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EVA and PVC Infusion Bags
Leachables Identification Case study

Released by:

Mark Jordi, Ph.D.
President

Job Number: J9163

CONFIDENTIAL

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200 Gilbert Street
Mansfield, MA 02048
P: (508) 966-1301
jordilabs.com

March 7, 2015

Client Name
Company Name
Address

Dear Valued Client,

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

1. EVA infusion bag
2. PVC infusion bag

The following tests were performed:

1. Gravimetric Analysis
2. Fourier Transform Infrared Spectroscopy (FTIR)
3. Pyrolysis Gas Chromatography Mass Spectrometry (PYMS)
4. Dynamic Headspace Gas Chromatography Mass Spectrometry (DHGCMS)
5. Gas Chromatography Mass Spectrometry (GCMS)
6. Liquid Chromatography Mass Spectrometry (LCMS)

Objective

The goal of this work was to compare an EVA and PVC infusion bag for its leachables profile.

Summary of Results

The chemical composition of samples *EVA infusion bag* and *PVC infusion bag* were determined using DHGCMS, PYMS and FTIR. The *EVA infusion bag was found to be consistent with an ethylenevinylacetate copolymer. No additional components were observed. The PVC infusion bag was found to be consistent with poly(vinylchloride) plasticized with dioctylphthalate.*

Sample *EVA infusion bag* and *PVC infusion bag were* extracted in water and Sample *EVA infusion bag* was extracted in saline. The leachables were subsequently analyzed by GC-MS and LC-MS. Leachables found in samples *EVA infusion bag* and *PVC infusion bag* are summarized in **Table 1**. The EVA infusion bag was found to show few types of leachables as compared to the PVC bag.

Table 1 **Leachables found from *PVC* and *EVA infusion bags***				
Chemical Name	**CAS**	***PVC infusion bag***	***EVA infusion bag***	***EVA infusion bag***
Solvent		**Water**	**Water**	**Saline**
Hydrazinecarboxamide	57-56-7		X	
Isosorbide	652-67-5		X	
Diethyl Phthalate	84-66-2		X	X
Cyclohexanone	108-94-1	X	X	X
Butylated Hydroxytoluene	128-37-0	X	X	X
Cyclopentanone, 2-methyl-	1120-72-5		X	X
7-Oxooctanoic acid	14112-98-2		X	
9-Oxononanoic acid	2553-17-5		X	
Oligomers of polyethylene glycol		X	X	X
Phthalic acid	88-99-3	X		
Diisooctyl phthalate	27554-26-3	X		
Octadecanoic acid, octyl ester	109-36-4	X		
Octadecanoic acid, 10-oxo-, methyl ester	870-10-0	X		
Octadecanoic acid, 9-oxo-, methyl ester	1842-70-2	X		
Phthalic anhydride	85-44-9	X		
Dibutyl phthalate	84-74-2	X		
8-Methoxy-8-oxooctyl methyl suberate		X		
Dimethyl 7-methylene-8-oxopentadecanedioate		X		
Oxononanoic acid	13139-94-1	X		
Mono(2-ethylhexyl)phthalate [MEHP]	224-477-1	X		
Dimethyl 7-methylene-8-oxopentadecanedioate		X		
Methyl (10E)-9-hydroxy-11-(3-pentyl-2-oxiranyl)- 10-undecenoate		X		
Trihydroxyoctadecenoic acid		X		
Methyl (9E)-8,11,12-trihydroxy-9-octadecenoate		X		
2-[(2-Octanyloxy)carbonyl]benzoic acid		X		
Methyl 9,10-Dihydroxystearate		X		
2-(Decanoylamino)propionic acid				X

Next Steps

The leachables identified in **Table 1** should be quantified using a combination of HPLC, LCMS and GCMS to allow for a toxicological risk assessment.

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.

Gravimetric Analysis

Sample preparation

The *EVA infusion bag* sample provided was found to contain two distinct layers (**Figure 1**). One side of the bag was found to be relatively clear (outside portion), while the opposite side of the bag was found to be opaque (inside portion).

The *PVC infusion bag* sample provided was also found to contain two sides (**Figure 2**). One side of the bag was found to be white (white portion), while the opposite side of the bag was found to be clear (clear portion).

The provided devices were extracted with water and or saline solutions. The extractions were performed at 37°C (±1°C) for a total of 72 hours. The extracts were agitated through the use of a shaker oven. **Table 2** showed the residue mass following the extraction and the percent leachables as a function of the weight of the original bag.

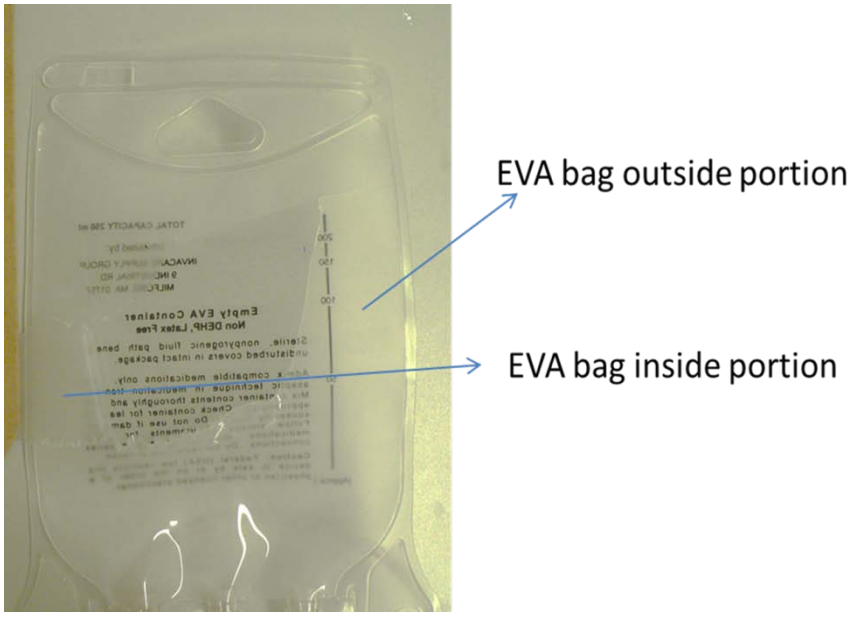


Figure 1- EVA infusion bag sample analyzed (arrows pointed to inside portion and outside portion).

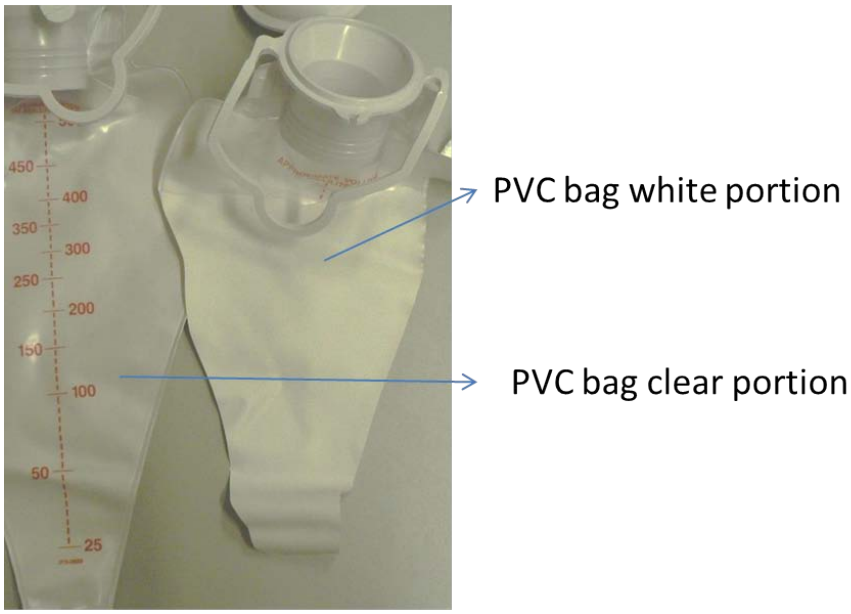


Figure 2- PVC infusion bag sample analyzed, left: white portion, right: clear portion.

Table 2: Residual Mass of Extracted Components				
Sample	**Infusion bag Mass (g)**	**Water amount (ml)**	**Residual Mass (mg)**	**% Leachables**
EVA infusion bag	21.6977	50	1.0	0.0046
PVC infusion bag	49.3393	50	1.4	0.0028
Water blank	-	50	0.3	-

FTIR

The *EVA infusion bag* (inside portion and outside portion) and *PVC infusion bag* (white portion and clear portion) were analyzed directly by FTIR in attenuated total reflectance (ATR) mode. The FTIR spectra for both the inside portion and outside portion were found to be nearly identical and an overlay of FTIR spectra from the inside portion of the *EVA infusion bag* (red) and an EVA reference material (blue) is shown in **Figure 3**. The FTIR peaks and assignments are listed in **Table 3**. A search of our FTIR spectral database produced Ethylene/Vinyl acetate copolymer as the best match.

The FTIR spectra of the white and clear portions of the sample *PVC bag* are nearly identical and an overlay of the FTIR spectrum from the white portion of the *PVC infusion bag* (purple) and a PVC reference material (red) is shown in **Figure 4**. The FTIR peaks and assignments are listed in **Table 4**. A search of our FTIR spectral database produced commercial PVC as the best match. A large peak at 1730 cm^{-1} suggests the presence of an ester plasticizer (phthalate).

Table 3 **FTIR Peaks and Identifications for EVA bags**		
IR Frequency (cm^{-1})		**Functional Group**
EVA- *inside portion*	EVA-*outside portion*	
2917	2916	CH_2 stretch, asymmetrical
2849	2849	CH_2 stretch, symmetrical
1738	1738	C=O stretch
1465	1467	C-H bend
1370	1370	CH_2 wag
1239	1239	C-H wag
1020	1020	C-O stretch
956	956	Chain stretch
720	720	C-H rock

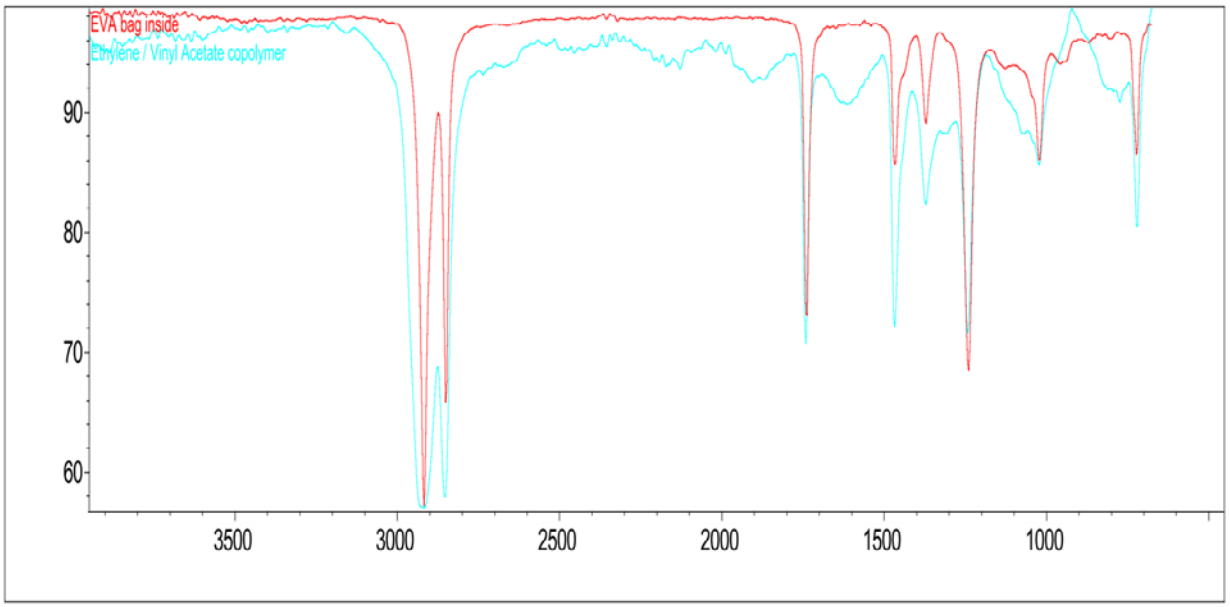


Figure 3– Overlay FTIR spectrum from inside portion of *EVA infusion bag* (red) and EVA reference material (blue).

Table 4 **FTIR Peaks and Identifications for PVC bags**		
IR Frequency (cm^{-1})		**Functional Group**
PVC- white portion	*PVC-clear portion*	
2958	2958	C-H stretch
2927	2927	CH_2 stretch, asymmetrical
2859	2859	CH_2 stretch, symmetrical
1730	1730	C=O stretch
1599	1599	C-C stretch
1580	1580	C-C stretch
1461	1461	C-H bend
1428	1428	CH_2 bend
1380	1381	CH_2 wag
1332	1332	C-H bend
1259	1259	C-O-C stretch
1197	1198	C-O-C stretch
1124	1124	Parallel chain stretch
1073	1073	C-O-C stretch
958	958	Chain stretch
834	834	Chain stretch
743	734	C-H rock
690	698	C-Cl stretch

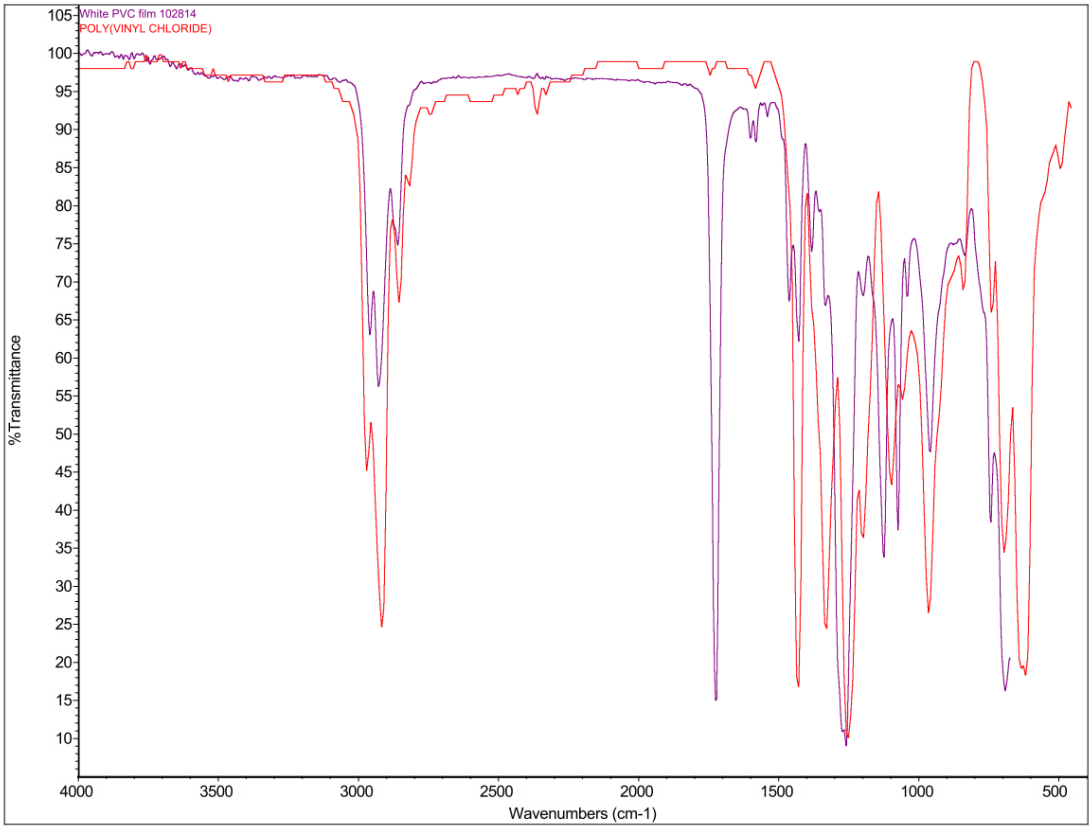


Figure 4– Overlay FTIR spectrum from white portion of *PVC infusion bag* (purple) and PVC reference material (red). Note that additional bands observed in the sample spectrum near 1730 cm^{-1} are due to phthalate plasticizers.

PYMS

Analysis by PY-GCMS was conducted using a double shot technique. The double shot experiment consists of heating a sample to release volatiles which were then cryogenically trapped and analyzed by GCMS. Following completion of the 1st pass analysis, the remaining portion of the sample was then heated above the decomposition temperature rapidly and pyrolyzed components were passed into a gas chromatography column and analyzed by mass spectroscopy.

Prominent peaks found in PY-GCMS typically include fragments of the polymer as well as monomer, antioxidants and other additives. Sample peaks were compared with over 796,613 reference compounds using the NIST/EPA/NIH mass spectral search program.

Results

Figure 5 and **Figure 6** show overlays of the PYMS 1st and 2nd pass chromatograms from the sample *EVA infusion bag*. The results were found to be most consistent with EVA based upon the presence of acetic acid and various alkane fragments.

During the 1st pass a series of linear alkanes ranging from approximately C_4-C_{20} were detected. The most intense peak in the chromatogram at retention time 1.127 minutes belongs to acetic acid. During the second heating a series of alkenes were also detected between 2 and 16 minutes retention time.

Figure 7and **Figure 8** show overlays of the PYMS 1st and 2nd pass chromatograms from the sample *PVC infusion bag*. HCl, Phthalic acid, Bis(2-ethylhexyl) adipate (DEHA), and diisooctyl phthalate are observed during the 1st pass. During the second heating, a series of alkenes were also detected between 2 and 16 minutes retention time. The HCl observed in the 1st pass and these alkenes are characteristic fragments from PVC pyrolysis.

