

Company Name
Contact Name

Released by:

Mark Jordi, Ph.D.
President

Job Number: J8674

COMPANY
CONFIDENTIAL

Date

Contact

P: ###-###-####

Company

E: email address

Street Address

City, State Zip

Dear Contact,

Please find enclosed the test results for your sample described as:

1. *Beer - India Pale Ale (IPA)*

The following test was performed:

1. Dynamic Headspace Gas Chromatography Mass Spectroscopy (DHGCMS)

Objective

The goal of this analysis was to demonstrate the quantitative recovery of two compounds known to impair the taste and smell of beverages from a complicated beer matrix by performing DHGCMS. For the purpose of this study, benzaldehyde, known to give an almond-like flavor to beer and wine, and trans-2-nonenal, a compound that gives stale beer a cardboard-like taste, will be spiked into a beer matrix at known concentrations. The structures are presented in **Figure 1**.

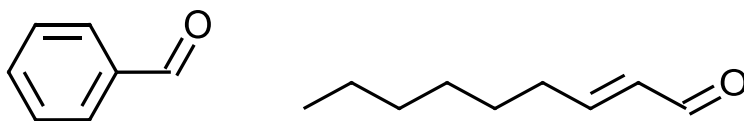


Figure 1. Structures of *benzaldehyde* (left) and *trans-2-nonenal* (right)

Summary of Results

Both benzaldehyde and trans-2-nonenal have been successfully detected in a beer matrix at 10 ppb and 50 ppb respectively. The compounds were quantitated at a level of 10 ppm with a recovery of 84.1% and 122.7% respectively. Quantitation data is presented in **Table 2**. Peaks consistent with numerous alcohols, esters and aromatics were also detected, and the major components identified in the *Beer (IPA)* have been compiled in **Table 1**.

Individual Test Results

A summary of the individual test results is provided below. All accompanying data, including spectra, has been included in the data section of this report.

DHGCMS

Sample Preparation

In order to perform the quantitation experiment, five 20 mL headspace sampling vials containing 2 mL of fresh *Beer (IPA)* with no added benzaldehyde or trans-2-nonenal (below the limit of detection of 10 ppb and 50 ppb respectively) were spiked with both compounds at a known concentration (10 ppm) and sealed. An unspiked *Beer (IPA)* sample was also prepared in order to confirm that both compounds of interest were absent from the sample *before* spiking.

Five headspace sampling vials were prepared consisting of both compounds at concentrations ranging from 50 ppm to 100 ppb. An internal standard of 1,4-dichlorobenzene-D₄ (10 µL of a 10 mg/mL solution in dichloromethane, DCM) was also included in each headspace sampling vial in order to adjust for injection-to-injection retention time variability.

All samples were then subjected to thermal desorption using the conditions outlined in the Analysis Conditions section of the report.

Results

An overlay of the DHGCMS chromatograms is presented in **Figure 2**. The major peak (between 9 and 10 minutes) is consistent with ethanol. The remaining peaks are consistent with additional alcohols, esters and aromatic compounds, and the deuterated internal standard (RT of 19.63 minutes). Peaks present in the control blank (air, DCM, siloxane) were subtracted. The benzaldehyde and trans-2-nonenal were only observed in the *Spike Beer (IPA)* sample at retention times of 19.26 and 21.54 minutes respectively (highlighted in **Figure 2**). All major peaks and their identifications are presented in **Table 1**.

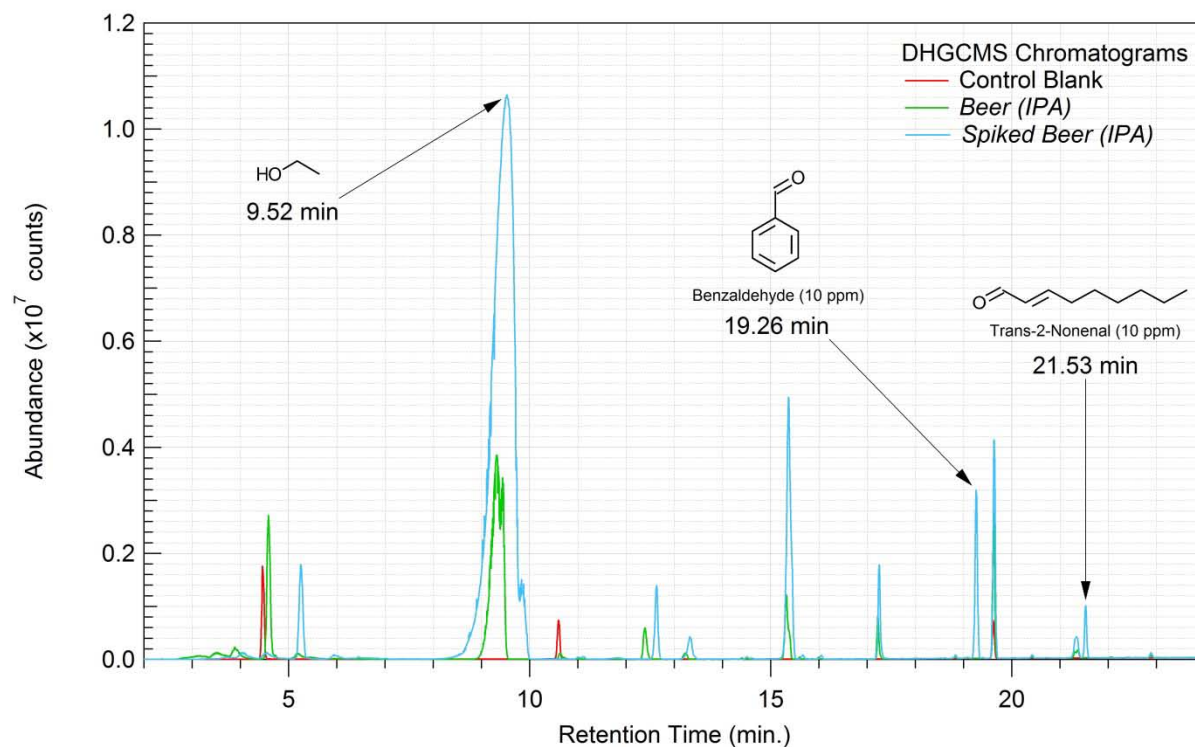


Figure 1. DHGCMS chromatographic overlay of *Beer (IPA)*, *Beer (IPA)* spiked with benzaldehyde and trans-2-nonenal, and a control blank

Table 1. Compounds Identified in Beer (IPA) and Spiked Beer (IPA)					
Retention Time (min)	Possible ID	CAS #	Structure	Detected	
				Beer (IPA)	Spiked Beer (IPA)
0.18, 4.58, 5.25	Oxygen	7782-44-7	<chem>O=O</chem>	✓	✓
3.88, 4.54, 5.19, 5.95, 6.02, 6.44, 9.32, 9.53	Ethanol	64-17-5	<chem>CCO</chem>	✓	✓
11.74, 11.85	1-Propanol	71-23-8	<chem>CCCO</chem>	✓	✓
12.39, 12.63	Ethyl Acetate	141-78-6	<chem>CC(=O)OCC</chem>	✓	✓
13.22, 13.32	2-Methyl-1-Propanol	78-83-1	<chem>CC(C)CO</chem>	✓	✓
14.41, 14.51	Ethyl propionate	105-37-3	<chem>CCC(=O)OCC</chem>	✓	✓
14.50, 14.60	n-Propyl acetate	109-60-4	<chem>CC(=O)OCCC</chem>	✓	✓
15.32, 15.37	3-Methyl-1-butanol	123-51-3	<chem>CC(C)CCO</chem>	✓	✓
16.00, 16.05	Ethyl butyrate	105-54-4	<chem>CCCC(=O)OCC</chem>	✓	✓
17.22, 17.25	Isoamyl acetate	123-92-2	<chem>CC(C)CCOC(=O)C</chem>	✓	✓
18.83, 18.84	Ethyl hexanoate	123-66-0	<chem>CCCCCC(=O)OCC</chem>	✓	✓
19.26	Benzaldehyde	100-52-7	<chem>c1ccccc1C=O</chem>	ND	✓
19.62, 19.63	1,4-Dichlorobenzene-D ₄	3855-82-1	<chem>ClC1=CC(=CC(=C1)Cl)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4</chem>	✓	✓
21.34, 21.37	Phenethyl alcohol	60-12-8	<chem>c1ccccc1CCO</chem>	✓	✓
21.54	Trans-2-nonenal	18829-56-6	<chem>CCCCCCC/C=C\C=O</chem>	ND	✓
22.88, 22.89	Phenethyl acetate	103-45-7	<chem>c1ccccc1CCOC(=O)C</chem>	✓	✓

✓ - Detected

ND - Not detected above LOD of 10 ppb (benzaldehyde) / 50 ppb (trans-2-nonenal)

Formal Quantitation of Benzaldehyde and Trans-2-Nonenal

In order to formally quantitate the benzaldehyde and trans-2-nonenal present in the *Spiked Beer (IPA)* sample, peaks from the five injections of each compound at a known concentration (50, 10, 1, 0.5 and 0.1 ppm) were integrated. The areas of these peaks (taken from EICs generated using the ions highlighted in **Table 2**) were used to generate a calibration curve of peak area vs. concentration for each compound. The R^2 values of the linear regression lines for the benzaldehyde and trans-2-nonenal calibration curves were 0.991 and 0.999 respectively. The peak areas for these compounds in the spiked *Beer (IPA)* sample were then converted to concentration values (in ppm) using the calibration curves. Both curves are presented in the data section of this report.

Both benzaldehyde and trans-2-nonenal were successfully detected in the beer. Using the formal quantitation method described above, the concentration of benzaldehyde was calculated to be 12.27 ppm, resulting in a 122.7% recovery. The concentration of trans-2-nonenal was calculated to be 8.41 ppm, resulting in an 84.1% recovery. The quantitation data is presented in **Table 2**.

Table 2. Peak Area and Quantification Data from Spiked Beer (IPA) Sample					
Compound	Ions (for EIC*)	Spiked Conc. (ppm)	Peak Response	Calculated Conc. (ppm)	% Recovery
Benzaldehyde	51, 77, 106	10	23,371,908	12.27	122.7
Trans-2-nonenal	41 , 55, 70	10	3,007,608	8.41	84.1

* Ions in **bold** used for formal quantitation

Conclusion

A quick and facile method for the formal quantitation of benzaldehyde and Trans-2-nonenal from Beer has been demonstrated. Reasonable recovery was obtained for both compounds.

Analysis Conditions

Gerstel Thermal Desorption DHGCMS

This section of a Jordi report provides information on the methods used including instrument type, temperatures, solvents, sample preparation, etc. The specific conditions have been removed for this case study.

Closing Comments

Deformulation of an unknown material is intended to provide a best estimate of the chemical nature of the sample. All chemical structures are supported by the evidence presented but are subject to revision upon receipt of additional evidence. Additional factors such as material processing conditions may also affect final material properties.

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Jordi Labs specializes in polymer testing and has 30 years experience doing complete polymer deformulations. We are one of the few labs in the country specialized in this type of testing. We will work closely with you to help explain your test results and solve your problem. We appreciate your business and are looking forward to speaking with you concerning these results.

Sincerely,

Anthony Grice

Anthony Grice, Ph.D.
Senior Scientist
Jordi Labs LLC

Oliver Palardy

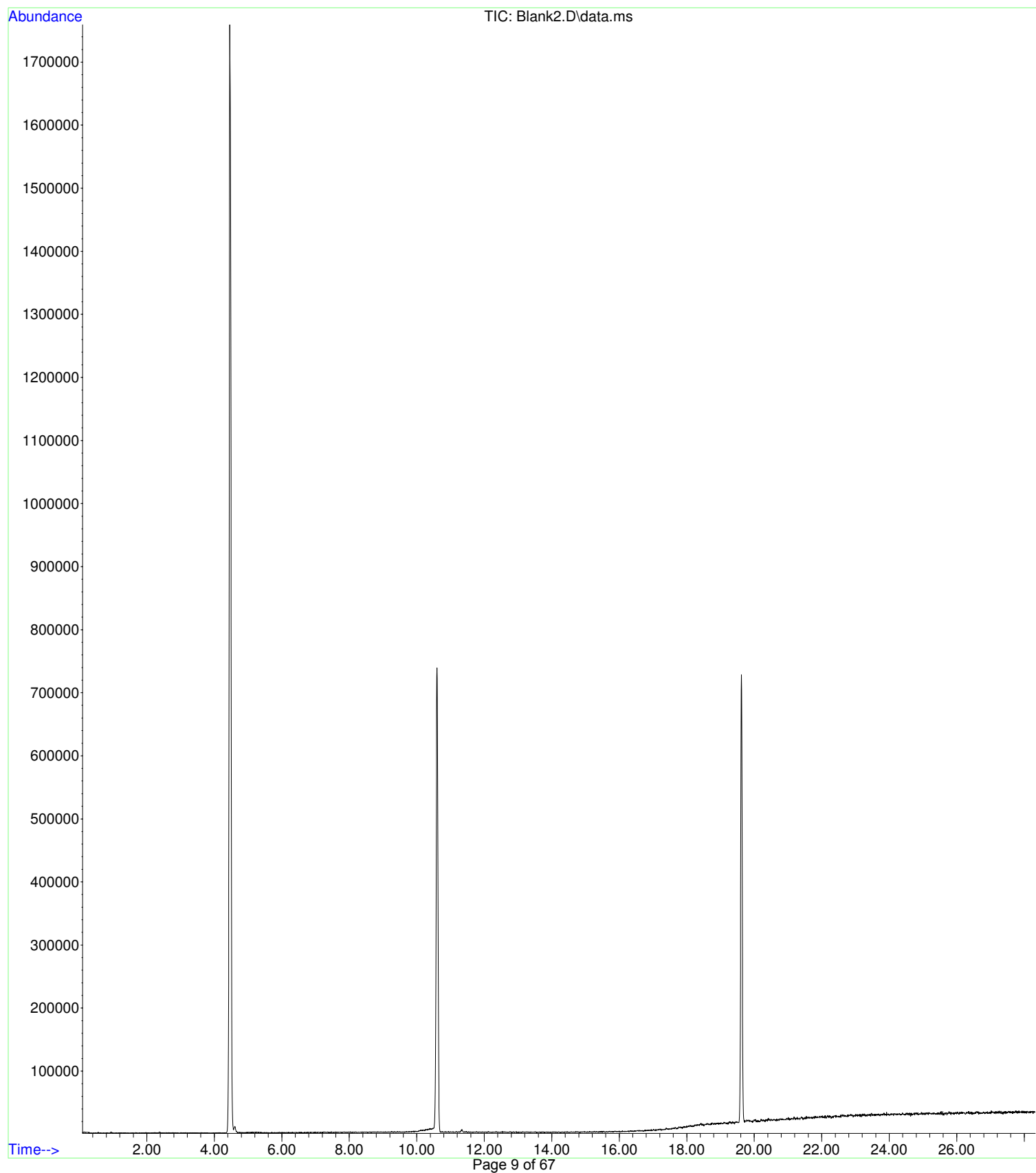
Oliver Palardy
Chemist
Jordi Labs LLC

Mark Jordi

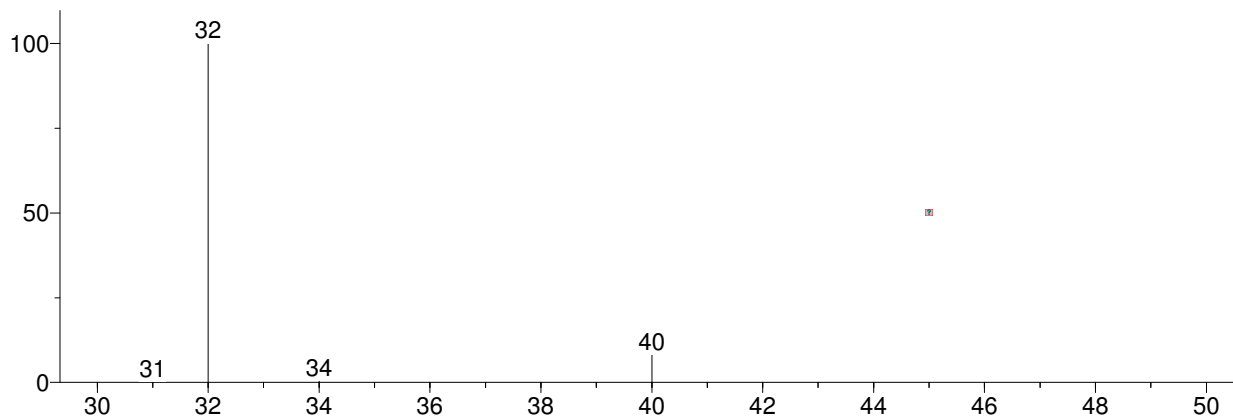
Mark Jordi, Ph.D.
President
Jordi Labs LLC

DHGCMS

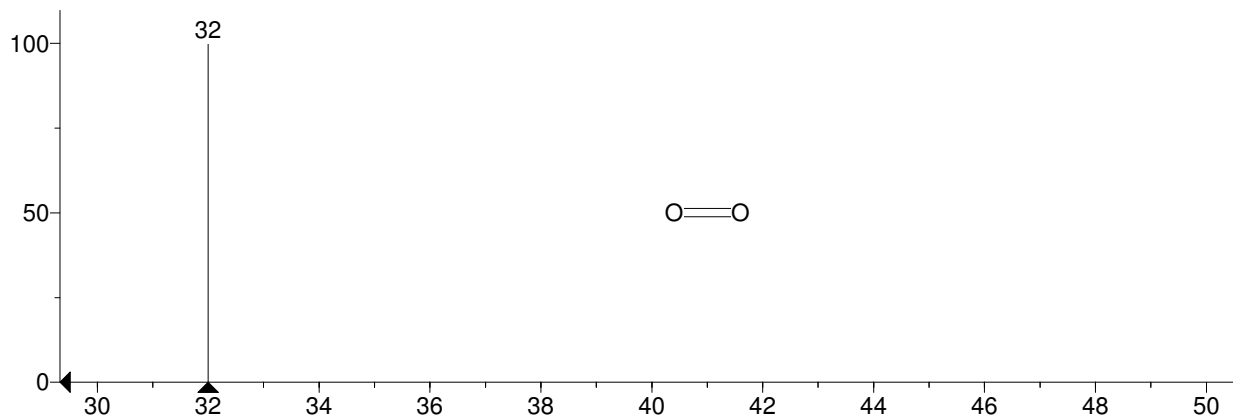
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Vial Number: 28



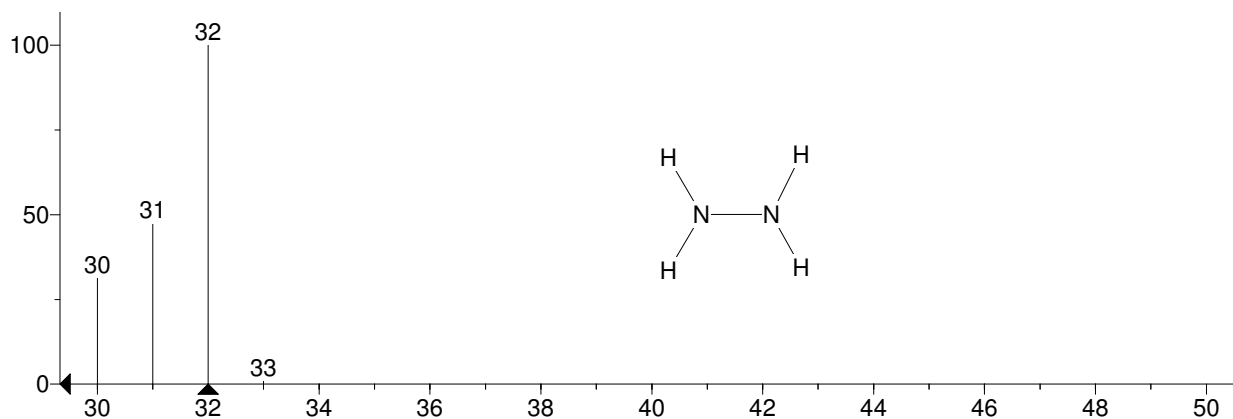
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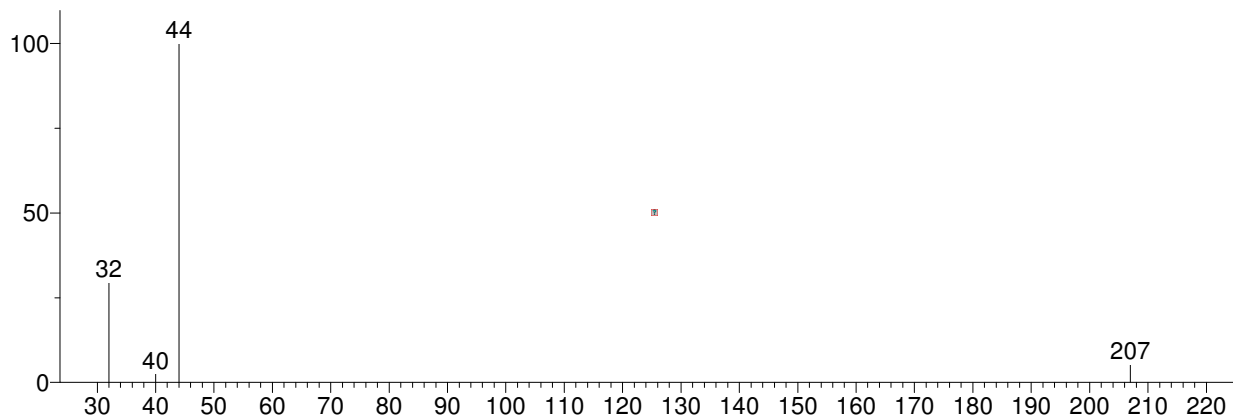
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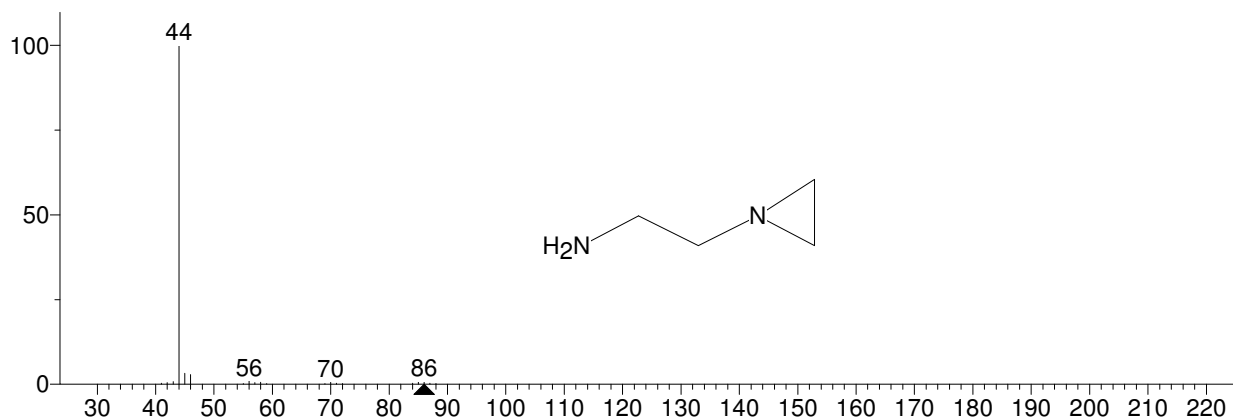
Hit 2 : Hydrazine
H₄N₂; MF: 443; RMF: 488; Prob 0.98%; CAS: 302-01-2; Lib: mainlib; ID: 1453.



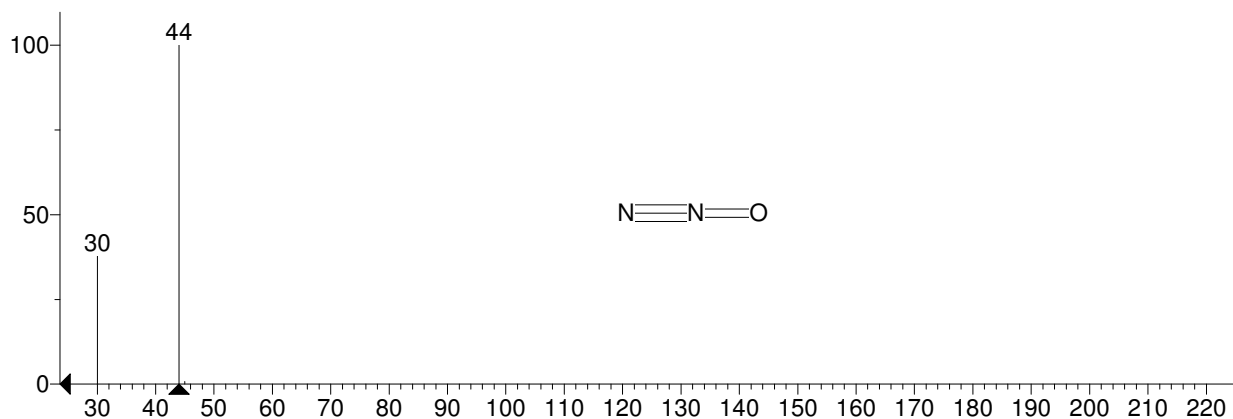
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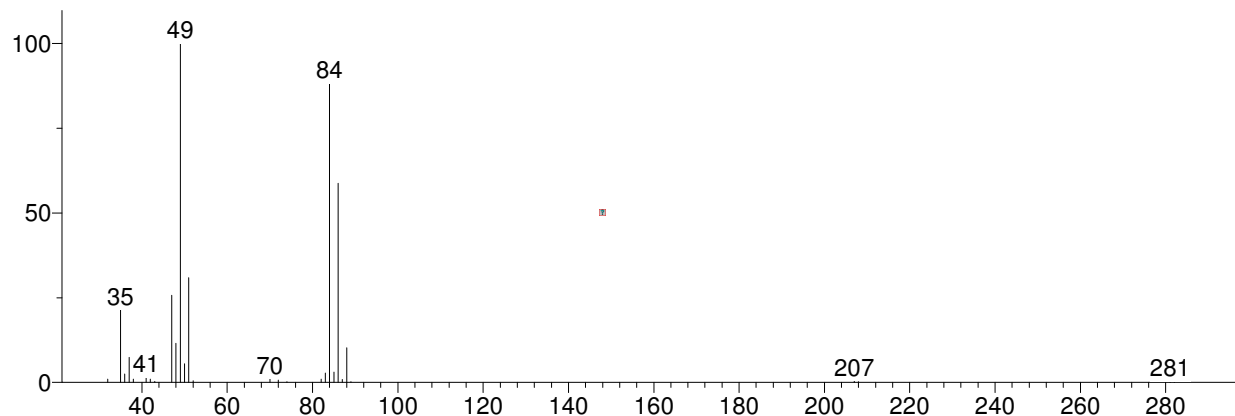
Hit 1 : (2-Aziridinylethyl)amine
C4H10N2; MF: 702; RMF: 874; Prob 58.0%; CAS: 4025-37-0; Lib: mainlib; ID: 14057.



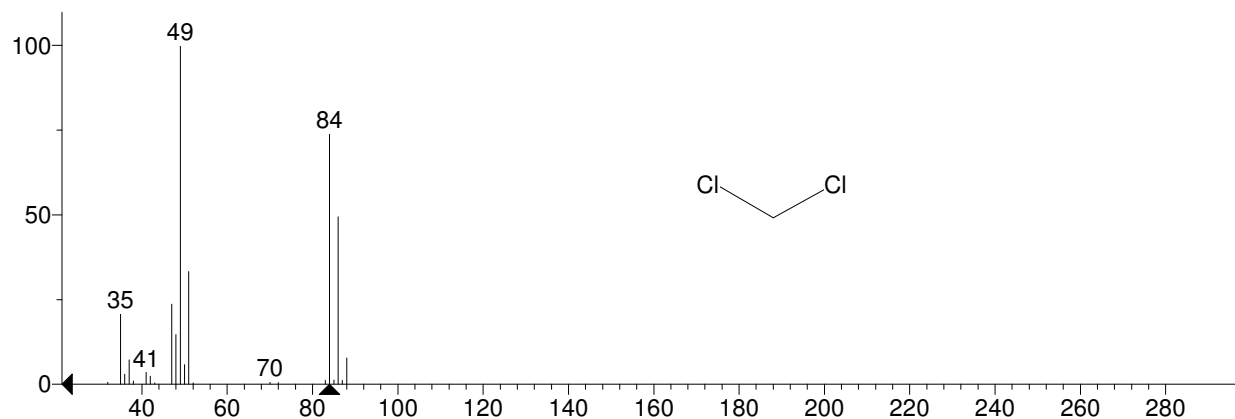
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N2O; MF: 670; RMF: 992; Prob 15.5%; CAS: 10024-97-2; Lib: replib; ID: 3180.



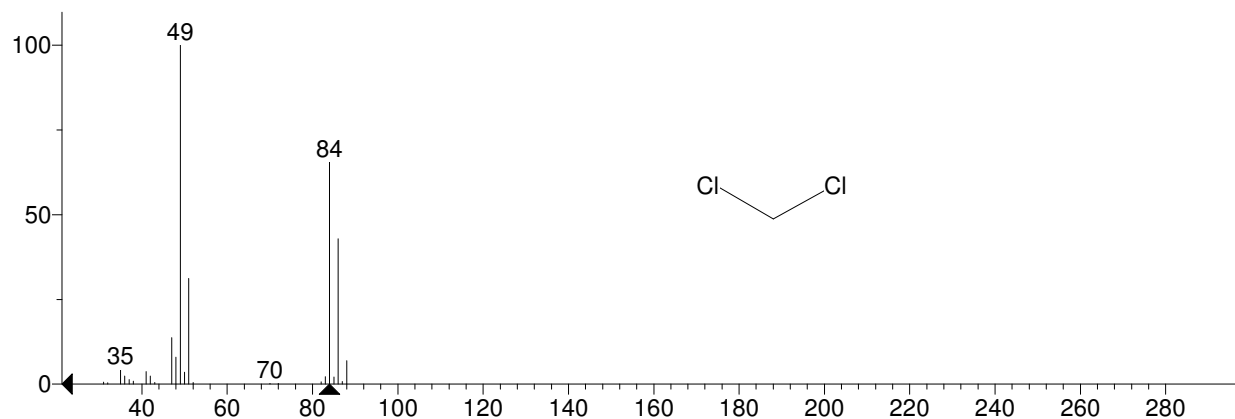
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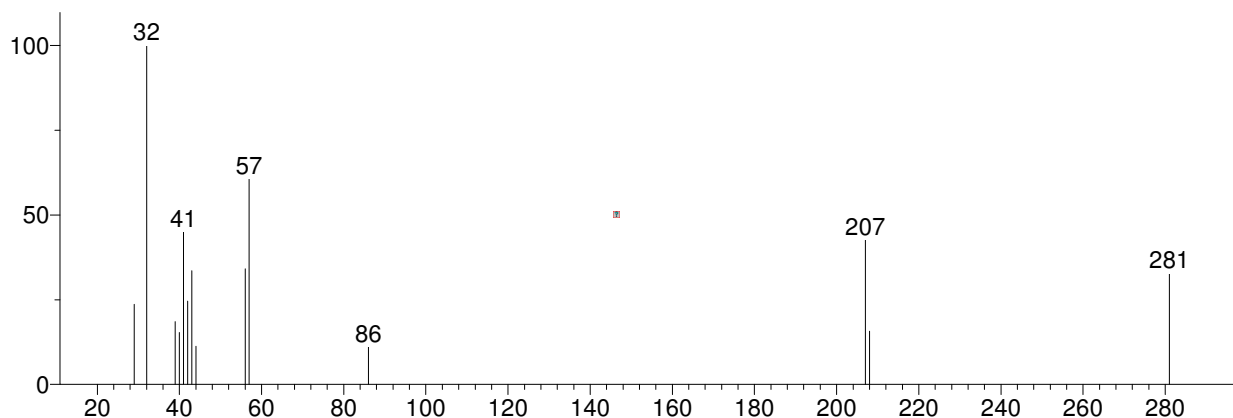
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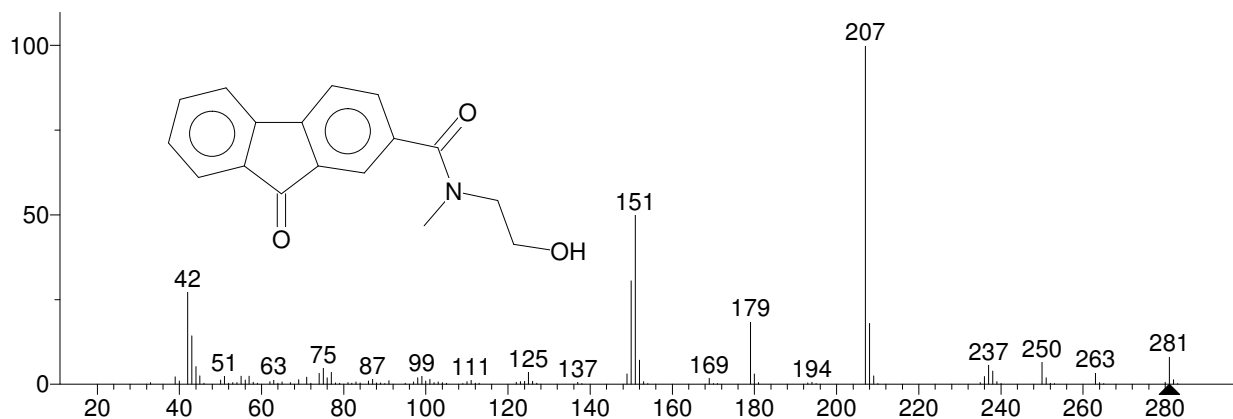
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CH2Cl2; MF: 885; RMF: 887; Prob 97.4%; CAS: 75-09-2; Lib: mainlib; ID: 16363.



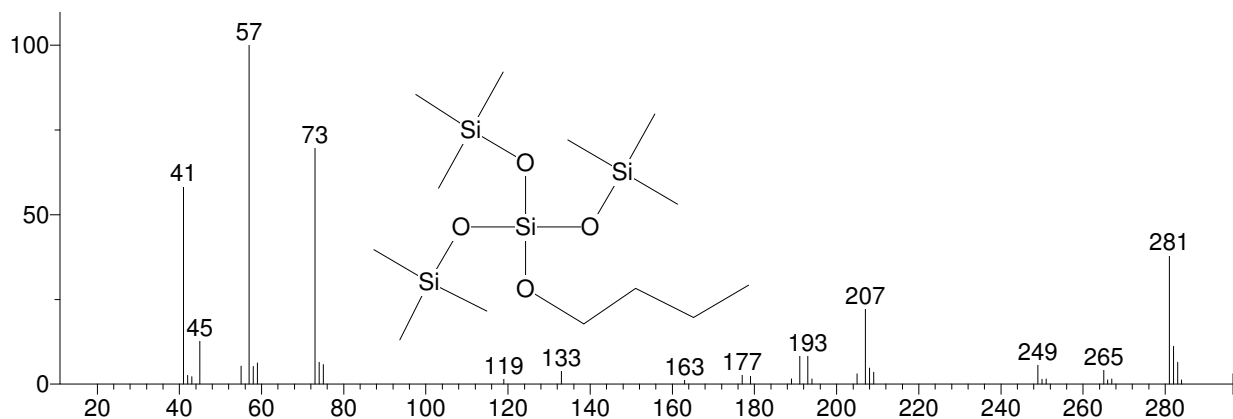
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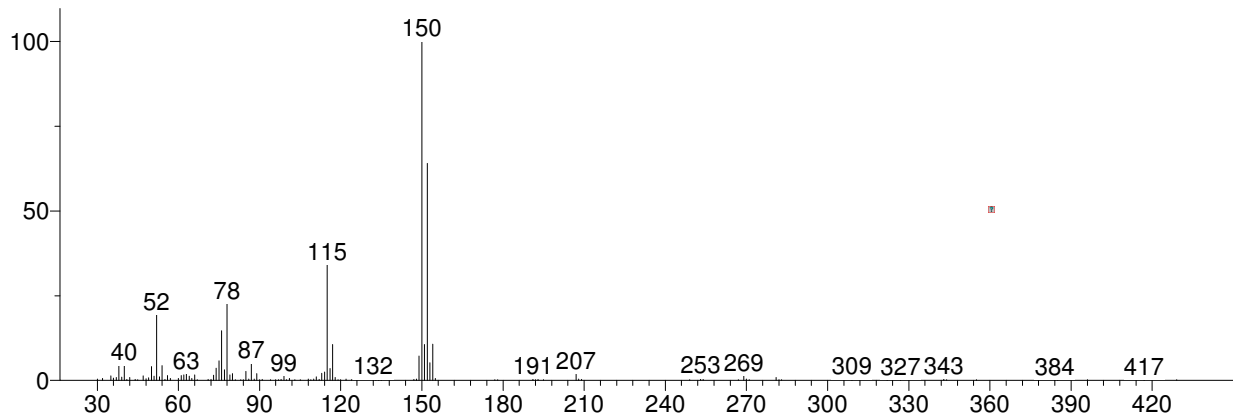
Hit 1 : 9H-Fluorene-2-carboxylic acid, 9-oxo-, (2-hydroxyethyl)(methyl)amide
C₁₇H₁₅NO₃; MF: 465; RMF: 478; Prob 9.72%; Lib: mainlib; ID: 148984.



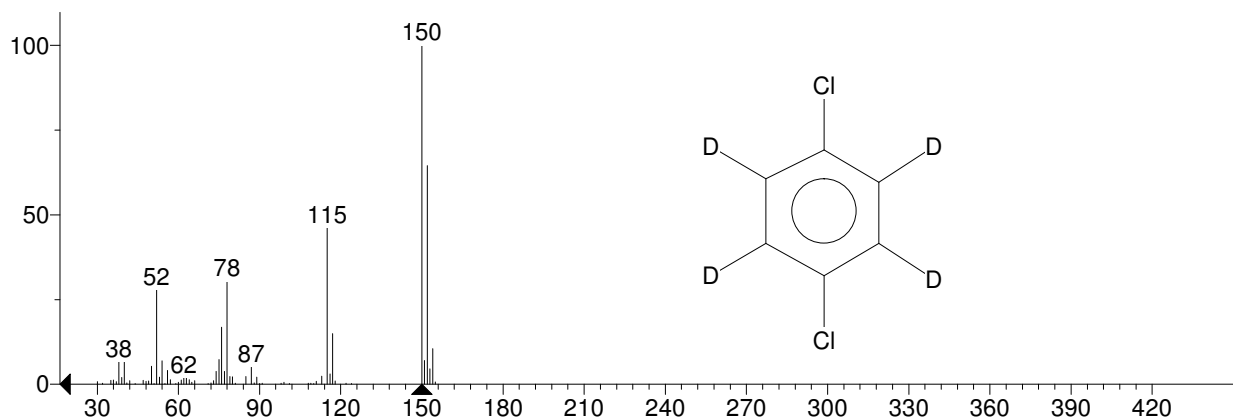
Hit 2 : 3-Butoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)trisiloxane
C₁₃H₃₆O₄Si₄; MF: 462; RMF: 491; Prob 8.59%; CAS: 87867-97-8; Lib: mainlib; ID: 22940.



