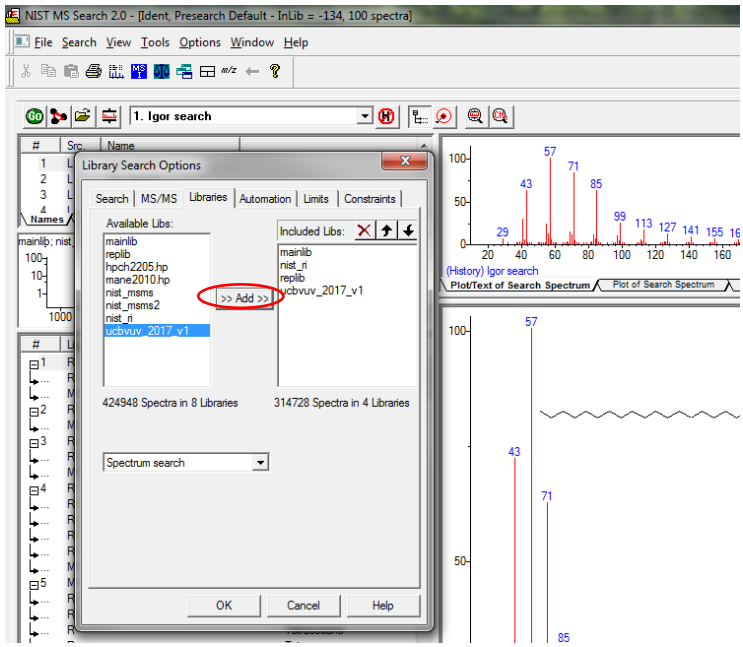


Table S1. Major families of molecular formulas, those with ≥5 homologues, Kendrick Mass Defect (KMD) and number observed matched to EI MS library with confirmation by VUV MS data (EI) and assigned molecular formulas from the observed molecular ion (VUV). Identified compound names from EI MS library matching are also shown for each family. The shaded areas correspond to the most abundant 6 families.

Family Formula	KMD	Frequency		Compound Names from EI library Matching
		EI	VUV	
$C_nH_{2n-4}O_2$	0.073	22	32	2(5H)-Furanone; 2(3H)-Furanone, 5-methyl-; 1,3-Cyclopentanedione; 1,3-Cyclopentanedione; 2(5H)-Furanone, 5-methyl; 2(5H)-Furanone, 5,5-dimethyl-;2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2,5-dimethyl-;2(5H)-Furanone, 3-methyl-;2-Furanone, 2,5-dihydro-3,5-dimethyl;3,4-Dihydro-6-methyl-2H-pyran-2-one;2-Cyclopenten-1-one, 2-hydroxy-3-methyl-;2(3H)-Furanone, 5-ethenyldihydro-5-methyl-;4-Methyl-5H-furan-2-one;2-Furanone, 2,5-dihydro-3,5-dimethyl;2(5H)-Furanone, 3,5,5-trimethyl-;2,3-Dimethyl-4-hydroxy-2-butenoic lactone;2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-;Cyclohexanone, 2-acetyl-2-Oxabicyclo[2.2.2]octan-6-one, 1,3,3-trimethyl-;5H-Inden-5-one, octahydro-1-hydroxy-7a-methyl-;2-Oxabicyclo[3.2.1]nonan-7-one, 1,5-dimethyl-;Spiro(2-oxabicyclo[2.1.0]pentane)-3,2'-oxetane, 1,5,5,3',3',4',4'-heptamethyl-
$C_nH_{2n-4}O$	0.050	28	16	Furan, 2-ethyl-5-methyl-; trans,trans-3,5-Heptadien-2-one;2-Cyclopenten-1-one;2,4-Hexadienal, (E,E)-; Cyclopentanecarboxaldehyde, 2-methyl-3-methylene-;Bicyclo[3.1.0]exan-3-one;2-Cyclohexen-1-one;trans,trans-3,5-Heptadien-2-one;2-Cyclopenten-1-one, 3-methyl-;3-Methyl-3-cyclohexen-1-one;Bicyclo[2.2.1]heptan-2-one, 3,3-dimethyl-;4-Acetyl-1-methylcyclohexene;4-Isopropenylcyclohexanone;2-Cyclopenten-1-one, 3,4-dimethyl-;2-Cyclopenten-1-one, 2,3-dimethyl-;3-Cyclohexene-1-carboxaldehyde, 4-methyl-; 3-Ethenyl-3-methylcyclopentanone;3-Isopropylidene-5-methyl-hex-4-en-2-one;3-Cyclohexen-1-carboxaldehyde, 3,4-dimethyl-;2-Cyclopenten-1-one, 3-(1-methylethyl)-;Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-;Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)-;Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-;2-Cyclohexen-1-one, 4-(1-methylethyl)-;Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl-, [1R-(1à,4á,6à)]-;Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-;1-Cyclohexene-1-methanol, 4-(1-methylethenyl)-;2-Isopropylidene-5-methylhex-4-enal
$C_nH_{2n-6}O_2$	0.086	13	29	3-Furaldehyde; 4-Cyclopentene-1,3-dione;1-(2,4-Dimethyl-furan-3-yl)-ethanone; 1,4-Cyclohex-2-enedione; 2-Acetyl-4,4-dimethyl-cyclopent-2-enone; Phenol, 2-methoxy-; 5-Ethyl-2-furaldehyde; 4-Cyclopentene-1,3-dione, 4-propyl-; 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-; 1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-; 5H-3,5a-Epoxynaphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-tetramethyl-, [3S-(3à,5aà,7aà,11aá,11bà)]-; 5H-3,5a-Epoxynaphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-tetramethyl-, [3S-(3à,5aà,7aà,11aá,11bà)]-; Sclareolide
$C_nH_{2n-2}O_2$	0.059	20	20	2,5-Hexanedione;3-Pentenoic acid, 4-methyl-;2H-Pyran-2-one, tetrahydro-;2H-Pyran-2-one, tetrahydro-6-methyl-;2(3H)-Furanone, dihydro-5-propyl-;2H-Pyran-2-one, 6 ethyltetrahydro-;2(3H)-Furanone, dihydro-5-butyl-;2(3H)-Furanone, dihydro-5-pentyl-;2H-Pyran-2-one, 6-butyltetrahydro-;2H-Pyran-2-one, 6-pentyltetrahydro-;2H-Pyran-2-one, 6-hexyltetrahydro-;2H-Pyran-2-one, 6-heptyltetrahydro-;Z-11-Tetradecenoic acid;cis-9-Hexadecenoic acid;2(3H)-Furanone,dihydro-X-methyl-5-nonyl;2H-Pyran-2-one, 6-nonyltetrahydro-;Oxacycloheptadecan-2-one;cis-Vaccenic acid;cis-13-Octadecenoic acid;cis-13-Eicosenoic acid
$C_nH_{2n-6}O$	0.063	16	12	Phenol, 3,5-dimethyl-;Cyclopentanone, 3,4-bis(methylene)-;Phenol, 2-methyl-;Benzene, 2-methoxy-1,3,4-trimethyl-;Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-; 4,4-Dimethylcyclohexadienone;5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde;Phenol, 3-(1-methylethyl)-;Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-; 2-Caren-10-al;p-Cymen-7-ol;Phenol, 2-methyl-5-(1-methylethyl)-;Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-;Butylated Hydroxytoluene; 1-Oxaspiro[2.5]octane, 5,5-dimethyl-4-(3-methyl-1,3-butadienyl)-; 14-Oxatricyclo[9..2.1.0(1,10)]tetradecane, 2,6,6,10,11-pentamethyl
$C_nH_{2n-2}O$	0.036	13	8	3-Buten-2-one, 3-methyl-;2-Butenal, 2-methyl-, (E)-;Furan, 2,3-dihydro-4-methyl-;2-Butenal, 3-methyl-;Cyclopentanone;3-Penten-2-one, 4-methyl-;3-Pentenal, 4-methyl-; 3-Penten-2-one, 3,4-dimethyl-;Cyclohexanone;Bicyclo[2.2.2]octan-1-ol, 4-methyl-;5-Hepten-2-one, 6-methyl-;2-Dodecenal, (E)-;2-Tridecenal, (E)-
C_nH_{2n+2}	-0.013	8	11	Dodecane;Tridecane;Tetradecane;Hexadecane;Heptadecane, 9-octyl-;Heneicosane;Tetracosane;Heptacosane
$C_nH_{2n-6}O_3$	0.109	2	17	2,5-Furandione, 3,4-dimethyl-;2-Furanpropionic acid
C_nH_{2n-6}	0.040	11	2	Toluene;p-Xylene;3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene;Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)-;1,3,5-Cycloheptatriene, 3,7,7-trimethyl-;Benzene, 1-ethyl-4-methyl-;2,6-Dimethyl-1,3,5,7-octatetraene, E,E-;Benzene, 1-ethyl-2-methyl-;o-Cymene;Benzene, 1-ethyl-2-methyl-
$C_nH_{2n}O$	0.023	6	6	2-Heptanone, 6-methyl-;2-Octanone;2-Pentadecanone;2-Hexadecanone;2-Pentadecanone, 6,10,14-trimethyl-;2-Heptadecanone
$C_nH_{2n-4}O_3$	0.096	2	10	Pinonic acid; Cyclooctanone, 5-(acetyloxy)-
$C_nH_{2n-8}O$	0.077	7	5	Benzaldehyde;Ethanone, 1-(3,4-dimethylphenyl)-;Benzaldehyde, 4-(1-methylethyl)-;2-Allyl-4-methylphenol;Ethanone, 1-(3-methylphenyl)-;Benzaldehyde, 4-(1-methylethyl)-;Ethanone, 1-(2,4-dimethylphenyl)-
$C_nH_{2n}O_2$	0.046	4	4	Tridecanoic acid, 12-methyl-, methyl ester; i-Propyl 12-methyl-tridecanoate; Hexadecanoic acid, methyl ester; Tetracosanoic acid, methyl ester
$C_nH_{2n-10}O_2$	0.113	7	0	2(3H)-Benzofuranone, 3-methyl-;2(3H)-Benzofuranone, 3-methyl-;1(3H)-Isobenzofuranone;Hydrocoumarin;3(2H)-Benzofuranone, 5-methyl-;Ethanone, 1,1'-(1,4-phenylene)bis-;Ethanone, 1,1'-(1,4-phenylene)bis-
$C_nH_{2n-8}O_2$	0.099	3	3	Ethanone, 1-[4-(1-hydroxy-1-methylethyl)phenyl]-;2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylpropyl)-;3,5-di-tert-Butyl-4-hydroxybenzaldehyde
$C_nH_{2n-12}O_2$	0.126	3	3	1H-Indene-1,3(2H)-dione;Coumarin, 8-methyl-;Methyl dehydroabietate
C_nH_{2n}	0.000	0	5	
$C_nH_{2n-8}O_3$	0.122	3	2	Vanillin;Apocynin;2-Ethylhexyl salicylate

Figure S1. Linear regression of I_1 (first dimension Kovats retention indices) from this work and the NIST database (bottom). The residual ($I_{1(\text{ this work})} - I_{1\ (\text{NIST})}$) of the linear regression demonstrates the degree of agreement. The datapoints are numerically labelled, which uniquely identifies each point to the corresponding chromatographic peak. The shaded area represents the boundary of what was considered a reasonable agreement and data outside of this area was excluded. This boundary was chosen empirically but is reasonable given the reported differences in I_1 by different groups reporting data used in the NIST GC retention time database and the variability in retention values resulting from differing chromatographic conditions and columns from various manufacturers due to differences in the polymeric structure of columns, e.g., 5 type columns (i.e., RTX-5, DB-5, CPSil-5) are not the same.

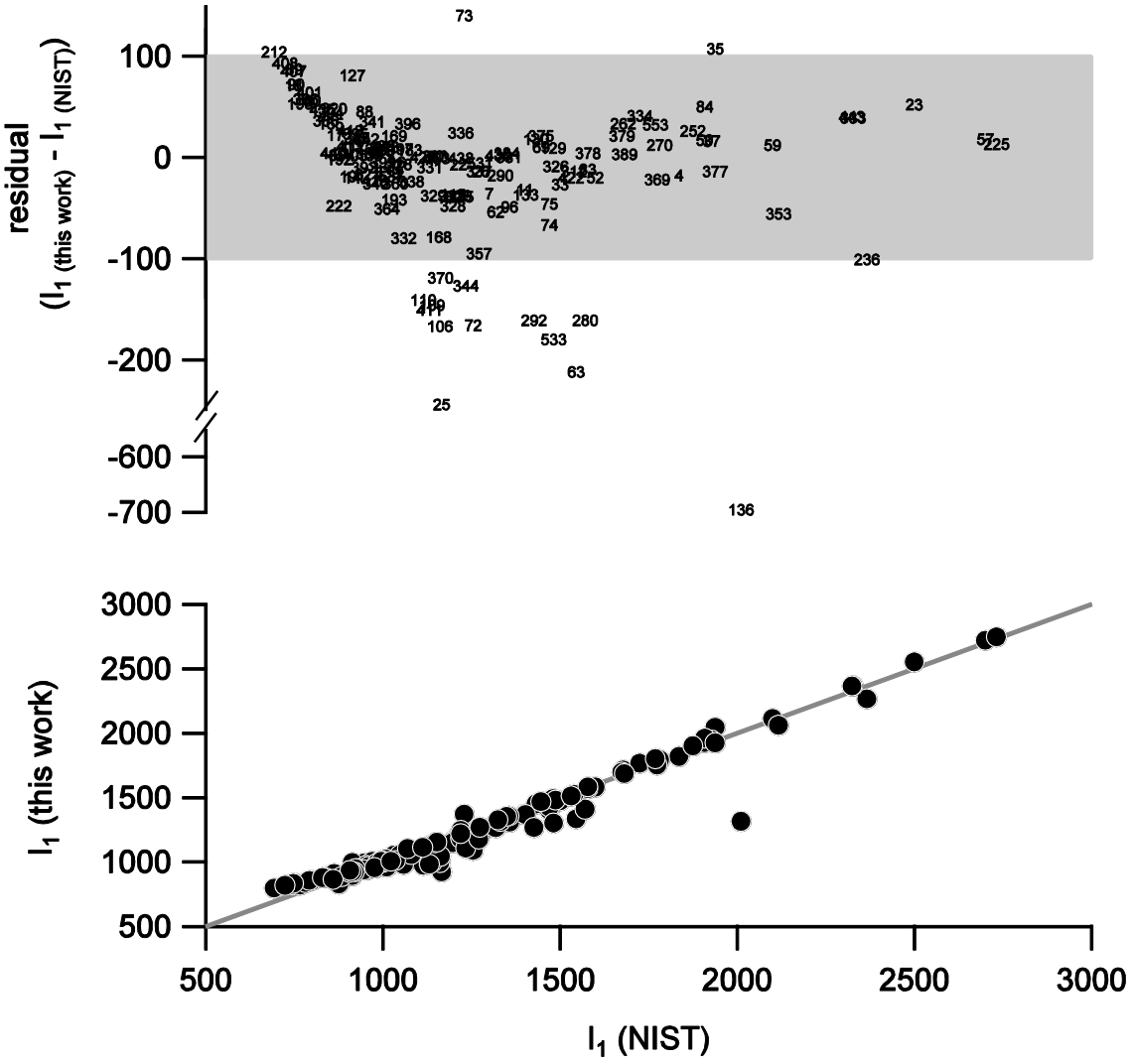


Figure S2. Relationship between measured Kovats index (I_1) and molecular weight (MW) determined from molecular formula for all species with the formula $C_nH_{2n-2}O_2$. Text symbols represent carbon number. This plot is used to check the assigned molecular formulas. For correctly identified molecular formulas within a family, molecular weight and carbon number are expected to increase with increasing I_1. The datapoint highlighted by red circle is an outlier as it does not conform to this indicating that a fragment has been mis-assigned as the molecular ion.

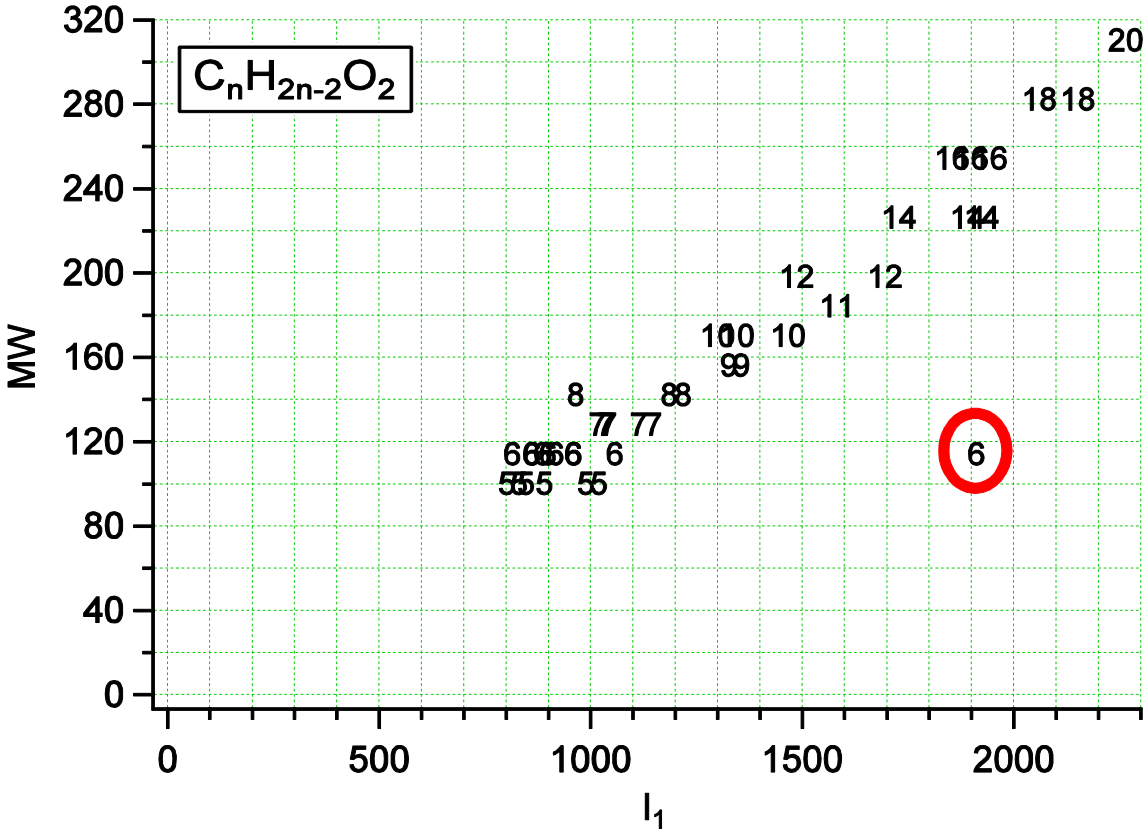


Figure S3. Comparison of number of peaks identified by EI only (left panel) and identified by EI and VUV (right panel) as a function of the forward matching statistic (FM) returned from the NIST MS search program.

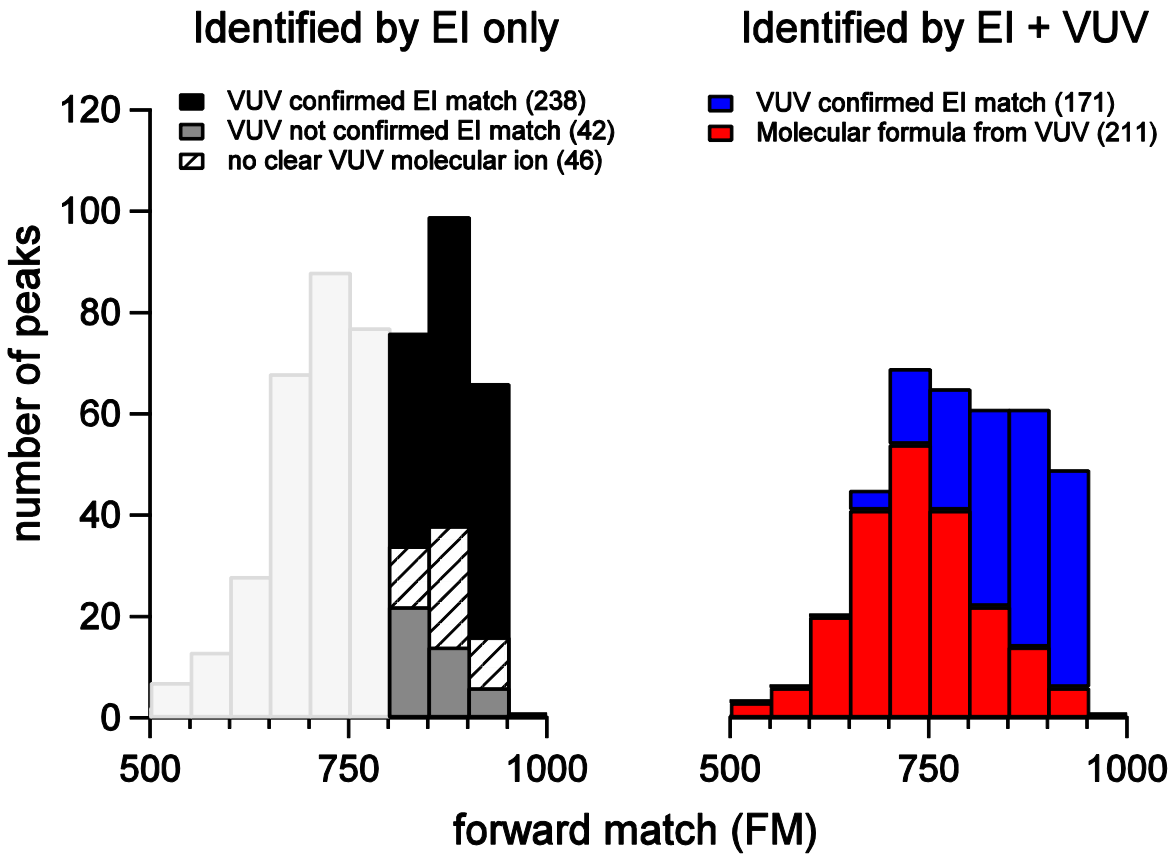


Figure S4. Kendrick mass defect plot showing identification of homologous series. The six most populous groups are indicated with the formula family based on identified EI and assigned VUV formulas.

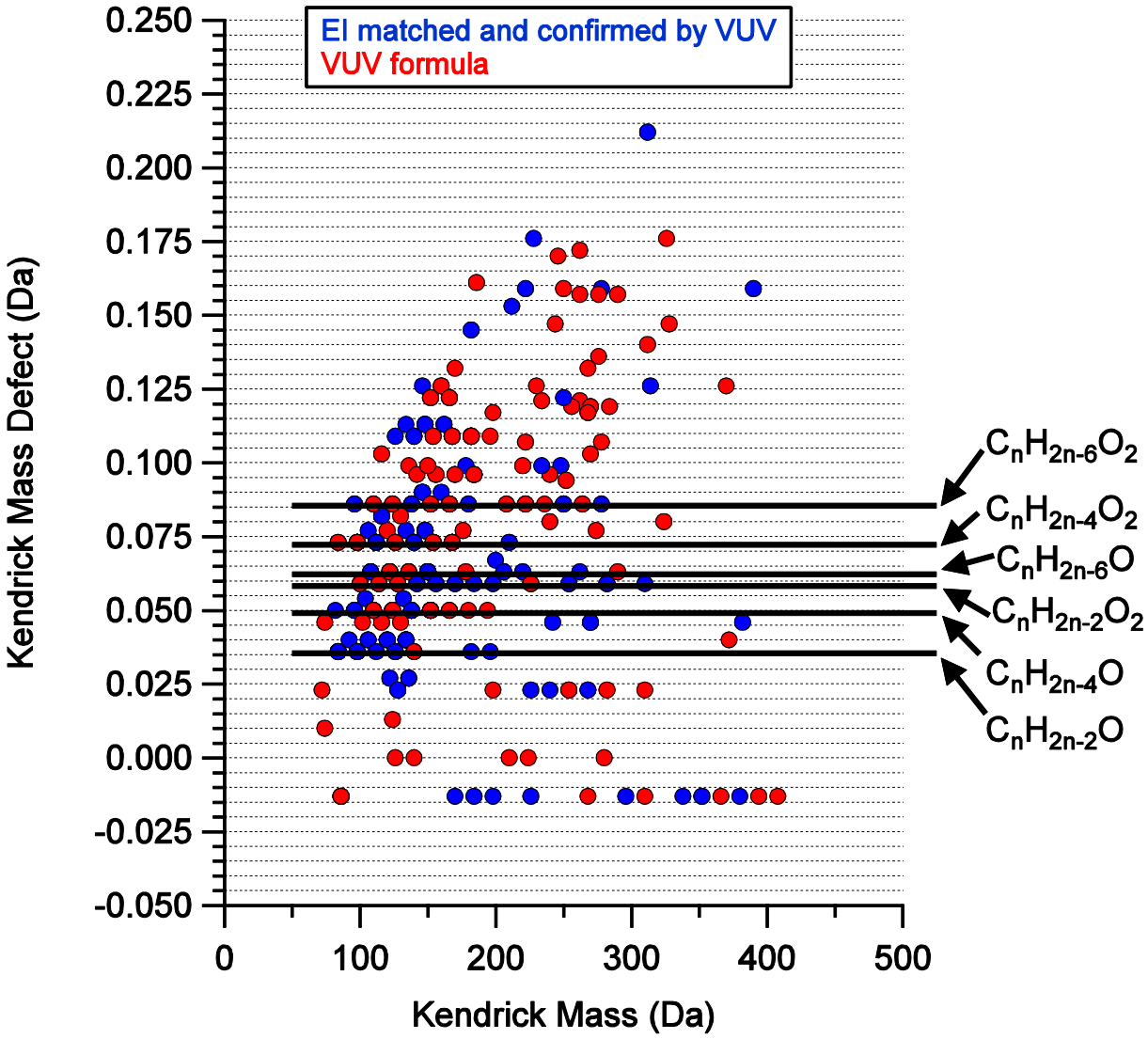


Figure S5. Relationship between measured Kovats index (I_1) and molecular weight (MW) determined from the identified molecular formula from high resolution VUV MS for the six homologous series shown in Figure S2. Text symbols represent carbon number.