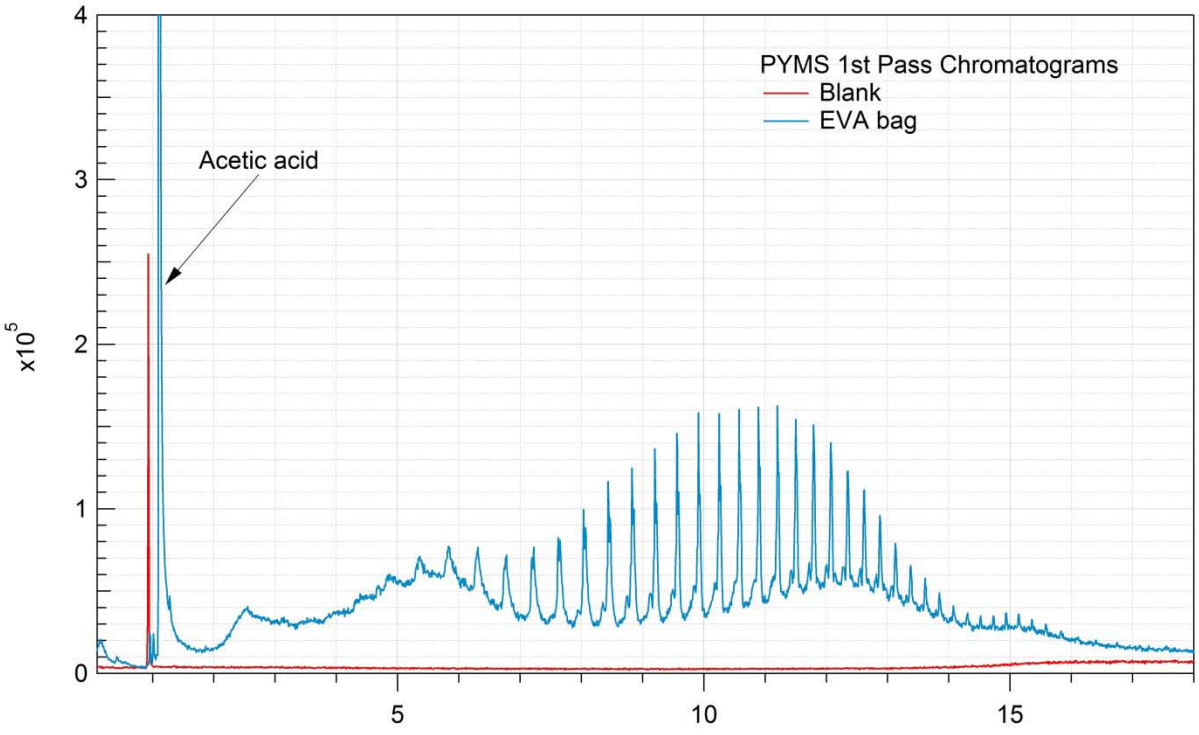


Figure 5- PYMS 1st pass chromatograms from sample *EVA infusion bag*.

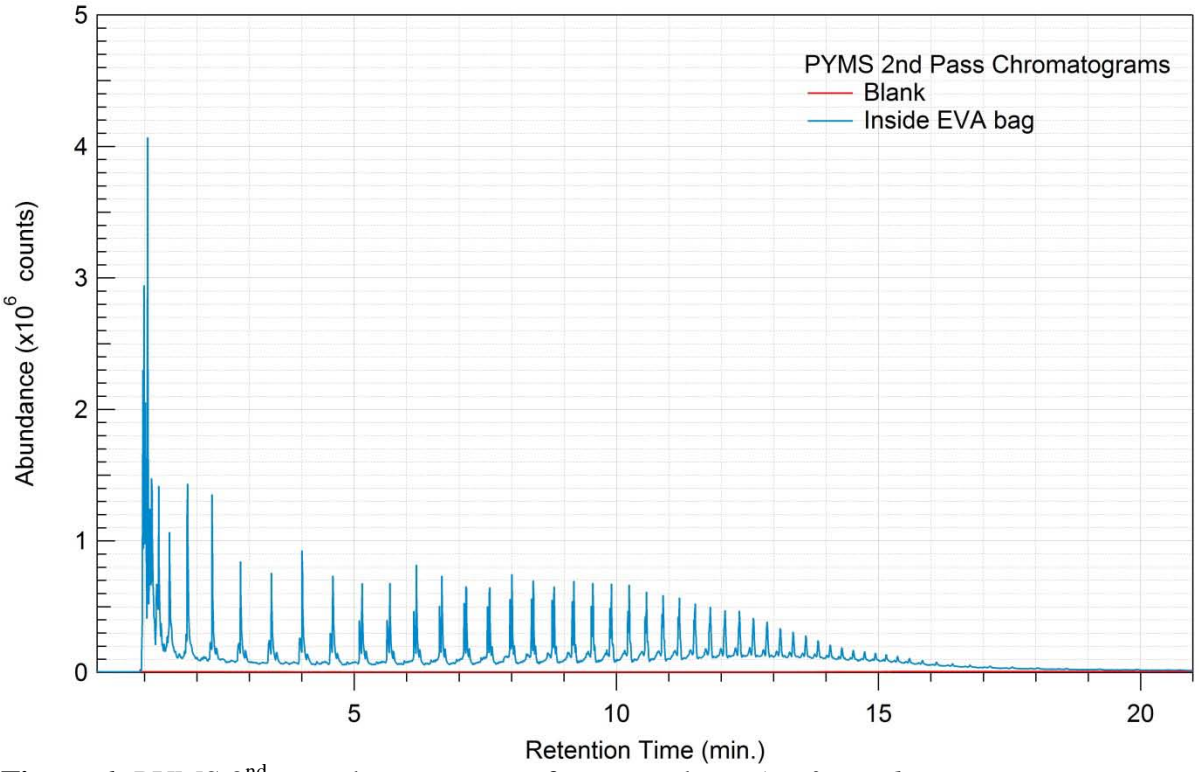


Figure 6- PYMS 2nd pass chromatograms from sample *EVA infusion bag*.

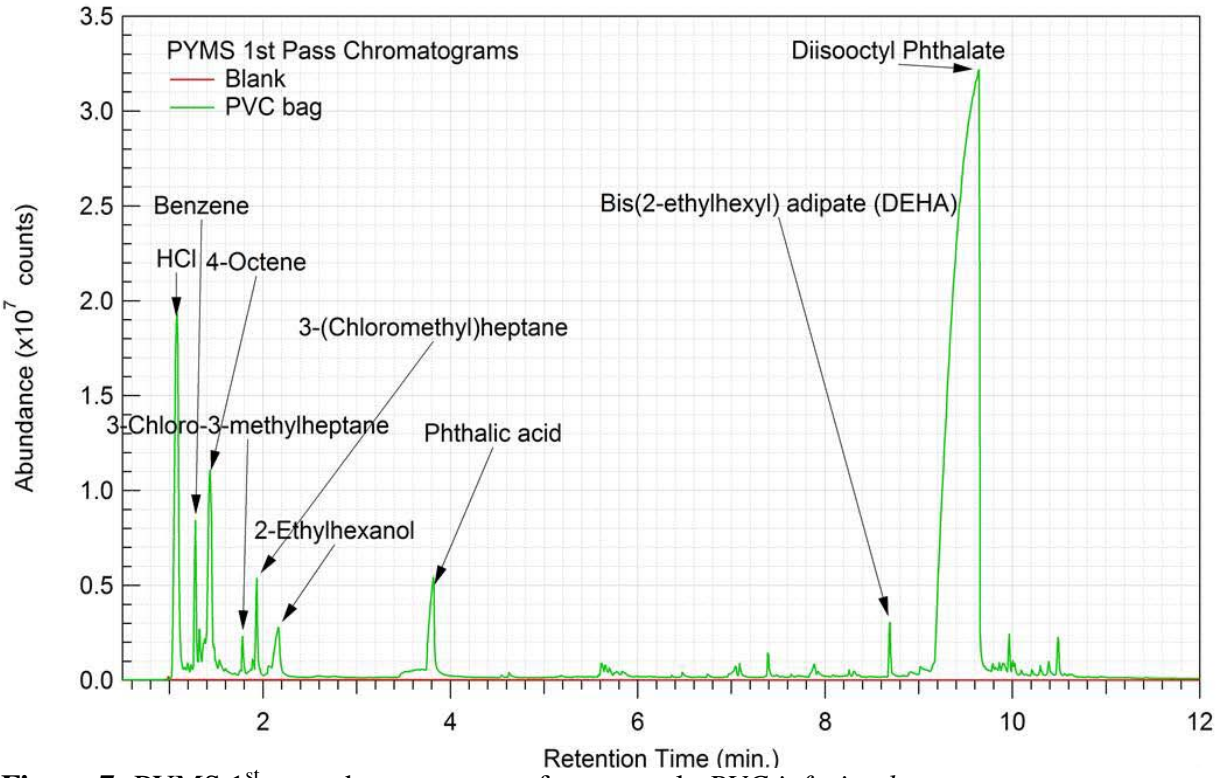


Figure 7- PYMS 1st pass chromatograms from sample *PVC infusion bag*.

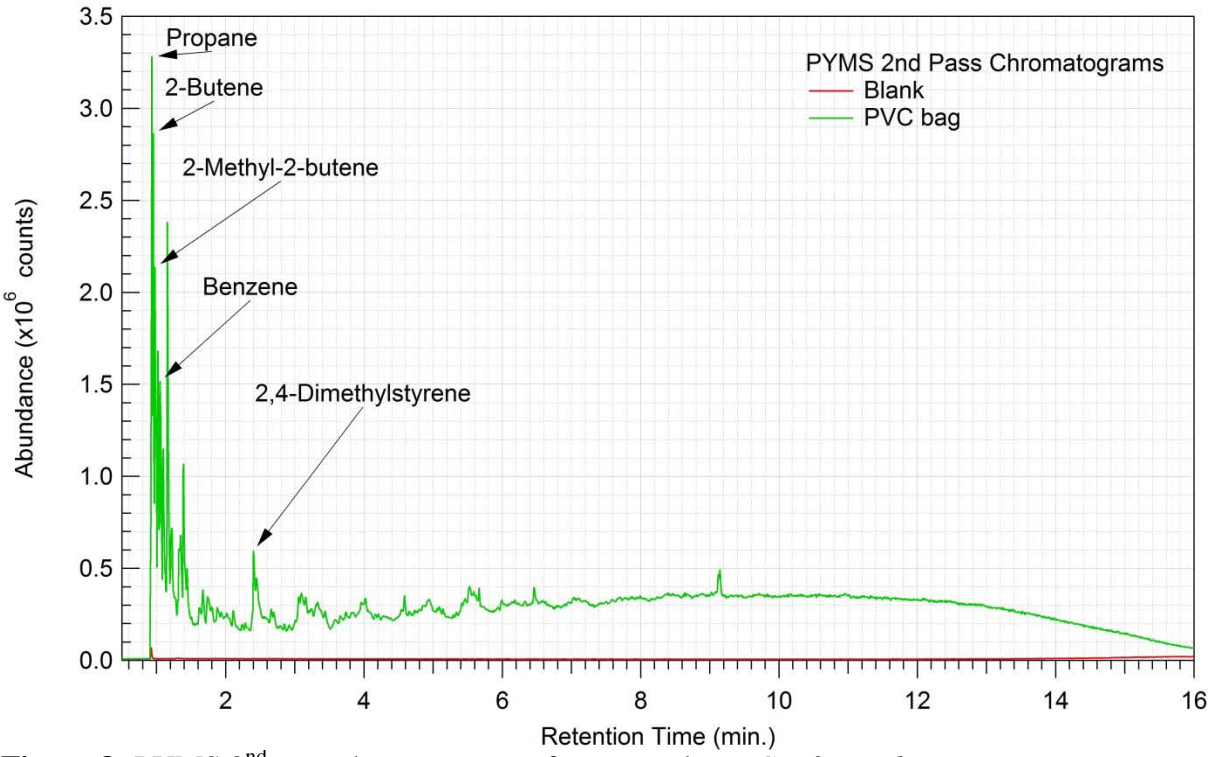


Figure 8- PYMS 2nd pass chromatograms from sample *PVC infusion bag*.

DHGCMS

Samples were analyzed directly by DHGCMS in order to investigate the volatile components which are present in the infusion bags. **Figure 9** and **Figure 10** include the collected chromatograms for sample *EVA infusion bag* and *PVC infusion bag*, respectively. The mass spectra observed were searched against the NIST mass spectral database. The resulting best matching compounds are summarized in **Table 5** and **Table 6** respectively.

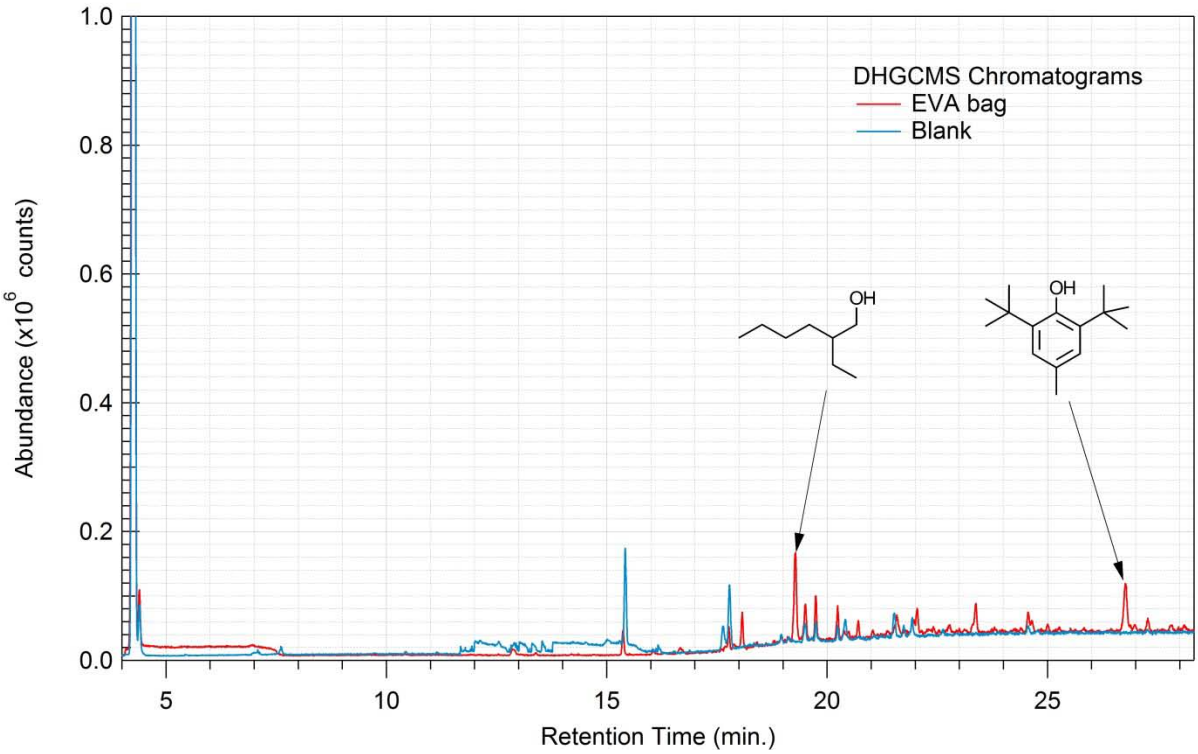


Figure 9- DHGCMS chromatograms collected from sample *EVA infusion bag*.

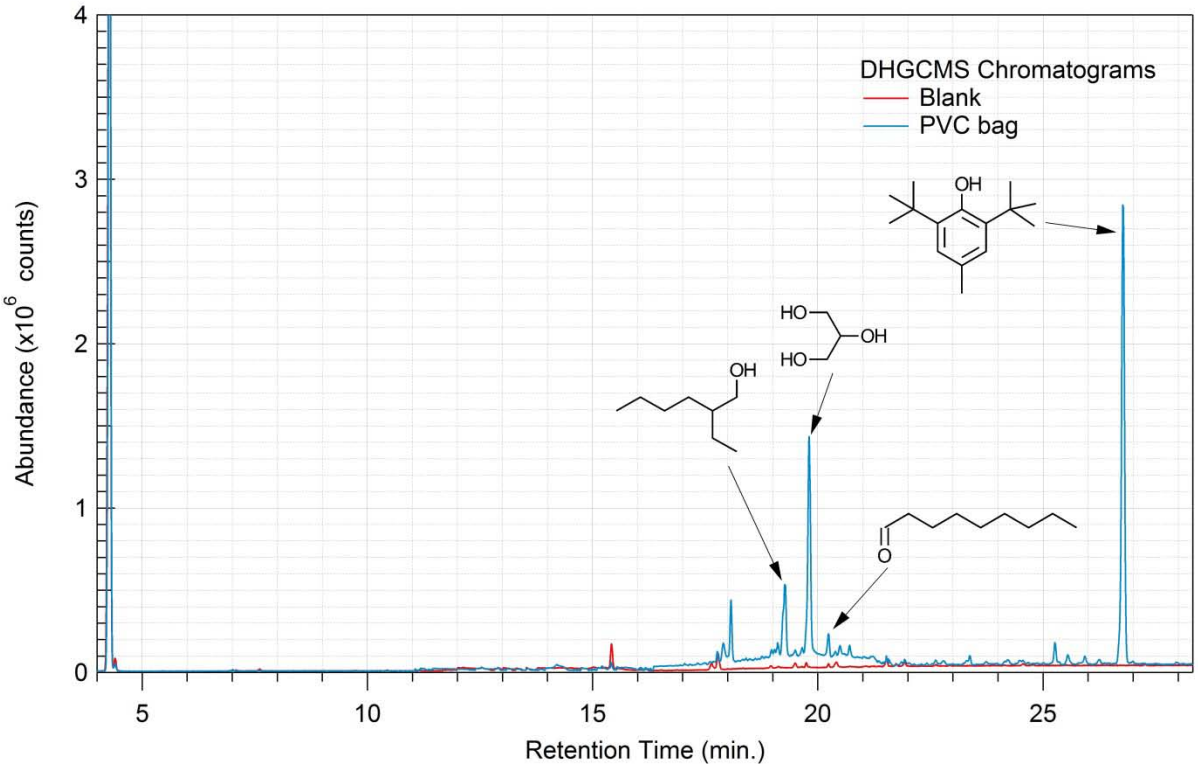


Figure 10- DHGCMS chromatograms collected from sample *PVC infusion bag*.

Table 5 **DHGCMS Results summary from Sample *EVA Infusion Bag***	
Chemical Name	CAS
Acetic acid	64-19-7
Hexanal	66-25-1
Diethyl Phthalate	84-66-2
Cyclohexanone	108-94-1
2-Ethyl-1-hexanol	104-76-7
Phenol	108-95-2
1,3-bis(1,1-dimethylethyl)-Benzene	1014-60-4
Butylated Hydroxytoluene	128-37-0
Cyclopentanone, 2-methyl-	1120-72-5
Nonanal	124-19-6

Table 6 **DHGCMS Results summary from Sample *PVC Infusion Bag***	
Chemical Name	CAS
2-Ethyl-1-hexanol	104-76-7
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester	74381-40-1
Cyclohexanone	108-94-1
Glycerin	56-81-5
Nonanal	124-19-6
Octane, 3-ethyl-	5881-17-4
Butylated Hydroxytoluene	128-37-0
Tetradecane	629-59-4

GCMS

The water and saline extracts were dried at approximately 50°C using a Pierce Reacti-Therm instrument under a gentle stream of nitrogen and reconstituted into approximately 2 mL of distilled dichloromethane. The reconstituted extracts were subjected to GCMS analysis. From the results shown in **Figure 11** and **Figure 12**, very few compounds were detected by GCMS. For sample *EVA infusion bag*, only hydrazinecarboxamide was detected. For sample *PVC infusion bag*, 2-ethyl-1-hexanol, phthalic anhydride and isosorbide were observed.

