

## 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)

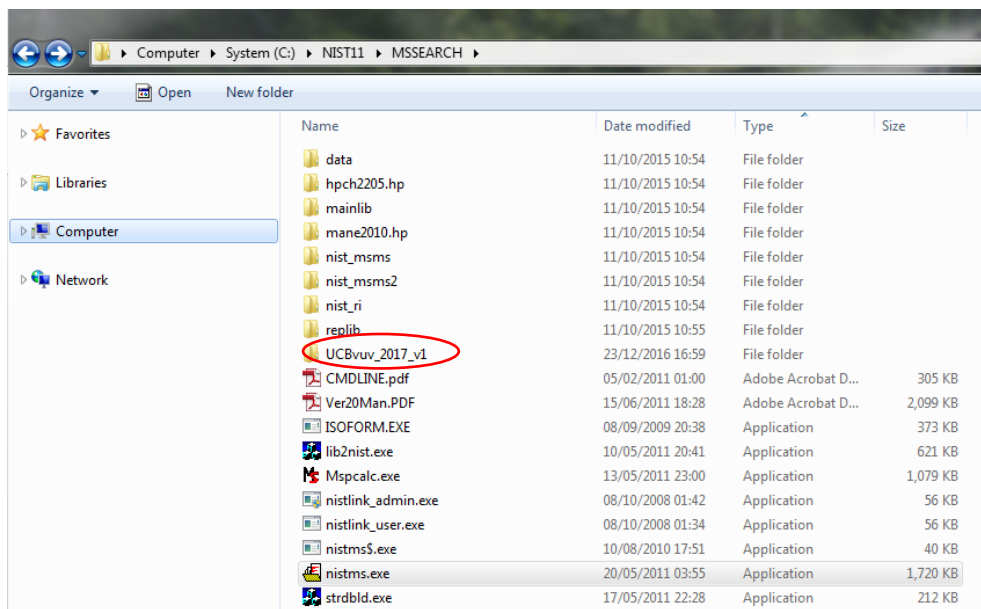
A searchable EI mass spectral library specifically generated with atmospherically relevant compounds of interest from this work in a format compatible with the NIST MSSEARCH program is available to download from:

[https://nature.berkeley.edu/ahg/MSLibrary/UCB\\_VUV\\_Lib\\_v1](https://nature.berkeley.edu/ahg/MSLibrary/UCB_VUV_Lib_v1).

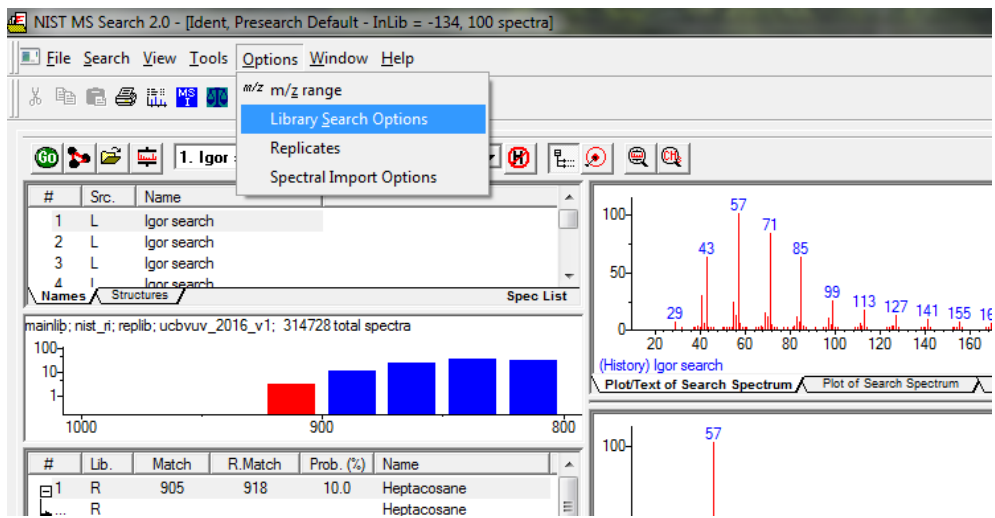
## Instructions on how to use the EI MS library generated from this work (UCBvuv\_2017\_v1)

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).

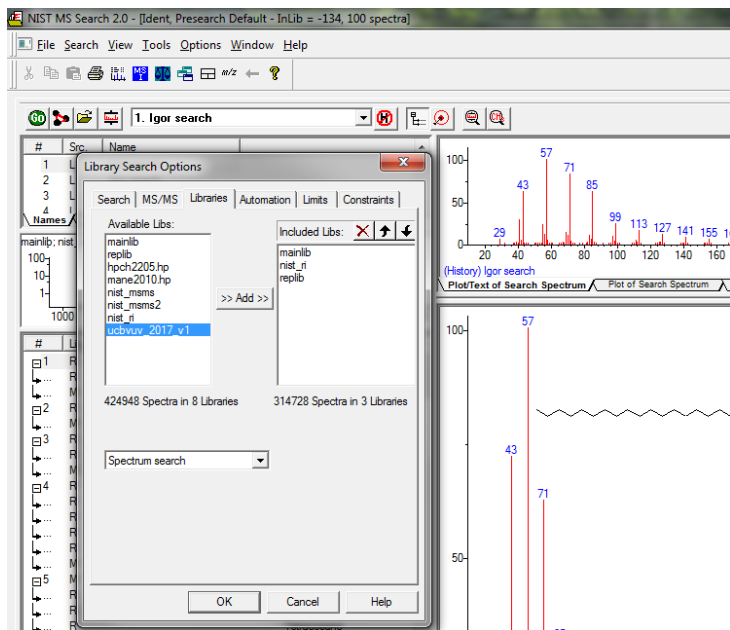
1. Copy the UCBvuv\_2017\_v1 into the NIST\MSSEARCH folder on the C:\ drive. This is the folder that contains the nistms.exe programme.



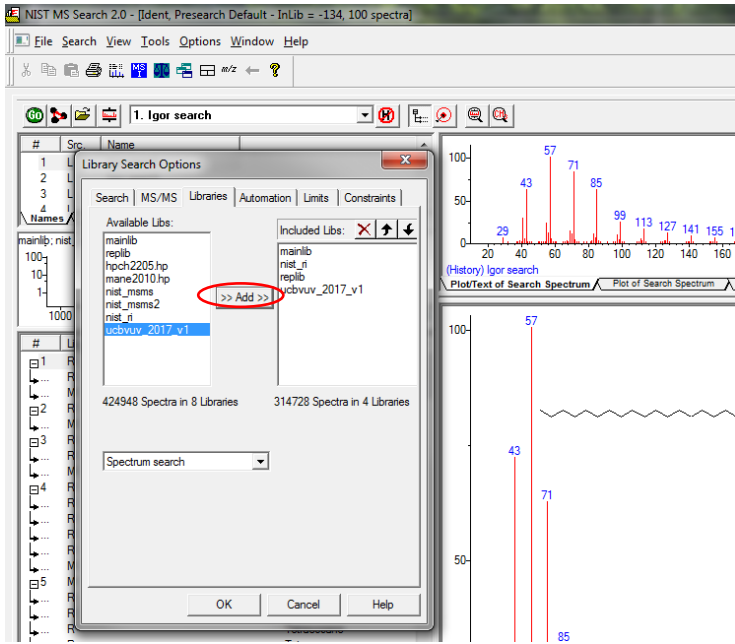
2. Open the nistms.exe programme and select the Options\Library Search Options.



3. Select the Libraries tab and you will see the UCBvuv\_2017\_v1 library as one of the available libraries.



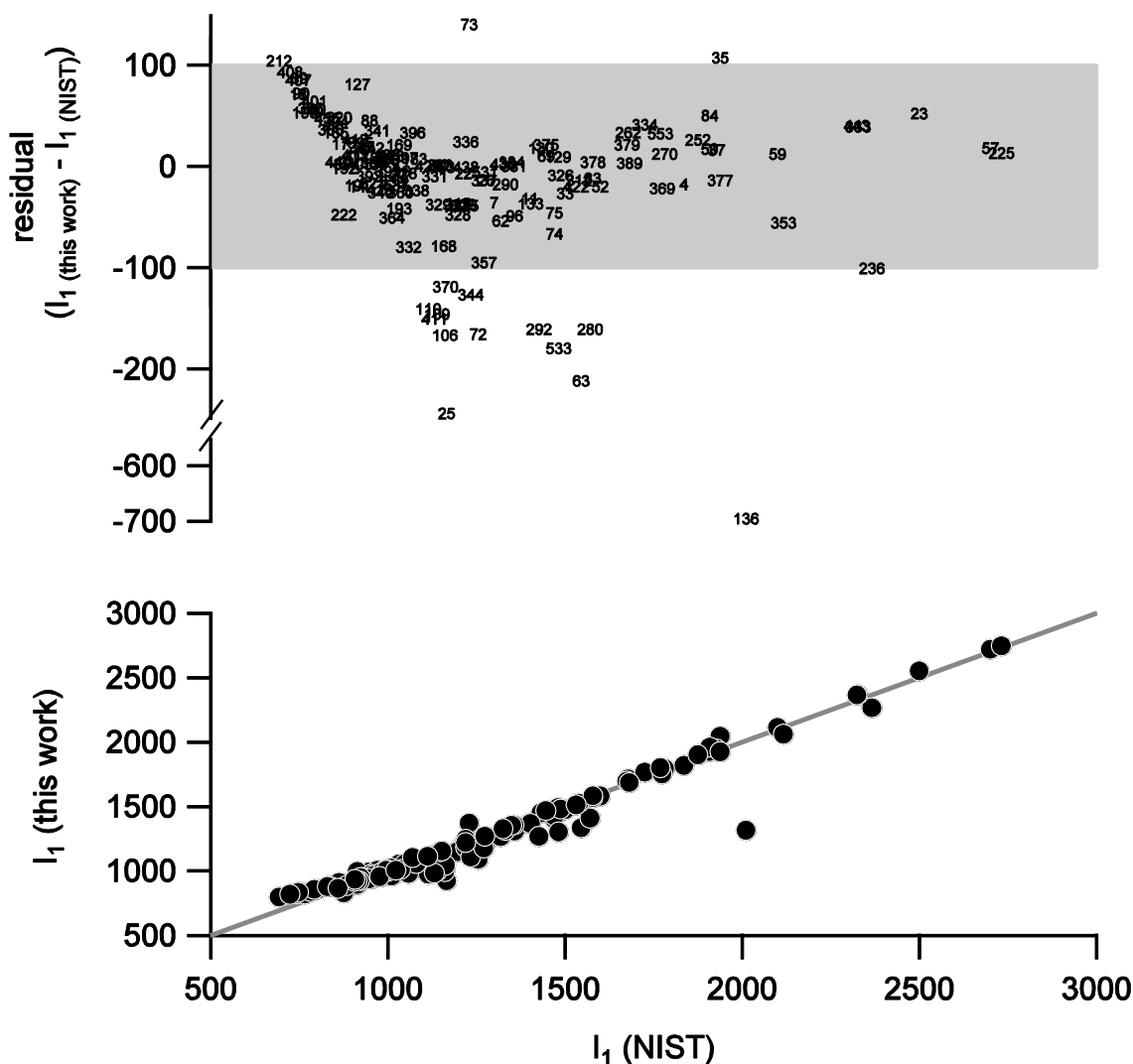
4. Add the UCBvuv\_2017\_v1 library to the included library list and click OK.



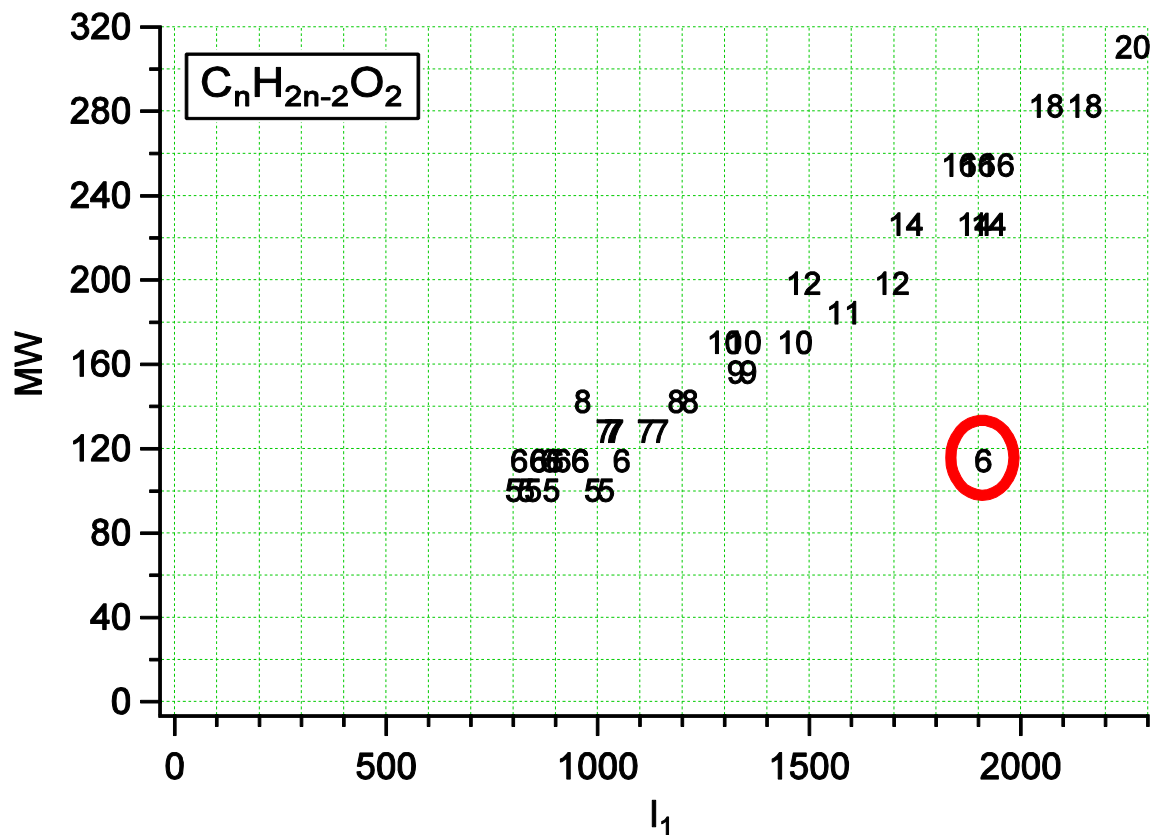
**Table S1.** Major families of molecular formulas, those with  $\geq 5$  homologues, Kendrick Mass Defect (KMD) and number observed matched to EI MS library with confirmation by VUV MS data (EI) and assigned molecular formulas from the observed molecular ion (VUV). Identified compound names from EI 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-butenone 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]hexan-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-(1a,4a,6a)]-; 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-Epoxy-naphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-tetramethyl-, [3S-(3a,5aa,7aa,11aa,11bb)]-; 5H-3,5a-Epoxy-naphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-tetramethyl-, [3S-(3a,5aa,7aa,11aa,11bb)]-; 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-yl-p-Cymen-7-yl; 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-Pentalen, 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-oxetyl-; 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

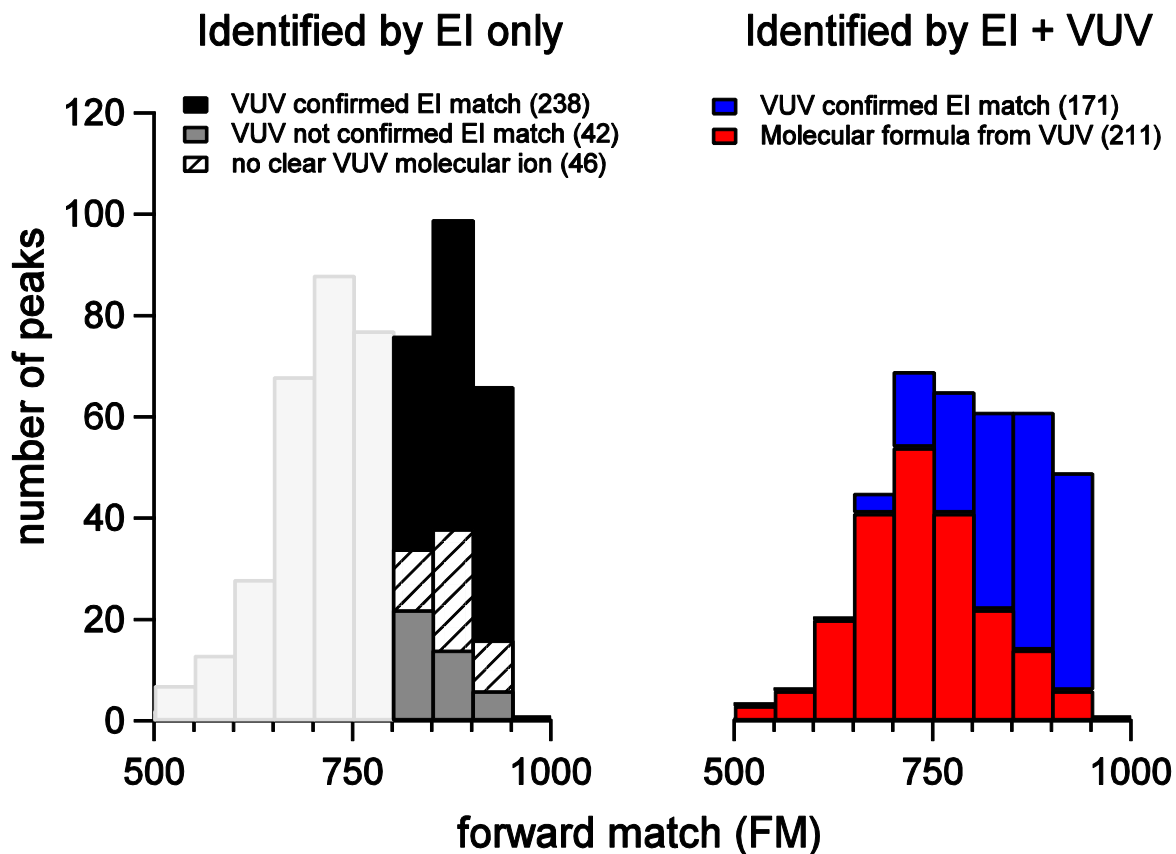
**Figure S1.** Linear regression of  $I_1$  (first dimension Kovats retention indices) from this work and the NIST database (bottom). The residual ( $I_{1(\text{this work})} - I_{1(\text{NIST})}$ ) of the linear regression demonstrates the degree of agreement. The datapoints are numerically labelled, 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.

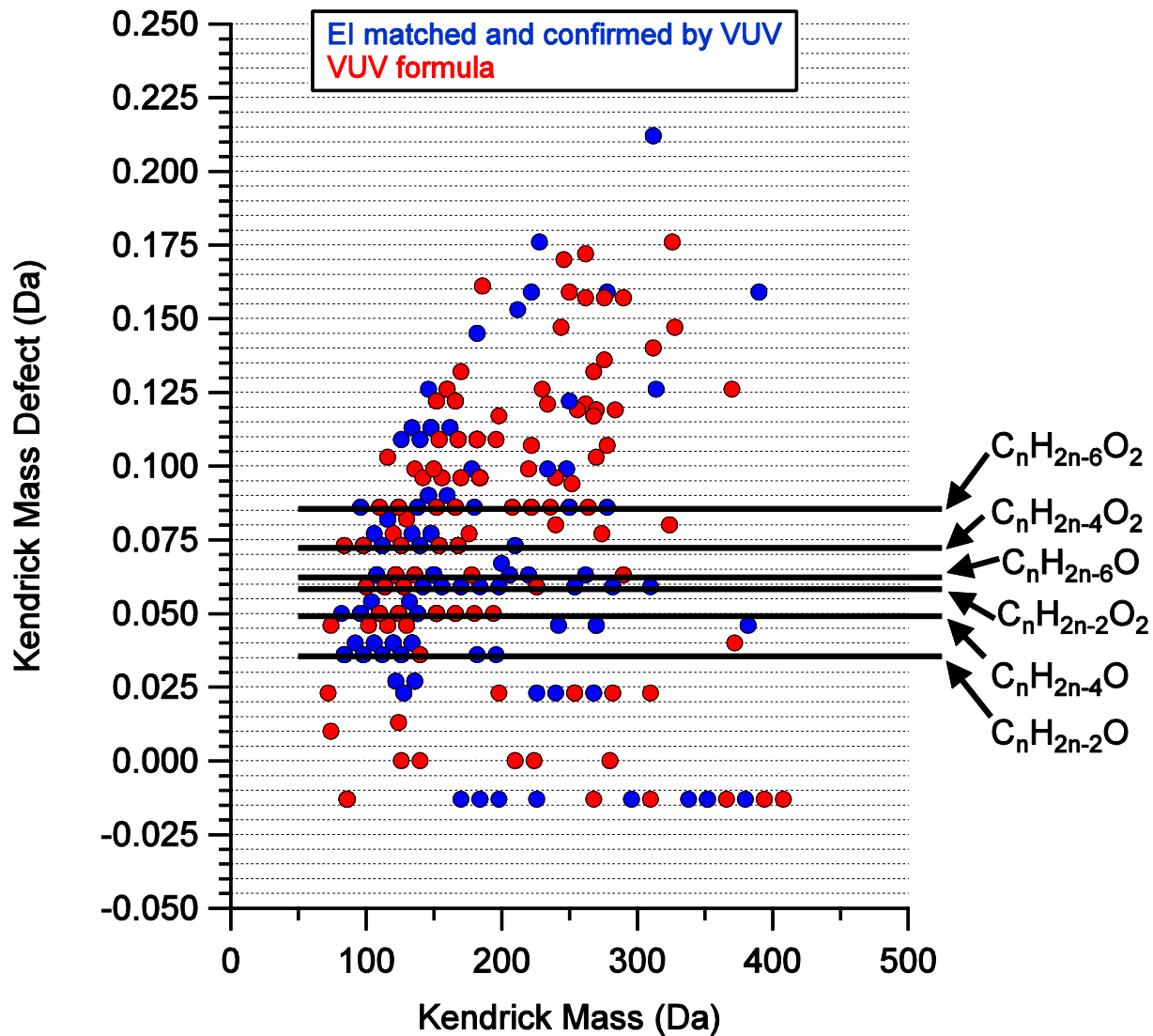


**Figure S3.** Comparison of number of peaks identified by EI only (left panel) and identified by EI and VUV (right panel) as a function of the forward matching statistic (FM) returned from the NIST MS search program.

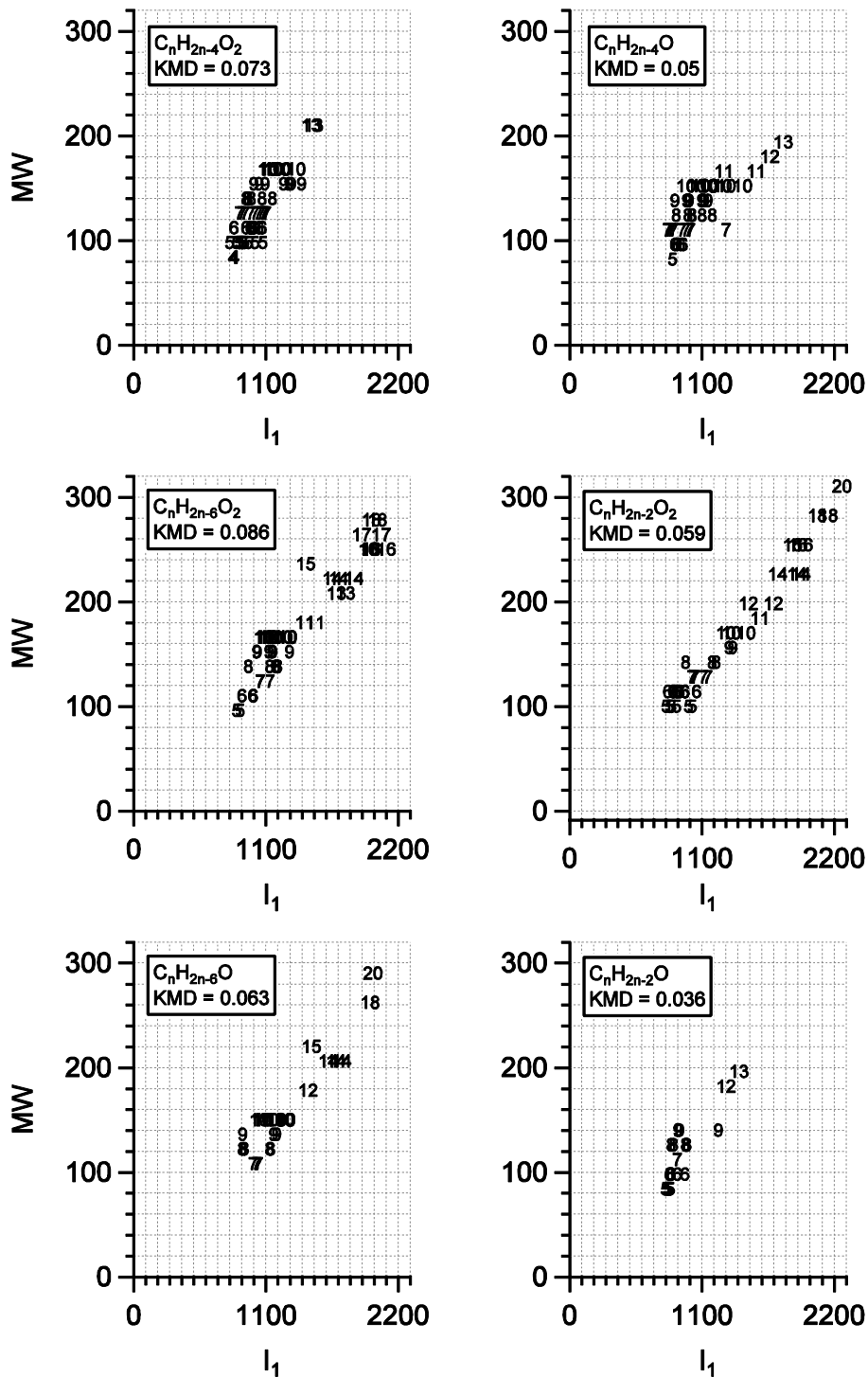




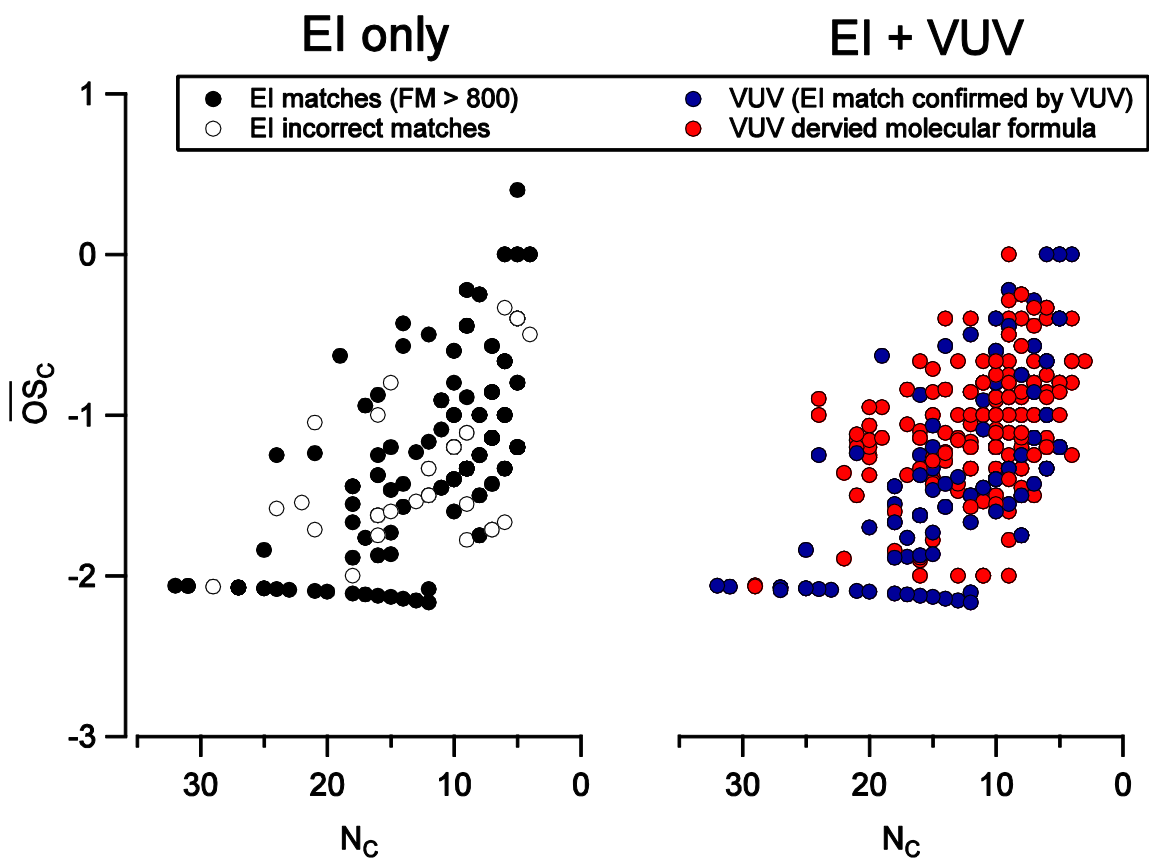
**Figure S4.** Kendrick mass defect plot showing identification of homologous series. The six most populous groups are indicated with the formula family based on identified EI and assigned VUV formulas.