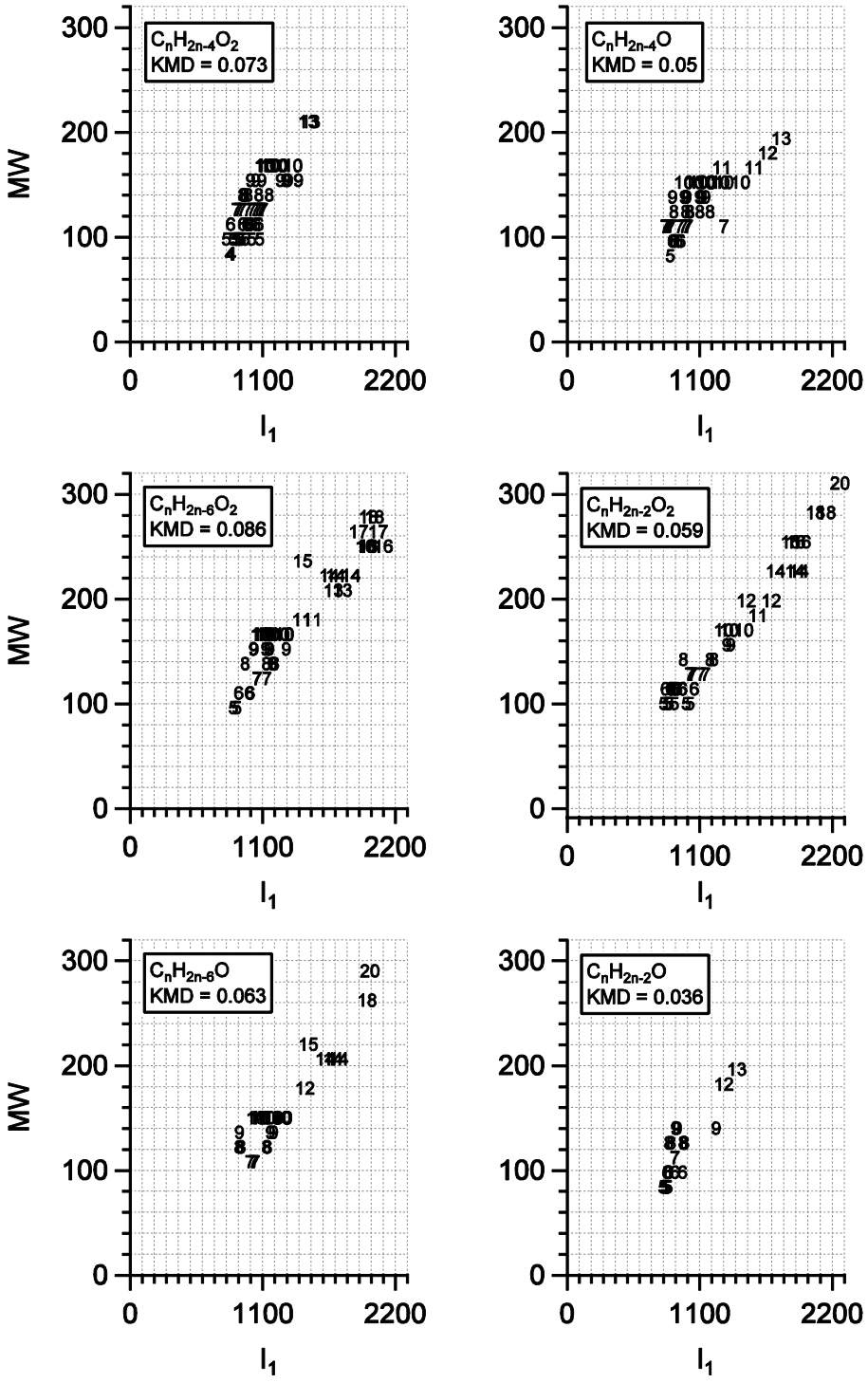
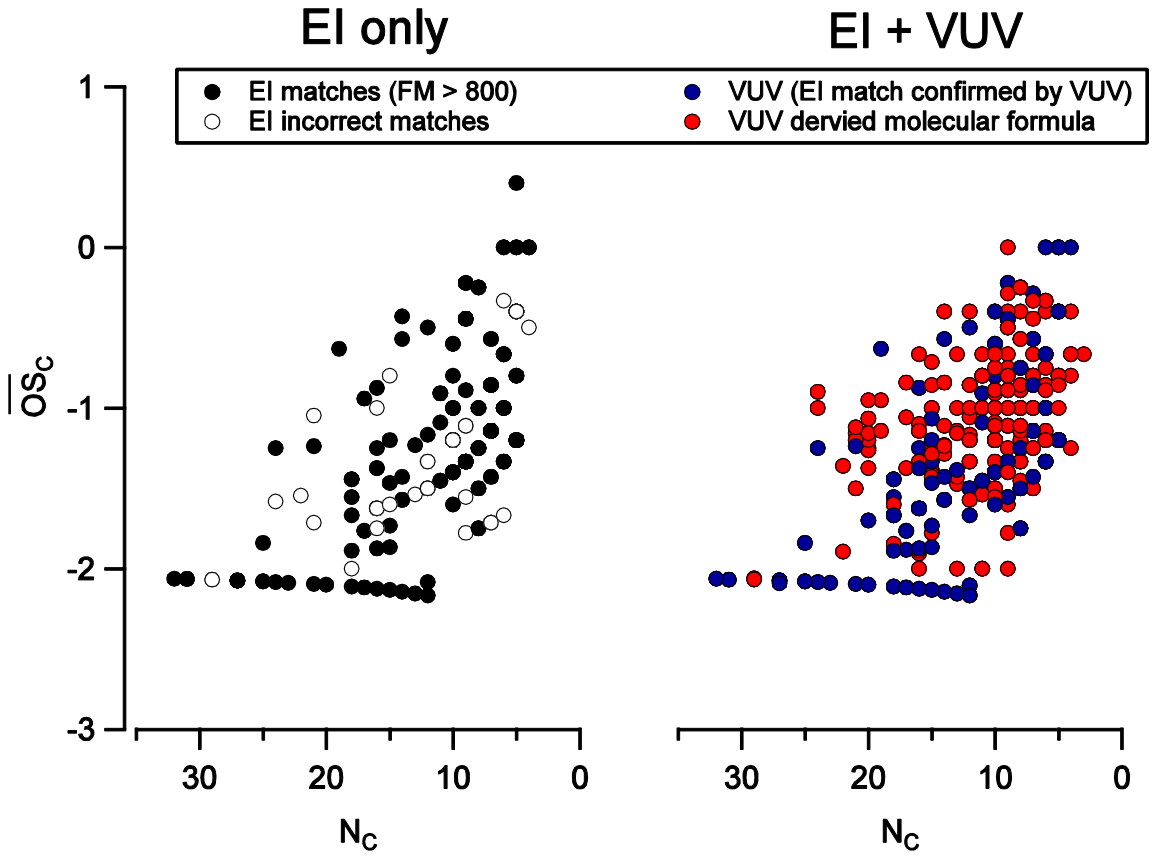
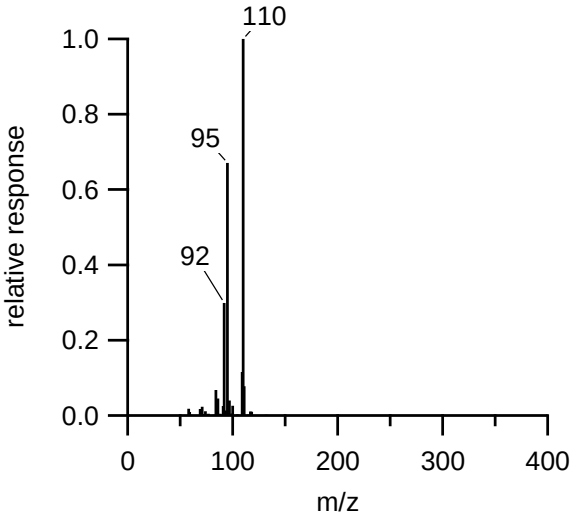


Figure S6. Average carbon oxidation state ($\overline{OSc}$) versus carbon number (N_C) for an EI only and an EI + VUV approach. The EI only approach includes only those compounds that had forward matching (FM) statistics of > 800 (filled black circles). Those which were not confirmed by VUV MS data (thus considered incorrectly identified) are shown as open circles. All molecular formulas containing only carbon (C), hydrogen (H) and oxygen (O) are included here ($C_xH_yO_z$) due to the nature of the calculation of OSc (2*O:C – H:C).

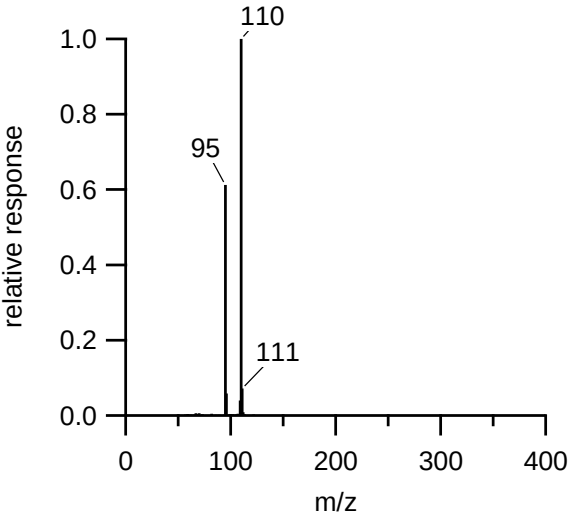


Appendix of VUV (10.5 eV) Mass Spectra

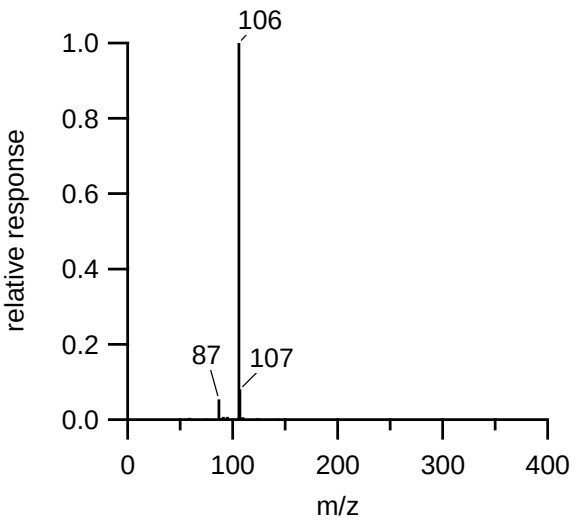
Furan, 2-ethyl-5-methyl-
CAS #1703-52-2, MW=110.07 (28 ppm)



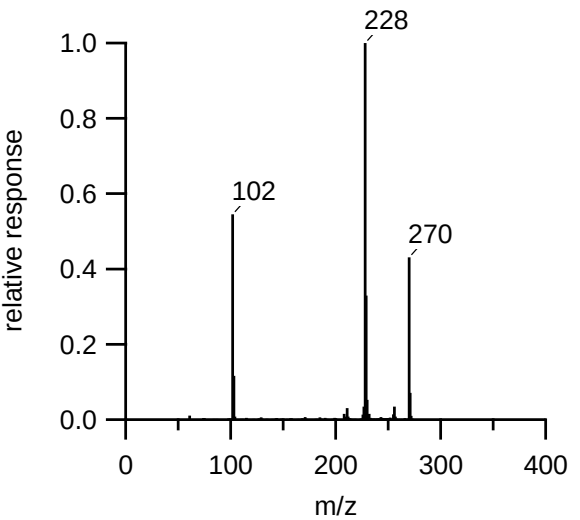
trans,trans-3,5-Heptadien-2-one
CAS #18402-90-9, MW=110.07 (28 ppm)



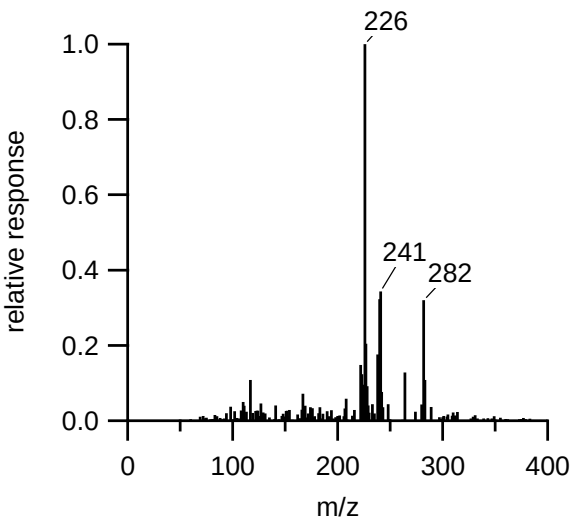
m-Xylene
CAS #108-38-3, MW=106.08 (14 ppm)



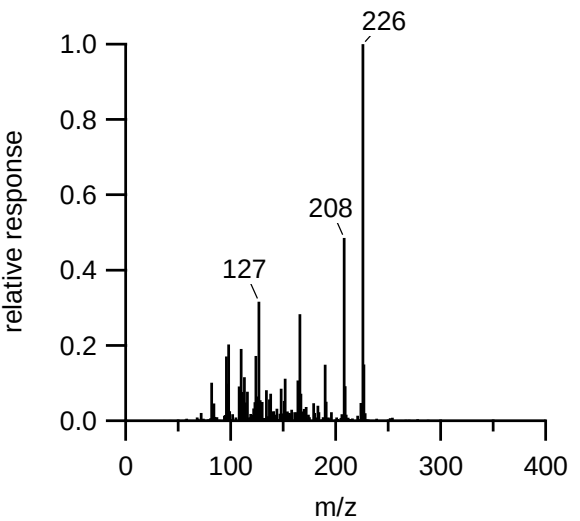
i-Propyl 12-methyl-tridecanoate
CAS #110-27-0, MW=270.26 (3 ppm)



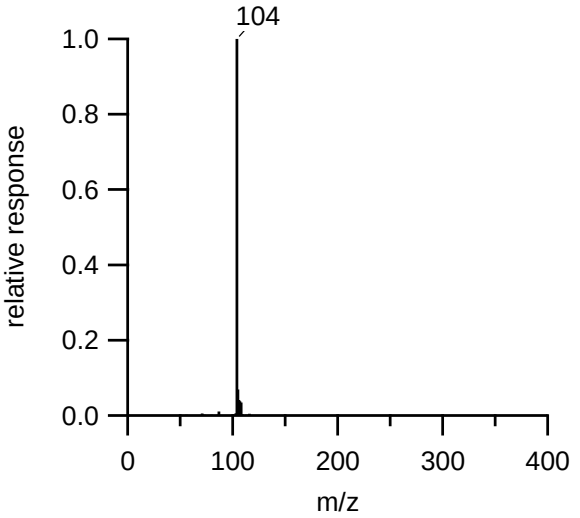
cis-13-Octadecenoic acid
CAS #112-79-8, MW=282.26 (18 ppm)



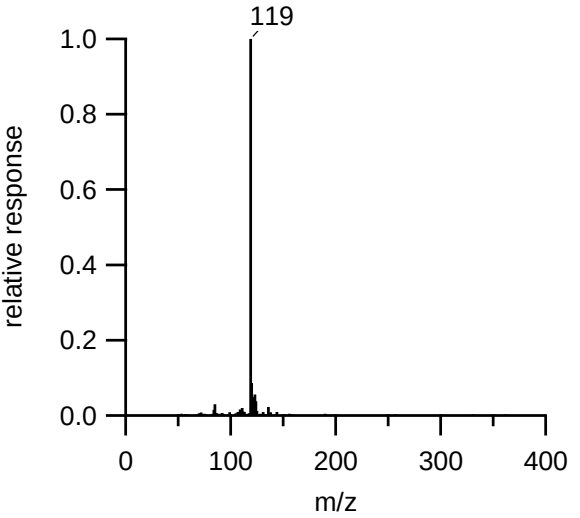
Z-11-Tetradecenoic acid
CAS #0-00-0, MW=226.19 (52 ppm)



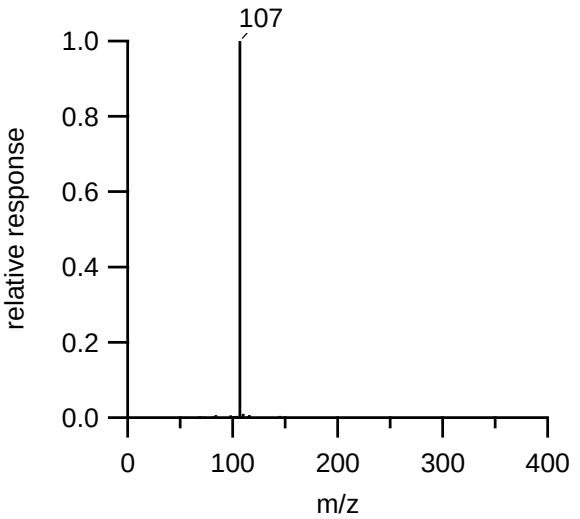
Styrene
CAS #100-42-5, MW=104.06 (9 ppm)



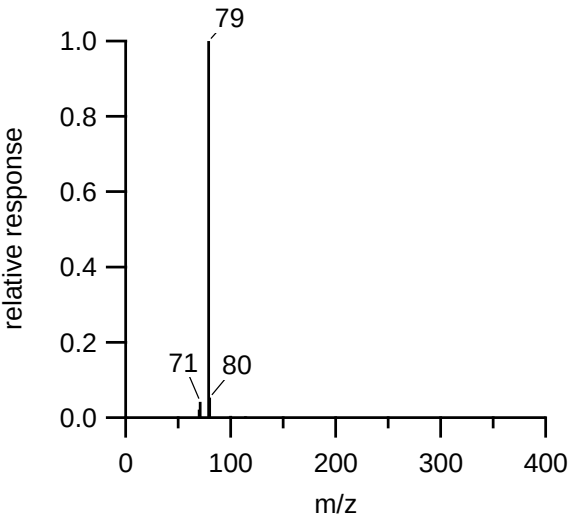
Pyridine, 5-ethenyl-2-methyl-
CAS #140-76-1, MW=119.07 (42 ppm)



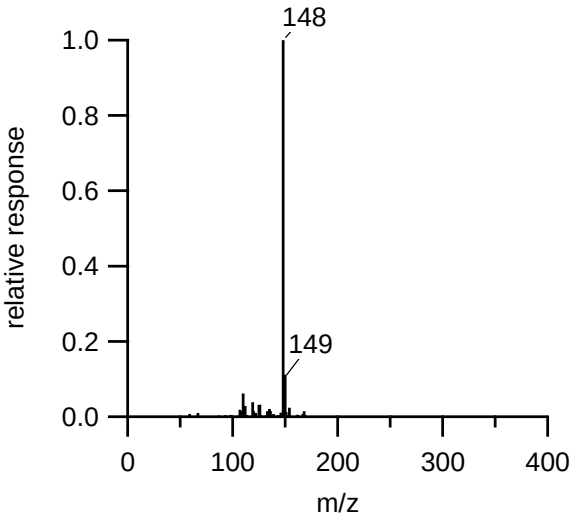
Pyridine, 2,6-dimethyl-
CAS #108-48-5, MW=107.07 (59 ppm)



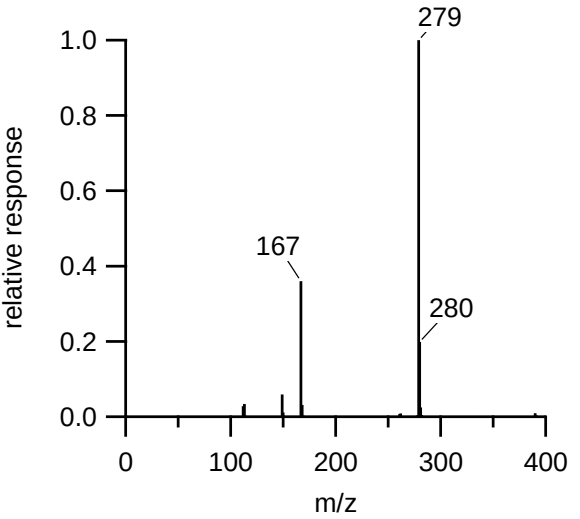
Pyridine
CAS #110-86-1, MW=79.042 (2 ppm)

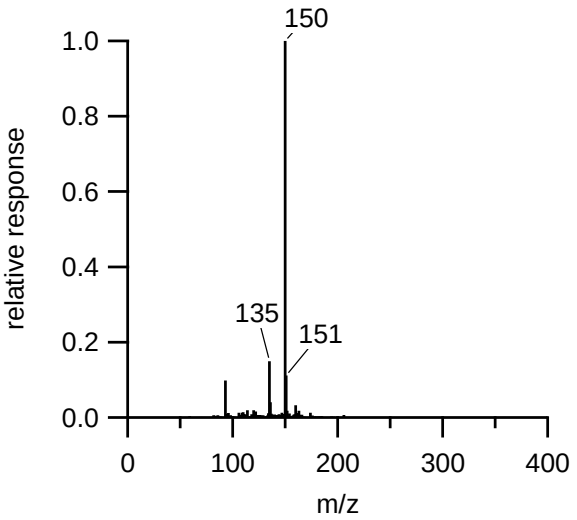


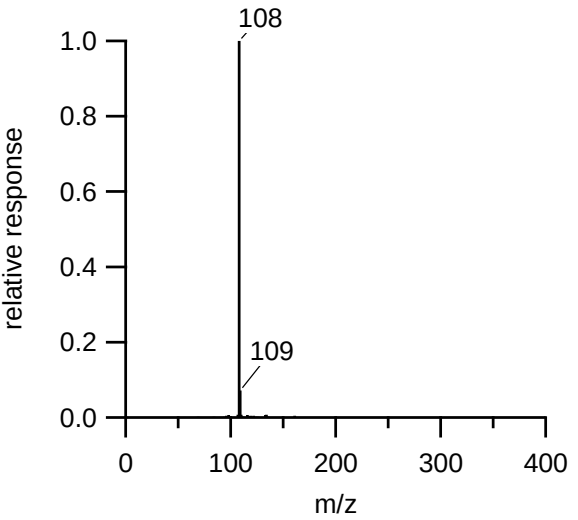
Benzaldehyde, 4-(1-methylethyl)-
CAS #122-03-2, MW=148.09 (44 ppm)

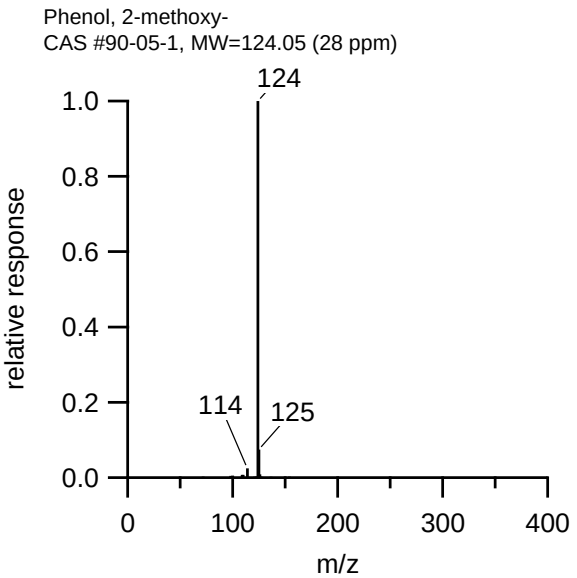


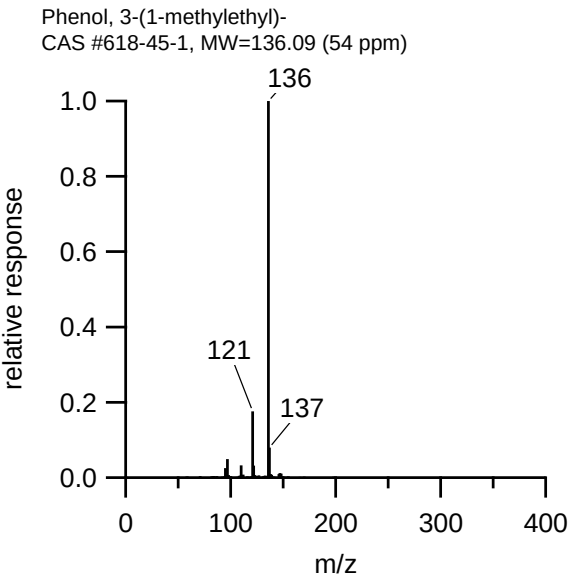
Phthalic acid, di(2-propylpentyl) ester
CAS #117-81-7, MW=390.28 (41 ppm)

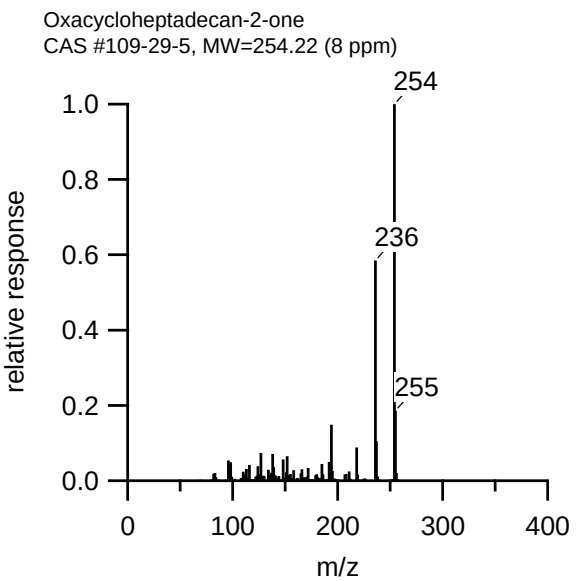


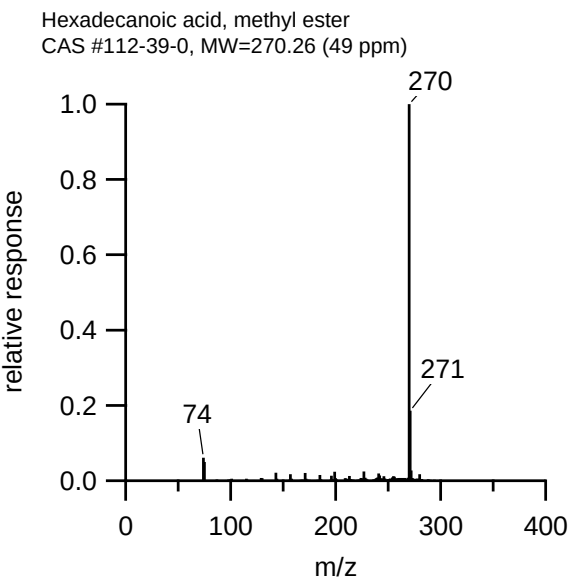

Phenol, 2-methyl-5-(1-methylethyl)-
CAS #499-75-2, MW=150.1 (35 ppm)
150
135
151
relative response
m/z


Phenol, 2-methyl-
CAS #95-48-7, MW=108.06 (47 ppm)
108
109
relative response
m/z

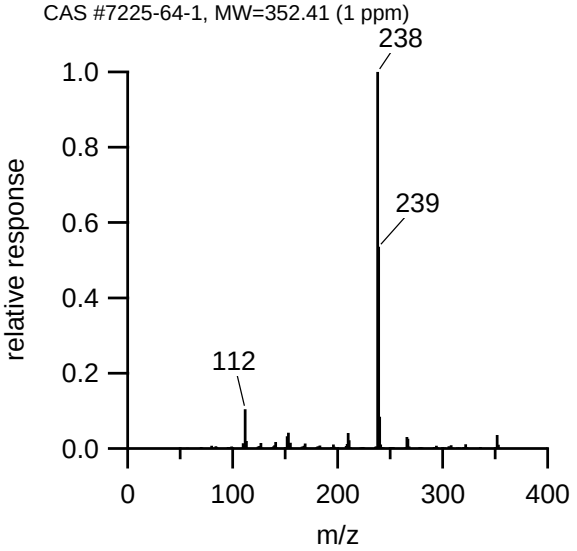

Phenol, 2-methoxy-
CAS #90-05-1, MW=124.05 (28 ppm)
124
114
125
relative response
m/z


Phenol, 3-(1-methylethyl)-
CAS #618-45-1, MW=136.09 (54 ppm)
136
121
137
relative response
m/z