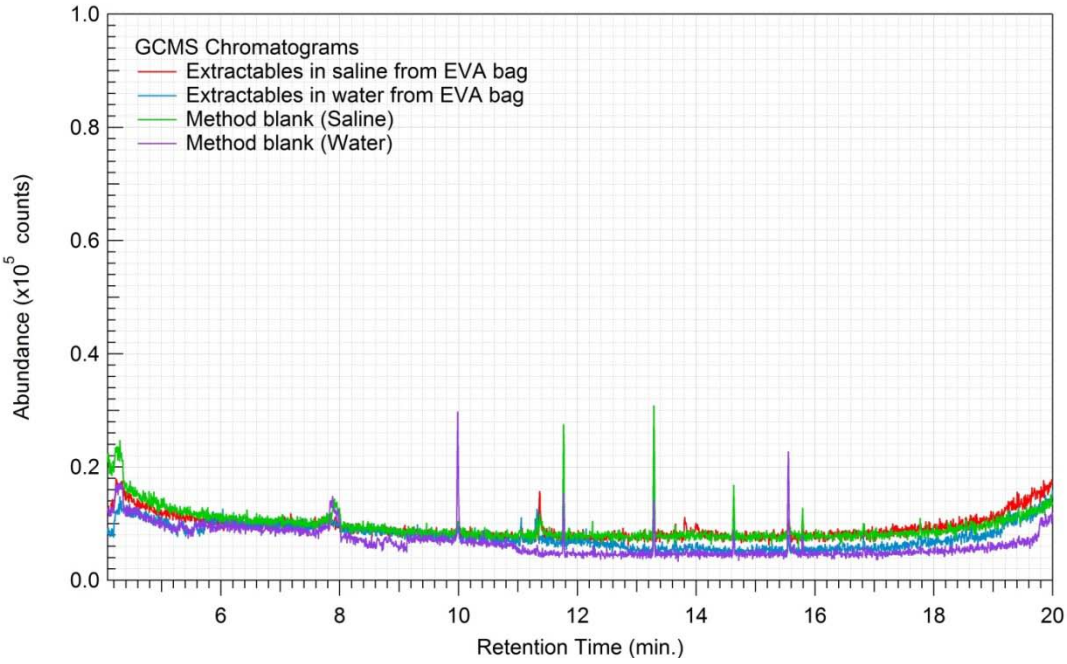


Figure 11- GCMS chromatograms collected from the leachables extracted with water or saline solution from sample EVA bag.

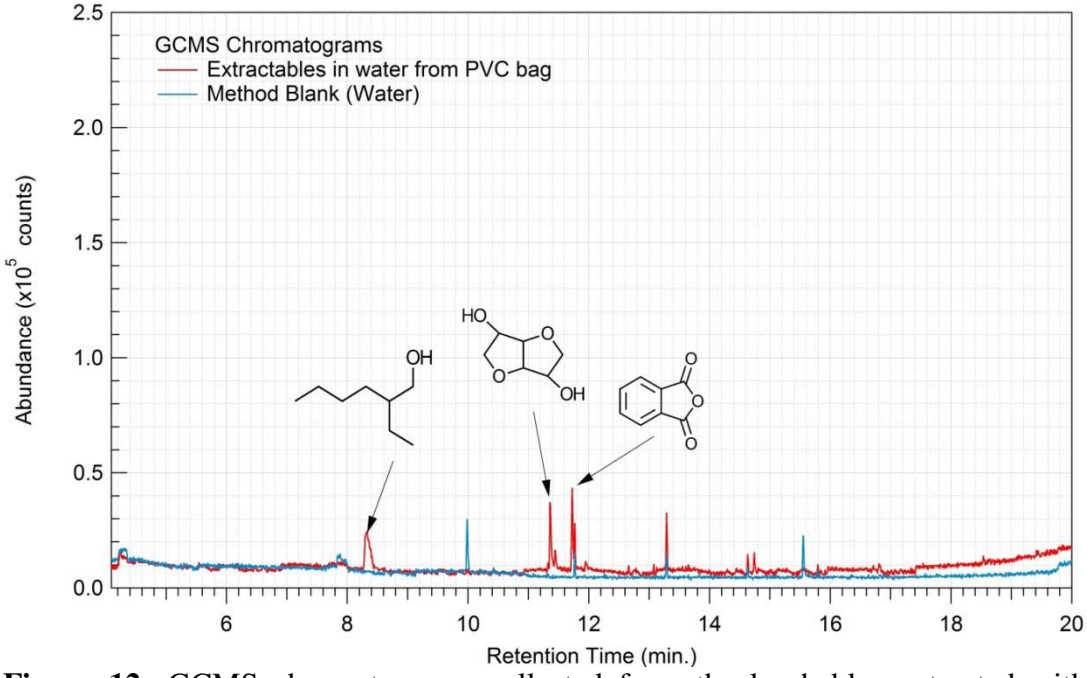


Figure 12- GCMS chromatograms collected from the leachables extracted with water from sample *PVC bag*.

LCMS

Background: QTOF-LCMS combines high mass accuracy time of flight mass spectroscopy with the power of a liquid chromatography separation to provide detailed information about the elemental composition of unknowns.

The presence of an additional quadrupole mass spectrometer (Q) provides the added capability to perform fragmentation experiments. This increases the confidence of unknown identification. It is preferable that a standard of the suspected unknown be analyzed under identical conditions as the sample. If the fragmentation patterns, high accuracy mass data, isotope patterns and LC retention times match for the unknown and standard then there is a very high probability that the identification is correct. It is possible to gain significant information about the structure of an unknown, even in cases in which standards are not available by using the molecular formula generation (MFG) algorithms contained in the Mass Hunter qualitative software.

LCMS requires that the molecule of interest be ionized. Thus, data is typically plotted in positive and negative modes indicating the charge on the ions. Ion formation is accomplished through the formation of a molecular adduct using a charge carrying species. Typical charge carriers in positive ion mode include H^+, Na^+, K^+, NH_4+ etc. Thus the observed mass is typically the mass of the compound plus the mass of the charge carrier.

The nature of the mobile phase and the ionization conditions determine the ions formed. In negative ion, the loss of hydrogen is generally observed which results in the loss of one mass unit (1.0078 amu). Other transformations are also possible including dehydration, dimer formation, etc.

A number of plots are used to aid in interpreting QTOF-LCMS data. This includes Base Peak Chromatograms (BPC), Extracted Ion Chromatograms (EIC), Extracted Compound Chromatogram (ECC), Mass spectra (MS) and Product Ion Spectra (MSMS). A BPC is formed by plotting the most intense ion at a given retention time. This spectrum is particularly useful for identifying the retention time of unknowns. EICs are formed by plotting a single mass at all retention times. This could be considered a plot of peak intensity (~compound concentration) for a single compound (and its isomers) versus retention time. ECC's are the sum of all the ions determined to be related to a single compound.

MS spectra plot the observed masses and their intensities at a single retention time. MS/MS spectra show the fragmentation pattern for a single compound. Mass Spectra plot the mass to charge ratio (m/z) and not the mass of the compound.

All structures indicated represent best estimates based on the data observed. In most cases the MS/MS fragmentation spectra have been consulted briefly to aid in identification of possible structures.

Results

Sample solutions were dried at approximately 50°C using a Pierce Reacti-Therm instrument under a gentle stream of nitrogen and reconstituted into approximately 500 µL of 80:20 methanol/isopropanol solution. The 80:20 methanol/isopropanol solution was taken through the same process and used as a control solution (Blank).

The summary of LCMS identification results both in positive mode and negative mode are listed in **Table 7** and **Table 8** for *EVA infusion bag* and *PVC infusion bag*, respectively. The overlays of the LCMS Base Peak Chromatograms (BPC) of the sample *EVA infusion bag* and the associated method blank in both positive mode and negative mode are shown in **Figures 13-14**. As shown, ions consistent with 7-Oxooctanoic acid, 9-Oxononanoic acid, 2-(Decanoylamino) propionic acid and oligomers from polyethylene glycol are observed.

The overlays of the LCMS Base Peak Chromatograms (BPC) of the sample *PVC infusion bag* and the associated method blank in both positive mode and negative mode are shown in **Figures 15-16**. As shown, ions consistent with 3,5-Bis(tert-butyl)toluene, Dibutyl phthalate, 8-Methoxy-8-oxooctyl methyl suberate, acids, Mono(2-ethylhexyl)phthalate [MEHP], Methyl 9,10-Dihydroxystearate, Diisooctyl phthalate and oligomers from polyethylene glycol are observed. The phthalates are consistent with plasticizers commonly used in PVC.

Table 7
Summary of LCMS Results – EVA infusion bag

RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
4.639	239.1496, 261.1309, 256.1760		238.1420	$C_{10}H_{22}O_6$	98.22	-1.66	Oligomer of polyethylene glycol
4.905	283.1757, 305.1576, 300.2024		282.1686	$C_{12}H_{26}O_7$	97.29	-2.71	Oligomer of polyethylene glycol
5.170	327.2025, 349.1834, 344.2284		326.1947	$C_{14}H_{30}O_8$	97.79	-1.96	Oligomer of polyethylene glycol
5.370	371.2283, 393.2101, 388.2547		370.221	$C_{16}H_{34}O_9$	97.94	-1.9	Oligomer of polyethylene glycol
5.569	415.2539, 437.2355, 432.2817		414.2477	$C_{18}H_{38}O_{10}$	96.03	-2.96	Oligomer of polyethylene glycol
5.768	385.2435, 407.2248, 402.2703		384.2157	$C_{17}H_{36}O_9$	98.16	-1.63	Oligomer of polyethylene glycol
6.033	429.2701, 446.2976		428.2636	$C_{19}H_{40}O_{10}$	94.59	-3.36	Oligomer of polyethylene glycol
6.232	399.2593, 421.2409, 416.2859		398.2523	$C_{18}H_{38}O_9$	97.67	-1.76	Oligomer of polyethylene glycol

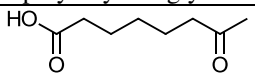
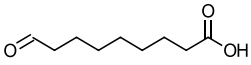
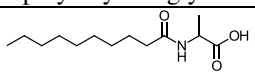
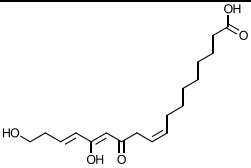
Table 7 Summary of LCMS Results – EVA infusion bag							
RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
6.365	465.2658, 460.3121		442.2784	$C_{20}H_{40}O_{10}$	98.13	-1.42	Oligomer of polyethylene glycol
6.498	509.2930, 504.3383		486.3047	$C_{22}H_{46}O_{11}$	98.16	-1.4	Oligomer of polyethylene glycol
6.631	553.3187, 548.3646		530.3310	$C_{24}H_{50}O_{12}$	97.82	-1.46	Oligomer of polyethylene glycol
6.692		157.0864	158.0938	$C_8H_{14}O_3$	97.74	3.35	 7-Oxooctanoic acid
6.764	430.3015		412.2678	$C_{19}H_{40}O_9$	98.53	-1.42	Oligomer of polyethylene glycol
6.963	474.3284		456.2944	$C_{21}H_{44}O_{10}$	97.61	-2.14	Oligomer of polyethylene glycol
7.162	562.3801		544.3462	$C_{25}H_{52}O_{12}$	99.53	-0.68	Oligomer of polyethylene glycol
7.560	620.4226		602.3888	$C_{28}H_{58}O_{13}$	97.62	-1.81	Oligomer of polyethylene glycol
7.627	664.4487		646.4149	$C_{30}H_{62}O_{14}$	97.87	-1.45	Oligomer of polyethylene glycol
7.892	451.3085		900.6019	$C_{45}H_{88}O_{17}$	98.55	0.29	Oligomer of polyethylene glycol
8.091	671.4384		1306.8083	$C_{60}H_{122}O_{29}$	98.84	-0.85	Oligomer of polyethylene glycol
8.224	524.3557		1046.6961	$C_{52}H_{102}O_{20}$	98.84	0.31	Oligomer of polyethylene glycol
8.290	546.3691		1090.7232	$C_{54}H_{106}O_{21}$	99.27	-0.45	Oligomer of polyethylene glycol
8.484		171.1022	172.1094	$C_9H_{16}O_3$	98.14	2.93	 9-Oxononanoic acid
8.556	538.3487		1040.6292	$C_{55}H_{92}O_{18}$	98.09	-0.83	Oligomer of polyethylene glycol
8.821	626.4237		1250.8319	$C_{62}H_{122}O_{24}$	98.73	0.54	Oligomer of polyethylene glycol
8.888	582.3974		1162.7795	$C_{58}H_{114}O_{22}$	98.63	0.56	Oligomer of polyethylene glycol
9.153	699.4699		1362.8707	$C_{64}H_{130}O_{29}$	98.81	-0.67	Oligomer of polyethylene glycol
9.215	242.1761		243.1833	$C_{13}H_{25}NO_3$	98.57	0.5	 2-(Decanoylamino)propionic acid
10.941		323.1891	324.1959	$C_{18}H_{28}O_5$	72.12	-6.76	 14,18-Dihydroxy-12-oxo-9,13,15-

Table 7 Summary of LCMS Results – EVA infusion bag							
RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
							octadecatrienoic acid

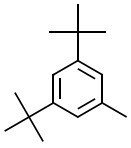
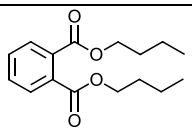
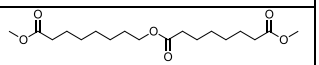
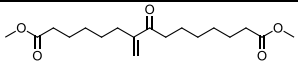
Table 8 Summary of LCMS Results – PVC infusion bag							
RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
4.500	227.1758		204.1865	$C_{15}H_{24}$	87.88	6.5	 3,5-Bis(*tert*-butyl)toluene
5.363	223.1542		222.1461	$C_{10}H_{22}O_5$	70.39	2.79	Oligomer of polyethylene glycol
5.496	267.1812		267.1812	$C_{12}H_{26}O_6$	95.99	-3.07	Oligomer of polyethylene glycol
5.828	267.1806, 289.1631		266.1734	$C_{12}H_{26}O_6$	98.82	-1.72	Isomer of polyethylene glycol
6.160	311.2072		310.2000	$C_{14}H_{30}O_7$	97.09	-2.71	Oligomer of polyethylene glycol
6.359	335.2335		354.2262	$C_{16}H_{34}O_8$	97.33	-2.49	Oligomer of polyethylene glycol
6.624	399.2601, 416.2860, 421.2406		398.2520	$C_{18}H_{38}O_9$	98.09	-0.96	Oligomer of polyethylene glycol
6.956	296.1861		278.1521	$C_{16}H_{22}O_4$	99.30	-1.15	 Dibutyl phthalate
7.421	441.2695, 463.2521, 458.2962		440.2620	$C_{20}H_{40}O_{10}$	96.64	0.27	Oligomer of polyethylene glycol
7.620	321.1906, 343.1724, 338.2168		320.1833	$C_{15}H_{28}O_7$	99.19	0.73	Derivatives of polyethylene glycol
7.753	365.2179, 387.1990, 382.2442		364.2103	$C_{17}H_{32}O_8$	98.83	-1.71	Derivatives of polyethylene glycol
7.886	409.2438, 431.2256, 426.2713		408.2367	$C_{19}H_{36}O_9$	96.37	-1.89	Derivatives of polyethylene glycol
8.284	345.2271, 367.2095, 362.2519		344.2199	$C_{18}H_{32}O_6$	85.84	-0.08	 8-Methoxy-8-oxooctyl methyl suberate
8.483	327.2161		326.2088	$C_{18}H_{30}O_5$	84.31	1.7	 Dimethyl 7-methylene-8-oxopentadecanedioate

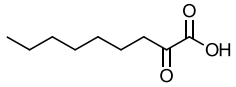
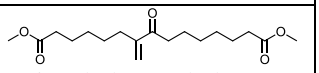
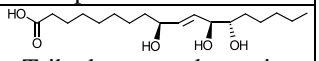
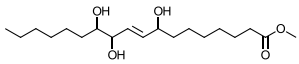
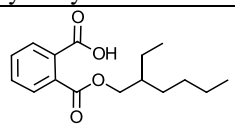
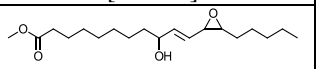
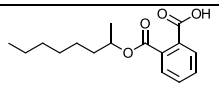
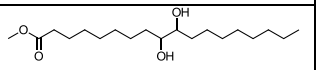
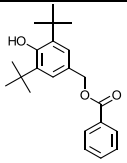
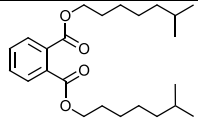
Table 8 Summary of LCMS Results – PVC infusion bag							
RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
8.491		171.1023	172.1095	$C_9H_{16}O_3$	97.81	2.51	 Oxononanoic acid
9.241	341.2326		340.2253	$C_{19}H_{32}O_5$	93.33	-0.99	 Dimethyl 7-methylene-8-oxopentadecanedioate
9.752	331.2485, 353.2312, 348.2749	329.2344	330.2416	$C_{18}H_{34}O_5$	95.56	-2.86	 Trihydroxyoctadecenoic acid
10.143	353.2314, 348.2743	329.2342	352.2240	$C_{18}H_{34}O_5$	92.92	-4.37	Isomer of Trihydroxyoctadecenoic acid
10.342	345.2642		344.2570	$C_{19}H_{36}O_5$	98.42	-1.99	 Methyl (9E)-8,11,12-trihydroxy-9-octadecenoate
10.748	279.1802	277.1451	278.1731	$C_{16}H_{22}O_4$	95.43	-0.47	 Mono(2-ethylhexyl)phthalate [MEHP]
11.139	327.2527, 349.2336, 344.2807		326.2466	$C_{19}H_{34}O_4$	95.25	-2.71	 Methyl (10E)-9-hydroxy-11-(3-pentyl-2-oxiranyl)-10-undecenoate
11.279		277.1438	278.1513	$C_{16}H_{22}O_4$	82.61	1.73	 2-[(2-Octanyloxy)carbonyl]benzoic acid
11.405	331.2843		330.2764	$C_{19}H_{38}O_4$	87.68	1.85	 Methyl 9,10-Dihydroxystearate
11.611		339.1996	340.2065	$C_{22}H_{28}O_3$	68.45	-7.68	 3,5-di-tert-butyl-4-hydroxybenzyl benzoate