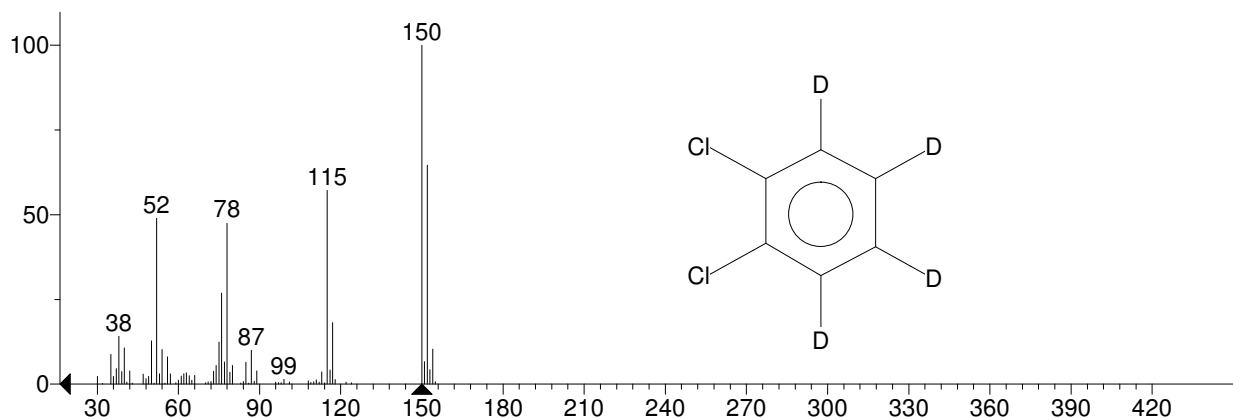
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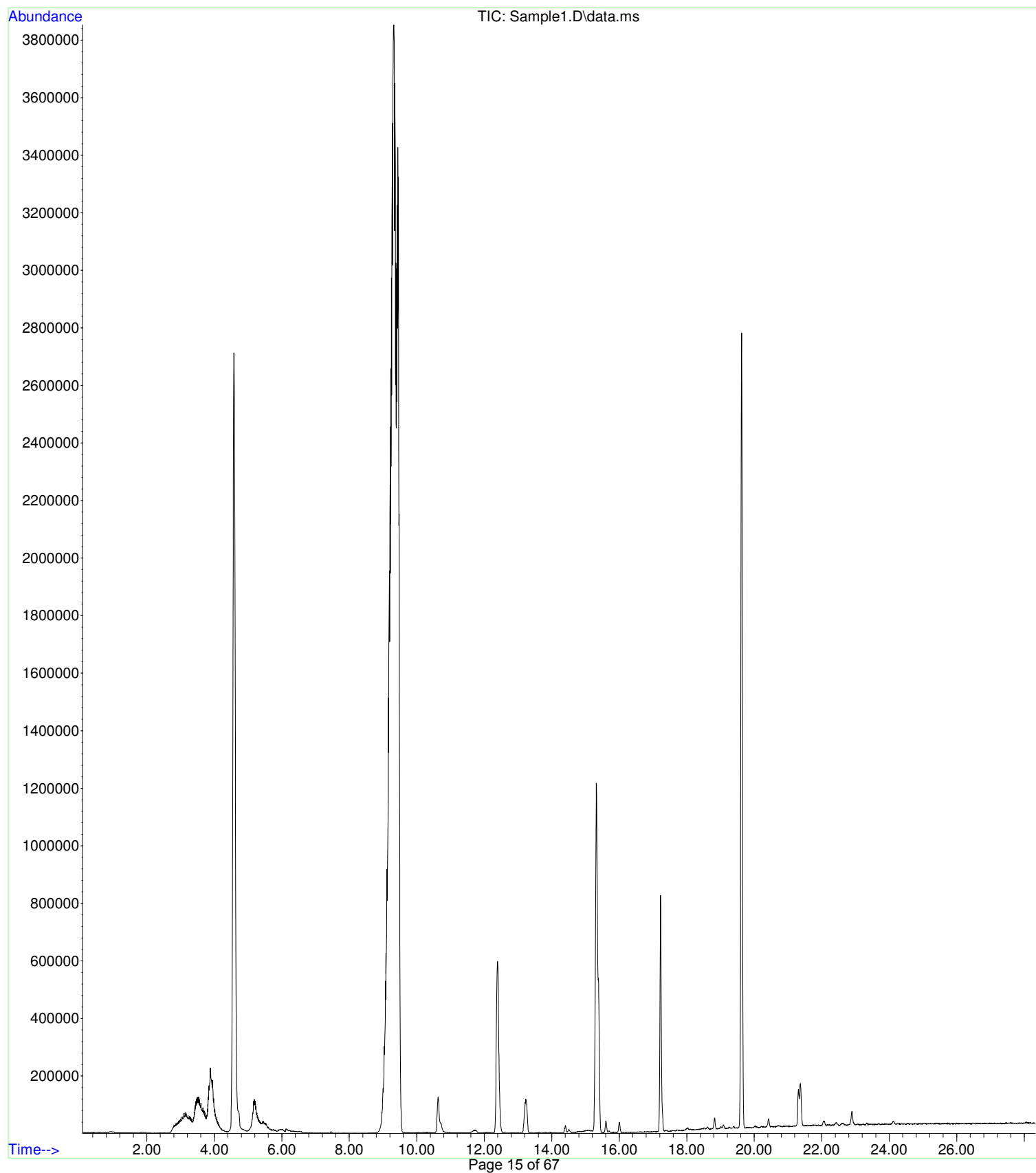
Hit 1 : 1,4-Dichlorobenzene-D4
C6Cl2D4; MF: 860; RMF: 894; Prob 61.4%; CAS: 3855-82-1; Lib: mainlib; ID: 111936.



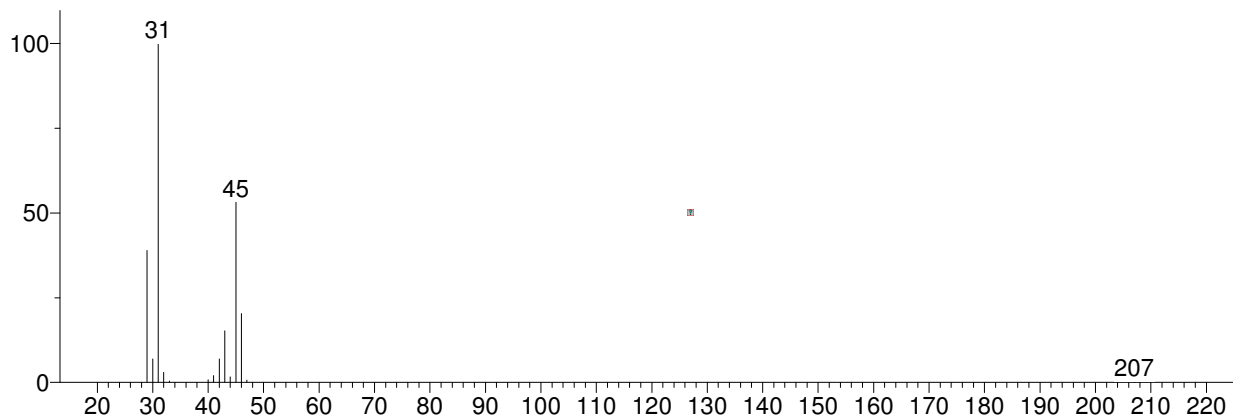
Hit 2 : 1,2-Dichlorobenzene-D4
C6Cl2D4; MF: 845; RMF: 876; Prob 37.2%; CAS: 2199-69-1; Lib: mainlib; ID: 111935.



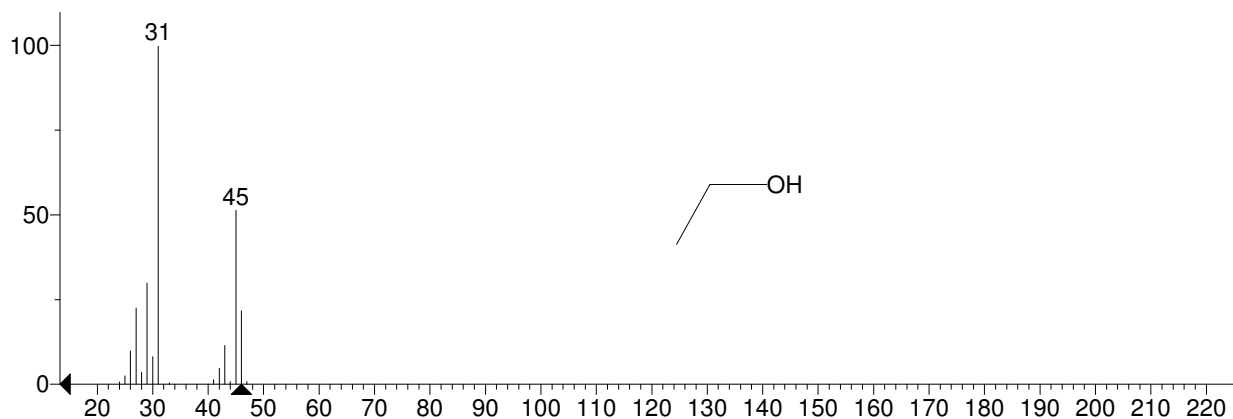
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Vial Number: 23



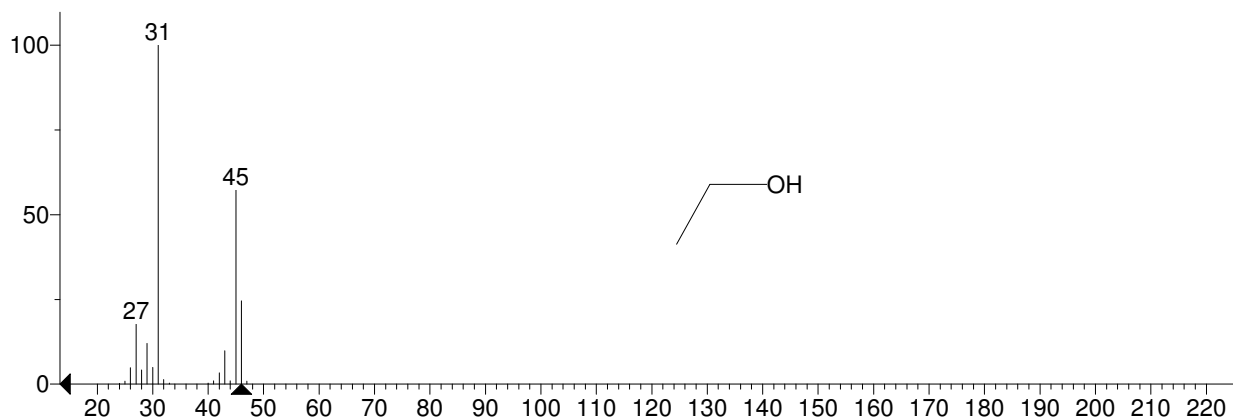
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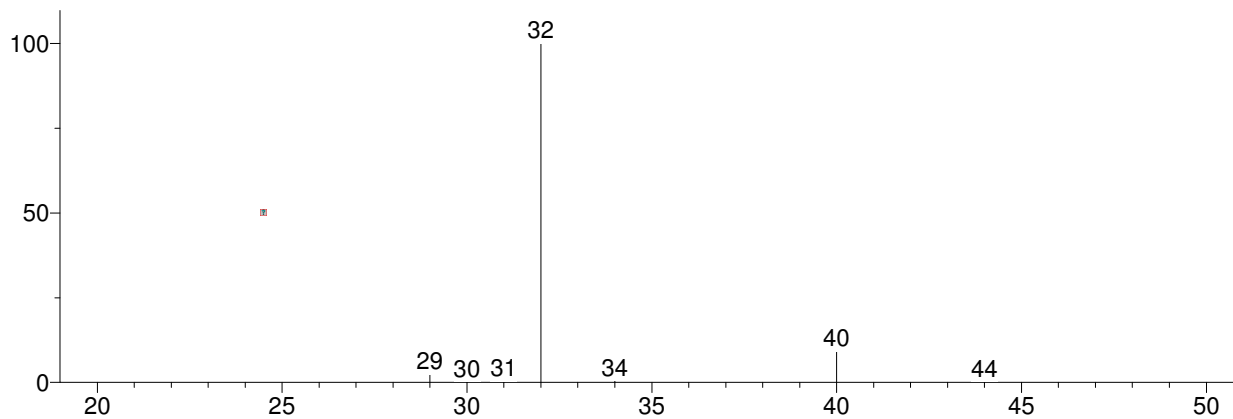
Hit 1 : Ethanol
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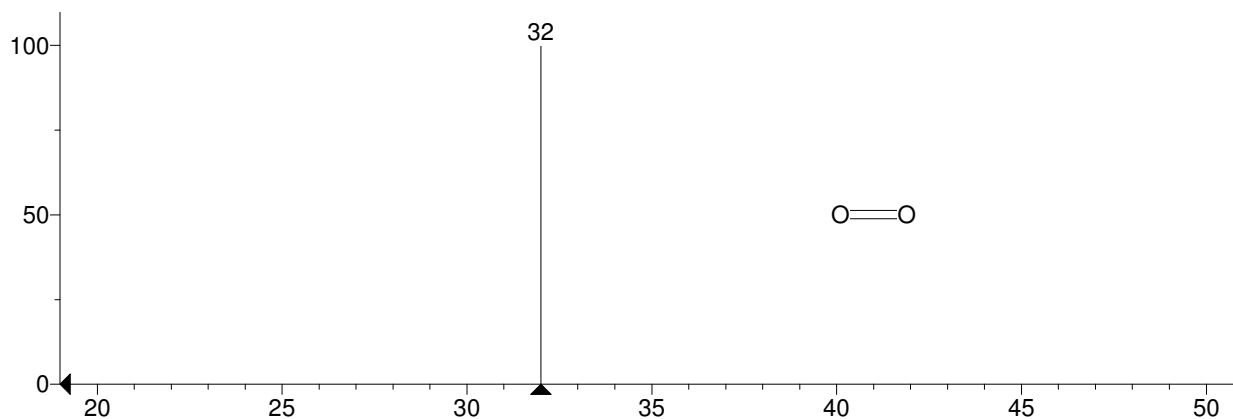
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C₂H₆O; MF: 897; RMF: 899; Prob 96.9%; CAS: 64-17-5; Lib: replib; ID: 573.



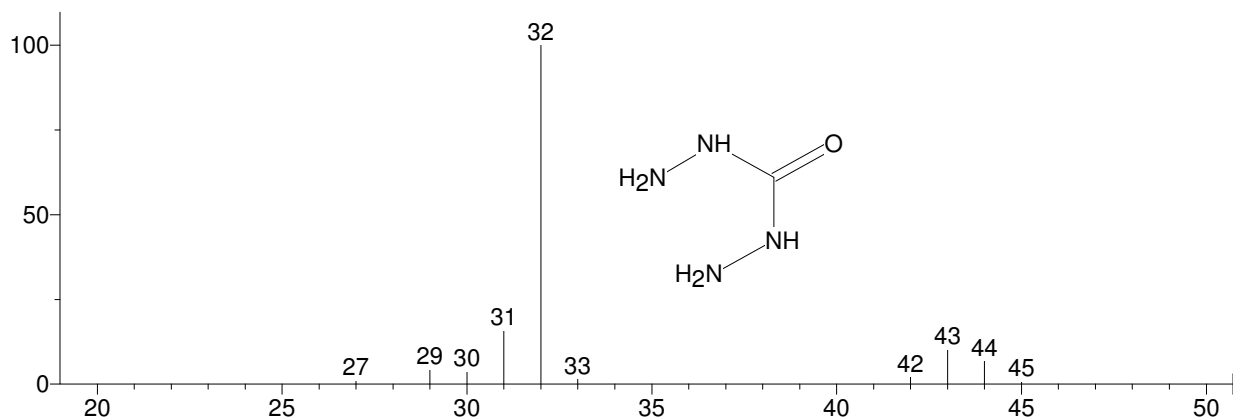
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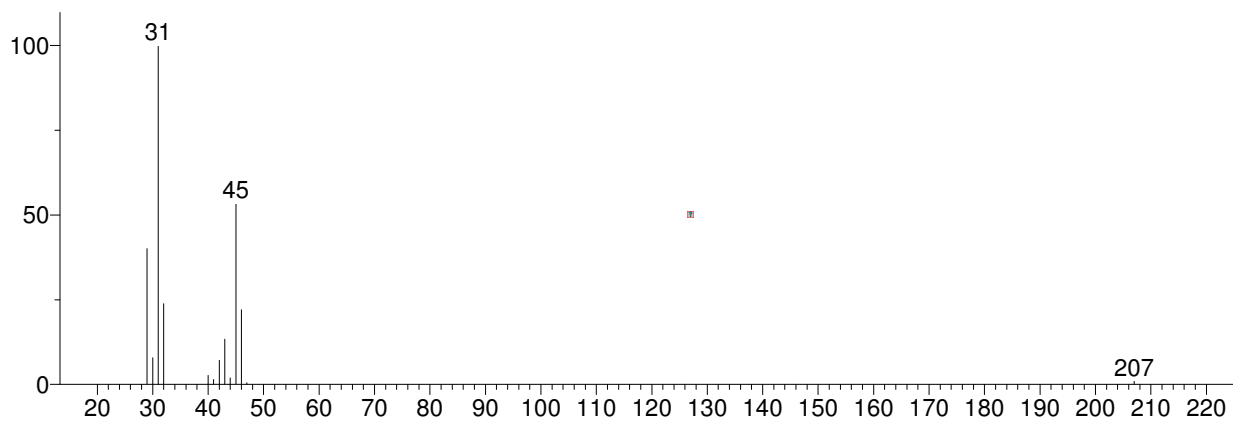
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O₂; MF: 876; RMF: 999; Prob 97.6%; CAS: 7782-44-7; Lib: mainlib; ID: 1449.



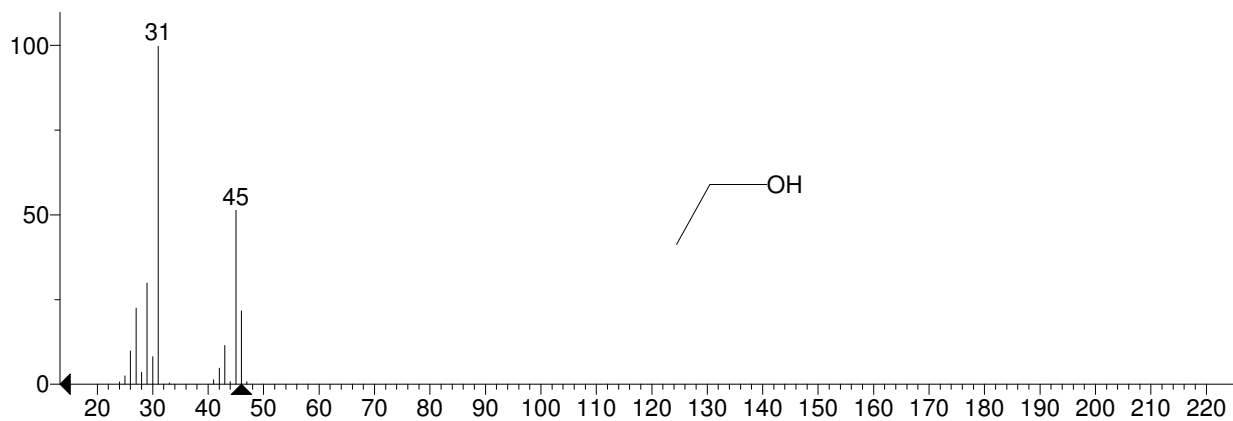
Hit 2 : Carbamic dihydrazide
CH₆N₄O; MF: 473; RMF: 513; Prob 0.97%; CAS: 497-18-7; Lib: replib; ID: 616.



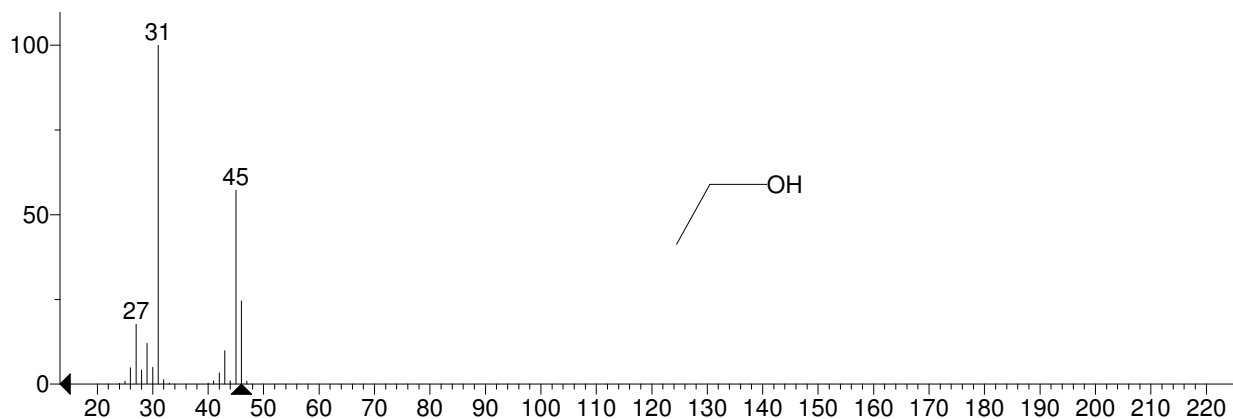
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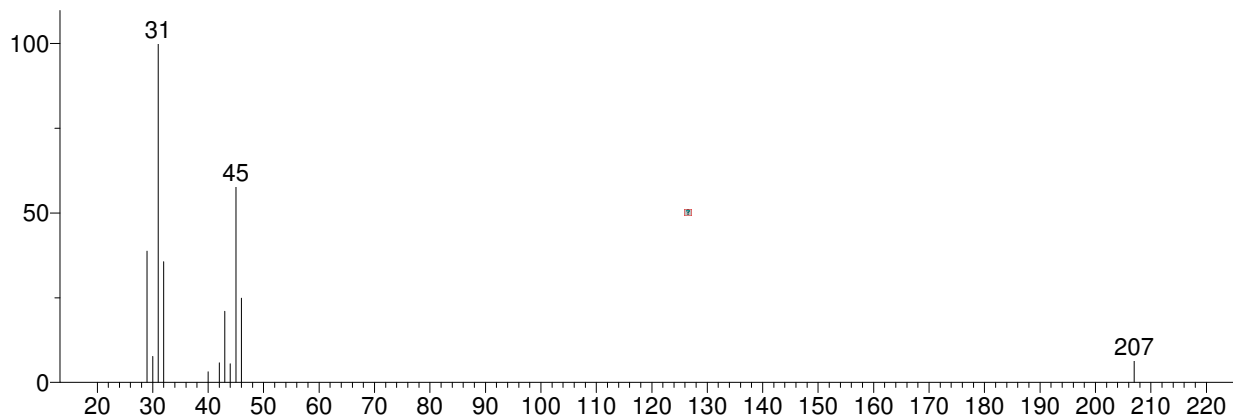
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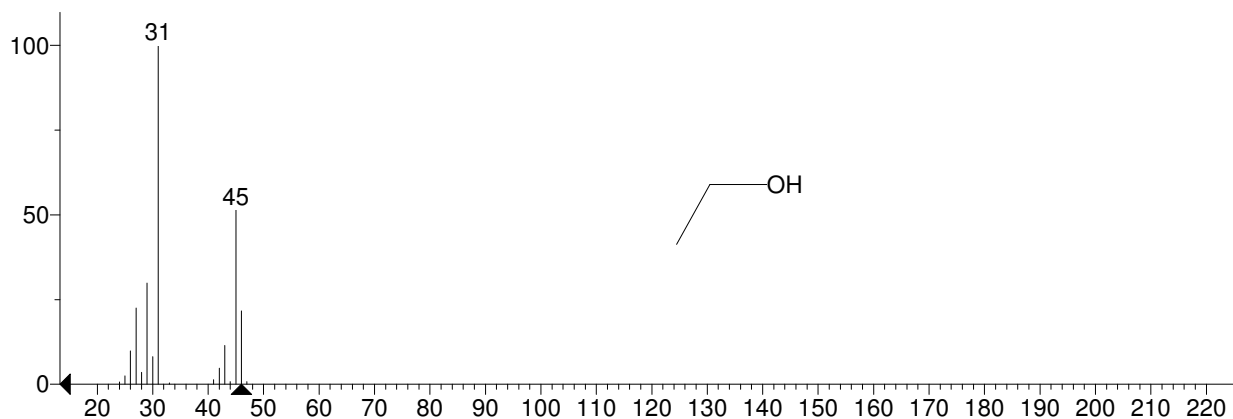
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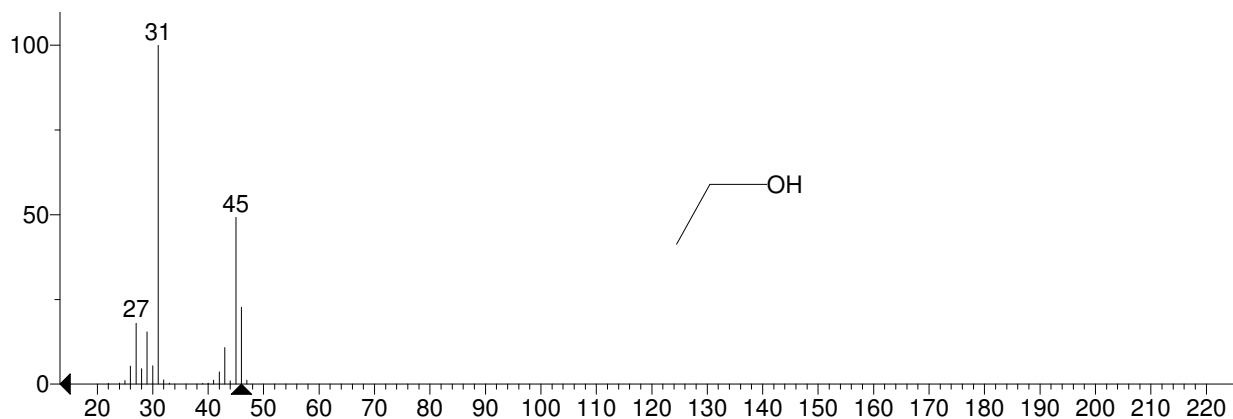
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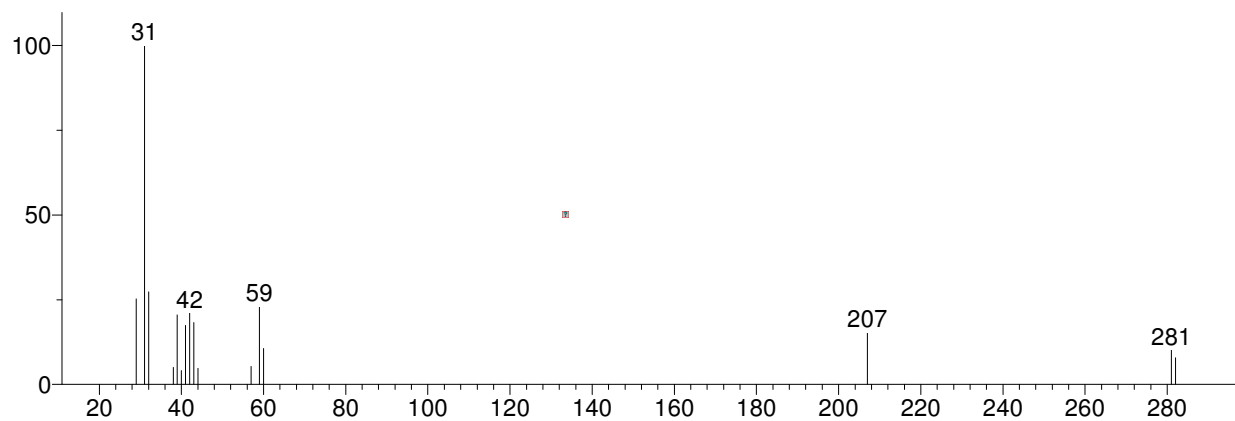
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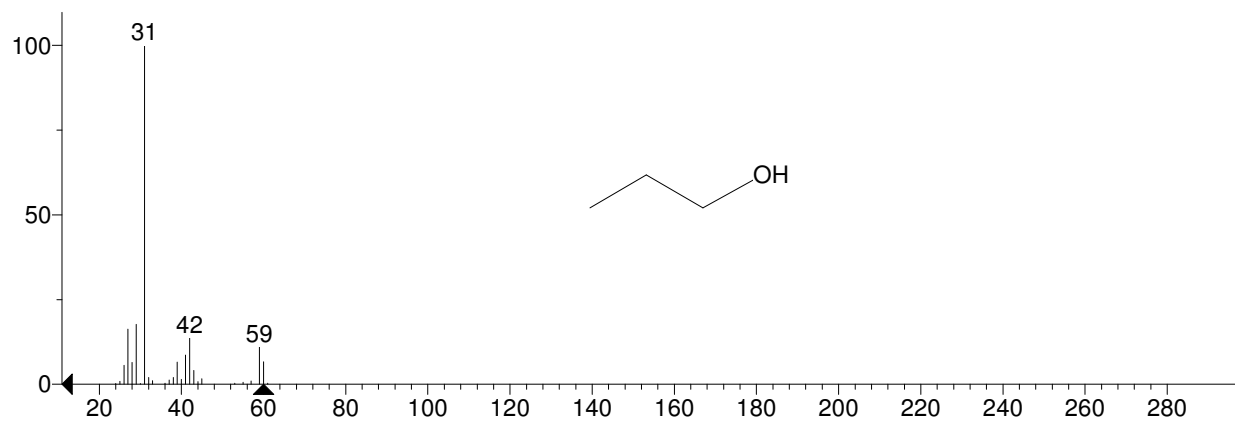
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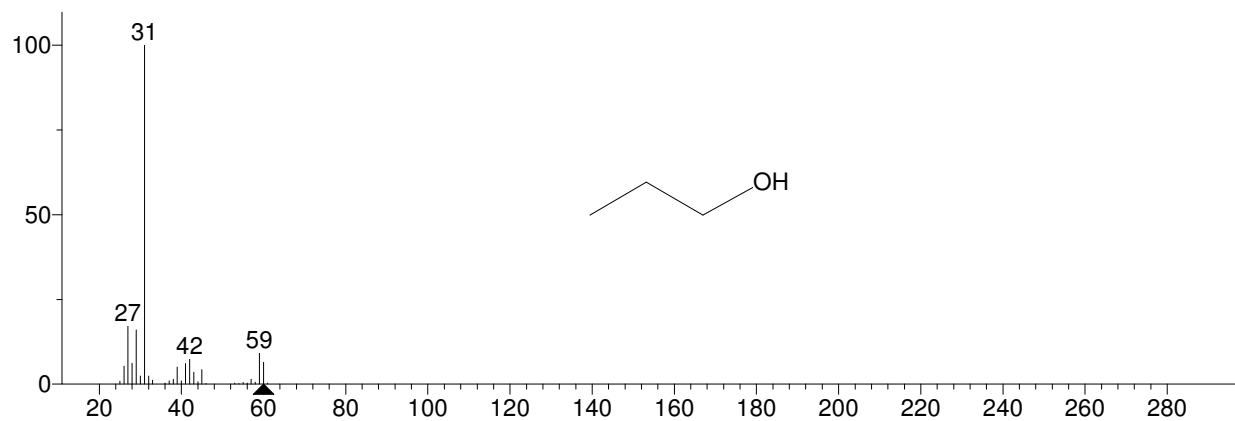
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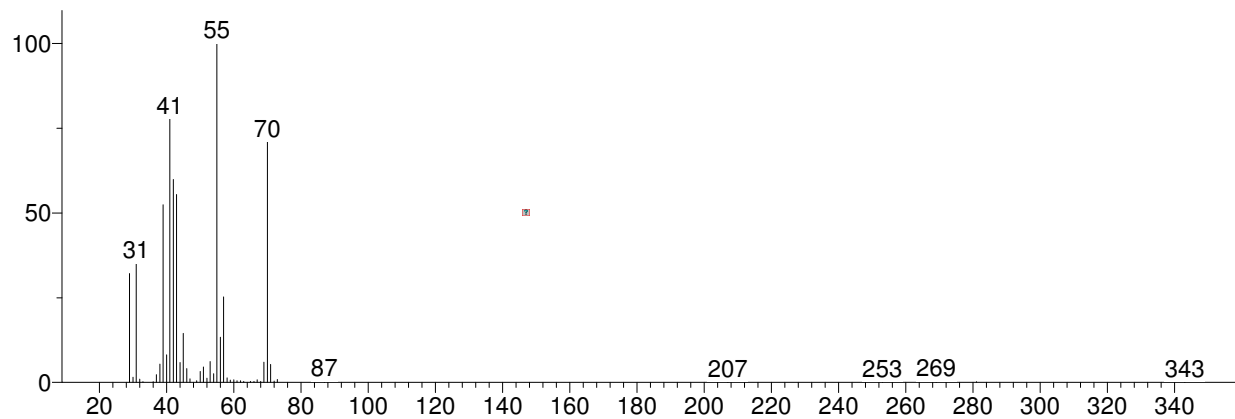
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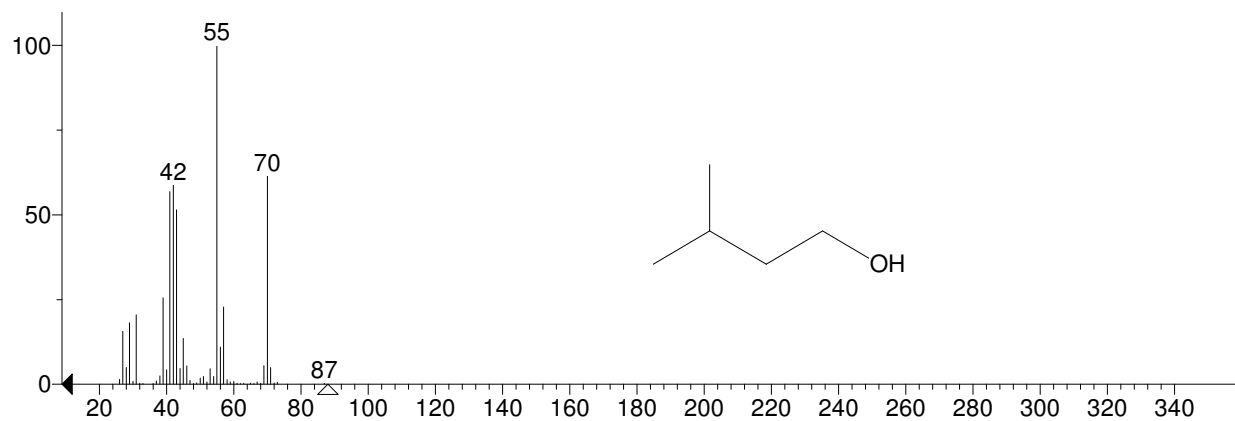
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C₃H₈O; MF: 600; RMF: 823; Prob 74.2%; CAS: 71-23-8; Lib: replib; ID: 540.



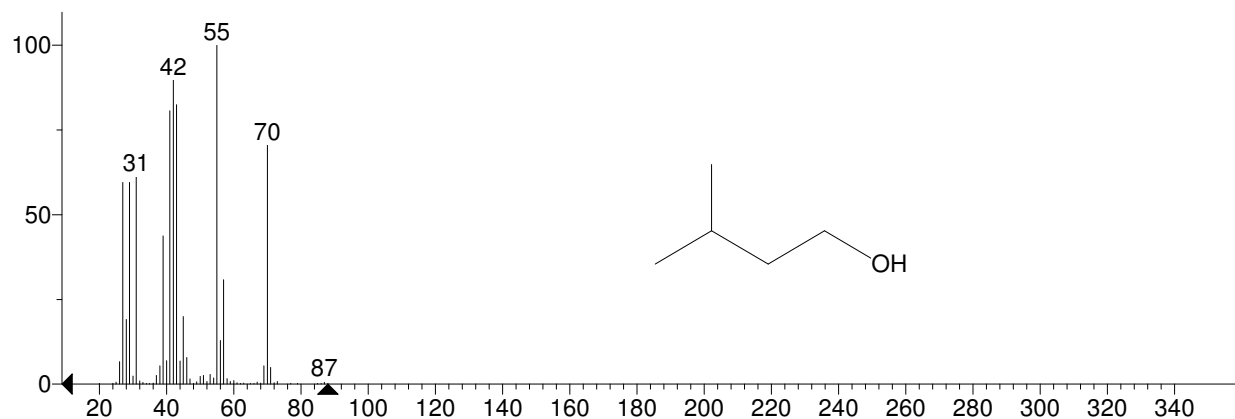
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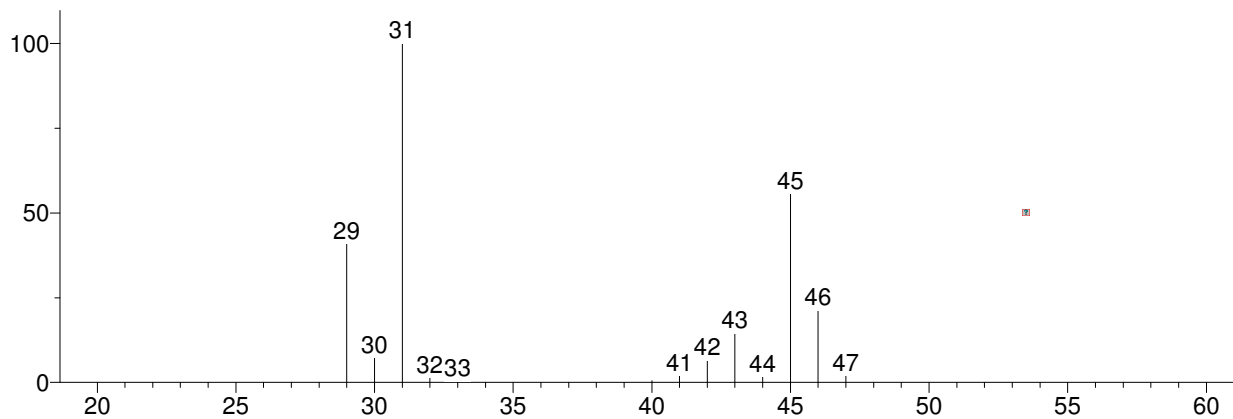
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C₅H₁₂O; MF: 930; RMF: 931; Prob 69.8%; CAS: 123-51-3; Lib: replib; ID: 4529.