**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.

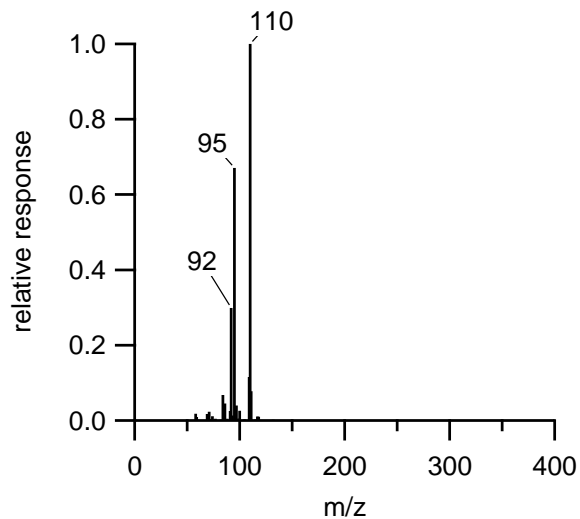


**Figure S6.** Average carbon oxidation state ( $\overline{\text{OSc}}$ ) versus carbon number ( $N_C$ ) for an EI only and an EI + VUV approach. The EI only approach includes only those compounds that had forward matching (FM) statistics of  $> 800$  (filled black circles). Those which were not confirmed 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 ( $\text{C}_x\text{H}_y\text{O}_z$ ) due to the nature of the calculation of  $\overline{\text{OSc}}$  ( $2*\text{O}:\text{C} - \text{H}:\text{C}$ ).

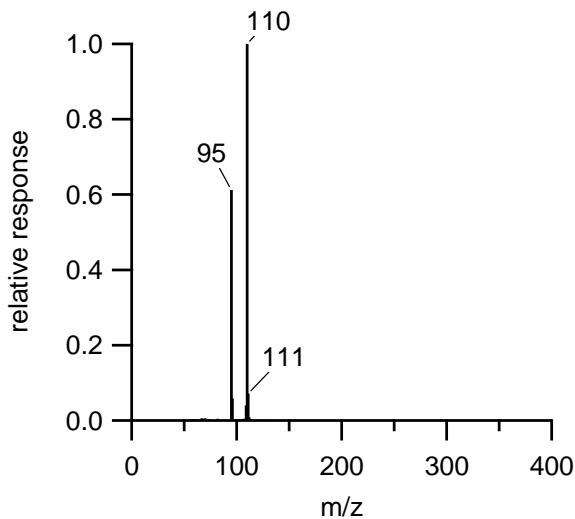


# **Appendix of VUV (10.5 eV) Mass Spectra**

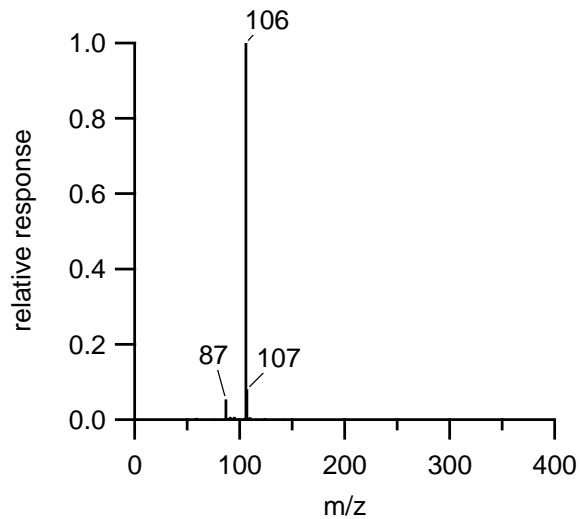
Furan, 2-ethyl-5-methyl-  
CAS #1703-52-2, MW=110.07 (28 ppm)



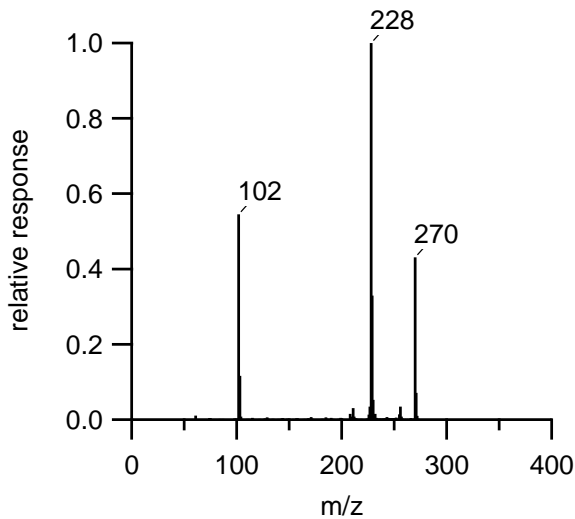
trans,trans-3,5-Heptadien-2-one  
CAS #18402-90-9, MW=110.07 (28 ppm)



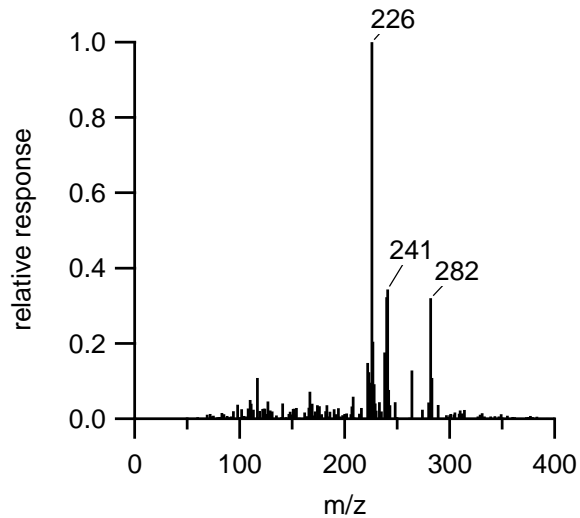
m-Xylene  
CAS #108-38-3, MW=106.08 (14 ppm)



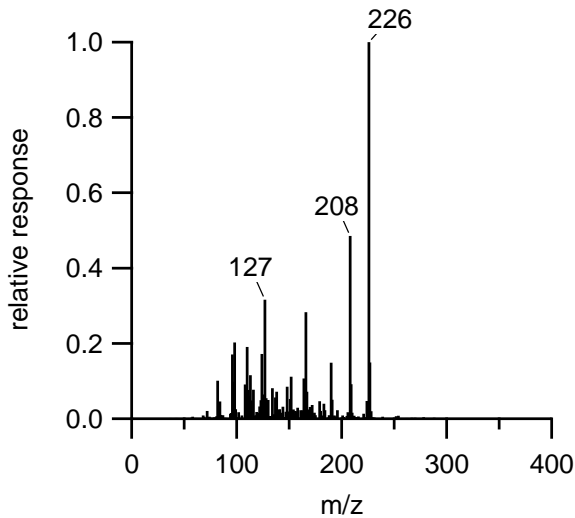
i-Propyl 12-methyl-tridecanoate  
CAS #110-27-0, MW=270.26 (3 ppm)



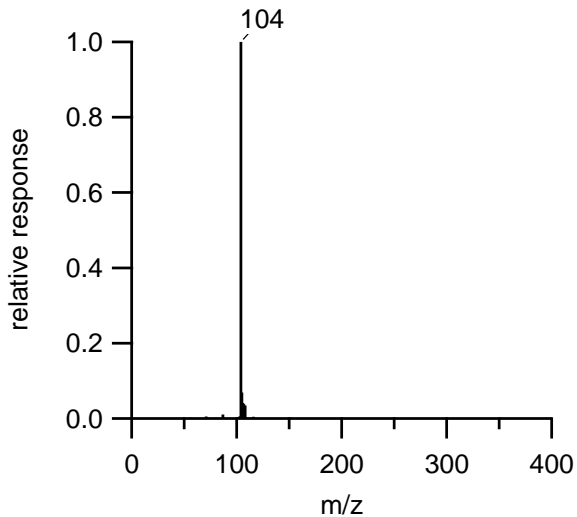
cis-13-Octadecenoic acid  
CAS #112-79-8, MW=282.26 (18 ppm)



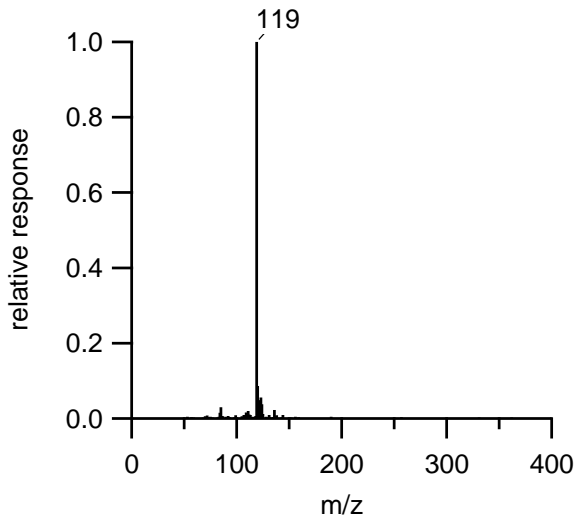
Z-11-Tetradecenoic acid  
CAS #0-00-0, MW=226.19 (52 ppm)



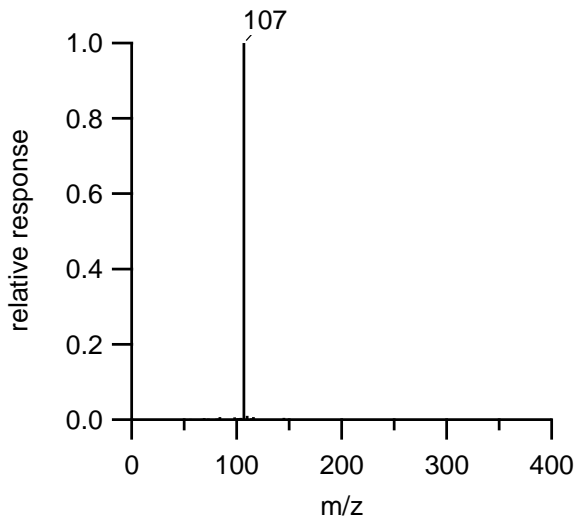
Styrene  
CAS #100-42-5, MW=104.06 (9 ppm)



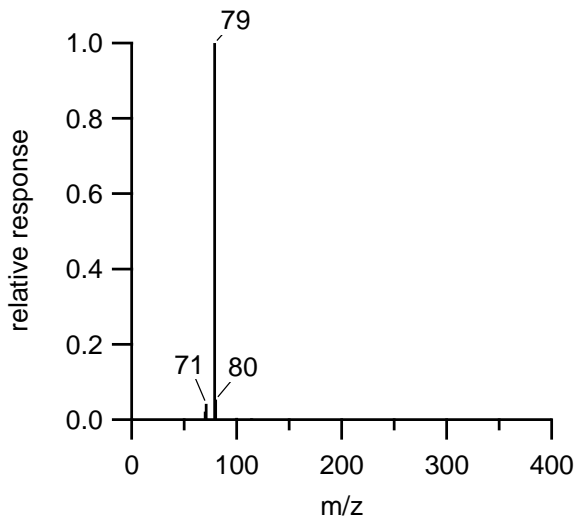
Pyridine, 5-ethenyl-2-methyl-  
CAS #140-76-1, MW=119.07 (42 ppm)



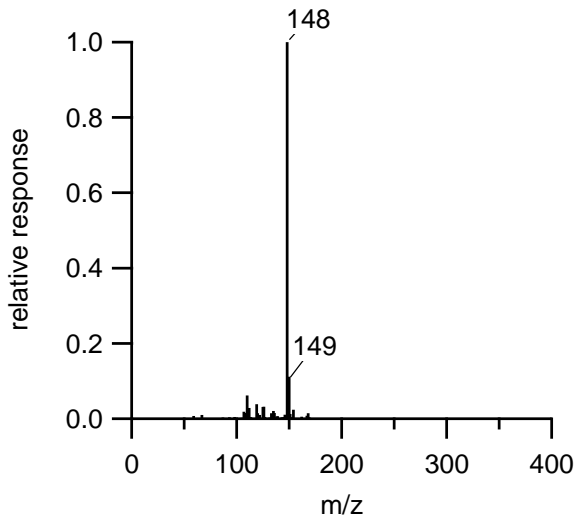
Pyridine, 2,6-dimethyl-  
CAS #108-48-5, MW=107.07 (59 ppm)



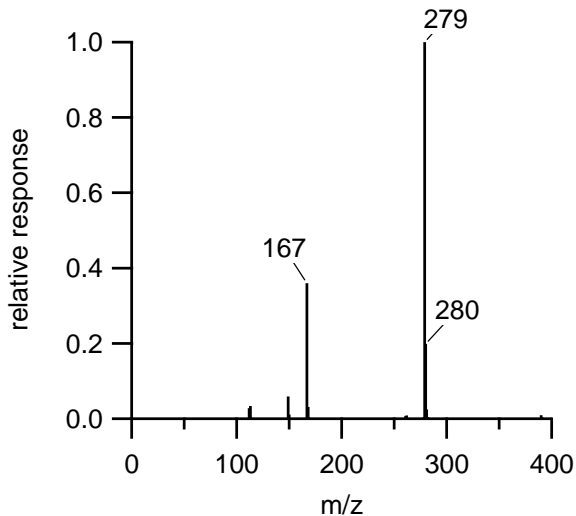
Pyridine  
CAS #110-86-1, MW=79.042 (2 ppm)



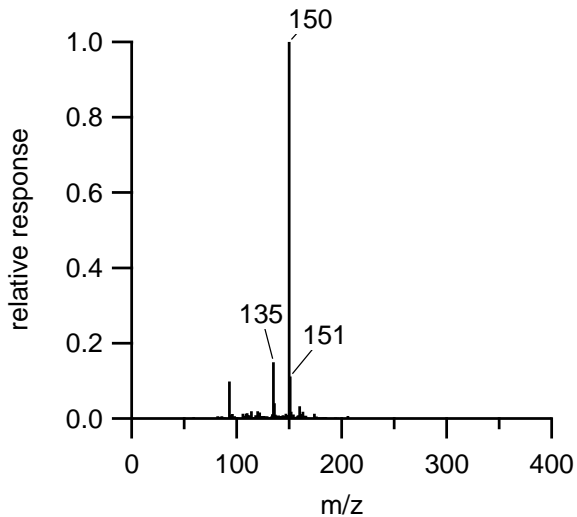
Benzaldehyde, 4-(1-methylethyl)-  
CAS #122-03-2, MW=148.09 (44 ppm)



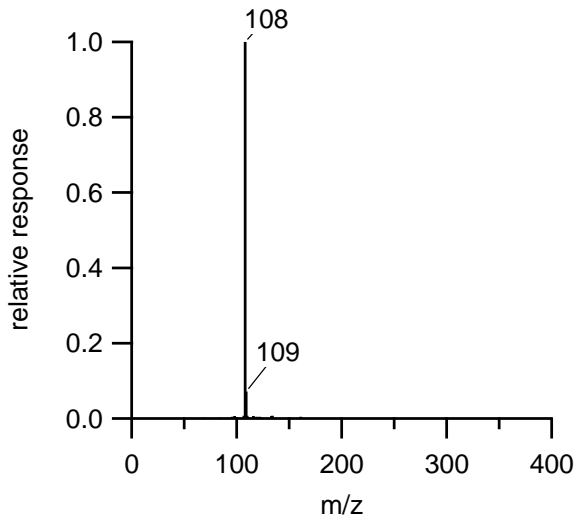
Phthalic acid, di(2-propylpentyl) ester  
CAS #117-81-7, MW=390.28 (41 ppm)



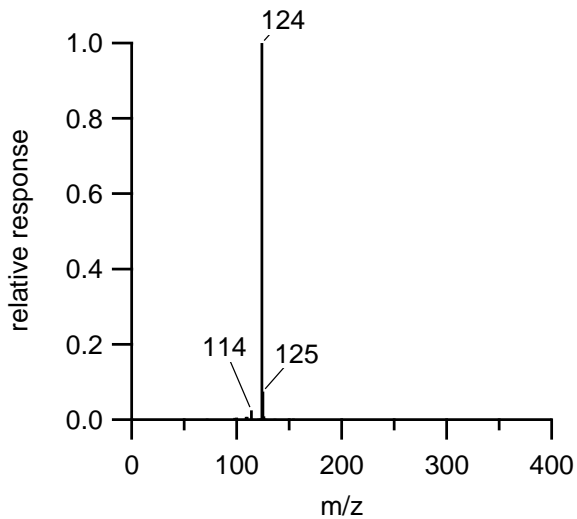
Phenol, 2-methyl-5-(1-methylethyl)-  
CAS #499-75-2, MW=150.1 (35 ppm)



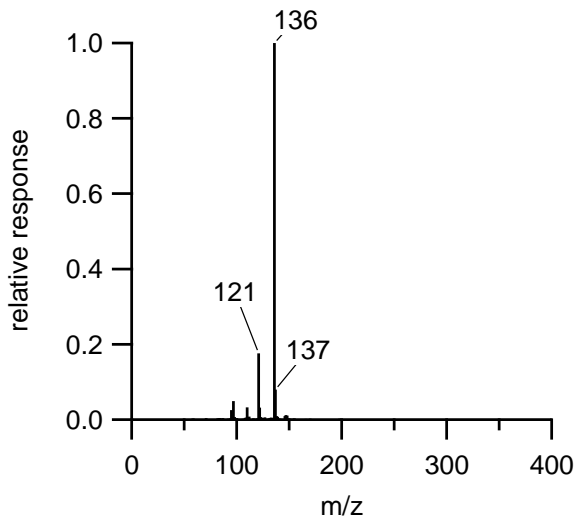
Phenol, 2-methyl-  
CAS #95-48-7, MW=108.06 (47 ppm)



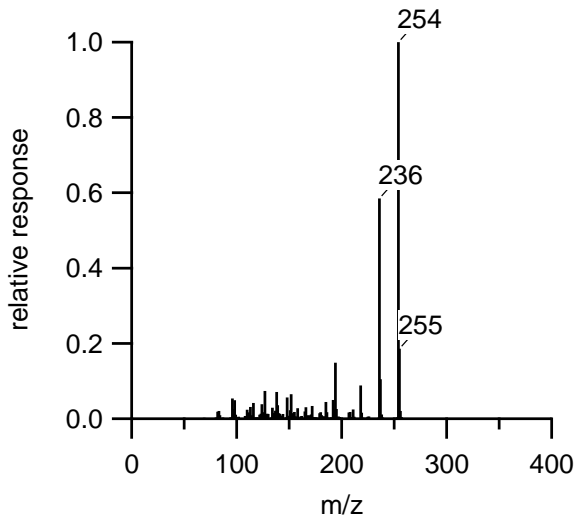
Phenol, 2-methoxy-  
CAS #90-05-1, MW=124.05 (28 ppm)



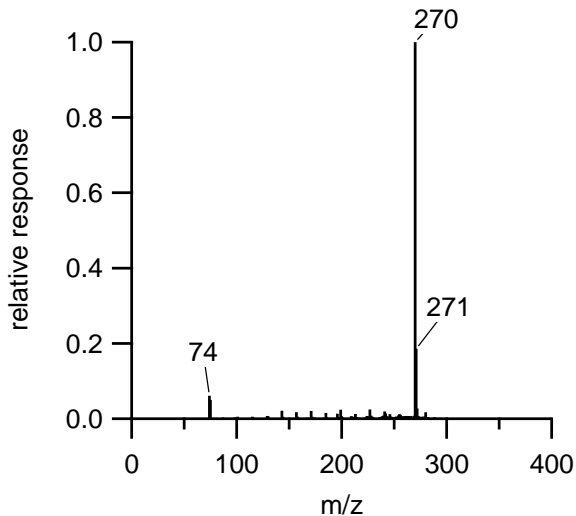
Phenol, 3-(1-methylethyl)-  
CAS #618-45-1, MW=136.09 (54 ppm)



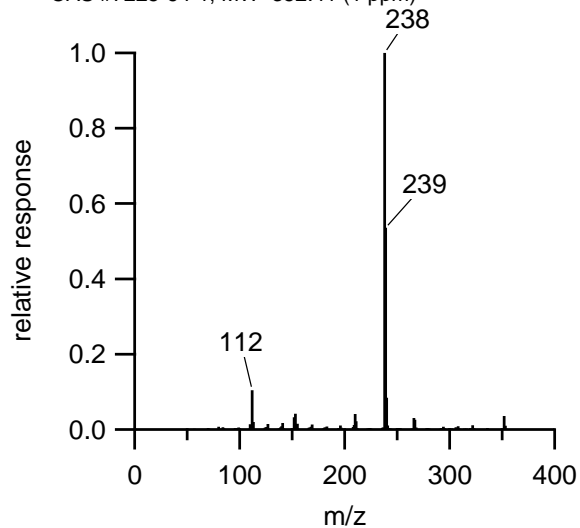
Oxacycloheptadecan-2-one  
CAS #109-29-5, MW=254.22 (8 ppm)



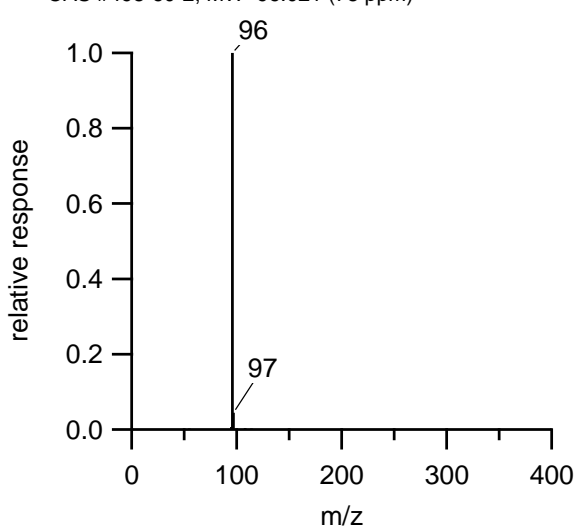
Hexadecanoic acid, methyl ester  
CAS #112-39-0, MW=270.26 (49 ppm)



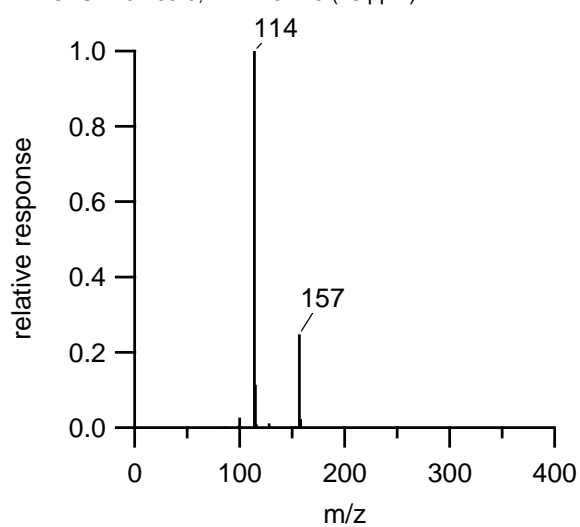
Heptadecane, 9-octyl-  
CAS #7225-64-1, MW=352.41 (1 ppm)



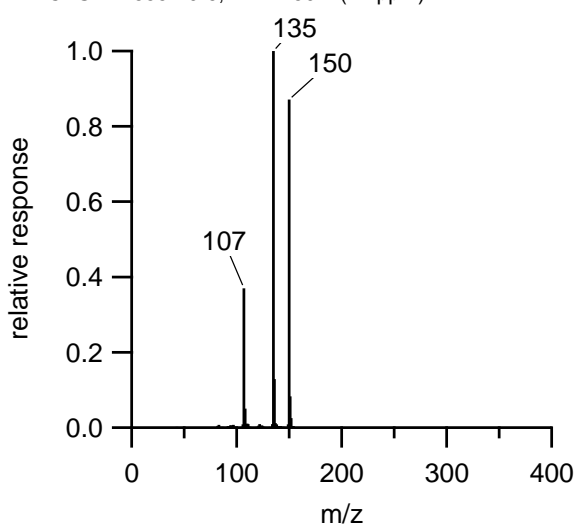
3-Furaldehyde  
CAS #498-60-2, MW=96.021 (78 ppm)