Table 8 Summary of LCMS Results – PVC infusion bag							
RT	*Positive m/z*	*Negative m/z*	Mass	Best Match	Score	Diff.	Possible ID
12.334	391.2863		390.279	$C_{24}H_{38}O_4$	89.37	-4.97	 Diisooctyl phthalate

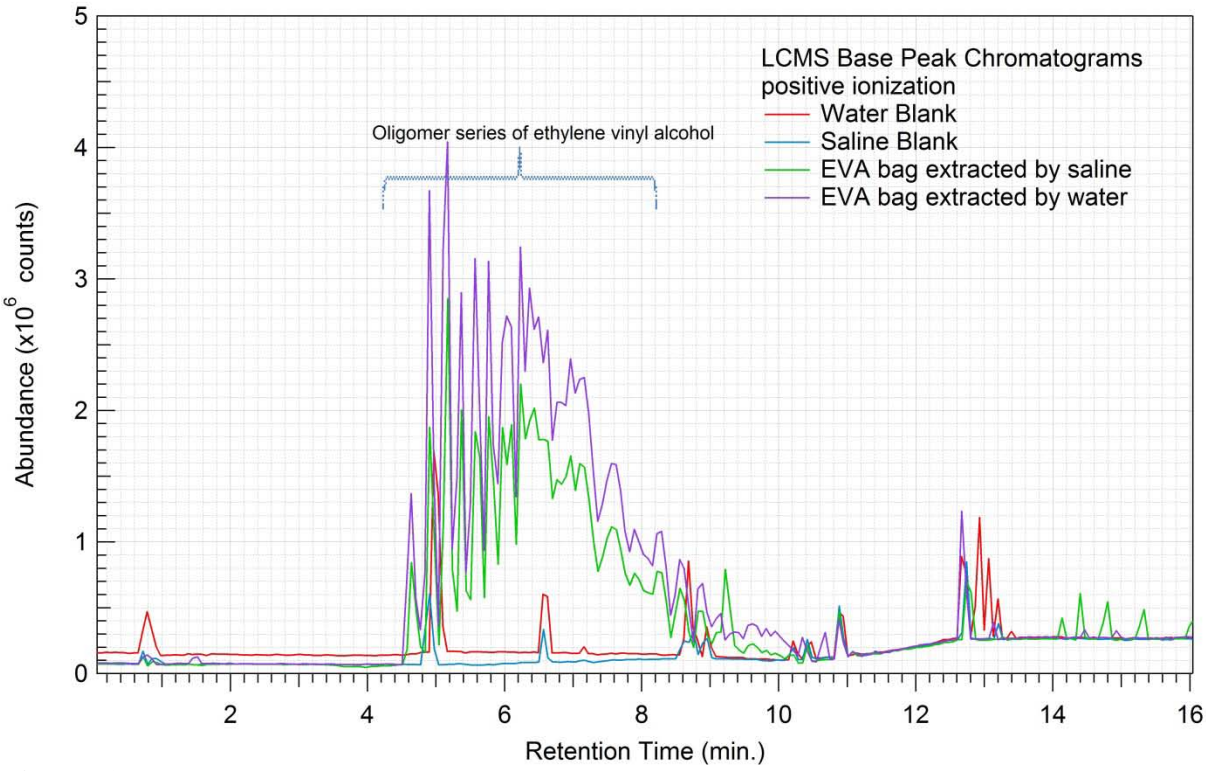


Figure 13- Overlay of LCMS base peak chromatograms, positive ionization from sample *EVA bag*.

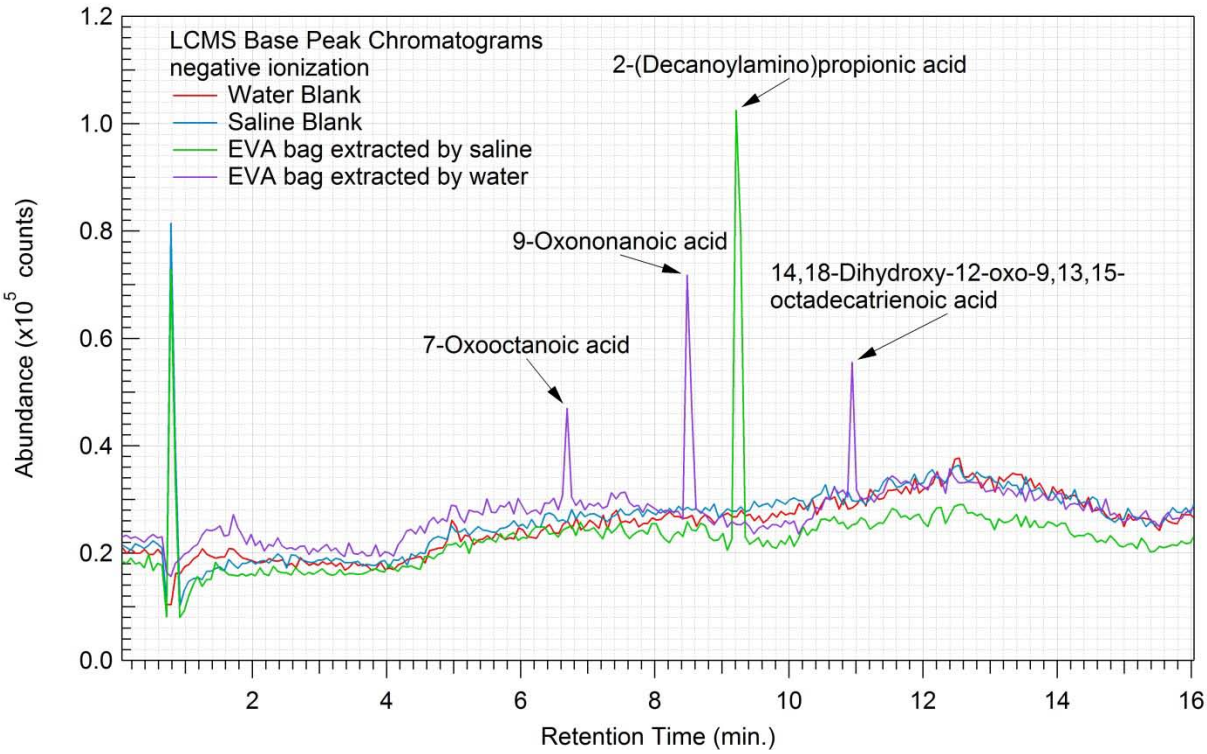


Figure 14- Overlay of LCMS base peak chromatograms, negative ionization from sample *EVA bag*.

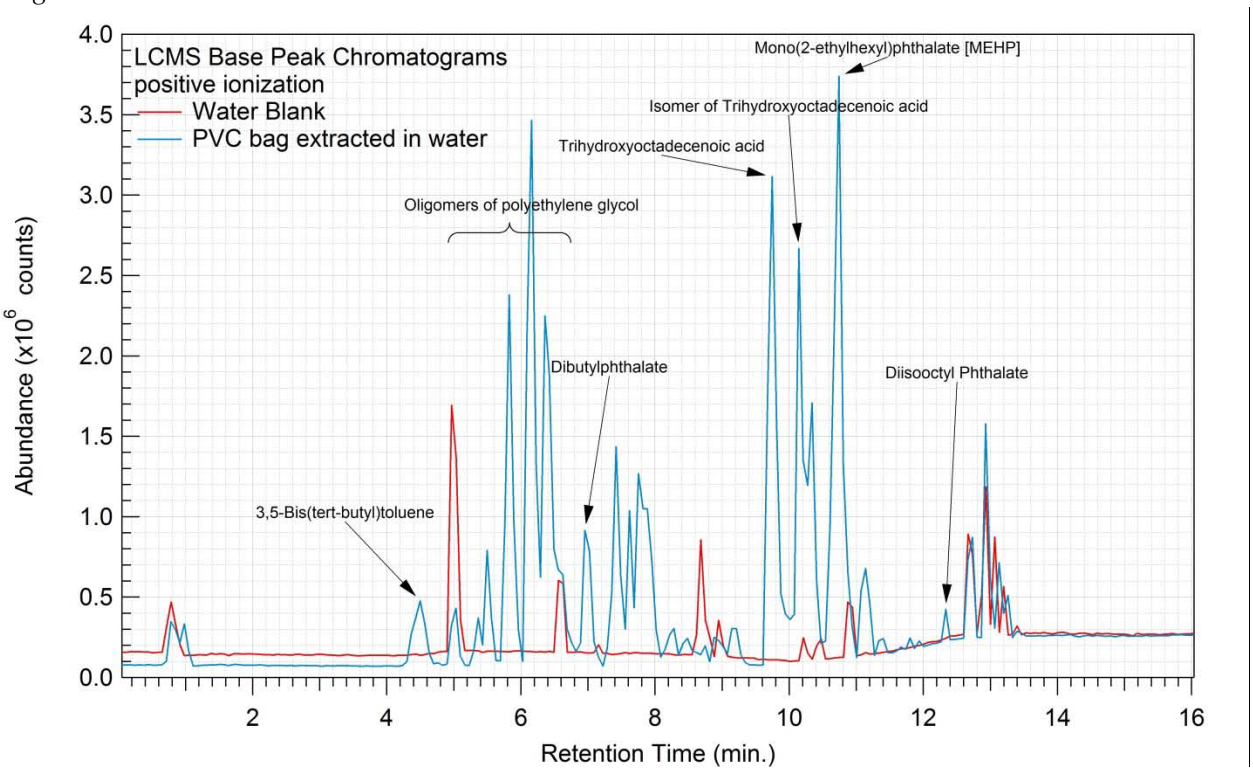


Figure 15- Overlay of LCMS base peak chromatograms, positive ionization from sample *PVC bag*.

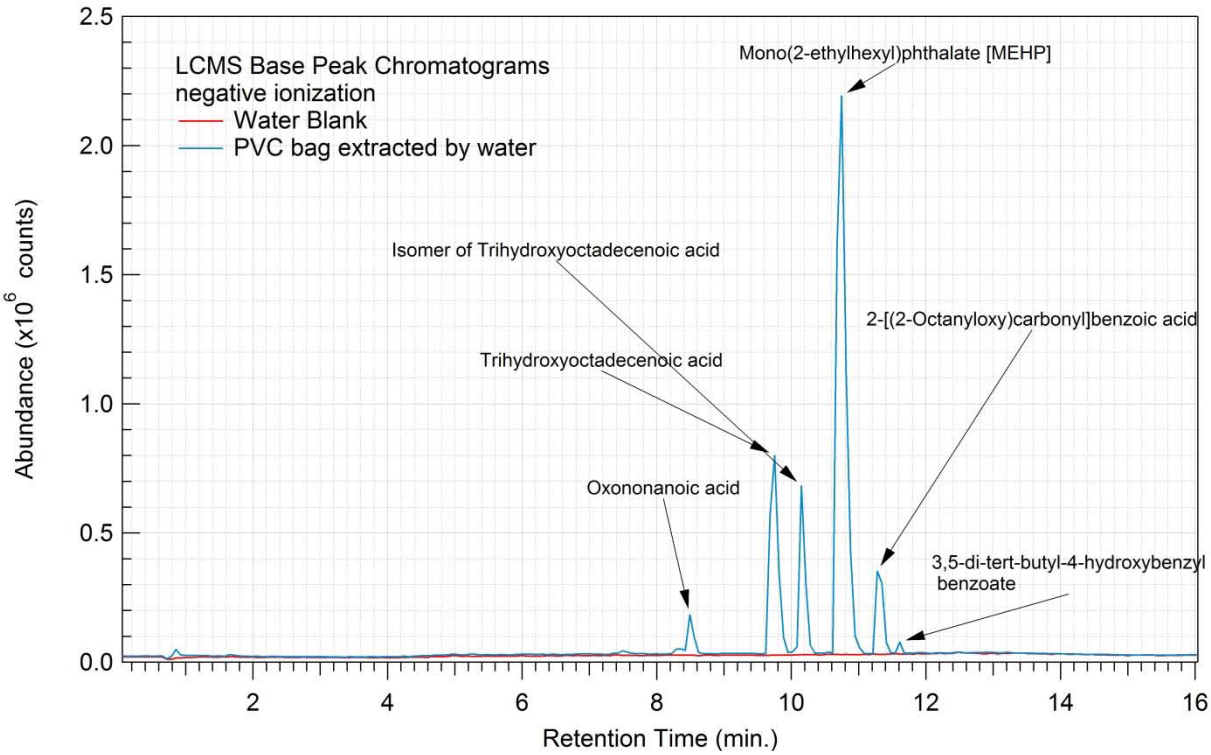


Figure 16- Overlay of LCMS base peak chromatograms, negative ionization from sample *PVC bag*.

Analysis Conditions

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

Jordi Labs' reports are issued solely for the use of the clients to whom they are addressed. No quotations from reports or use of the Jordi name is permitted except as authorized in writing. The liability of Jordi Labs with respect to the services rendered shall be limited to the amount of consideration paid for such services and do not include any consequential damages.

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,

Longxi Xiao

Longxi Xiao, Ph. D.
Senior Chemist
Jordi Labs LLC

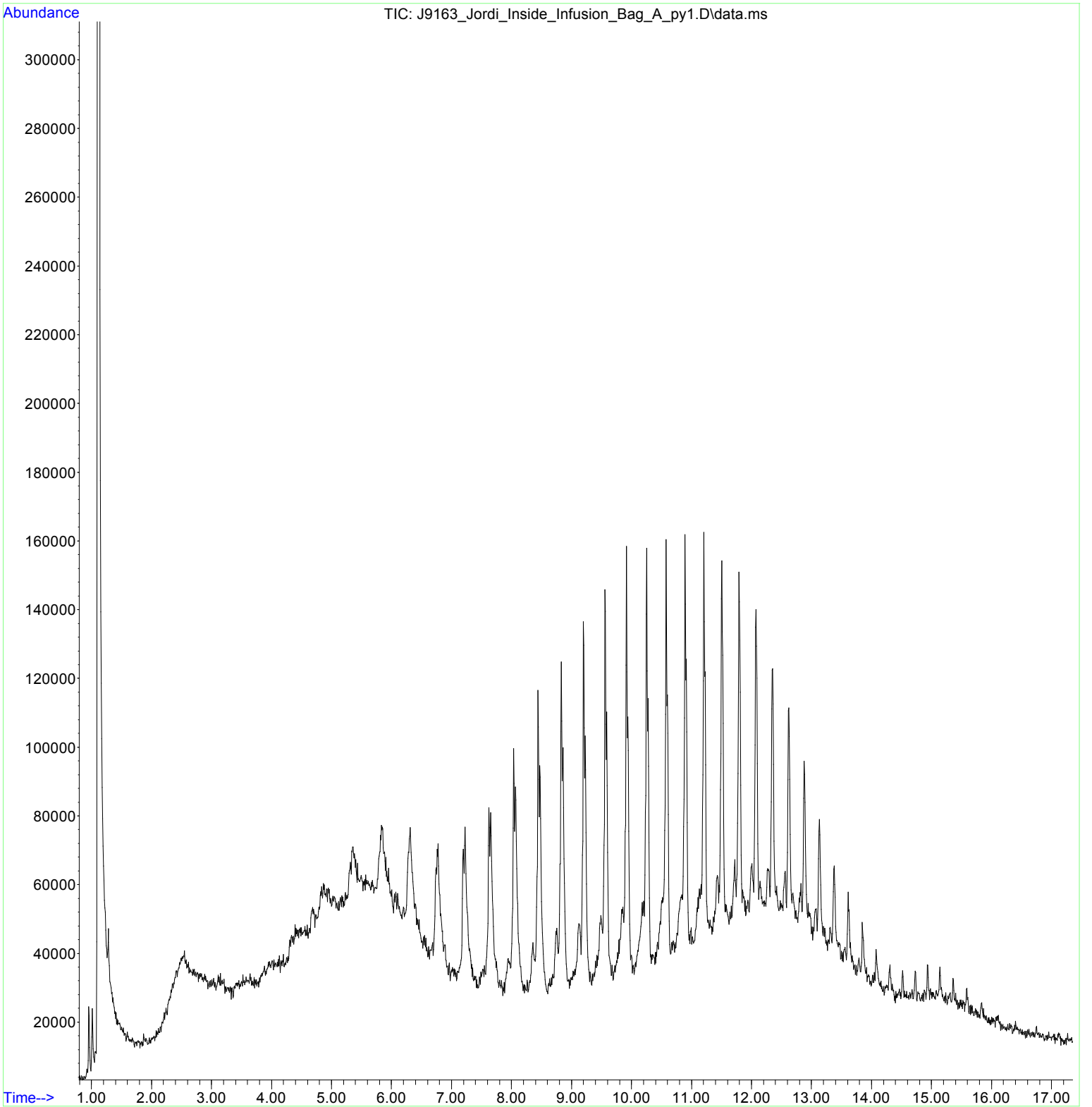
Mark Jordi

Mark Jordi, Ph. D.
President
Jordi Labs LLC

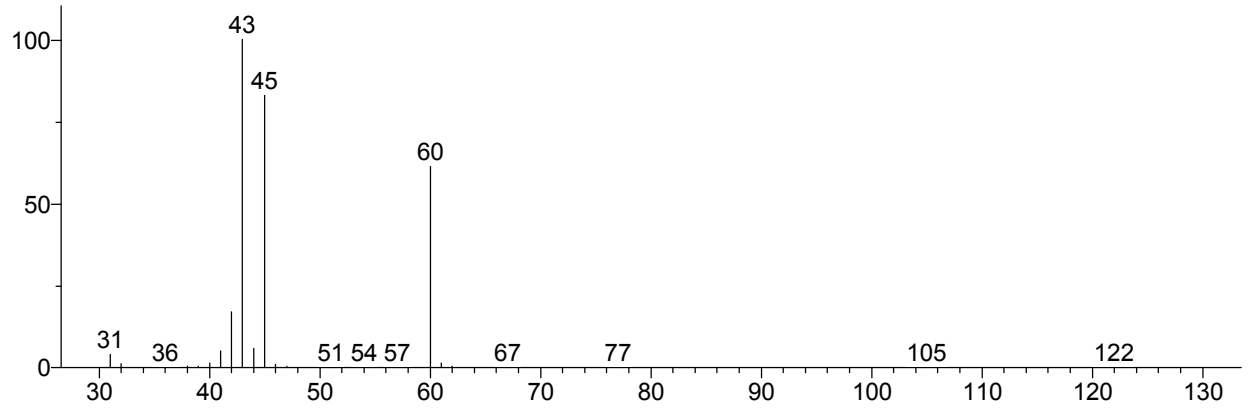
Appendix

PYMS Data

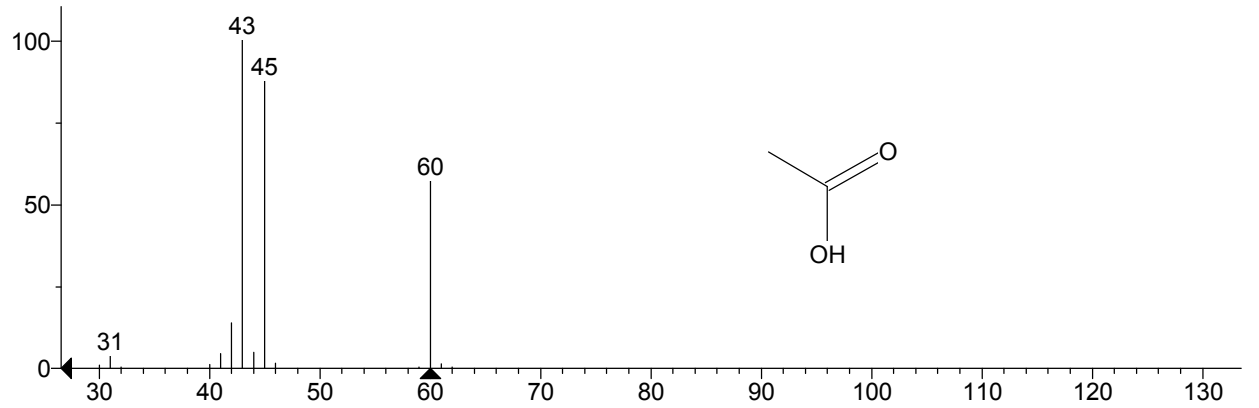
File :C:\msdchem\1\DATA\2014\Temp\102014\J9163_Jordi_Inside_Infusi
... on_Bag_A_py1.D
Operator : Julia Berk
Instrument : Instrument #1
Acquired : 21 Oct 2014 14:59 using AcqMethod PYMSSP30.M
Sample Name: J9163 Jordi Inside Infusion Bag
Misc Info : J9163 Jordi Inside Infusion Bag