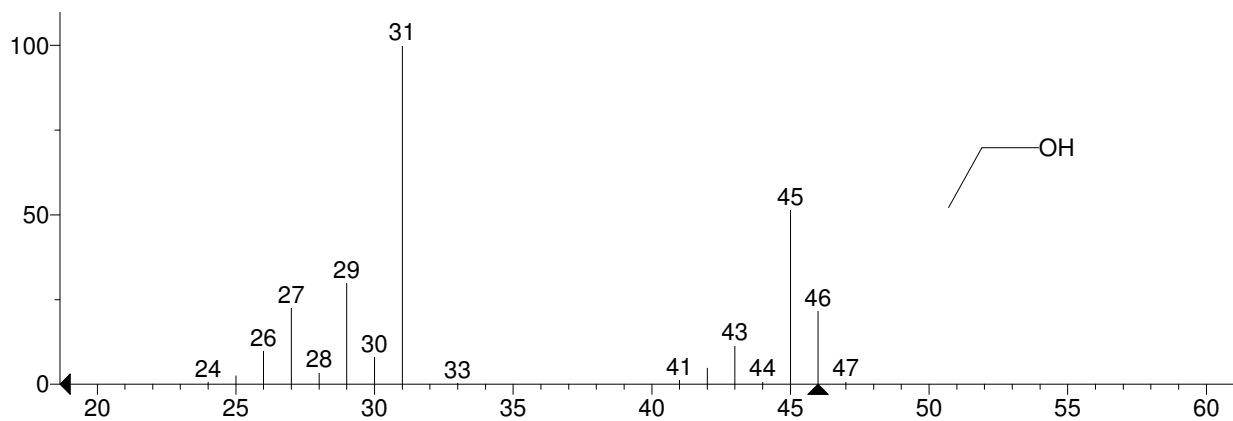
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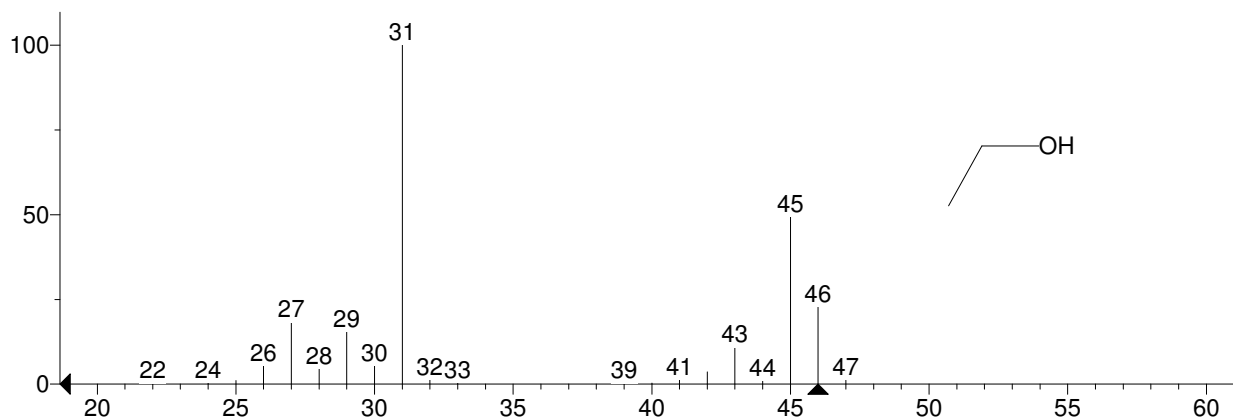
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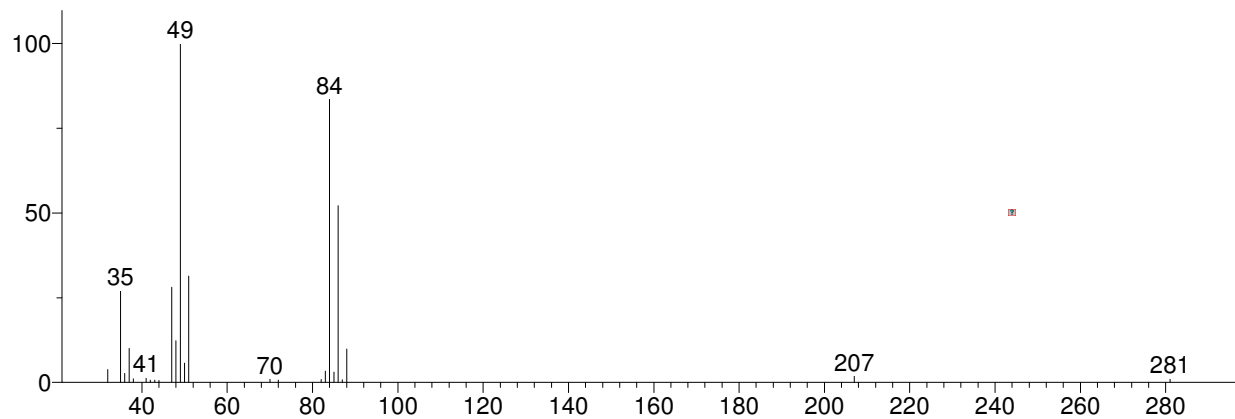
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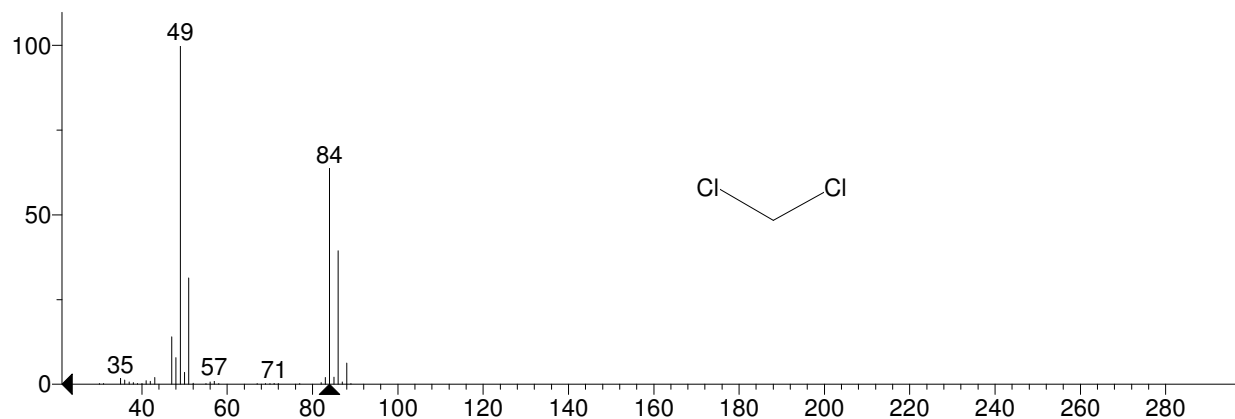
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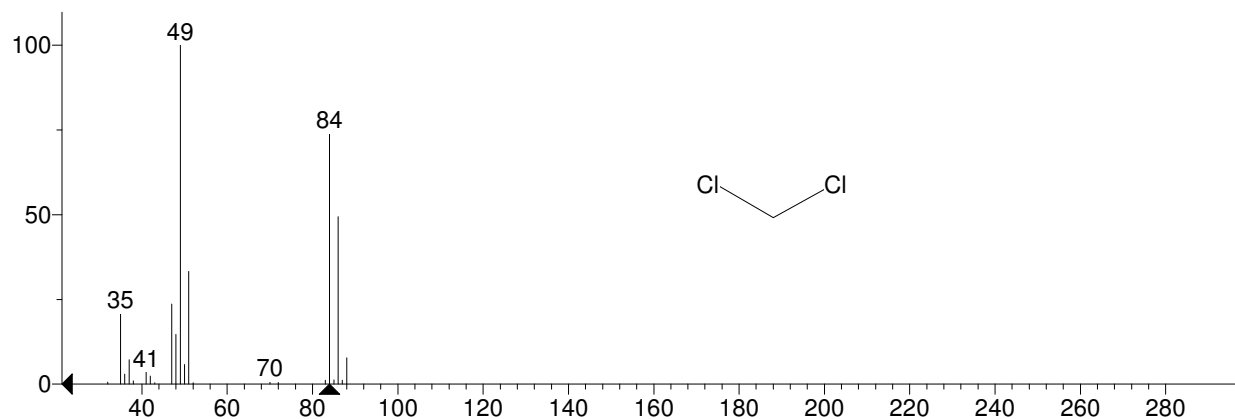
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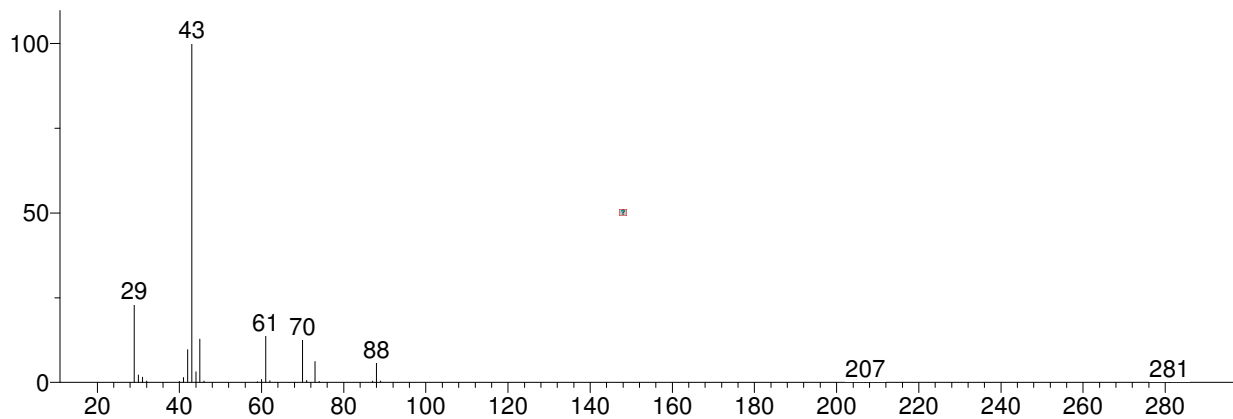
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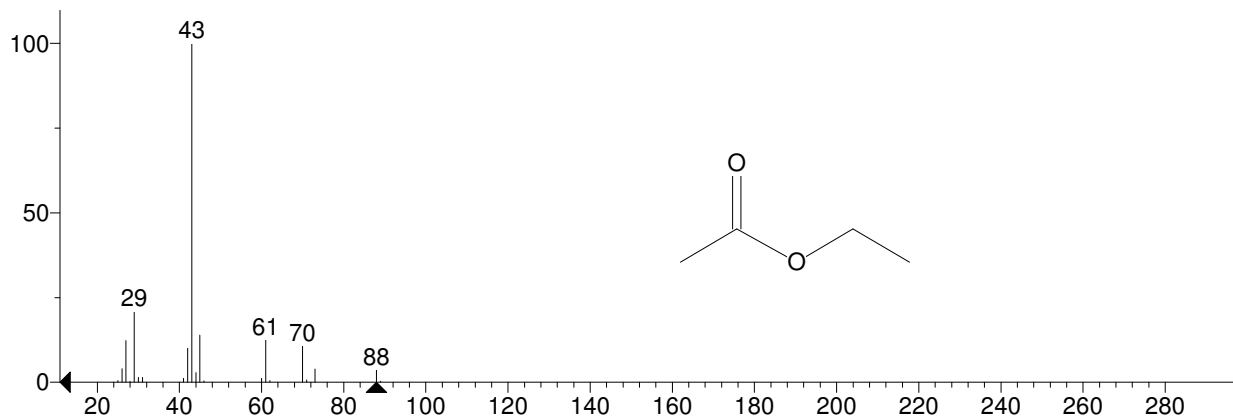
Hit 2 : Methylene Chloride
CH2Cl2; MF: 864; RMF: 881; Prob 96.5%; CAS: 75-09-2; Lib: replib; ID: 3894.



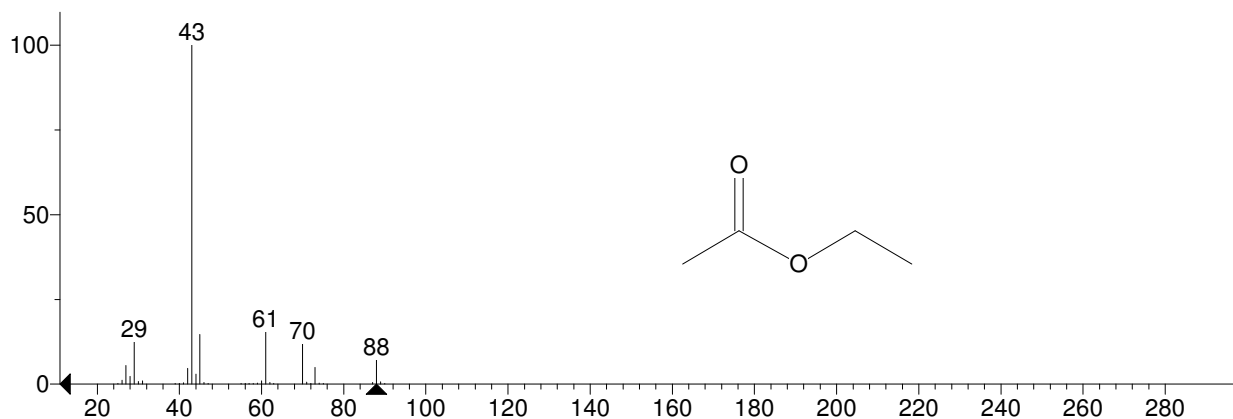
Unknown: Scan 2069 (12.390 min): Sample1.D\data.ms
Compound in Library Factor = 457



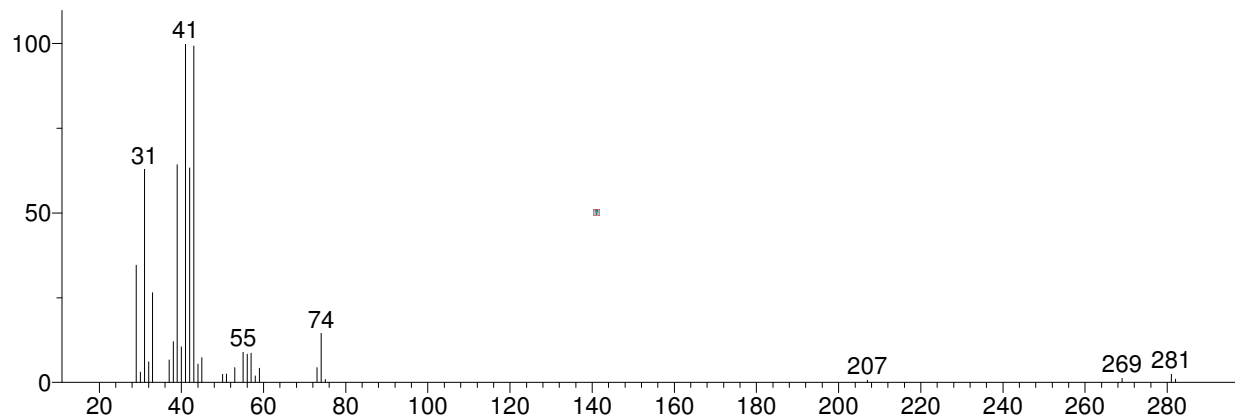
Hit 1 : Ethyl Acetate
C₄H₈O₂; MF: 943; RMF: 946; Prob 94.9%; CAS: 141-78-6; Lib: replib; ID: 1575.



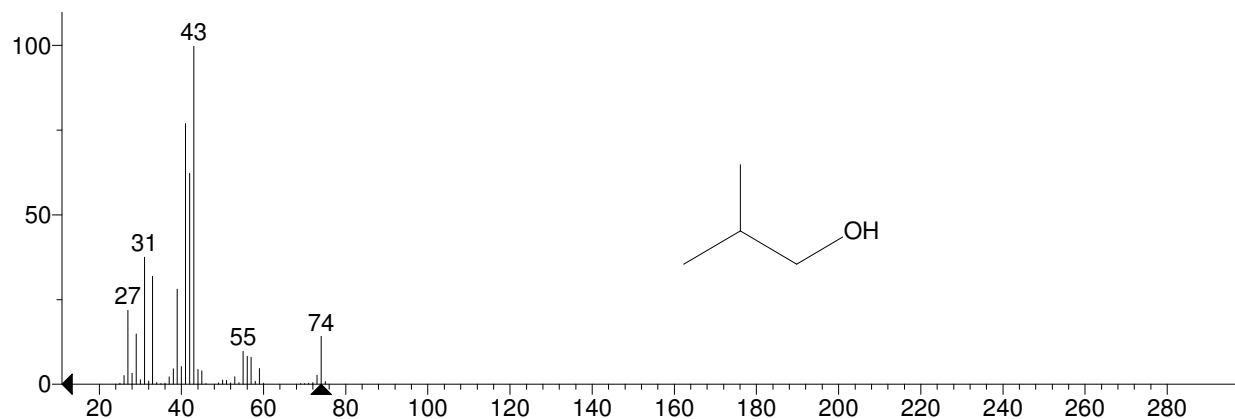
Hit 2 : Ethyl Acetate
C₄H₈O₂; MF: 929; RMF: 929; Prob 94.9%; CAS: 141-78-6; Lib: mainlib; ID: 7691.



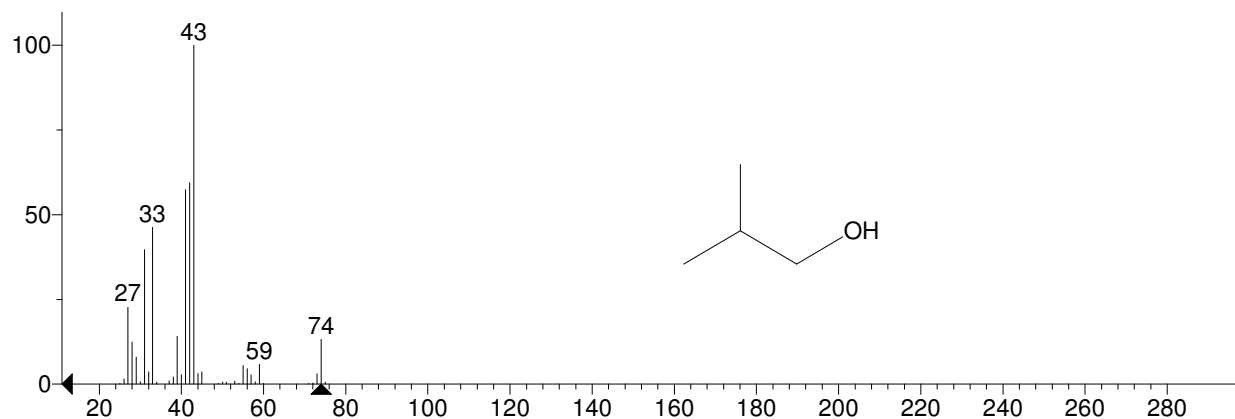
Unknown: Scan 2209 (13.222 min): Sample1.D\data.ms
Compound in Library Factor = 253



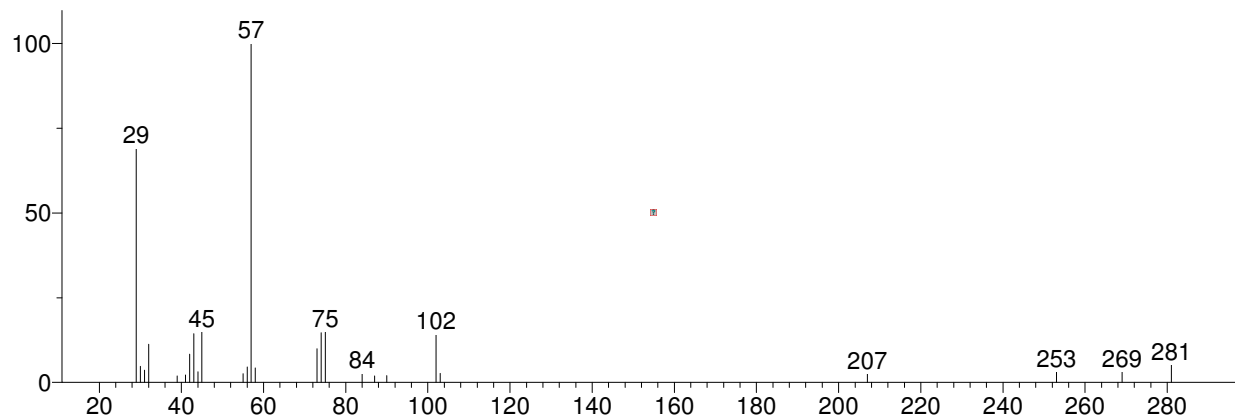
Hit 1 : 1-Propanol, 2-methyl-
C₄H₁₀O; MF: 875; RMF: 910; Prob 89.8%; CAS: 78-83-1; Lib: mainlib; ID: 5486.



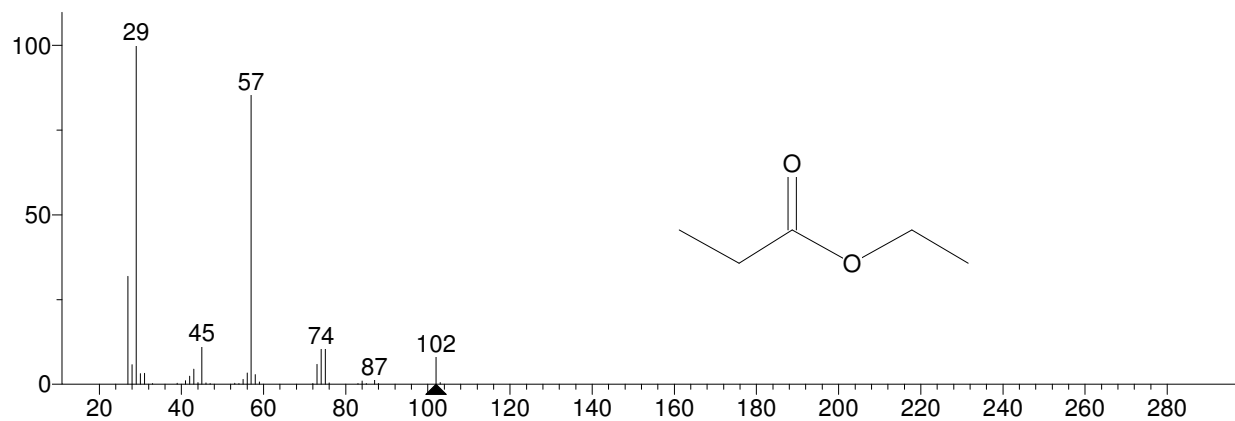
Hit 2 : 1-Propanol, 2-methyl-
C₄H₁₀O; MF: 840; RMF: 871; Prob 89.8%; CAS: 78-83-1; Lib: replib; ID: 1820.



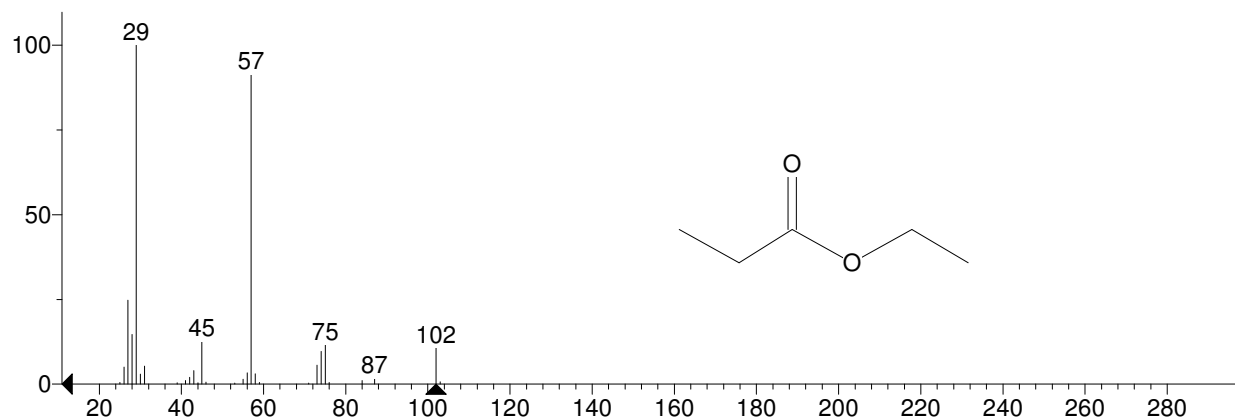
Unknown: Scan 2408 (14.405 min): Sample1.D\data.ms
Compound in Library Factor = -209



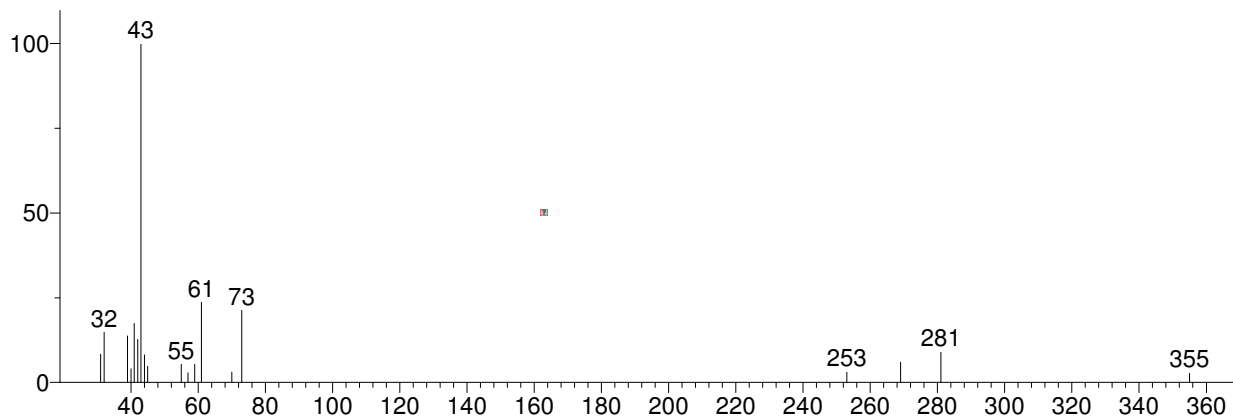
Hit 1 : Propanoic acid, ethyl ester
C₅H₁₀O₂; MF: 755; RMF: 871; Prob 81.8%; CAS: 105-37-3; Lib: replib; ID: 201.



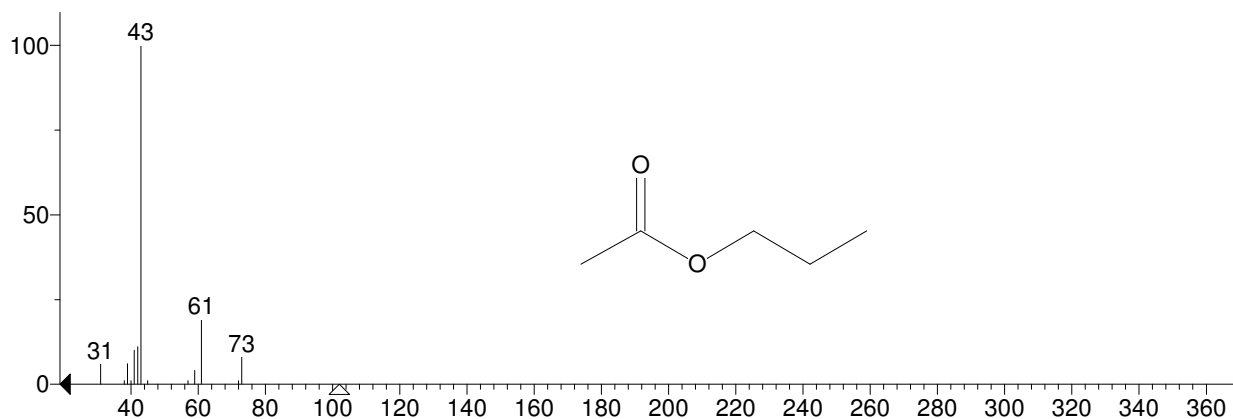
Hit 2 : Propanoic acid, ethyl ester
C₅H₁₀O₂; MF: 746; RMF: 861; Prob 81.8%; CAS: 105-37-3; Lib: replib; ID: 202.



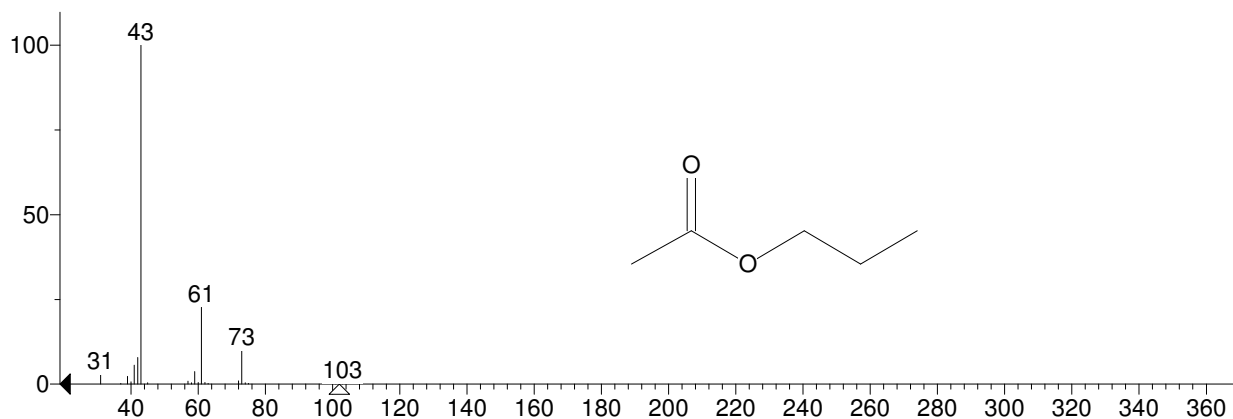
Unknown: Scan 2424 (14.500 min): Sample1.D\data.ms
Compound in Library Factor = -550



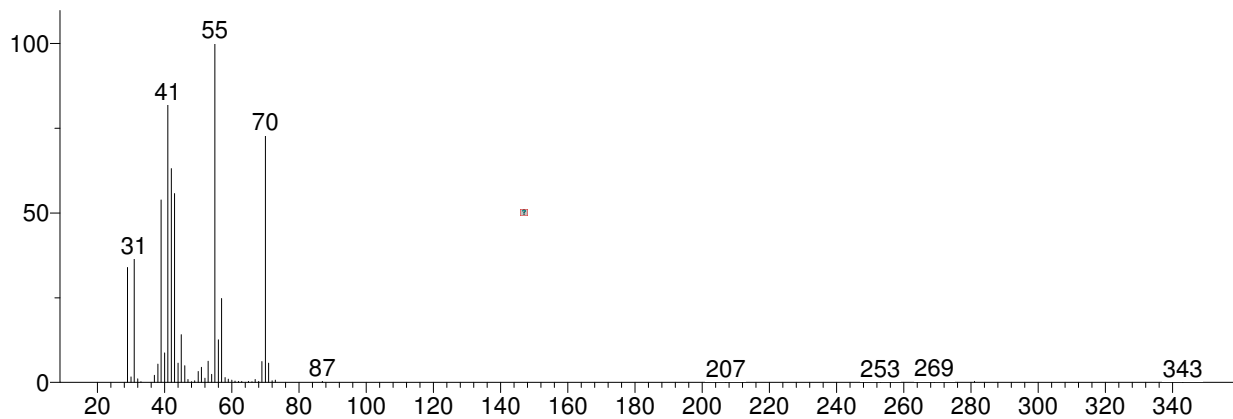
Hit 1 : n-Propyl acetate
C5H10O2; MF: 644; RMF: 901; Prob 51.3%; CAS: 109-60-4; Lib: replib; ID: 2272.



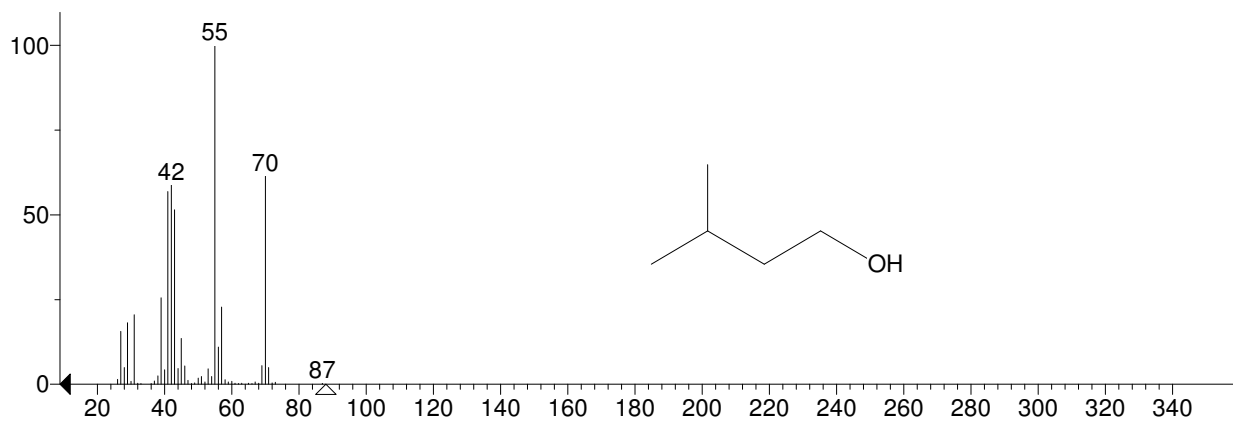
Hit 2 : n-Propyl acetate
C5H10O2; MF: 603; RMF: 884; Prob 51.3%; CAS: 109-60-4; Lib: replib; ID: 2284.



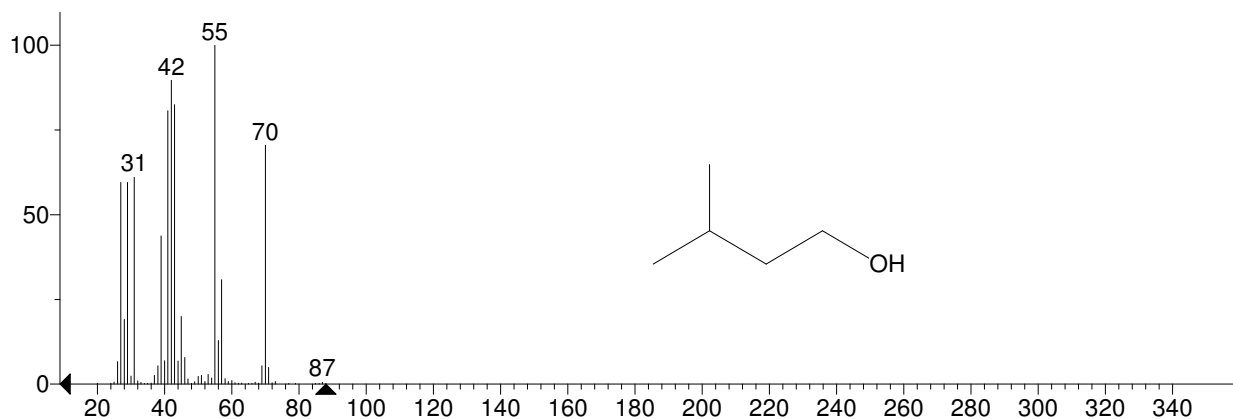
Unknown: Scan 2561 (15.315 min): Sample1.D\data.ms
Compound in Library Factor = 184



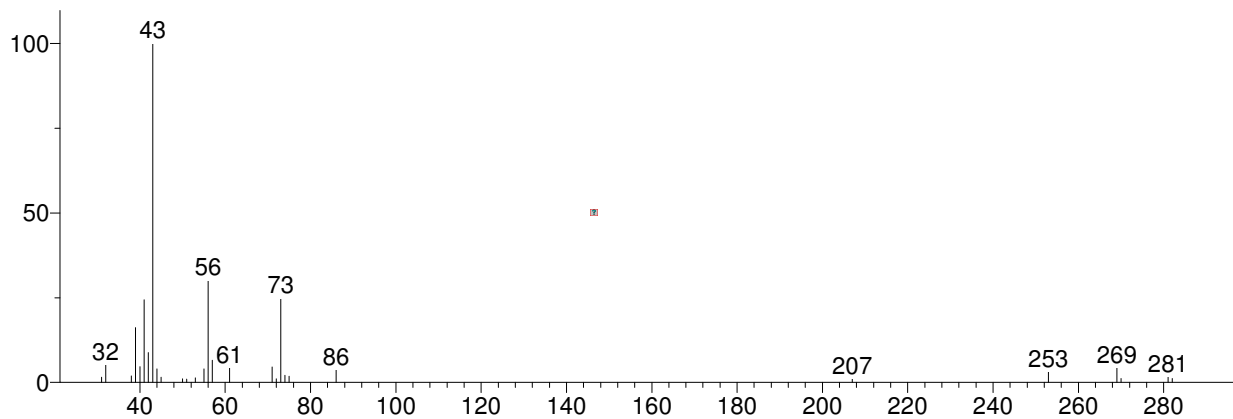
Hit 1 : 1-Butanol, 3-methyl-
C₅H₁₂O; MF: 939; RMF: 941; Prob 70.1%; CAS: 123-51-3; Lib: replib; ID: 4529.



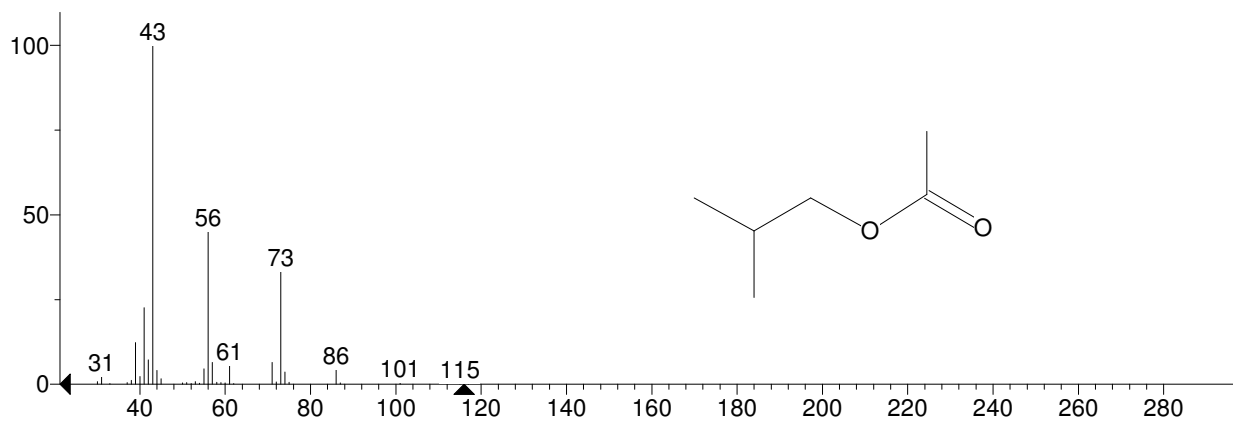
Hit 2 : 1-Butanol, 3-methyl-
C₅H₁₂O; MF: 917; RMF: 918; Prob 70.1%; CAS: 123-51-3; Lib: mainlib; ID: 17753.



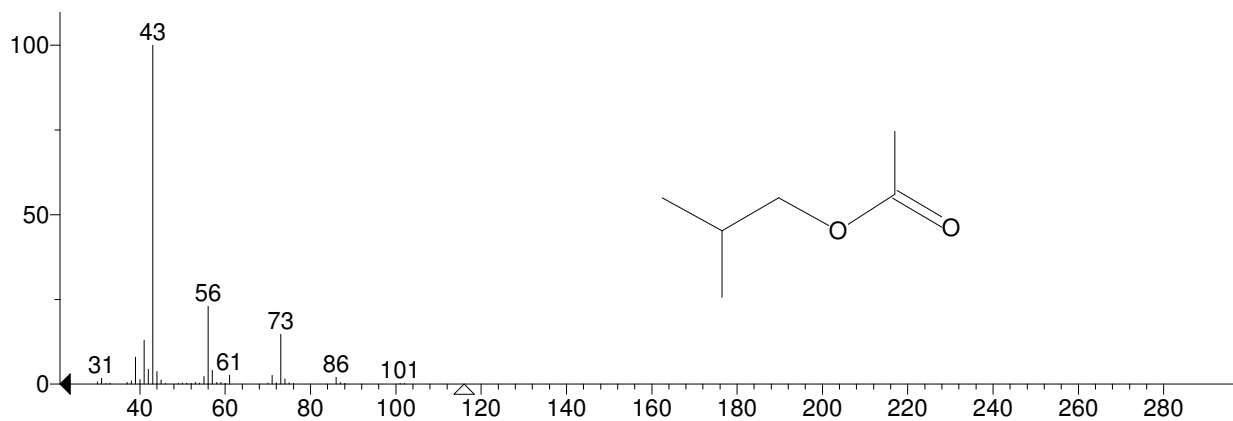
Unknown: Scan 2609 (15.600 min): Sample1.D\data.ms
Compound in Library Factor = -168



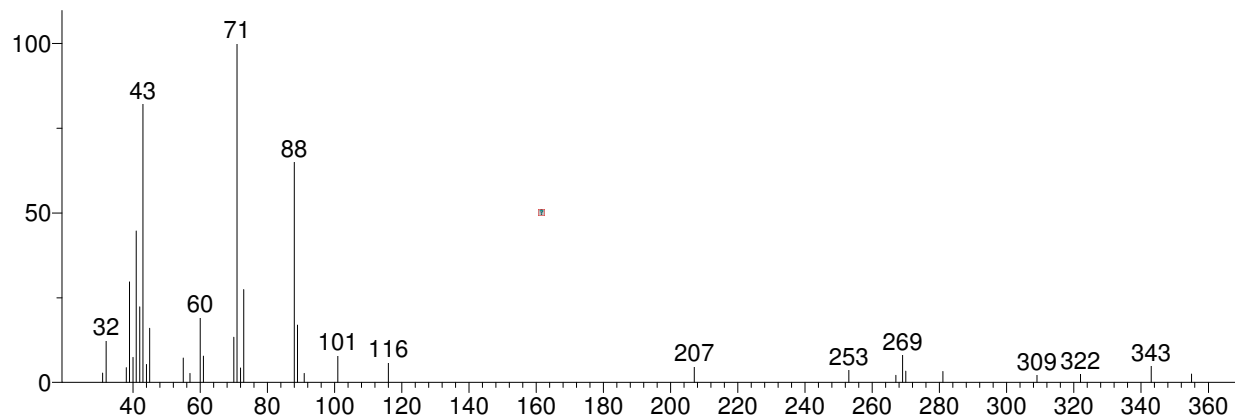
Hit 1 : Acetic acid, 2-methylpropyl ester
C₆H₁₂O₂; MF: 766; RMF: 879; Prob 67.9%; CAS: 110-19-0; Lib: mainlib; ID: 7062.