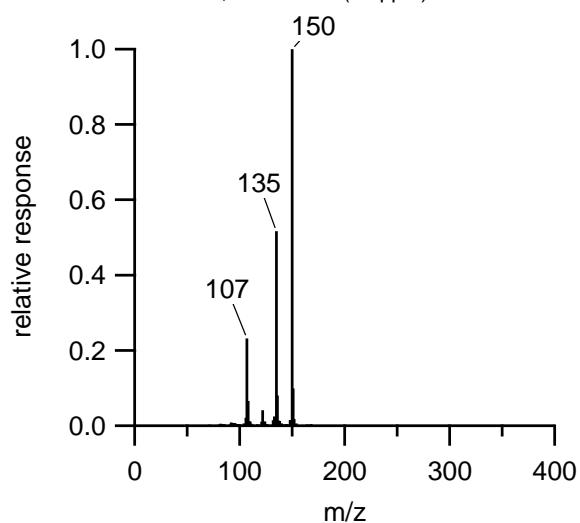
Formamide, N,N-dibutyl-  
CAS #761-65-9, MW=157.15 (48 ppm)



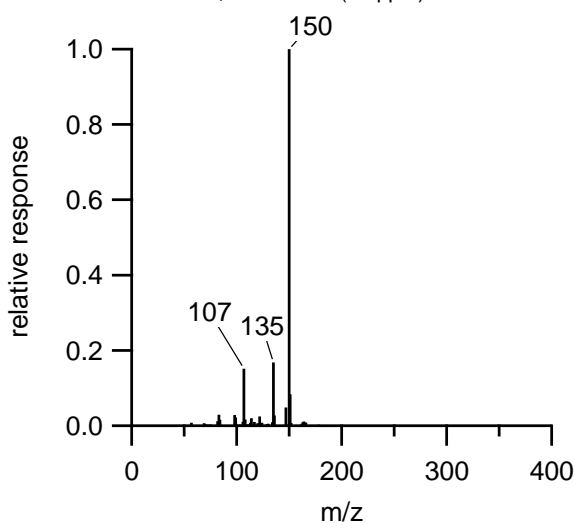
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-  
CAS #24555-40-6, MW=150.1 (27 ppm)



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

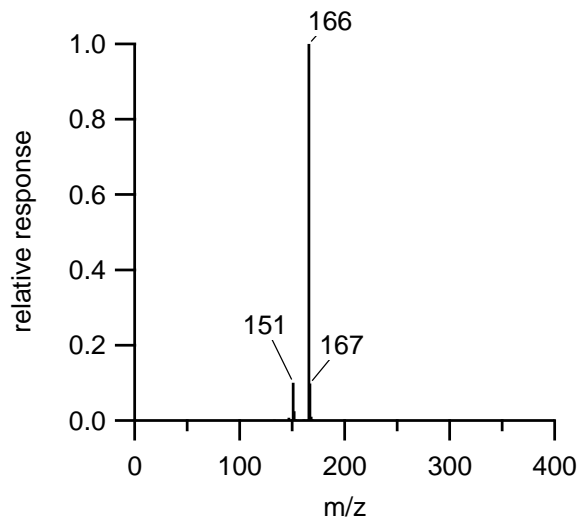


Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-  
CAS #24555-40-6, MW=150.1 (35 ppm)

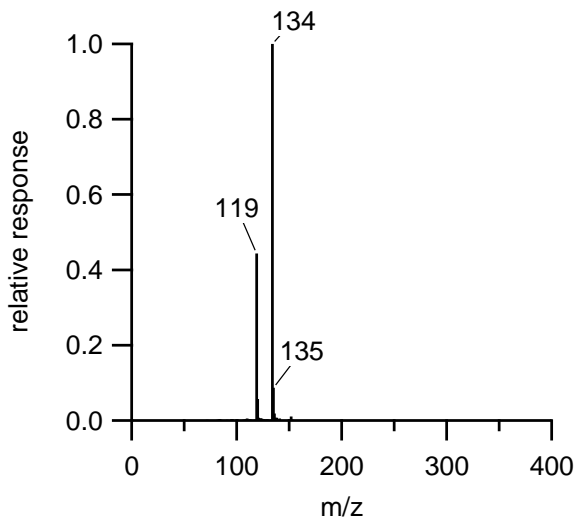




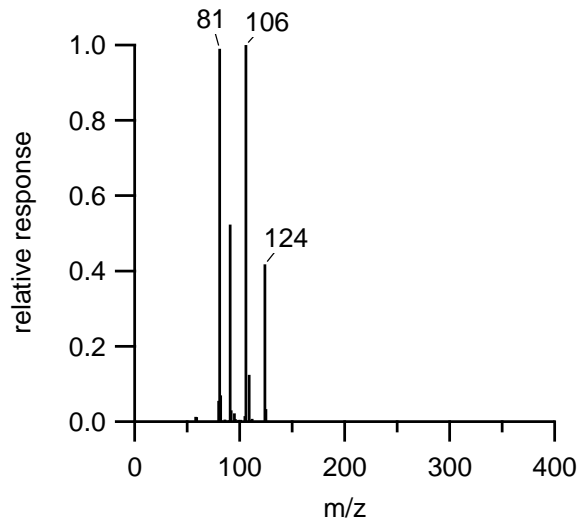
Apocynin  
CAS #498-02-2, MW=166.06 (21 ppm)



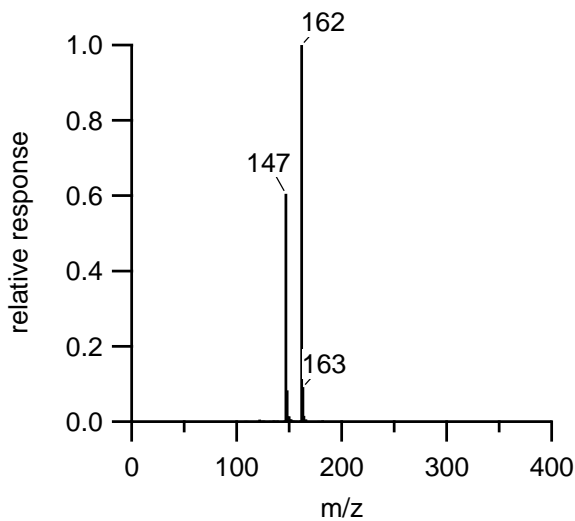
Ethanone, 1-(3-methylphenyl)-  
CAS #585-74-0, MW=134.07 (3 ppm)



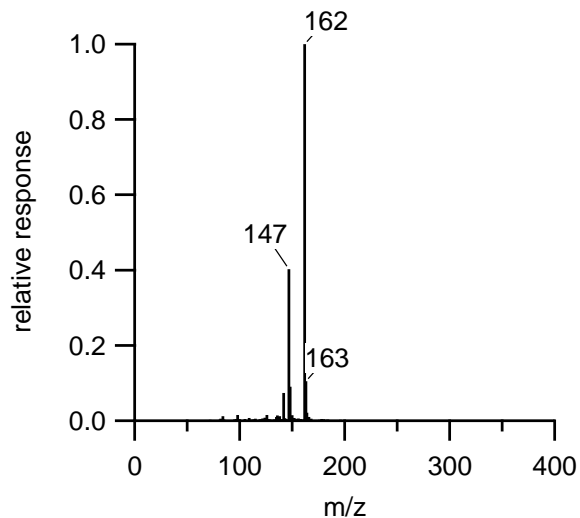
Cyclopentanecarboxaldehyde, 2-methyl-3-methylene-  
CAS #0-00-0, MW=124.09 (17 ppm)



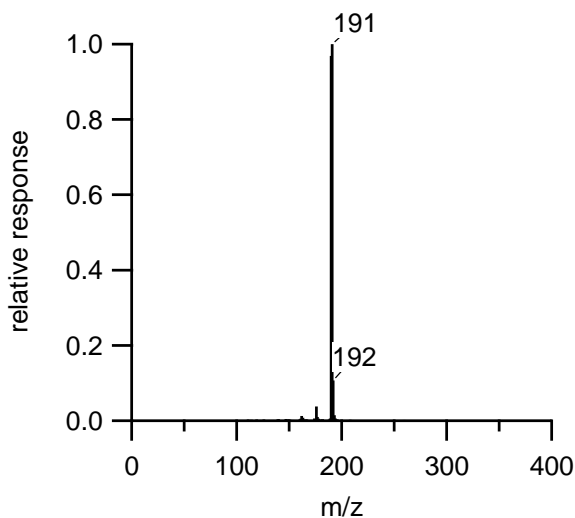
Ethanone, 1,1'-(1,4-phenylene)bis-  
CAS #1009-61-6, MW=162.07 (19 ppm)



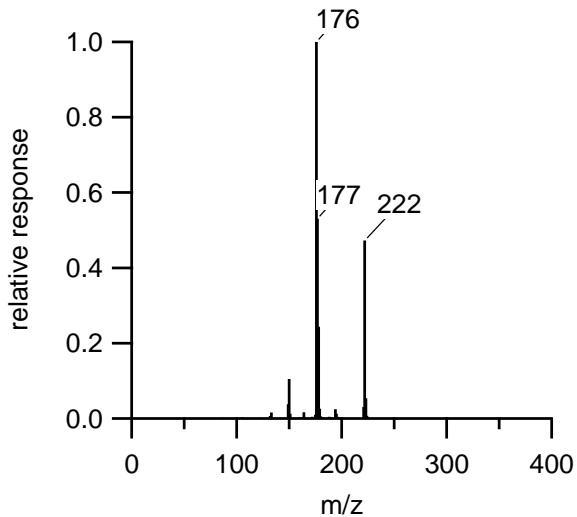
Ethanone, 1,1'-(1,4-phenylene)bis-  
CAS #1009-61-6, MW=162.07 (80 ppm)



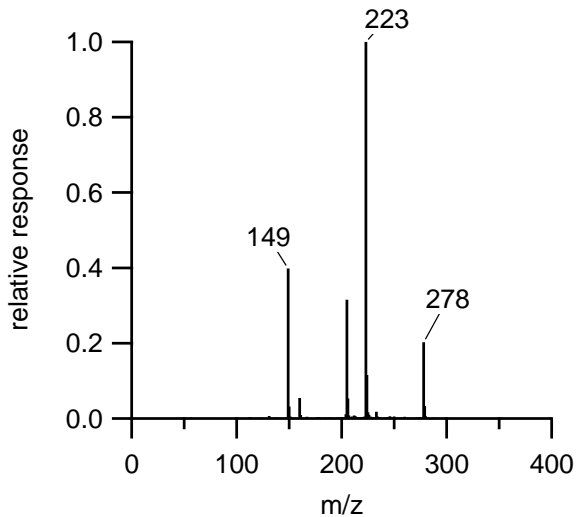
Benzamide, N,N-diethyl-4-methyl-  
CAS #2728-05-4, MW=191.13 (3 ppm)



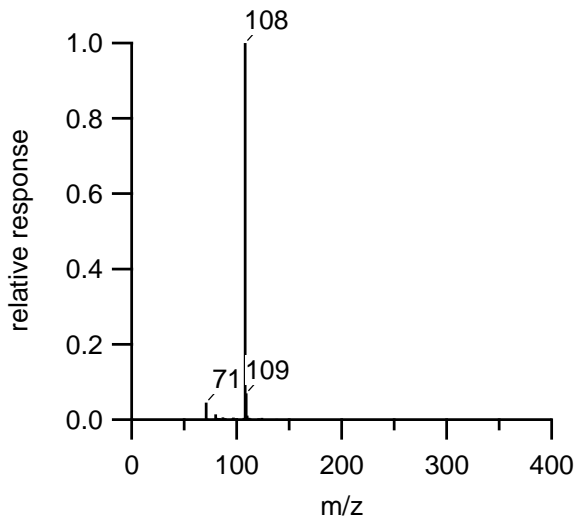
Diethyl Phthalate  
CAS #84-66-2, MW=222.09 (7 ppm)



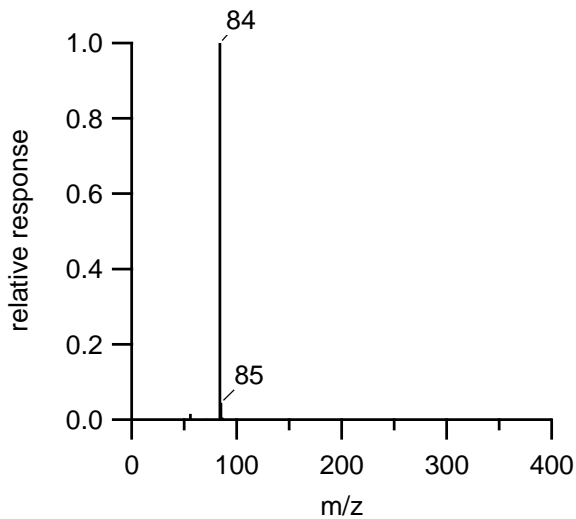
Dibutyl phthalate  
CAS #84-74-2, MW=278.15 (1 ppm)



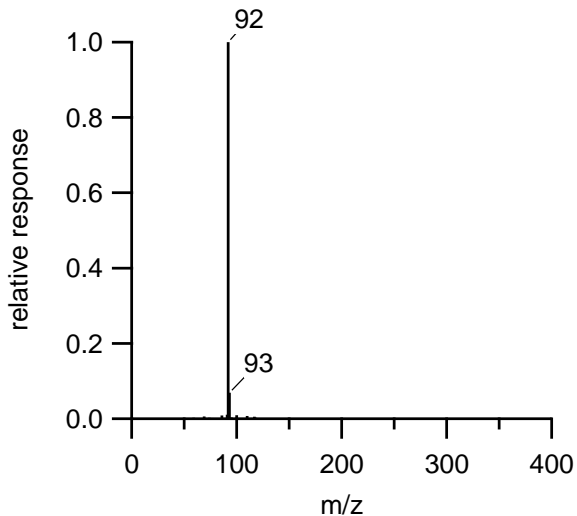
Cyclopentanone, 3,4-bis(methylene)-  
CAS #27646-73-7, MW=108.06 (98 ppm)



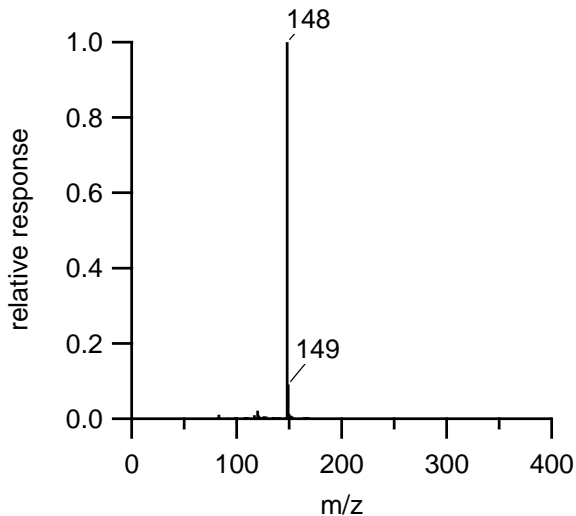
Cyclopentanone  
CAS #120-92-3, MW=84.058 (39 ppm)



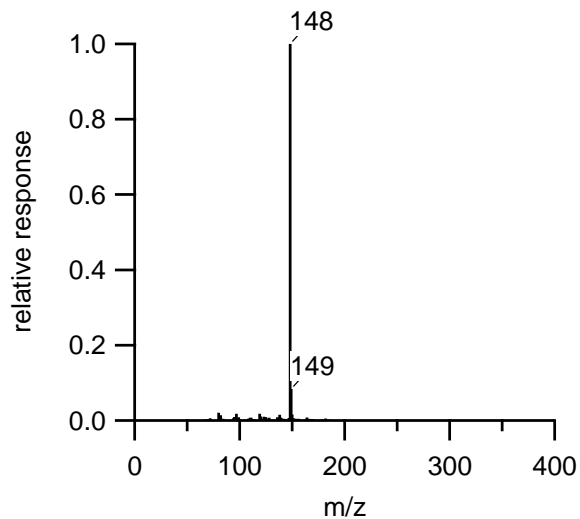
Toluene  
CAS #108-88-3, MW=92.063 (2 ppm)



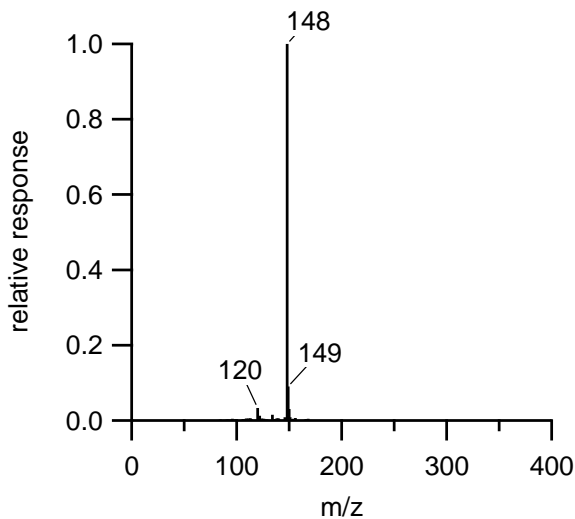
2(3H)-Benzofuranone, 3-methyl-  
CAS #32267-71-3, MW=148.05 (51 ppm)



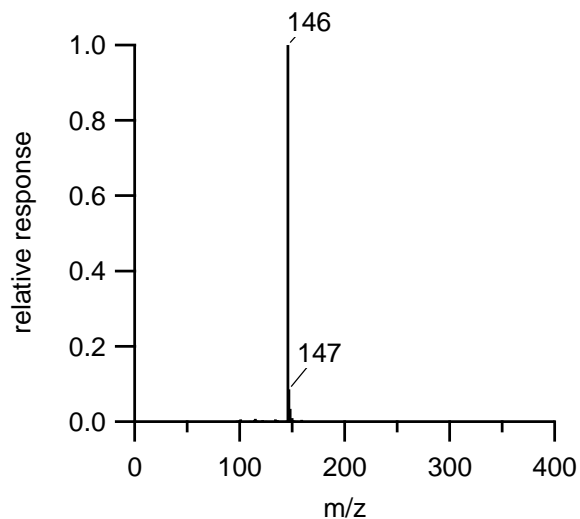
3(2H)-Benzofuranone, 5-methyl-  
CAS #54120-66-0, MW=148.05 (11 ppm)



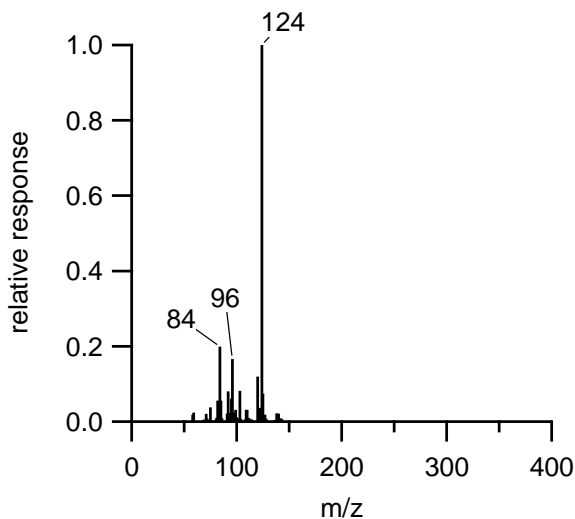
2(3H)-Benzofuranone, 3-methyl-  
CAS #32267-71-3, MW=148.05 (11 ppm)



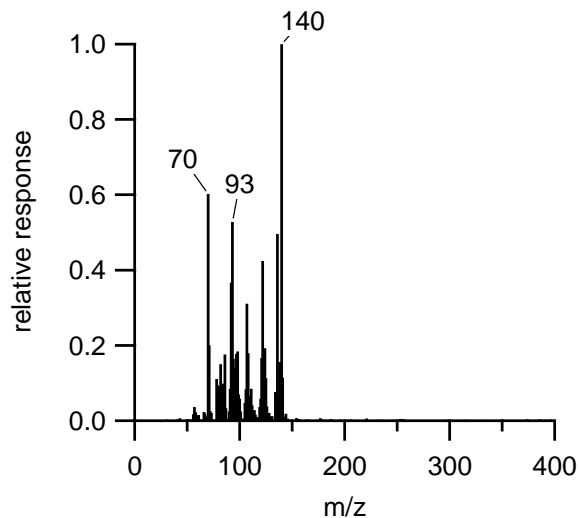
1H-Indene-1,3(2H)-dione  
CAS #606-23-5, MW=146.04 (21 ppm)



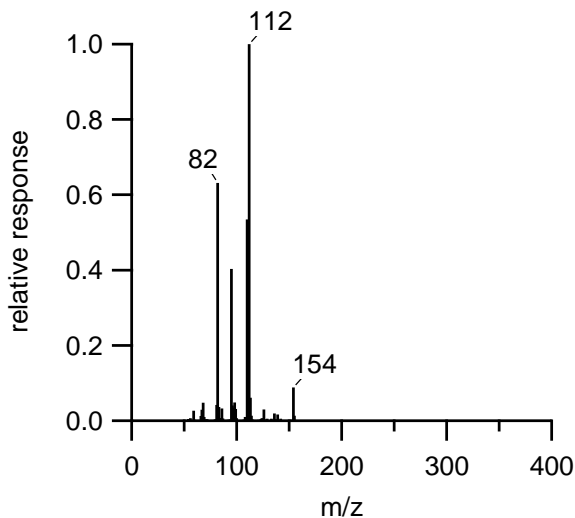
3-Cyclohexene-1-carboxaldehyde, 4-methyl-  
CAS #7560-64-7, MW=124.09 (17 ppm)



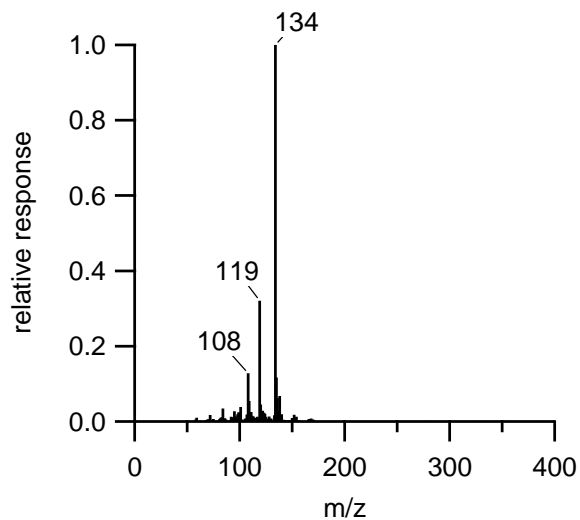
Bicyclo[2.2.2]octan-1-ol, 4-methyl-  
CAS #824-13-5, MW=140.12 (11 ppm)



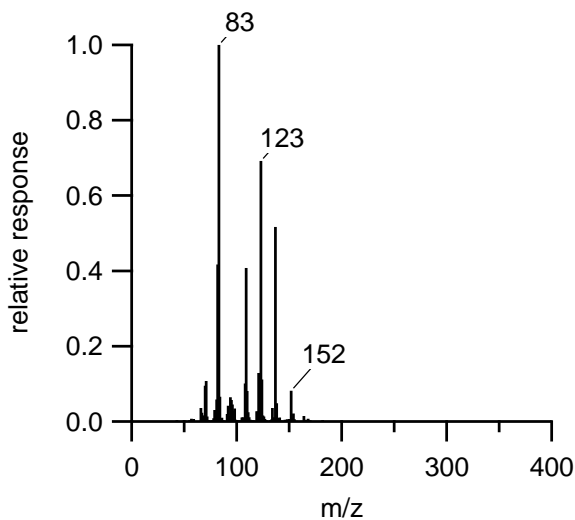
2-Oxabicyclo[3.2.1]nonan-7-one, 1,5-dimethyl-  
CAS #13747-98-3, MW=154.1 (26 ppm)



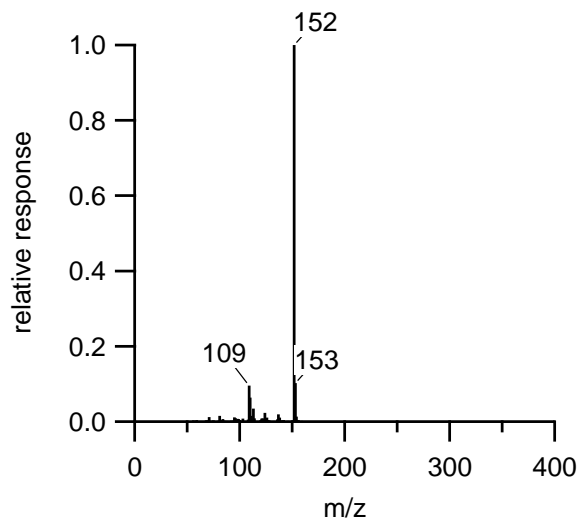
3-Cyclohexen-1-carboxaldehyde, 3,4-dimethyl-  
CAS #0-00-0, MW=138.1 (12 ppm)



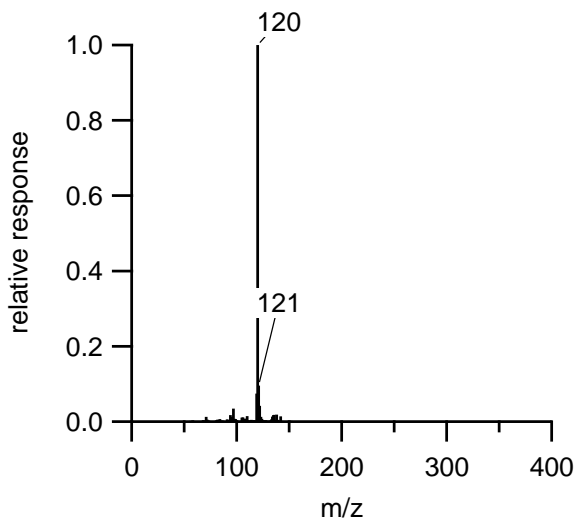
Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-  
CAS #4764-14-1, MW=152.12 (25 ppm)



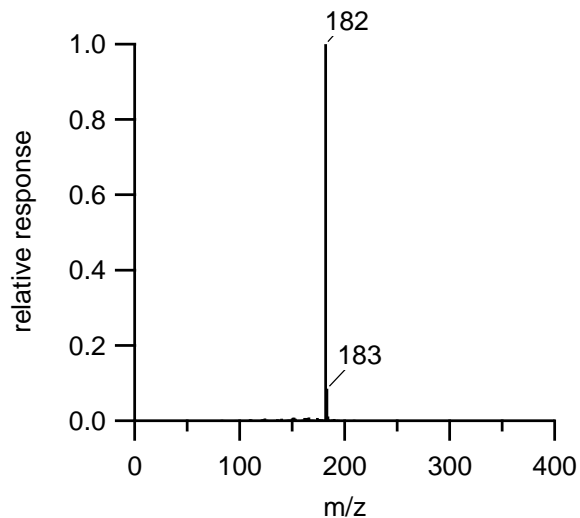
2-Acetyl-4,4-dimethyl-cyclopent-2-enone  
CAS #81979-96-6, MW=152.08 (19 ppm)