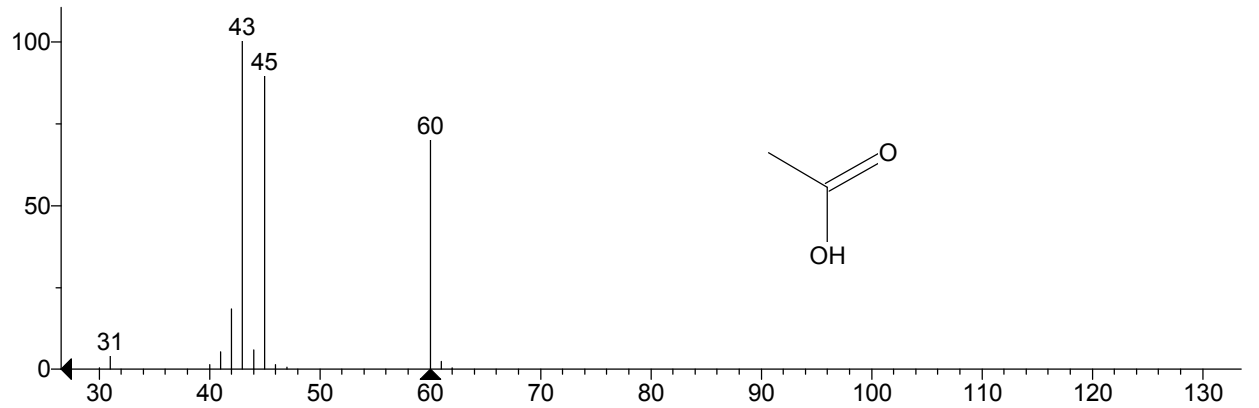
Unknown: Scan 138 (1.127 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = 584



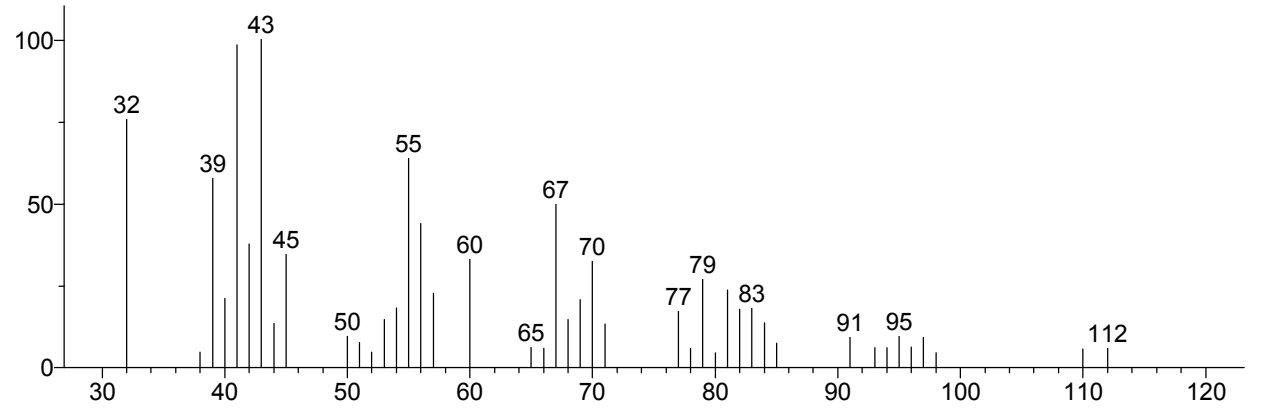
Hit 1 : Acetic acid
C2H4O2; MF: 953; RMF: 957; Prob 97.3%; CAS: 64-19-7; Lib: replib; ID: 1868.



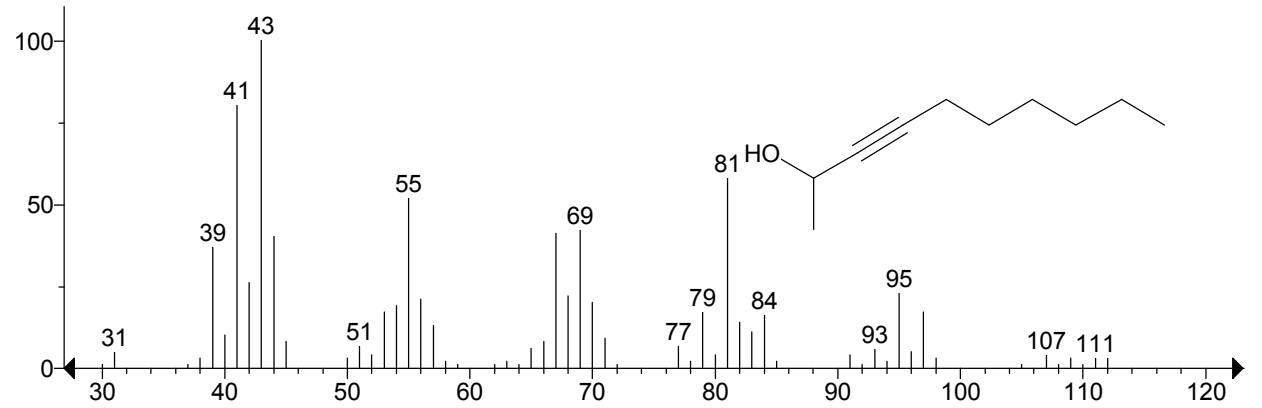
Hit 2 : Acetic acid
C2H4O2; MF: 943; RMF: 947; Prob 97.3%; CAS: 64-19-7; Lib: replib; ID: 1870.



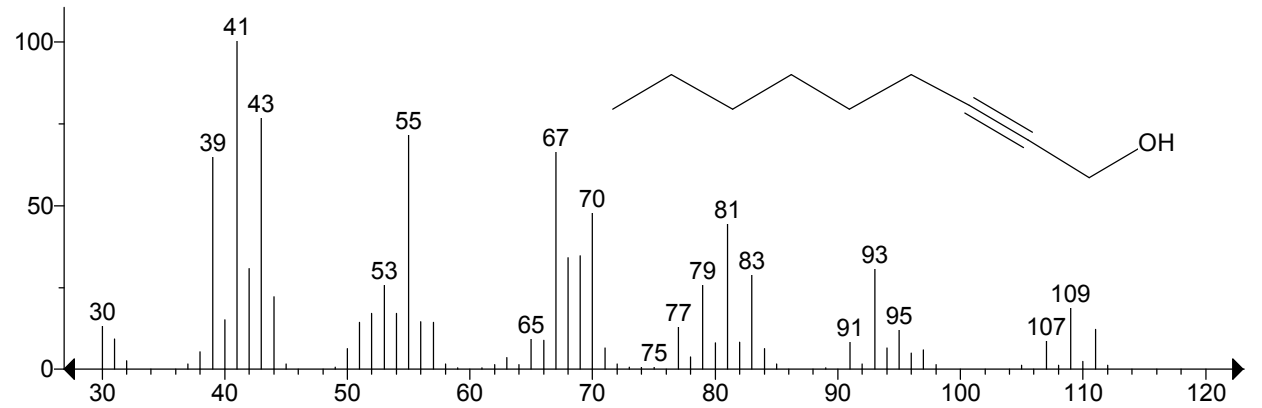
Unknown: Scan 326 (2.544 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -858



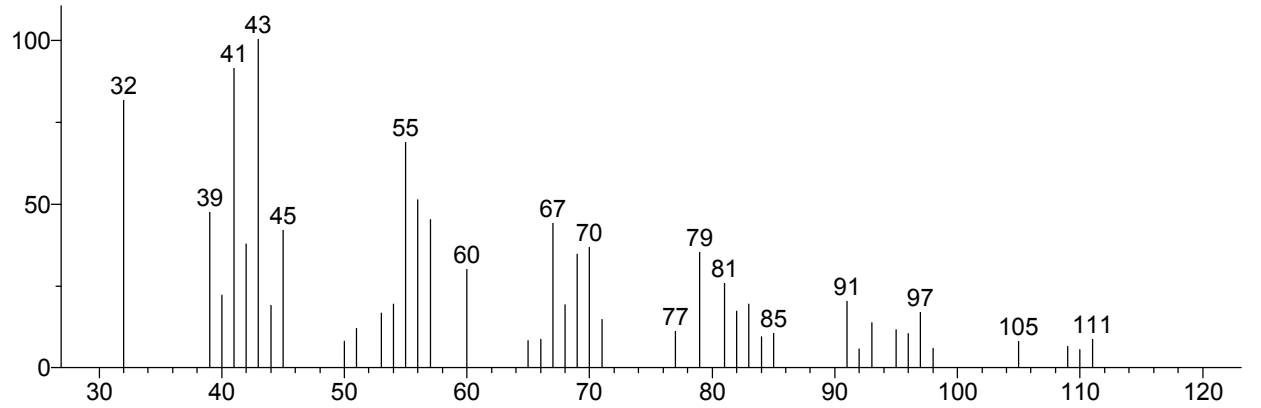
Hit 1 : 3-Decyn-2-ol
C10H18O; MF: 765; RMF: 802; Prob 4.82%; CAS: 69668-93-5; Lib: mainlib; ID: 5859.



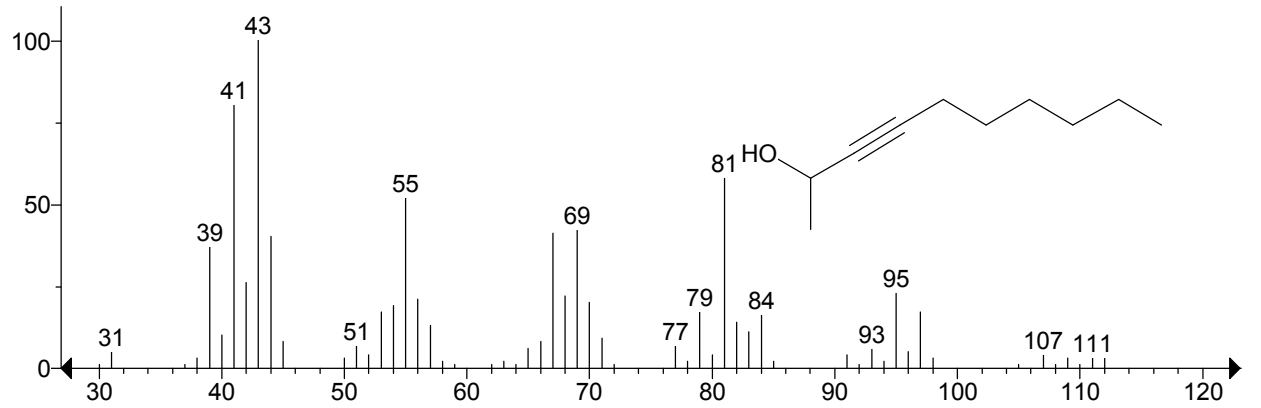
Hit 2 : 2-Nonyn-1-ol
C9H16O; MF: 759; RMF: 775; Prob 3.79%; CAS: 5921-73-3; Lib: replib; ID: 827.



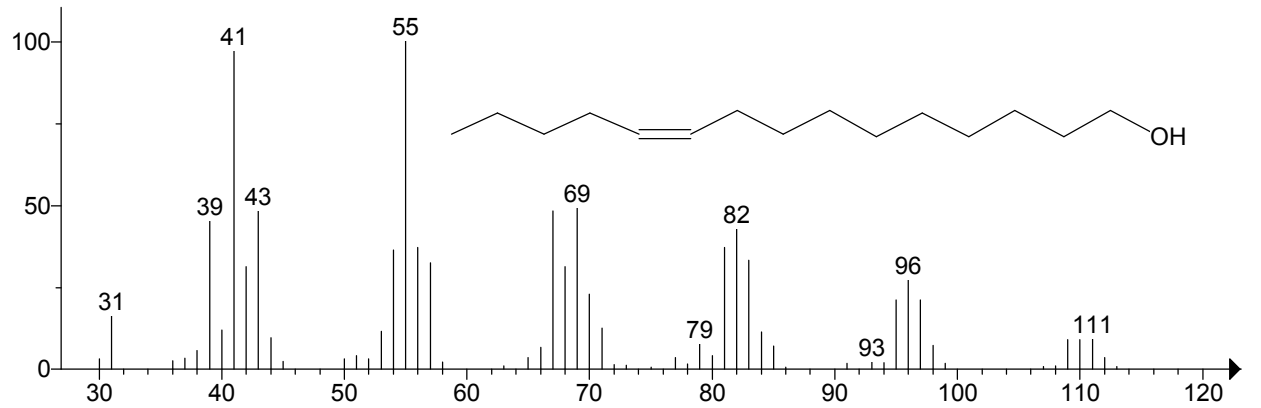
Unknown: Scan 408 (3.162 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -625



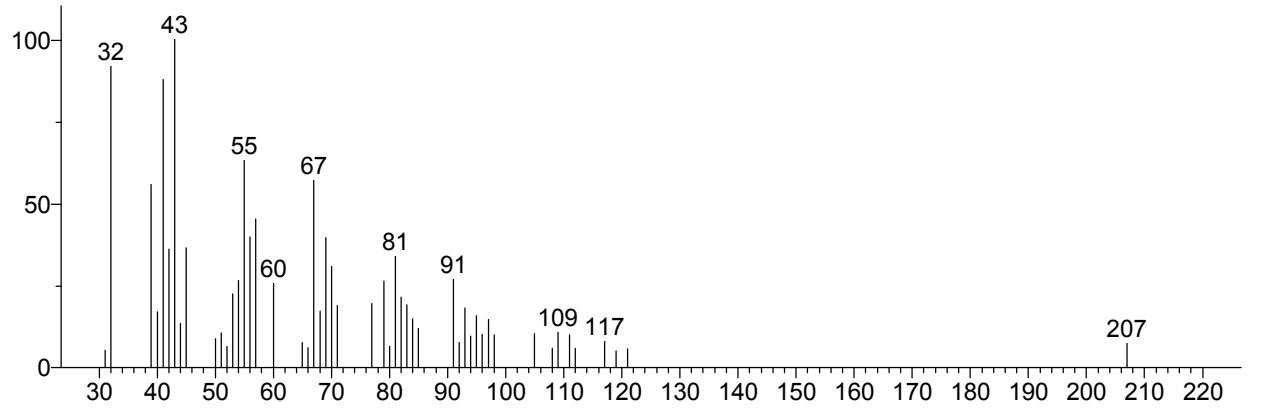
Hit 1 : 3-Decyn-2-ol
C10H18O; MF: 765; RMF: 798; Prob 6.00%; CAS: 69668-93-5; Lib: mainlib; ID: 5859.



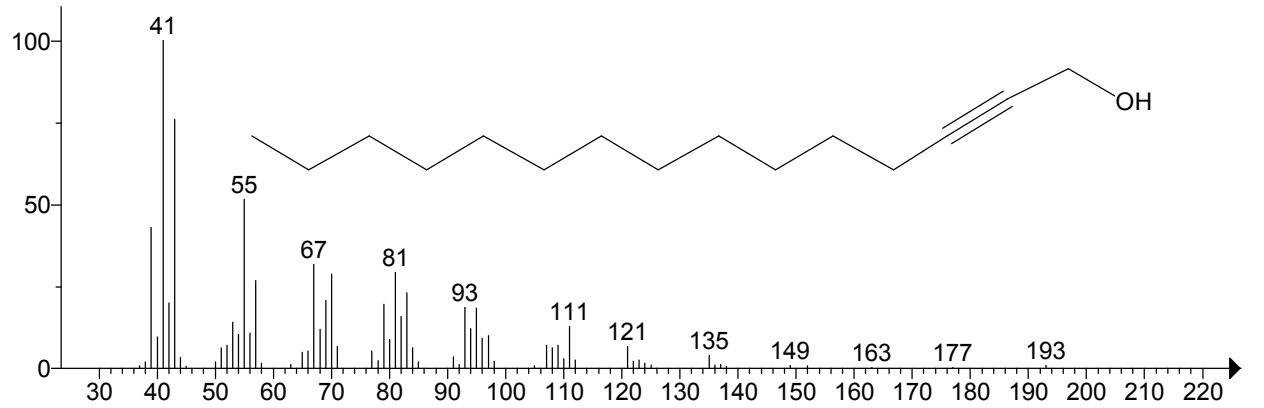
Hit 2 : Z-10-Pentadecen-1-ol
C15H30O; MF: 753; RMF: 794; Prob 3.99%; Lib: mainlib; ID: 17434.