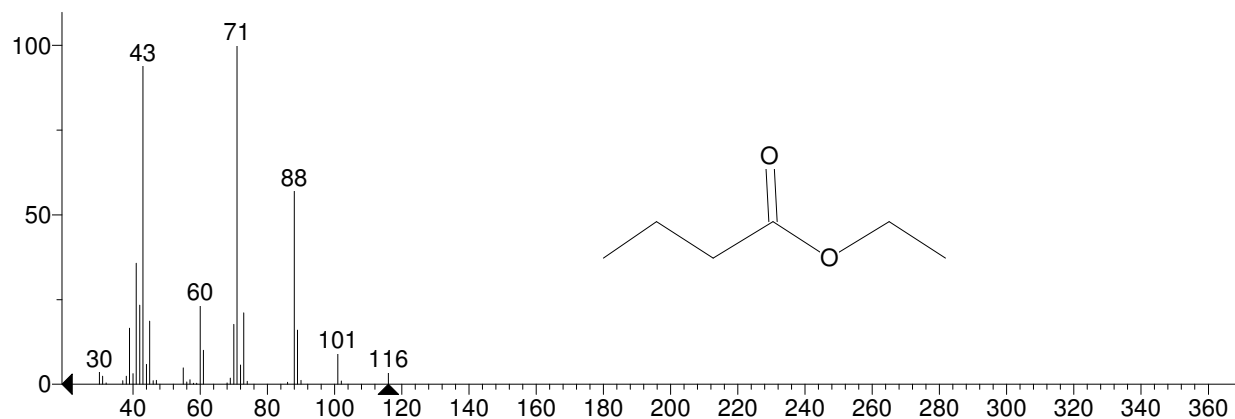
Hit 2 : Acetic acid, 2-methylpropyl ester
C₆H₁₂O₂; MF: 755; RMF: 862; Prob 67.9%; CAS: 110-19-0; Lib: replib; ID: 2007.



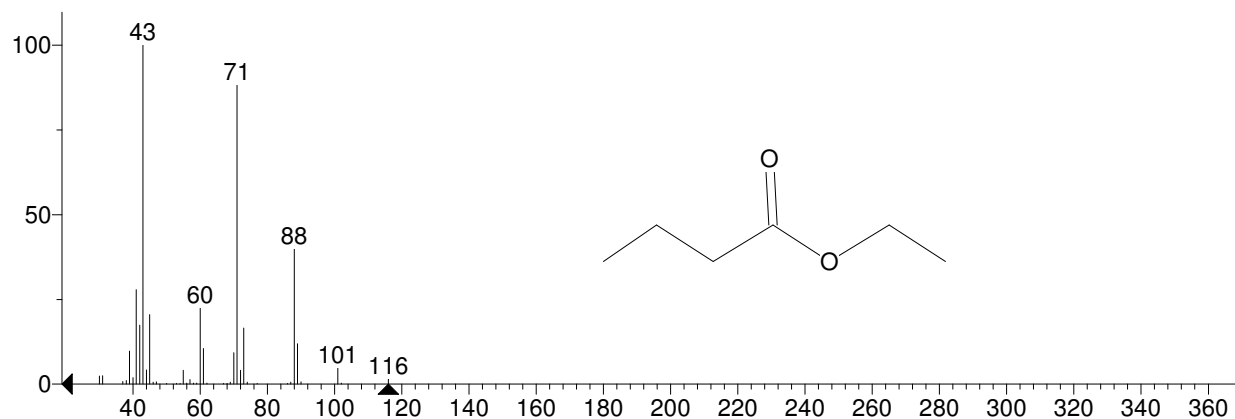
Unknown: Scan 2676 (15.999 min): Sample1.D\data.ms
Compound in Library Factor = -142



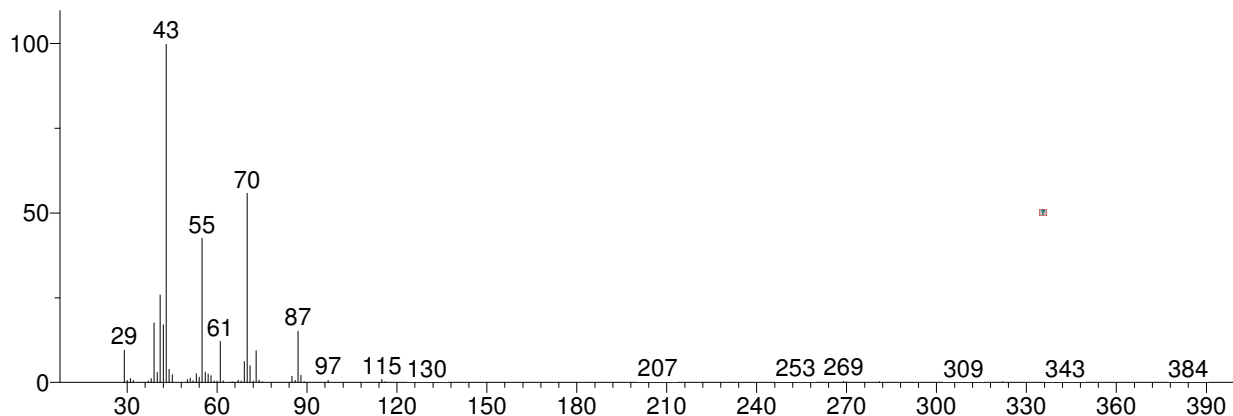
Hit 1 : Butanoic acid, ethyl ester
C₆H₁₂O₂; MF: 768; RMF: 923; Prob 90.4%; CAS: 105-54-4; Lib: mainlib; ID: 33076.



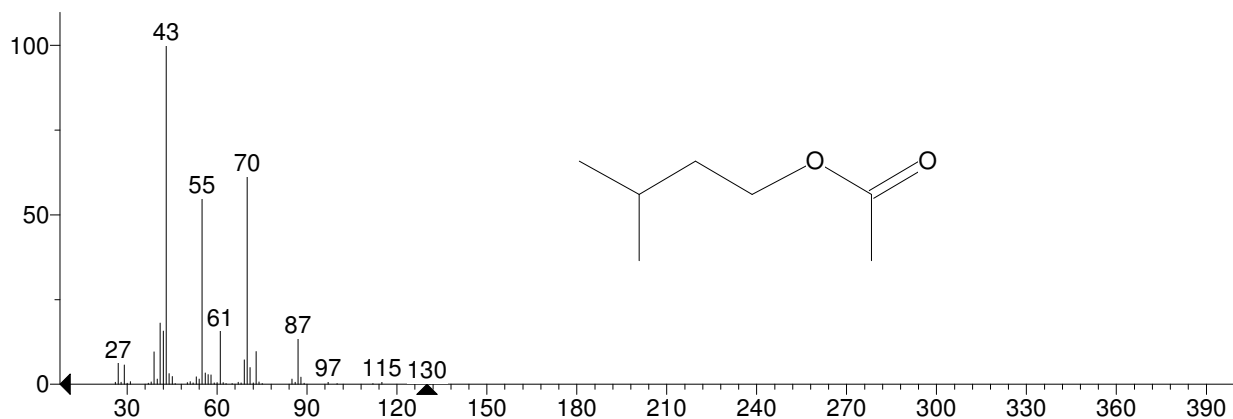
Hit 2 : Butanoic acid, ethyl ester
C₆H₁₂O₂; MF: 758; RMF: 921; Prob 90.4%; CAS: 105-54-4; Lib: replib; ID: 2399.



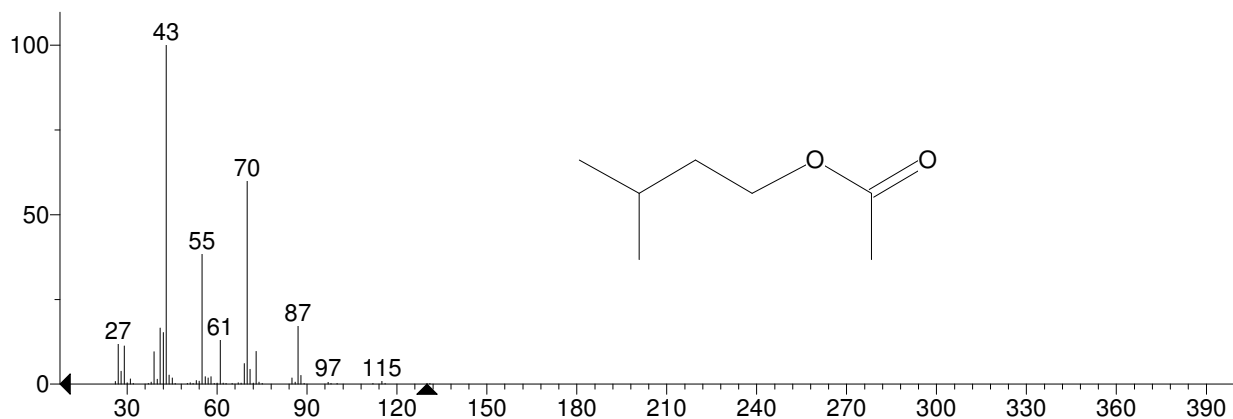
Unknown: Scan 2882 (17.224 min): Sample1.D\data.ms
Compound in Library Factor = 244



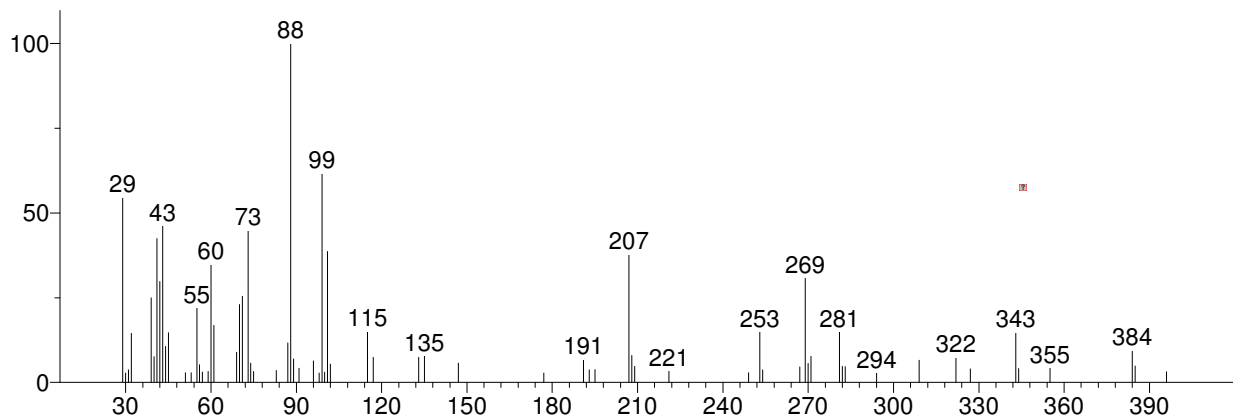
Hit 1 : 1-Butanol, 3-methyl-, acetate
C₇H₁₄O₂; MF: 942; RMF: 948; Prob 88.5%; CAS: 123-92-2; Lib: mainlib; ID: 8018.



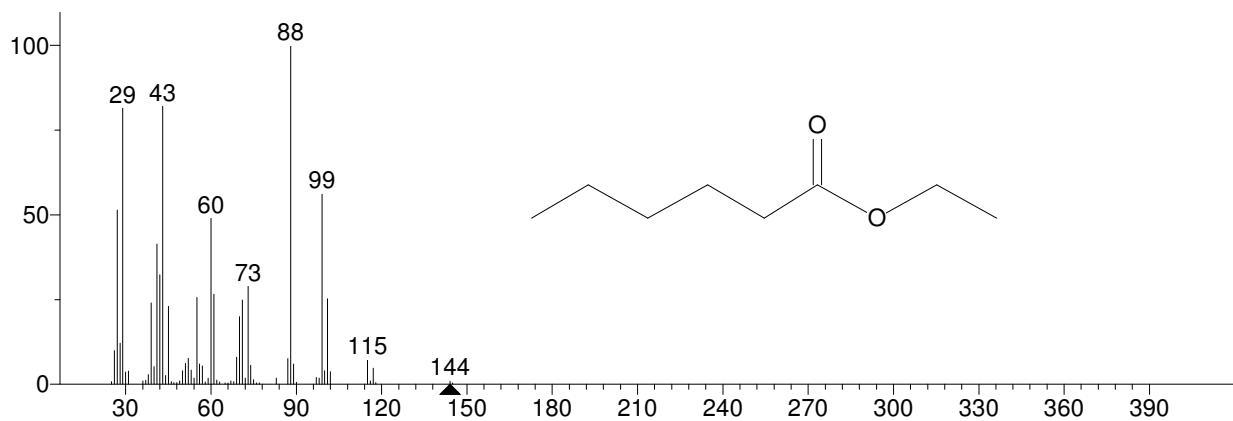
Hit 2 : 1-Butanol, 3-methyl-, acetate
C₇H₁₄O₂; MF: 917; RMF: 924; Prob 88.5%; CAS: 123-92-2; Lib: replib; ID: 2361.



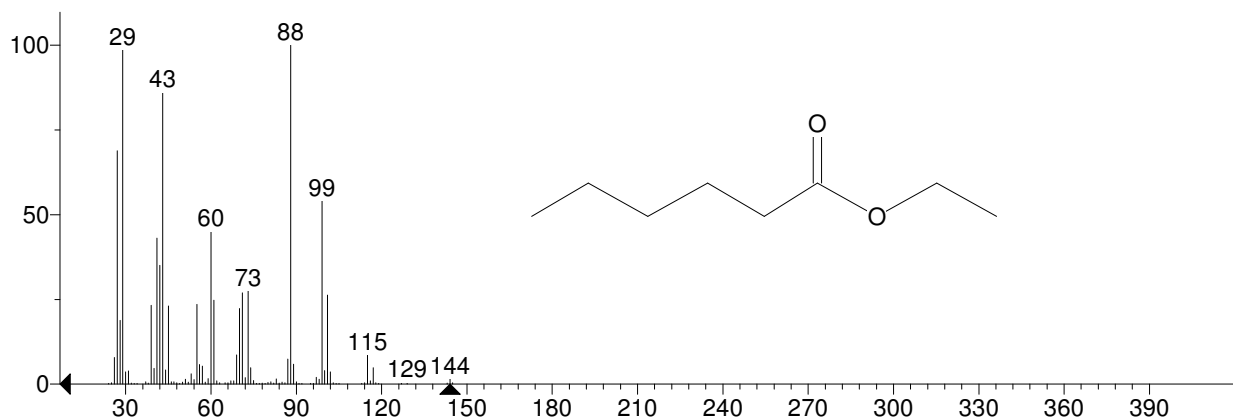
Unknown: Scan 3152 (18.829 min): Sample1.D\data.ms
Compound in Library Factor = -1014



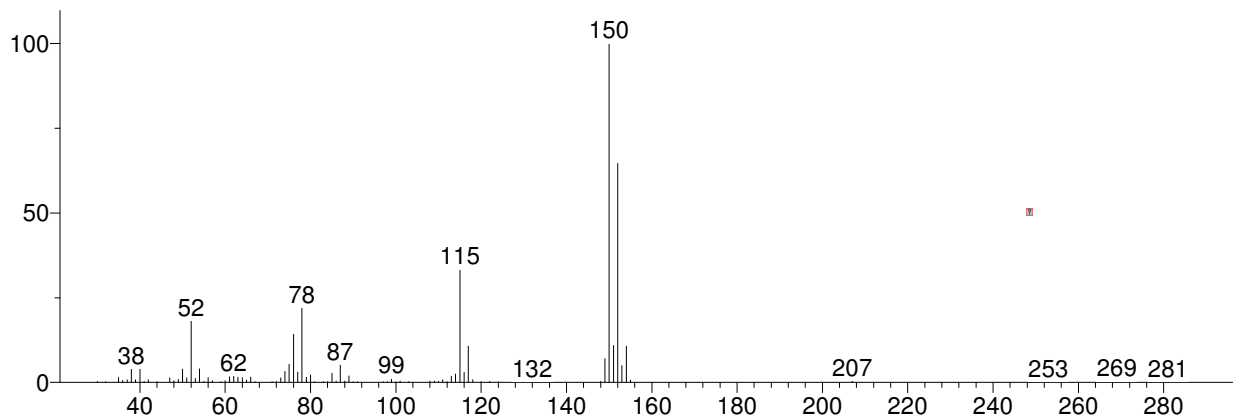
Hit 1 : Hexanoic acid, ethyl ester
C₈H₁₆O₂; MF: 566; RMF: 886; Prob 67.5%; CAS: 123-66-0; Lib: replib; ID: 11040.



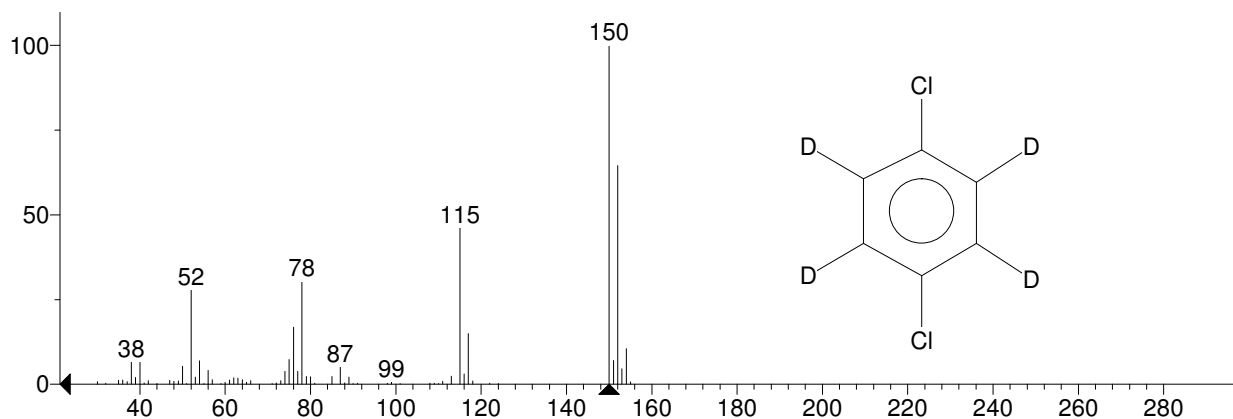
Hit 2 : Hexanoic acid, ethyl ester
C₈H₁₆O₂; MF: 552; RMF: 872; Prob 67.5%; CAS: 123-66-0; Lib: mainlib; ID: 49157.



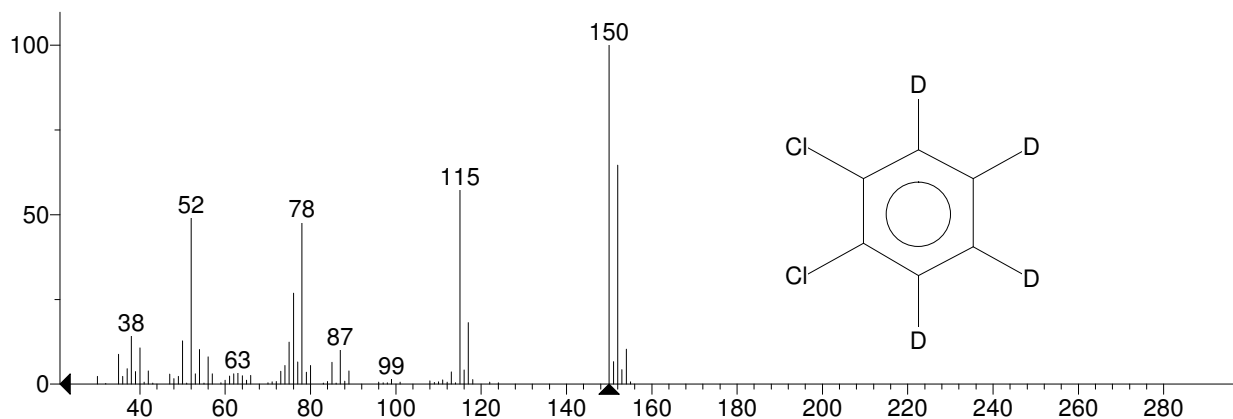
Unknown: Scan 3286 (19.626 min): Sample1.D\data.ms
Compound in Library Factor = 418



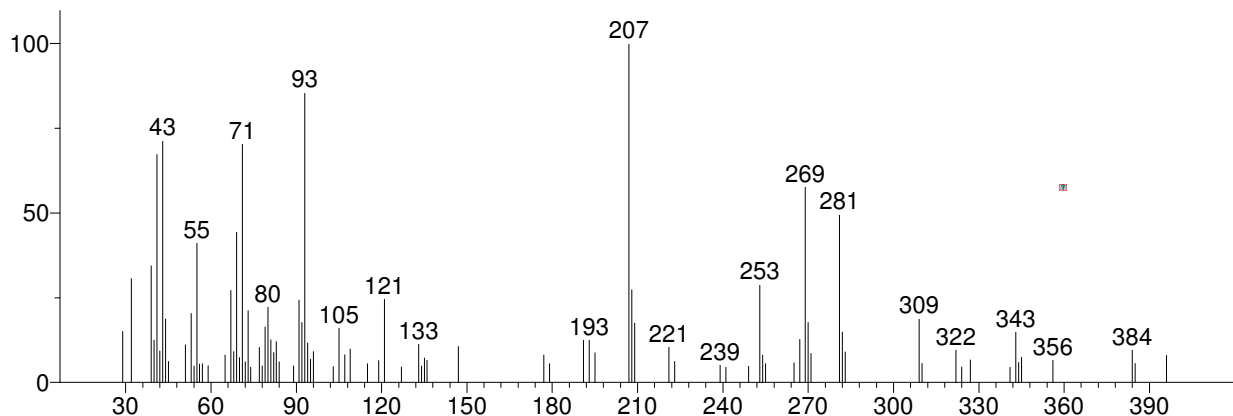
Hit 1 : 1,4-Dichlorobenzene-D4
C6Cl2D4; MF: 892; RMF: 909; Prob 79.5%; CAS: 3855-82-1; Lib: mainlib; ID: 111936.



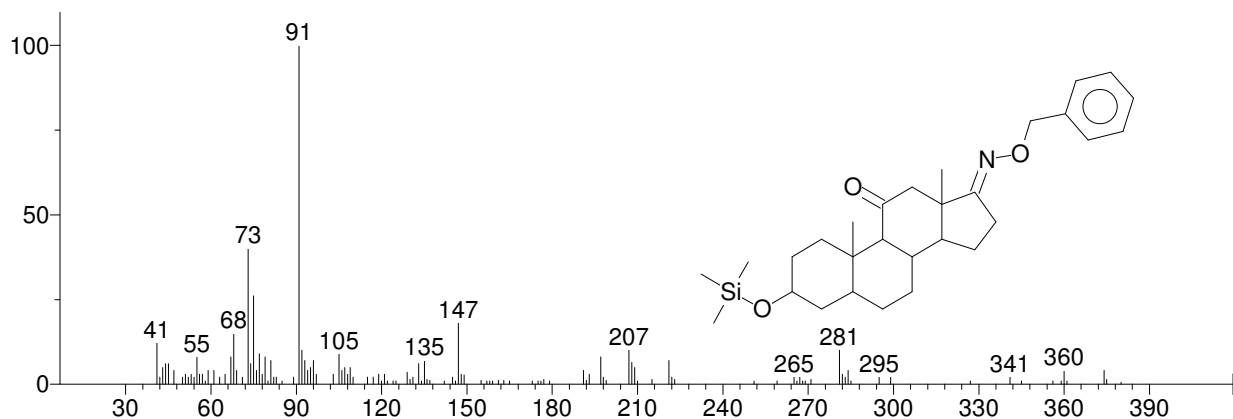
Hit 2 : 1,2-Dichlorobenzene-D4
C6Cl2D4; MF: 856; RMF: 870; Prob 19.7%; CAS: 2199-69-1; Lib: mainlib; ID: 111935.



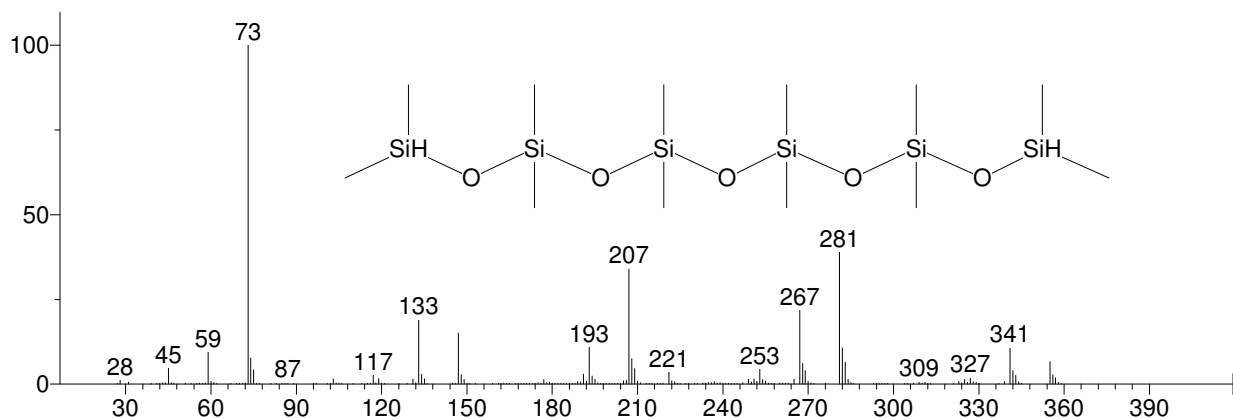
Unknown: Scan 3420 (20.423 min): Sample1.D\data.ms
Compound in Library Factor = -1558



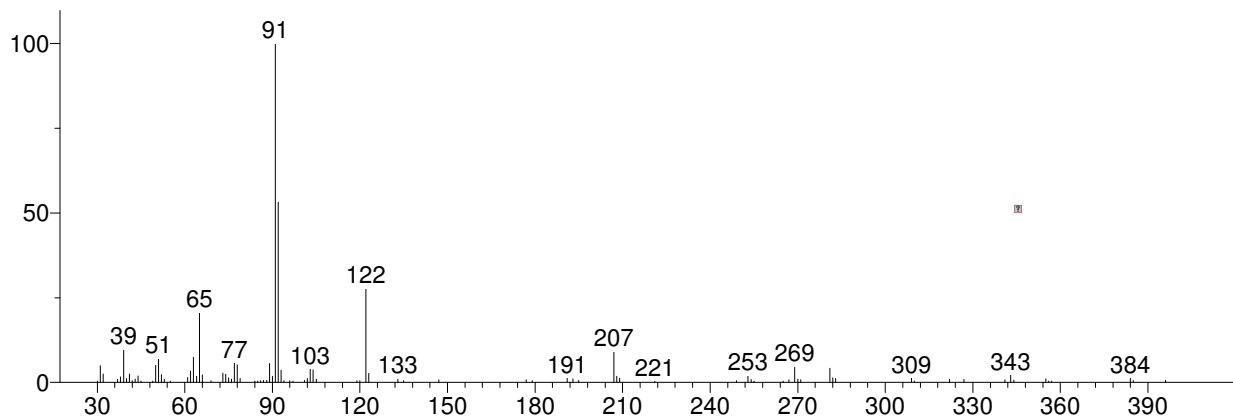
Hit 1 : Androstane-11,17-dione, 3-[(trimethylsilyl)oxy]-, 17-[O-(phenylmethyl)oxime], (3 α ,5 α)-
C₂₉H₄₃NO₃Si; MF: 493; RMF: 569; Prob 19.6%; CAS: 57305-11-0; Lib: mainlib; ID: 51252.



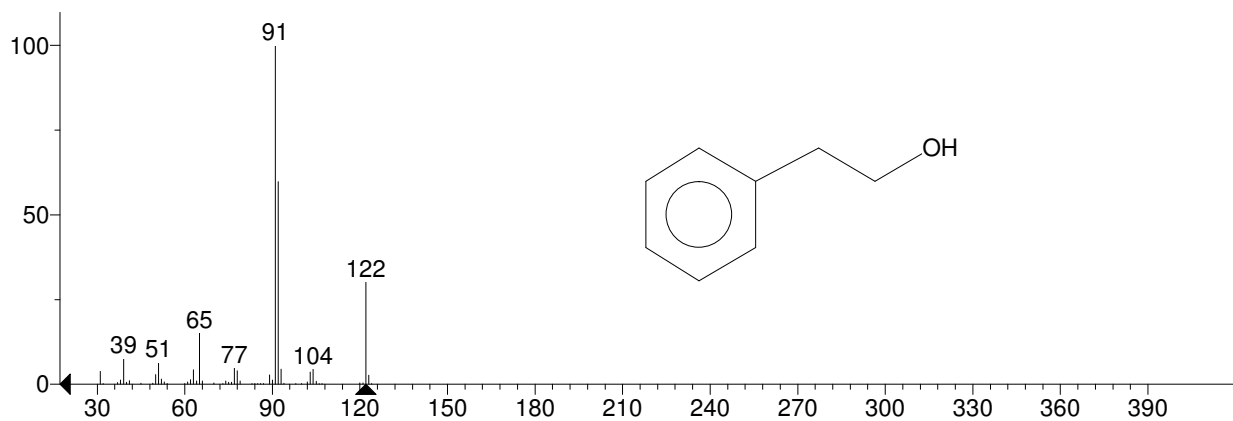
Hit 2 : Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
C₁₂H₃₈O₅Si₆; MF: 479; RMF: 563; Prob 12.2%; CAS: 995-82-4; Lib: mainlib; ID: 37488.



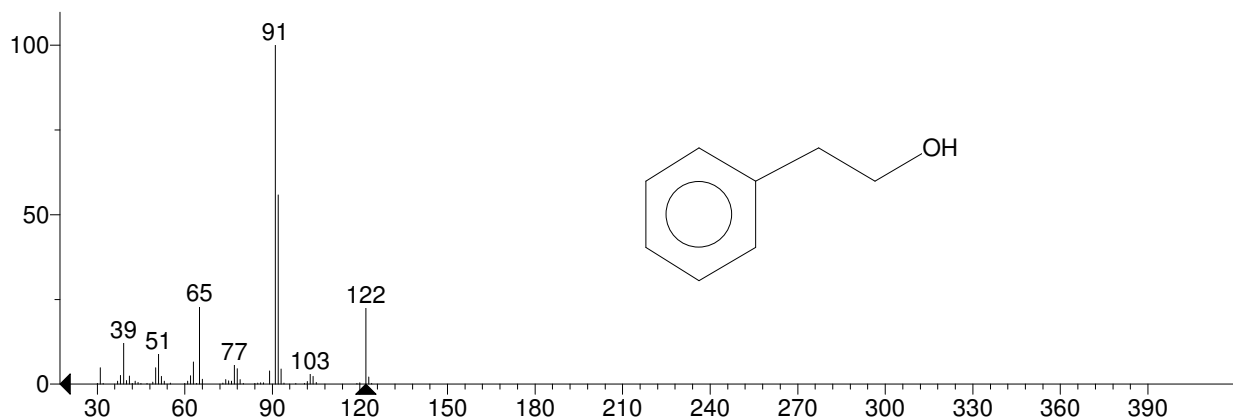
Unknown: Scan 3579 (21.368 min): Sample1.D\data.ms
Compound in Library Factor = -302



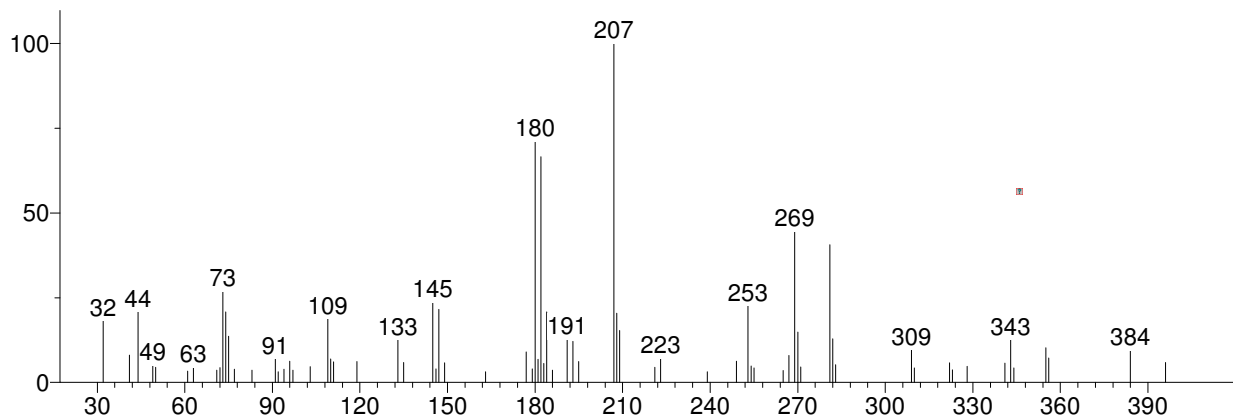
Hit 1 : Phenylethyl Alcohol
C₈H₁₀O; MF: 739; RMF: 914; Prob 59.9%; CAS: 60-12-8; Lib: replib; ID: 11425.



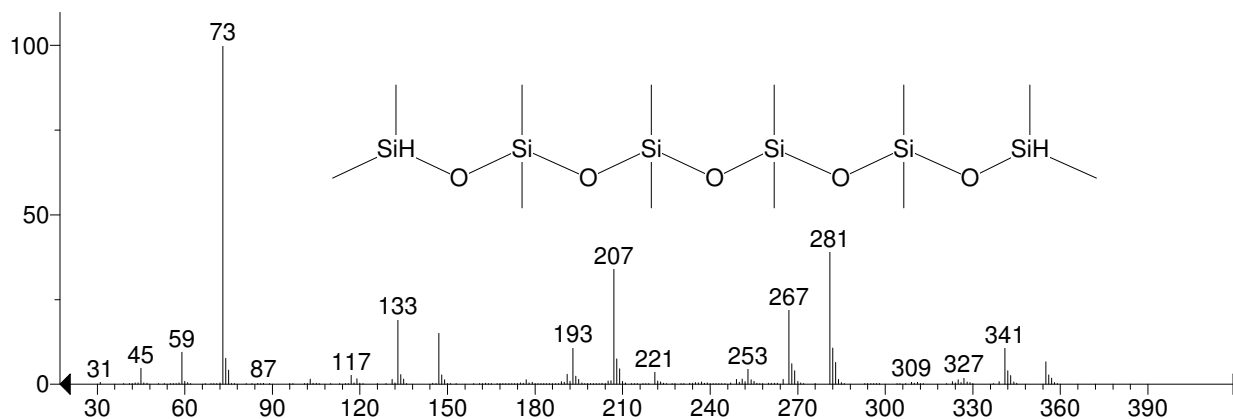
Hit 2 : Phenylethyl Alcohol
C₈H₁₀O; MF: 737; RMF: 919; Prob 59.9%; CAS: 60-12-8; Lib: mainlib; ID: 51691.



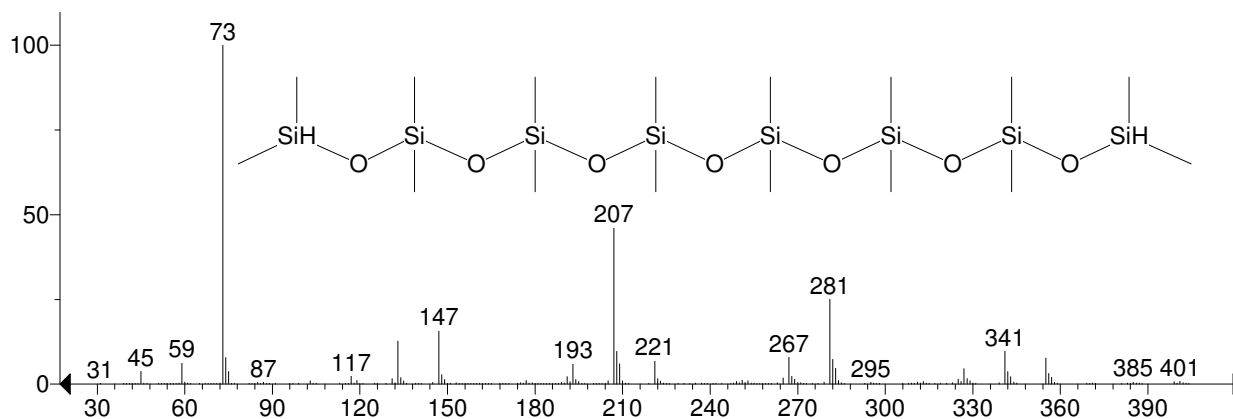
Unknown: Scan 3696 (22.064 min): Sample1.D\data.ms
Compound in Library Factor = -1558



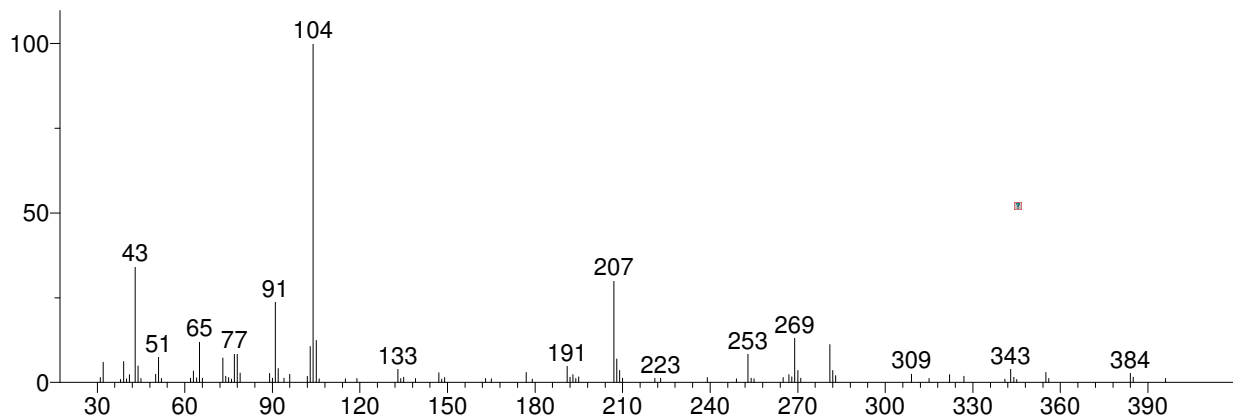
Hit 1 : Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
C12H38O5Si6; MF: 508; RMF: 567; Prob 30.4%; CAS: 995-82-4; Lib: mainlib; ID: 37488.