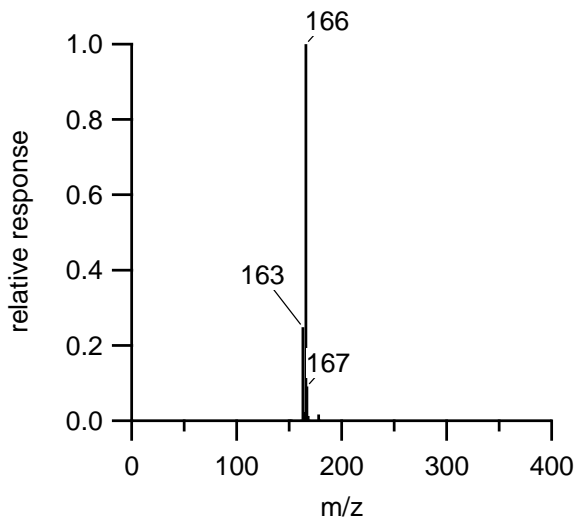
Benzene, 1-ethyl-2-methyl-  
CAS #98-86-2, MW=120.09 (18 ppm)



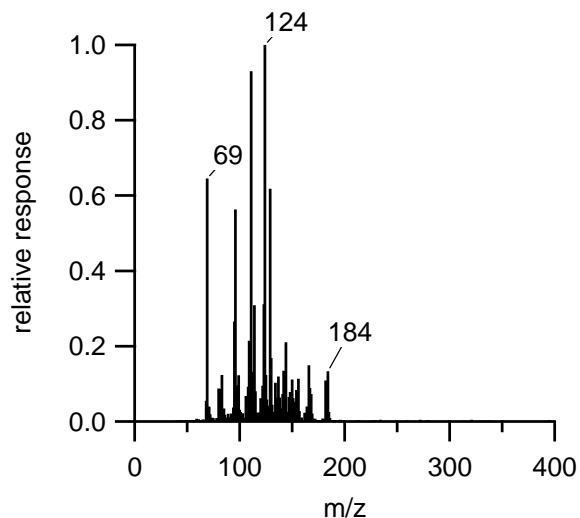
Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester  
CAS #3943-74-6, MW=182.06 (45 ppm)



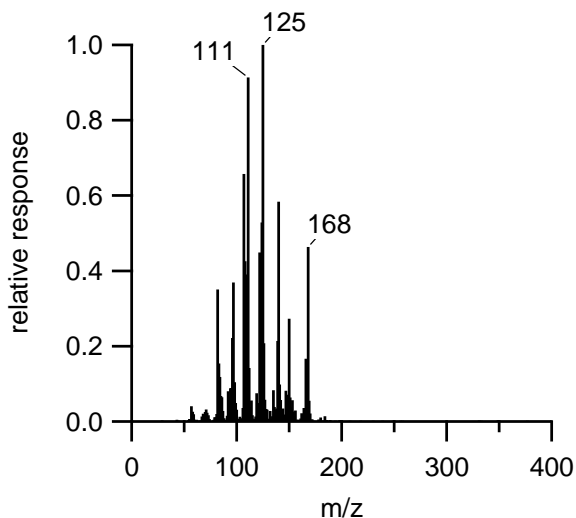
Ethanone, 1-[4-(1-hydroxy-1-methylethyl)phenyl]-  
CAS #54549-72-3, MW=178.1 (33 ppm)



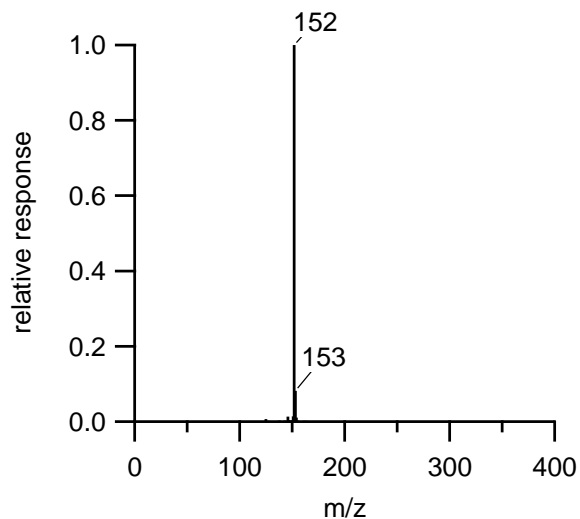
Cyclooctanone, 5-(acetyloxy)-  
CAS #22253-83-4, MW=184.11 (27 ppm)



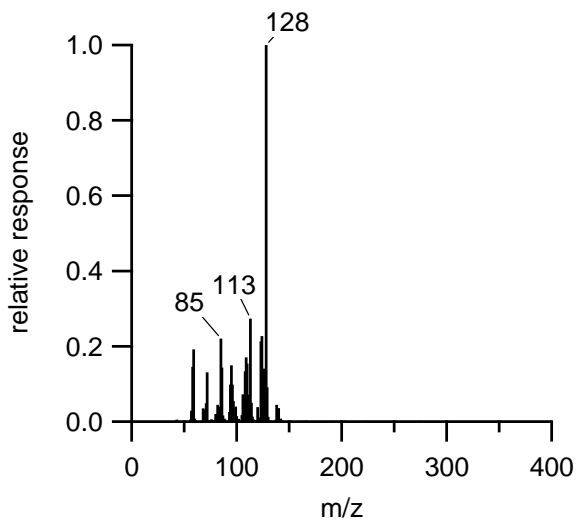
5H-Inden-5-one, octahydro-1-hydroxy-7a-methyl-  
CAS #42199-04-2, MW=168.12 (23 ppm)



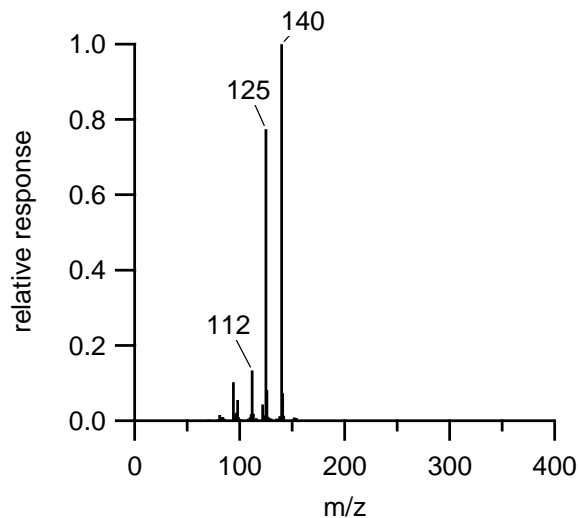
Vanillin  
CAS #121-33-5, MW=152.05 (46 ppm)



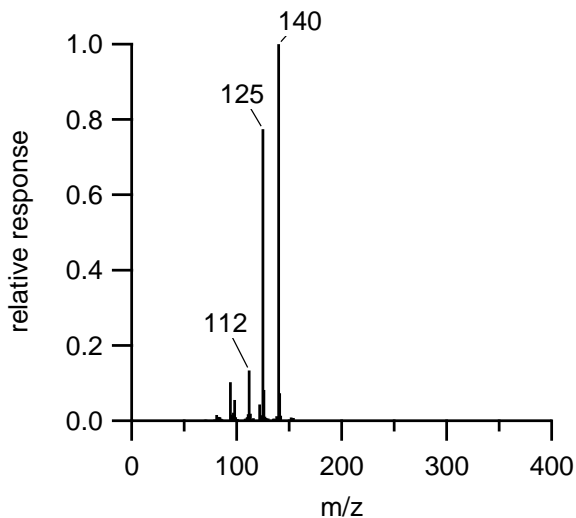
2-Octanone  
CAS #111-13-7, MW=128.12 (12 ppm)



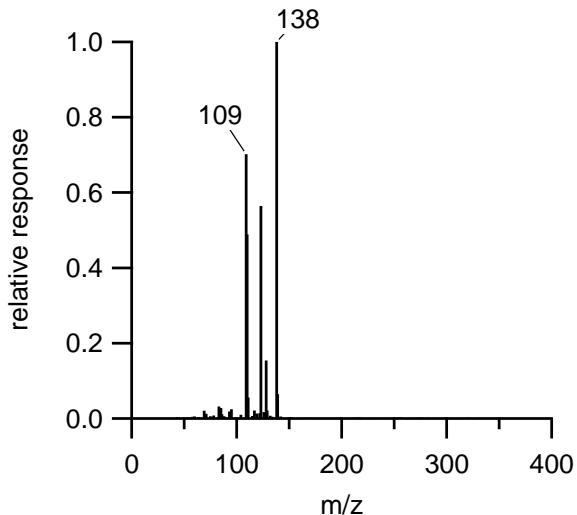
Cyclohexanone, 2-acetyl-  
CAS #874-23-7, MW=140.08 (29 ppm)



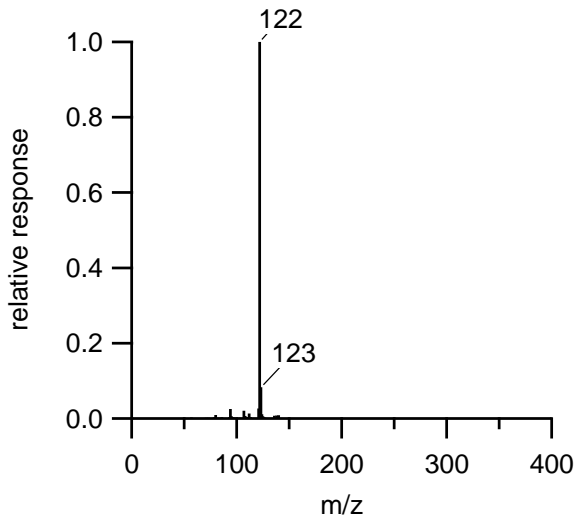
2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2,5-dimethyl-  
CAS #1920-21-4, MW=140.08 (38 ppm)



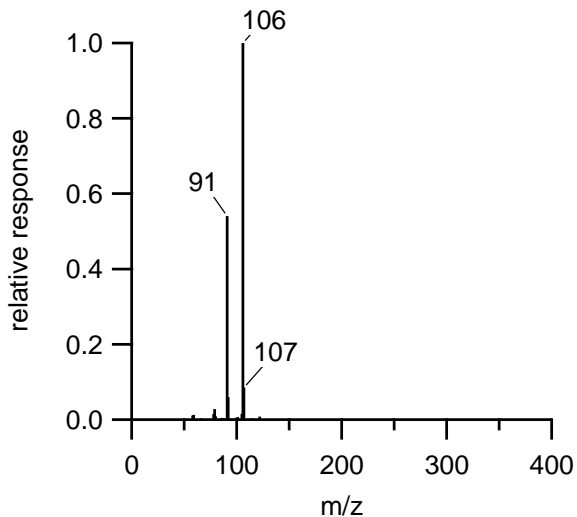
1-(2,4-Dimethyl-furan-3-yl)-ethanone  
CAS #32933-07-6, MW=138.07 (13 ppm)



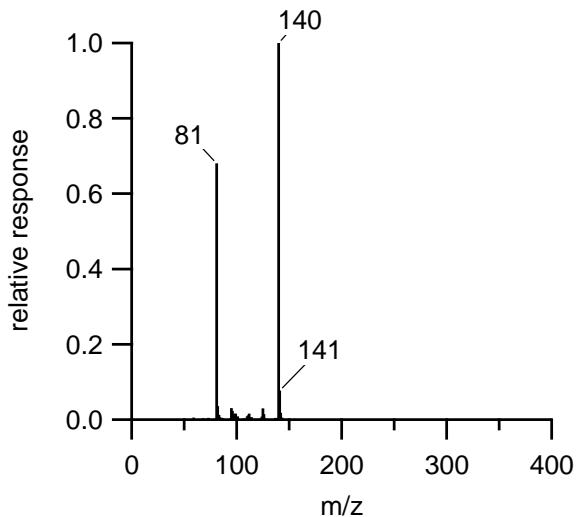
4,4-Dimethylcyclohexadienone  
CAS #1073-14-9, MW=122.07 (38 ppm)



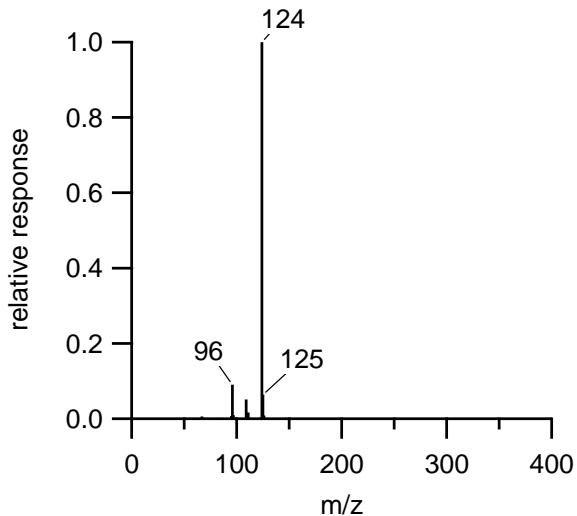
p-Xylene  
CAS #106-42-3, MW=106.08 (14 ppm)



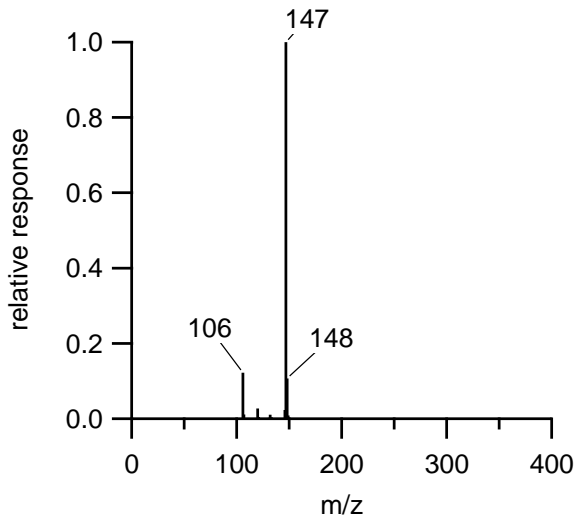
2-Furanpropionic acid  
CAS #935-13-7, MW=140.05 (31 ppm)



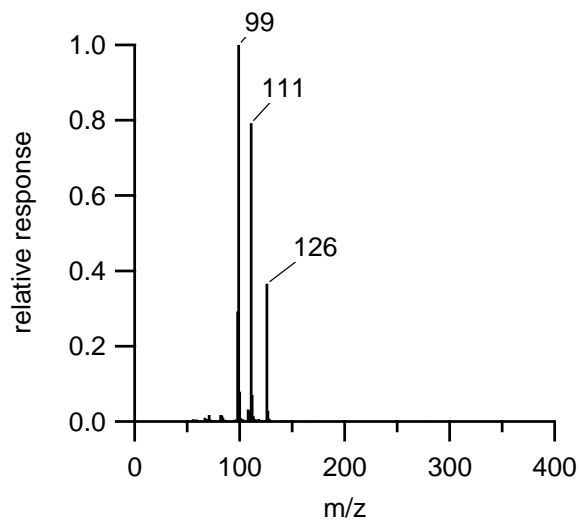
5-Ethyl-2-furaldehyde  
CAS #23074-10-4, MW=124.05 (28 ppm)



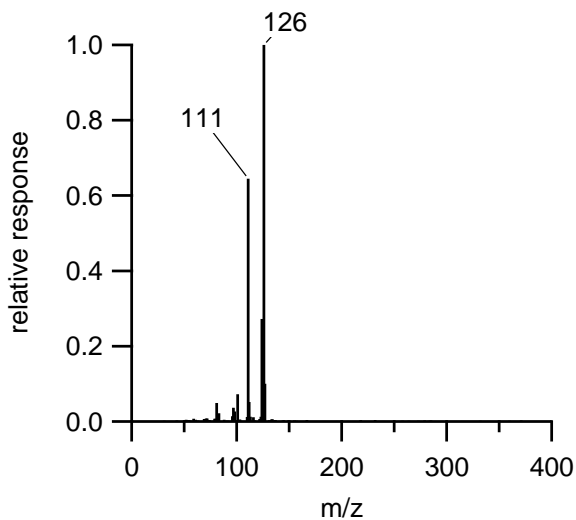
Benzenamine, 2-(1-methylcyclopropyl)-  
CAS #0-00-0, MW=147.1 (14 ppm)



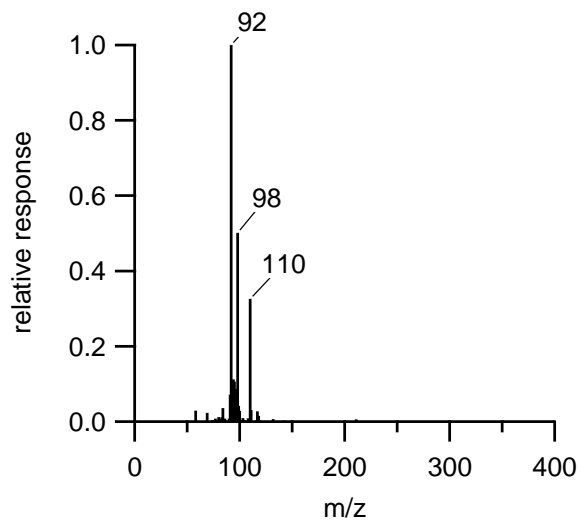
2(3H)-Furanone, 5-ethenyldihydro-5-methyl-  
CAS #1073-11-6, MW=126.07 (21 ppm)



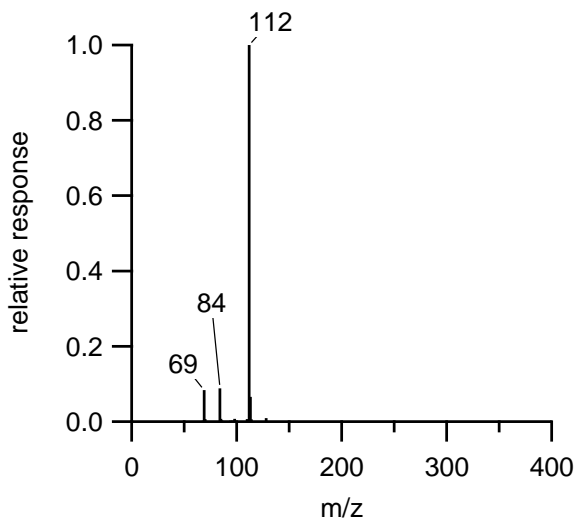
2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-  
CAS #21835-00-7, MW=126.07 (21 ppm)



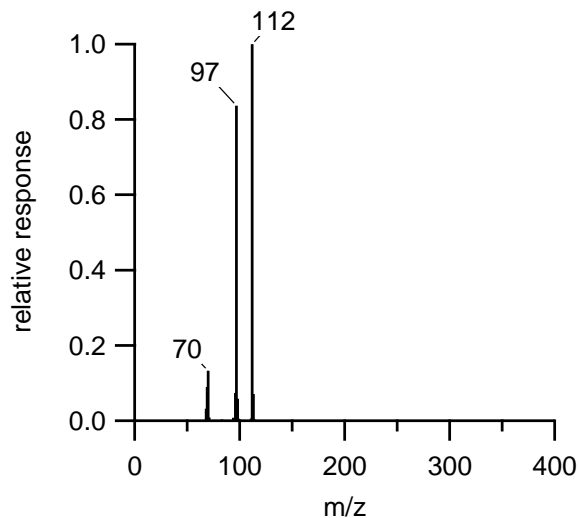
trans,trans-3,5-Heptadien-2-one  
CAS #18402-90-9, MW=110.07 (28 ppm)



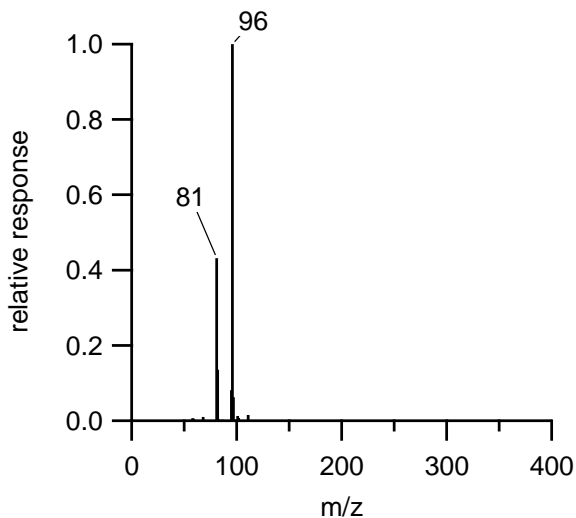
2-Furanone, 2,5-dihydro-3,5-dimethyl  
CAS #3212-68-8, MW=112.05 (55 ppm)



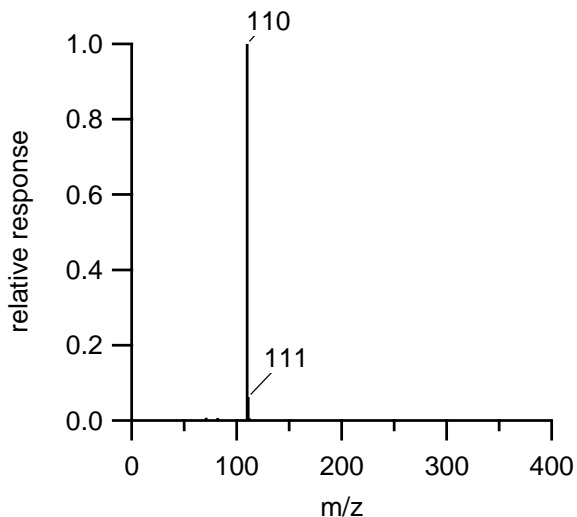
3-Penten-2-one, 3,4-dimethyl-  
CAS #5166-53-0, MW=112.09 (56 ppm)



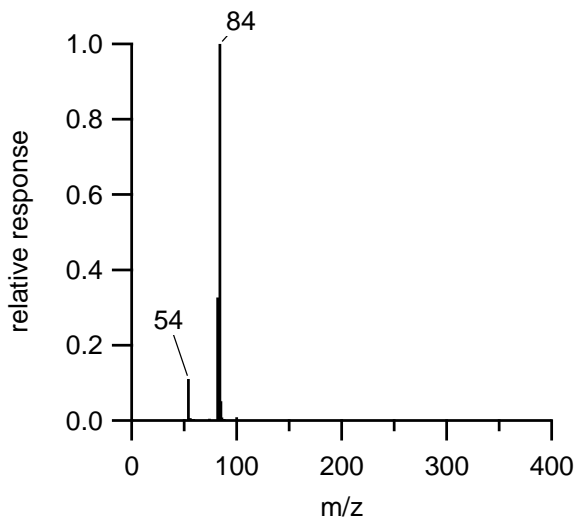
2,4-Hexadienal, (E,E)-  
CAS #3710-43-8, MW=96.058 (45 ppm)



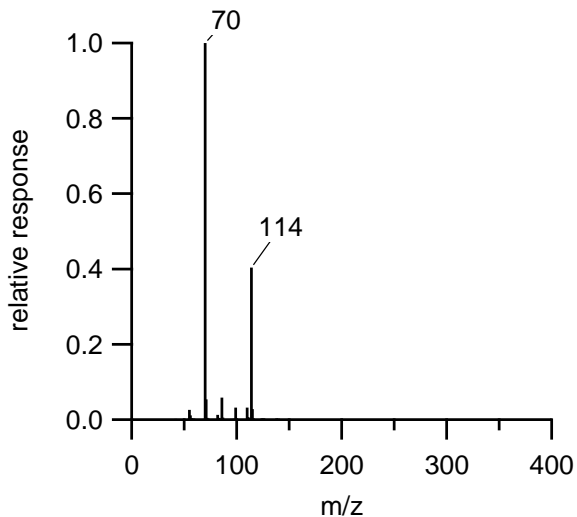
1,4-Cyclohex-2-enedione  
CAS #4505-38-8, MW=110.04 (20 ppm)



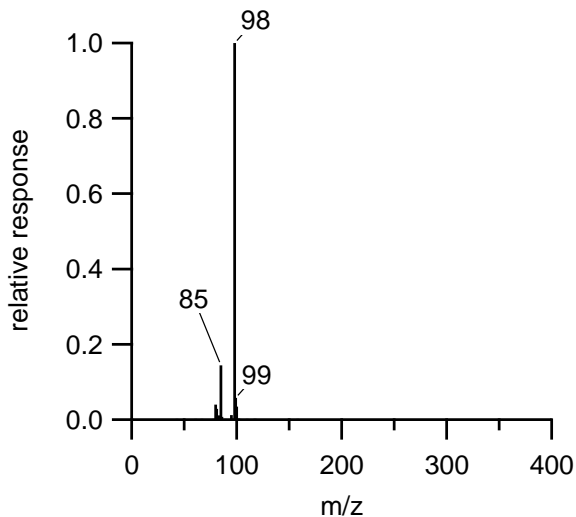
Furan, 2,3-dihydro-4-methyl-  
CAS #1115-11-3, MW=84.058 (39 ppm)



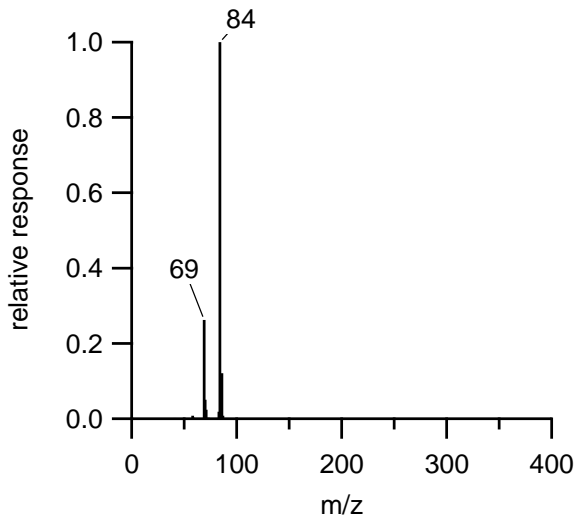
2H-Pyran-2-one, tetrahydro-6-methyl-  
CAS #823-22-3, MW=114.07 (28 ppm)