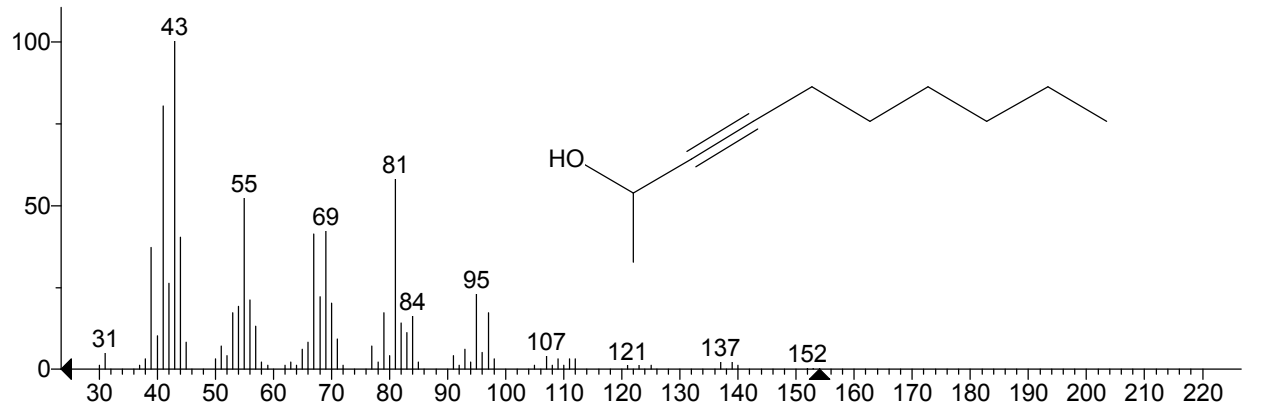
Unknown: Scan 523 (4.028 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -625



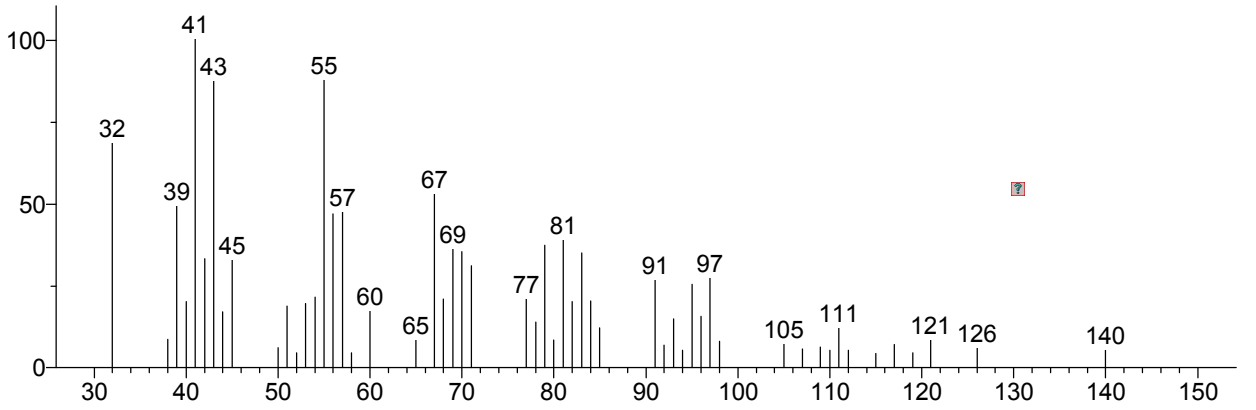
Hit 1 : 2-Pentadecyn-1-ol
C15H28O; MF: 763; RMF: 792; Prob 8.17%; CAS: 2834-00-6; Lib: mainlib; ID: 2205.



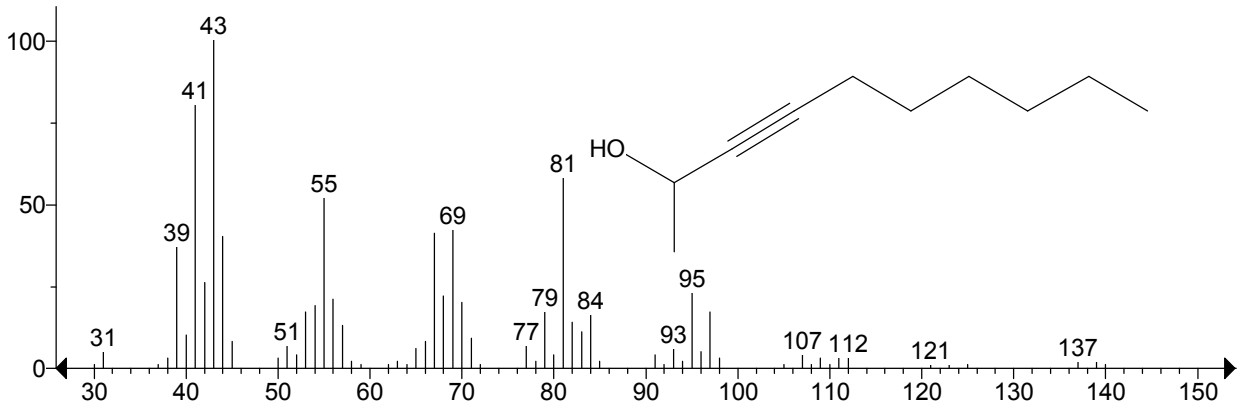
Hit 2 : 3-Decyn-2-ol
C10H18O; MF: 760; RMF: 808; Prob 7.22%; CAS: 69668-93-5; Lib: mainlib; ID: 5859.



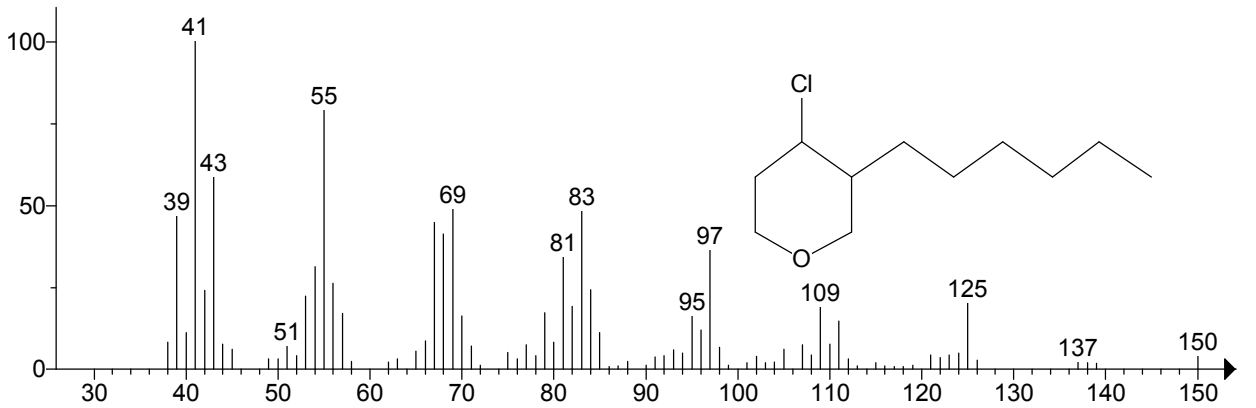
Unknown: Scan 578 (4.443 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -811



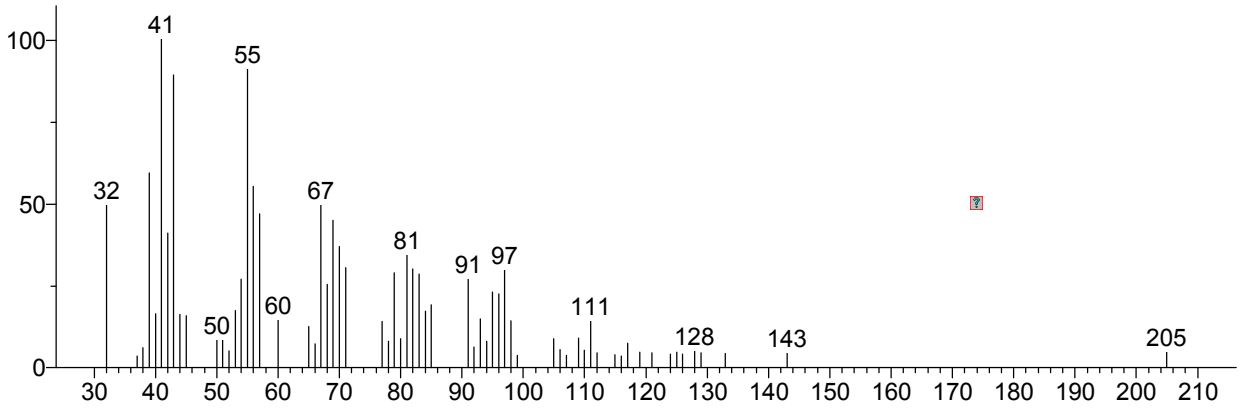
Hit 1 : 3-Decyn-2-ol
C10H18O; MF: 777; RMF: 811; Prob 6.31%; CAS: 69668-93-5; Lib: mainlib; ID: 5859.



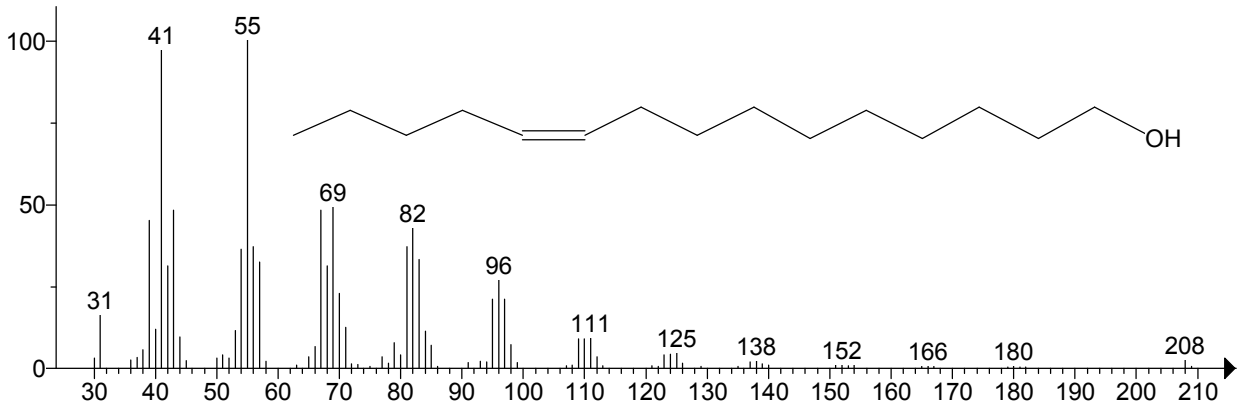
Hit 2 : 4-Chloro-3-n-hexyltetrahydropyran
C11H21ClO; MF: 776; RMF: 786; Prob 6.07%; CAS: 66555-66-6; Lib: mainlib; ID: 2467.



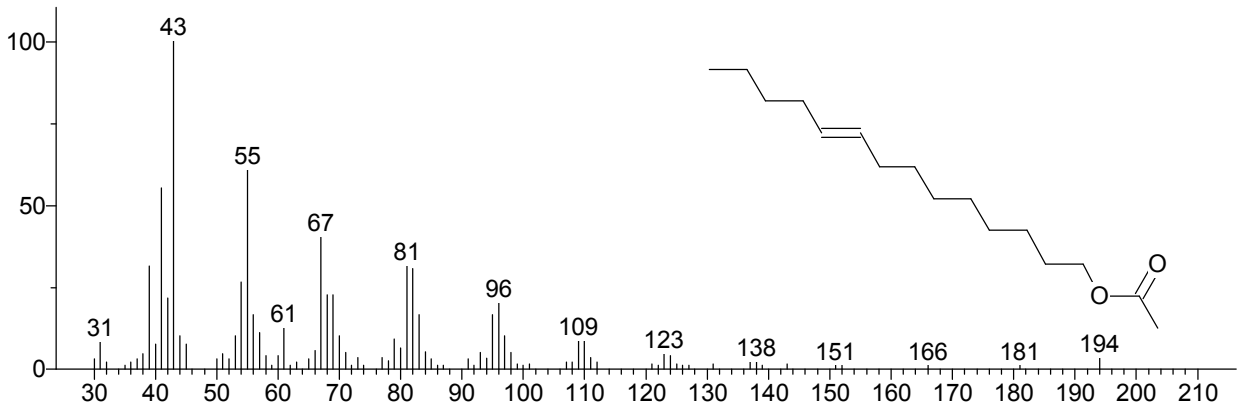
Unknown: Scan 637 (4.887 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -520



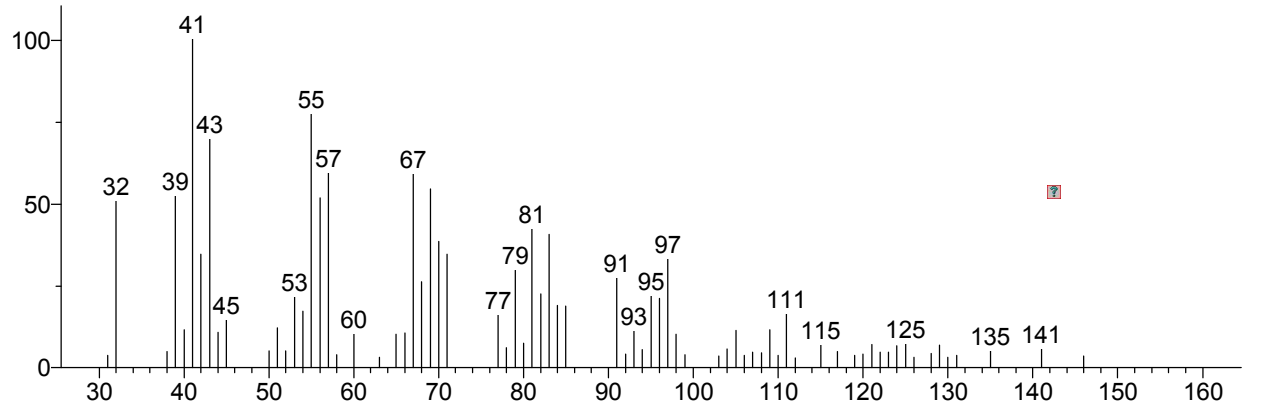
Hit 1 : Z-10-Pentadecen-1-ol
C15H30O; MF: 790; RMF: 842; Prob 7.26%; Lib: mainlib; ID: 17434.



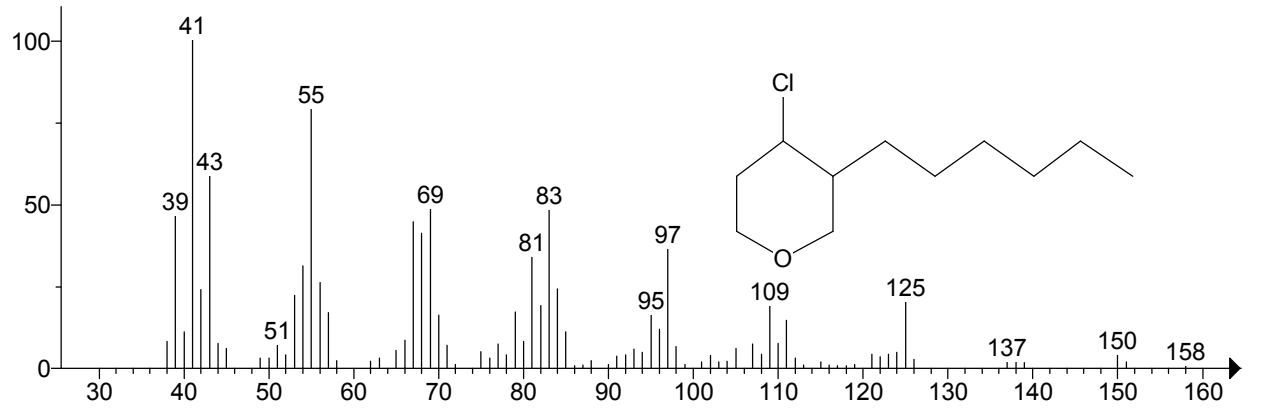
Hit 2 : 9-Tetradecen-1-ol, acetate, (E)-
C16H30O2; MF: 774; RMF: 807; Prob 4.18%; CAS: 23192-82-7; Lib: mainlib; ID: 6711.



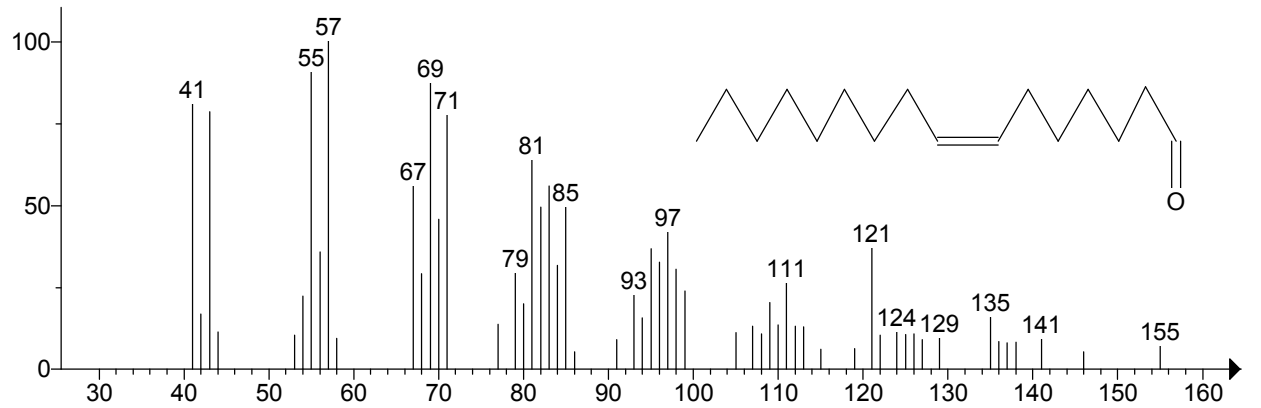
Unknown: Scan 701 (5.370 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -457



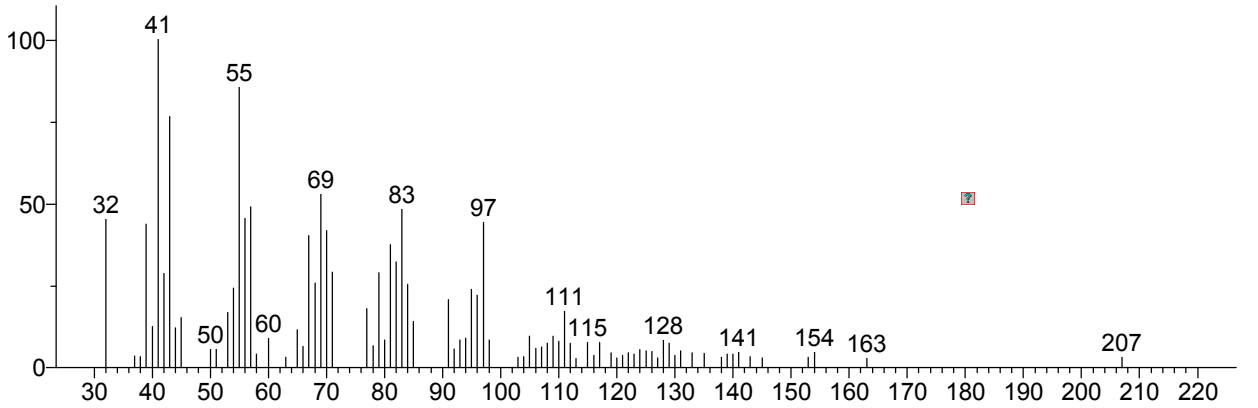
Hit 1 : 4-Chloro-3-n-hexyltetrahydropyran
C11H21ClO; MF: 802; RMF: 833; Prob 16.0%; CAS: 66555-66-6; Lib: mainlib; ID: 2467.