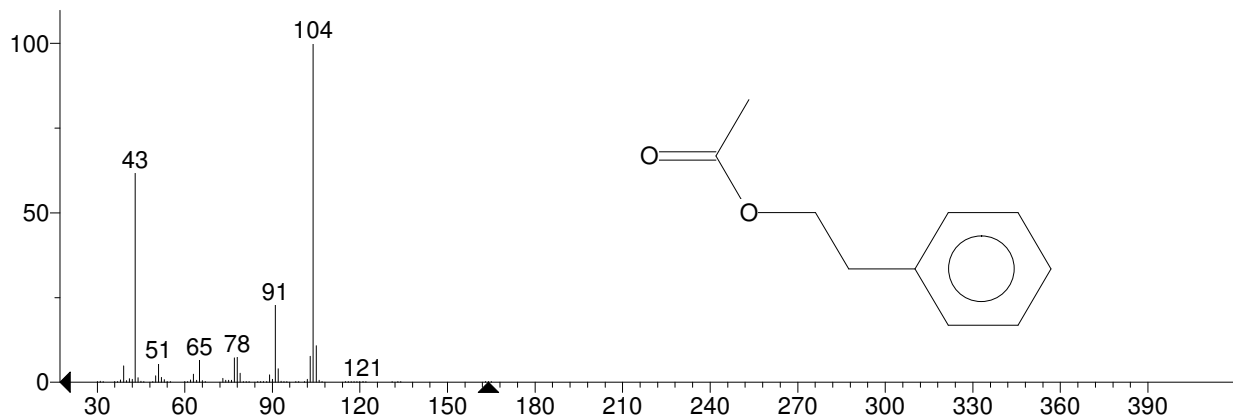
Hit 2 : Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
C16H50O7Si8; MF: 499; RMF: 555; Prob 22.1%; CAS: 19095-24-0; Lib: mainlib; ID: 37082.



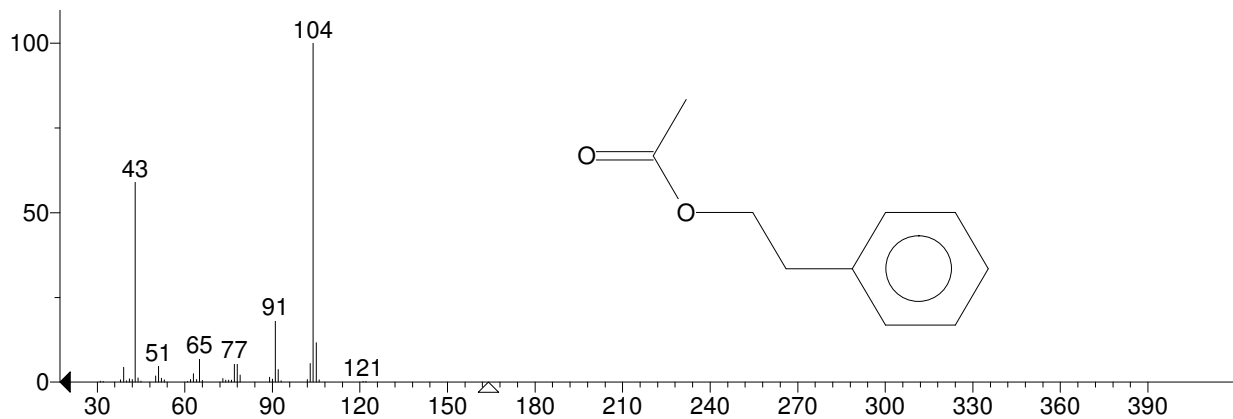
Unknown: Scan 3835 (22.890 min): Sample1.D\data.ms
Compound in Library Factor = -1014



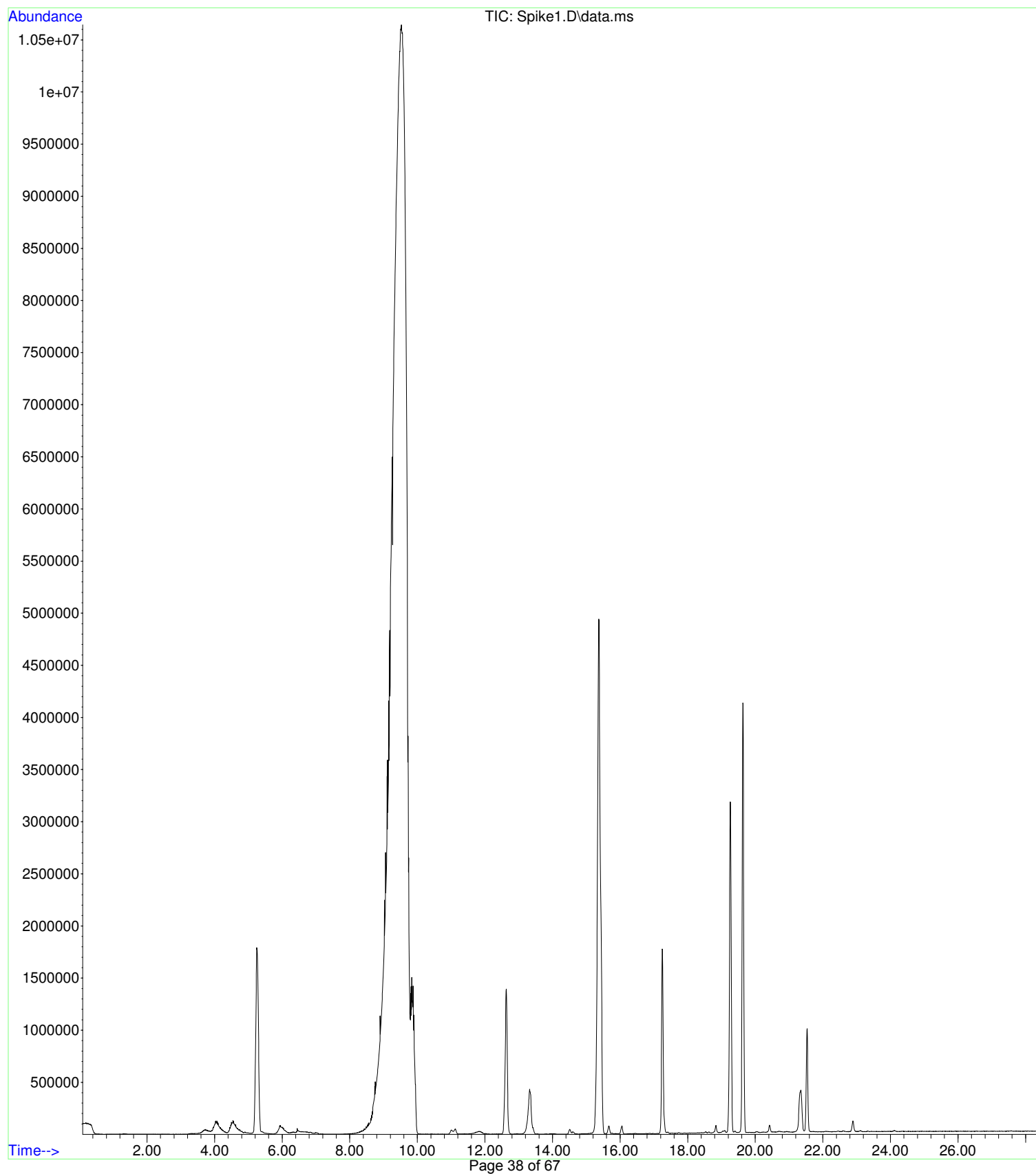
Hit 1 : Acetic acid, 2-phenylethyl ester
C₁₀H₁₂O₂; MF: 575; RMF: 903; Prob 21.3%; CAS: 103-45-7; Lib: replib; ID: 13444.



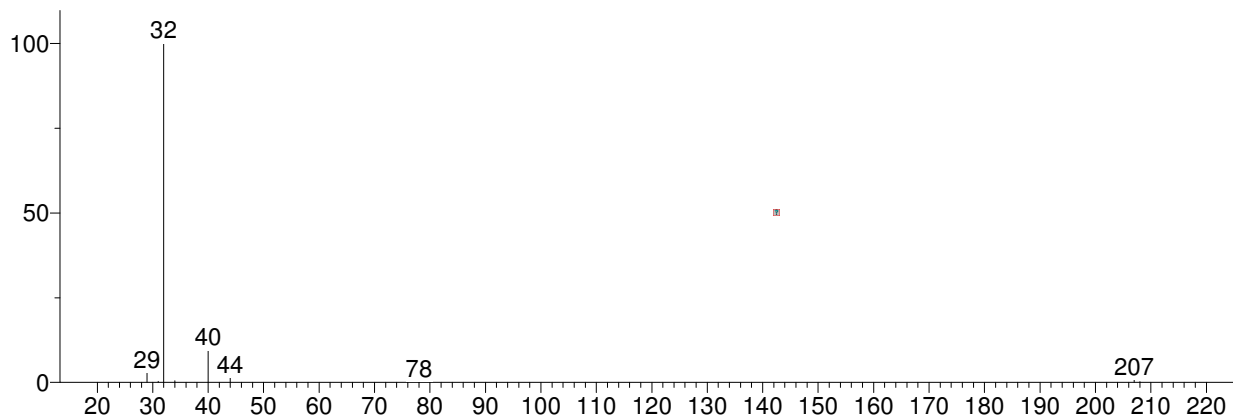
Hit 2 : Acetic acid, 2-phenylethyl ester
C₁₀H₁₂O₂; MF: 573; RMF: 889; Prob 21.3%; CAS: 103-45-7; Lib: mainlib; ID: 65178.



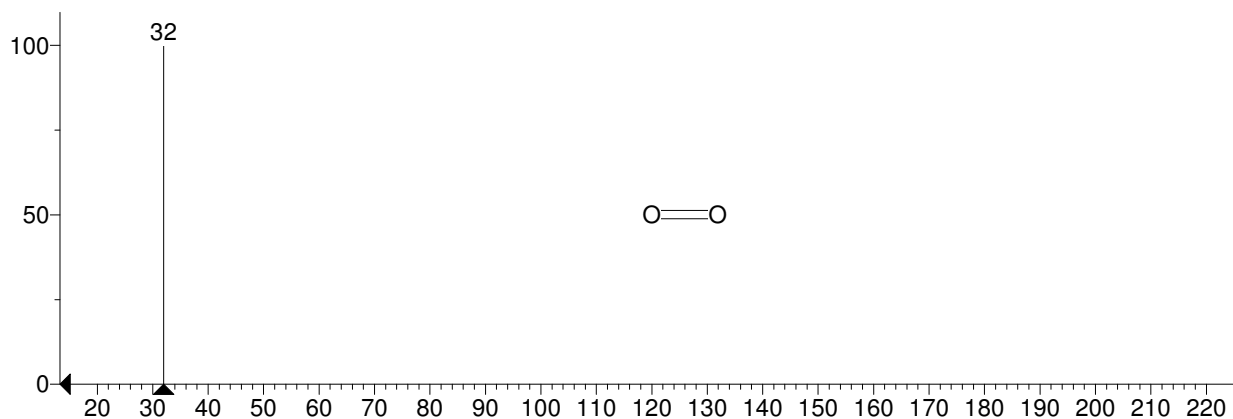
File :D:\msdchem\1\data\2014\J8675 DHS Beer\080314\Spike1.D
Operator : Oliver Palardy
Acquired : 5 Aug 2014 6:04 using AcqMethod DHSBeer_Sample.M
Instrument : 7890
Sample Name: Beer sample, spiked at 10ppm
Misc Info :
Vial Number: 25



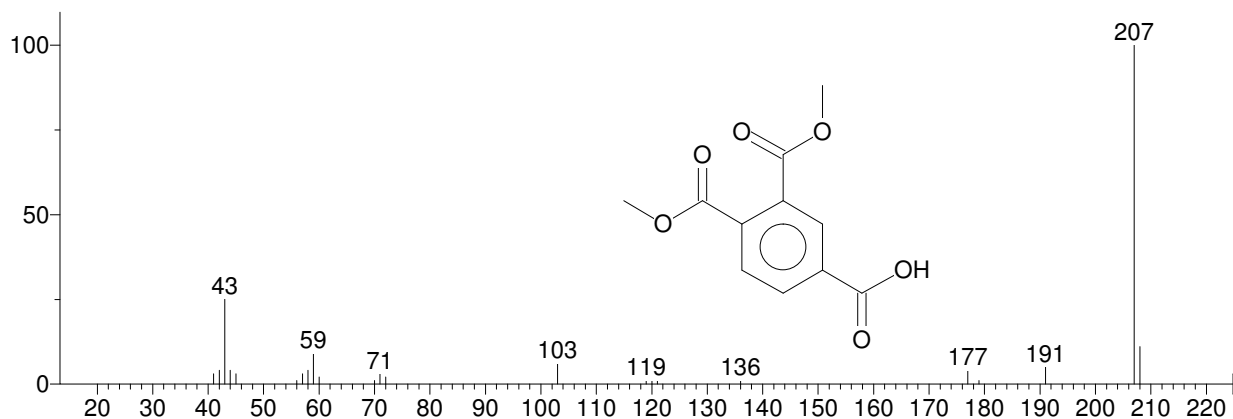
Unknown: Scan 17 (0.189 min): Spike1.D\data.ms
Compound in Library Factor = 137



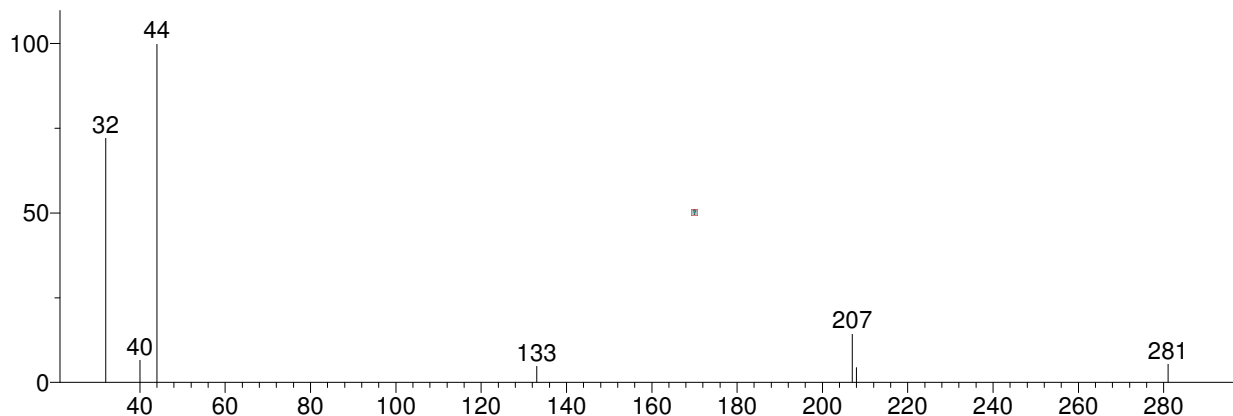
Hit 1 : Oxygen
O₂; MF: 826; RMF: 999; Prob 96.0%; CAS: 7782-44-7; Lib: mainlib; ID: 1449.



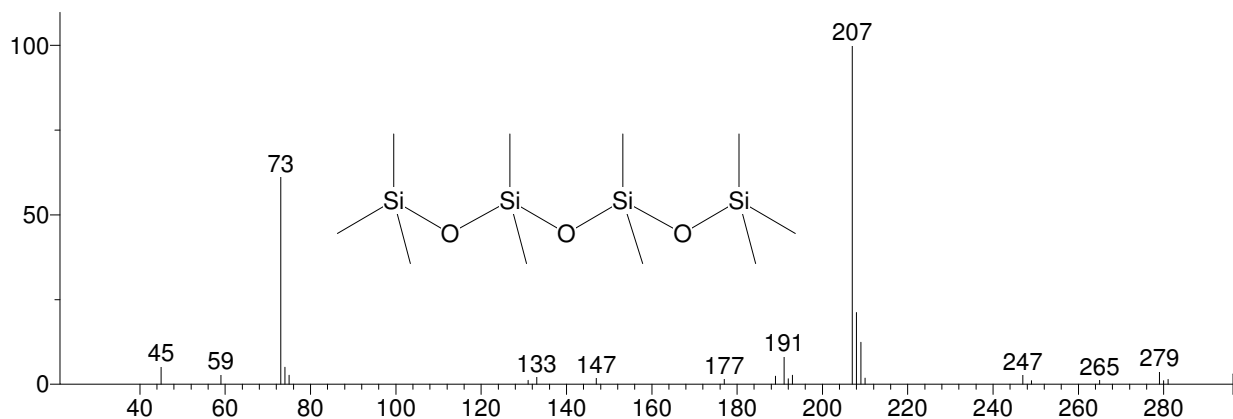
Hit 2 : 1,2,4-Benzenetricarboxylic acid, 1,2-dimethyl ester
C₁₁H₁₀O₆; MF: 692; RMF: 692; Prob 3.71%; CAS: 54699-35-3; Lib: mainlib; ID: 148837.



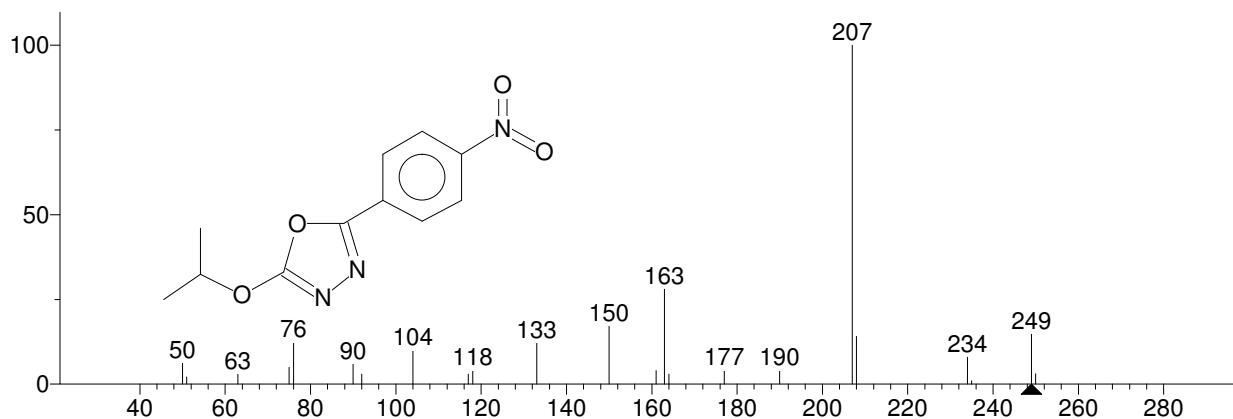
Unknown: Scan 203 (1.294 min): Spike1.D\data.ms
Compound in Library Factor = -817



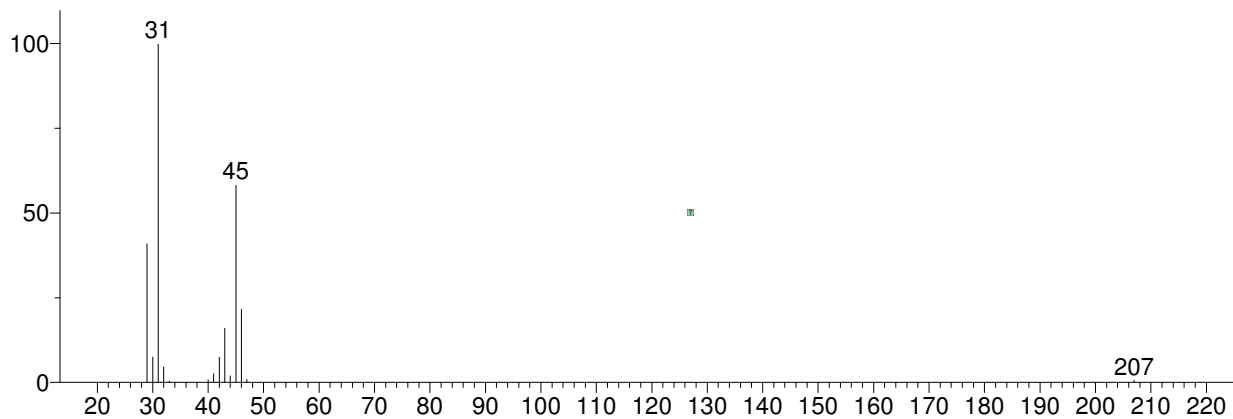
Hit 1 : Tetrasiloxane, decamethyl-
C₁₀H₃₀O₃Si₄; MF: 480; RMF: 480; Prob 39.5%; CAS: 141-62-8; Lib: replib; ID: 24667.



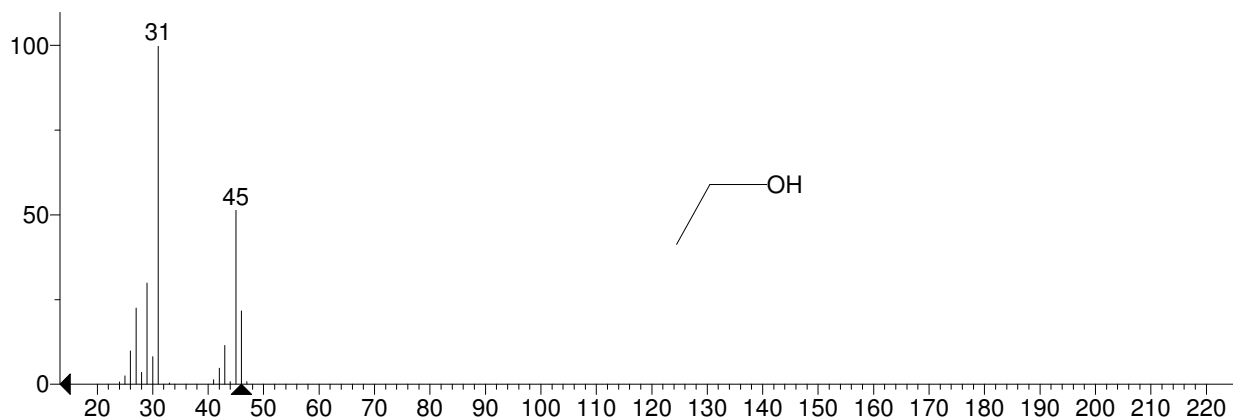
Hit 2 : 2-p-Nitrophenyl-5-isopropoxy-oxadiazole-1,3,4
C₁₁H₁₁N₃O₄; MF: 468; RMF: 567; Prob 26.3%; CAS: 41125-94-4; Lib: mainlib; ID: 149003.



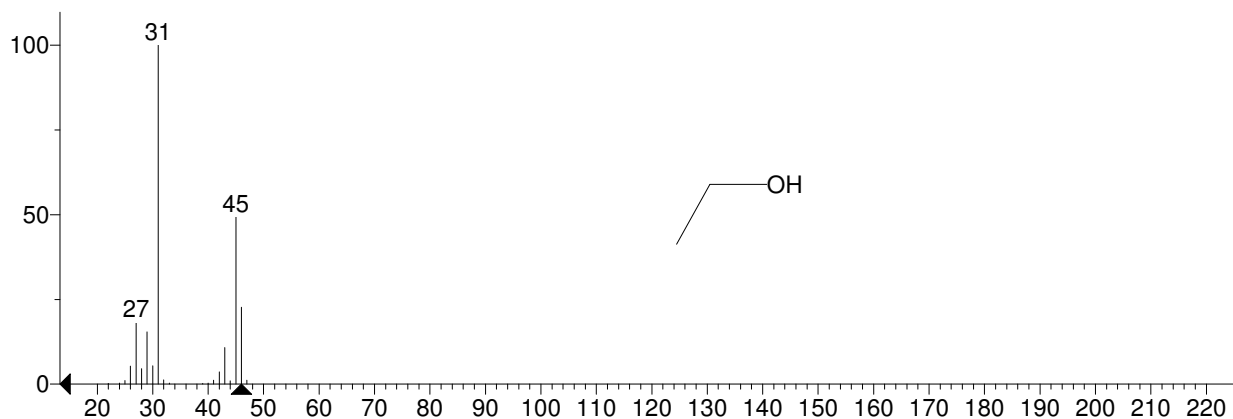
Unknown: Scan 749 (4.541 min): Spike1.D\data.ms
Compound in Library Factor = 447



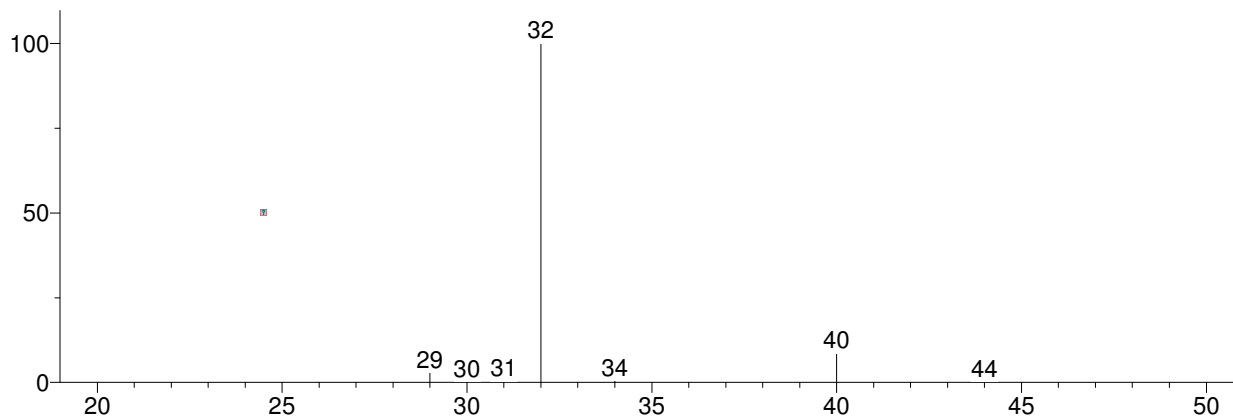
Hit 1 : Ethanol
C₂H₆O; MF: 919; RMF: 937; Prob 96.3%; CAS: 64-17-5; Lib: mainlib; ID: 1370.



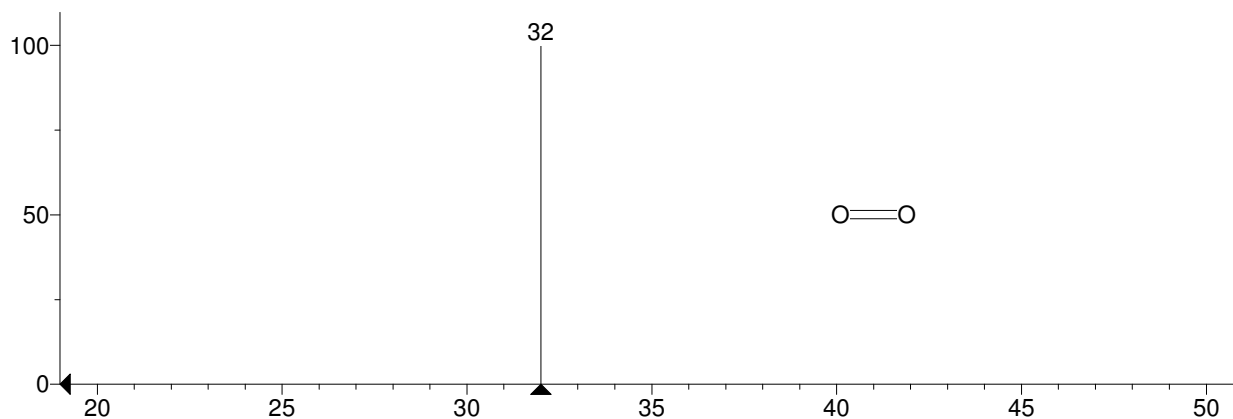
Hit 2 : Ethanol
C₂H₆O; MF: 880; RMF: 887; Prob 96.3%; CAS: 64-17-5; Lib: replib; ID: 572.



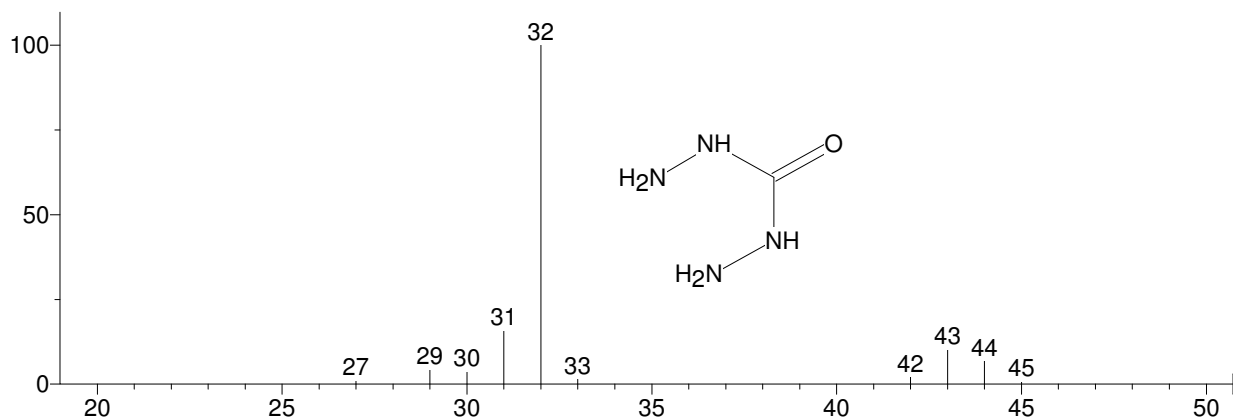
Unknown: Scan 868 (5.249 min): Spike1.D\data.ms
Compound in Library Factor = 759



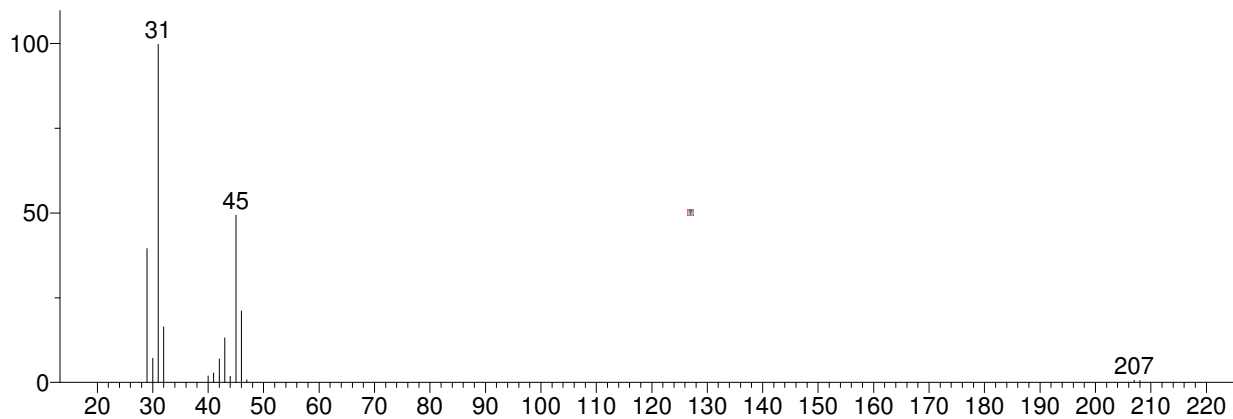
Hit 1 : Oxygen
O₂; MF: 880; RMF: 999; Prob 97.5%; CAS: 7782-44-7; Lib: mainlib; ID: 1449.



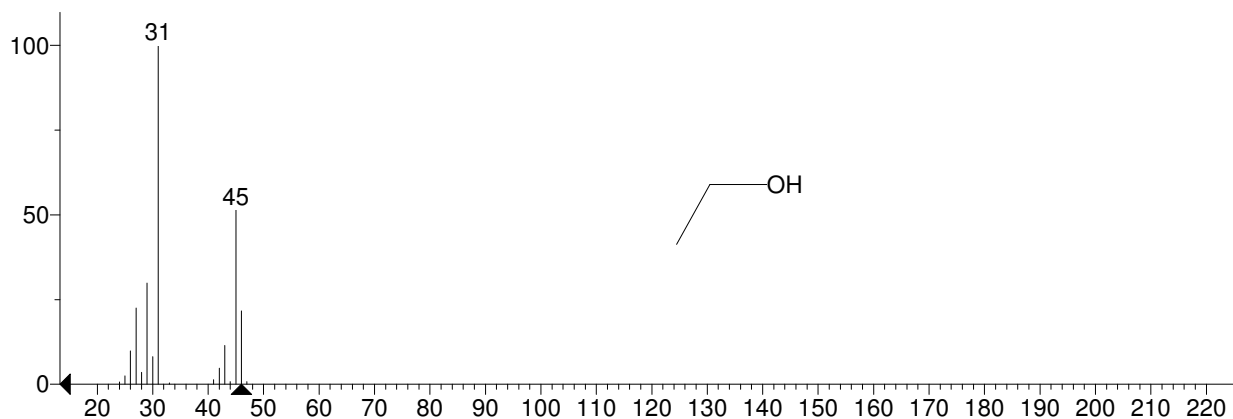
Hit 2 : Carbonic dihydrazide
CH₆N₄O; MF: 474; RMF: 511; Prob 0.97%; CAS: 497-18-7; Lib: replib; ID: 616.



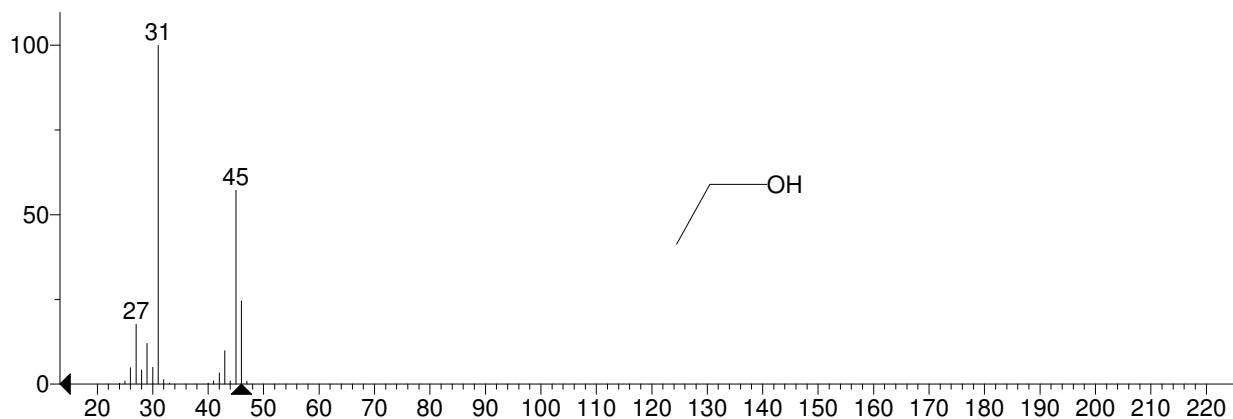
Unknown: Scan 986 (5.950 min): Spike1.D\data.ms
Compound in Library Factor = 232



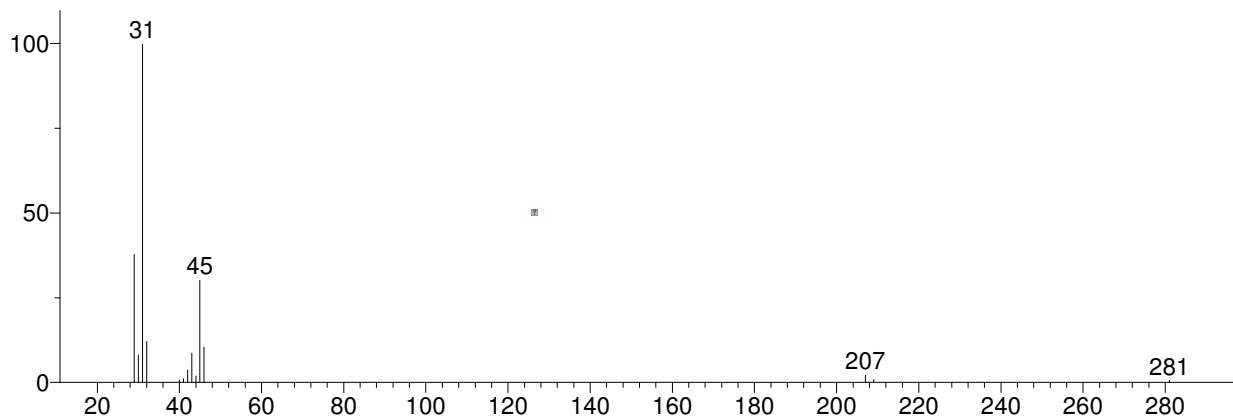
Hit 1 : Ethanol
C₂H₆O; MF: 877; RMF: 927; Prob 94.0%; CAS: 64-17-5; Lib: mainlib; ID: 1370.



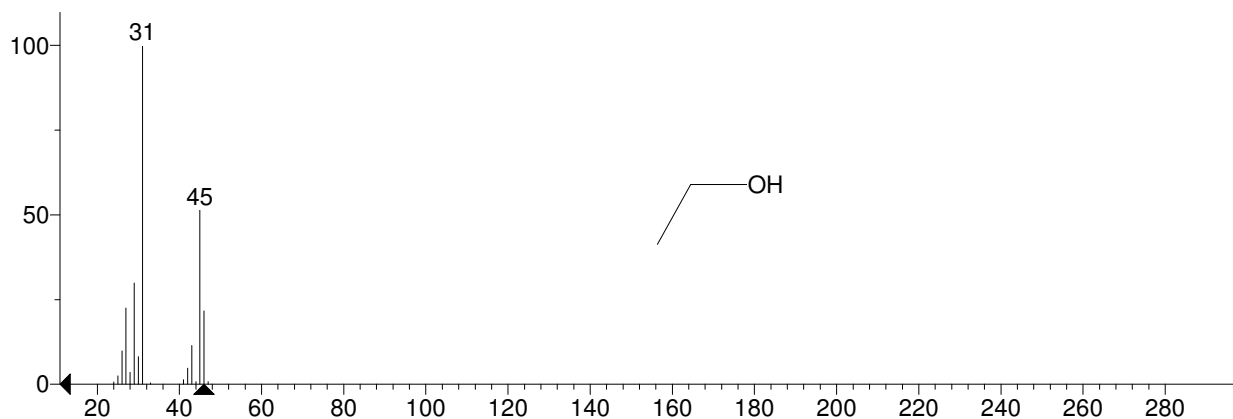
Hit 2 : Ethanol
C₂H₆O; MF: 843; RMF: 858; Prob 94.0%; CAS: 64-17-5; Lib: replib; ID: 573.