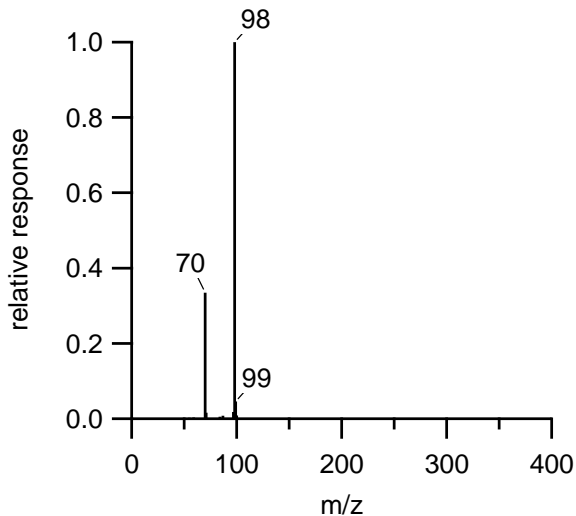
Cyclohexanone  
CAS #108-94-1, MW=98.073 (34 ppm)



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

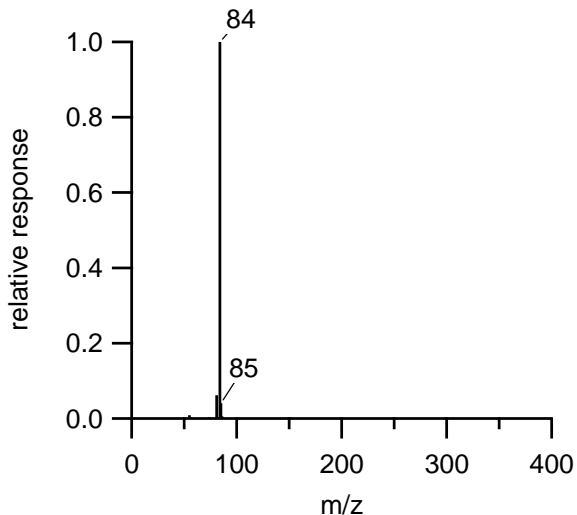


1,3-Cyclopentanedione  
CAS #3859-41-4, MW=98.037 (63 ppm)

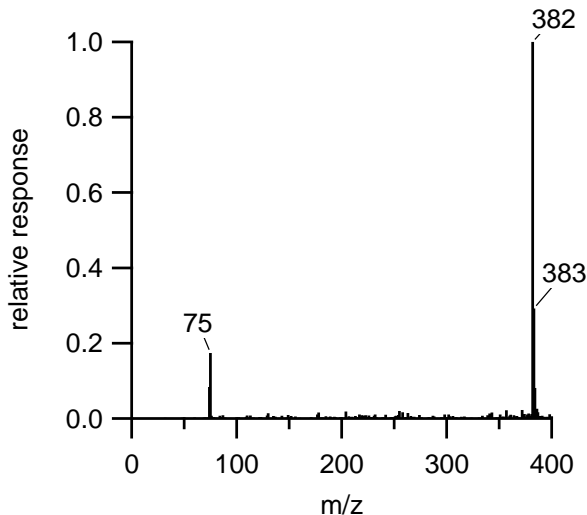




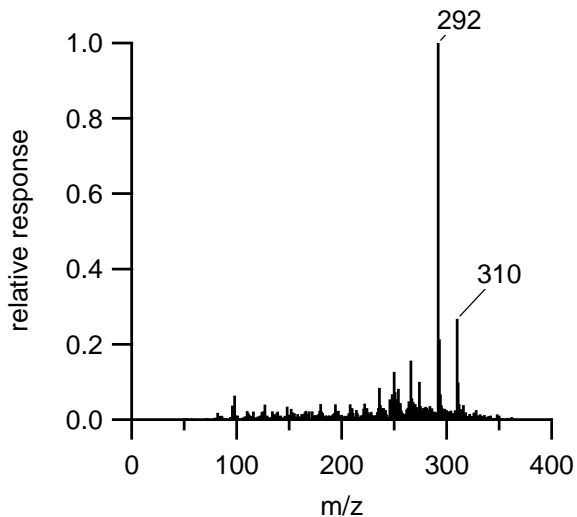
2(5H)-Furanone  
CAS #497-23-4, MW=84.021 (99 ppm)



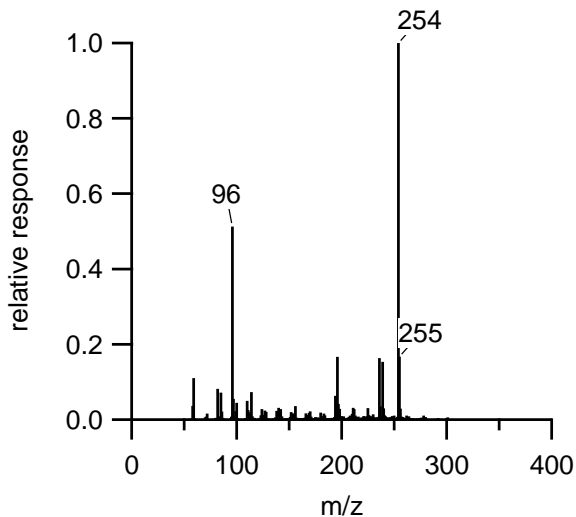
Tetracosanoic acid, methyl ester  
CAS #2442-49-1, MW=382.38 (12 ppm)



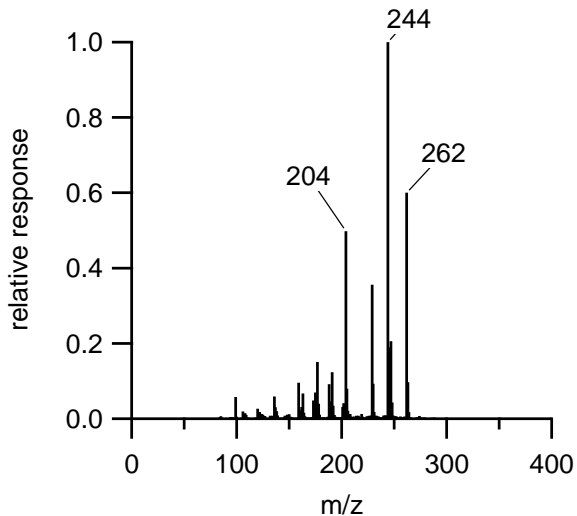
cis-13-Eicosenoic acid  
CAS #17735-94-3, MW=310.29 (77 ppm)



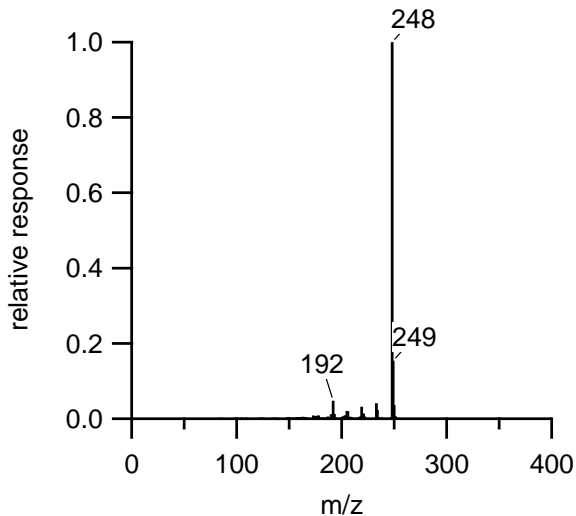
2-Heptadecanone  
CAS #2922-51-2, MW=254.26 (6 ppm)



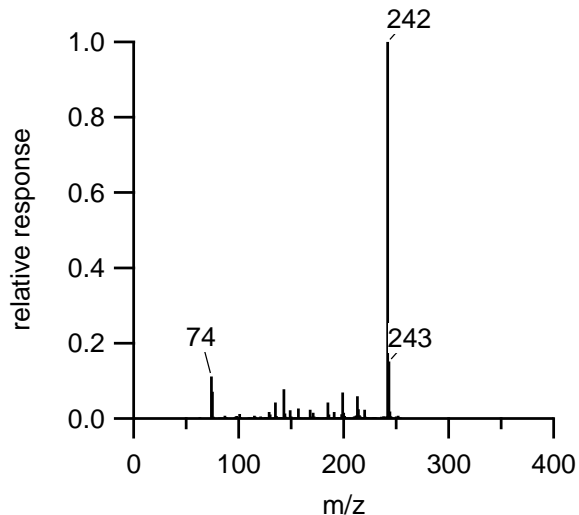
14-Oxatricyclo[9..2.1.0(1,10)]tetradecane, 2,6,6,10,11-pent  
CAS #0-00-0, MW=262.23 (18 ppm)



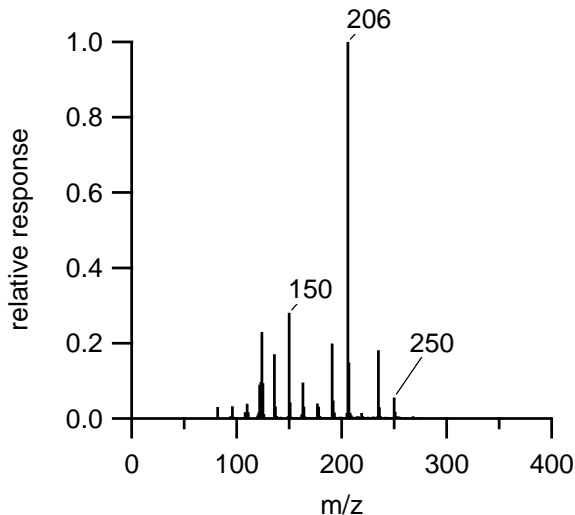
2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylpropyl)-  
CAS #4584-63-8, MW=248.18 (18 ppm)



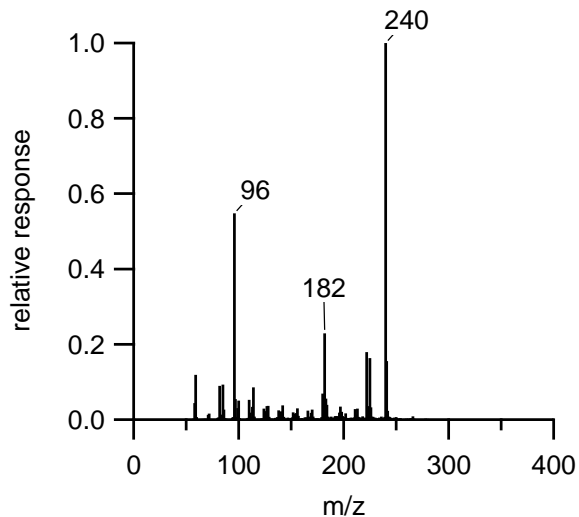
Tridecanoic acid, 12-methyl-, methyl ester  
CAS #5129-58-8, MW=242.22 (13 ppm)



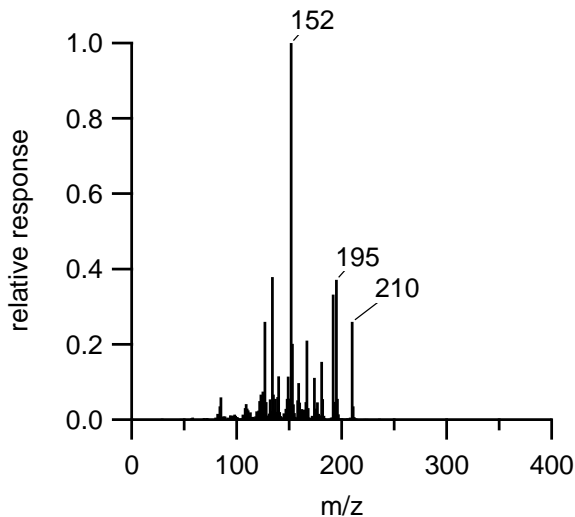
Sclareolide  
CAS #564-20-5, MW=250.19 (52 ppm)



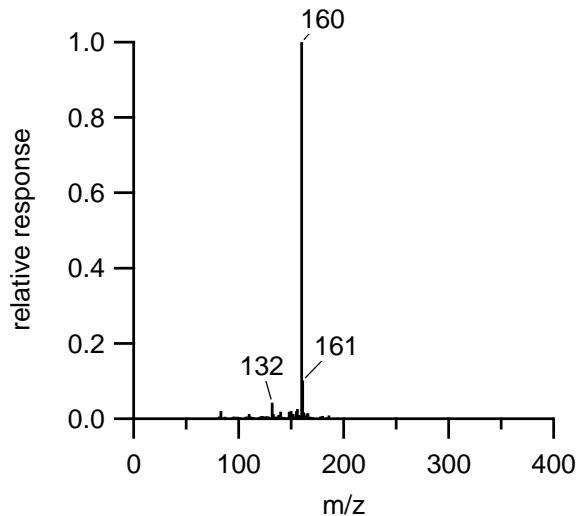
2-Hexadecanone  
CAS #18787-63-8, MW=240.25 (4 ppm)



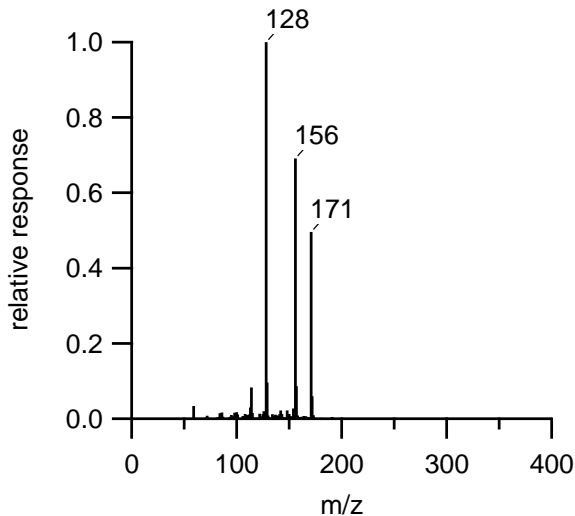
Spiro(2-oxabicyclo[2.1.0]pentane)-3,2'-oxetane, 1,5,5,3',4',  
CAS #0-00-0, MW=210.16 (21 ppm)



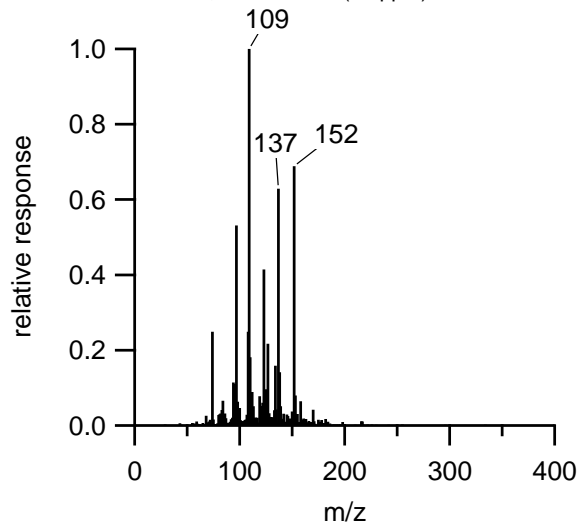
Coumarin, 8-methyl-  
CAS #1807-36-9, MW=160.05 (31 ppm)



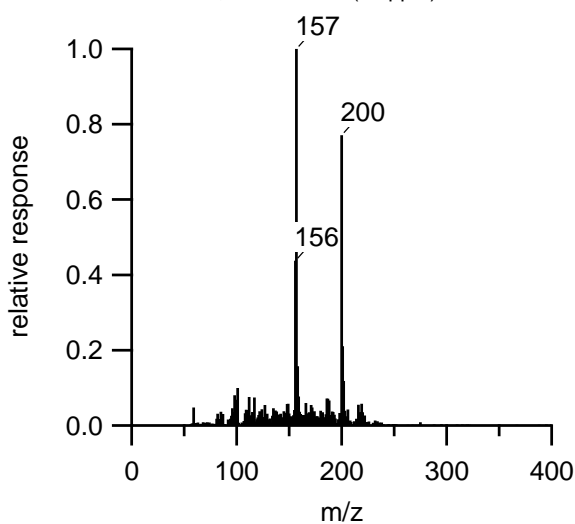
Acetamide, N,N-dibutyl-  
CAS #1563-90-2, MW=171.16 (18 ppm)



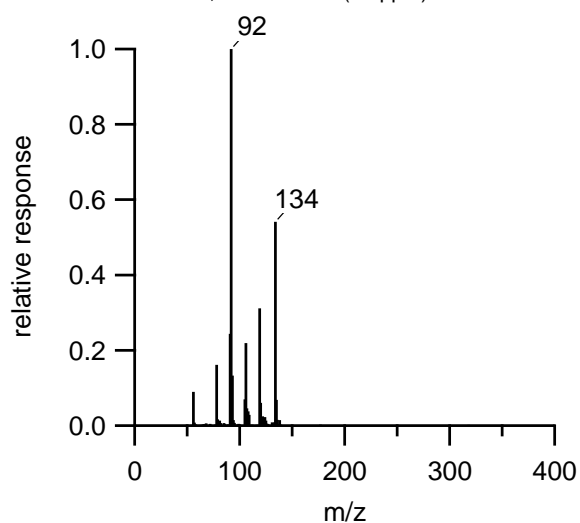
2-Isopropylidene-5-methylhex-4-enal  
CAS #3304-28-7, MW=152.12 (25 ppm)



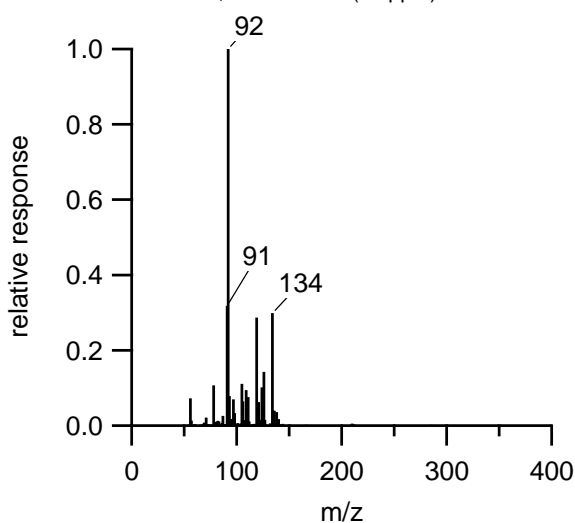
à-Calacorene  
CAS #21391-99-1, MW=200.16 (36 ppm)



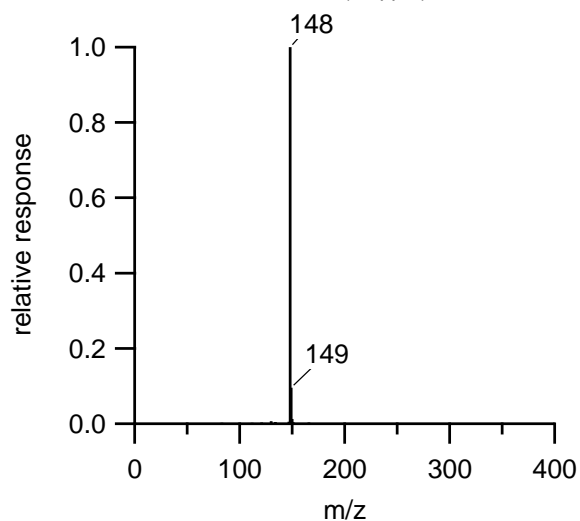
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene  
CAS #4488-57-7, MW=134.11 (17 ppm)



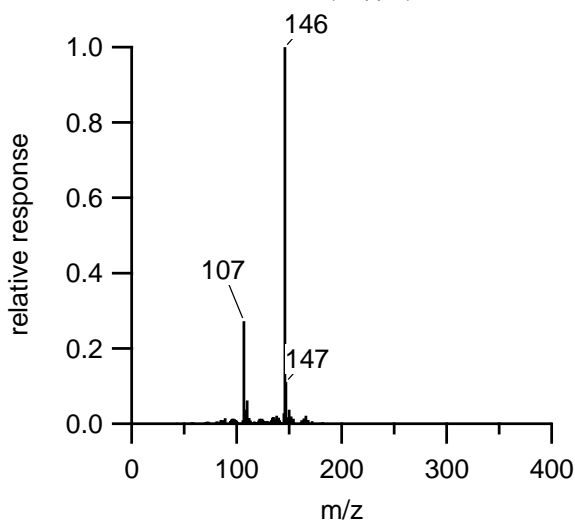
Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)-  
CAS #36262-09-6, MW=134.11 (17 ppm)



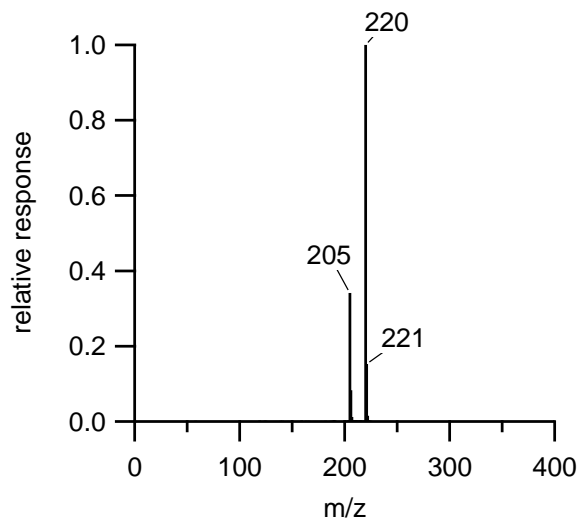
2-Allyl-4-methylphenol  
CAS #3354-58-3, MW=148.09 (35 ppm)



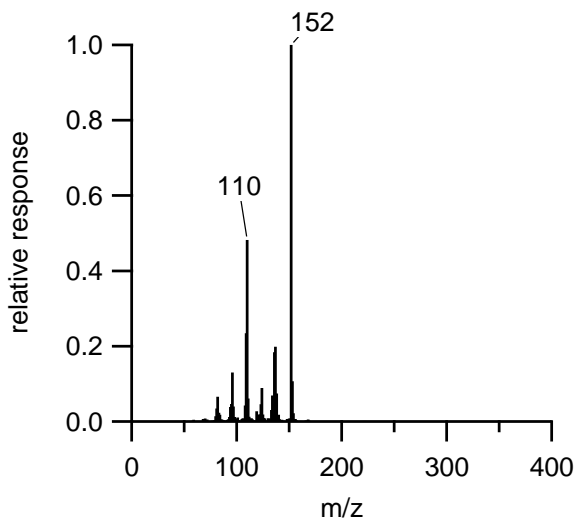
Cinnamaldehyde, à-methyl-  
CAS #101-39-3, MW=146.07 (52 ppm)



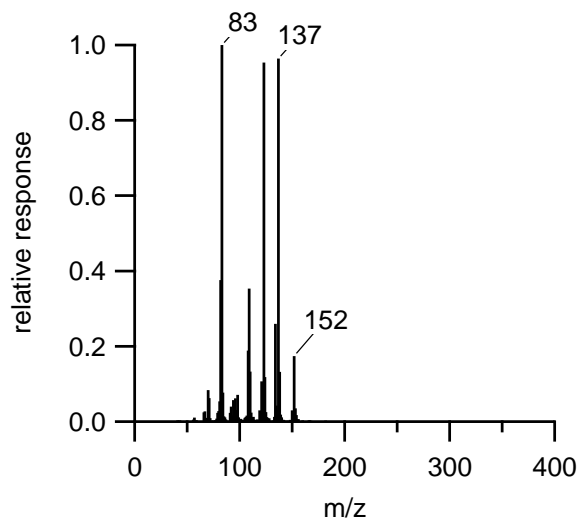
Butylated Hydroxytoluene  
CAS #128-37-0, MW=220.18 (28 ppm)



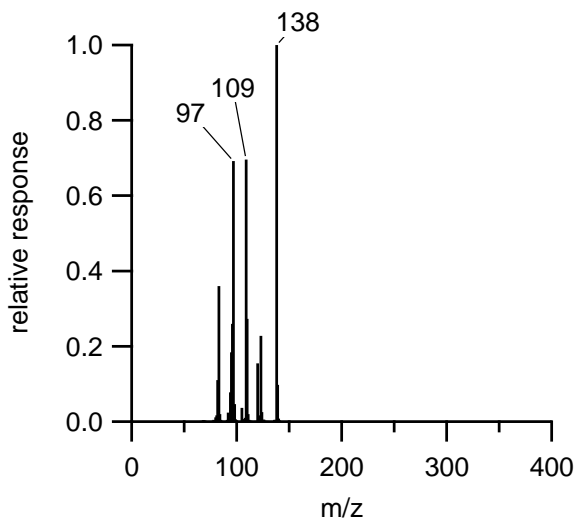
Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl-, [1R-(1à,4á,6à)]-  
CAS #4176-04-9, MW=152.12 (25 ppm)



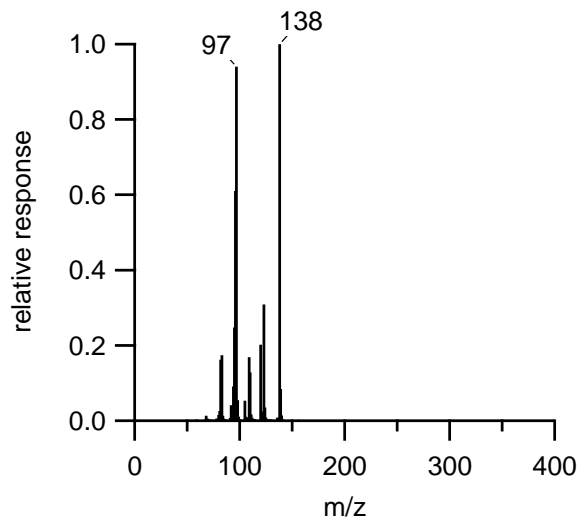
Bicyclo[3.1.1]heptane-2-carboxaldehyde, 6,6-dimethyl-  
CAS #4764-14-1, MW=152.12 (25 ppm)



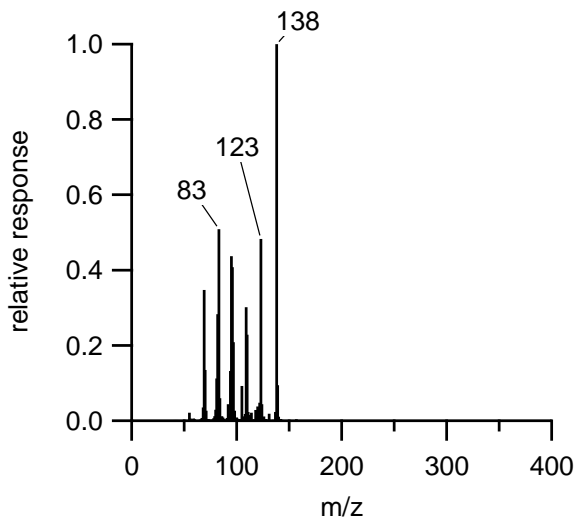
Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl-, (1R)-  
CAS #38651-65-9, MW=138.1 (12 ppm)