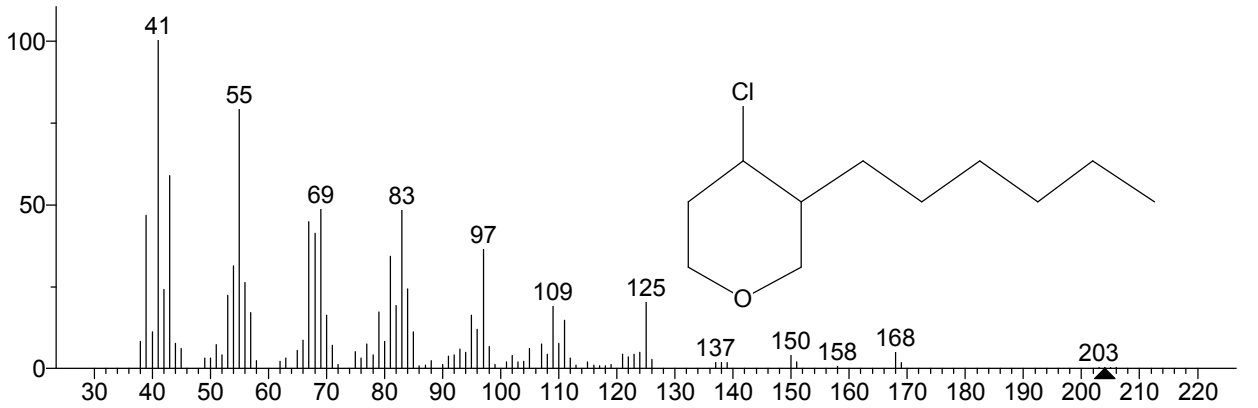
Hit 2 : 7-Hexadecenal, (Z)-
C16H30O; MF: 776; RMF: 828; Prob 4.78%; CAS: 56797-40-1; Lib: replib; ID: 5616.



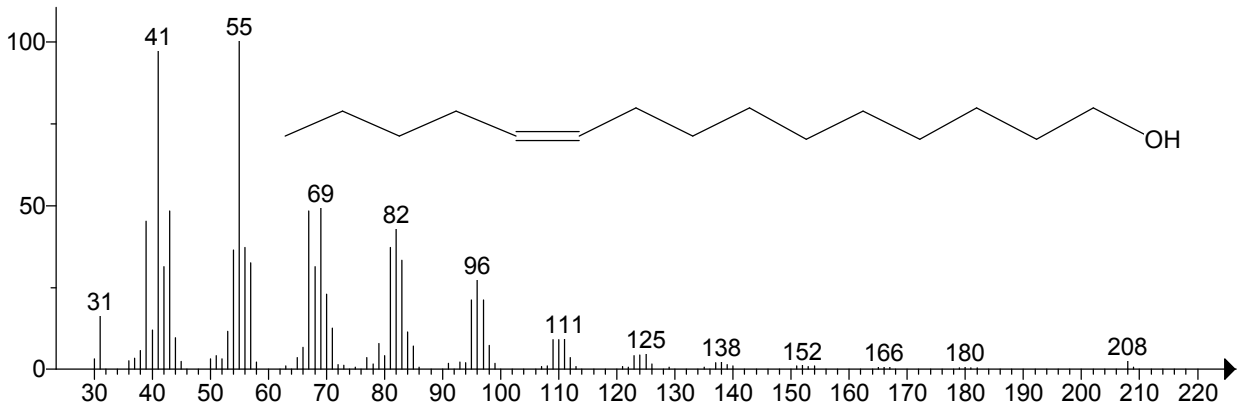
Unknown: Scan 763 (5.837 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -464



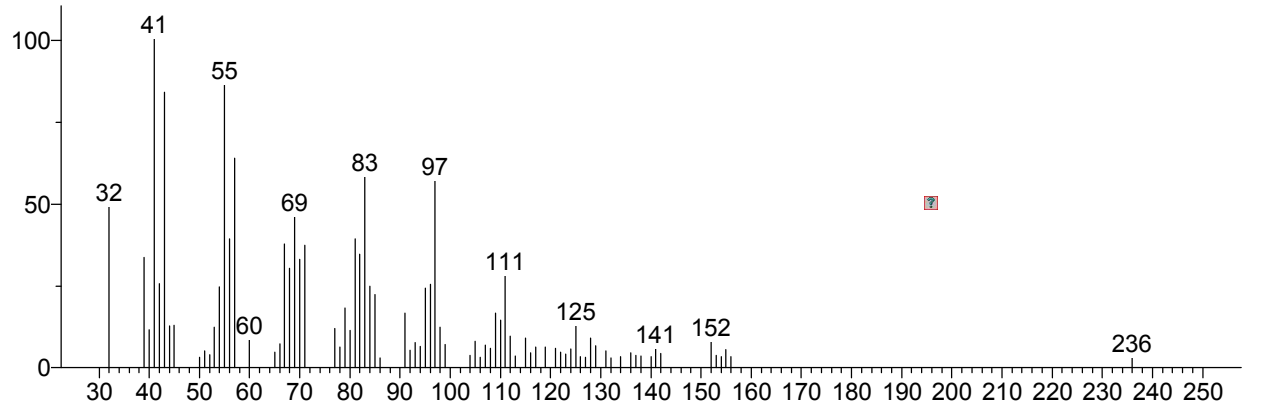
Hit 1 : 4-Chloro-3-n-hexyltetrahydropyran
C11H21ClO; MF: 792; RMF: 844; Prob 11.2%; CAS: 66555-66-6; Lib: mainlib; ID: 2467.



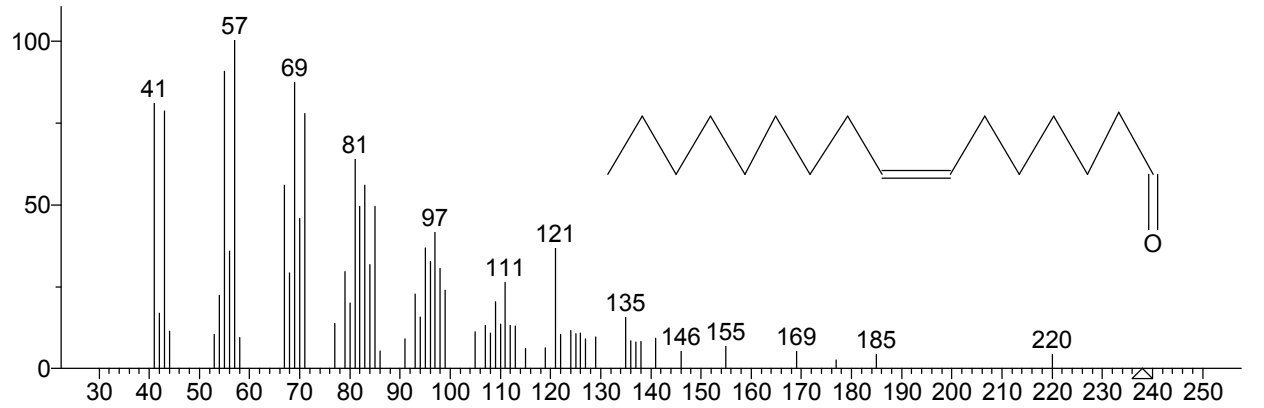
Hit 2 : Z-10-Pentadecen-1-ol
C15H30O; MF: 769; RMF: 837; Prob 4.10%; Lib: mainlib; ID: 17434.



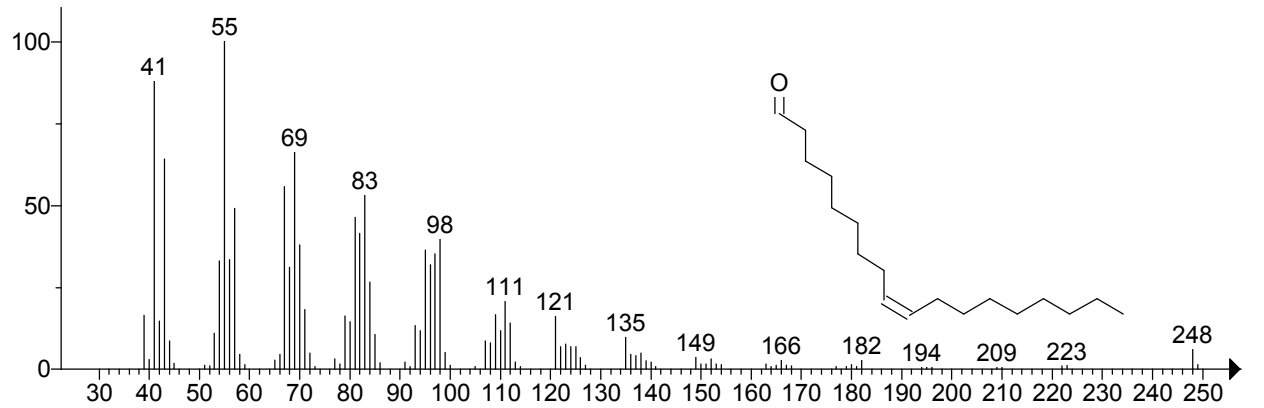
Unknown: Scan 827 (6.319 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -474



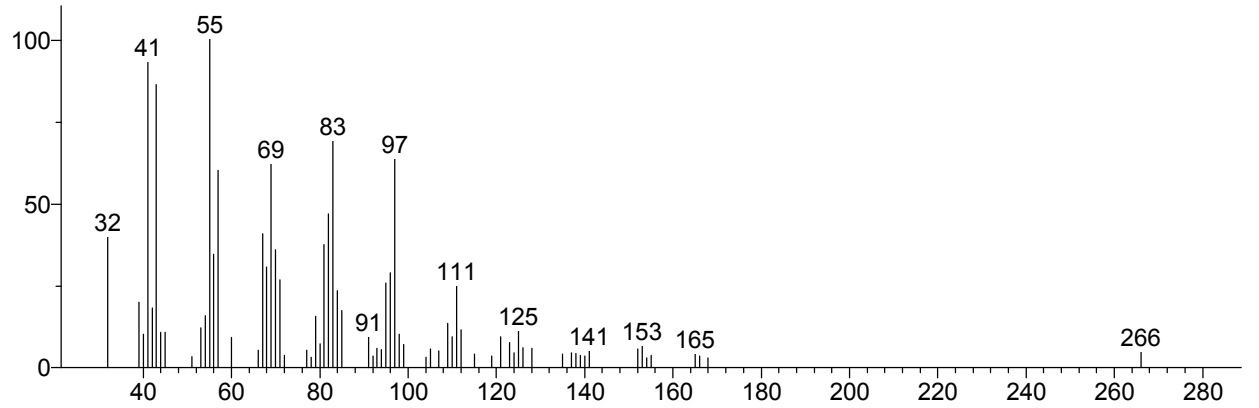
Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 789; RMF: 855; Prob 9.94%; CAS: 56797-40-1; Lib: replib; ID: 5616.



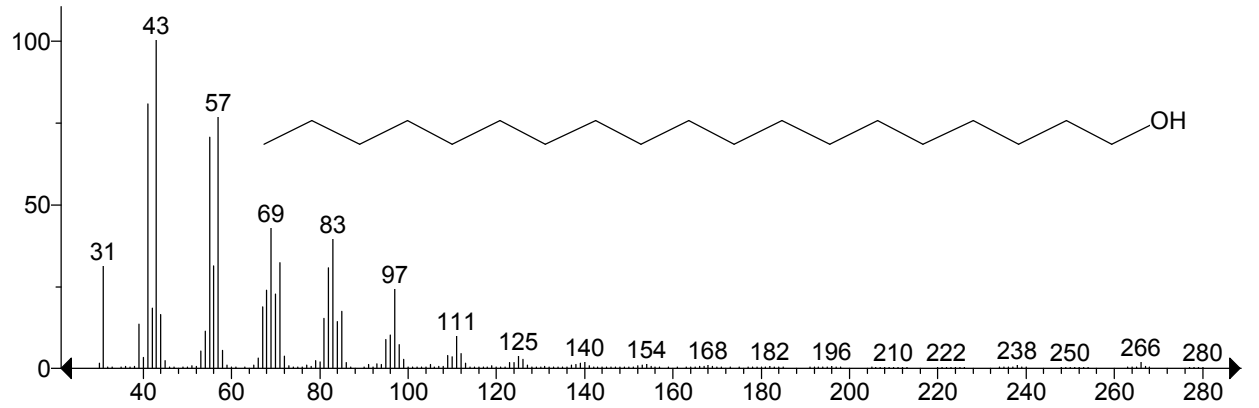
Hit 2 : 9-Octadecenal, (Z)-
C18H34O; MF: 767; RMF: 814; Prob 3.93%; CAS: 2423-10-1; Lib: mainlib; ID: 17466.



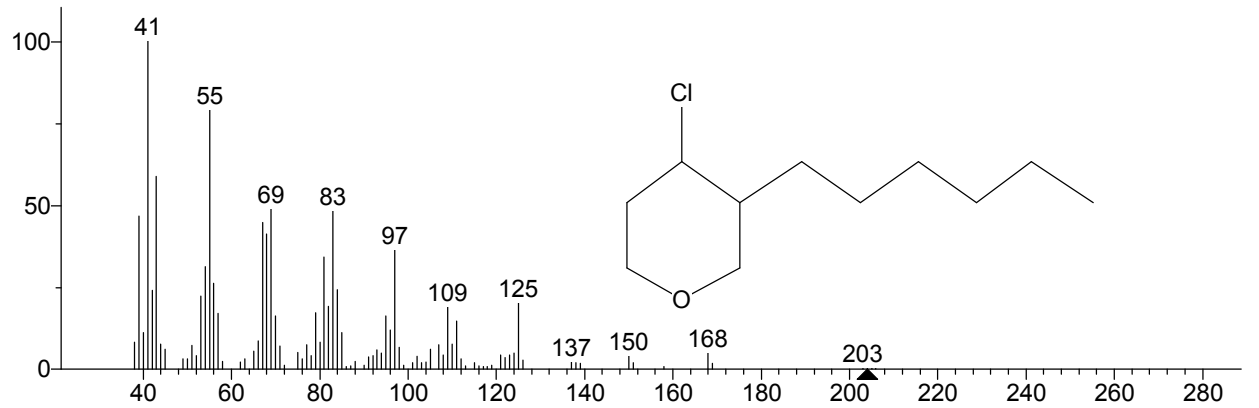
Unknown: Scan 887 (6.771 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -501



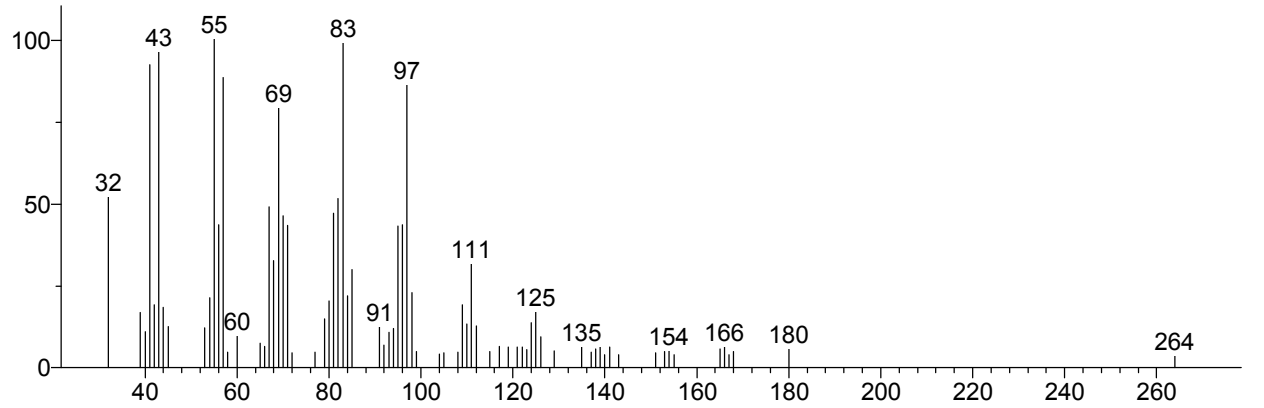
Hit 1 : n-Nonadecanol-1
C19H40O; MF: 809; RMF: 818; Prob 4.59%; CAS: 1454-84-8; Lib: replib; ID: 1706.



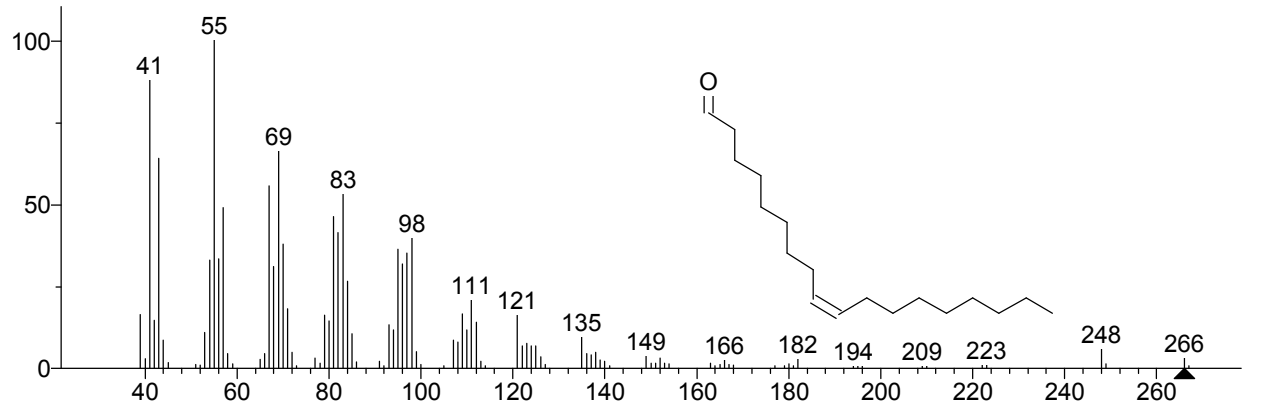
Hit 2 : 4-Chloro-3-n-hexyltetrahydropyran
C11H21ClO; MF: 799; RMF: 843; Prob 3.24%; CAS: 66555-66-6; Lib: mainlib; ID: 2467.