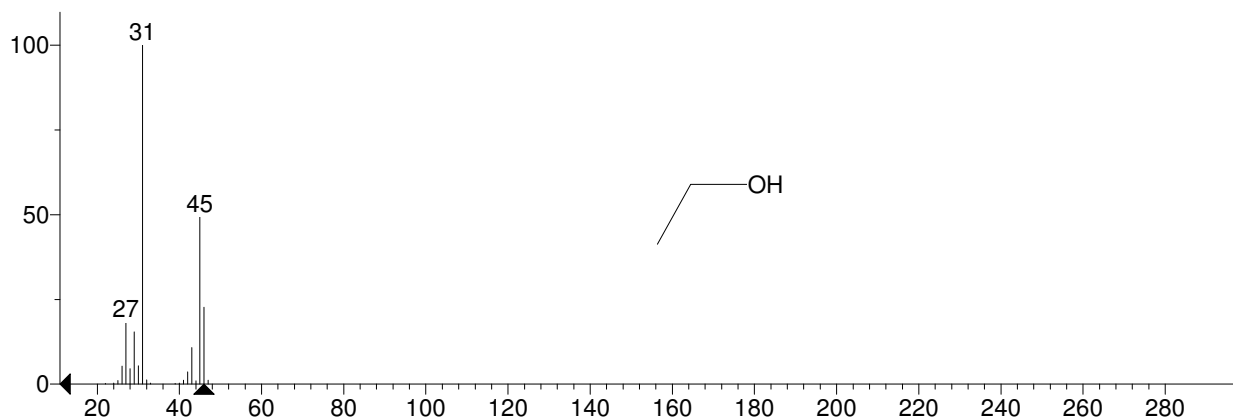
Unknown: Scan 1069 (6.444 min): Spike1.D\data.ms
Compound in Library Factor = -183



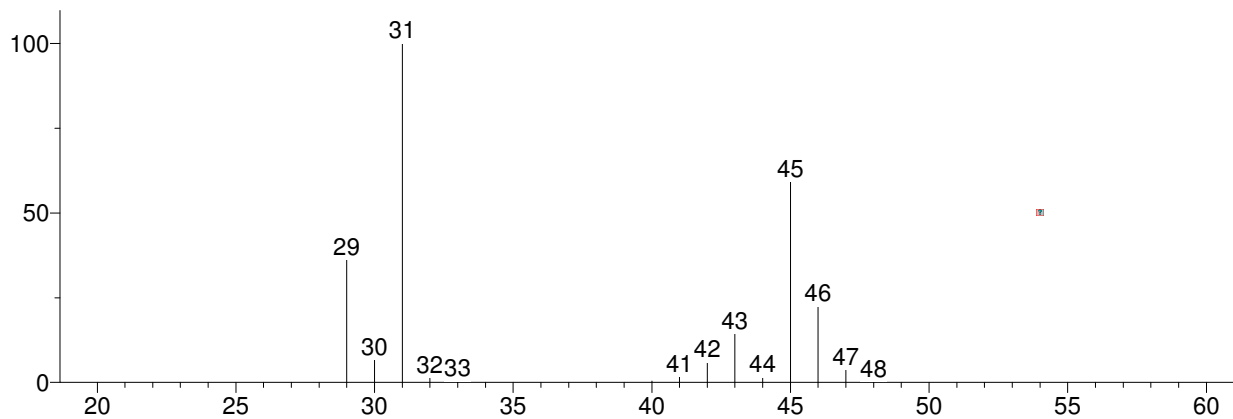
Hit 1 : Ethanol
C₂H₆O; MF: 819; RMF: 900; Prob 81.6%; CAS: 64-17-5; Lib: mainlib; ID: 1370.



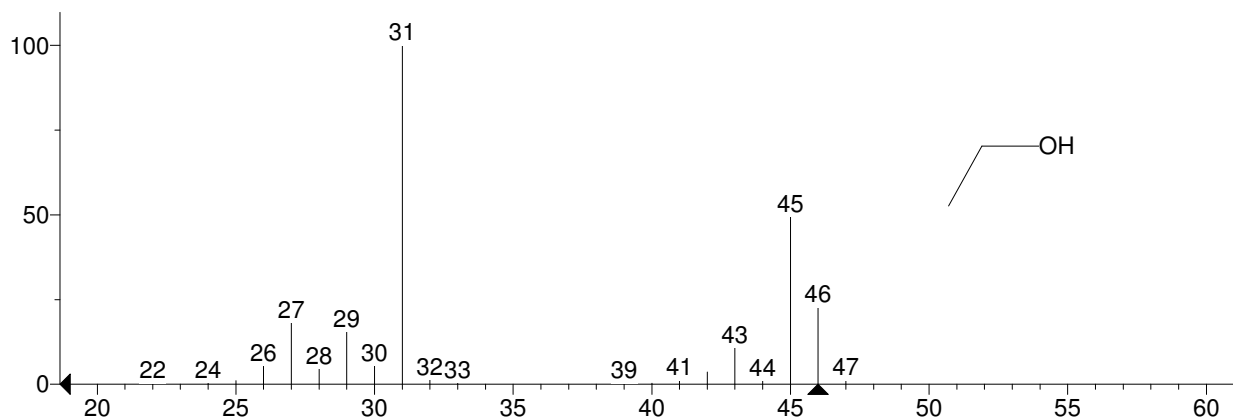
Hit 2 : Ethanol
C₂H₆O; MF: 777; RMF: 826; Prob 81.6%; CAS: 64-17-5; Lib: replib; ID: 572.



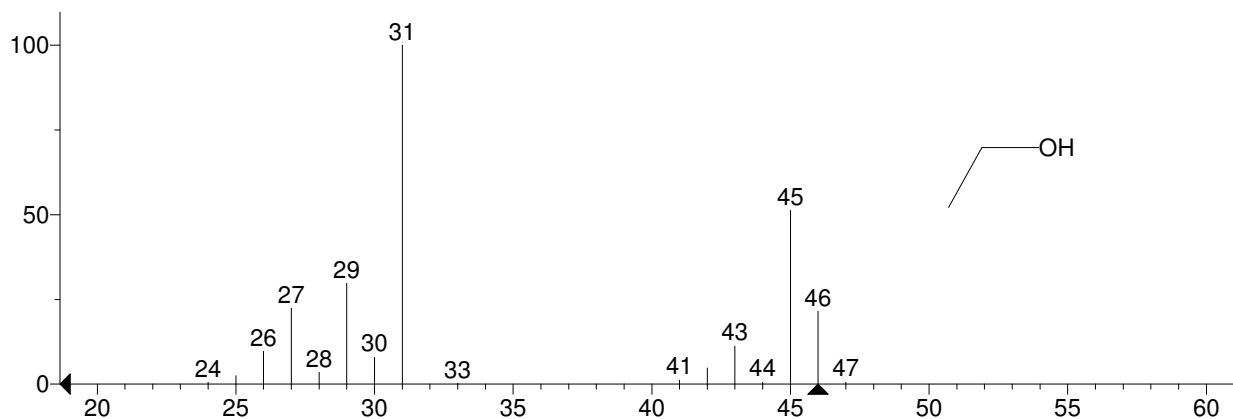
Unknown: Scan 1588 (9.530 min): Spike1.D\data.ms
Compound in Library Factor = 475



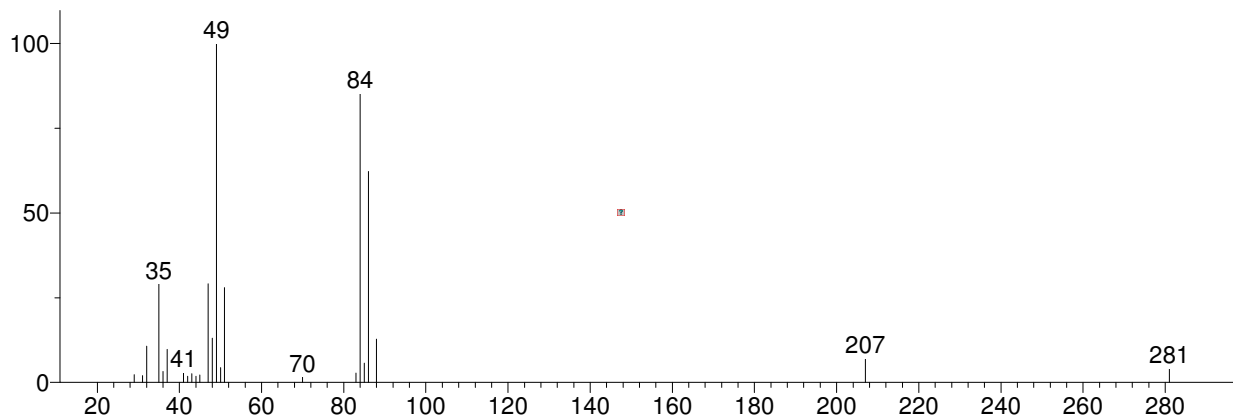
Hit 1 : Ethanol
C2H6O; MF: 929; RMF: 929; Prob 93.8%; CAS: 64-17-5; Lib: replib; ID: 572.



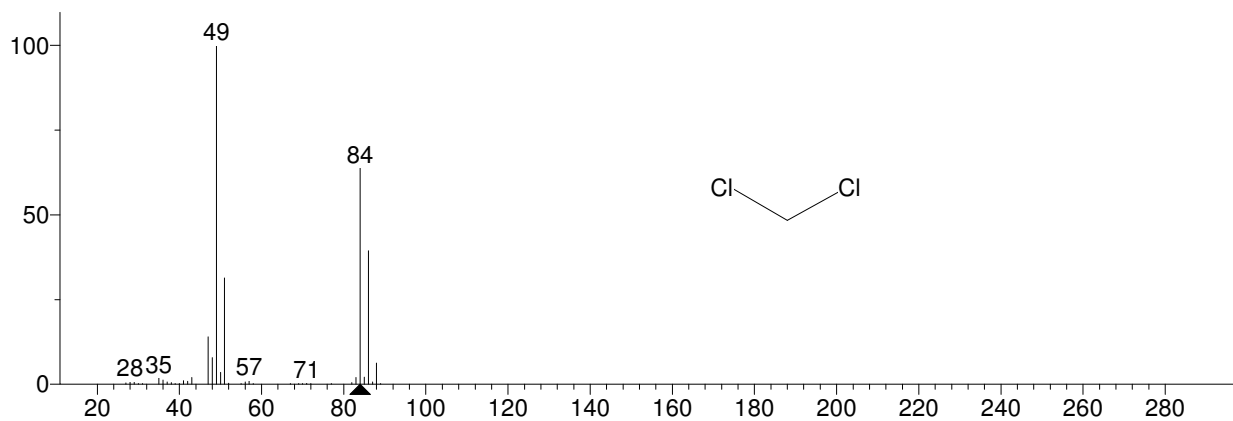
Hit 2 : Ethanol
C2H6O; MF: 918; RMF: 921; Prob 93.8%; CAS: 64-17-5; Lib: mainlib; ID: 1370.



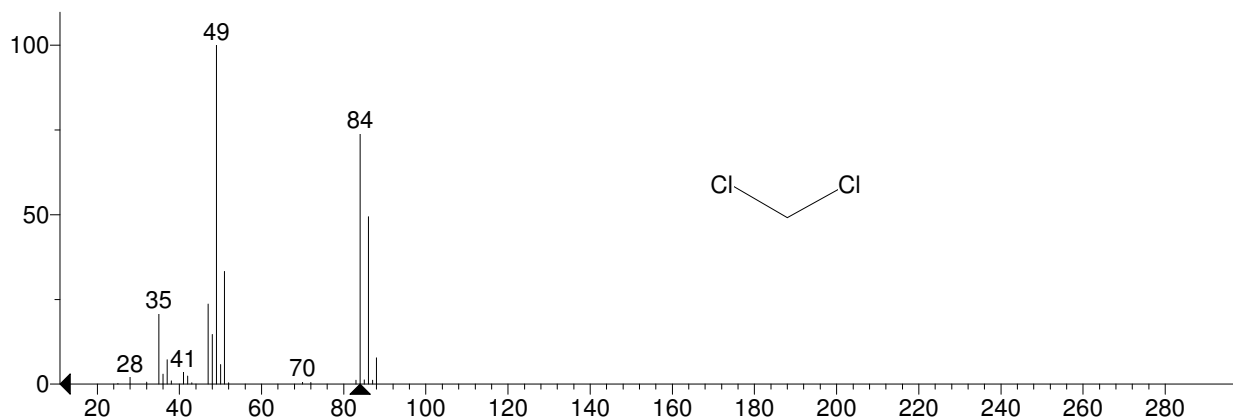
Unknown: Scan 1837 (11.010 min): Spike1.D\data.ms
Compound in Library Factor = 134



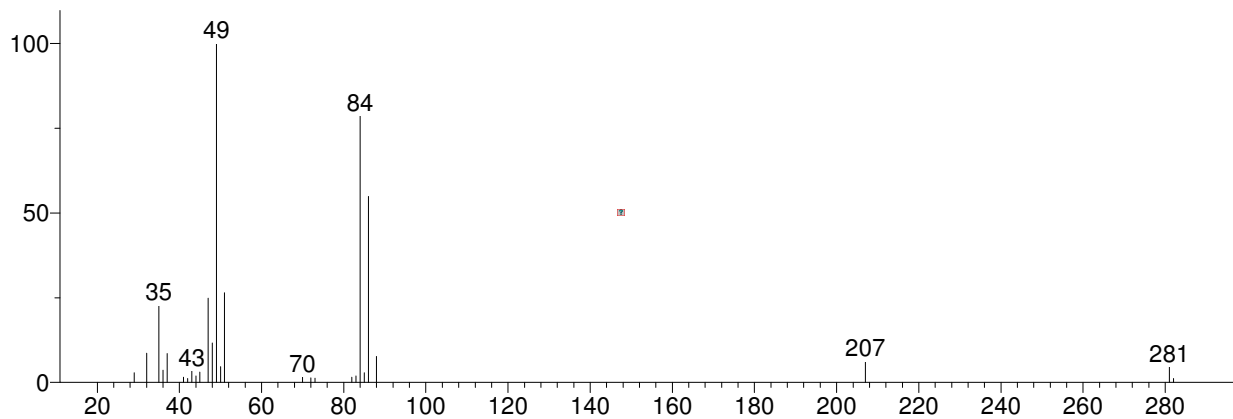
Hit 1 : Methylene Chloride
CH2Cl2; MF: 812; RMF: 877; Prob 96.6%; CAS: 75-09-2; Lib: replib; ID: 3893.



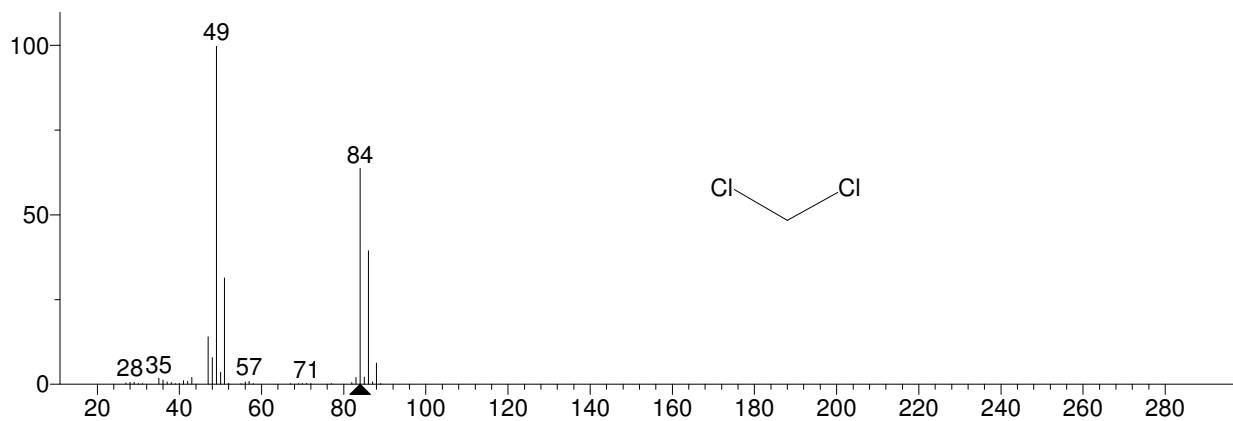
Hit 2 : Methylene Chloride
CH2Cl2; MF: 801; RMF: 860; Prob 96.6%; CAS: 75-09-2; Lib: replib; ID: 3894.



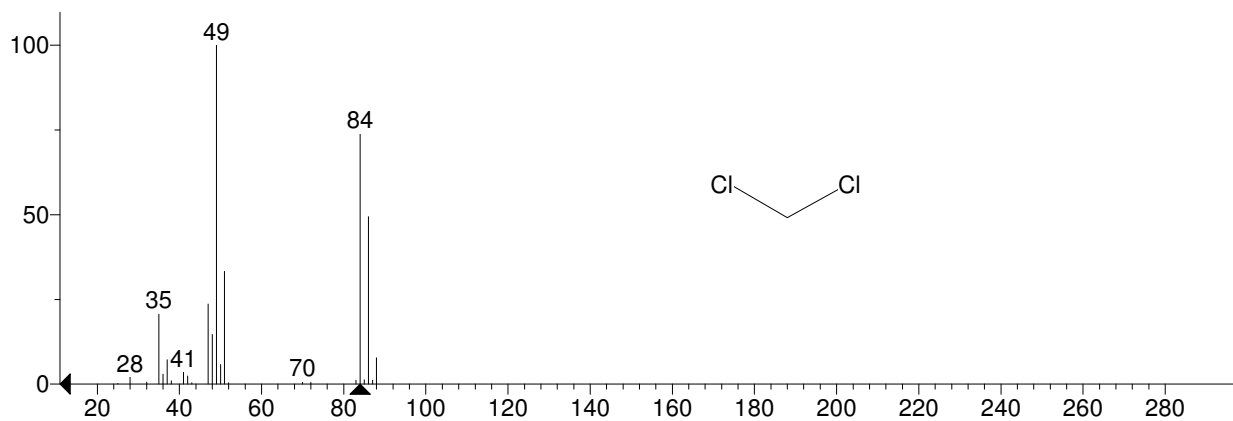
Unknown: Scan 1855 (11.117 min): Spike1.D\data.ms
Compound in Library Factor = 134



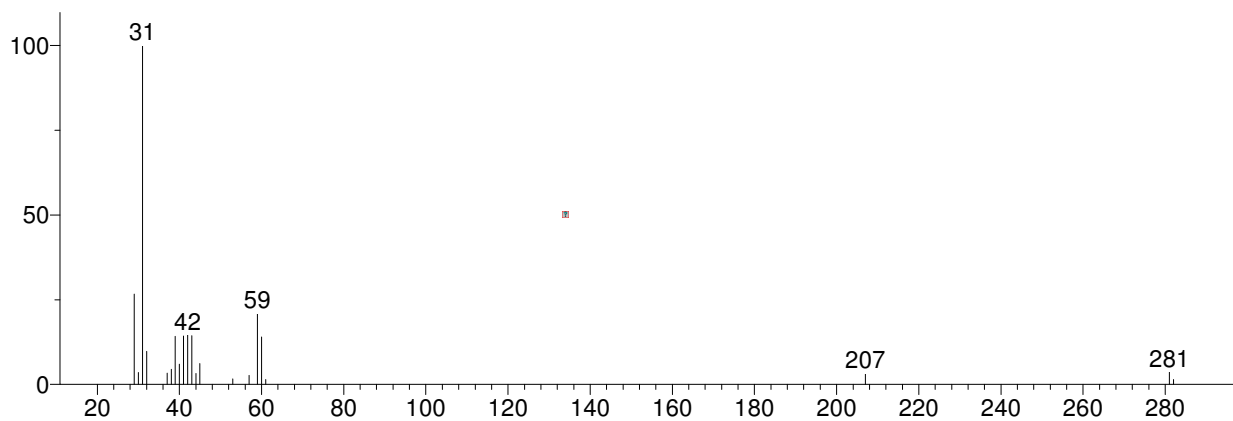
Hit 1 : Methylene Chloride
CH2Cl2; MF: 817; RMF: 896; Prob 96.9%; CAS: 75-09-2; Lib: replib; ID: 3893.



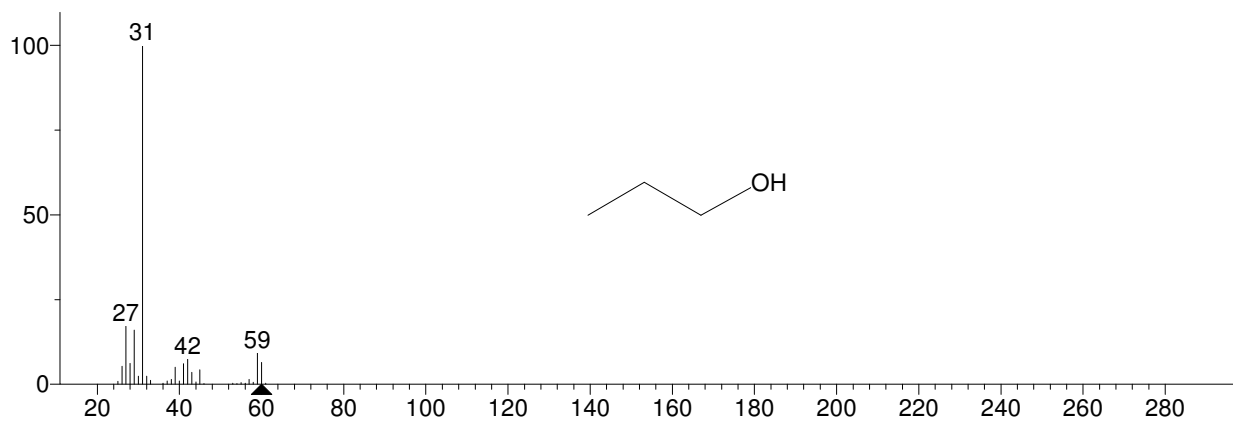
Hit 2 : Methylene Chloride
CH2Cl2; MF: 817; RMF: 892; Prob 96.9%; CAS: 75-09-2; Lib: replib; ID: 3894.



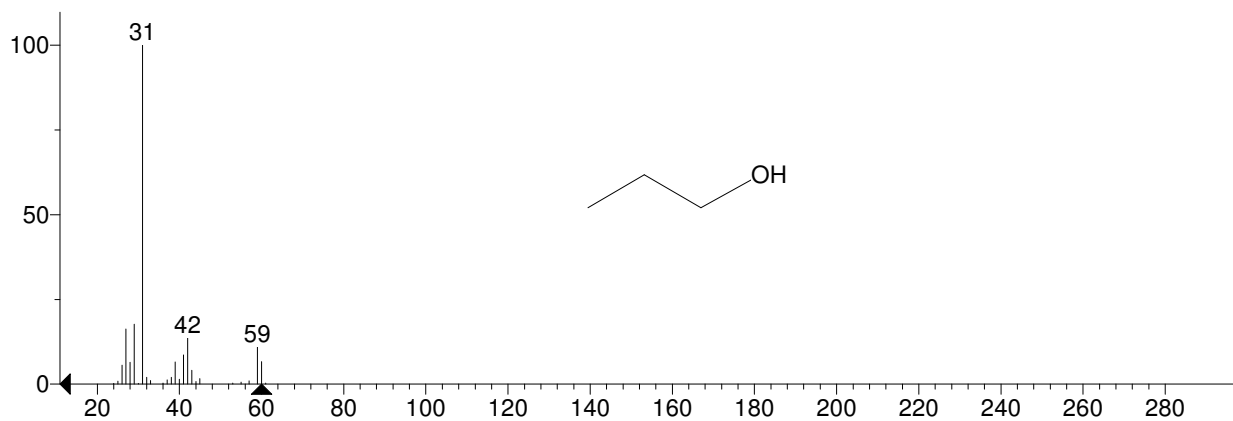
Unknown: Scan 1978 (11.849 min): Spike1.D\data.ms
Compound in Library Factor = -298



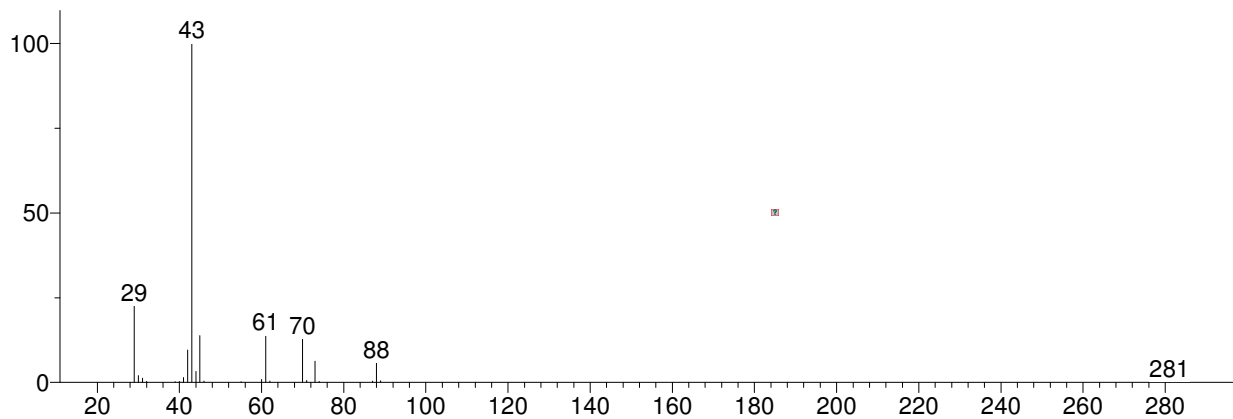
Hit 1 : 1-Propanol
C₃H₈O; MF: 750; RMF: 838; Prob 83.5%; CAS: 71-23-8; Lib: replib; ID: 540.



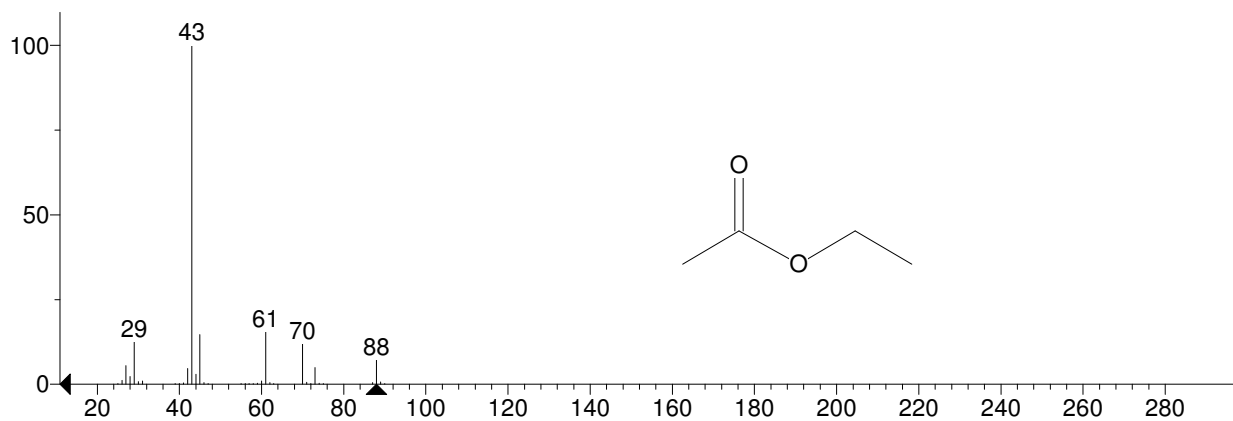
Hit 2 : 1-Propanol
C₃H₈O; MF: 742; RMF: 828; Prob 83.5%; CAS: 71-23-8; Lib: mainlib; ID: 1319.



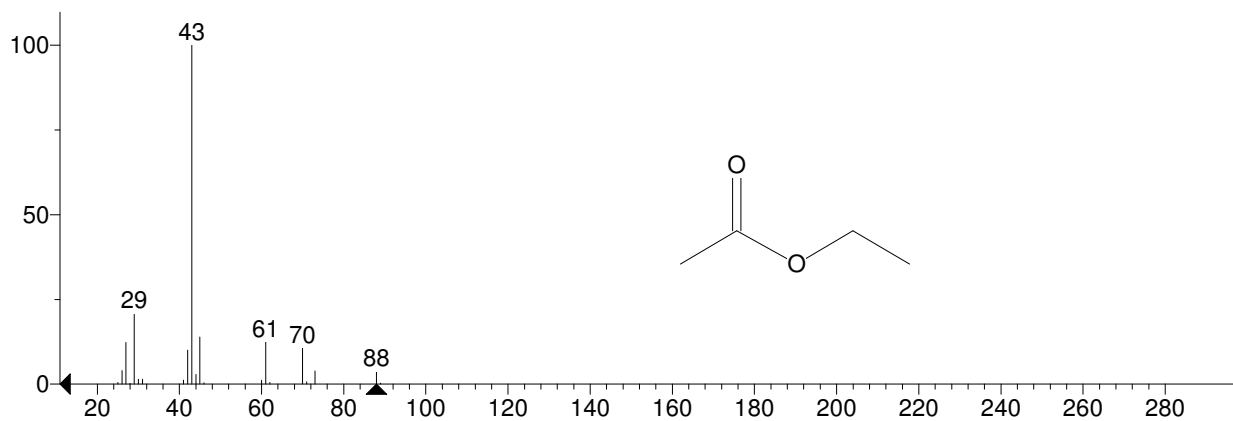
Unknown: Scan 2110 (12.633 min): Spike1.D\data.ms
Compound in Library Factor = 327



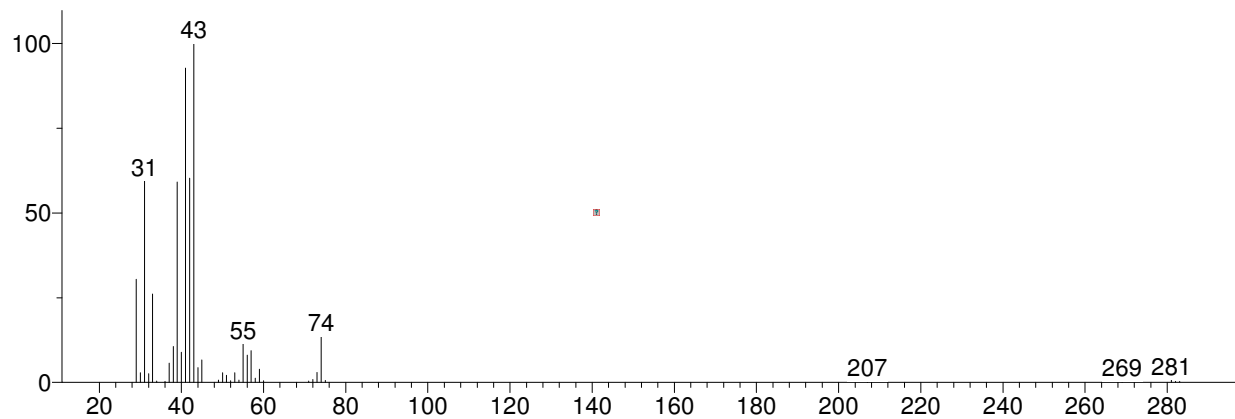
Hit 1 : Ethyl Acetate
C₄H₈O₂; MF: 934; RMF: 934; Prob 92.9%; CAS: 141-78-6; Lib: mainlib; ID: 7691.



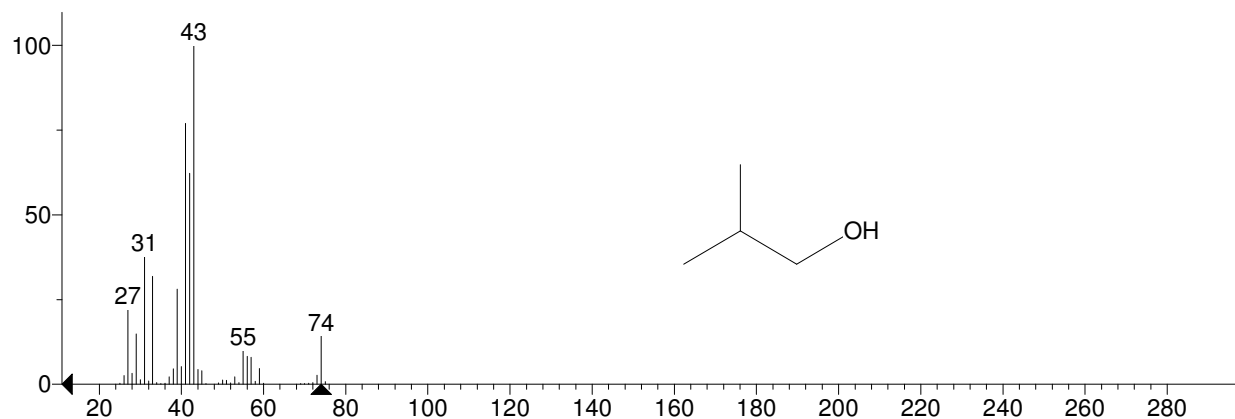
Hit 2 : Ethyl Acetate
C₄H₈O₂; MF: 927; RMF: 931; Prob 92.9%; CAS: 141-78-6; Lib: replib; ID: 1575.



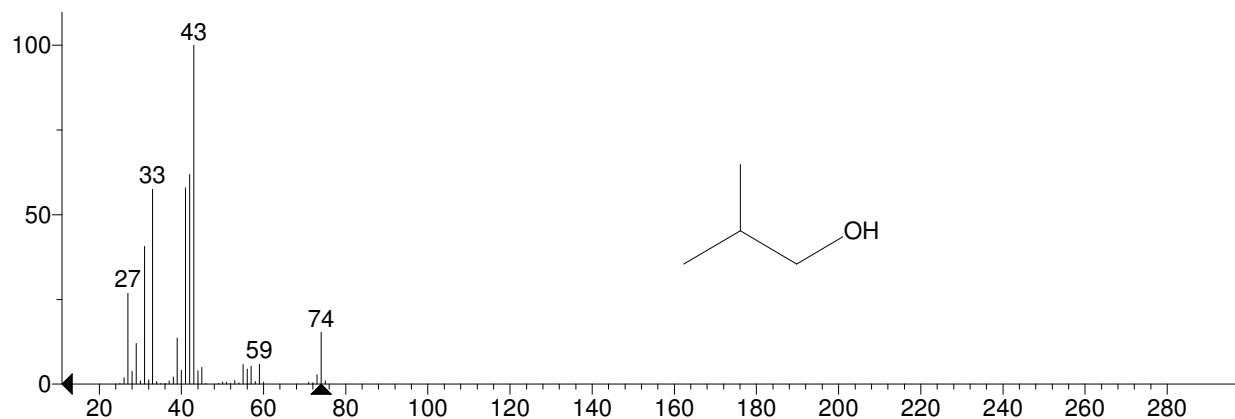
Unknown: Scan 2226 (13.323 min): Spike1.D\data.ms
Compound in Library Factor = 447



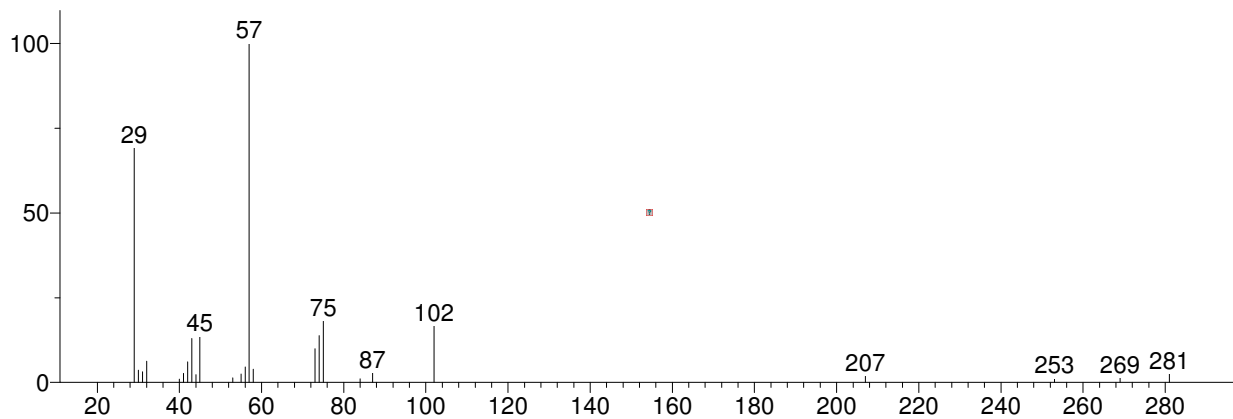
Hit 1 : 1-Propanol, 2-methyl-
C₄H₁₀O; MF: 913; RMF: 921; Prob 92.3%; CAS: 78-83-1; Lib: mainlib; ID: 5486.



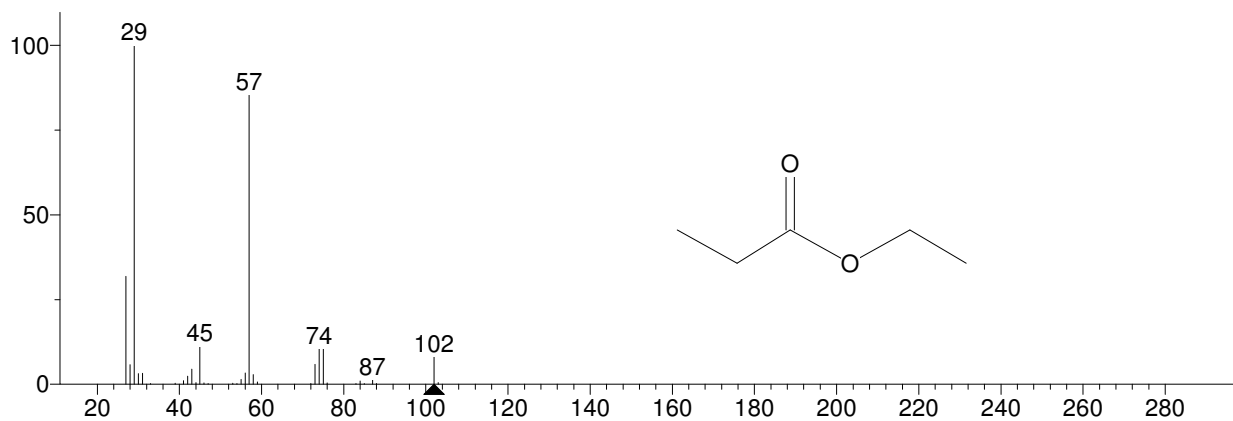
Hit 2 : 1-Propanol, 2-methyl-
C₄H₁₀O; MF: 863; RMF: 871; Prob 92.3%; CAS: 78-83-1; Lib: replib; ID: 1819.



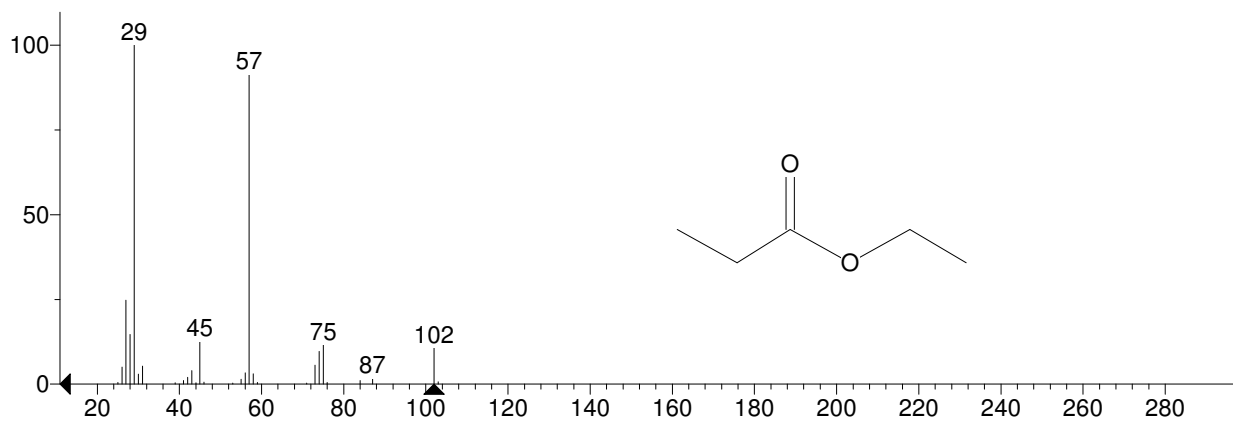
Unknown: Scan 2425 (14.506 min): Spike1.D\data.ms
Compound in Library Factor = 166



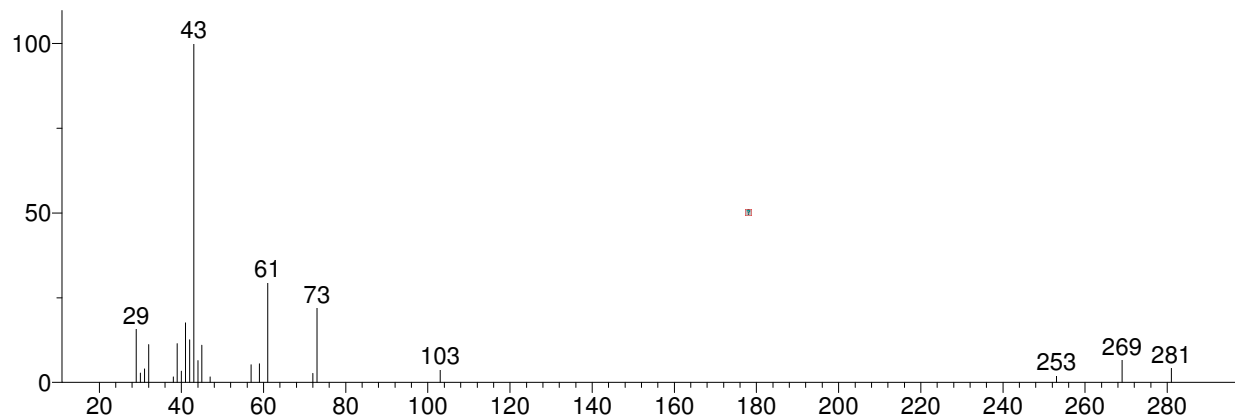
Hit 1 : Propanoic acid, ethyl ester
C5H10O2; MF: 841; RMF: 903; Prob 91.0%; CAS: 105-37-3; Lib: replib; ID: 201.