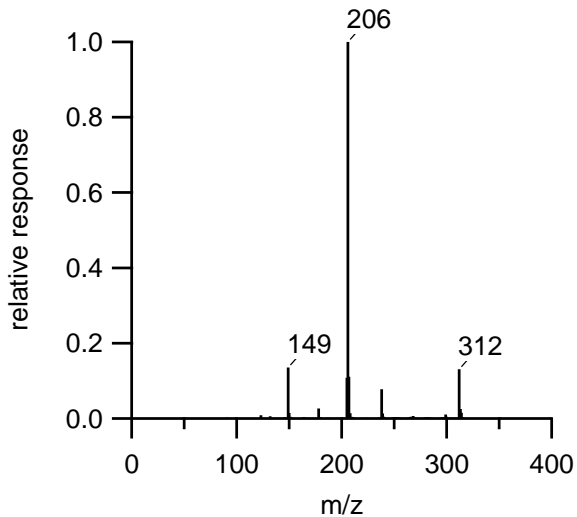
Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)-  
CAS #513-20-2, MW=138.1 (12 ppm)



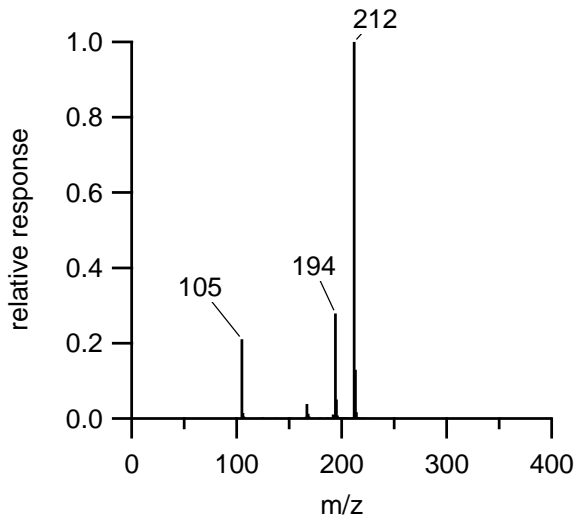
Bicyclo[2.2.1]heptan-2-one, 3,3-dimethyl-  
CAS #13211-15-9, MW=138.1 (12 ppm)



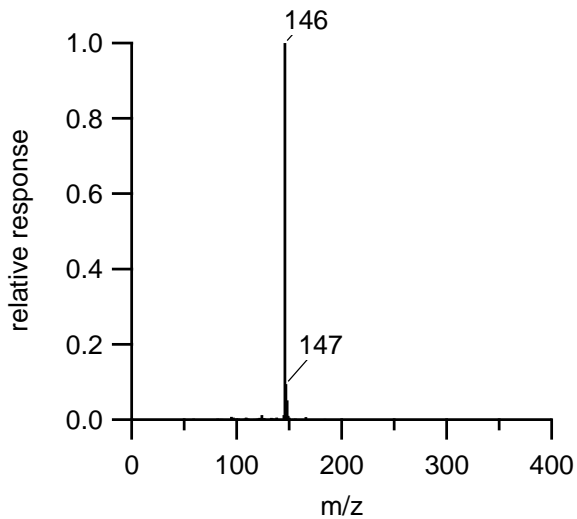
Benzyl butyl phthalate  
CAS #85-68-7, MW=312.14 (2 ppm)



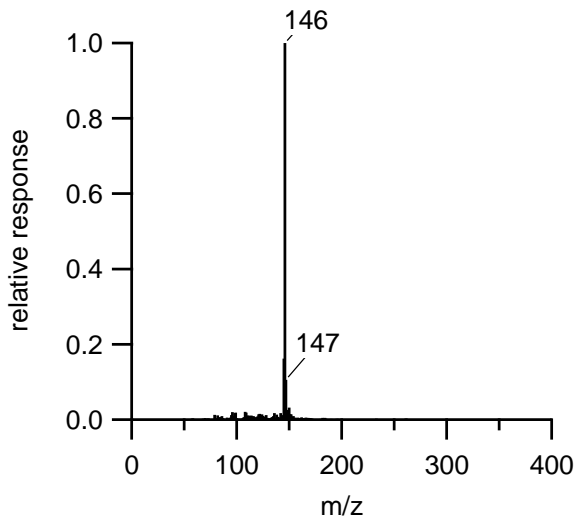
Benzyl Benzoate  
CAS #120-51-4, MW=212.08 (8 ppm)



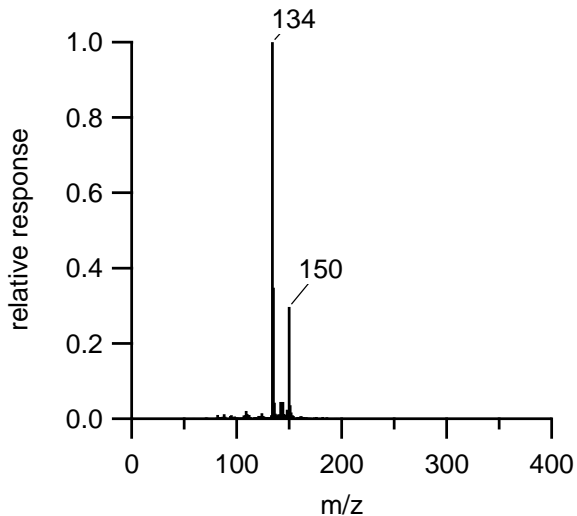
Benzofuran, 4,7-dimethyl-  
CAS #28715-26-6, MW=146.07 (52 ppm)



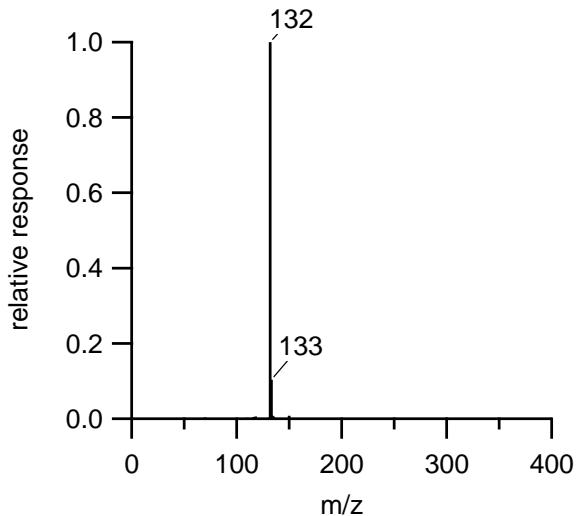
Benzofuran, 4,7-dimethyl-  
CAS #28715-26-6, MW=146.07 (42 ppm)



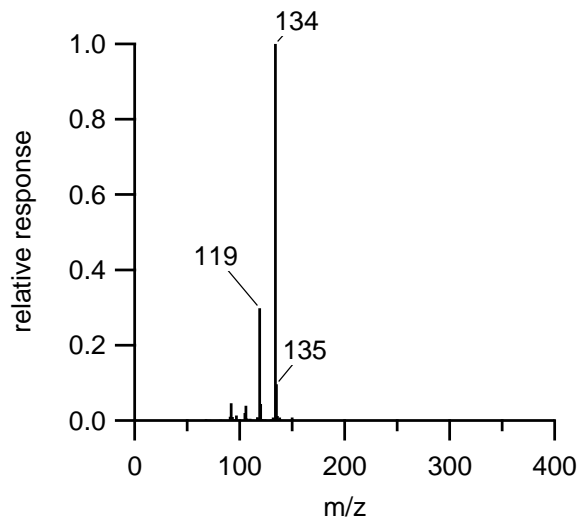
p-Cymen-7-ol  
CAS #536-60-7, MW=150.1 (35 ppm)



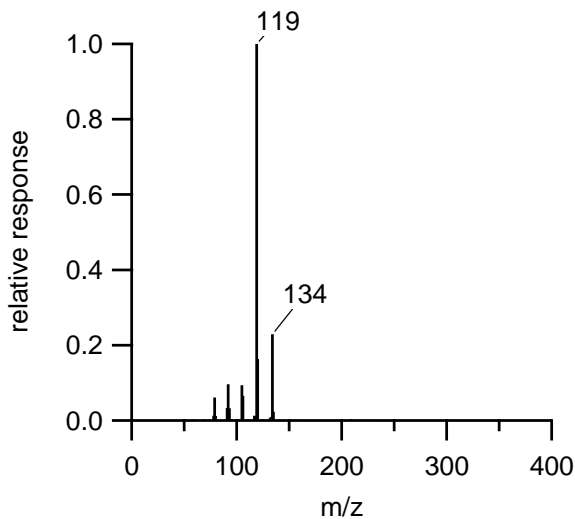
Benzene, 1-methyl-4-(1-methylethenyl)-  
CAS #1195-32-0, MW=132.09 (21 ppm)



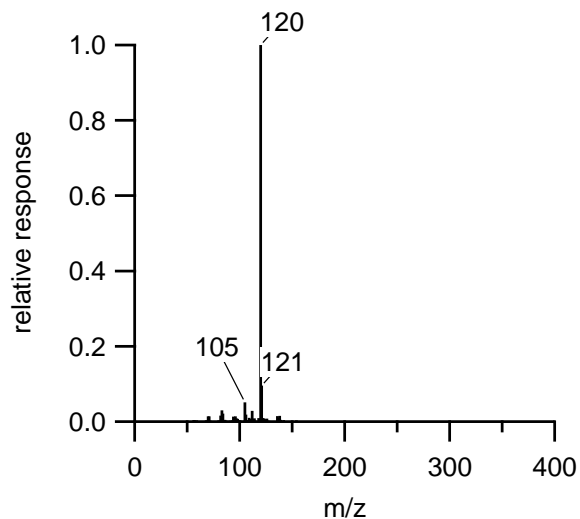
*o*-Cymene  
CAS #535-77-3, MW=134.11 (17 ppm)



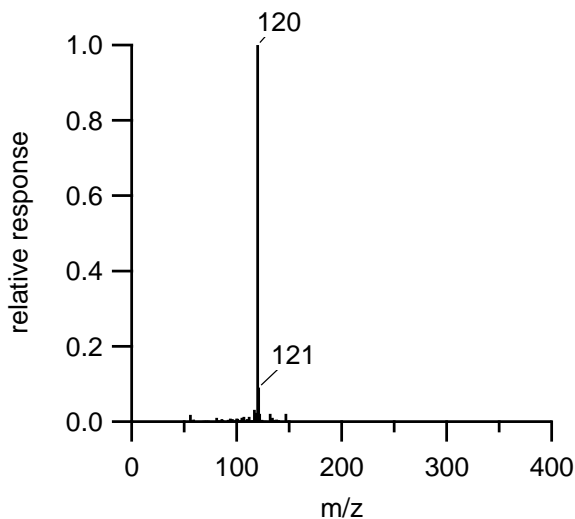
1,3,5-Cycloheptatriene, 3,7,7-trimethyl-  
CAS #3479-89-8, MW=134.11 (17 ppm)



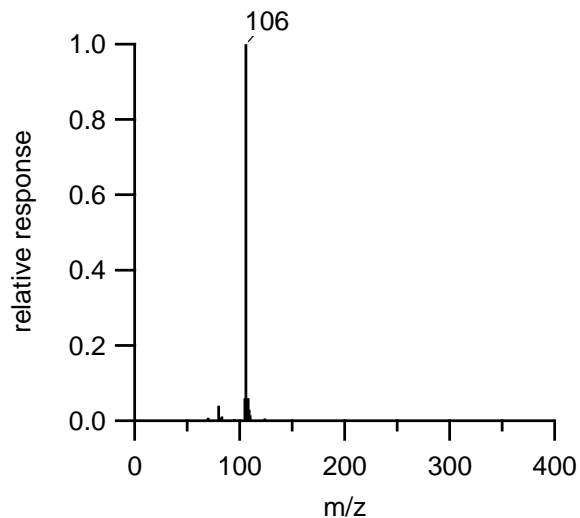
Benzene, 1-ethyl-2-methyl-  
CAS #98-82-8, MW=120.09 (18 ppm)



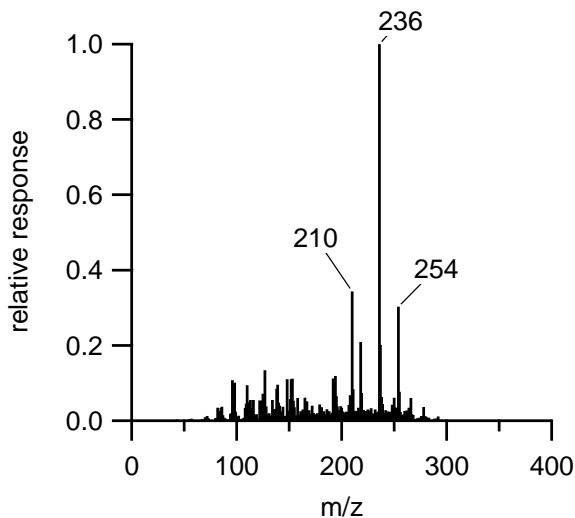
Benzene, 1-ethyl-4-methyl-  
CAS #98-82-8, MW=120.09 (18 ppm)



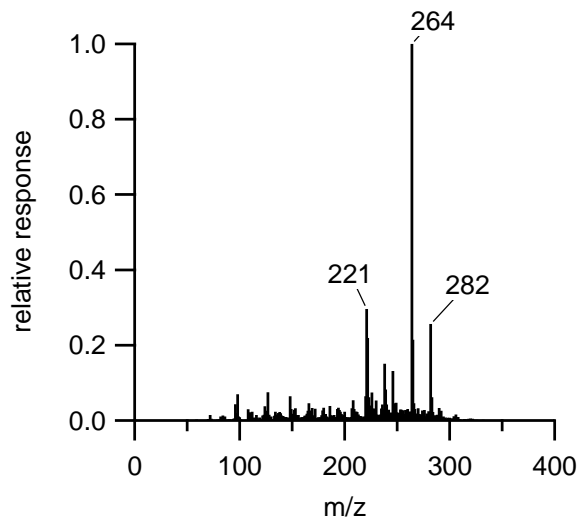
Benzaldehyde  
CAS #100-52-7, MW=106.04 (0 ppm)



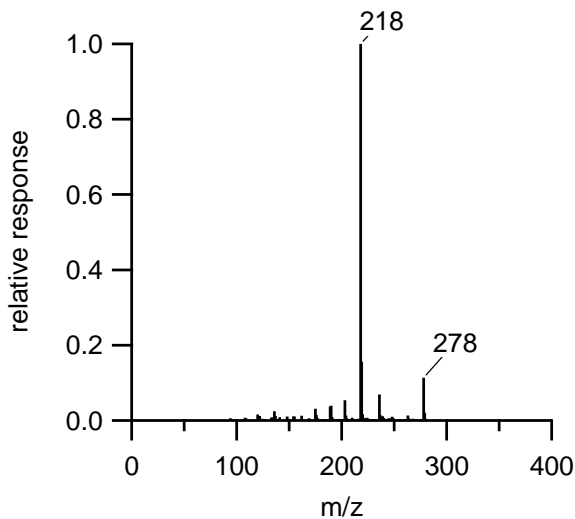
*cis*-9-Hexadecenoic acid  
CAS #2416-20-8, MW=254.22 (63 ppm)



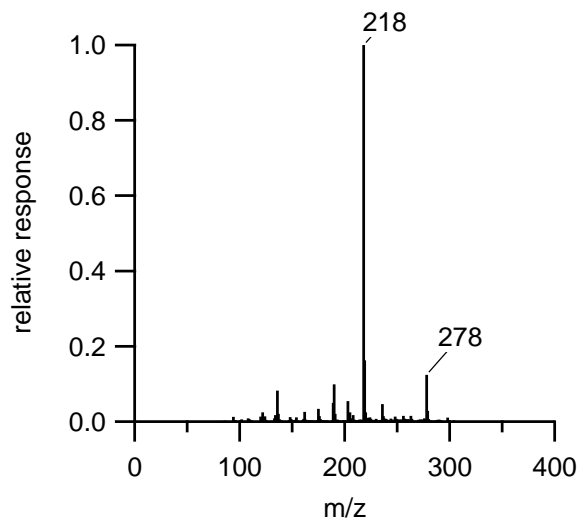
cis-Vaccenic acid  
CAS #506-17-2, MW=282.26 (38 ppm)



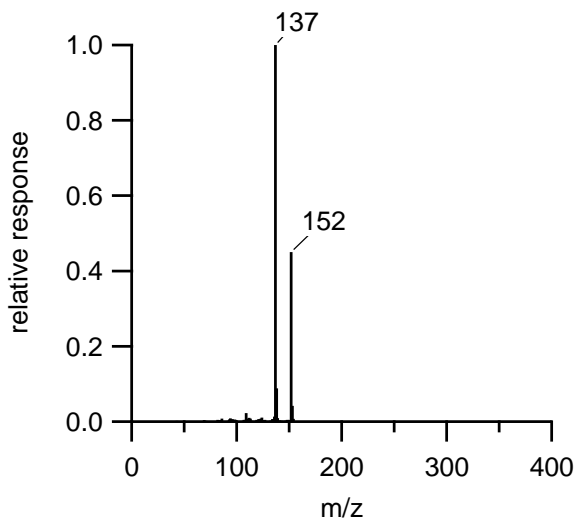
5H-3,5a-Epoxy-naphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-  
CAS #1153-34-0, MW=278.22 (31 ppm)



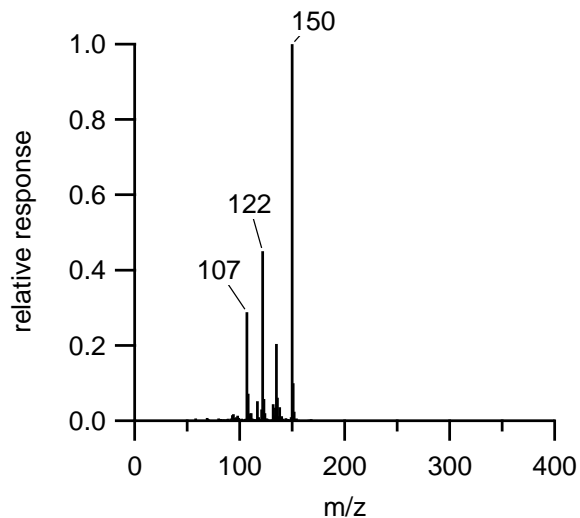
5H-3,5a-Epoxy-naphth[2,1-c]oxepin, dodecahydro-3,8,8,11a-  
CAS #1153-34-0, MW=278.22 (31 ppm)



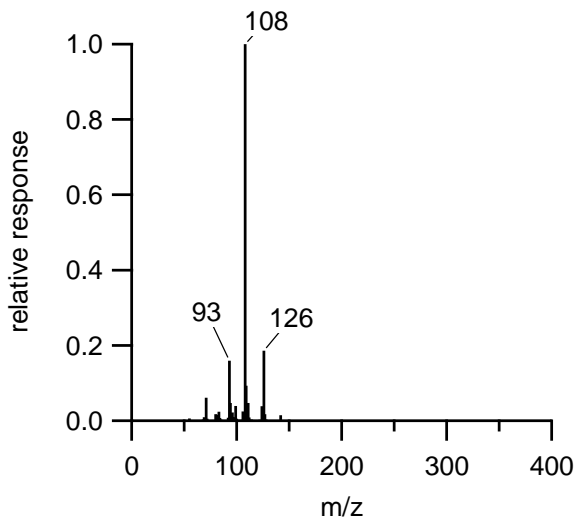
3-Isopropylidene-5-methyl-hex-4-en-2-one  
CAS #64149-32-2, MW=152.12 (17 ppm)



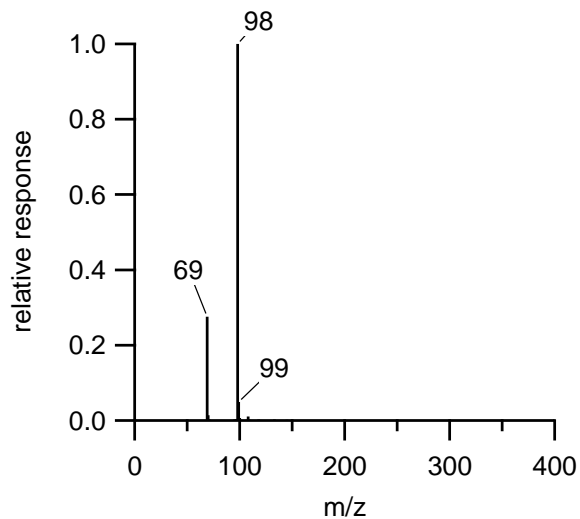
5-Isopropenyl-2-methylcyclopent-1-enecarboxaldehyde  
CAS #0-00-0, MW=150.1 (35 ppm)



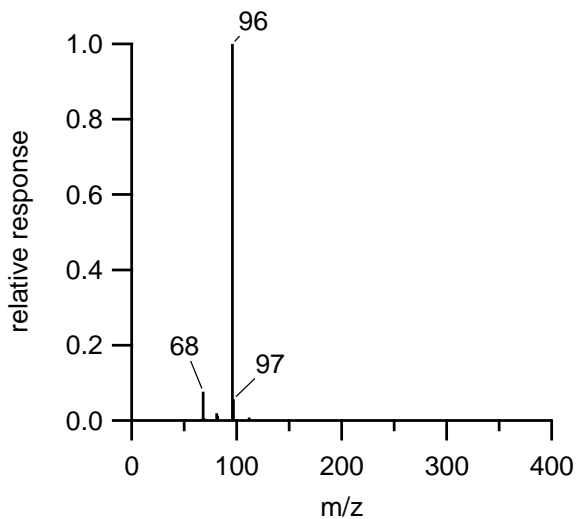
5-Hepten-2-one, 6-methyl-  
CAS #110-93-0, MW=126.1 (34 ppm)



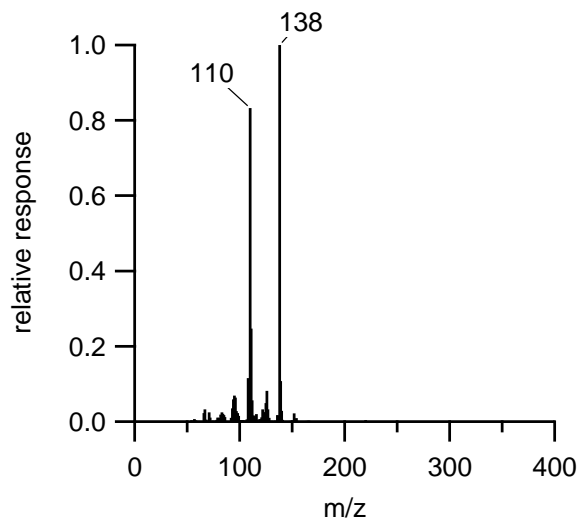
4-Methyl-5H-furan-2-one  
CAS #6124-79-4, MW=98.037 (63 ppm)



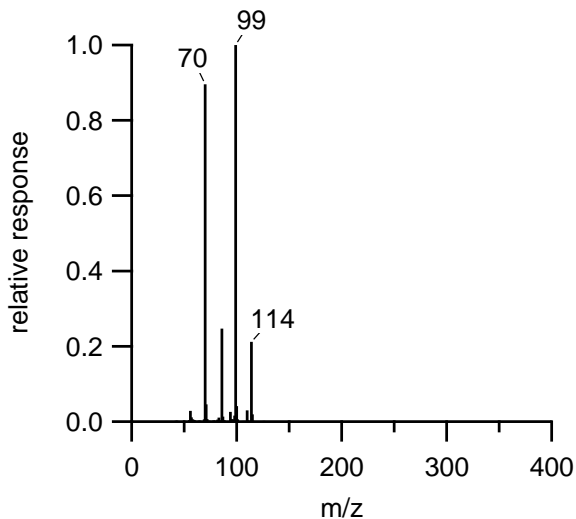
Bicyclo[3.1.0]hexan-3-one  
CAS #1755-04-0, MW=96.058 (45 ppm)



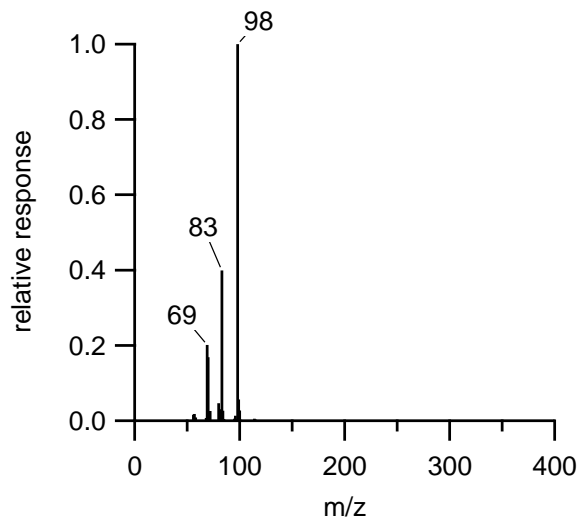
4-Cyclopentene-1,3-dione, 4-propyl-  
CAS #58940-74-2, MW=138.07 (13 ppm)



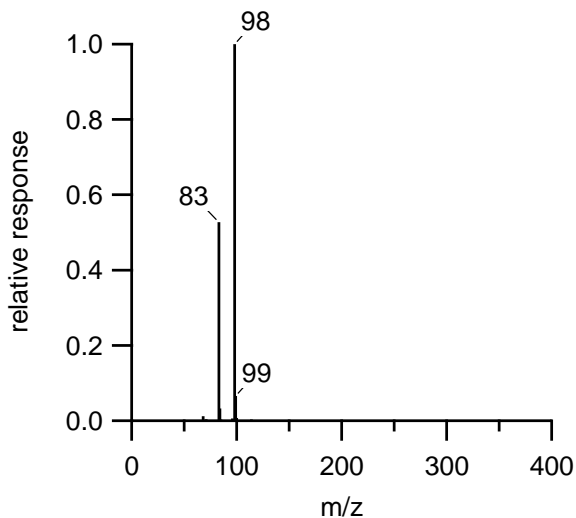
3-Pentenoic acid, 4-methyl-  
CAS #504-85-8, MW=114.07 (28 ppm)



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

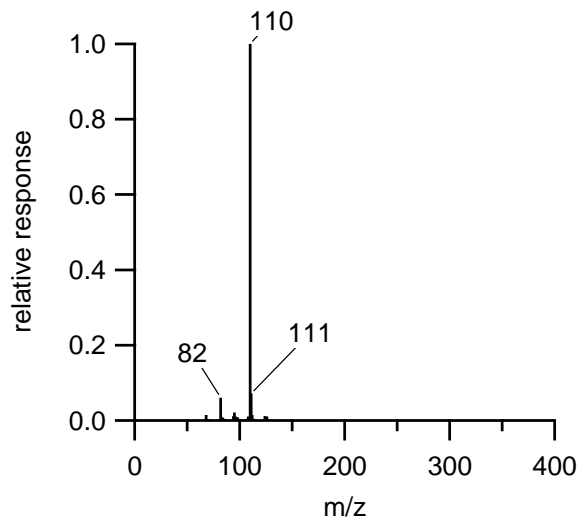


3-Penten-2-one, 4-methyl-  
CAS #141-79-7, MW=98.073 (34 ppm)