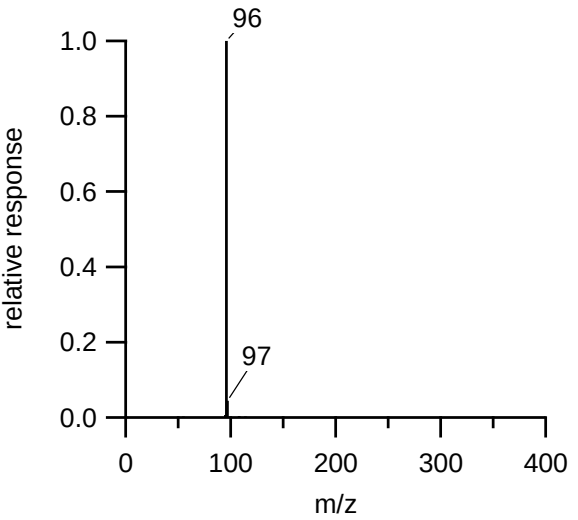

Oxacycloheptadecan-2-one
CAS #109-29-5, MW=254.22 (8 ppm)
254
236
255
relative response
m/z


Hexadecanoic acid, methyl ester
CAS #112-39-0, MW=270.26 (49 ppm)
270
271
74
relative response
m/z

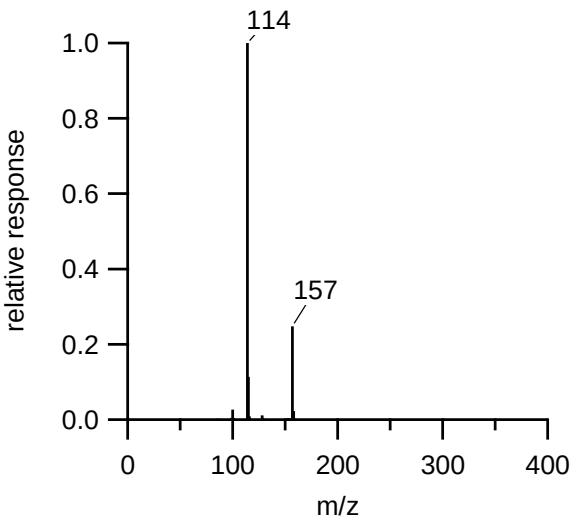
Heptadecane, 9-octyl-
CAS #7225-64-1, MW=352.41 (1 ppm)



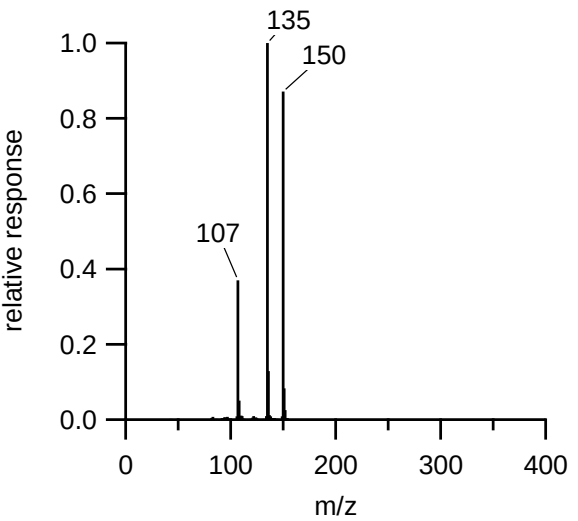
3-Furaldehyde
CAS #498-60-2, MW=96.021 (78 ppm)



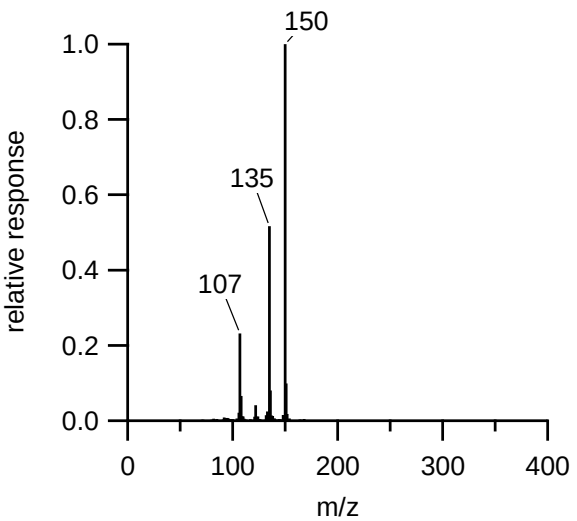
Formamide, N,N-dibutyl-
CAS #761-65-9, MW=157.15 (48 ppm)



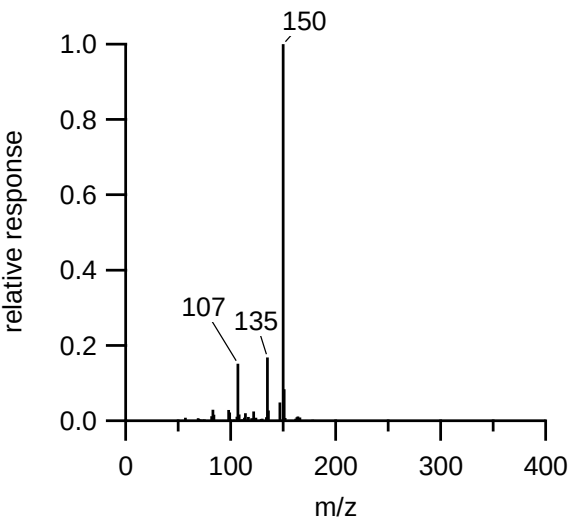
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-
CAS #24555-40-6, MW=150.1 (27 ppm)



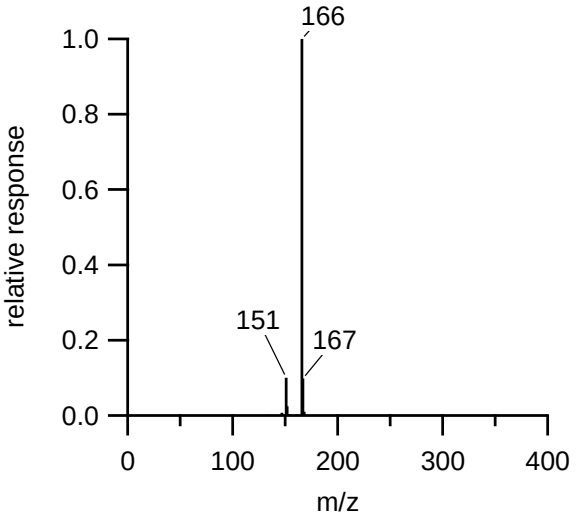
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-
CAS #24555-40-6, MW=150.1 (35 ppm)



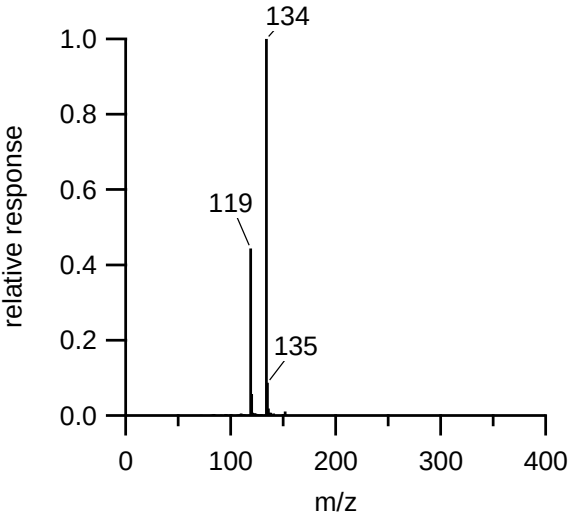
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-
CAS #24555-40-6, MW=150.1 (35 ppm)



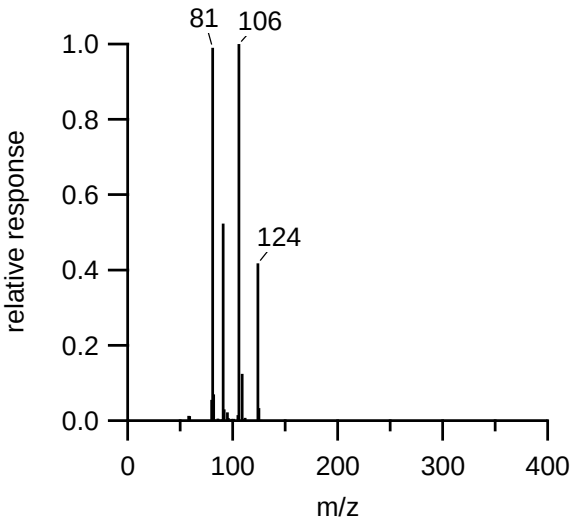
Apocynin
CAS #498-02-2, MW=166.06 (21 ppm)



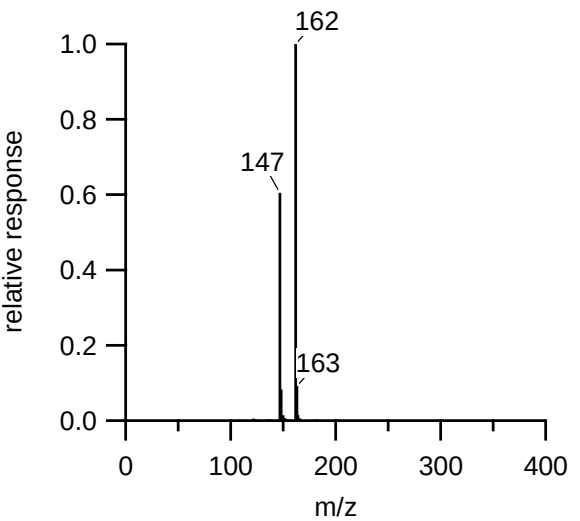
Ethanone, 1-(3-methylphenyl)-
CAS #585-74-0, MW=134.07 (3 ppm)



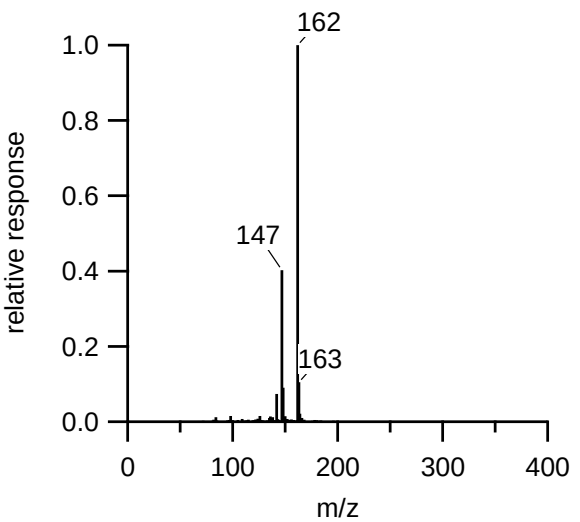
Cyclopentanecarboxaldehyde, 2-methyl-3-methylene-
CAS #0-00-0, MW=124.09 (17 ppm)



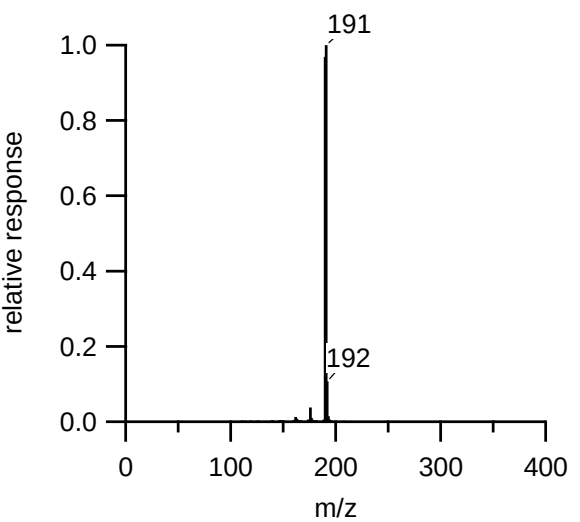
Ethanone, 1,1'-(1,4-phenylene)bis-
CAS #1009-61-6, MW=162.07 (19 ppm)



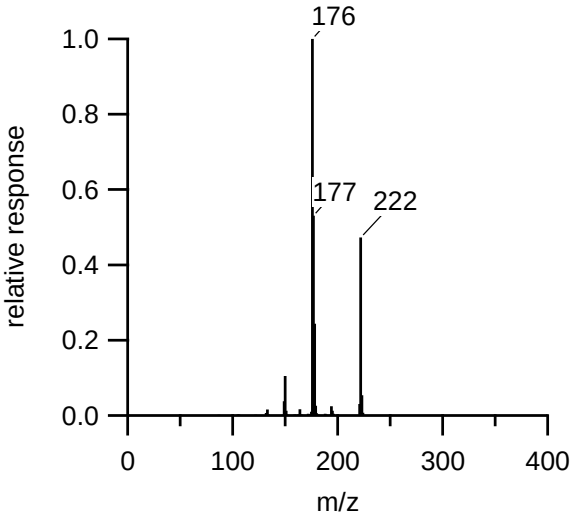
Ethanone, 1,1'-(1,4-phenylene)bis-
CAS #1009-61-6, MW=162.07 (80 ppm)



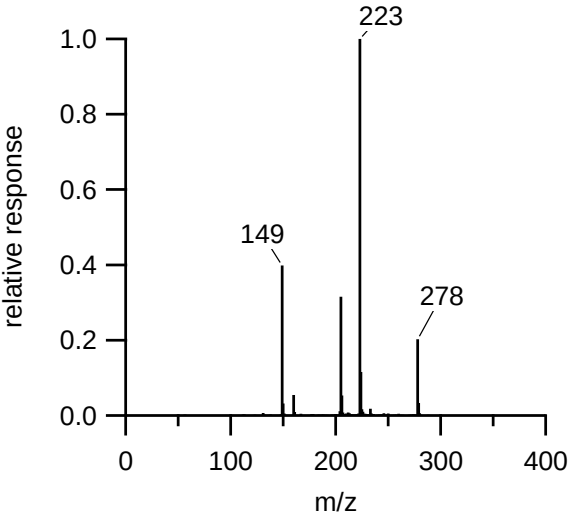
Benzamide, N,N-diethyl-4-methyl-
CAS #2728-05-4, MW=191.13 (3 ppm)



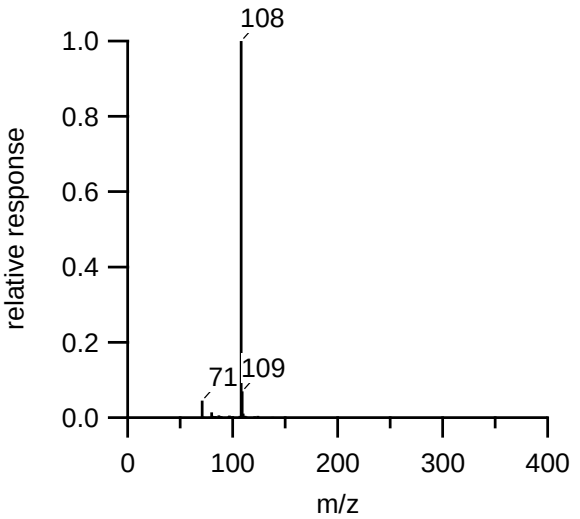
Diethyl Phthalate
CAS #84-66-2, MW=222.09 (7 ppm)



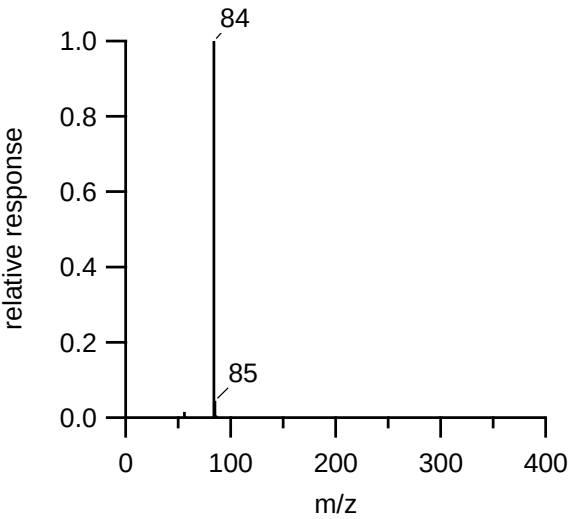
Dibutyl phthalate
CAS #84-74-2, MW=278.15 (1 ppm)



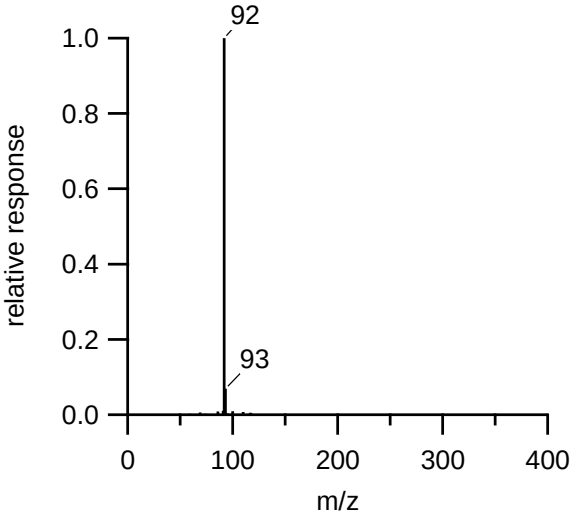
Cyclopentanone, 3,4-bis(methylene)-
CAS #27646-73-7, MW=108.06 (98 ppm)



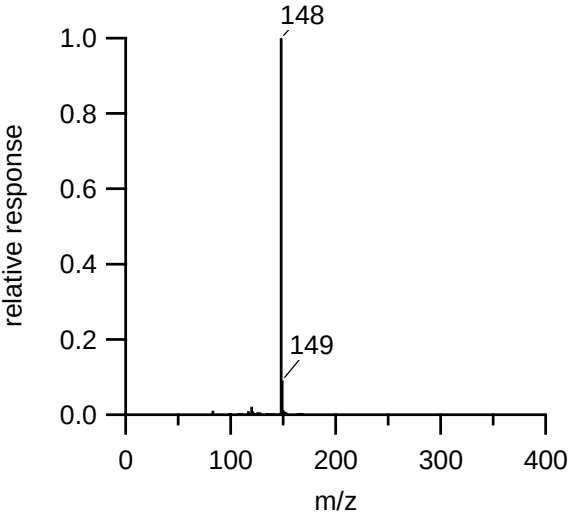
Cyclopentanone
CAS #120-92-3, MW=84.058 (39 ppm)



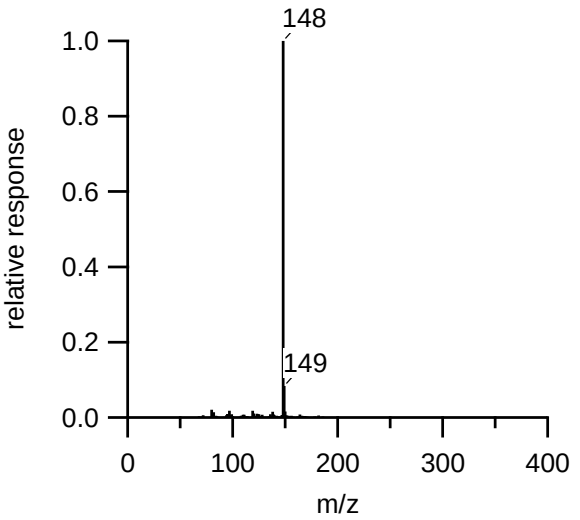
Toluene
CAS #108-88-3, MW=92.063 (2 ppm)



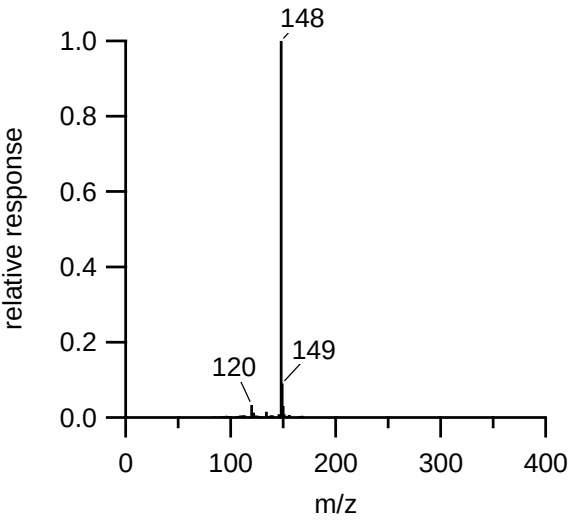
2(3H)-Benzofuranone, 3-methyl-
CAS #32267-71-3, MW=148.05 (51 ppm)



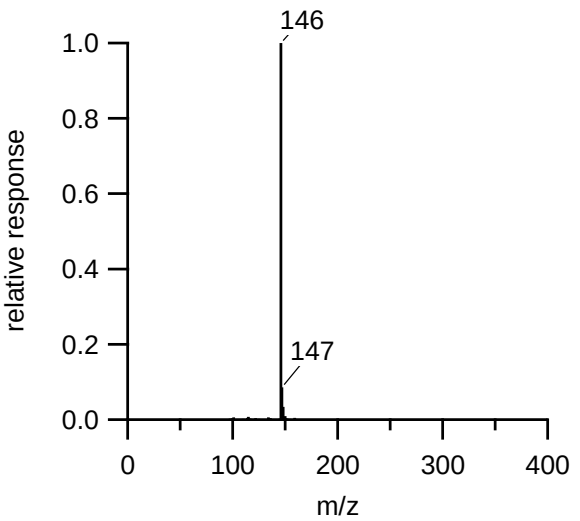
3(2H)-Benzofuranone, 5-methyl-
CAS #54120-66-0, MW=148.05 (11 ppm)



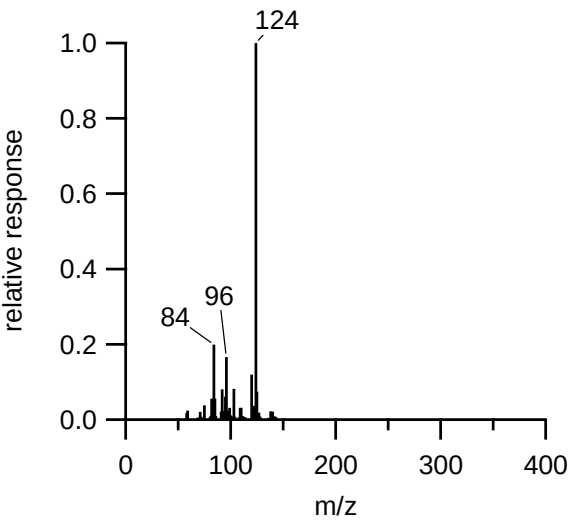
2(3H)-Benzofuranone, 3-methyl-
CAS #32267-71-3, MW=148.05 (11 ppm)



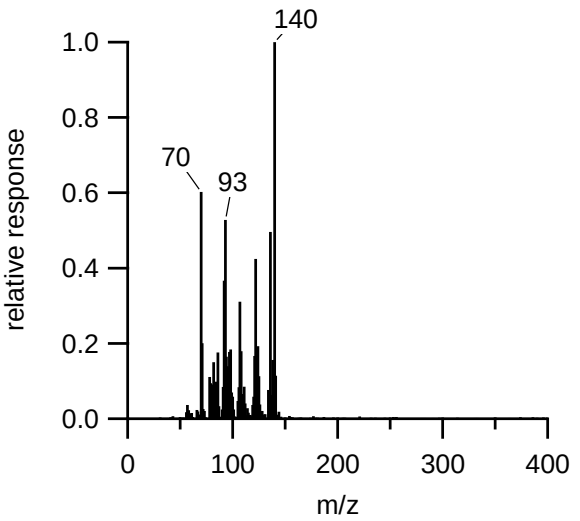
1H-Indene-1,3(2H)-dione
CAS #606-23-5, MW=146.04 (21 ppm)



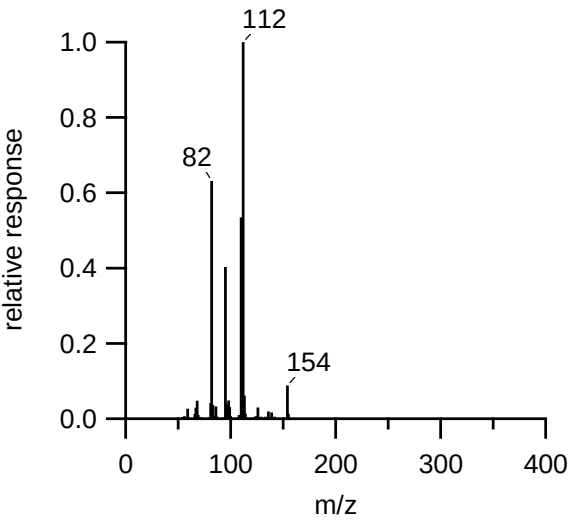
3-Cyclohexene-1-carboxaldehyde, 4-methyl-
CAS #7560-64-7, MW=124.09 (17 ppm)



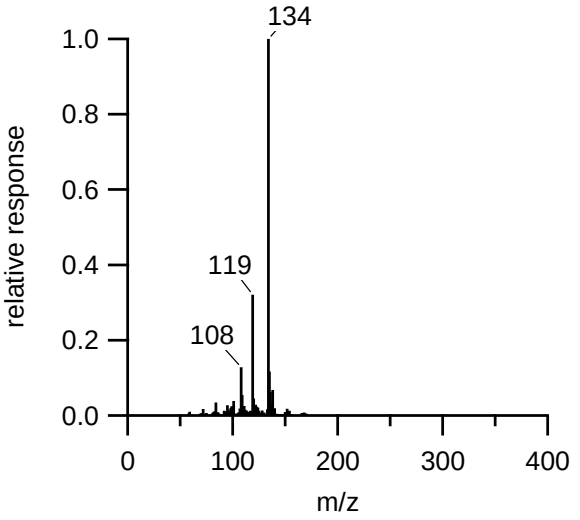
Bicyclo[2.2.2]octan-1-ol, 4-methyl-
CAS #824-13-5, MW=140.12 (11 ppm)



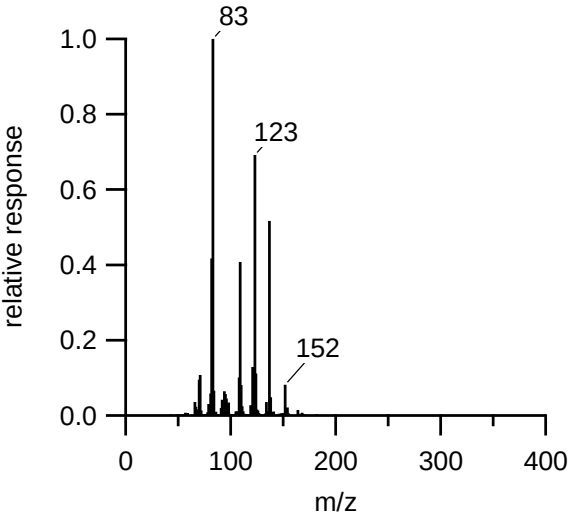
2-Oxabicyclo[3.2.1]nonan-7-one, 1,5-dimethyl-
CAS #13747-98-3, MW=154.1 (26 ppm)