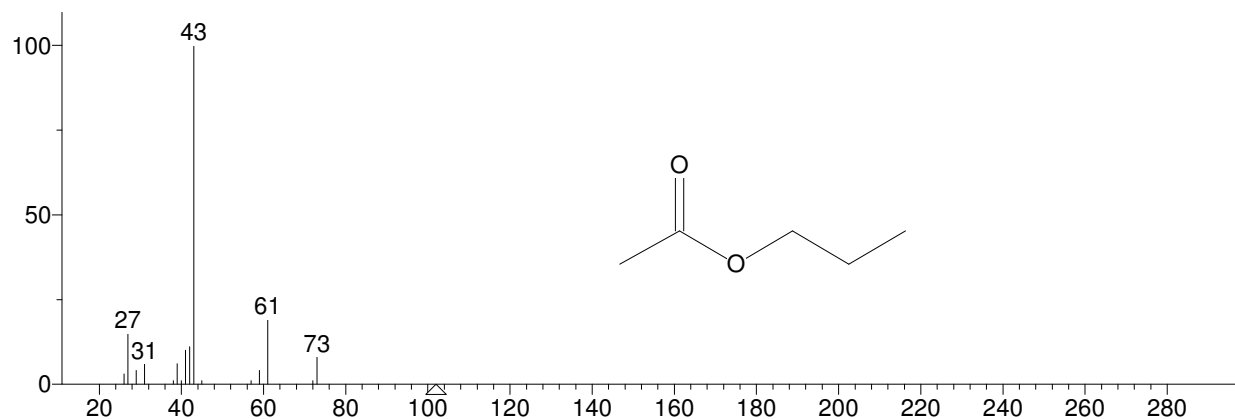
Hit 2 : Propanoic acid, ethyl ester
C5H10O2; MF: 835; RMF: 897; Prob 91.0%; CAS: 105-37-3; Lib: replib; ID: 202.



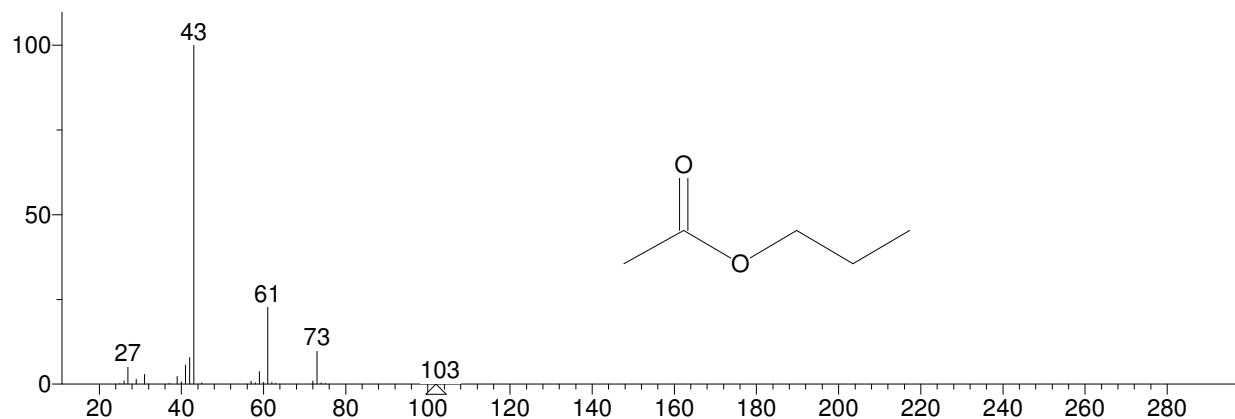
Unknown: Scan 2440 (14.596 min): Spike1.D\data.ms
Compound in Library Factor = -233



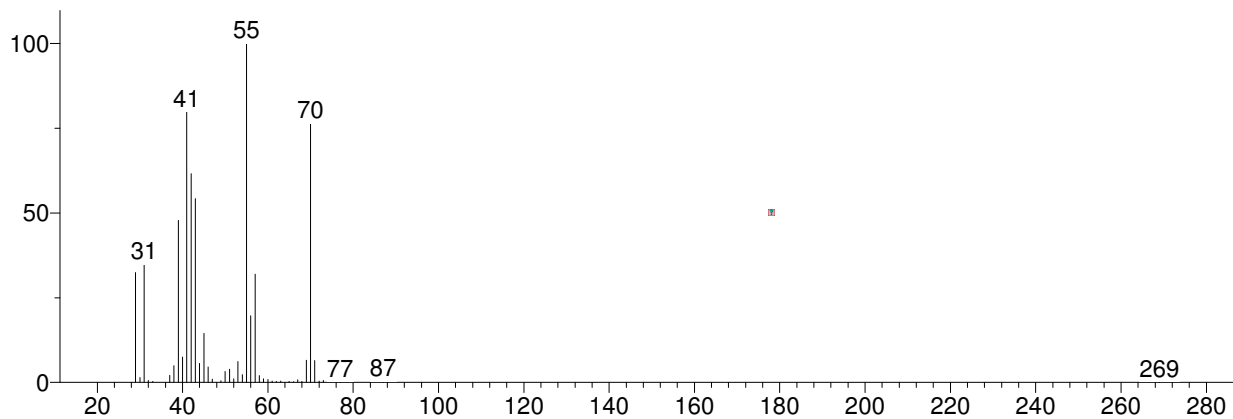
Hit 1 : n-Propyl acetate
C5H10O2; MF: 727; RMF: 891; Prob 68.5%; CAS: 109-60-4; Lib: replib; ID: 2272.



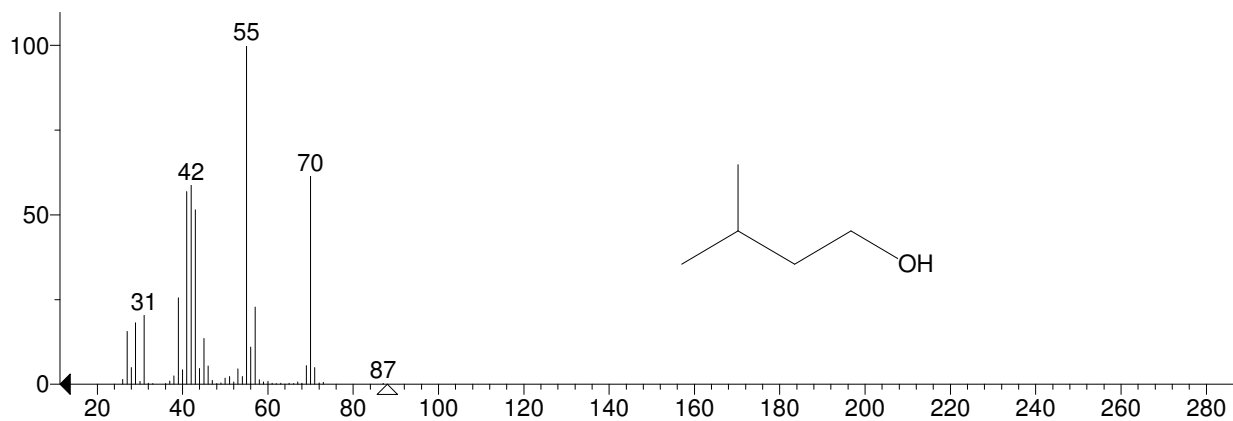
Hit 2 : n-Propyl acetate
C5H10O2; MF: 693; RMF: 866; Prob 68.5%; CAS: 109-60-4; Lib: replib; ID: 2284.



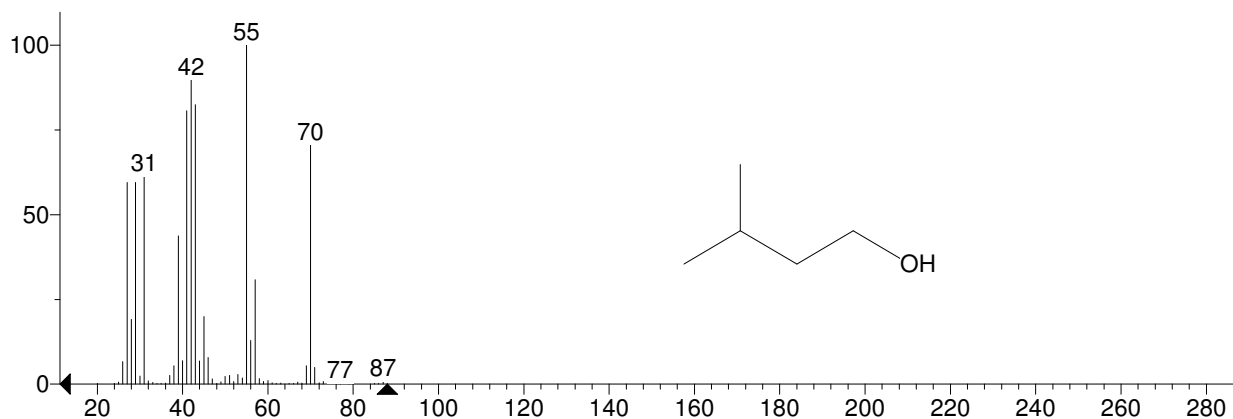
Unknown: Scan 2570 (15.369 min): Spike1.D\data.ms
Compound in Library Factor = 168



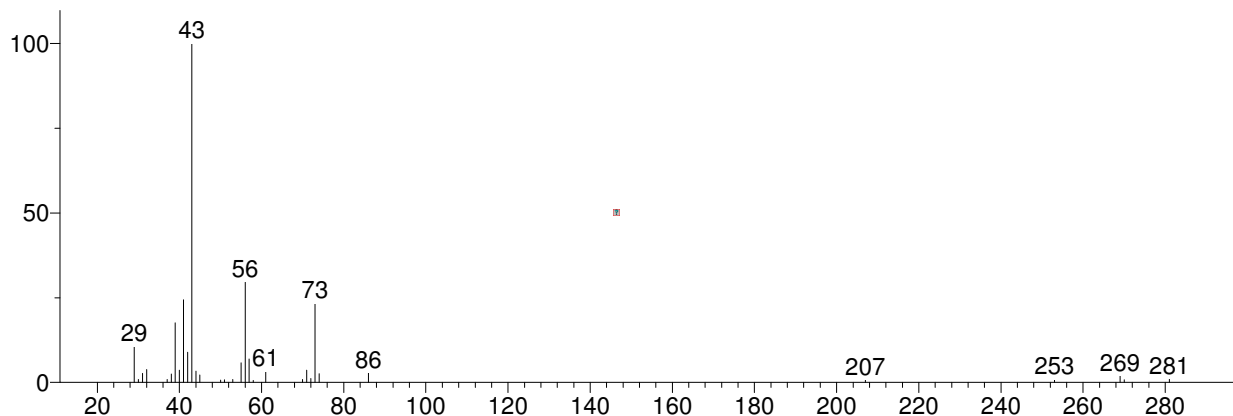
Hit 1 : 1-Butanol, 3-methyl-
C₅H₁₂O; MF: 951; RMF: 951; Prob 70.8%; CAS: 123-51-3; Lib: replib; ID: 4529.



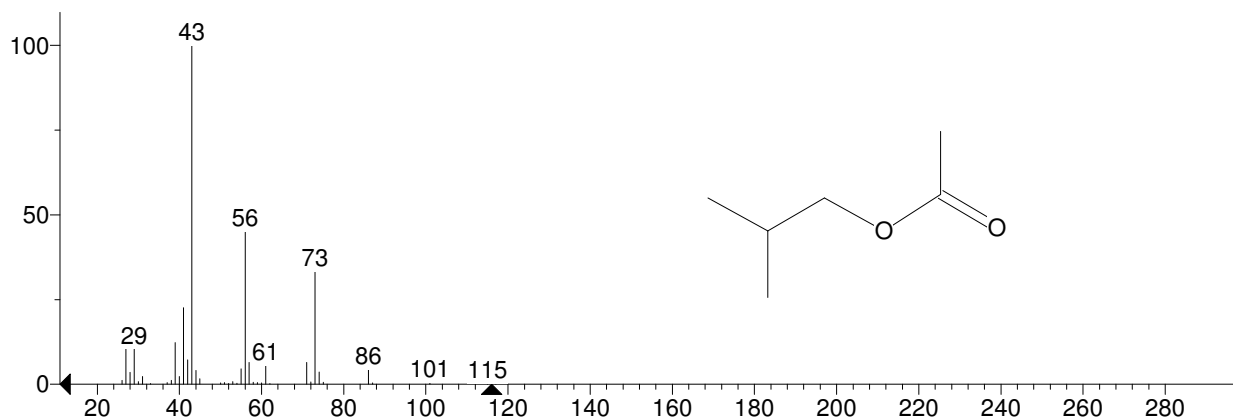
Hit 2 : 1-Butanol, 3-methyl-
C₅H₁₂O; MF: 927; RMF: 927; Prob 70.8%; CAS: 123-51-3; Lib: mainlib; ID: 17753.



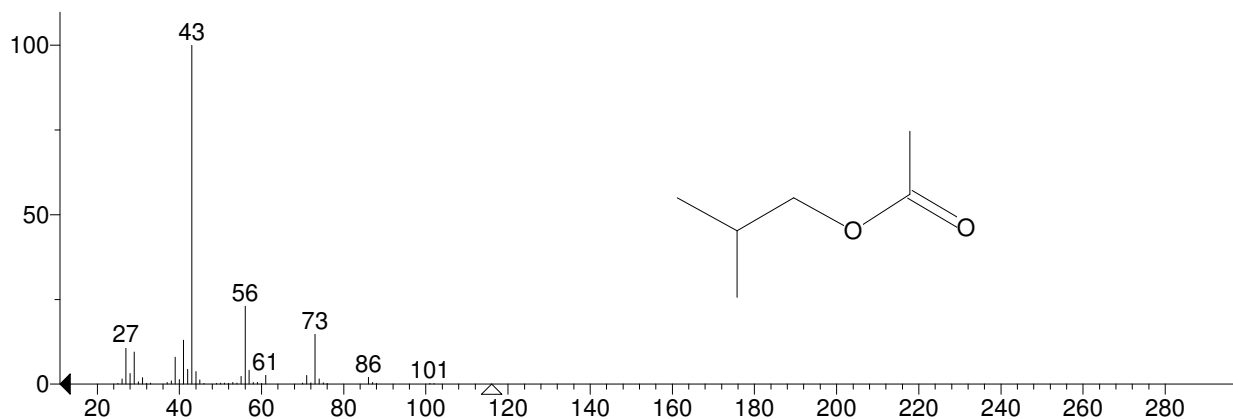
Unknown: Scan 2621 (15.672 min): Spike1.D\data.ms
Compound in Library Factor = 124



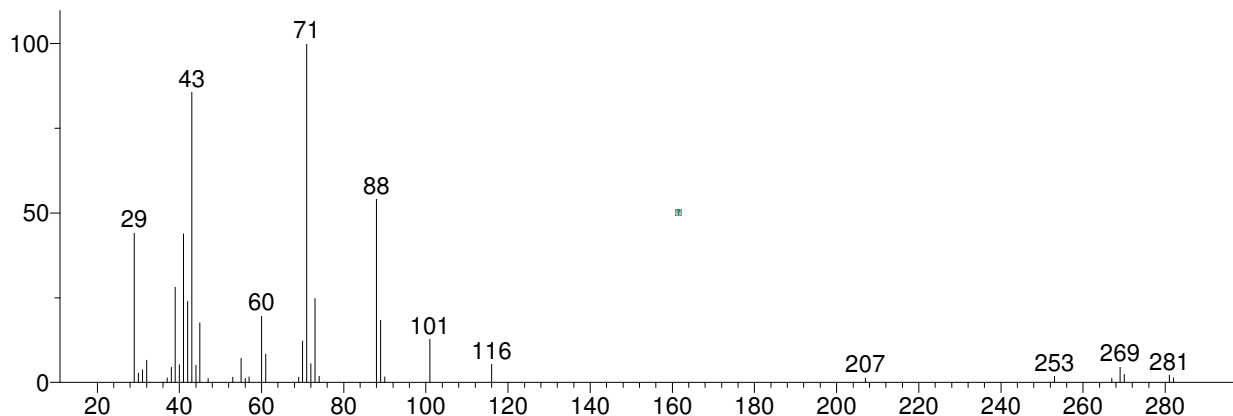
Hit 1 : Acetic acid, 2-methylpropyl ester
C₆H₁₂O₂; MF: 854; RMF: 911; Prob 72.8%; CAS: 110-19-0; Lib: mainlib; ID: 7062.



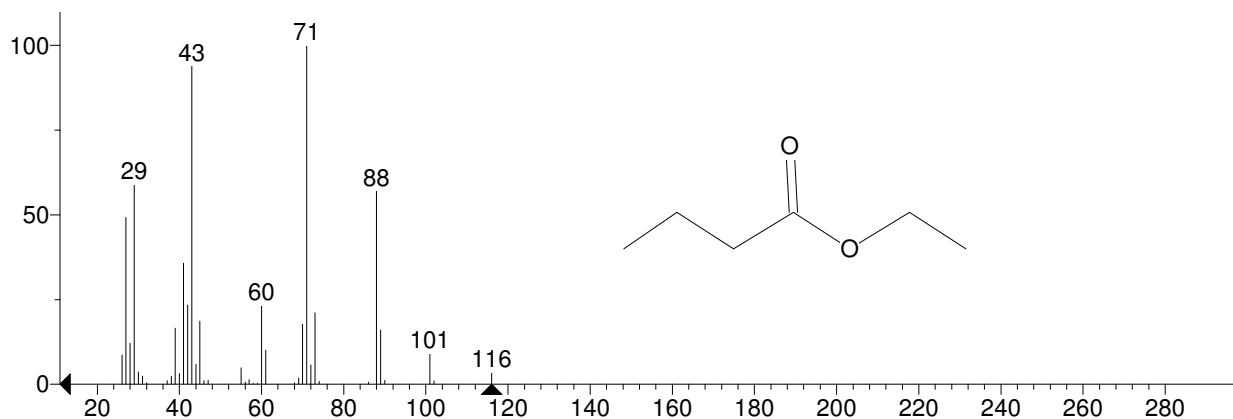
Hit 2 : Acetic acid, 2-methylpropyl ester
C₆H₁₂O₂; MF: 827; RMF: 874; Prob 72.8%; CAS: 110-19-0; Lib: replib; ID: 2007.



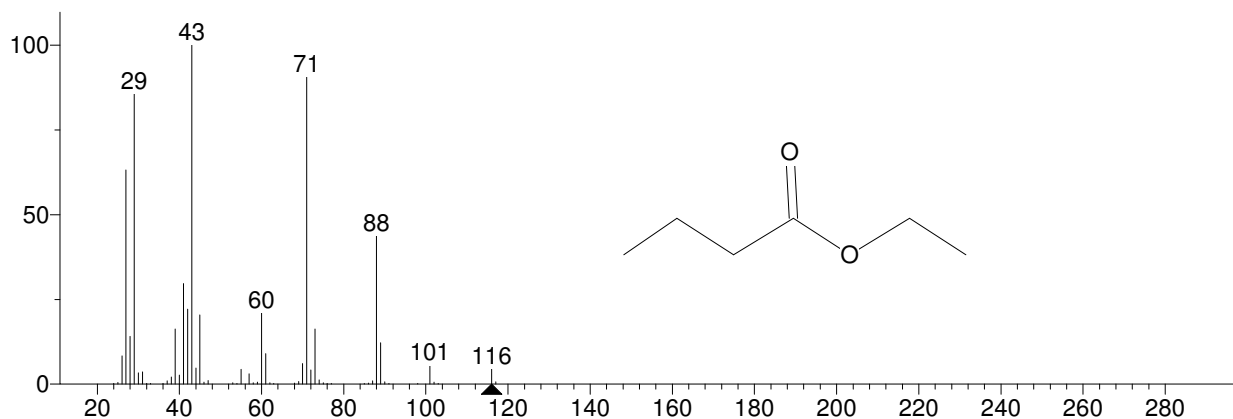
Unknown: Scan 2685 (16.052 min): Spike1.D\data.ms
Compound in Library Factor = 209



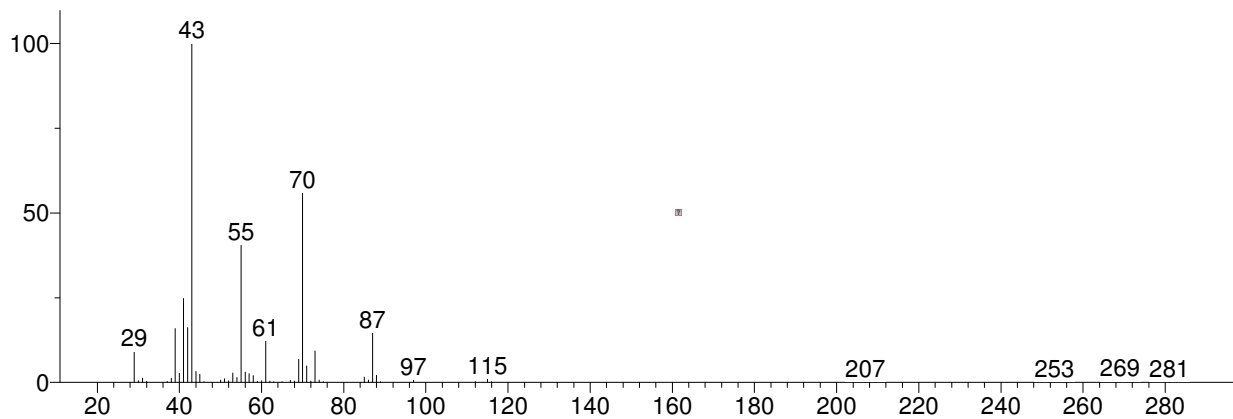
Hit 1 : Butanoic acid, ethyl ester
C₆H₁₂O₂; MF: 868; RMF: 930; Prob 92.1%; CAS: 105-54-4; Lib: mainlib; ID: 33076.



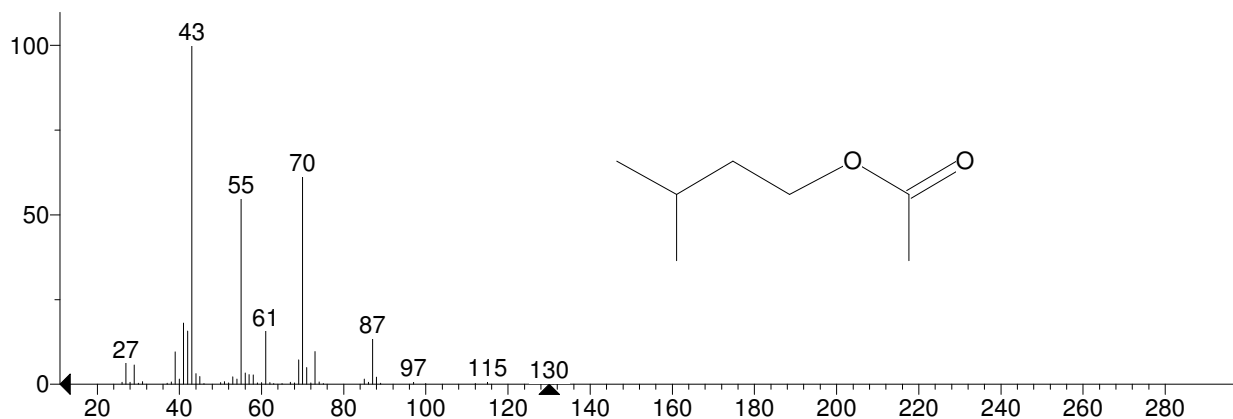
Hit 2 : Butanoic acid, ethyl ester
C₆H₁₂O₂; MF: 836; RMF: 896; Prob 92.1%; CAS: 105-54-4; Lib: replib; ID: 2398.



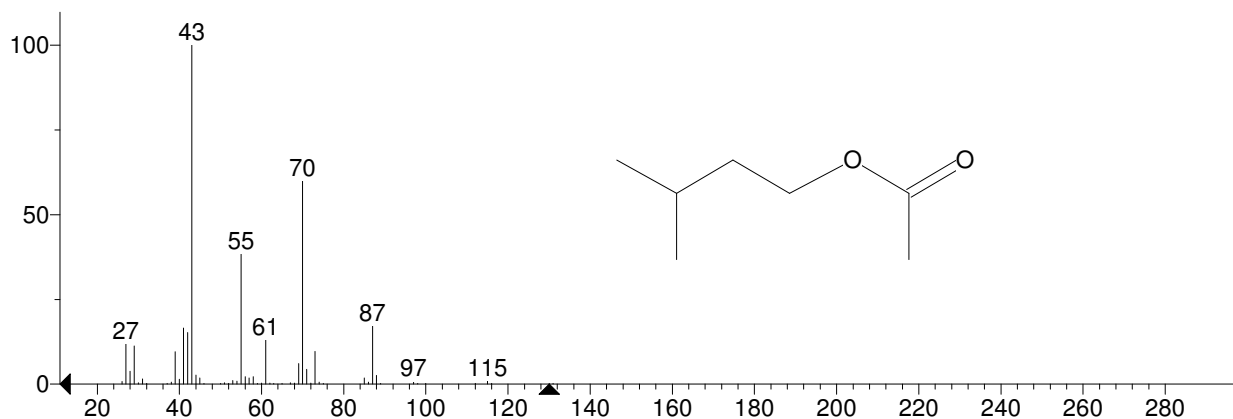
Unknown: Scan 2886 (17.248 min): Spike1.D\data.ms
Compound in Library Factor = 278



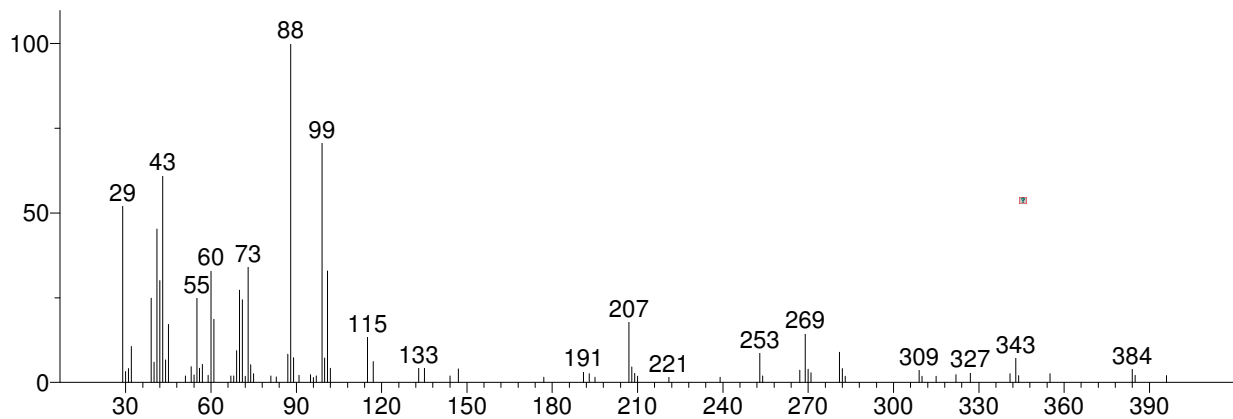
Hit 1 : 1-Butanol, 3-methyl-, acetate
C7H14O2; MF: 953; RMF: 955; Prob 89.0%; CAS: 123-92-2; Lib: mainlib; ID: 8018.



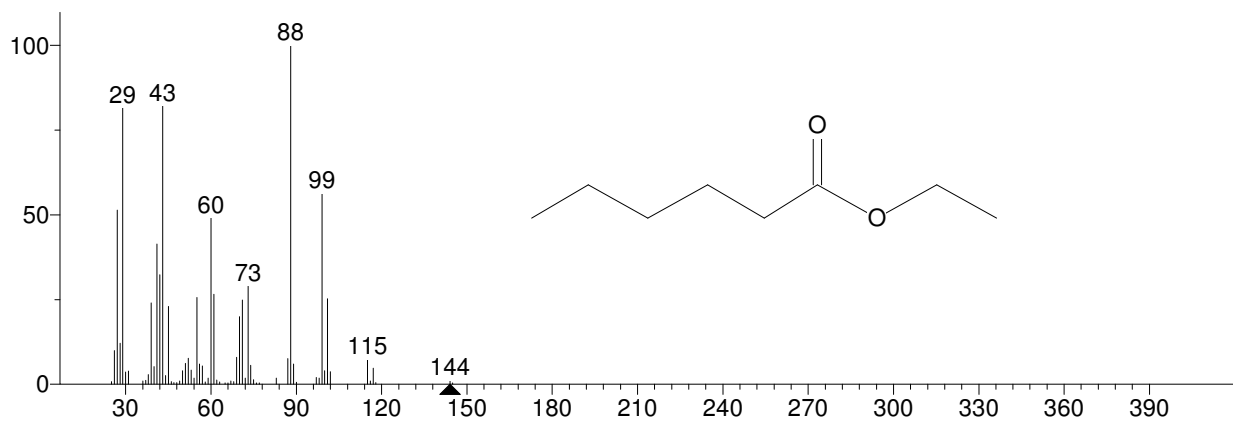
Hit 2 : 1-Butanol, 3-methyl-, acetate
C7H14O2; MF: 924; RMF: 927; Prob 89.0%; CAS: 123-92-2; Lib: replib; ID: 2361.



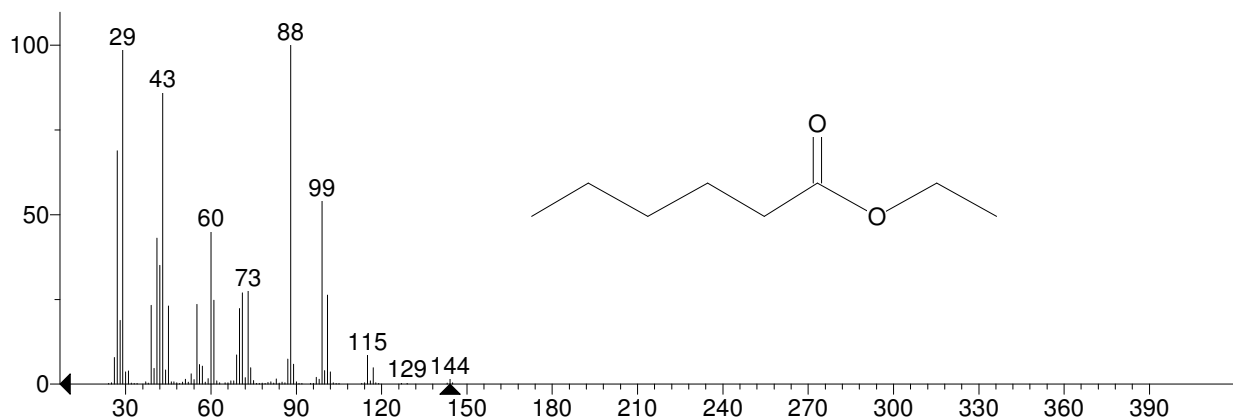
Unknown: Scan 3153 (18.835 min): Spike1.D\data.ms
Compound in Library Factor = -549



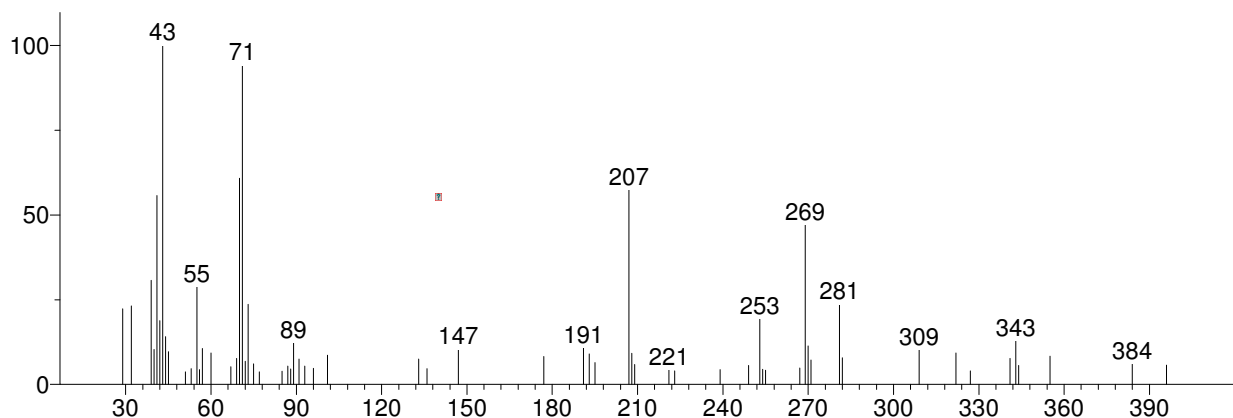
Hit 1 : Hexanoic acid, ethyl ester
C₈H₁₆O₂; MF: 675; RMF: 911; Prob 70.2%; CAS: 123-66-0; Lib: replib; ID: 11040.



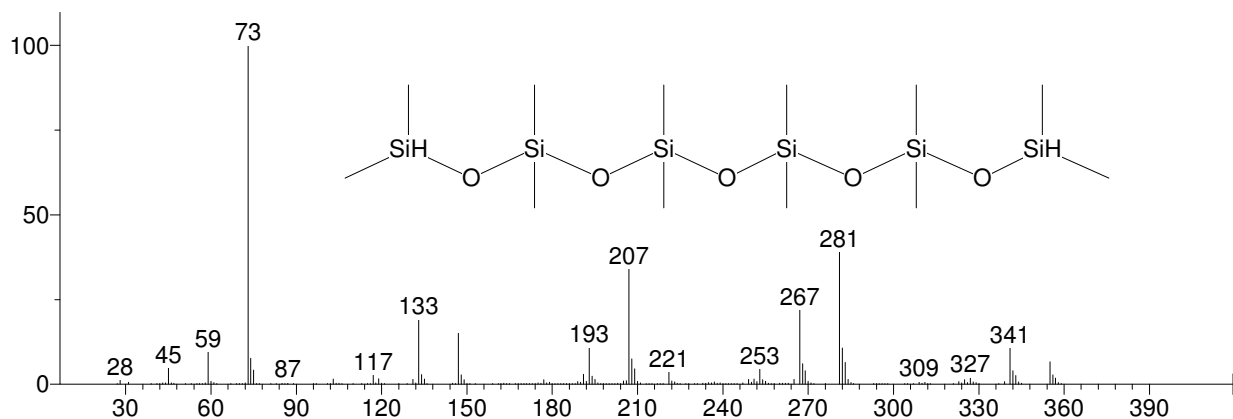
Hit 2 : Hexanoic acid, ethyl ester
C₈H₁₆O₂; MF: 666; RMF: 900; Prob 70.2%; CAS: 123-66-0; Lib: mainlib; ID: 49157.



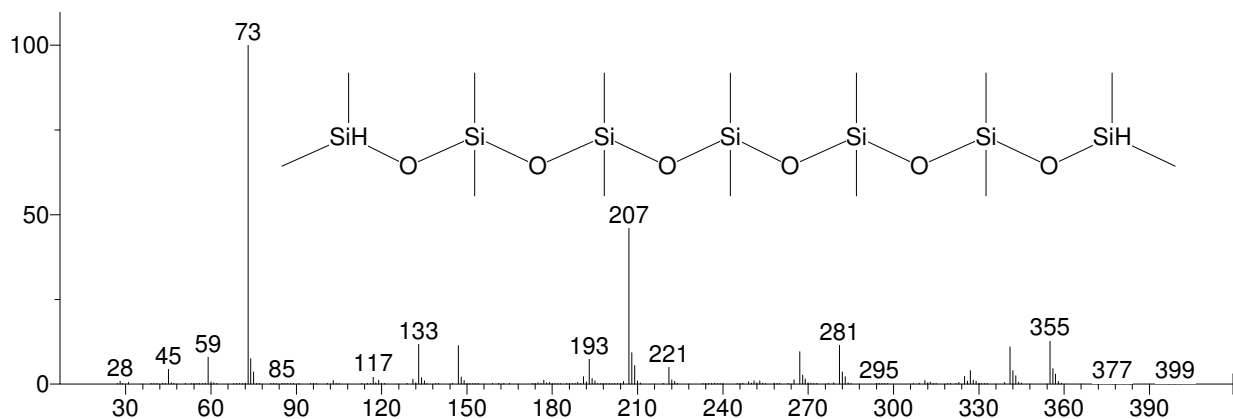
Unknown: Scan 3197 (19.097 min): Spike1.D\data.ms
Compound in Library Factor = -1774



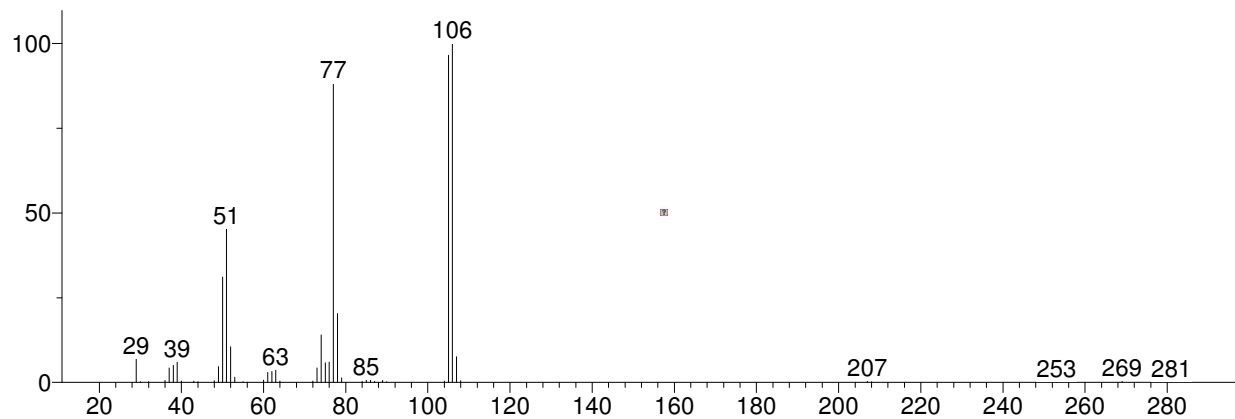
Hit 1 : Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
C₁₂H₃₈O₅Si₆; MF: 459; RMF: 517; Prob 9.76%; CAS: 995-82-4; Lib: mainlib; ID: 37488.