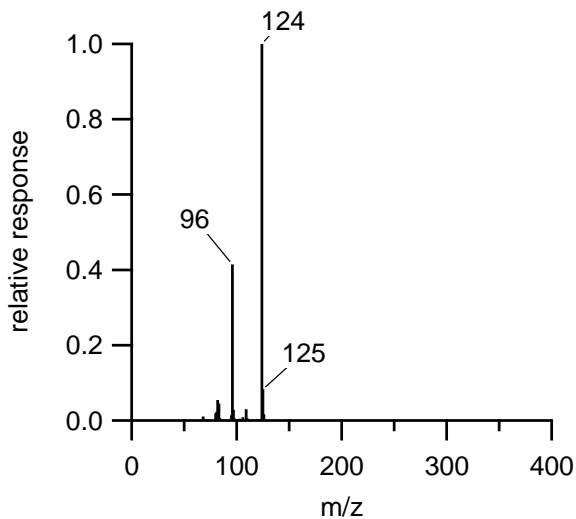




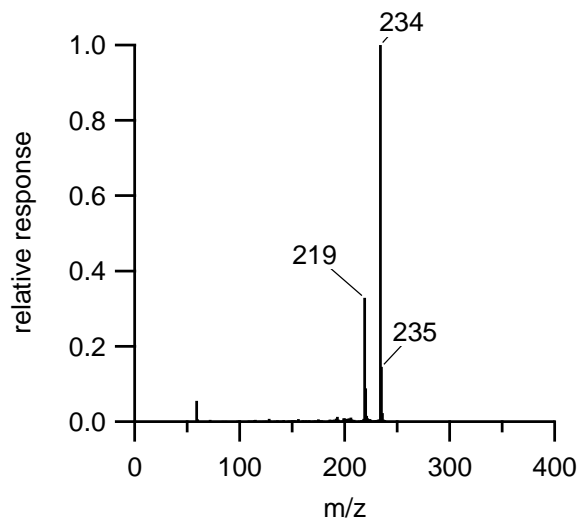
3-Methyl-3-cyclohexen-1-one  
CAS #31883-98-4, MW=110.07 (28 ppm)



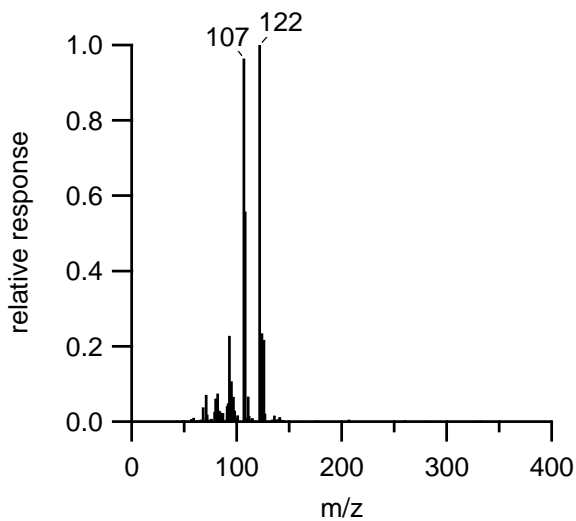
3-Ethenyl-3-methylcyclopentanone  
CAS #49664-66-6, MW=124.09 (17 ppm)



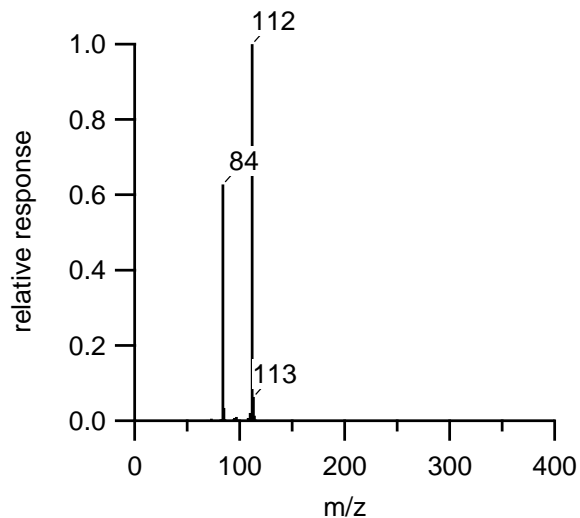
3,5-di-tert-Butyl-4-hydroxybenzaldehyde  
CAS #1620-98-0, MW=234.16 (38 ppm)



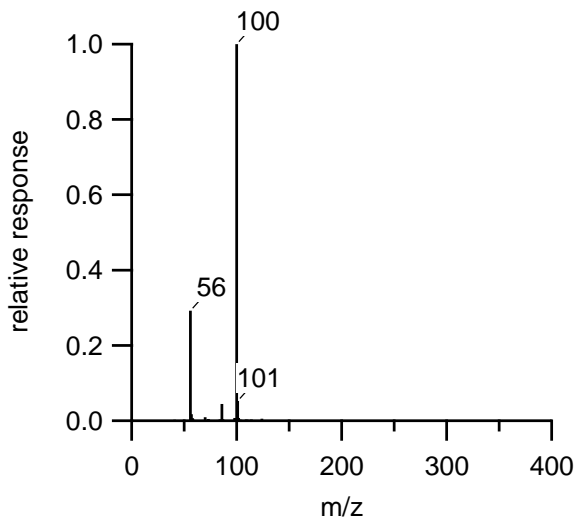
1,6-Dimethylhepta-1,3,5-triene  
CAS #0-00-0, MW=122.11 (29 ppm)



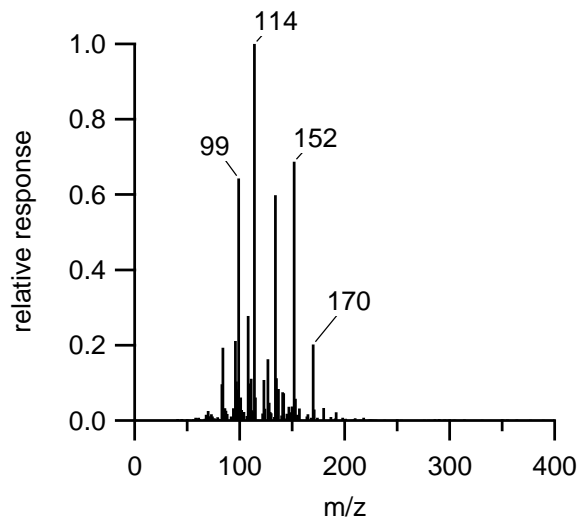
3,4-Dihydro-6-methyl-2H-pyran-2-one  
CAS #3740-59-8, MW=112.05 (52 ppm)



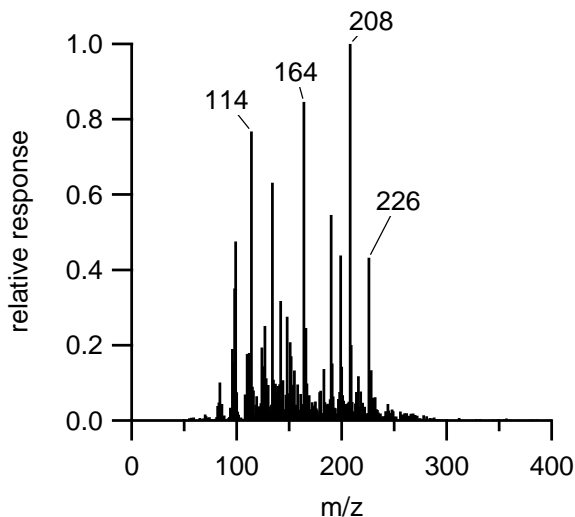
2H-Pyran-2-one, tetrahydro-  
CAS #542-28-9, MW=100.05 (32 ppm)



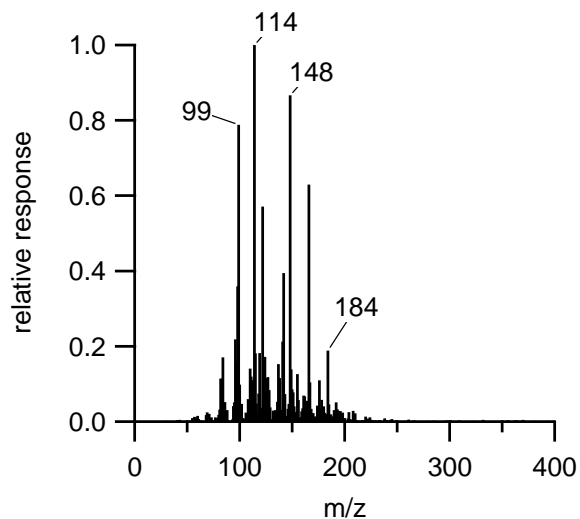
2H-Pyran-2-one, 6-pentyltetrahydro-  
CAS #705-86-2, MW=170.13 (9 ppm)



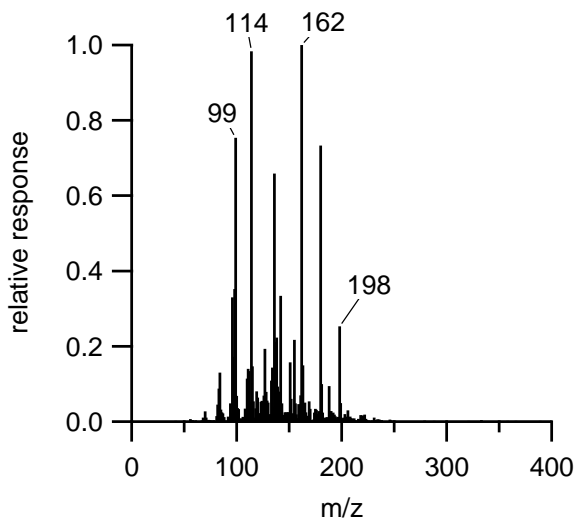
2H-Pyran-2-one, 6-nonyltetrahydro-  
CAS #2721-22-4, MW=226.19 (52 ppm)



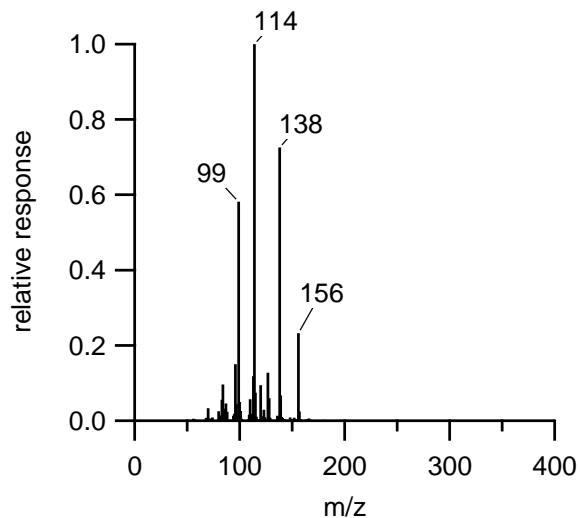
2H-Pyran-2-one, 6-hexyltetrahydro-  
CAS #710-04-3, MW=184.15 (42 ppm)



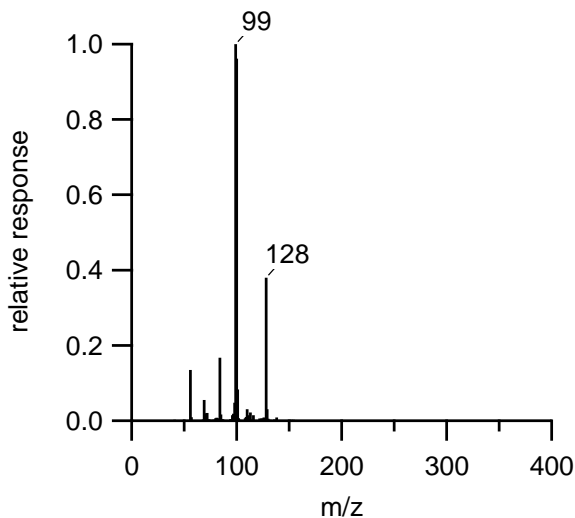
2H-Pyran-2-one, 6-heptyltetrahydro-  
CAS #713-95-1, MW=198.16 (19 ppm)



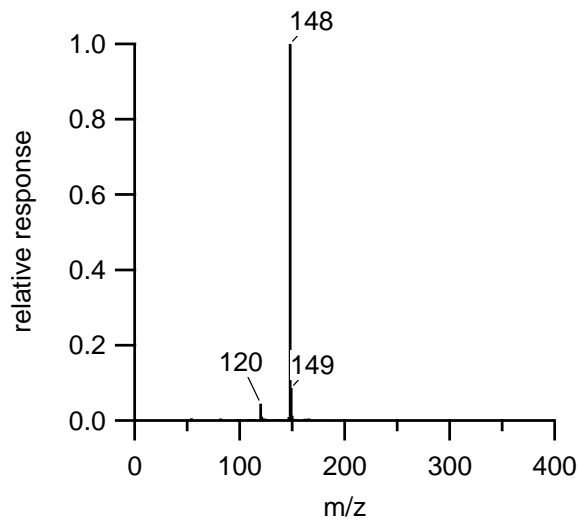
2H-Pyran-2-one, 6-butyltetrahydro-  
CAS #3301-94-8, MW=156.12 (44 ppm)



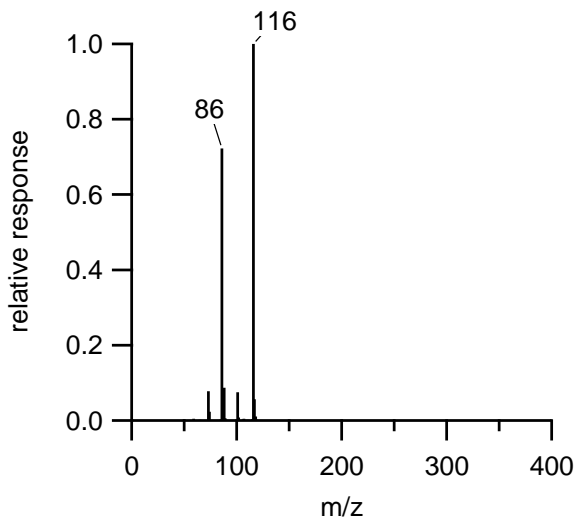
2H-Pyran-2-one, 6 ethyltetrahydro-  
CAS #3301-90-4, MW=128.08 (1 ppm)



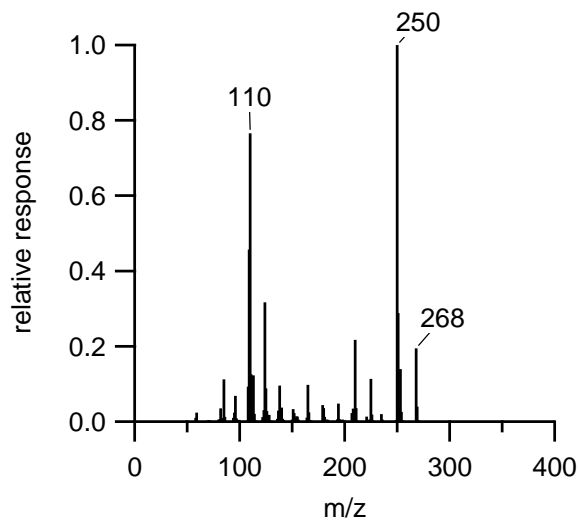
Hydrocoumarin  
CAS #119-84-6, MW=148.05 (11 ppm)



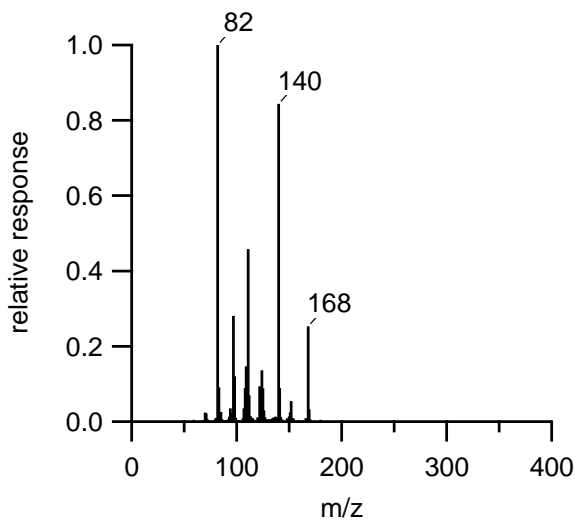
2-Propanone, 1-(acetyloxy)-  
CAS #592-20-1, MW=116.05 (45 ppm)



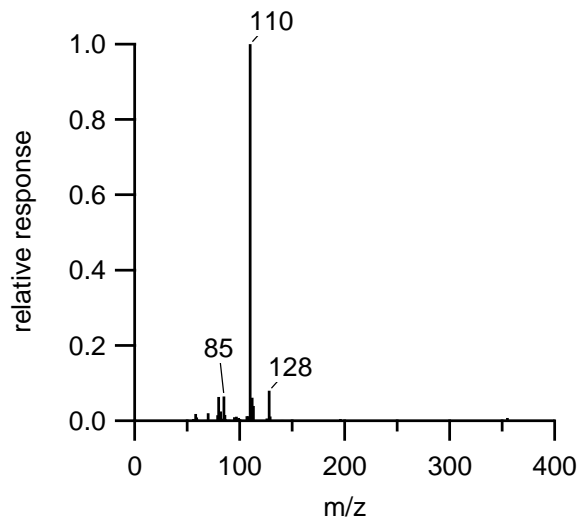
2-Pentadecanone, 6,10,14-trimethyl-  
CAS #502-69-2, MW=268.28 (21 ppm)



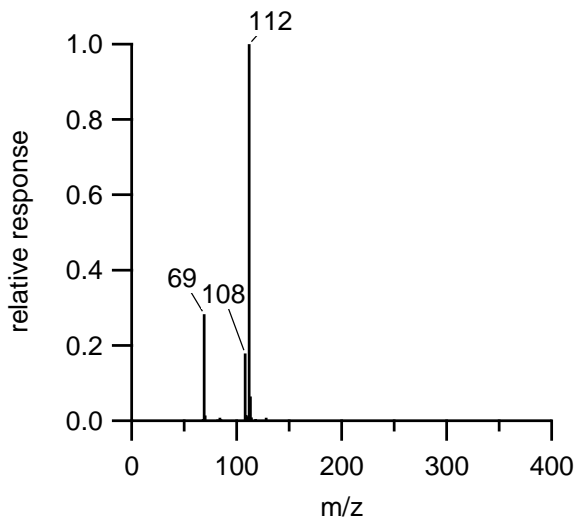
2-Oxabicyclo[2.2.2]octan-6-one, 1,3,3-trimethyl-  
CAS #107598-08-3, MW=168.12 (23 ppm)



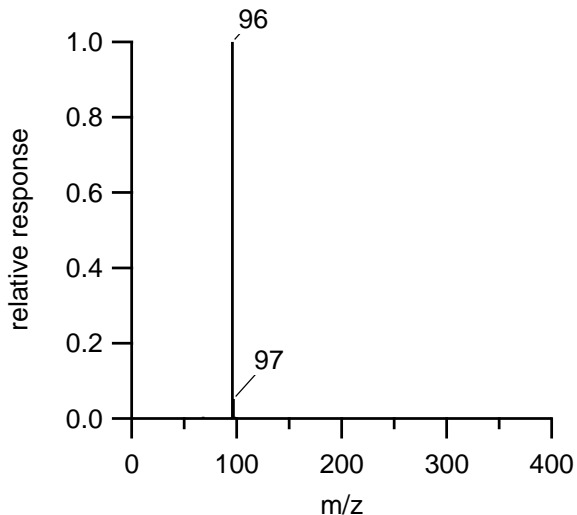
2-Heptanone, 6-methyl-  
CAS #928-68-7, MW=128.12 (88 ppm)



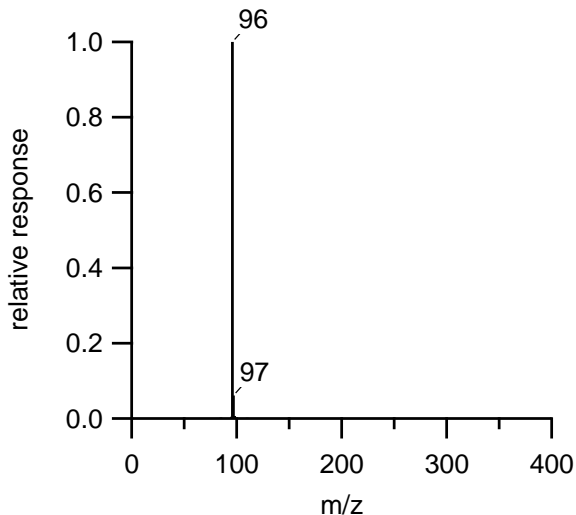
2-Furanone, 2,5-dihydro-3,5-dimethyl  
CAS #0-00-0, MW=112.05 (52 ppm)



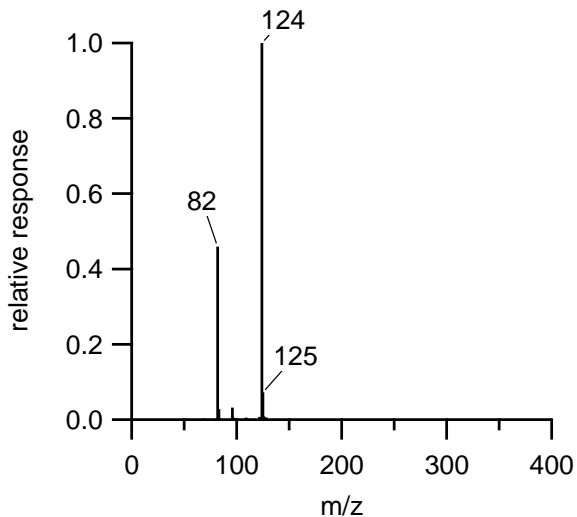
4-Cyclopentene-1,3-dione  
CAS #930-60-9, MW=96.021 (37 ppm)



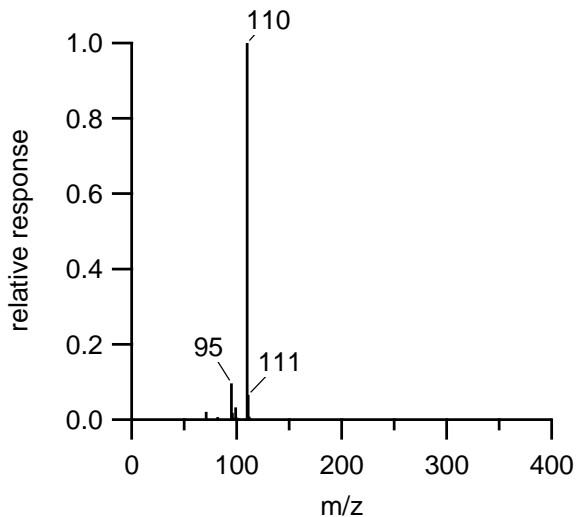
2-Cyclopenten-1-one, 3-methyl-  
CAS #2758-18-1, MW=96.058 (45 ppm)



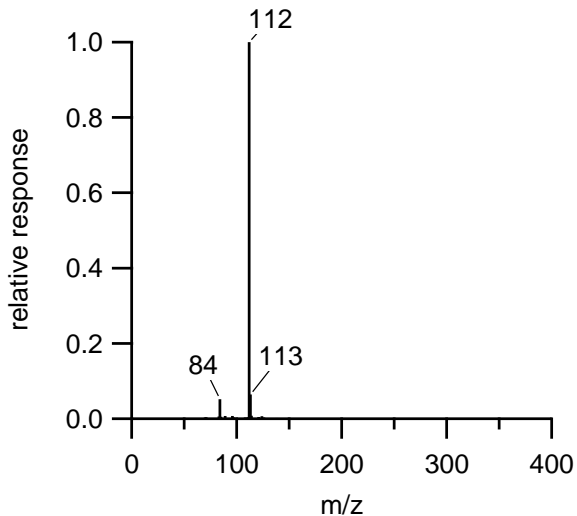
2-Cyclopenten-1-one, 3-(1-methylethyl)-  
CAS #1619-28-9, MW=124.09 (17 ppm)



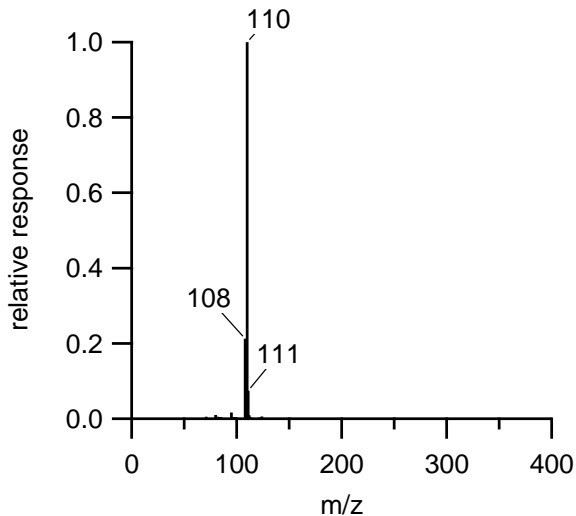
2-Cyclopenten-1-one, 3,4-dimethyl-  
CAS #30434-64-1, MW=110.07 (28 ppm)



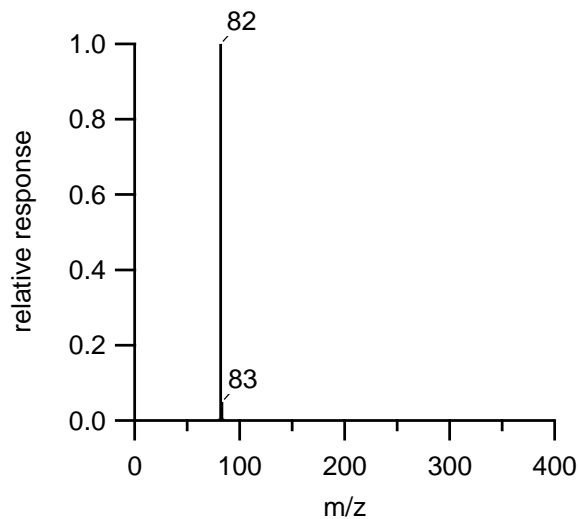
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-  
CAS #80-71-7, MW=112.05 (52 ppm)