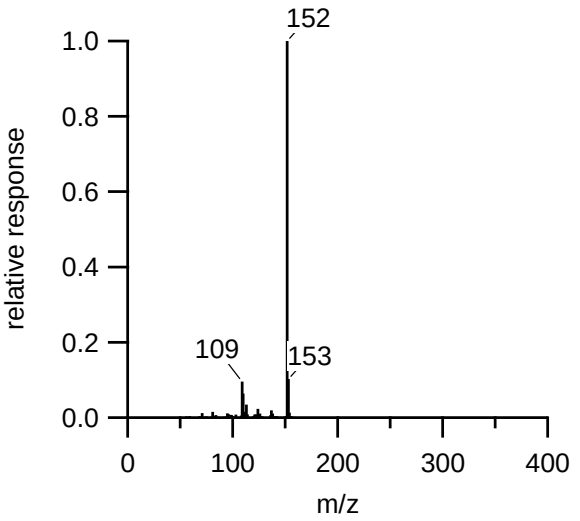
3-Cyclohexen-1-carboxaldehyde, 3,4-dimethyl-
CAS #0-00-0, MW=138.1 (12 ppm)



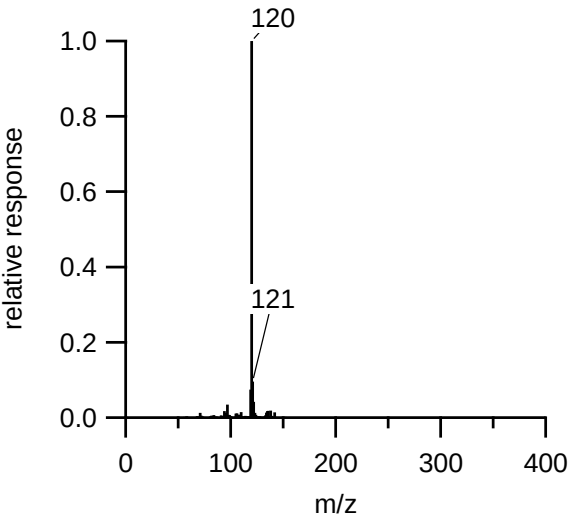
Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-
CAS #4764-14-1, MW=152.12 (25 ppm)



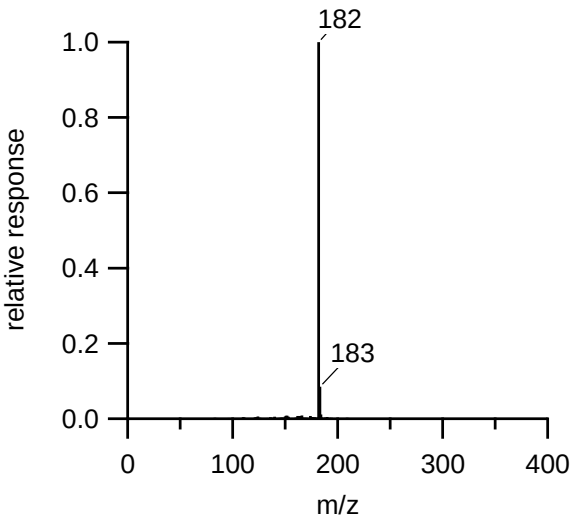
2-Acetyl-4,4-dimethyl-cyclopent-2-enone
CAS #81979-96-6, MW=152.08 (19 ppm)



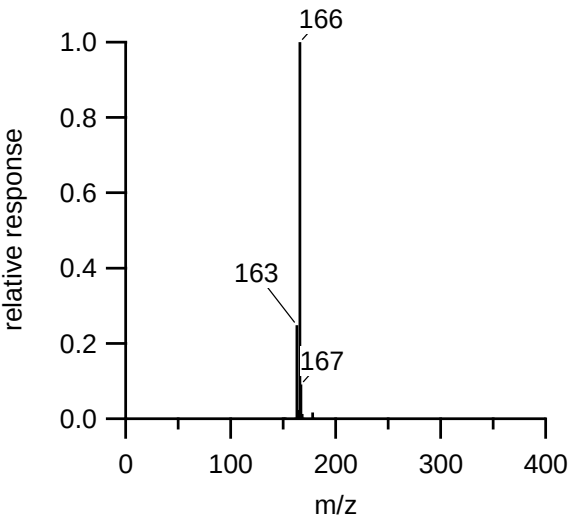
Benzene, 1-ethyl-2-methyl-
CAS #98-86-2, MW=120.09 (18 ppm)



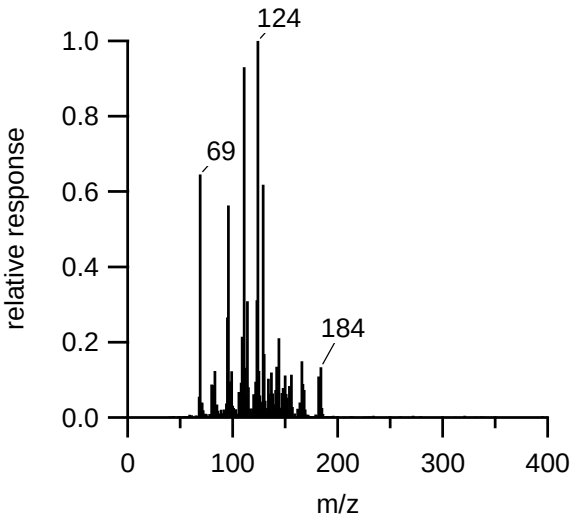
Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester
CAS #3943-74-6, MW=182.06 (45 ppm)



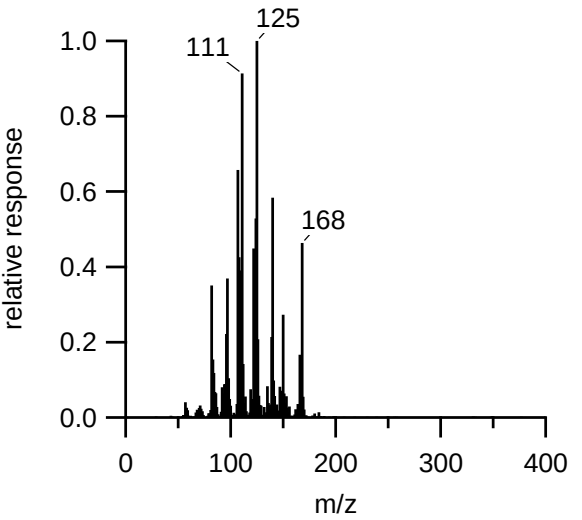
Ethanone, 1-[4-(1-hydroxy-1-methylethyl)phenyl]-
CAS #54549-72-3, MW=178.1 (33 ppm)



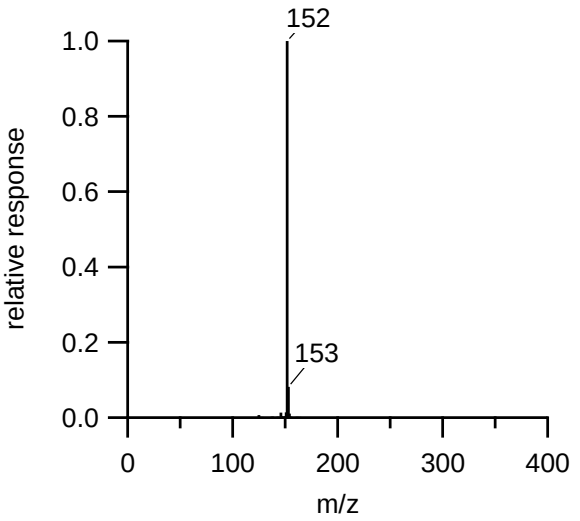
Cyclooctanone, 5-(acetyloxy)-
CAS #22253-83-4, MW=184.11 (27 ppm)



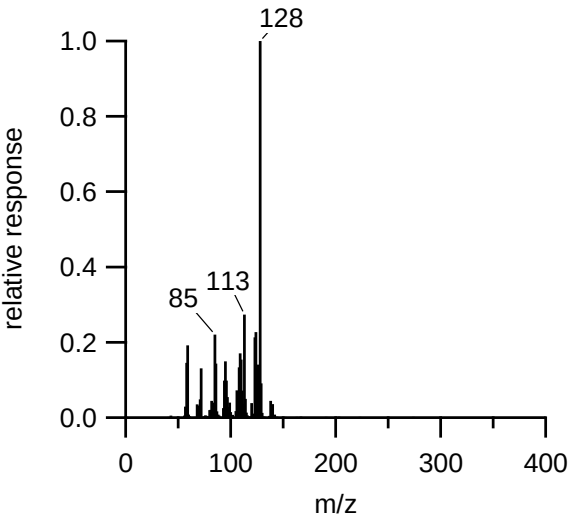
5H-Inden-5-one, octahydro-1-hydroxy-7a-methyl-
CAS #42199-04-2, MW=168.12 (23 ppm)



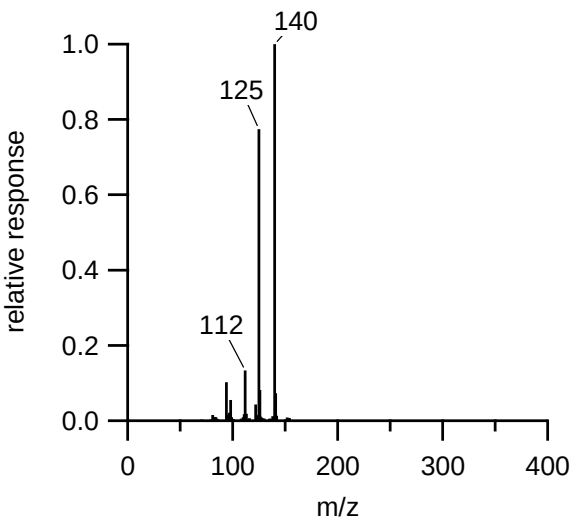
Vanillin
CAS #121-33-5, MW=152.05 (46 ppm)



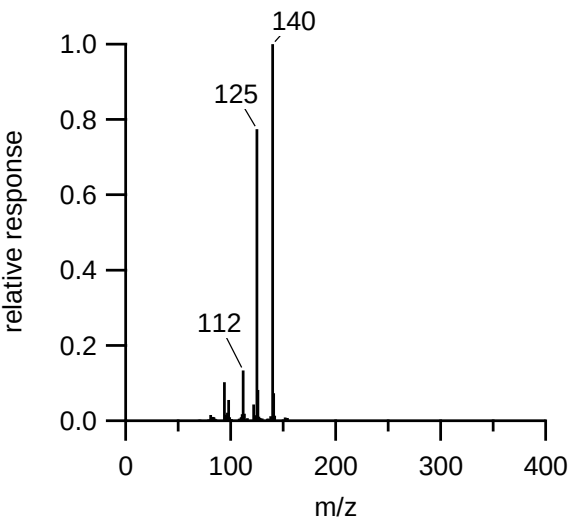
2-Octanone
CAS #111-13-7, MW=128.12 (12 ppm)



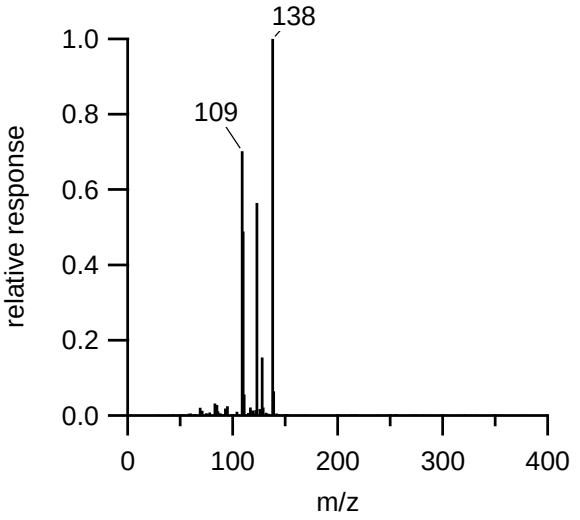
Cyclohexanone, 2-acetyl-
CAS #874-23-7, MW=140.08 (29 ppm)



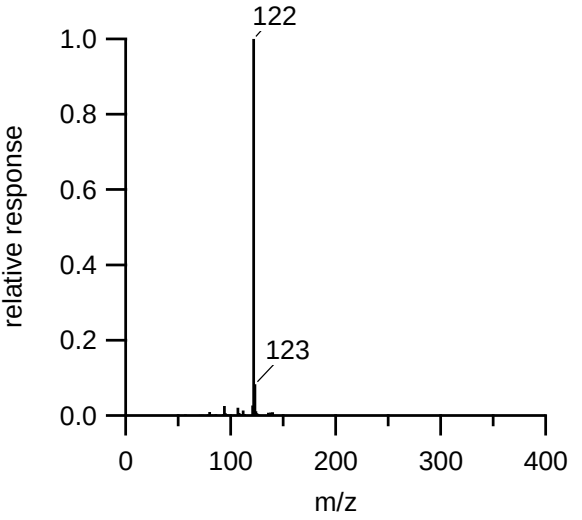
2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2,5-dimethyl-
CAS #1920-21-4, MW=140.08 (38 ppm)



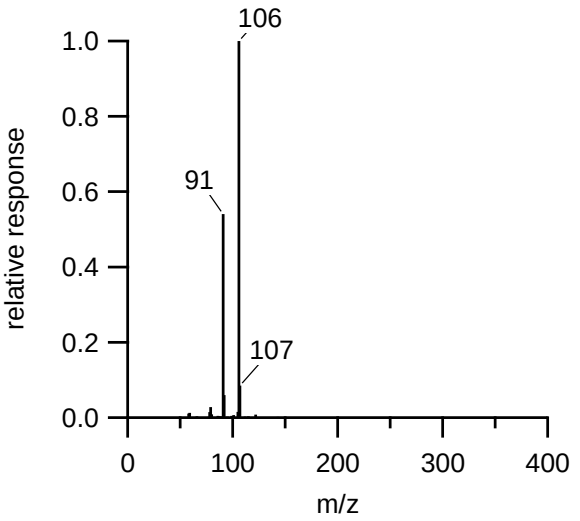
1-(2,4-Dimethyl-furan-3-yl)-ethanone
CAS #32933-07-6, MW=138.07 (13 ppm)



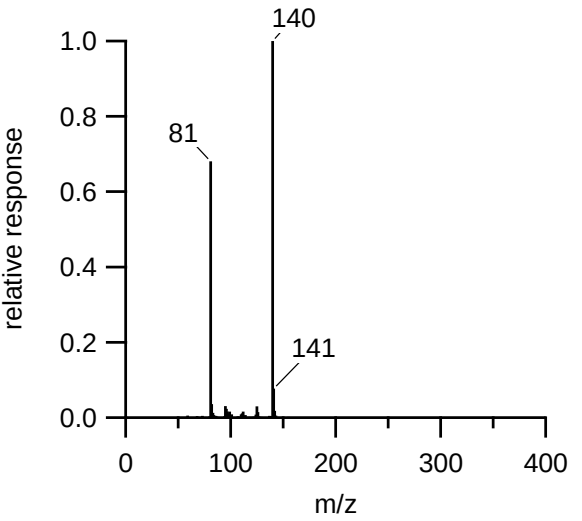
4,4-Dimethylcyclohexadienone
CAS #1073-14-9, MW=122.07 (38 ppm)



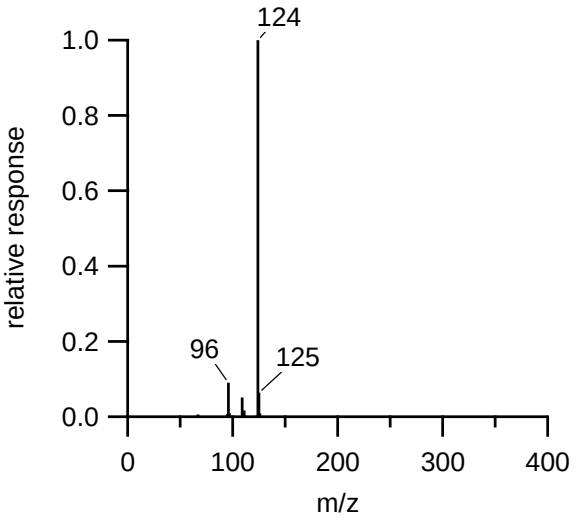
p-Xylene
CAS #106-42-3, MW=106.08 (14 ppm)



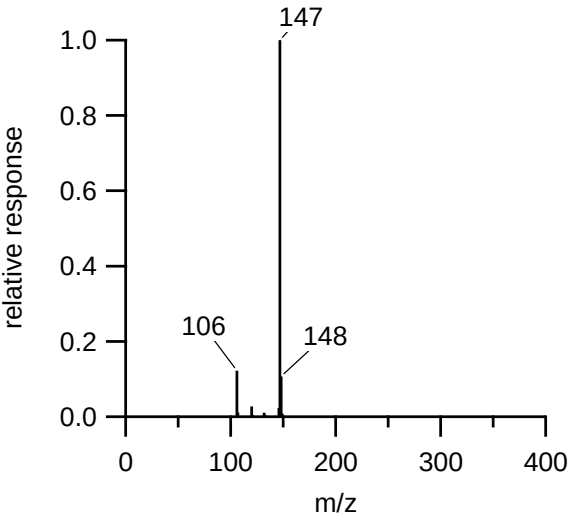
2-Furanpropionic acid
CAS #935-13-7, MW=140.05 (31 ppm)



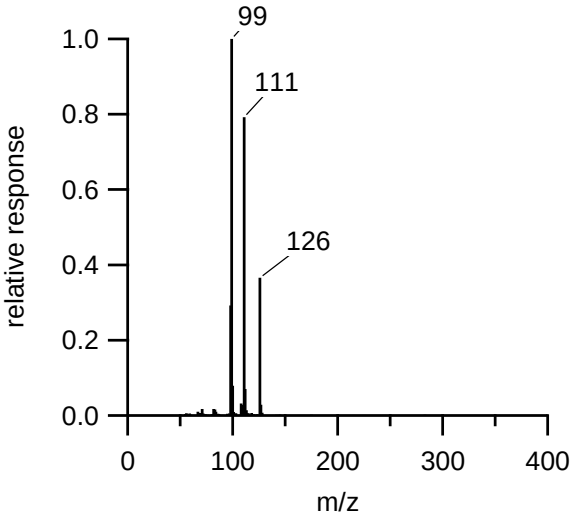
5-Ethyl-2-furaldehyde
CAS #23074-10-4, MW=124.05 (28 ppm)



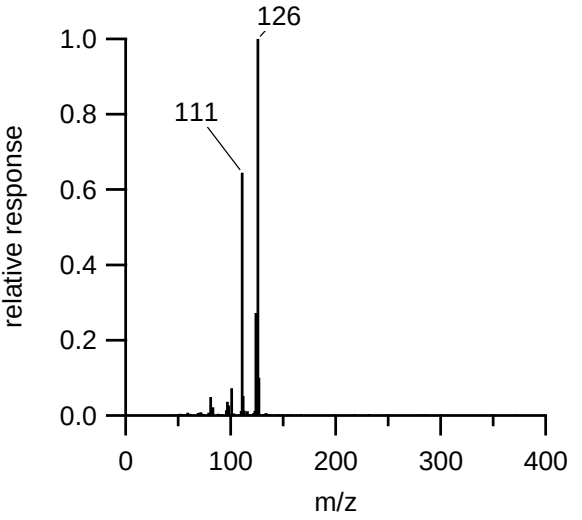
Benzenamine, 2-(1-methylcyclopropyl)-
CAS #0-00-0, MW=147.1 (14 ppm)



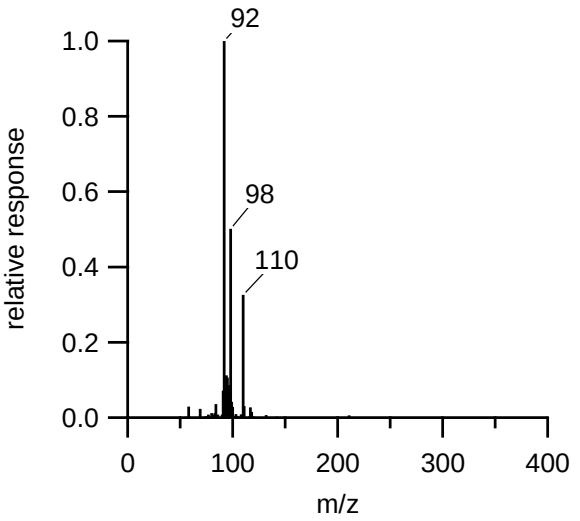
2(3H)-Furanone, 5-ethenyldihydro-5-methyl-
CAS #1073-11-6, MW=126.07 (21 ppm)



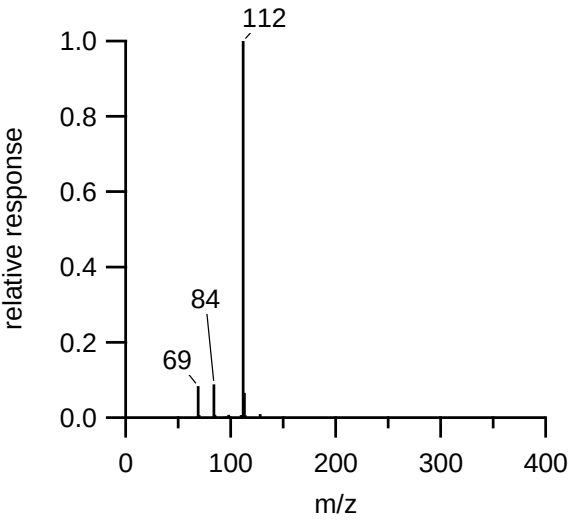
2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-
CAS #21835-00-7, MW=126.07 (21 ppm)



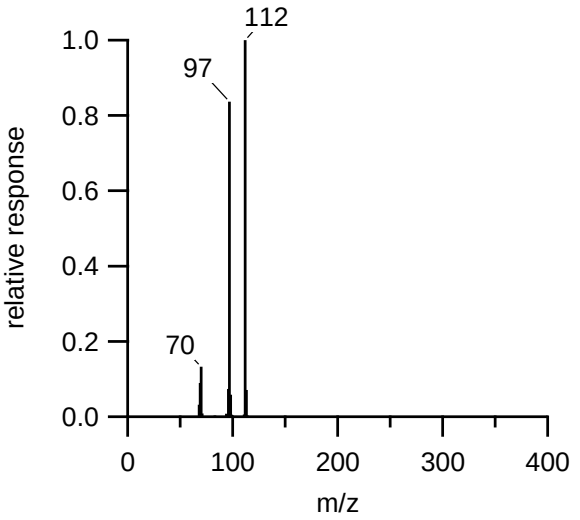
trans,trans-3,5-Heptadien-2-one
CAS #18402-90-9, MW=110.07 (28 ppm)



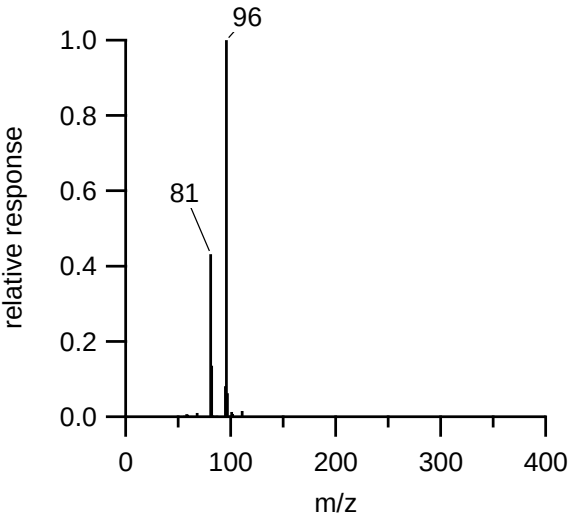
2-Furanone, 2,5-dihydro-3,5-dimethyl
CAS #3212-68-8, MW=112.05 (55 ppm)



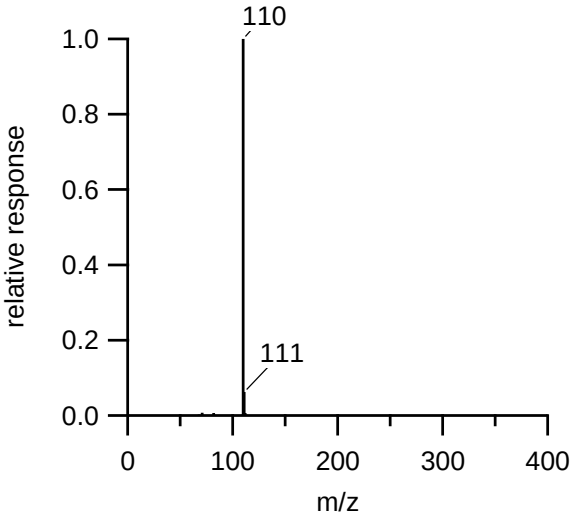
3-Penten-2-one, 3,4-dimethyl-
CAS #5166-53-0, MW=112.09 (56 ppm)



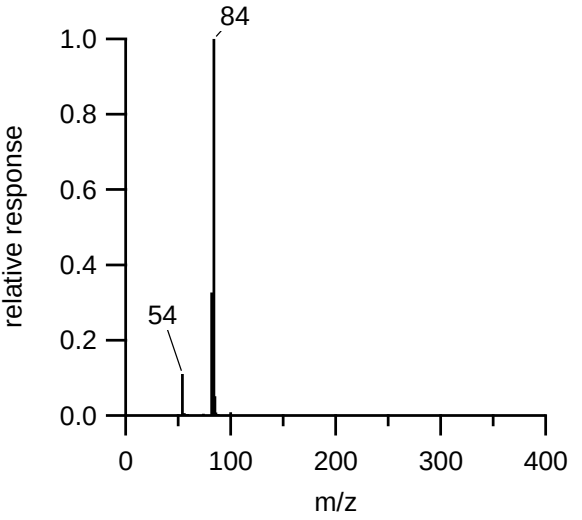
2,4-Hexadienal, (E,E)-
CAS #3710-43-8, MW=96.058 (45 ppm)



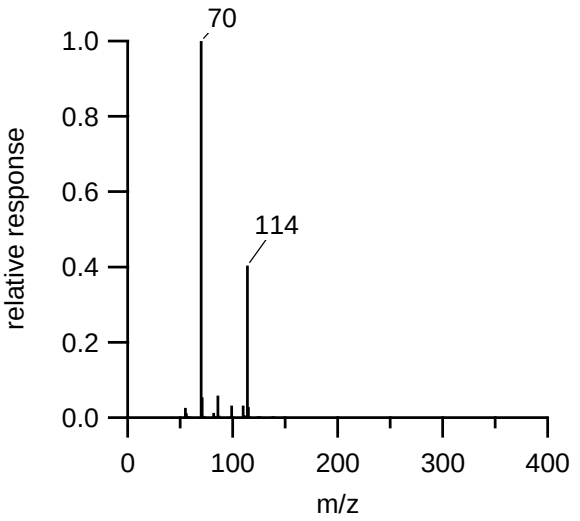
1,4-Cyclohex-2-enedione
CAS #4505-38-8, MW=110.04 (20 ppm)



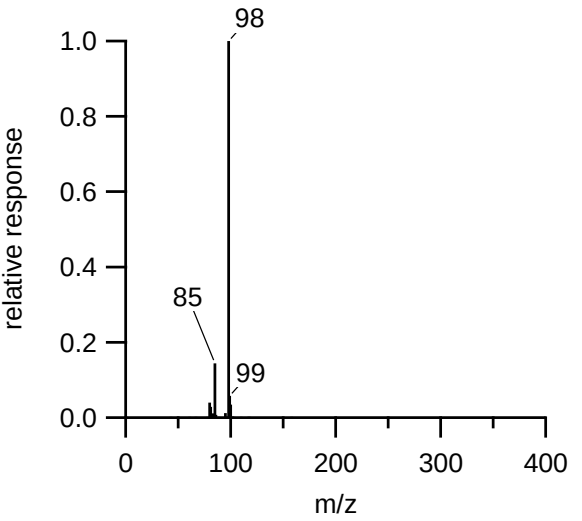
Furan, 2,3-dihydro-4-methyl-
CAS #1115-11-3, MW=84.058 (39 ppm)