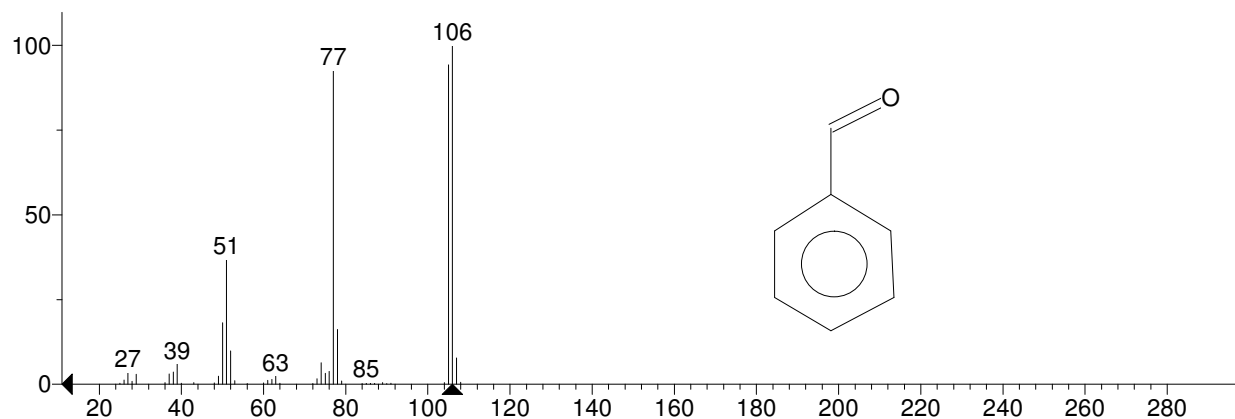
Hit 2 : Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
C₁₄H₄₄O₆Si₇; MF: 456; RMF: 513; Prob 8.63%; CAS: 19095-23-9; Lib: mainlib; ID: 37083.



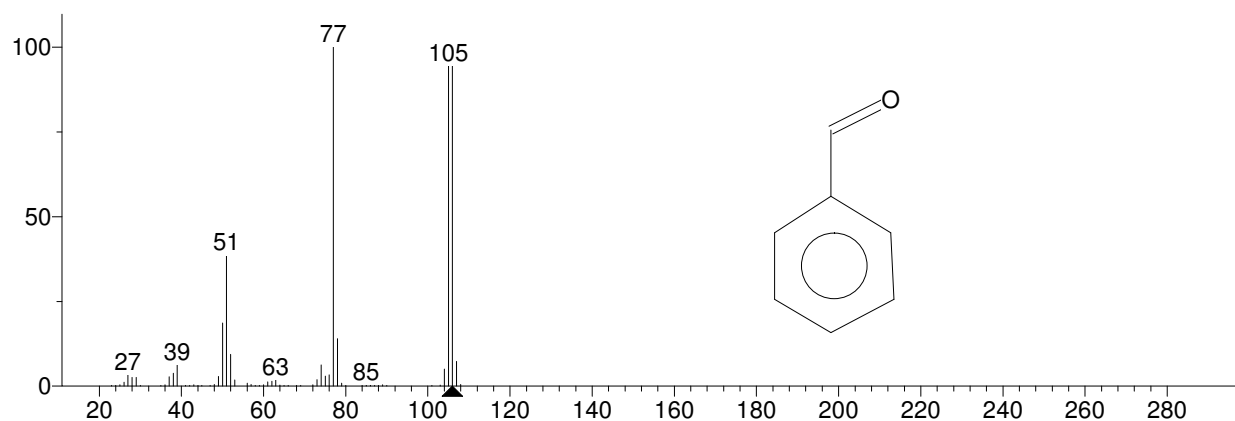
Unknown: Scan 3225 (19.263 min): Spike1.D\data.ms
Compound in Library Factor = 229



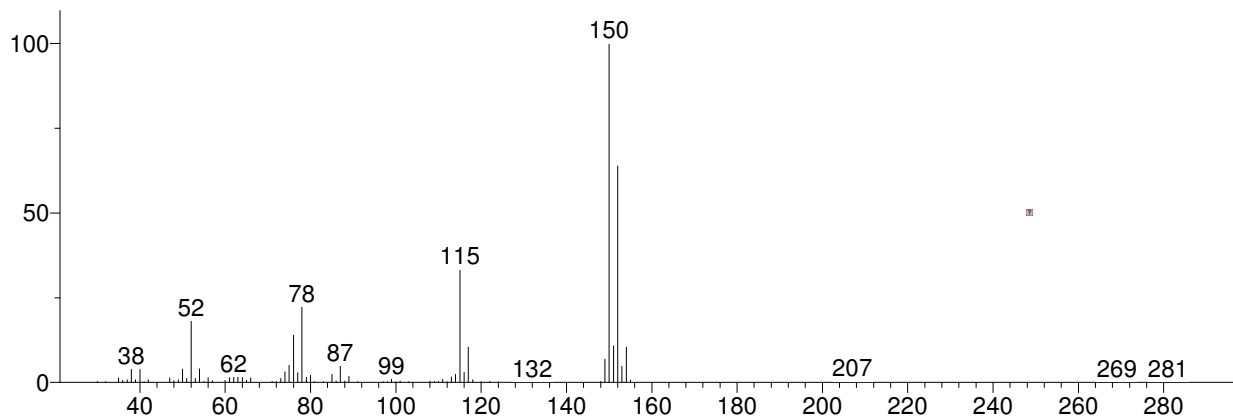
Hit 1 : Benzaldehyde
C7H6O; MF: 930; RMF: 933; Prob 77.5%; CAS: 100-52-7; Lib: replib; ID: 14266.



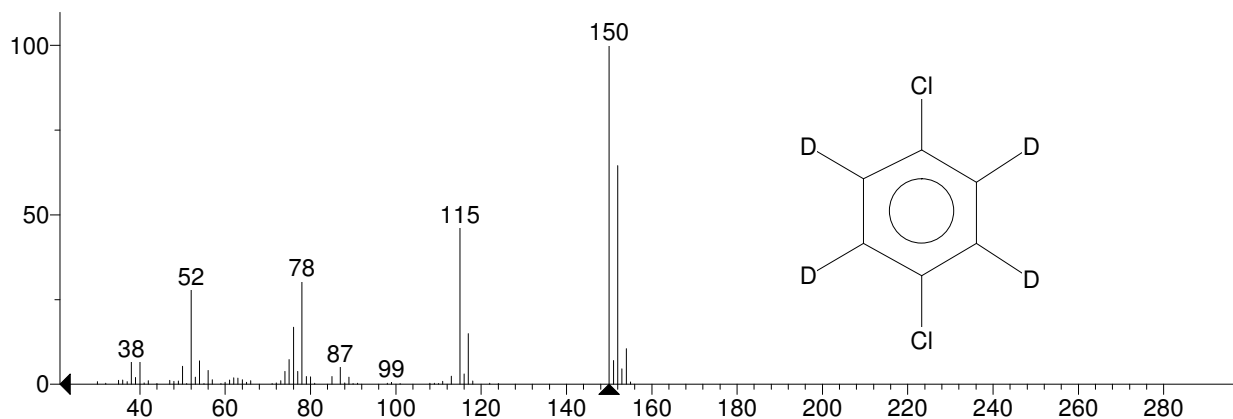
Hit 2 : Benzaldehyde
C7H6O; MF: 929; RMF: 931; Prob 77.5%; CAS: 100-52-7; Lib: replib; ID: 9456.



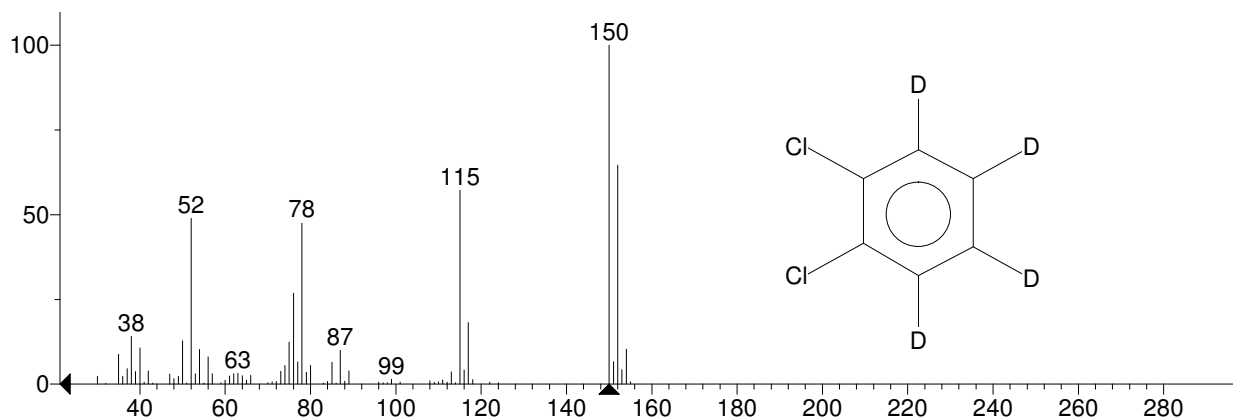
Unknown: Scan 3287 (19.632 min): Spike1.D\data.ms
Compound in Library Factor = 344



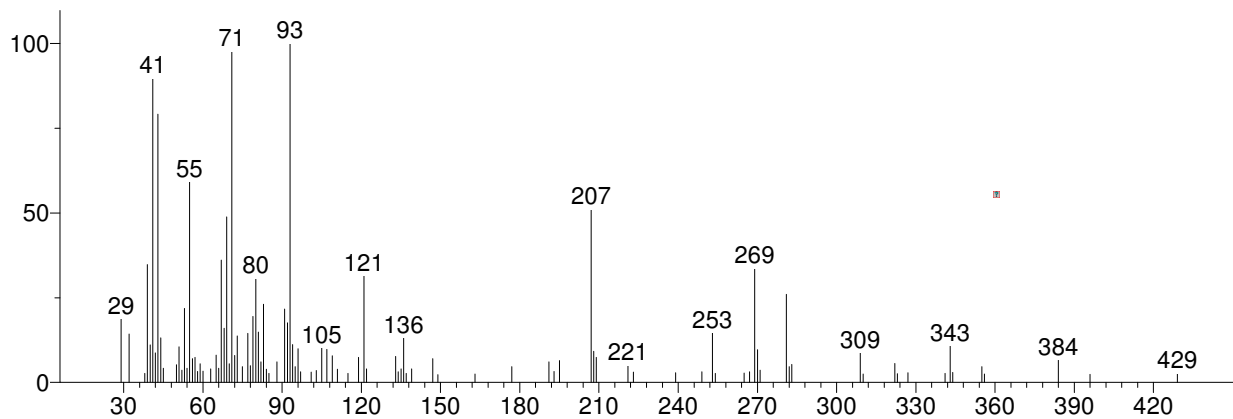
Hit 1 : 1,4-Dichlorobenzene-D4
C6Cl2D4; MF: 890; RMF: 906; Prob 72.6%; CAS: 3855-82-1; Lib: mainlib; ID: 111936.



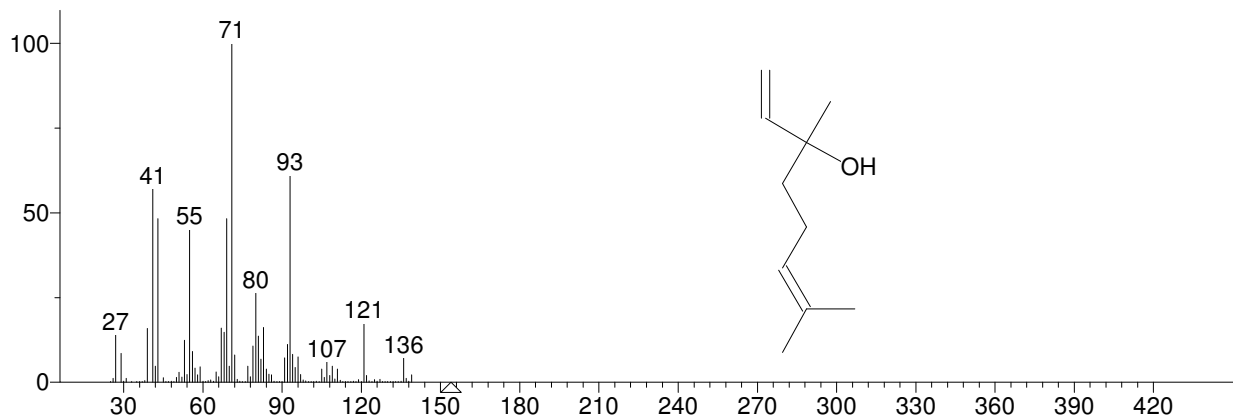
Hit 2 : 1,2-Dichlorobenzene-D4
C6Cl2D4; MF: 867; RMF: 880; Prob 26.5%; CAS: 2199-69-1; Lib: mainlib; ID: 111935.



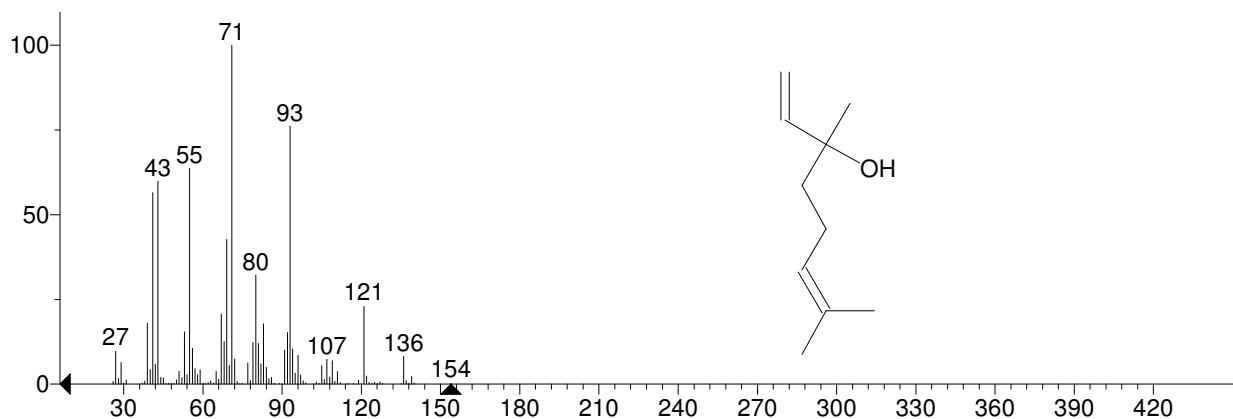
Unknown: Scan 3420 (20.423 min): Spike1.D\data.ms
Compound in Library Factor = -1421



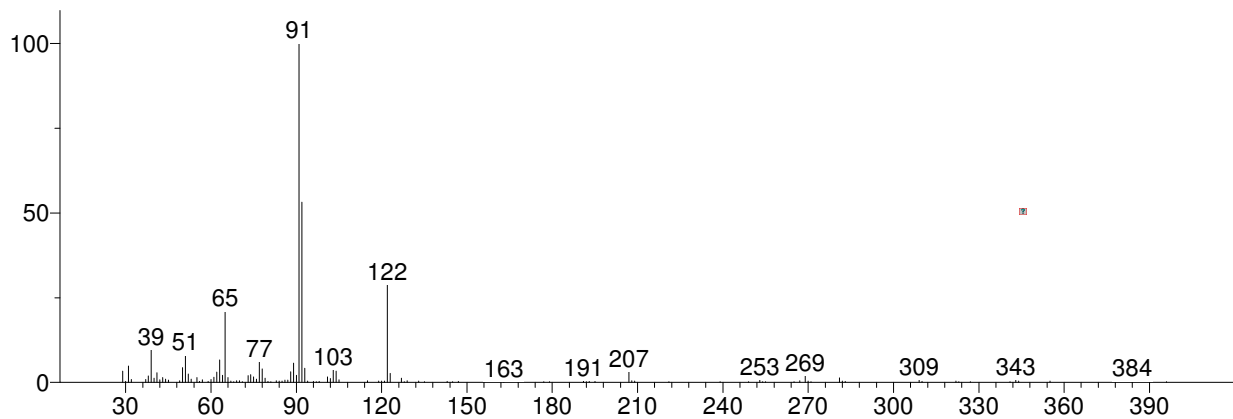
Hit 1 : 1,6-Octadien-3-ol, 3,7-dimethyl-
C₁₀H₁₈O; MF: 594; RMF: 864; Prob 17.8%; CAS: 78-70-6; Lib: replib; ID: 8149.



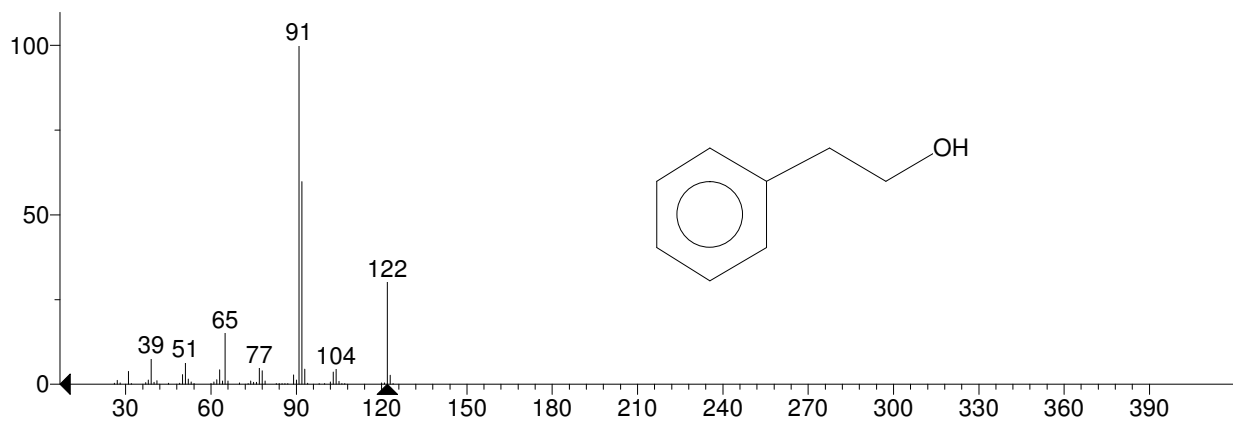
Hit 2 : 1,6-Octadien-3-ol, 3,7-dimethyl-
C₁₀H₁₈O; MF: 588; RMF: 847; Prob 17.8%; CAS: 78-70-6; Lib: mainlib; ID: 33714.



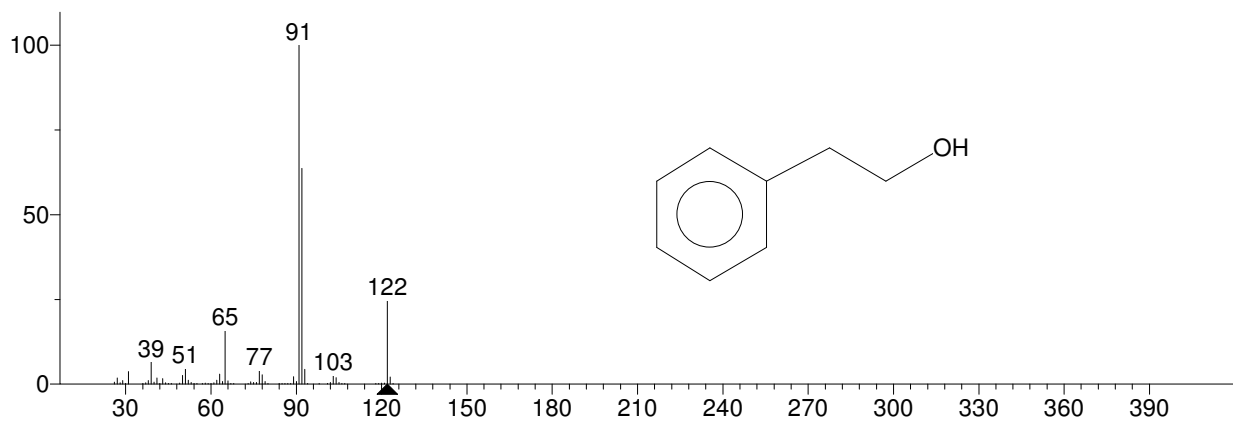
Unknown: Scan 3575 (21.344 min): Spike1.D\data.ms
Compound in Library Factor = -133



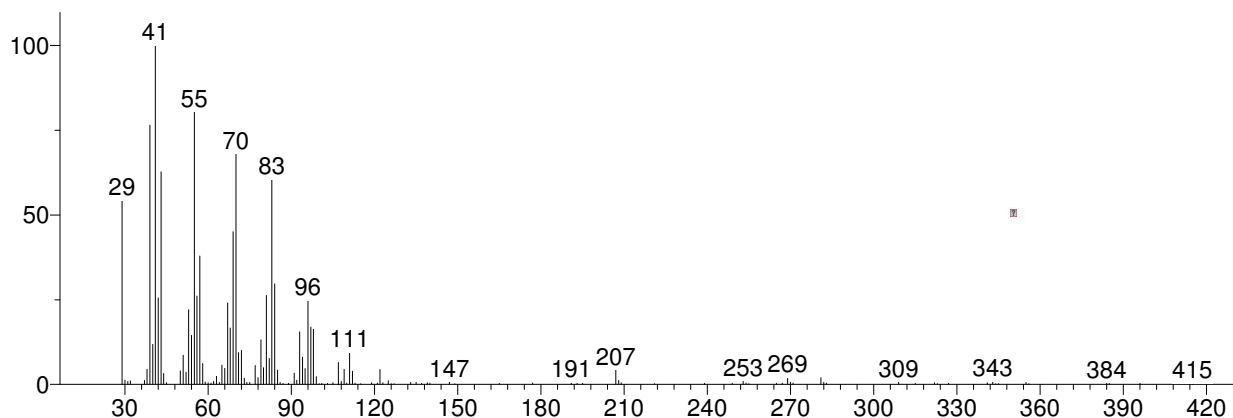
Hit 1 : Phenylethyl Alcohol
C₈H₁₀O; MF: 837; RMF: 917; Prob 74.9%; CAS: 60-12-8; Lib: replib; ID: 11425.



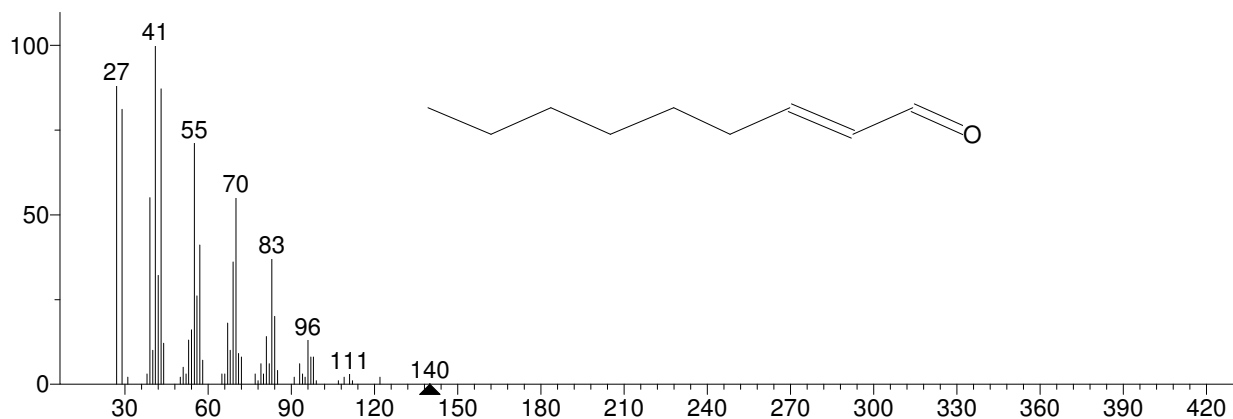
Hit 2 : Phenylethyl Alcohol
C₈H₁₀O; MF: 824; RMF: 901; Prob 74.9%; CAS: 60-12-8; Lib: replib; ID: 11424.



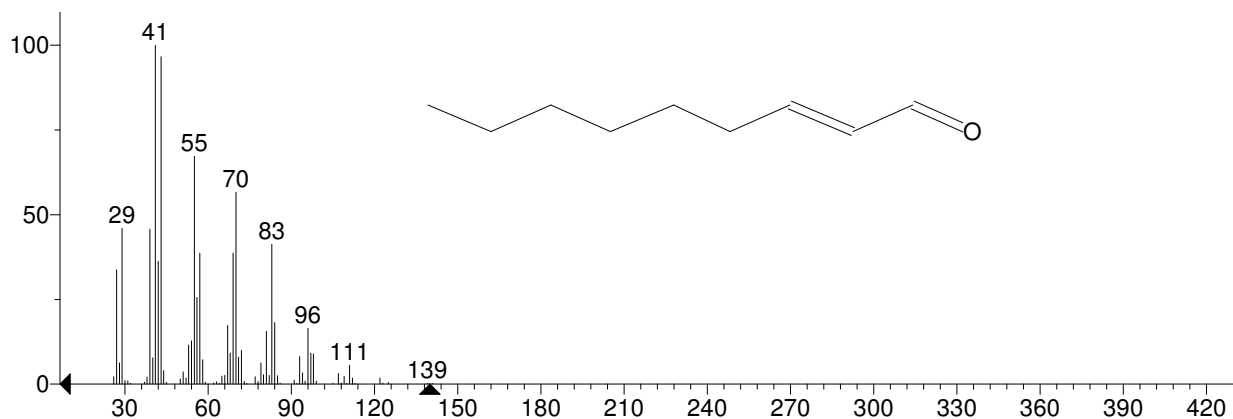
Unknown: Scan 3607 (21.535 min): Spike1.D\data.ms
Compound in Library Factor = -118



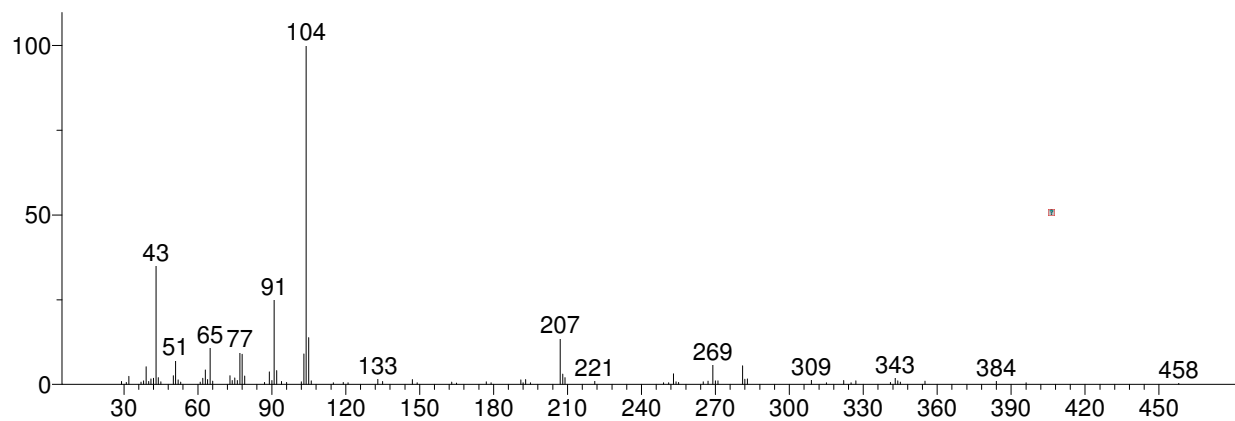
Hit 1 : 2-Nonenal, (E)-
C₉H₁₆O; MF: 887; RMF: 940; Prob 58.8%; CAS: 18829-56-6; Lib: replib; ID: 711.



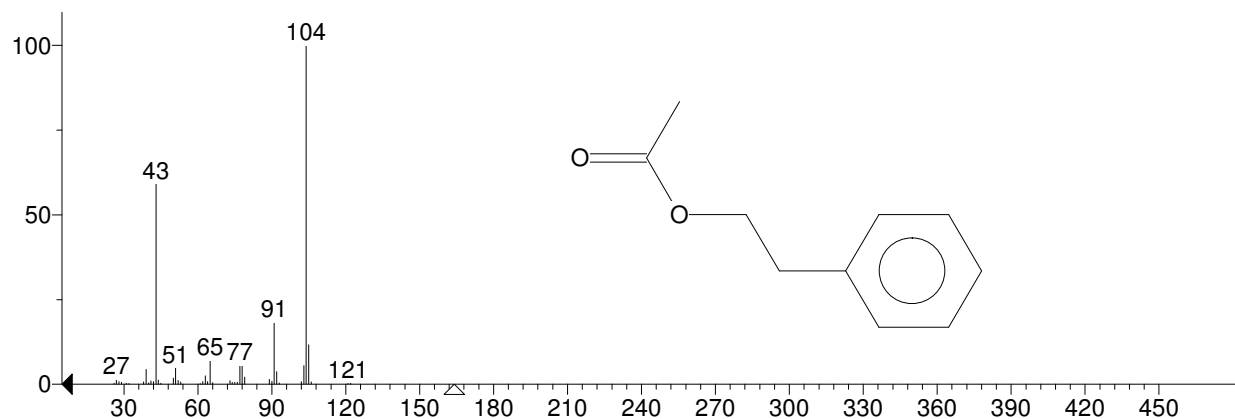
Hit 2 : 2-Nonenal, (E)-
C₉H₁₆O; MF: 864; RMF: 908; Prob 58.8%; CAS: 18829-56-6; Lib: replib; ID: 831.



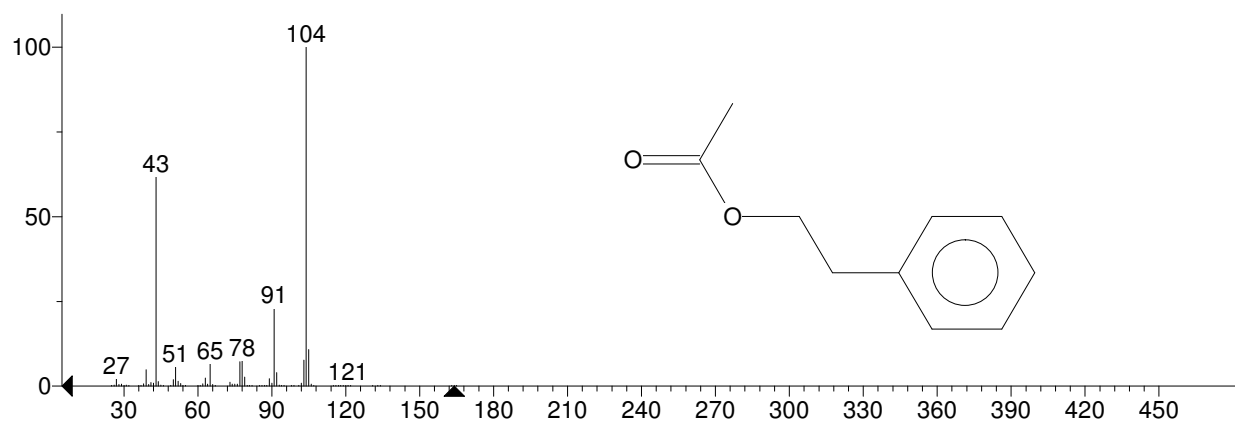
Unknown: Scan 3834 (22.884 min): Spike1.D\data.ms
Compound in Library Factor = -799



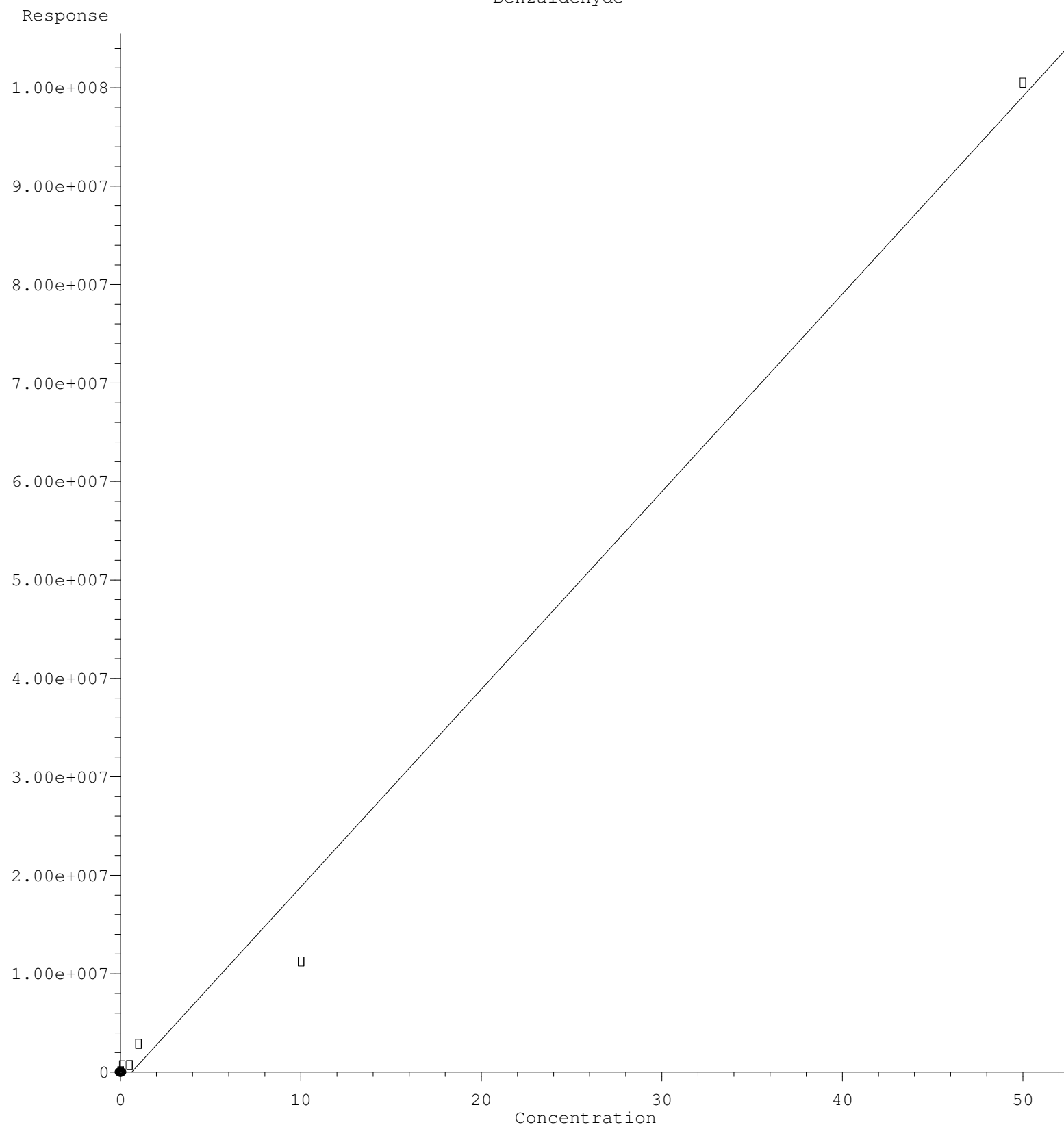
Hit 1 : Acetic acid, 2-phenylethyl ester
C₁₀H₁₂O₂; MF: 682; RMF: 898; Prob 32.3%; CAS: 103-45-7; Lib: mainlib; ID: 65178.

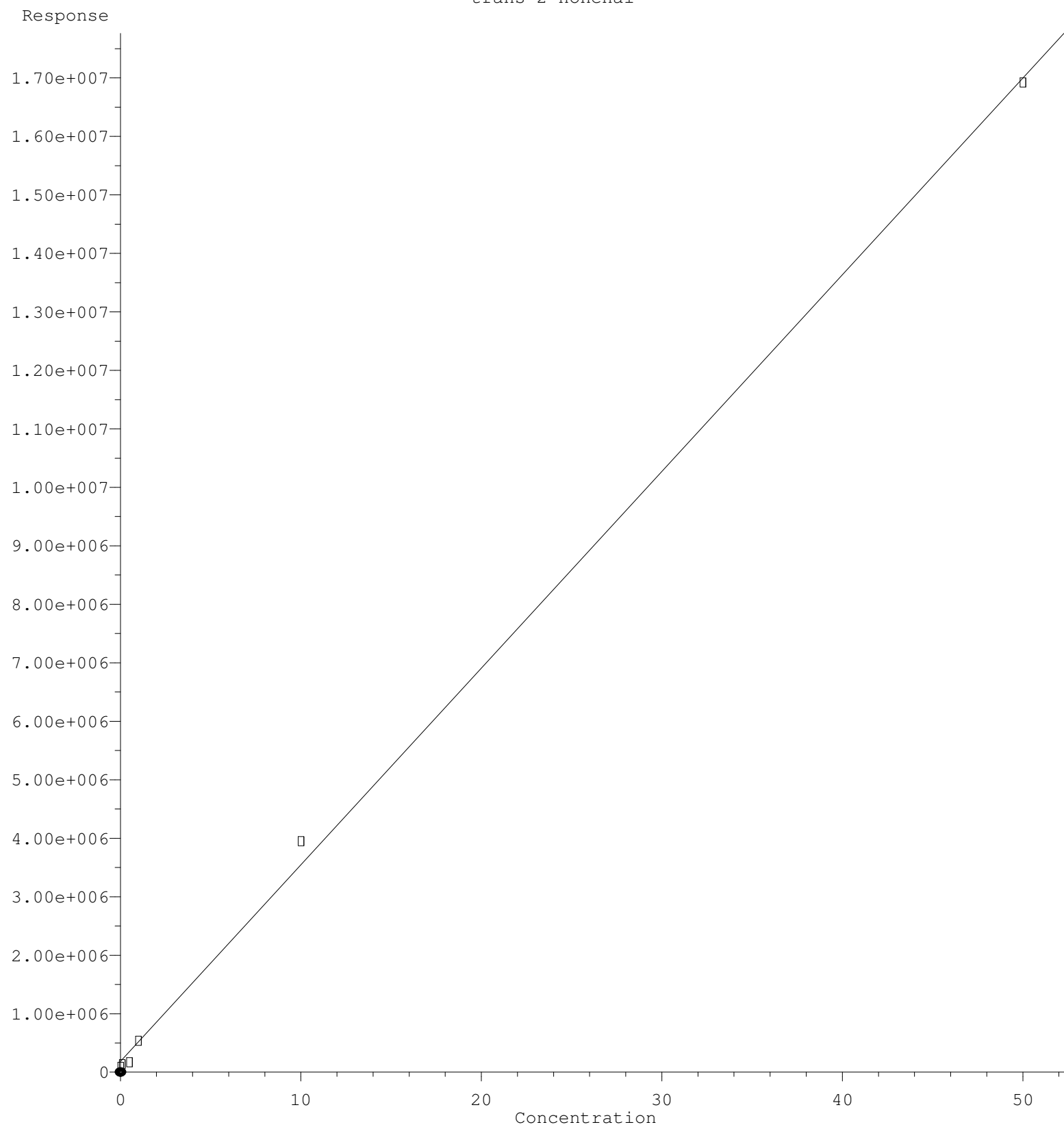


Hit 2 : Acetic acid, 2-phenylethyl ester
C₁₀H₁₂O₂; MF: 678; RMF: 893; Prob 32.3%; CAS: 103-45-7; Lib: replib; ID: 13444.



Benzaldehyde





Data Path : D:\msdchem\1\data\2014\J8675 DHS Beer\080314\
Data File : Spikel.D
Acq On : 5 Aug 2014 6:04
Operator : Oliver Palardy
Sample : Beer sample, spiked at 10ppm
Misc :
ALS Vial : 25 Sample Multiplier: 1

Quant Time: Sep 25 13:49:10 2014
Quant Method : D:\msdchem\1\methods\J8675.M
Quant Title :
QLast Update : Tue Aug 05 10:26:43 2014
Response via : Initial Calibration

Compound	R.T.	QIon	Response	Conc	Units	Dev(Min)

Internal Standards						
3) 1,4-Dichlorobenzene-d4	19.637	TIC	129467557	5.00	ug/mL	0.04
Target Compounds						
1) Benzaldehyde	19.266	106	23371908	12.27	ug/mL	100
2) trans-2-nonenal	21.534	41	3007608	8.41	ug/mL	100

(#) = qualifier out of range (m) = manual integration (+) = signals summed

J8675.M Thu Sep 25 13:49:10 2014 7890