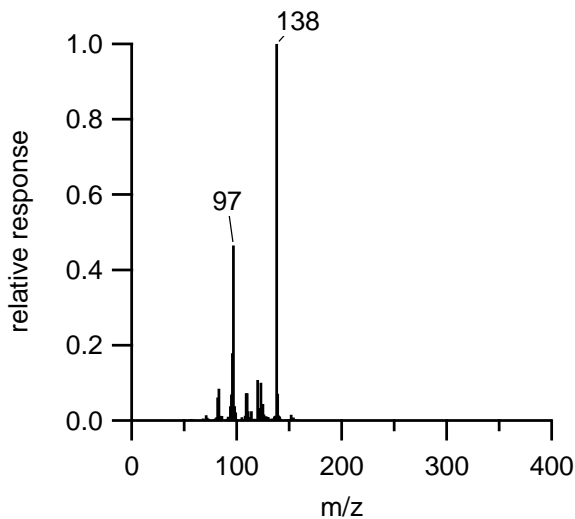
2-Cyclopenten-1-one, 2,3-dimethyl-  
CAS #1121-05-7, MW=110.07 (28 ppm)



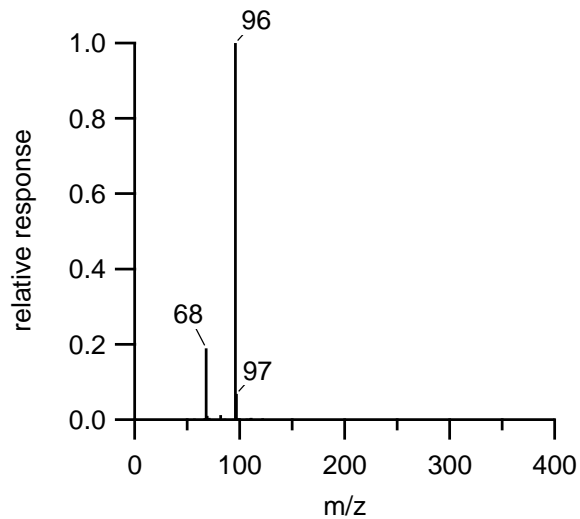
2-Cyclopenten-1-one  
CAS #930-30-3, MW=82.042 (14 ppm)



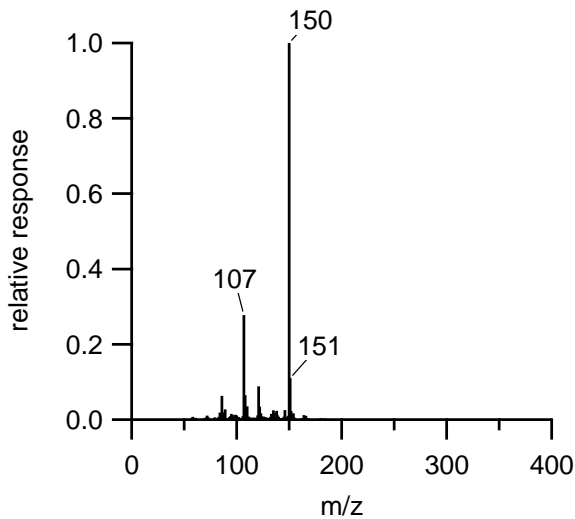
2-Cyclohexen-1-one, 4-(1-methylethyl)-  
CAS #500-02-7, MW=138.1 (21 ppm)



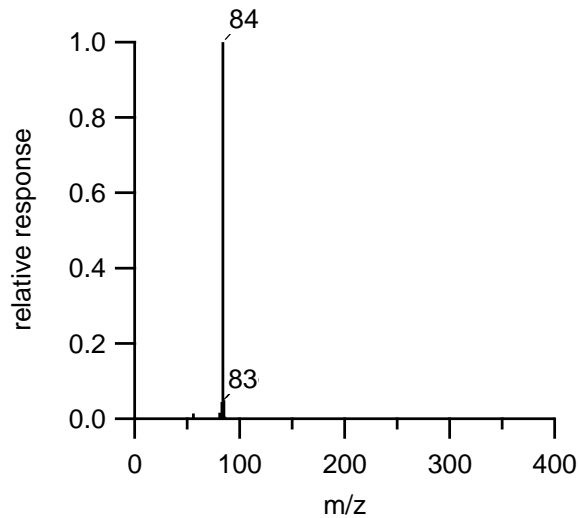
2-Cyclohexen-1-one  
CAS #930-68-7, MW=96.058 (45 ppm)



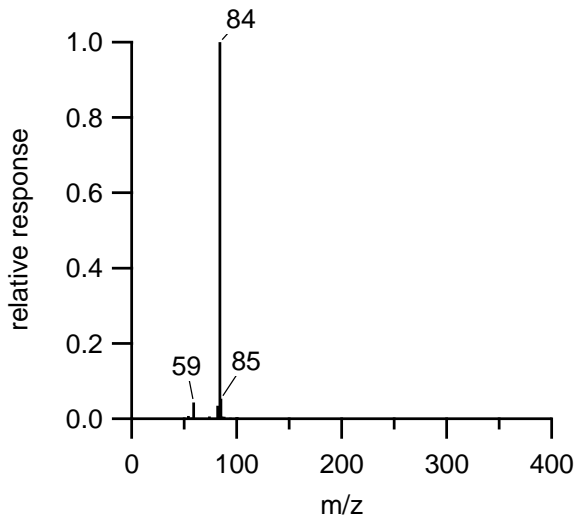
2-Caren-10-al  
CAS #0-00-0, MW=150.1 (35 ppm)



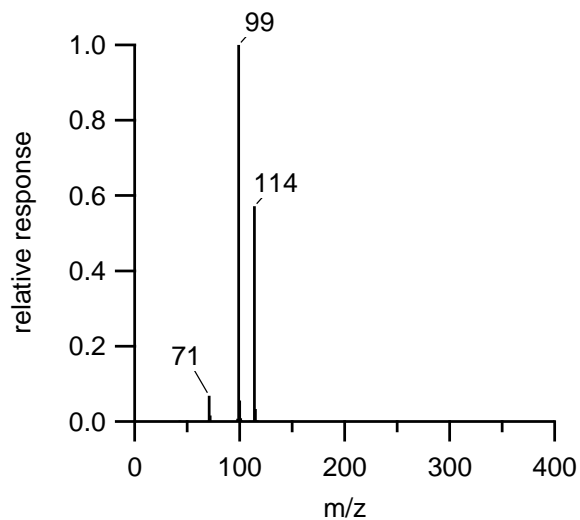
2-Butenal, 3-methyl-  
CAS #107-86-8, MW=84.058 (39 ppm)



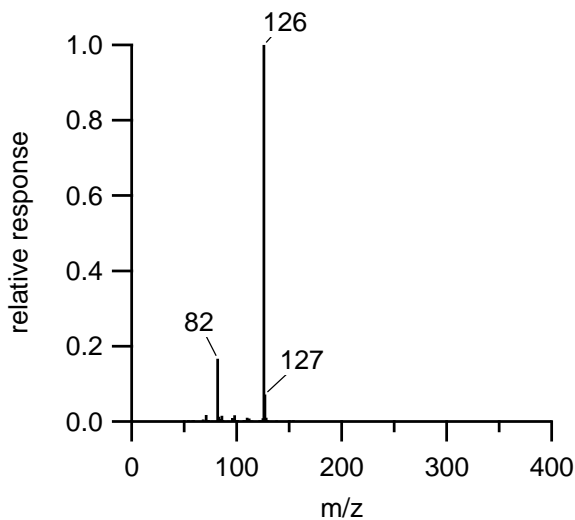
2-Butenal, 2-methyl-, (E)-  
CAS #497-03-0, MW=84.058 (39 ppm)



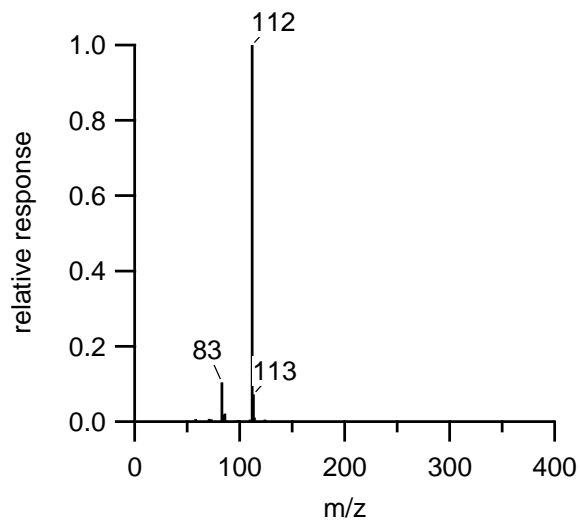
2,5-Hexanedione  
CAS #110-13-4, MW=114.07 (28 ppm)



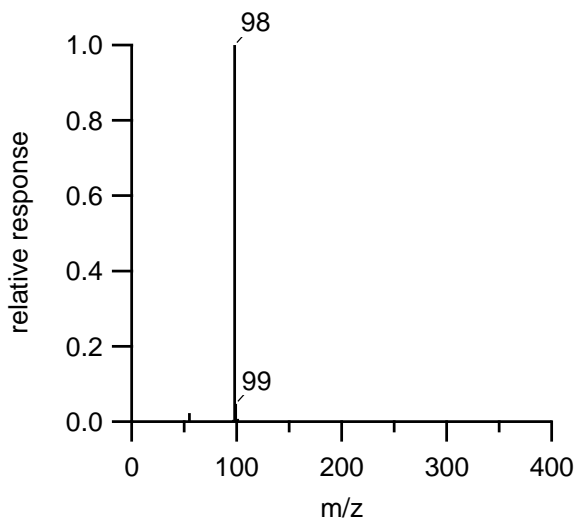
2,5-Furandione, 3,4-dimethyl-  
CAS #766-39-2, MW=126.03 (8 ppm)



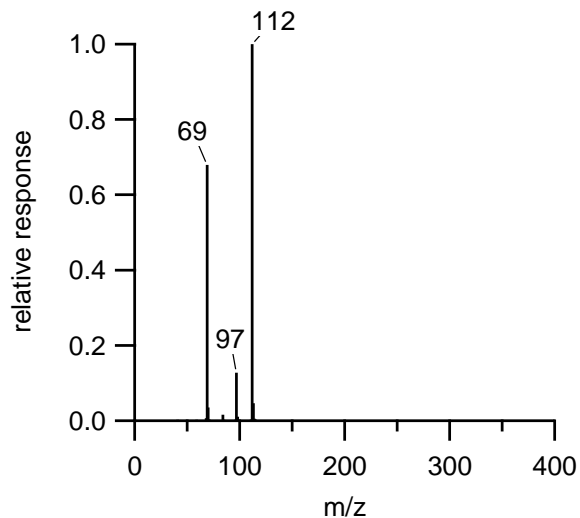
2,3-Dimethyl-4-hydroxy-2-butenic lactone  
CAS #1575-46-8, MW=112.05 (55 ppm)



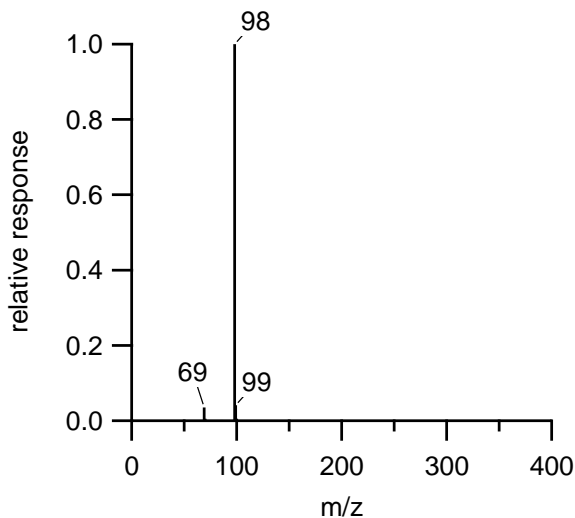
2(5H)-Furanone, 5-methyl-  
CAS #591-11-7, MW=98.037 (63 ppm)



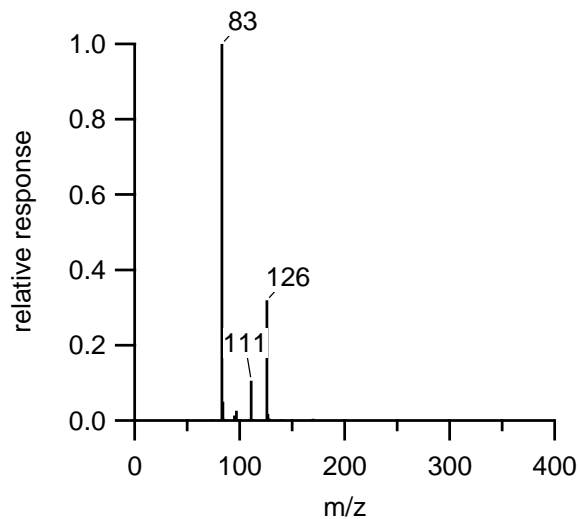
2(5H)-Furanone, 5,5-dimethyl-  
CAS #20019-64-1, MW=112.05 (52 ppm)



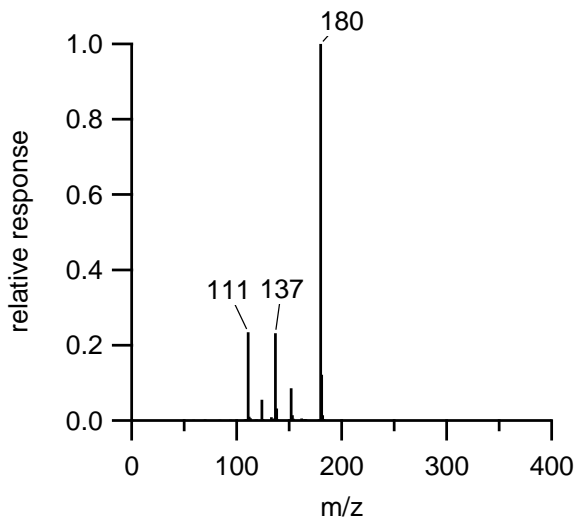
2(5H)-Furanone, 3-methyl-  
CAS #22122-36-7, MW=98.037 (63 ppm)



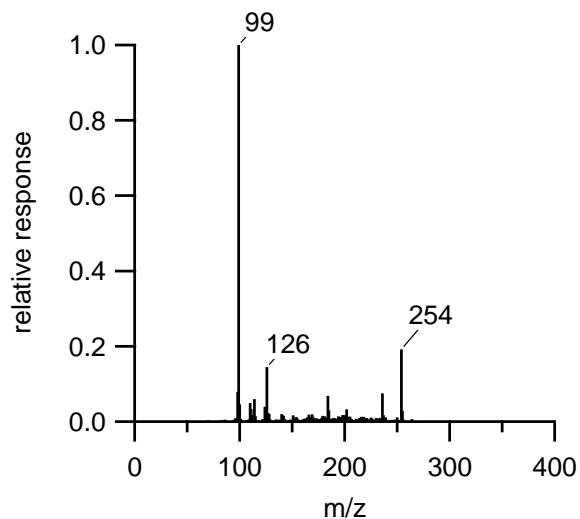
2(5H)-Furanone, 3,5,5-trimethyl-  
CAS #50598-50-0, MW=126.07 (21 ppm)



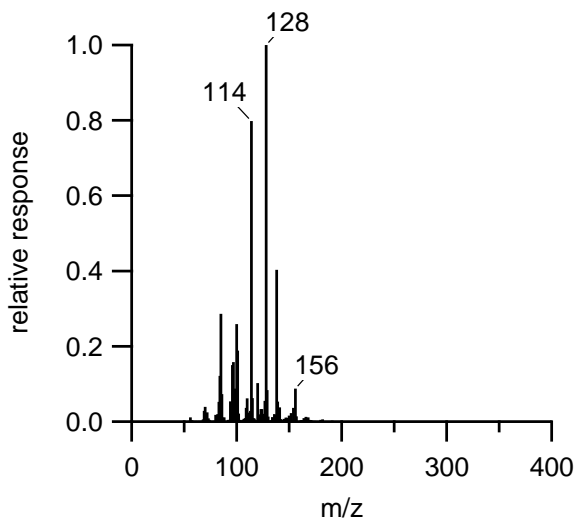
2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-,  
CAS #17092-92-1, MW=180.12 (26 ppm)



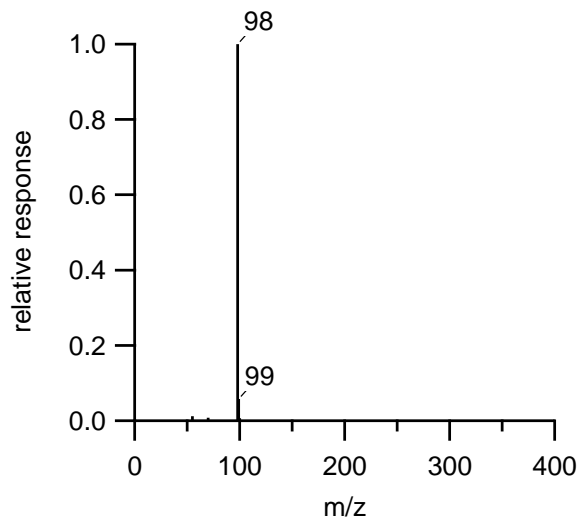
2(3H)-Furanone, dihydro-X-methyl-5-nonyl  
CAS #220904-24-5, MW=254.22 (8 ppm)



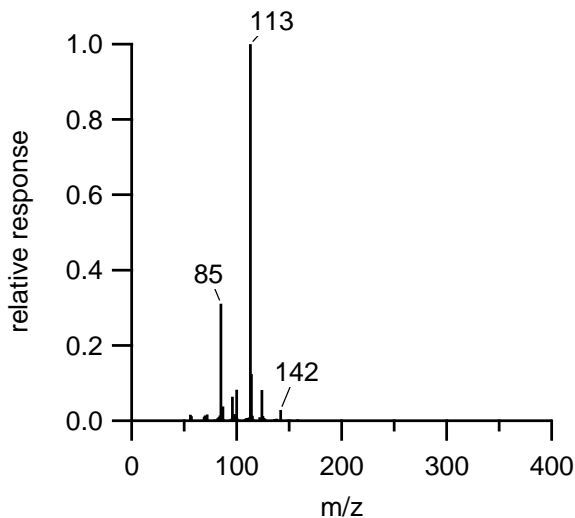
2(3H)-Furanone, dihydro-5-pentyl-  
CAS #104-61-0, MW=156.12 (46 ppm)



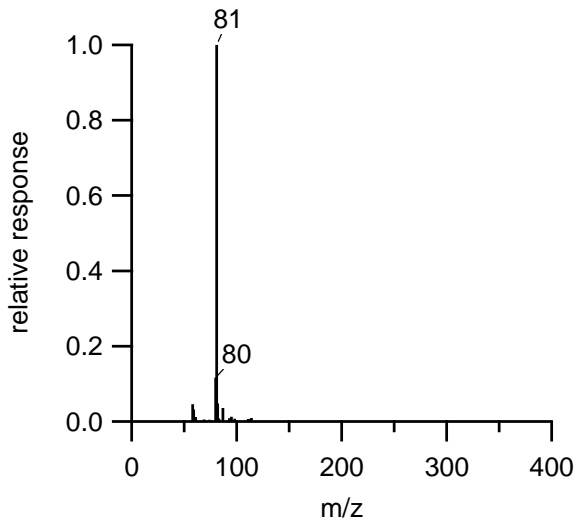
2(3H)-Furanone, 5-methyl-  
CAS #591-12-8, MW=98.037 (63 ppm)



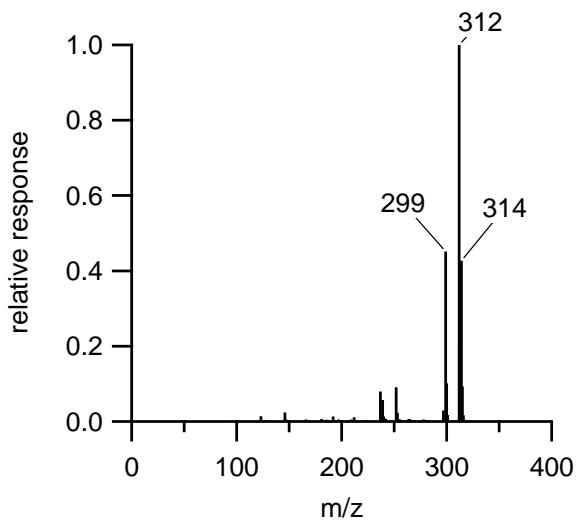
2(3H)-Furanone, dihydro-5-butyl-  
CAS #104-50-7, MW=142.1 (45 ppm)



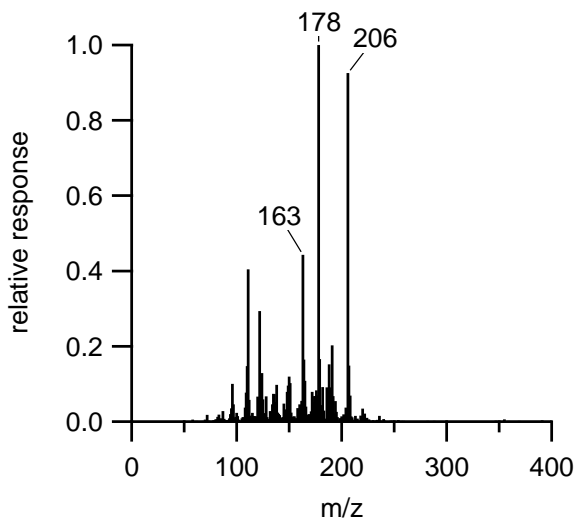
1H-Pyrrole, 2-methyl-  
CAS #616-43-3, MW=81.058 (72 ppm)



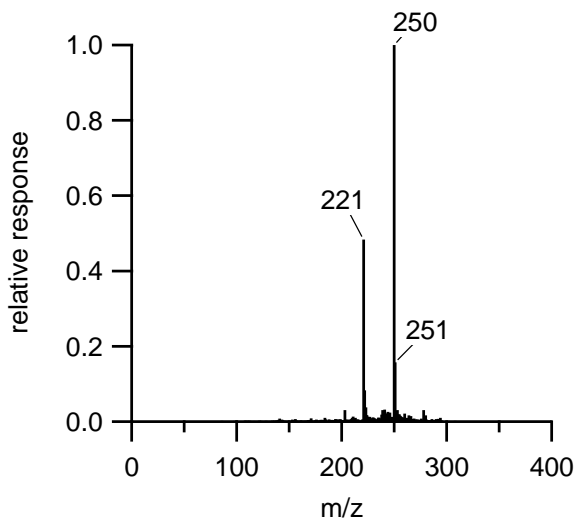
Methyl dehydroabietate  
CAS #1235-74-1, MW=314.22 (25 ppm)



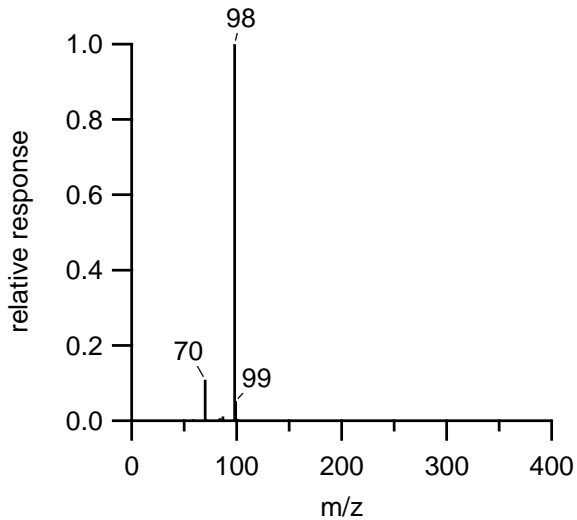
1-Oxaspiro[2.5]octane, 5,5-dimethyl-4-(3-methyl-1,3-butadienyl)-  
CAS #0-00-0, MW=206.17 (2 ppm)



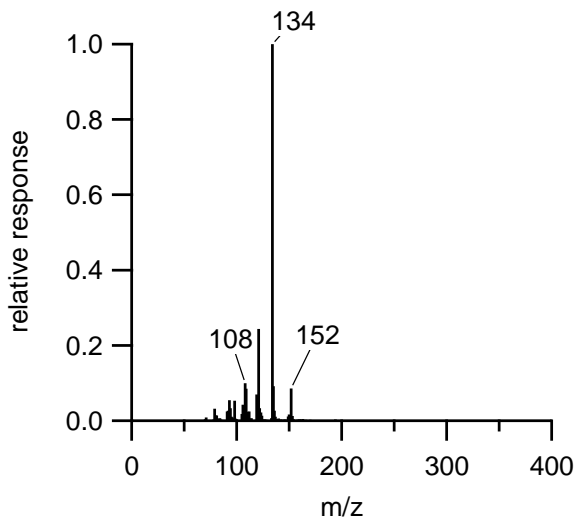
1,4-Benzenediol, 2,5-bis(1,1-dimethylpropyl)-  
CAS #79-74-3, MW=250.19 (18 ppm)



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

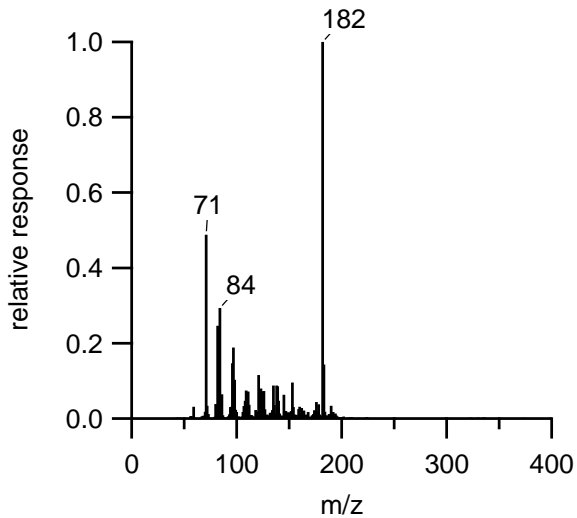


1-Cyclohexene-1-methanol, 4-(1-methylethenyl)-  
CAS #536-59-4, MW=152.12 (25 ppm)

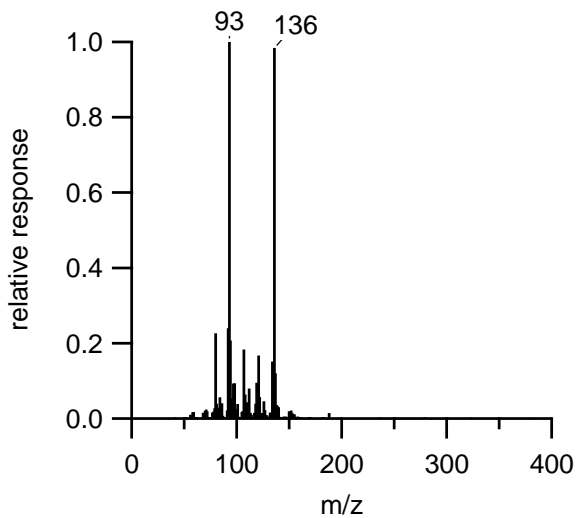




2-Dodecenal, (E)-  
CAS #20407-84-5, MW=182.17 (32 ppm)



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



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