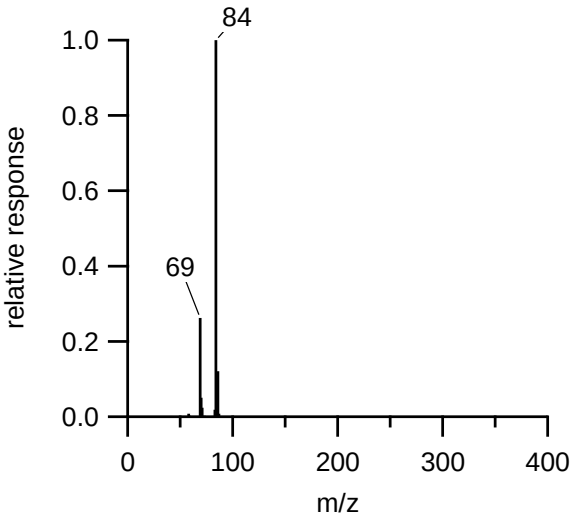
2H-Pyran-2-one, tetrahydro-6-methyl-
CAS #823-22-3, MW=114.07 (28 ppm)



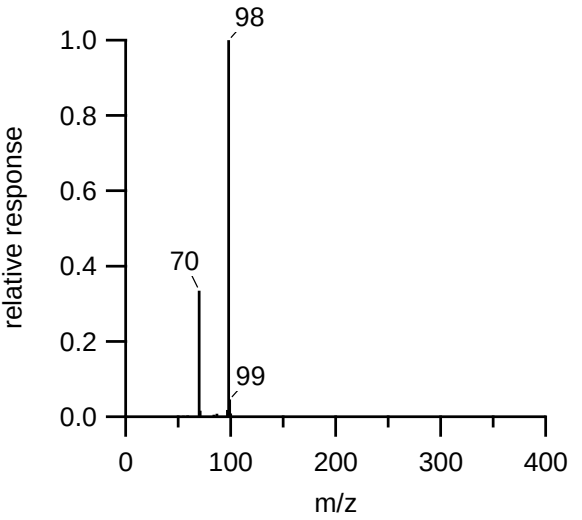
Cyclohexanone
CAS #108-94-1, MW=98.073 (34 ppm)



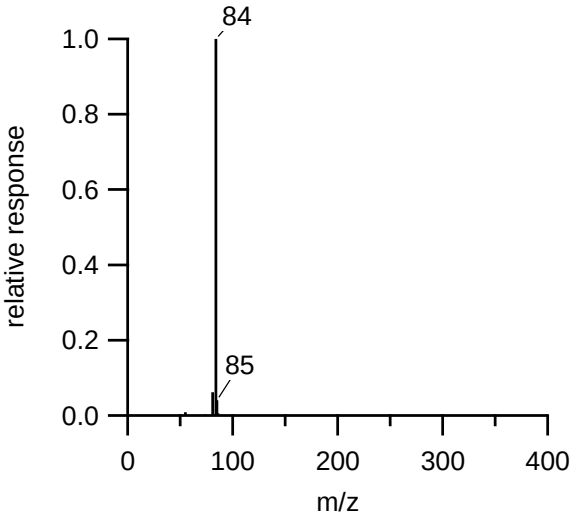
3-Buten-2-one, 3-methyl-
CAS #625-33-2, MW=84.058 (39 ppm)



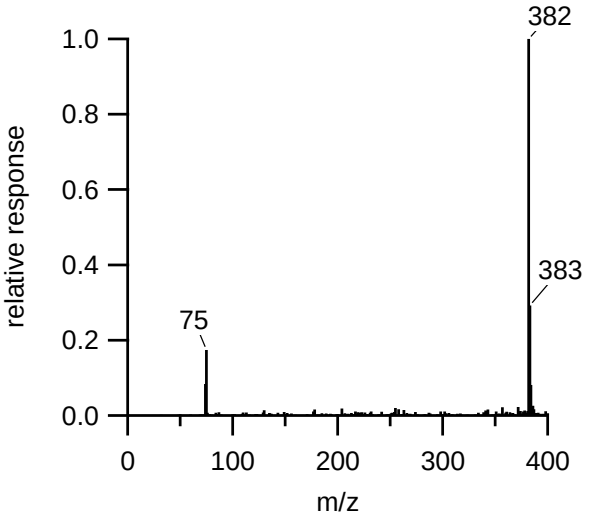
1,3-Cyclopentanedione
CAS #3859-41-4, MW=98.037 (63 ppm)



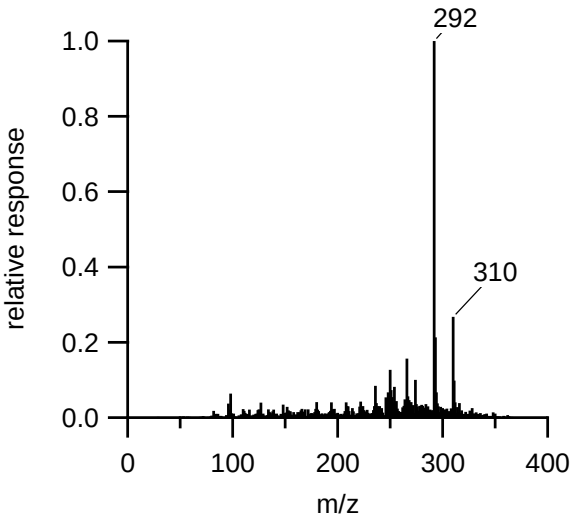
2(5H)-Furanone
CAS #497-23-4, MW=84.021 (99 ppm)



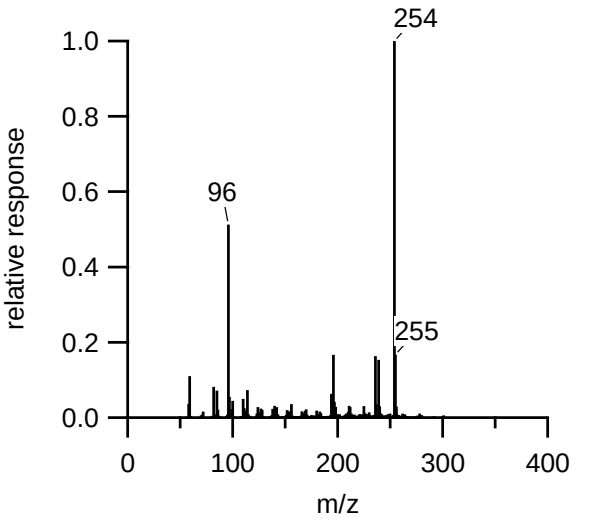
Tetracosanoic acid, methyl ester
CAS #2442-49-1, MW=382.38 (12 ppm)



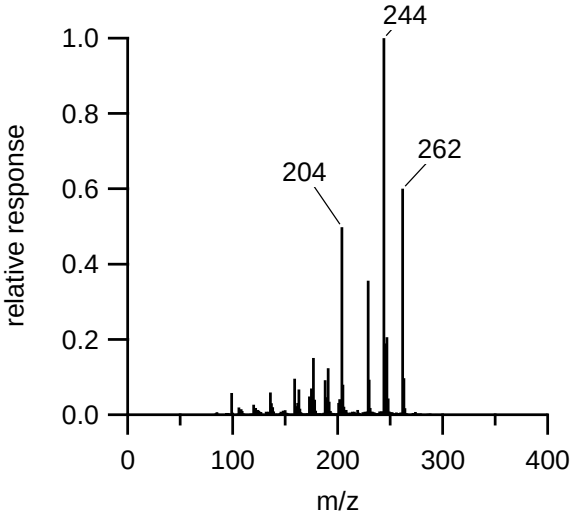
cis-13-Eicosenoic acid
CAS #17735-94-3, MW=310.29 (77 ppm)



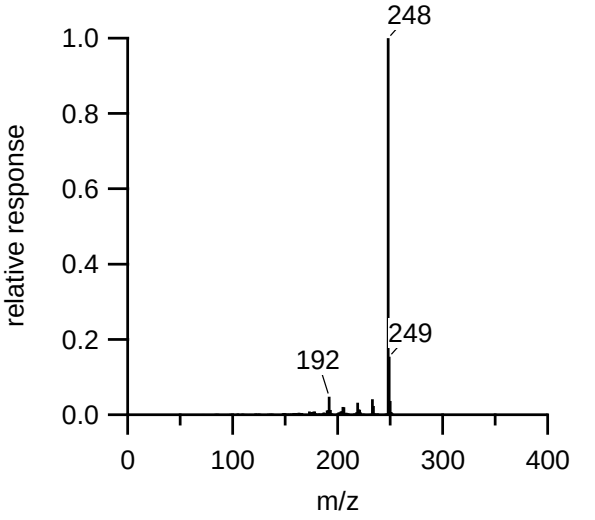
2-Heptadecanone
CAS #2922-51-2, MW=254.26 (6 ppm)



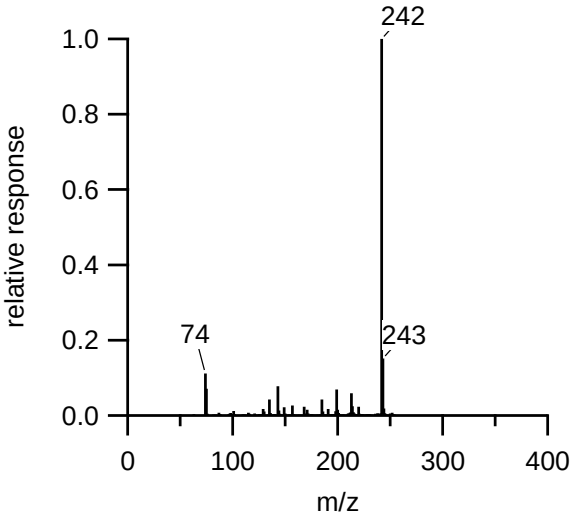
14-Oxatricyclo[9..2.1.0(1,10)]tetradecane, 2,6,6,10,11-pent
CAS #0-00-0, MW=262.23 (18 ppm)



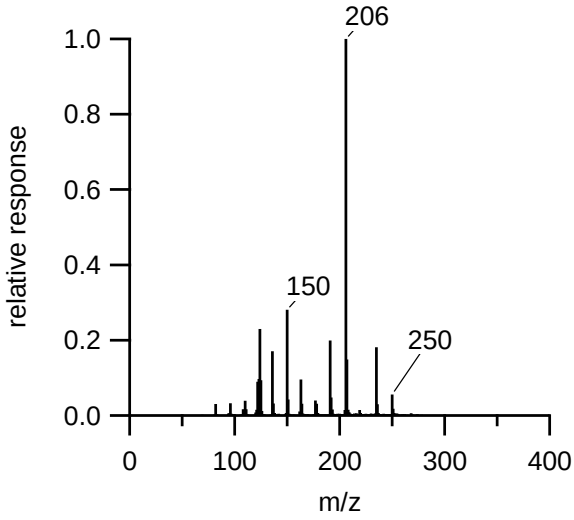
2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylpropyl)-
CAS #4584-63-8, MW=248.18 (18 ppm)



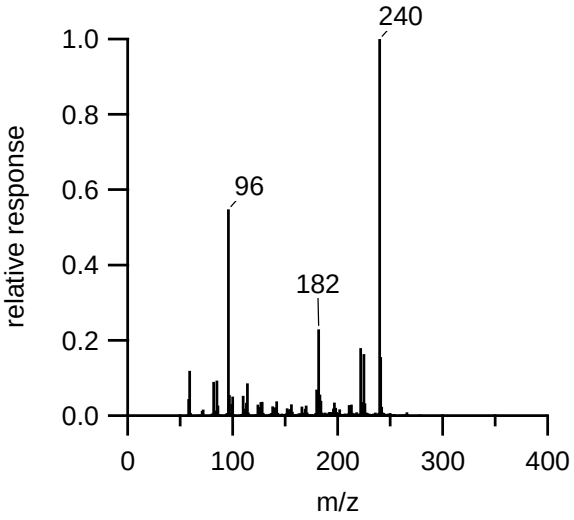
Tridecanoic acid, 12-methyl-, methyl ester
CAS #5129-58-8, MW=242.22 (13 ppm)



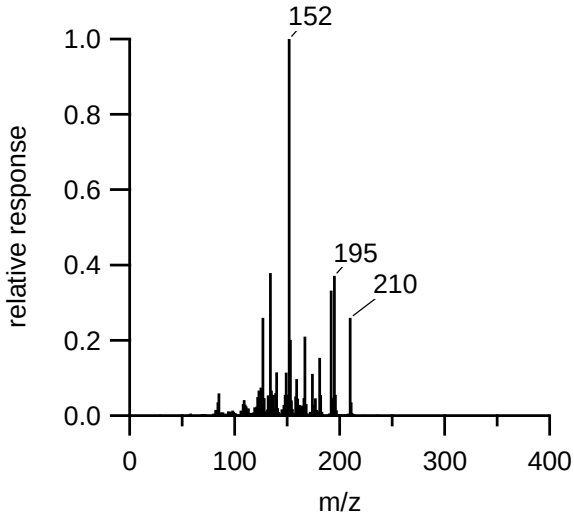
Sclareolide
CAS #564-20-5, MW=250.19 (52 ppm)



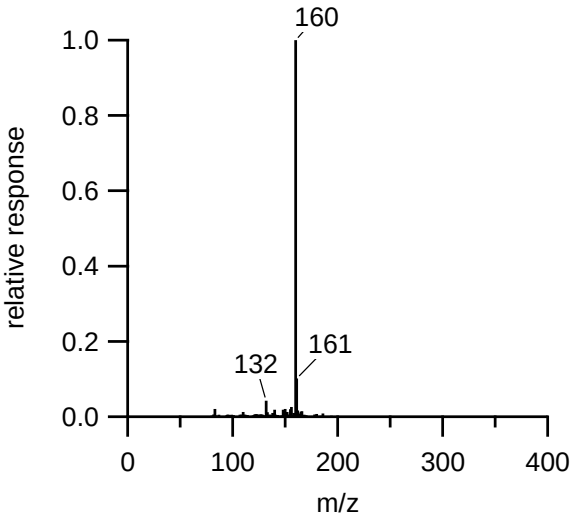
2-Hexadecanone
CAS #18787-63-8, MW=240.25 (4 ppm)



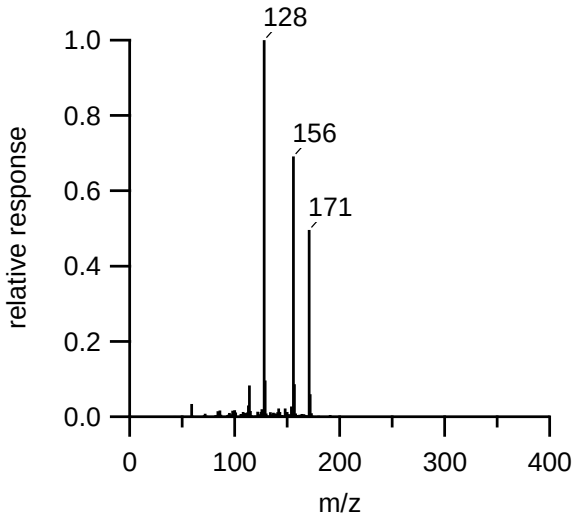
Spiro(2-oxabicyclo[2.1.0]pentane)-3,2'-oxetane, 1,5,5,3',3',4',
CAS #0-00-0, MW=210.16 (21 ppm)



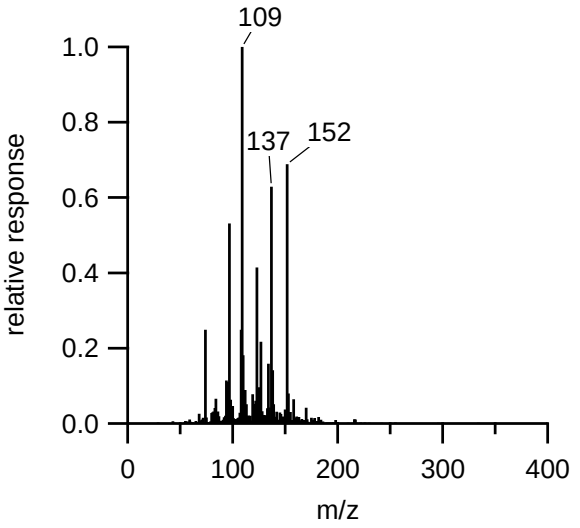
Coumarin, 8-methyl-
CAS #1807-36-9, MW=160.05 (31 ppm)



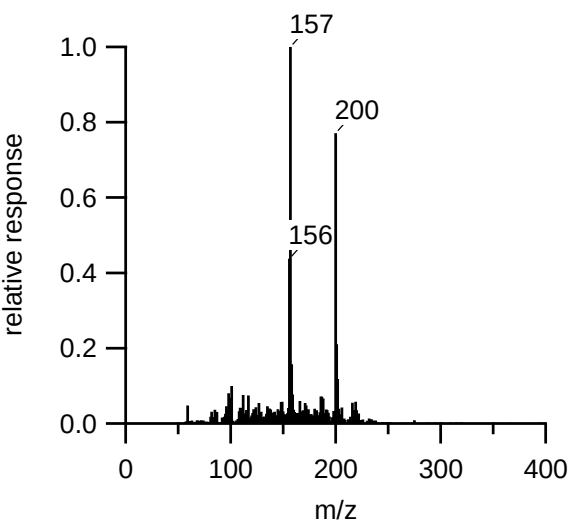
Acetamide, N,N-dibutyl-
CAS #1563-90-2, MW=171.16 (18 ppm)



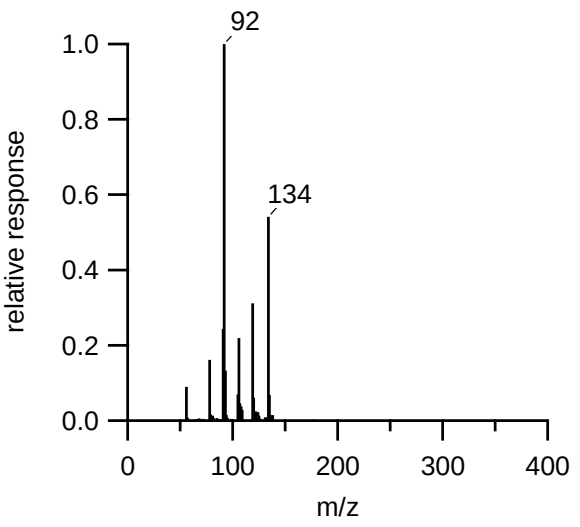
2-Isopropylidene-5-methylhex-4-enal
CAS #3304-28-7, MW=152.12 (25 ppm)



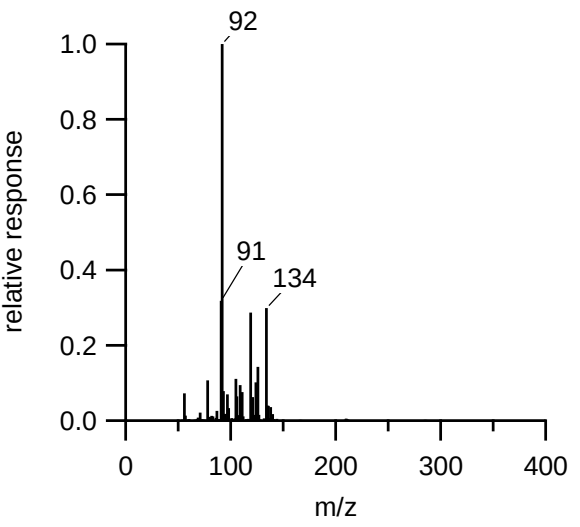
à-Calacorene
CAS #21391-99-1, MW=200.16 (36 ppm)



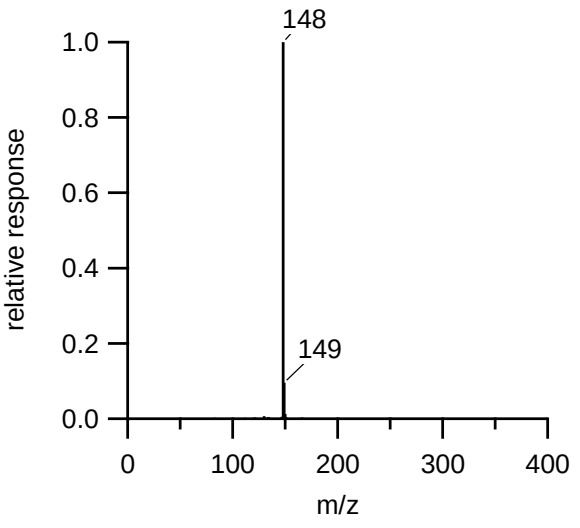
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene
CAS #4488-57-7, MW=134.11 (17 ppm)



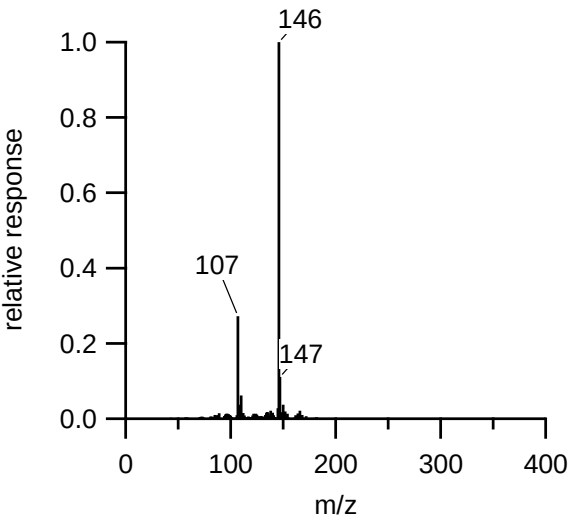
Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)-
CAS #36262-09-6, MW=134.11 (17 ppm)



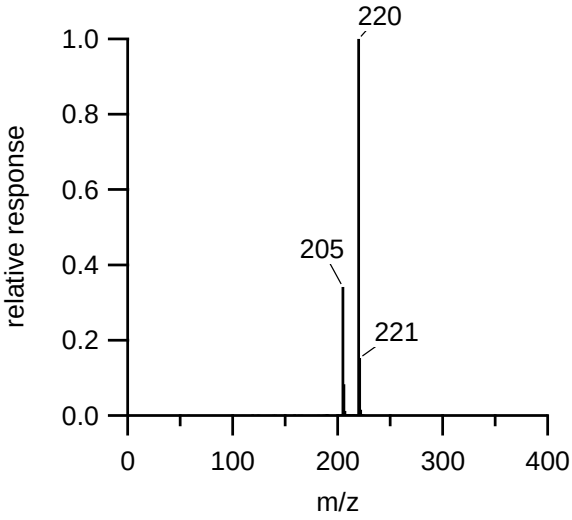
2-Allyl-4-methylphenol
CAS #3354-58-3, MW=148.09 (35 ppm)



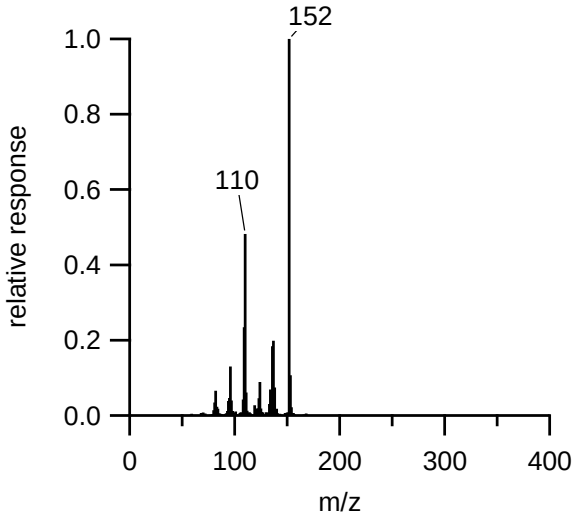
Cinnamaldehyde, á-methyl-
CAS #101-39-3, MW=146.07 (52 ppm)



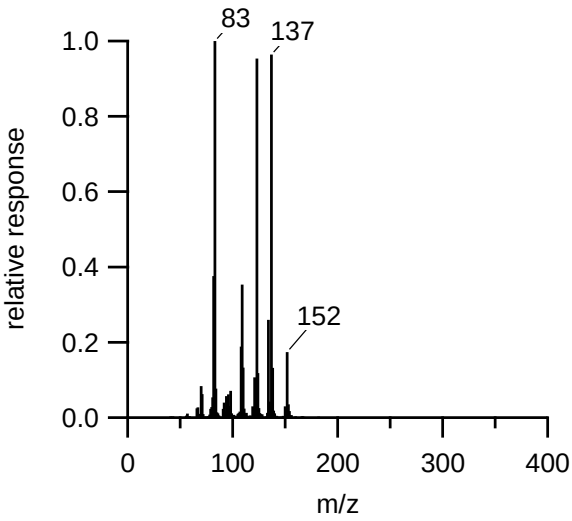
Butylated Hydroxytoluene
CAS #128-37-0, MW=220.18 (28 ppm)



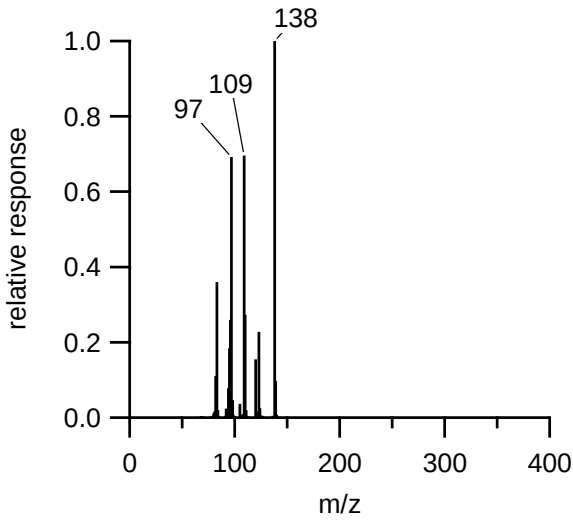
Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl-, [1R-(1à,4á,6à)]-
CAS #4176-04-9, MW=152.12 (25 ppm)



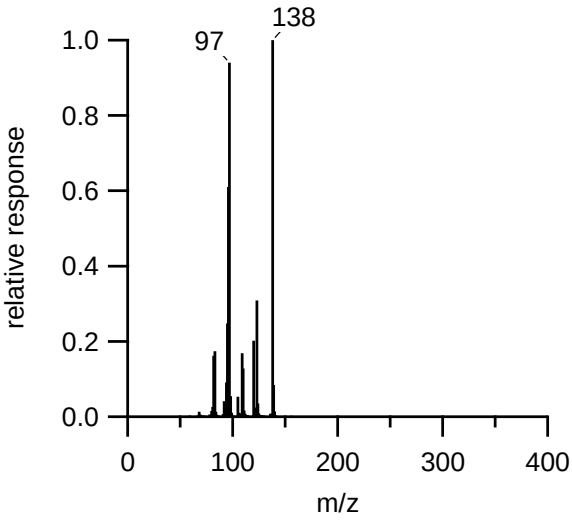
Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-
CAS #4764-14-1, MW=152.12 (25 ppm)



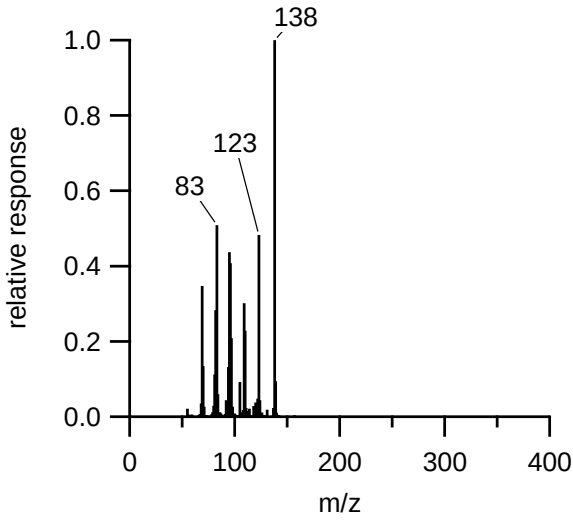
Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-
CAS #38651-65-9, MW=138.1 (12 ppm)



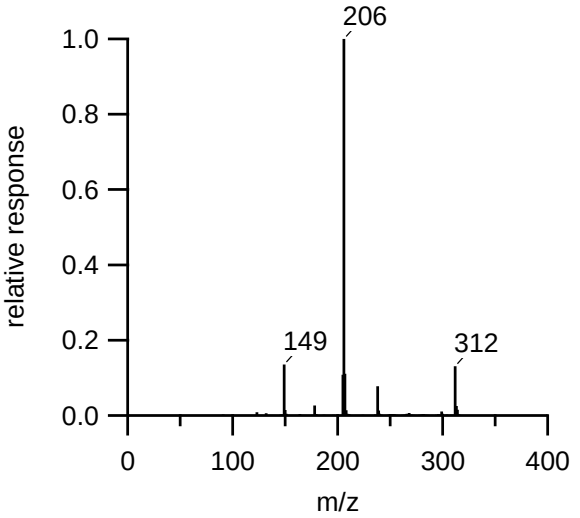
Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)-
CAS #513-20-2, MW=138.1 (12 ppm)



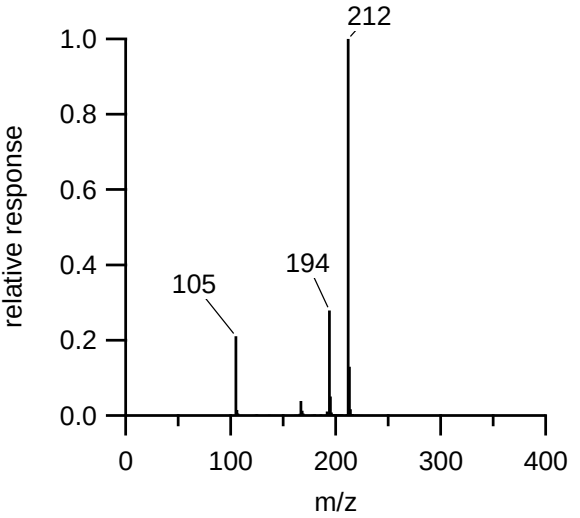
Bicyclo[2.2.1]heptan-2-one, 3,3-dimethyl-
CAS #13211-15-9, MW=138.1 (12 ppm)



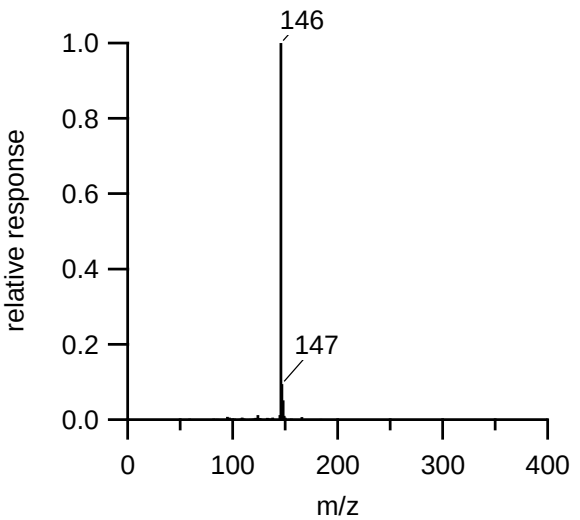
Benzyl butyl phthalate
CAS #85-68-7, MW=312.14 (2 ppm)



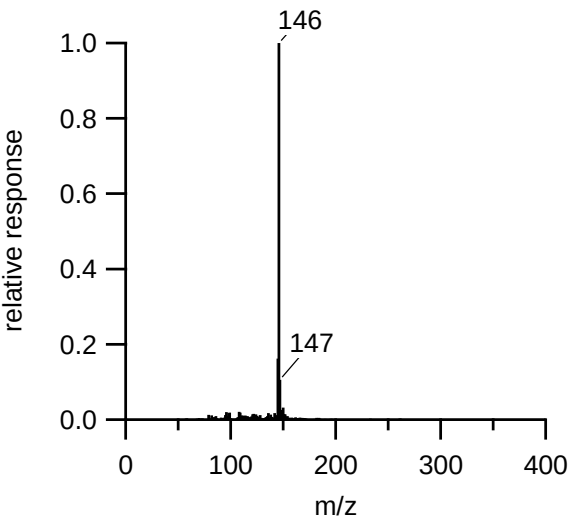
Benzyl Benzoate
CAS #120-51-4, MW=212.08 (8 ppm)



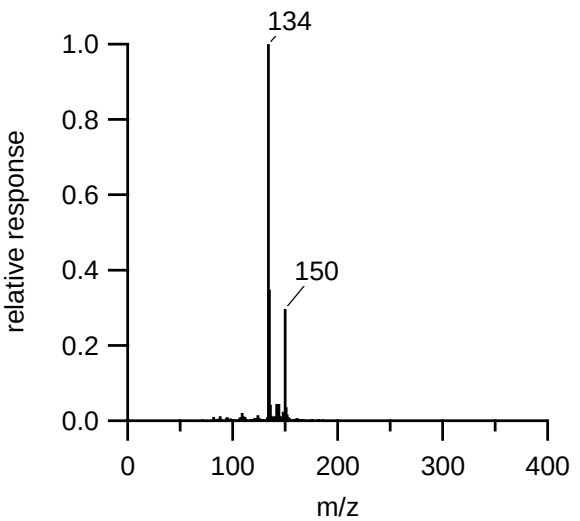
Benzofuran, 4,7-dimethyl-
CAS #28715-26-6, MW=146.07 (52 ppm)



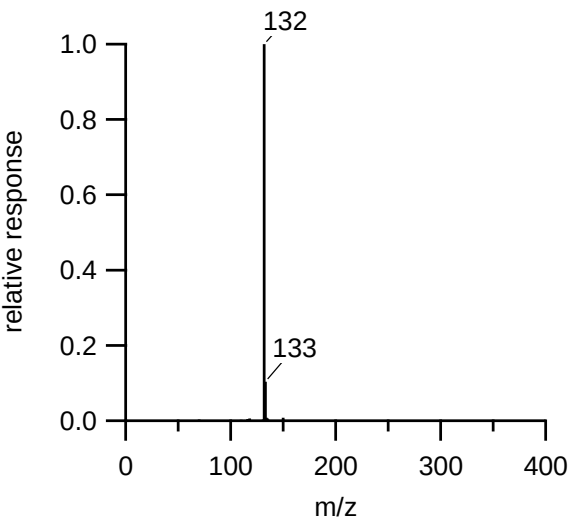
Benzofuran, 4,7-dimethyl-
CAS #28715-26-6, MW=146.07 (42 ppm)



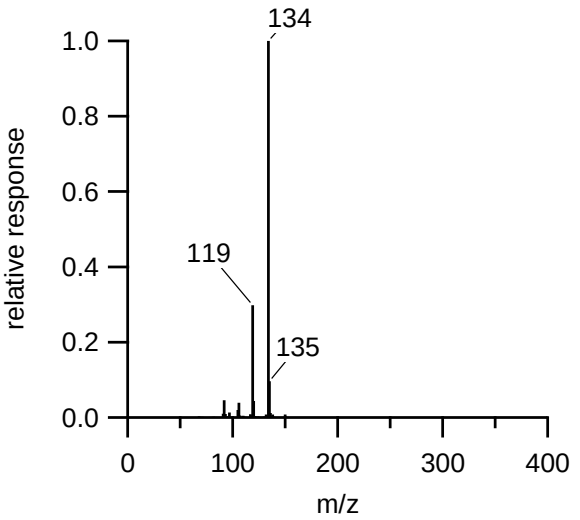
p-Cymen-7-ol
CAS #536-60-7, MW=150.1 (35 ppm)



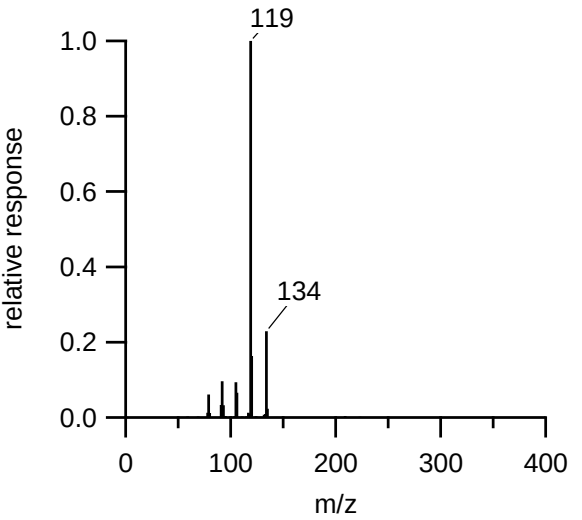
Benzene, 1-methyl-4-(1-methylethenyl)-
CAS #1195-32-0, MW=132.09 (21 ppm)



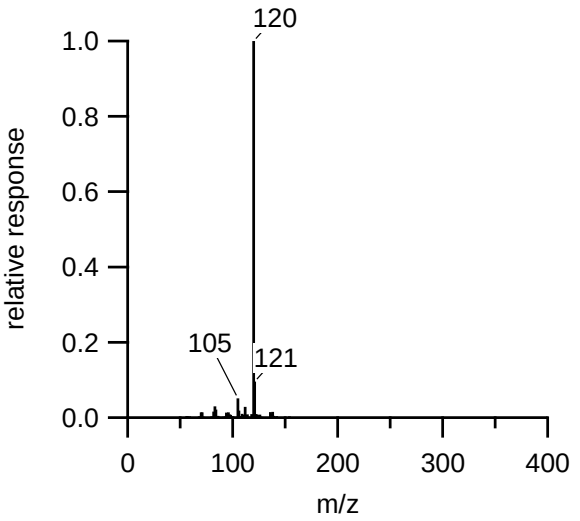
o-Cymene
CAS #535-77-3, MW=134.11 (17 ppm)



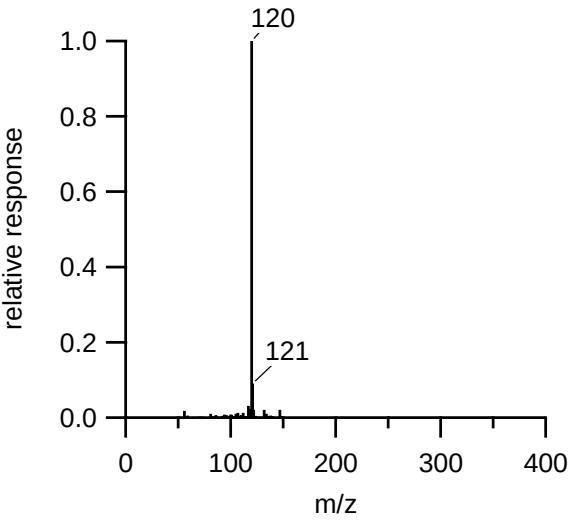
1,3,5-Cycloheptatriene, 3,7,7-trimethyl-
CAS #3479-89-8, MW=134.11 (17 ppm)



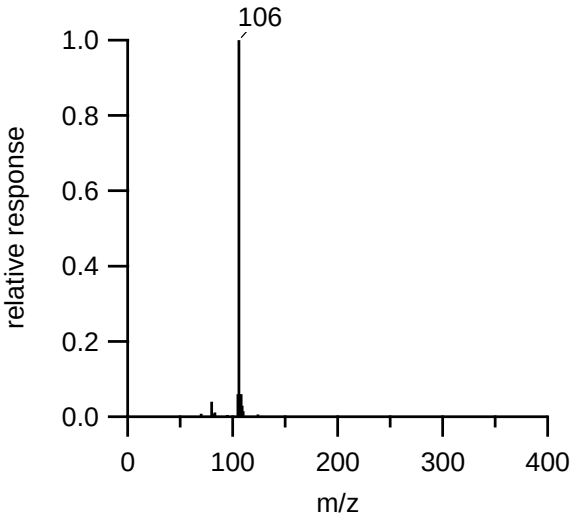
Benzene, 1-ethyl-2-methyl-
CAS #98-82-8, MW=120.09 (18 ppm)



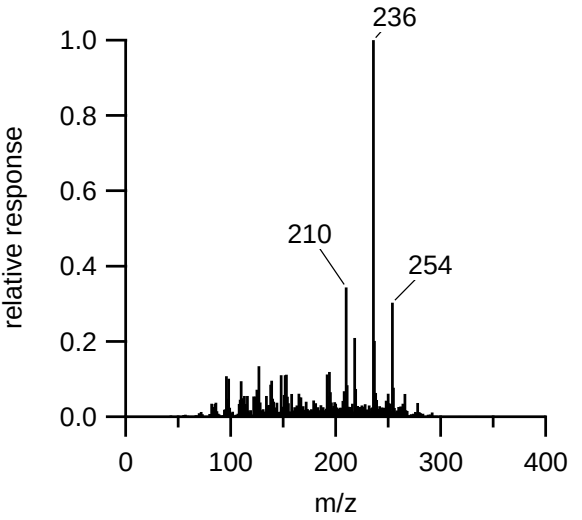
Benzene, 1-ethyl-4-methyl-
CAS #98-82-8, MW=120.09 (18 ppm)



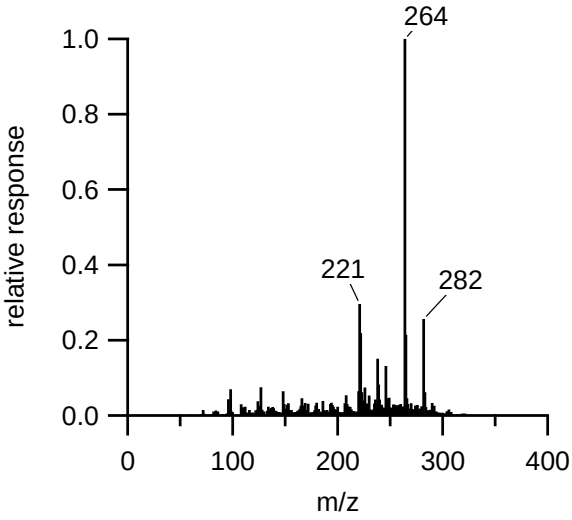
Benzaldehyde
CAS #100-52-7, MW=106.04 (0 ppm)



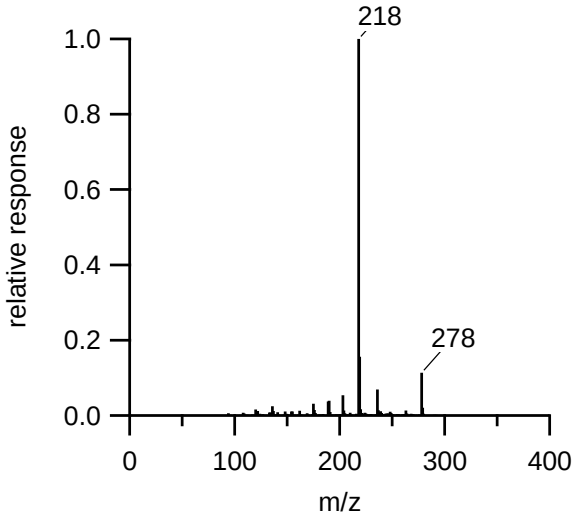
cis-9-Hexadecenoic acid
CAS #2416-20-8, MW=254.22 (63 ppm)



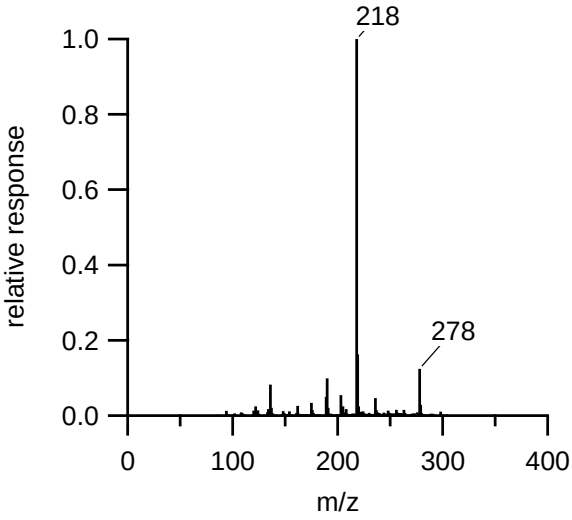
cis-Vaccenic acid
CAS #506-17-2, MW=282.26 (38 ppm)



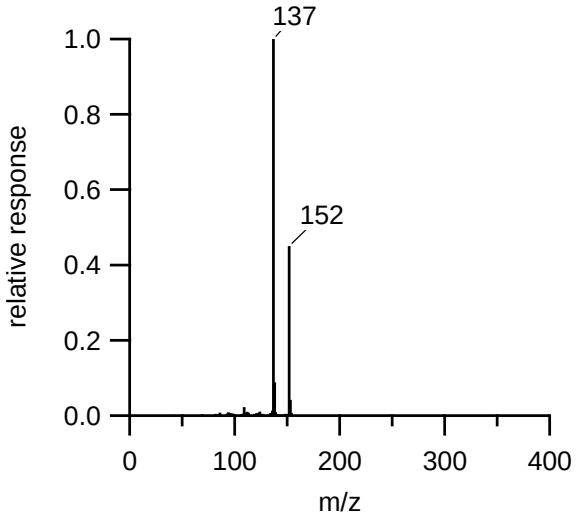
5H-3,5a-Epoxynaphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-t
CAS #1153-34-0, MW=278.22 (31 ppm)



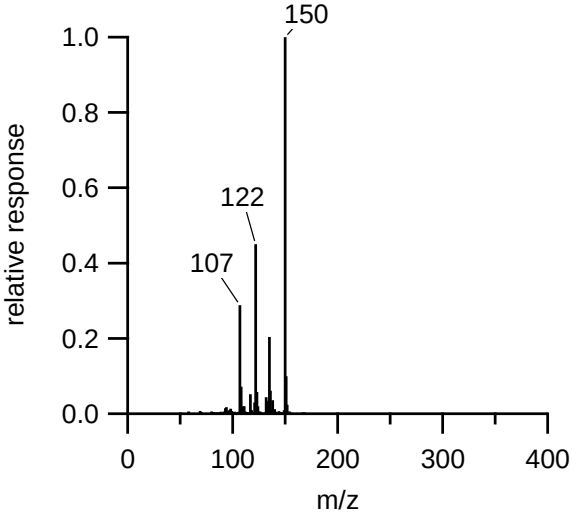
5H-3,5a-Epoxynaphth[2,1-c]oxepin, dodecahydro-3,8,8,11a
CAS #1153-34-0, MW=278.22 (31 ppm)



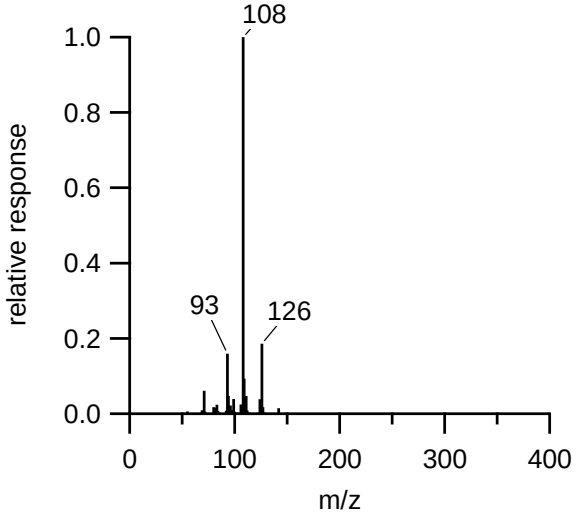
3-Isopropylidene-5-methyl-hex-4-en-2-one
CAS #64149-32-2, MW=152.12 (17 ppm)



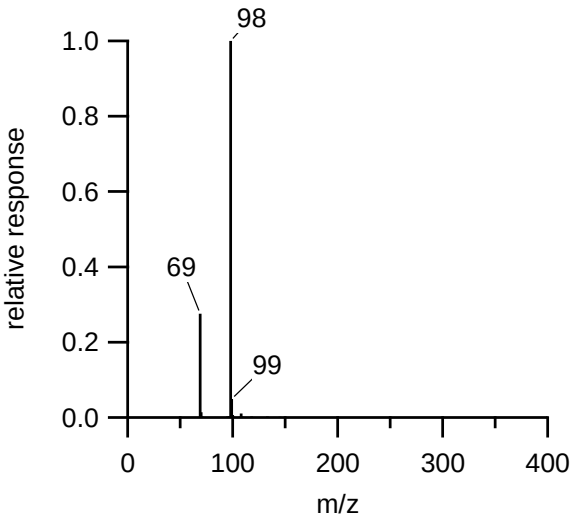
5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde
CAS #0-00-0, MW=150.1 (35 ppm)



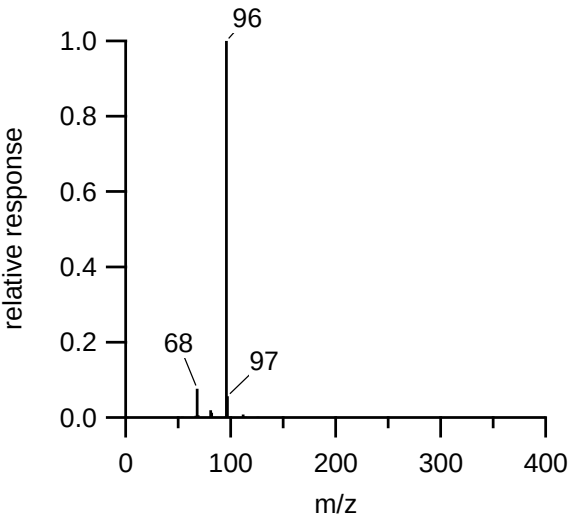
5-Hepten-2-one, 6-methyl-
CAS #110-93-0, MW=126.1 (34 ppm)



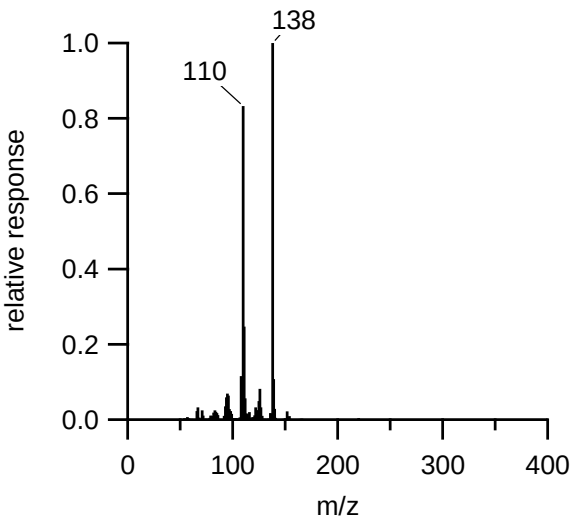
4-Methyl-5H-furan-2-one
CAS #6124-79-4, MW=98.037 (63 ppm)



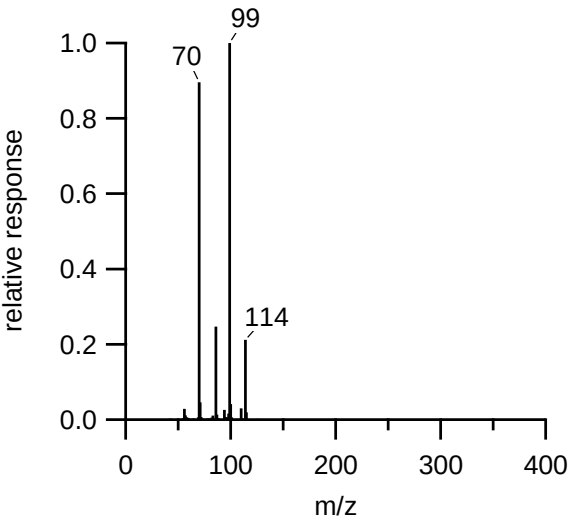
Bicyclo[3.1.0]hexan-3-one
CAS #1755-04-0, MW=96.058 (45 ppm)



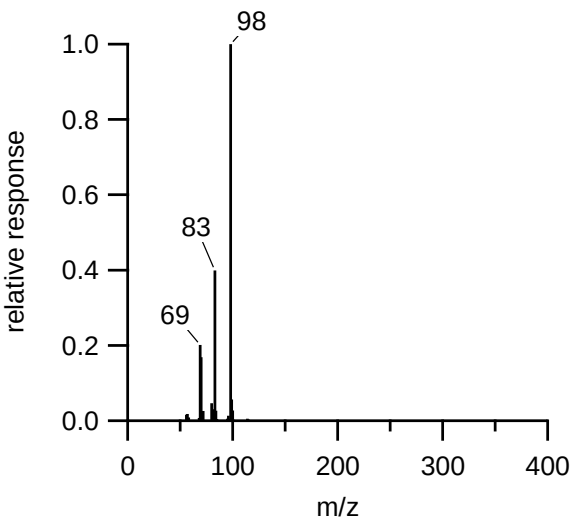
4-Cyclopentene-1,3-dione, 4-propyl-
CAS #58940-74-2, MW=138.07 (13 ppm)



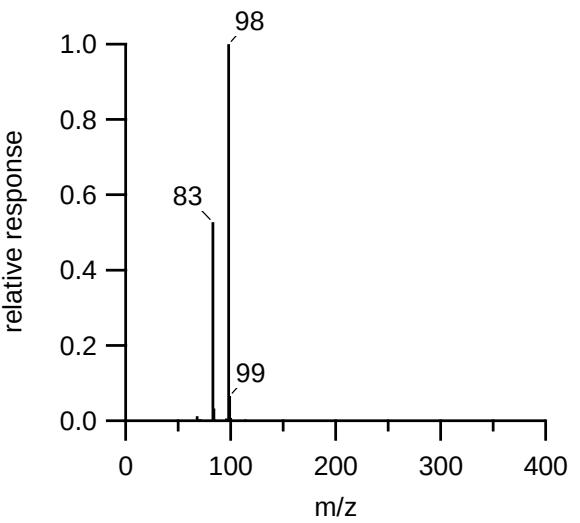
3-Pentenoic acid, 4-methyl-
CAS #504-85-8, MW=114.07 (28 ppm)



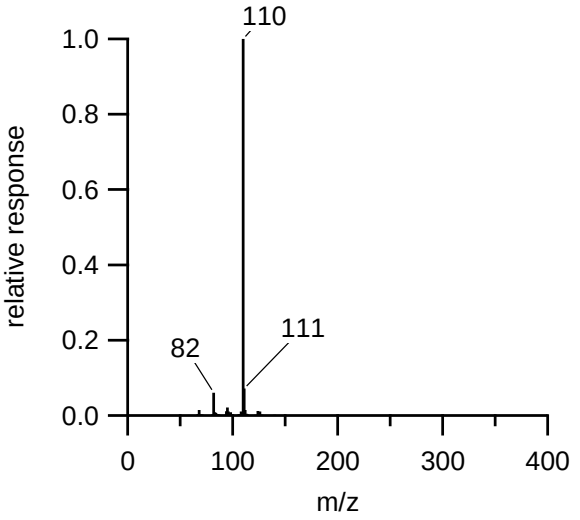
3-Pentenal, 4-methyl-
CAS #690-08-4, MW=98.073 (34 ppm)



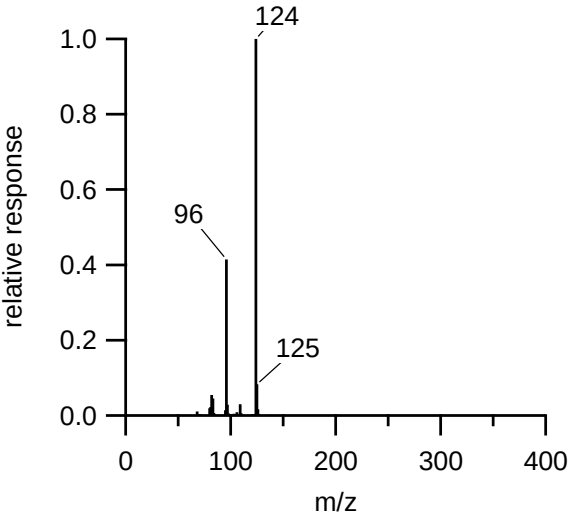
3-Penten-2-one, 4-methyl-
CAS #141-79-7, MW=98.073 (34 ppm)



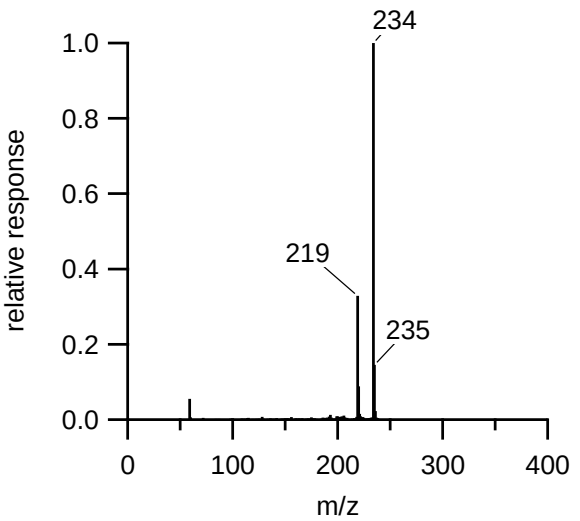
3-Methyl-3-cyclohexen-1-one
CAS #31883-98-4, MW=110.07 (28 ppm)



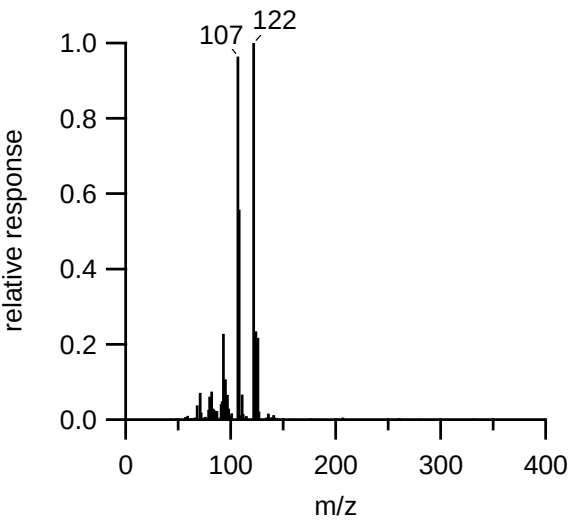
3-Ethenyl-3-methylcyclopentanone
CAS #49664-66-6, MW=124.09 (17 ppm)



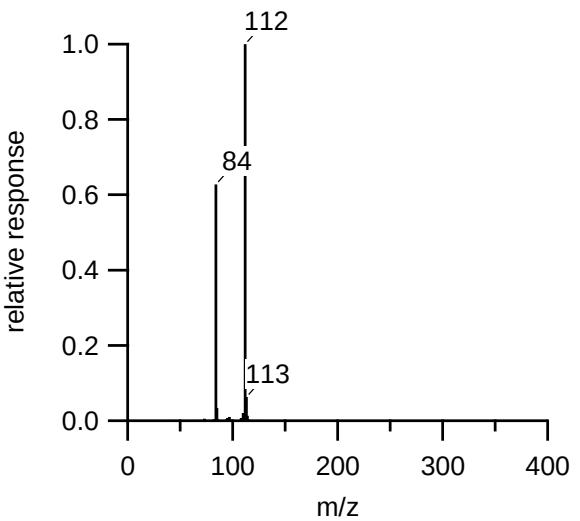
3,5-di-tert-Butyl-4-hydroxybenzaldehyde
CAS #1620-98-0, MW=234.16 (38 ppm)



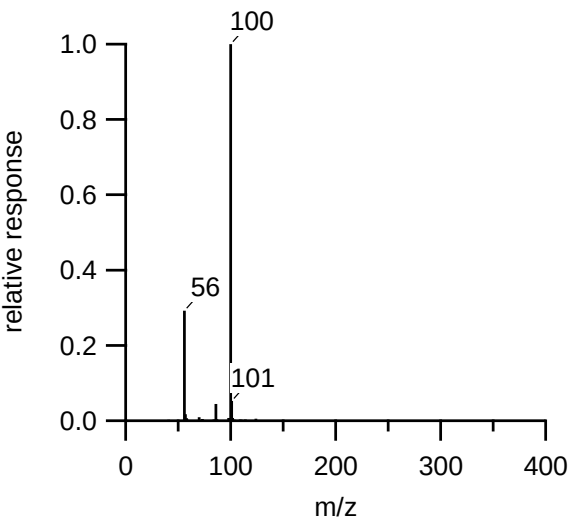
1,6-Dimethylhepta-1,3,5-triene
CAS #0-00-0, MW=122.11 (29 ppm)



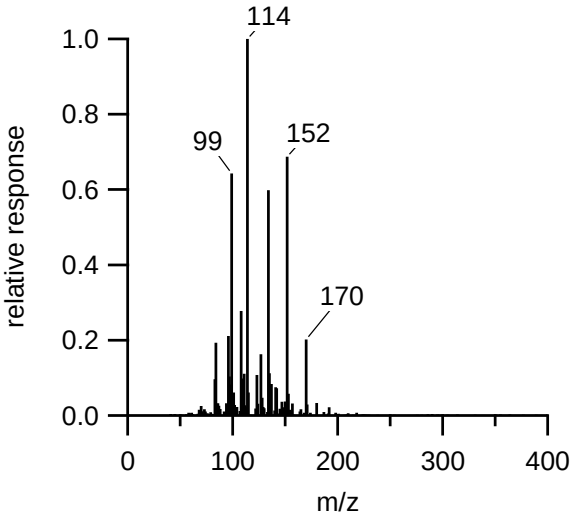
3,4-Dihydro-6-methyl-2H-pyran-2-one
CAS #3740-59-8, MW=112.05 (52 ppm)



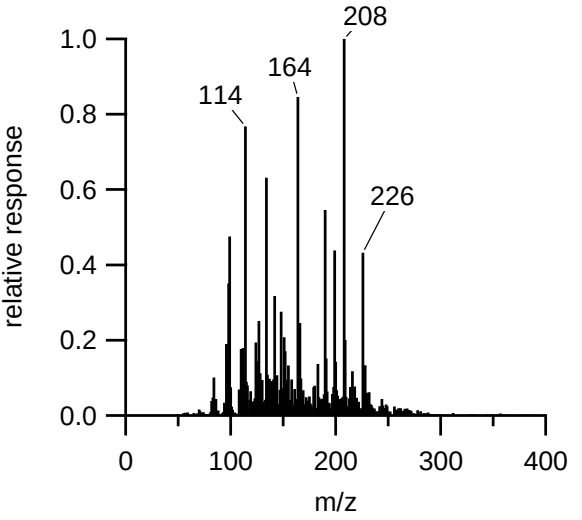
2H-Pyran-2-one, tetrahydro-
CAS #542-28-9, MW=100.05 (32 ppm)



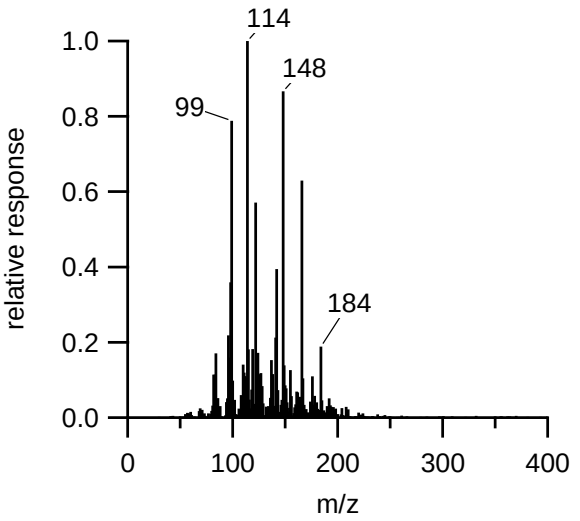
2H-Pyran-2-one, 6-pentyltetrahydro-
CAS #705-86-2, MW=170.13 (9 ppm)



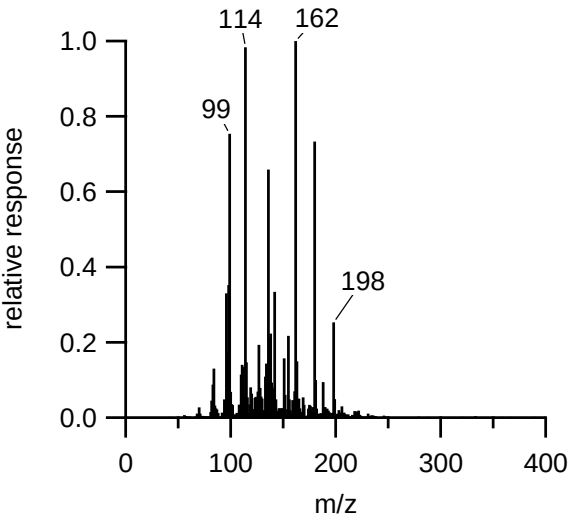
2H-Pyran-2-one, 6-nonyltetrahydro-
CAS #2721-22-4, MW=226.19 (52 ppm)



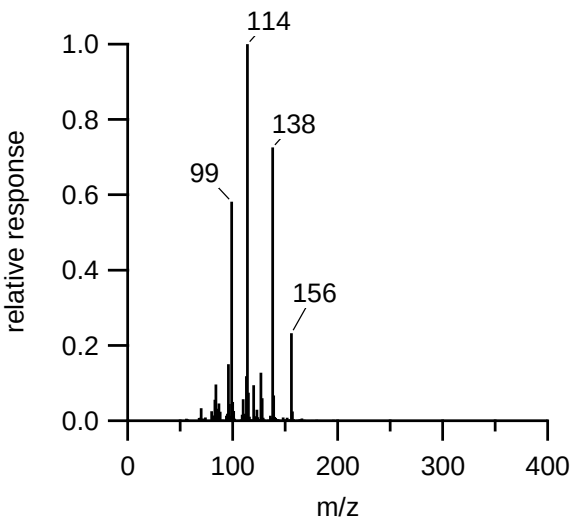
2H-Pyran-2-one, 6-hexyltetrahydro-
CAS #710-04-3, MW=184.15 (42 ppm)



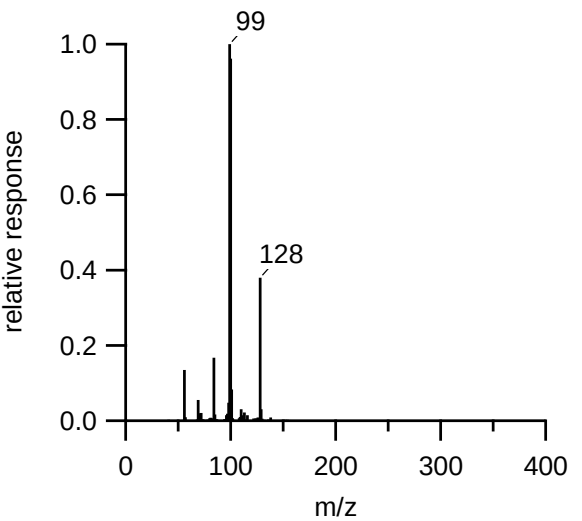
2H-Pyran-2-one, 6-heptyltetrahydro-
CAS #713-95-1, MW=198.16 (19 ppm)



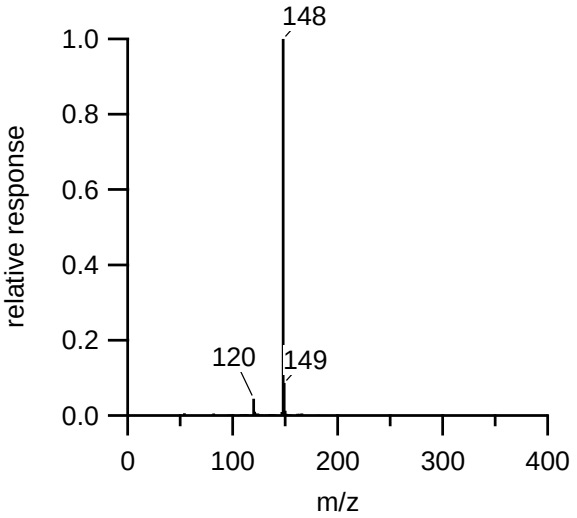
2H-Pyran-2-one, 6-butyltetrahydro-
CAS #3301-94-8, MW=156.12 (44 ppm)



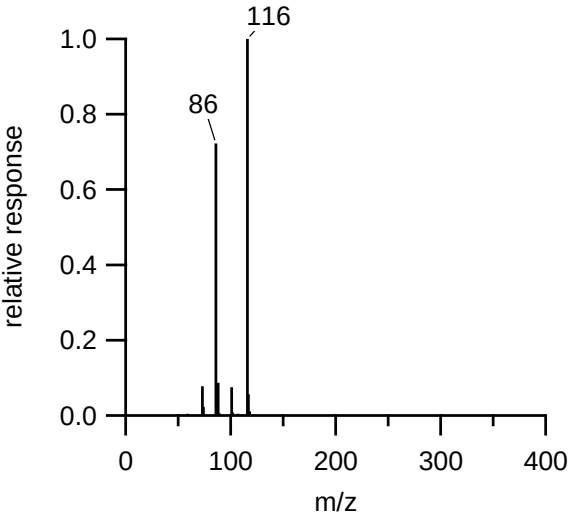
2H-Pyran-2-one, 6 ethyltetrahydro-
CAS #3301-90-4, MW=128.08 (1 ppm)



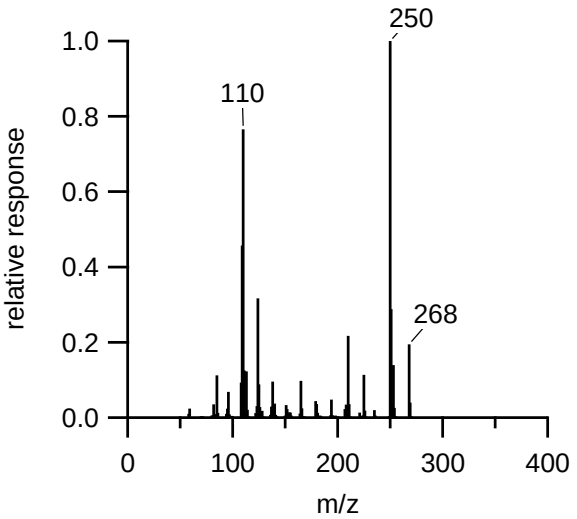
Hydrocoumarin
CAS #119-84-6, MW=148.05 (11 ppm)



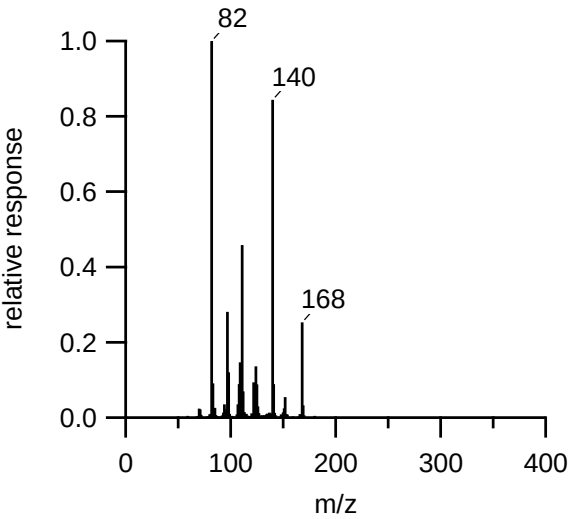
2-Propanone, 1-(acetyloxy)-
CAS #592-20-1, MW=116.05 (45 ppm)



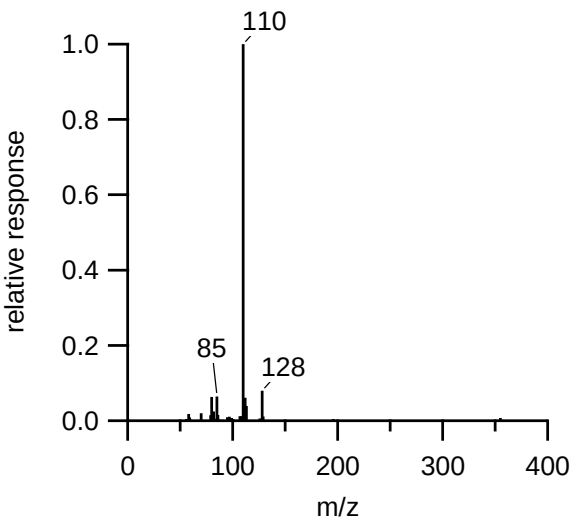
2-Pentadecanone, 6,10,14-trimethyl-
CAS #502-69-2, MW=268.28 (21 ppm)



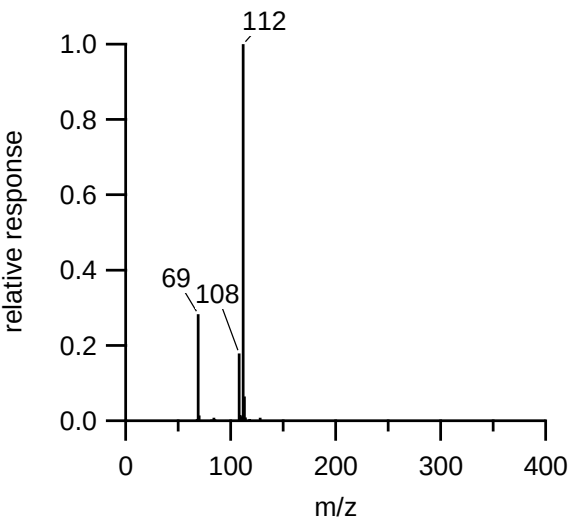
2-Oxabicyclo[2.2.2]octan-6-one, 1,3,3-trimethyl-
CAS #107598-08-3, MW=168.12 (23 ppm)



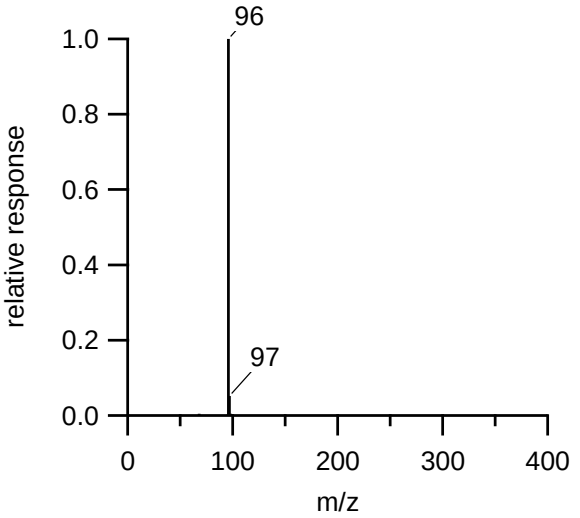
2-Heptanone, 6-methyl-
CAS #928-68-7, MW=128.12 (88 ppm)



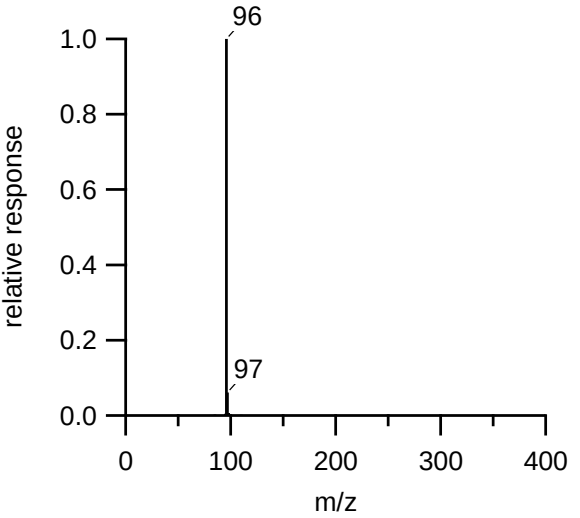
2-Furanone, 2,5-dihydro-3,5-dimethyl
CAS #0-00-0, MW=112.05 (52 ppm)



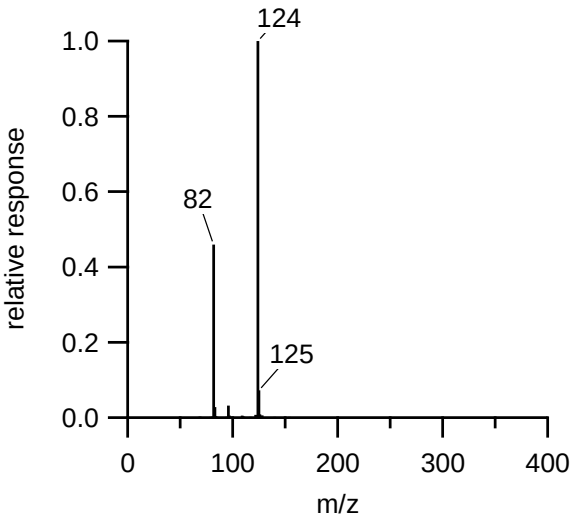
4-Cyclopentene-1,3-dione
CAS #930-60-9, MW=96.021 (37 ppm)



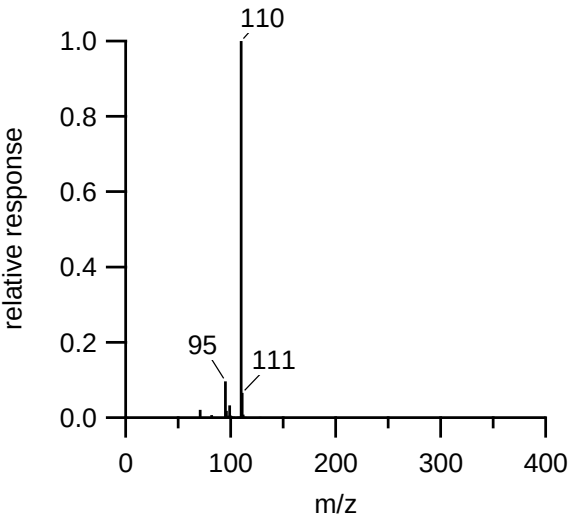
2-Cyclopenten-1-one, 3-methyl-
CAS #2758-18-1, MW=96.058 (45 ppm)



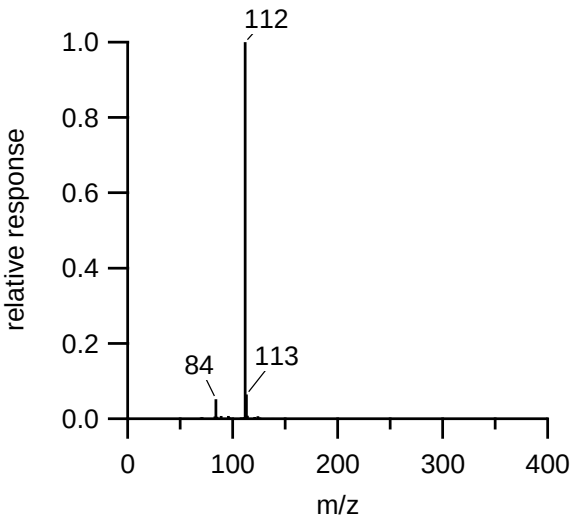
2-Cyclopenten-1-one, 3-(1-methylethyl)-
CAS #1619-28-9, MW=124.09 (17 ppm)



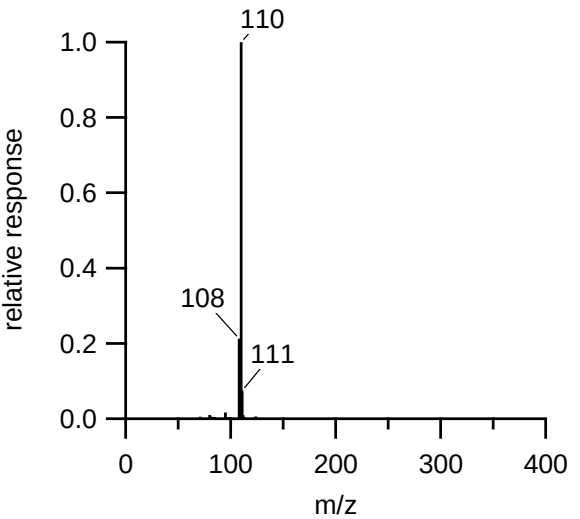
2-Cyclopenten-1-one, 3,4-dimethyl-
CAS #30434-64-1, MW=110.07 (28 ppm)



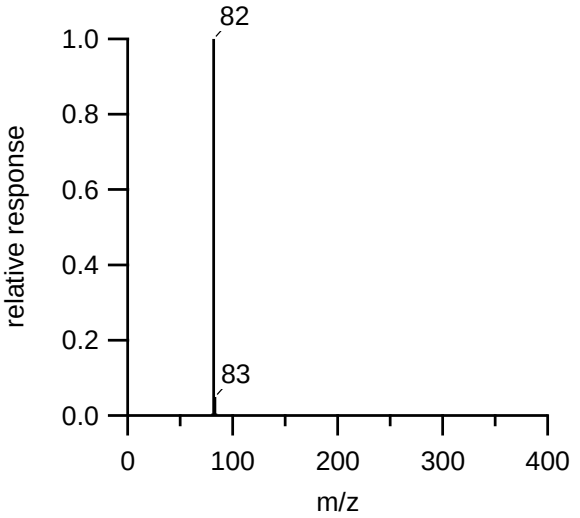
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-
CAS #80-71-7, MW=112.05 (52 ppm)



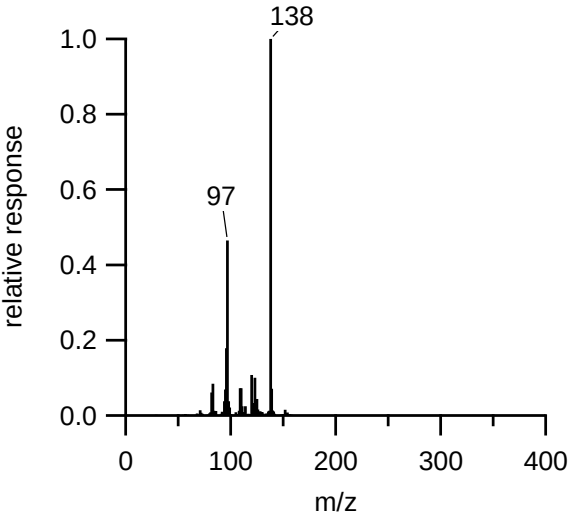
2-Cyclopenten-1-one, 2,3-dimethyl-
CAS #1121-05-7, MW=110.07 (28 ppm)



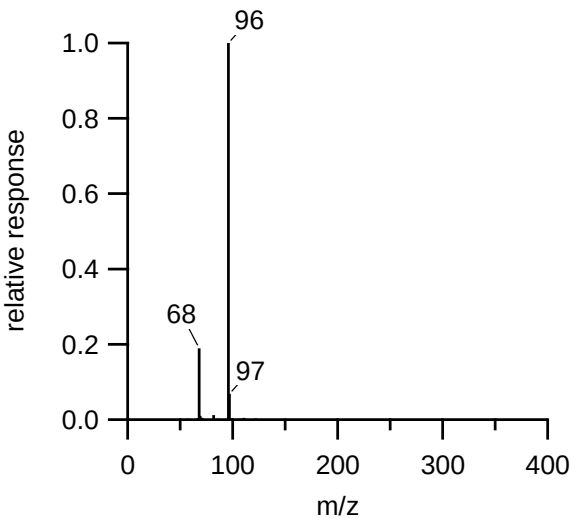
2-Cyclopenten-1-one
CAS #930-30-3, MW=82.042 (14 ppm)



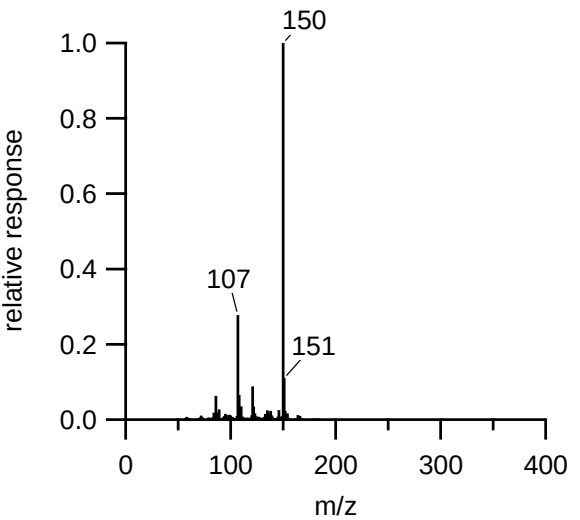
2-Cyclohexen-1-one, 4-(1-methylethyl)-
CAS #500-02-7, MW=138.1 (21 ppm)



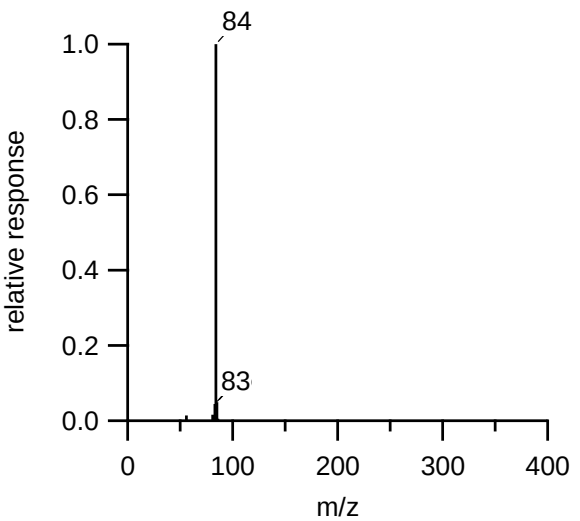
2-Cyclohexen-1-one
CAS #930-68-7, MW=96.058 (45 ppm)



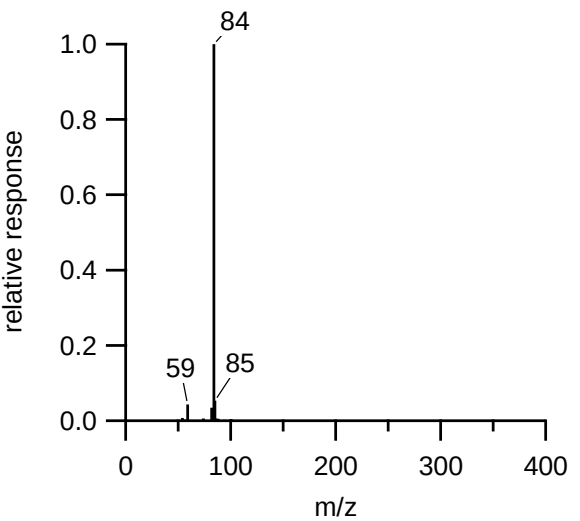
2-Caren-10-al
CAS #0-00-0, MW=150.1 (35 ppm)



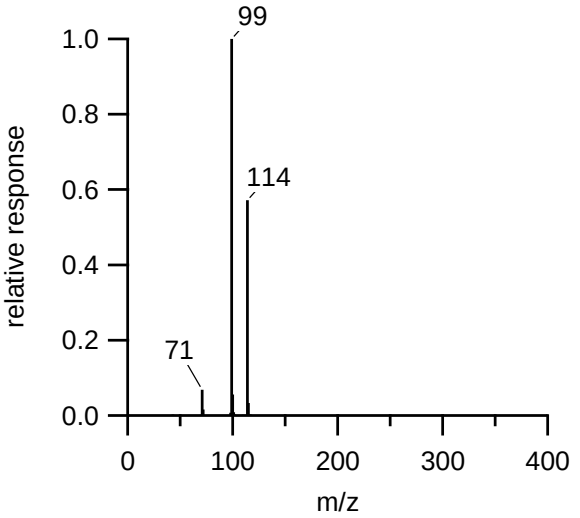
2-Butenal, 3-methyl-
CAS #107-86-8, MW=84.058 (39 ppm)



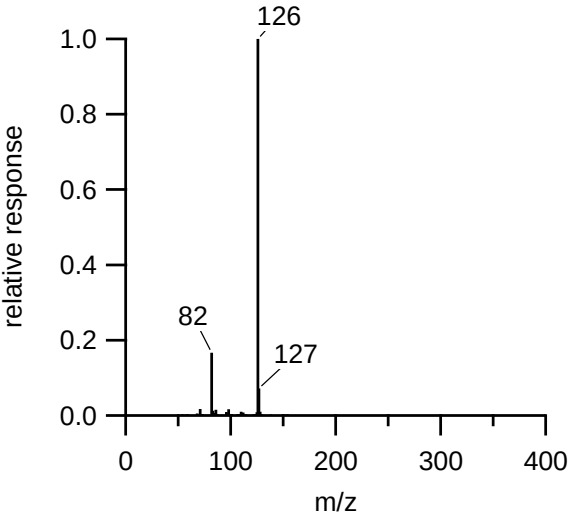
2-Butenal, 2-methyl-, (E)-
CAS #497-03-0, MW=84.058 (39 ppm)



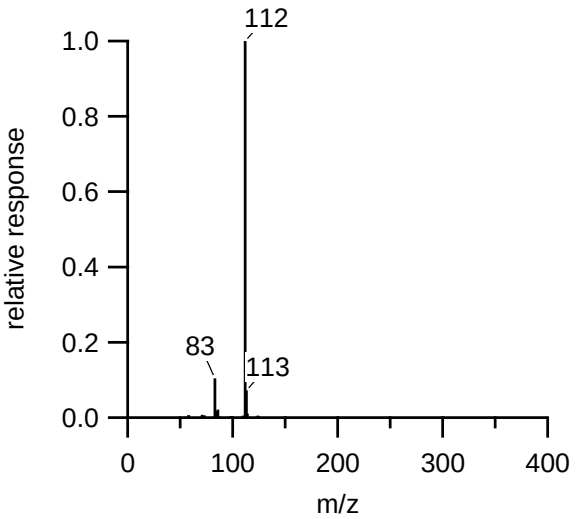
2,5-Hexanedione
CAS #110-13-4, MW=114.07 (28 ppm)



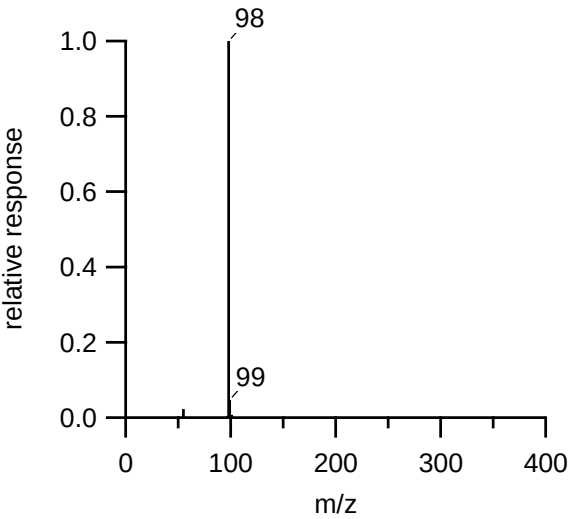
2,5-Furandione, 3,4-dimethyl-
CAS #766-39-2, MW=126.03 (8 ppm)



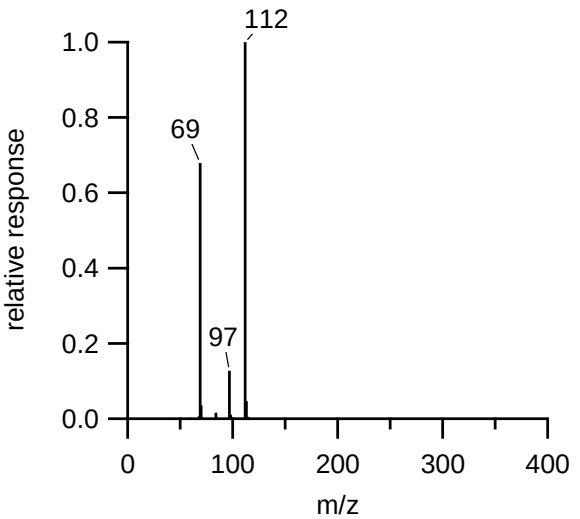
2,3-Dimethyl-4-hydroxy-2-butenoic lactone
CAS #1575-46-8, MW=112.05 (55 ppm)



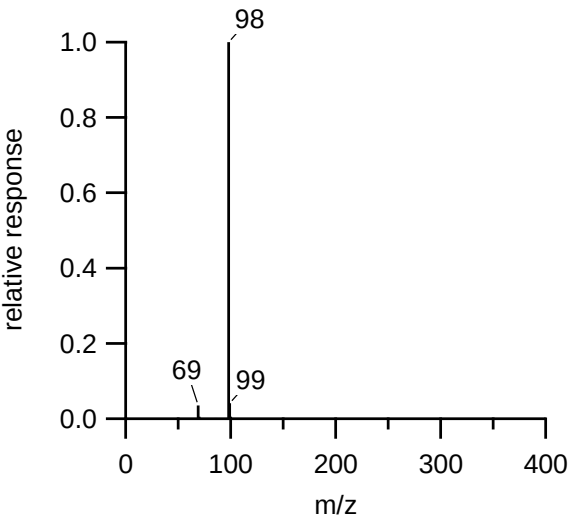
2(5H)-Furanone, 5-methyl-
CAS #591-11-7, MW=98.037 (63 ppm)



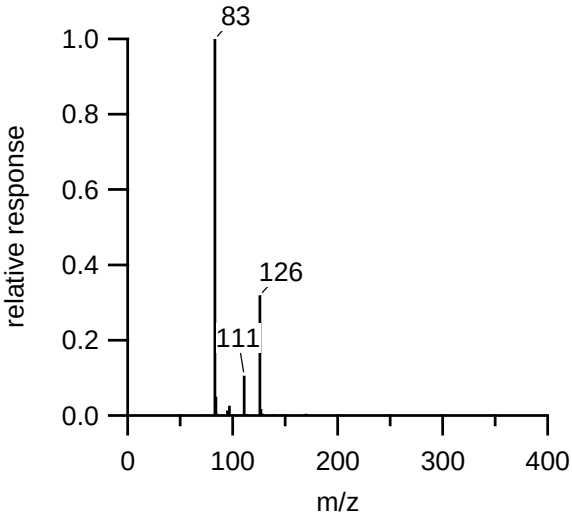
2(5H)-Furanone, 5,5-dimethyl-
CAS #20019-64-1, MW=112.05 (52 ppm)



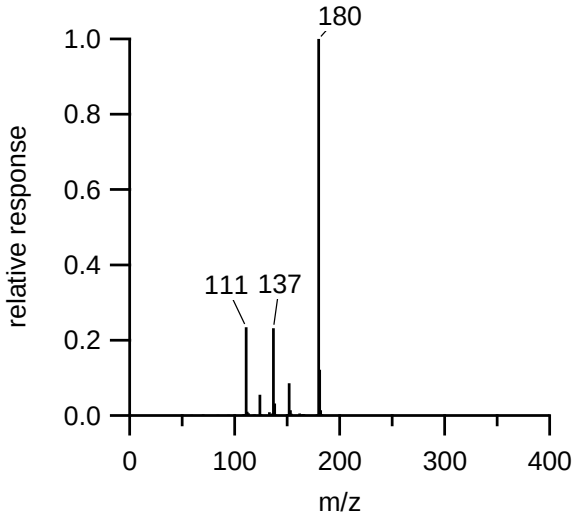
2(5H)-Furanone, 3-methyl-
CAS #22122-36-7, MW=98.037 (63 ppm)



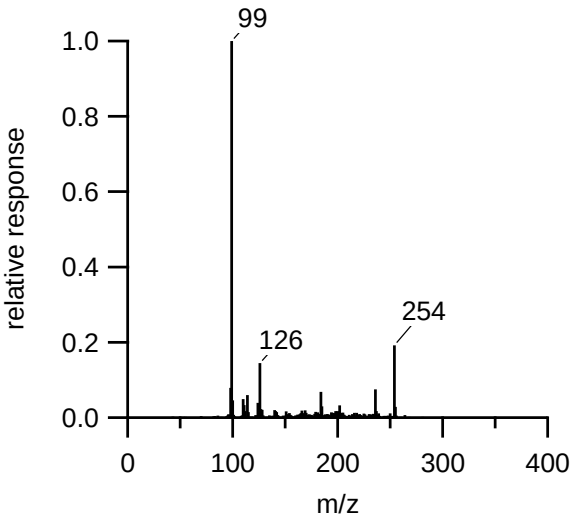
2(5H)-Furanone, 3,5,5-trimethyl-
CAS #50598-50-0, MW=126.07 (21 ppm)



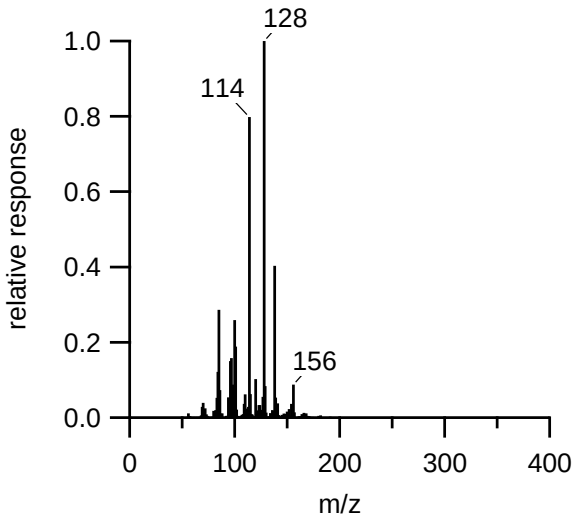
2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-,
CAS #17092-92-1, MW=180.12 (26 ppm)



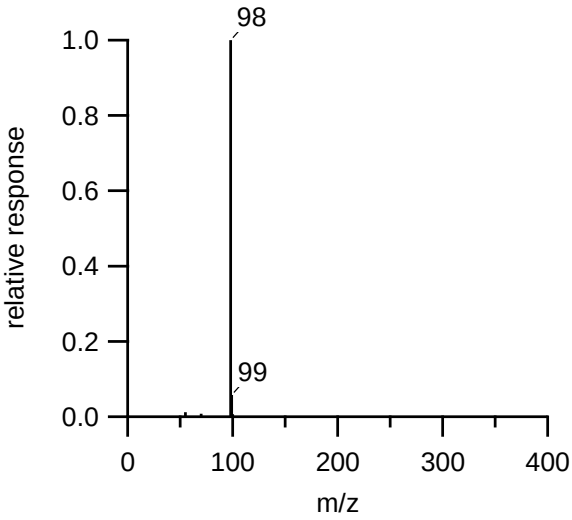
2(3H)-Furanone,dihydro-X-methyl-5-nonyl
CAS #220904-24-5, MW=254.22 (8 ppm)



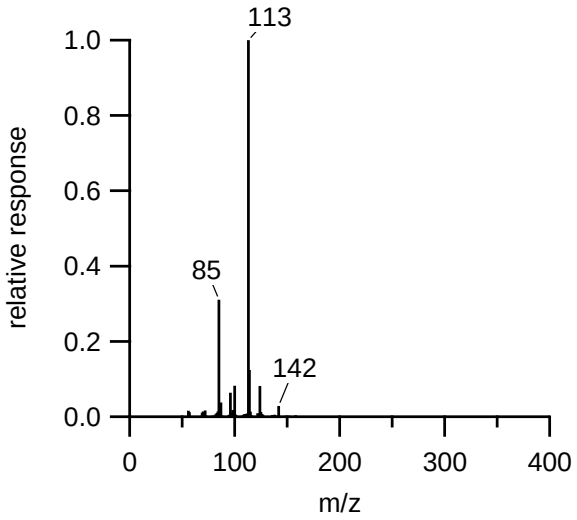
2(3H)-Furanone, dihydro-5-pentyl-
CAS #104-61-0, MW=156.12 (46 ppm)



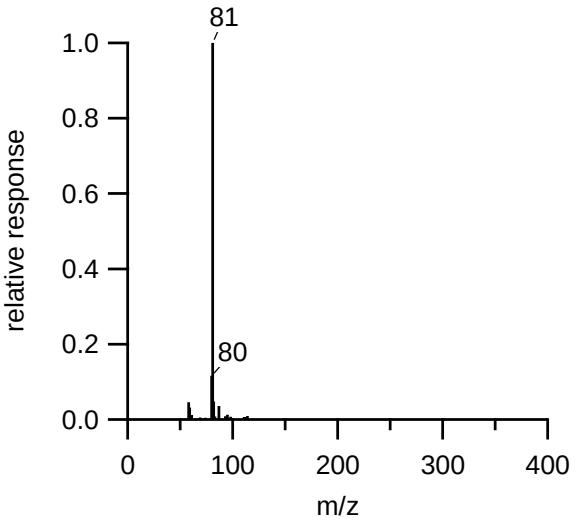
2(3H)-Furanone, 5-methyl-
CAS #591-12-8, MW=98.037 (63 ppm)



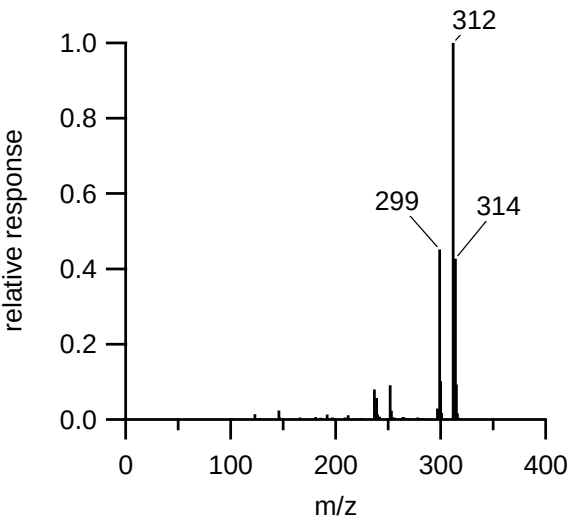
2(3H)-Furanone, dihydro-5-butyl-
CAS #104-50-7, MW=142.1 (45 ppm)



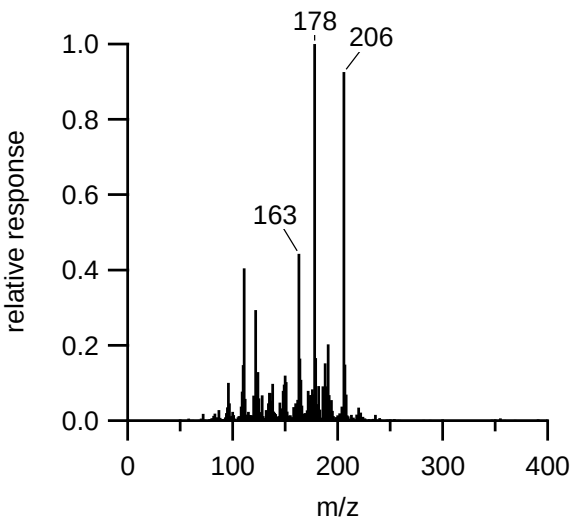
1H-Pyrrole, 2-methyl-
CAS #616-43-3, MW=81.058 (72 ppm)



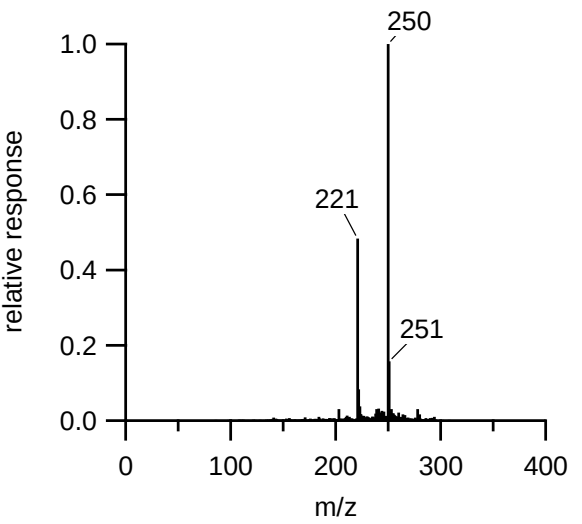
Methyl dehydroabietate
CAS #1235-74-1, MW=314.22 (25 ppm)



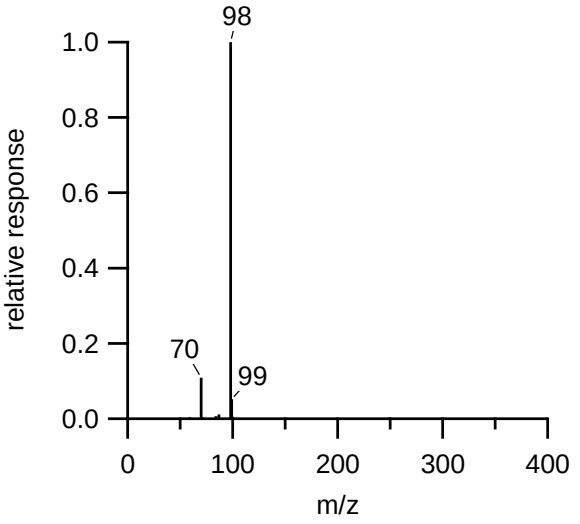
1-Oxaspiro[2.5]octane, 5,5-dimethyl-4-(3-methyl-1,3-butadi
CAS #0-00-0, MW=206.17 (2 ppm)



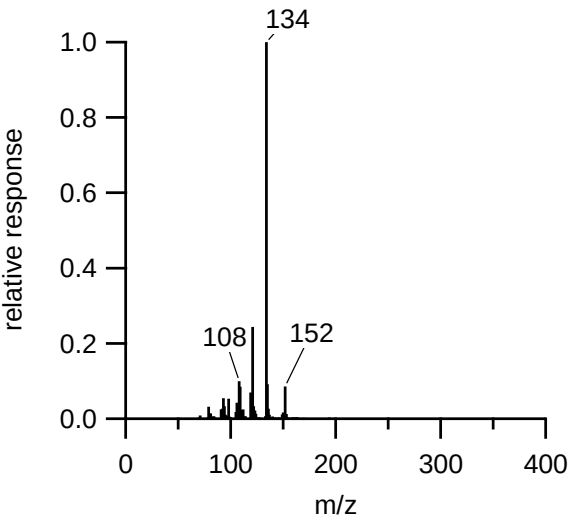
1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-
CAS #79-74-3, MW=250.19 (18 ppm)



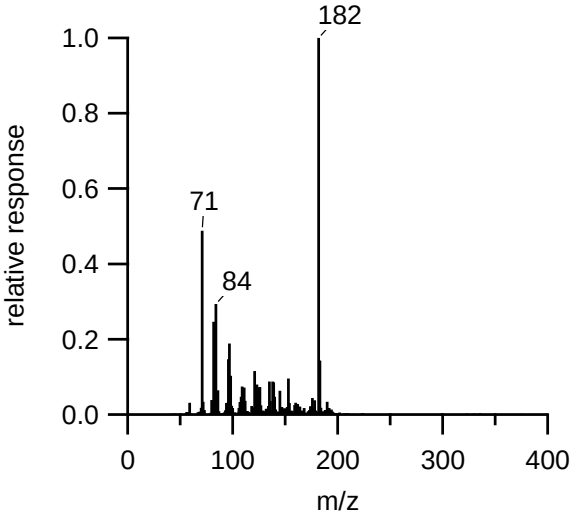
1,3-Cyclopentanedione
CAS #3859-41-4, MW=98.037 (63 ppm)



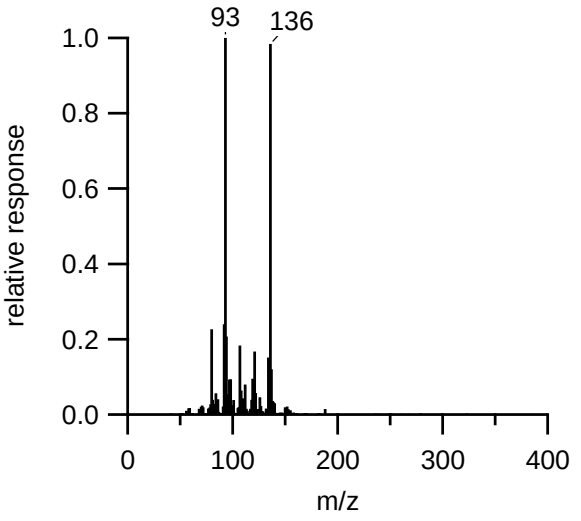
1-Cyclohexene-1-methanol, 4-(1-methylethenyl)-
CAS #536-59-4, MW=152.12 (25 ppm)



2-Dodecenal, (E)-
CAS #20407-84-5, MW=182.17 (32 ppm)



á-Phellandrene
CAS #555-10-2, MW=136.13 (28 ppm)



2-Ethylhexyl salicylate
CAS #118-60-5, MW=250.16 (16 ppm)