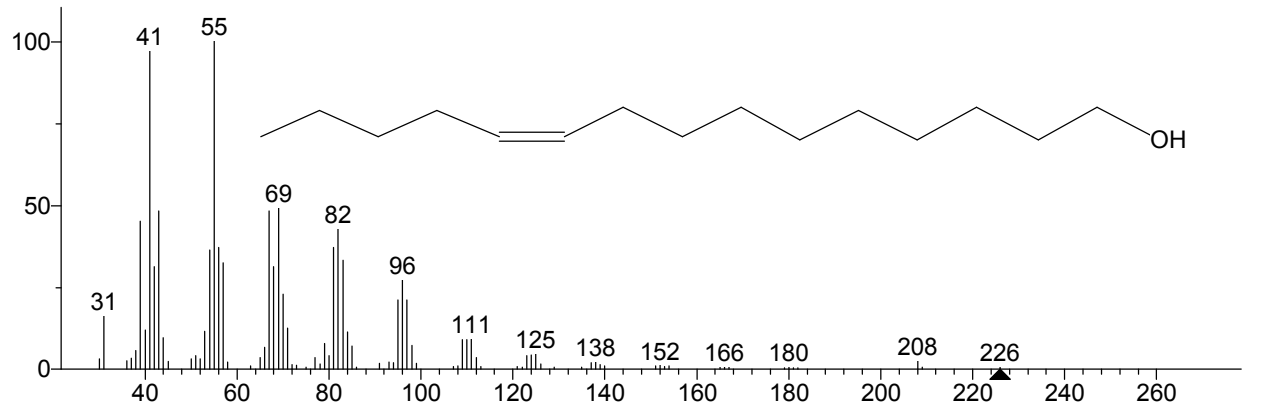
Unknown: Scan 946 (7.216 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -698



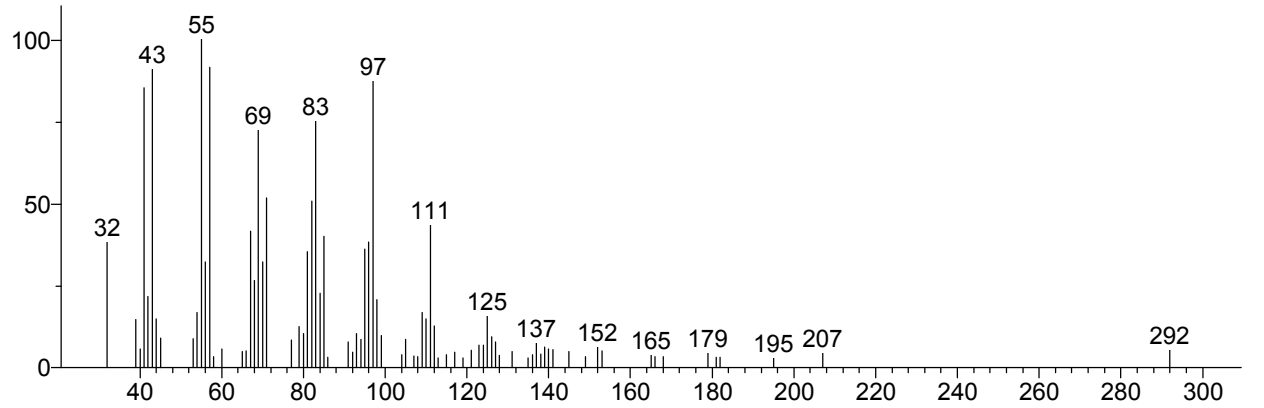
Hit 1 : 9-Octadecenal, (Z)-
C18H34O; MF: 798; RMF: 820; Prob 3.82%; CAS: 2423-10-1; Lib: mainlib; ID: 17466.



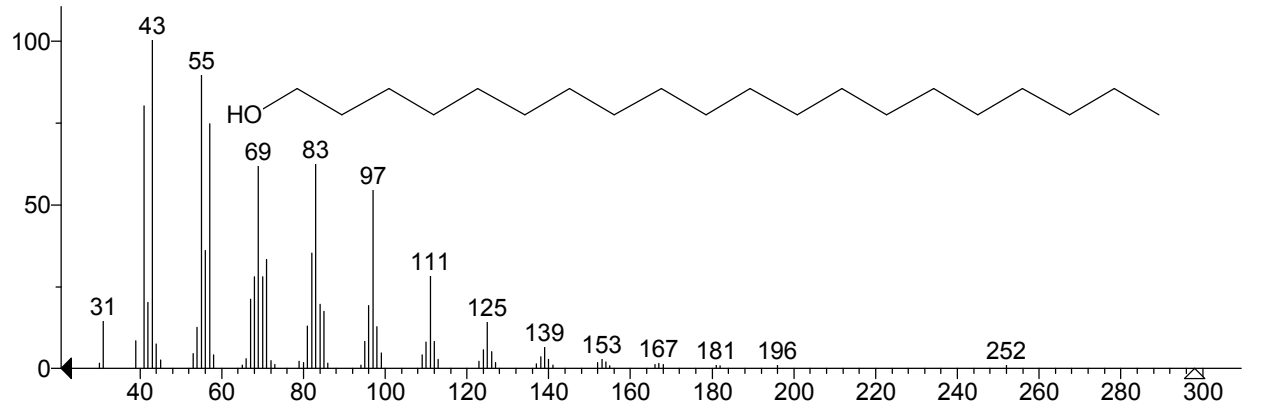
Hit 2 : Z-10-Pentadecen-1-ol
C15H30O; MF: 790; RMF: 827; Prob 2.85%; Lib: mainlib; ID: 17434.



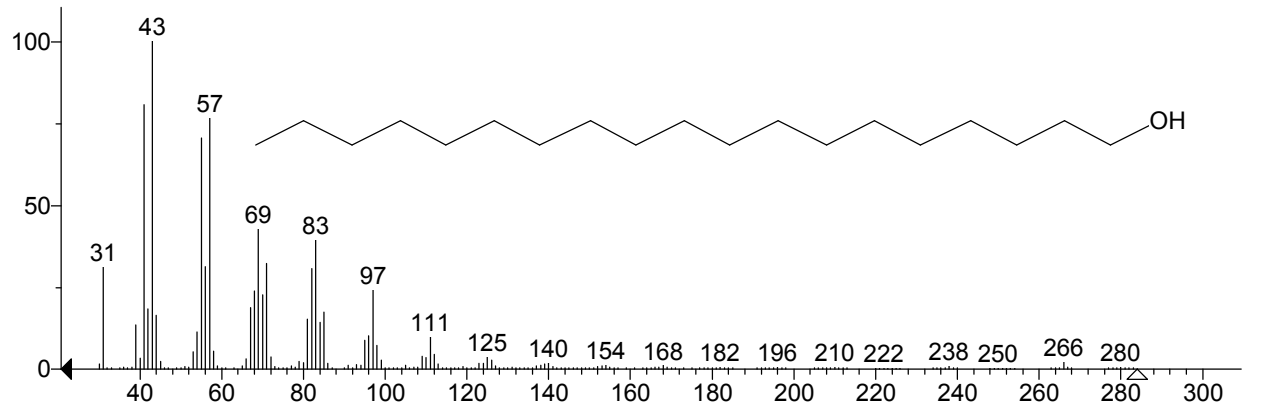
Unknown: Scan 1004 (7.653 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -509



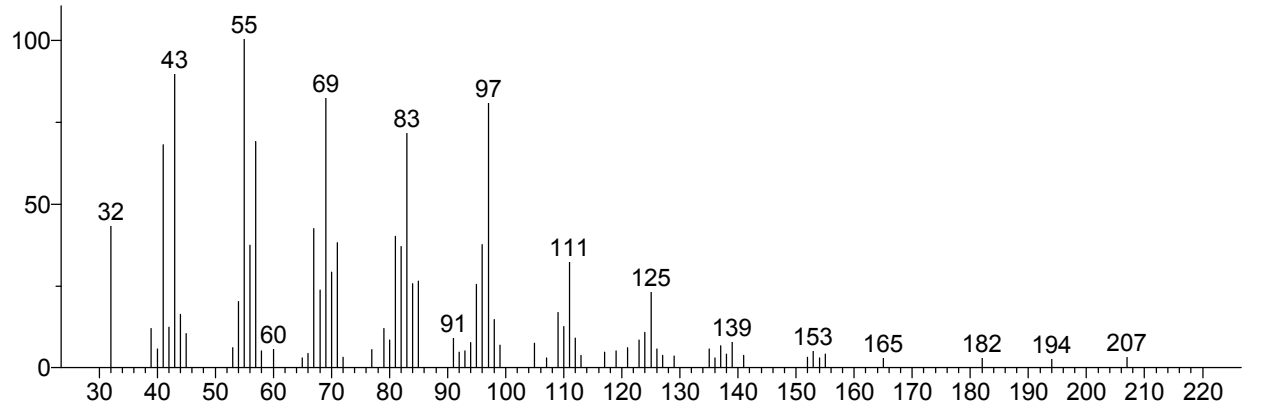
Hit 1 : 1-Eicosanol
C20H42O; MF: 800; RMF: 870; Prob 4.32%; CAS: 629-96-9; Lib: replib; ID: 1938.



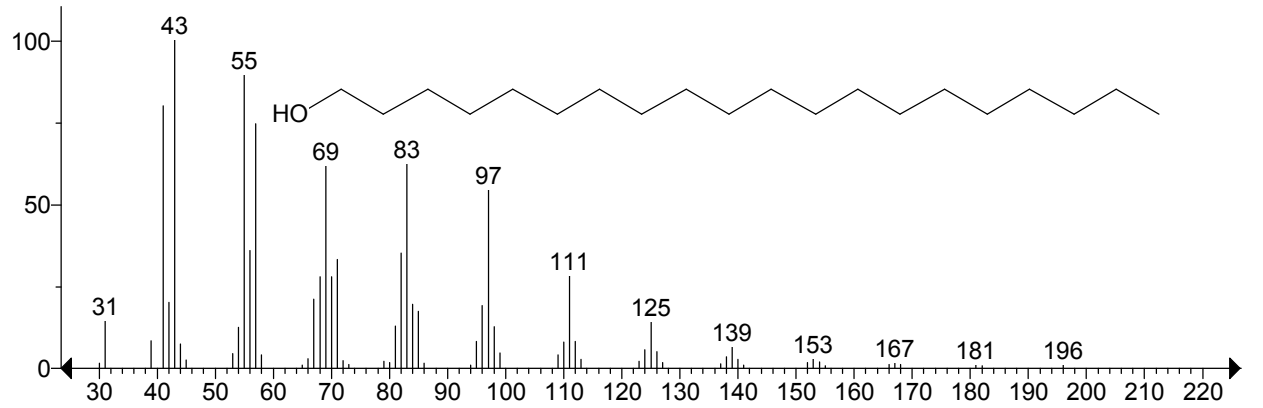
Hit 2 : n-Nonadecanol-1
C19H40O; MF: 800; RMF: 818; Prob 4.32%; CAS: 1454-84-8; Lib: replib; ID: 1706.



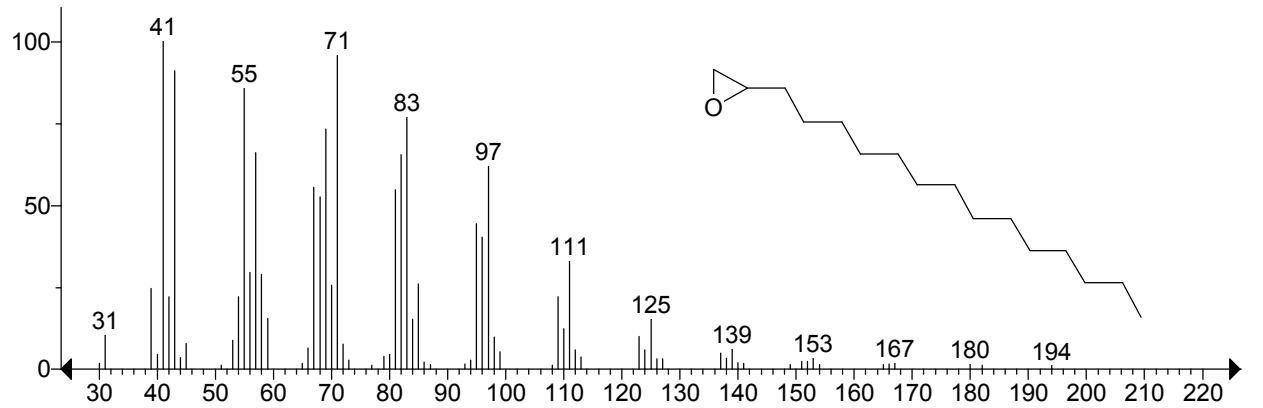
Unknown: Scan 1057 (8.052 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -367



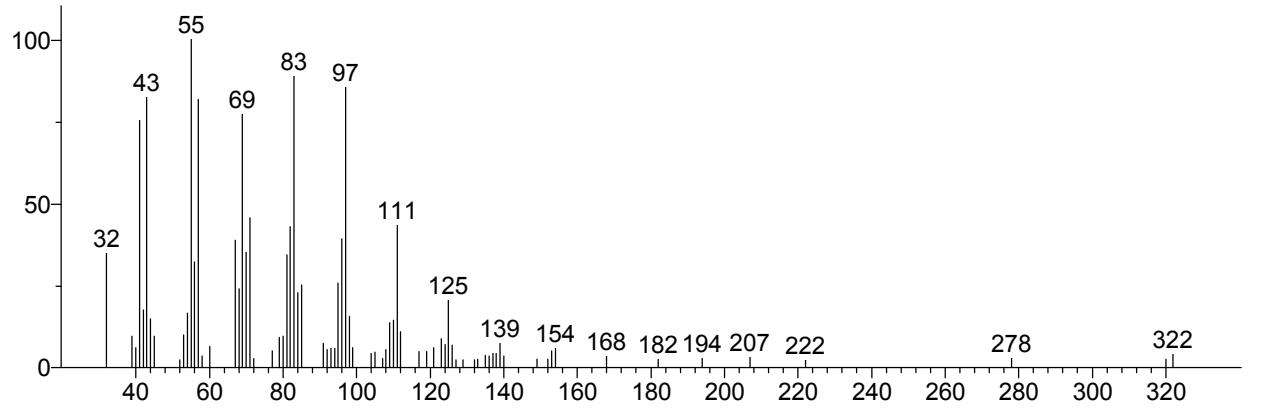
Hit 1 : 1-Eicosanol
C20H42O; MF: 823; RMF: 874; Prob 6.02%; CAS: 629-96-9; Lib: replib; ID: 1938.



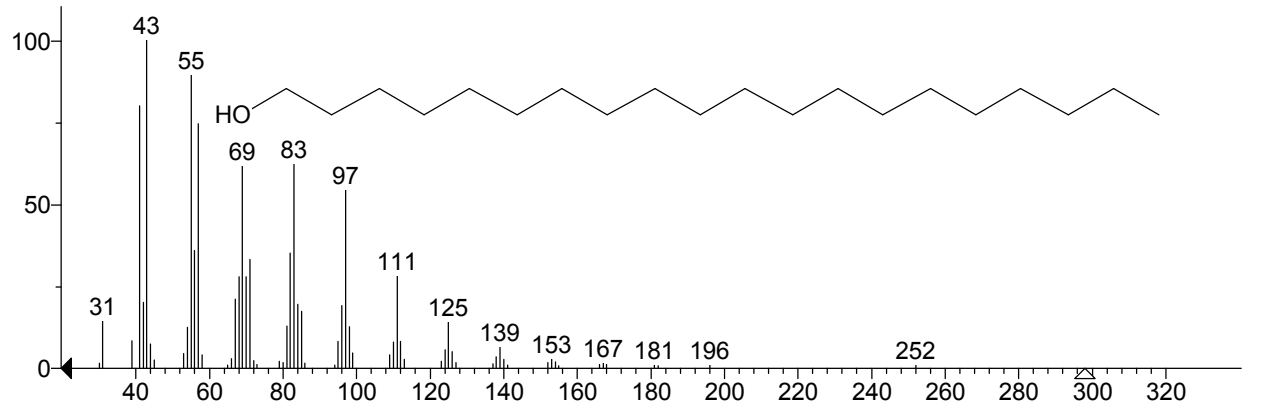
Hit 2 : Oxirane, tetradecyl-
C16H32O; MF: 821; RMF: 864; Prob 5.55%; CAS: 7320-37-8; Lib: replib; ID: 1171.



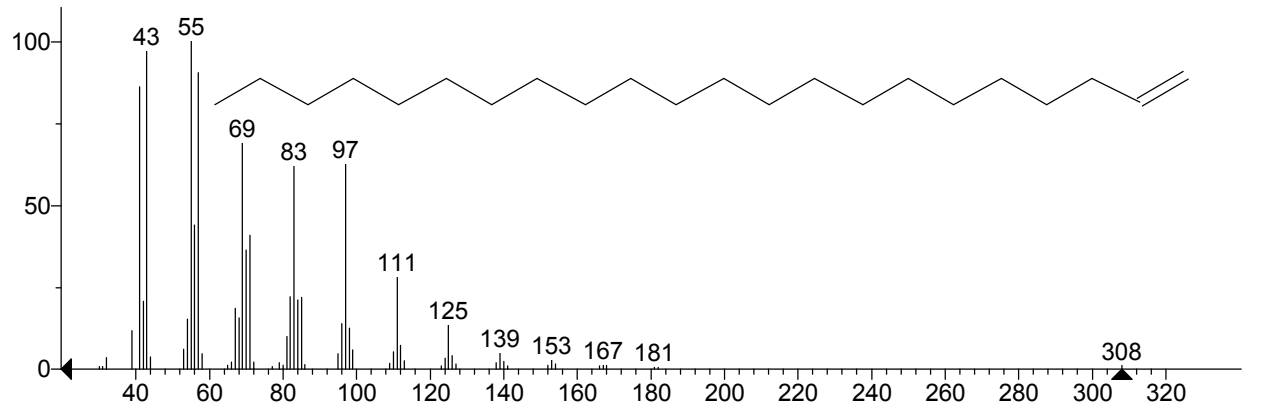
Unknown: Scan 1110 (8.452 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -334



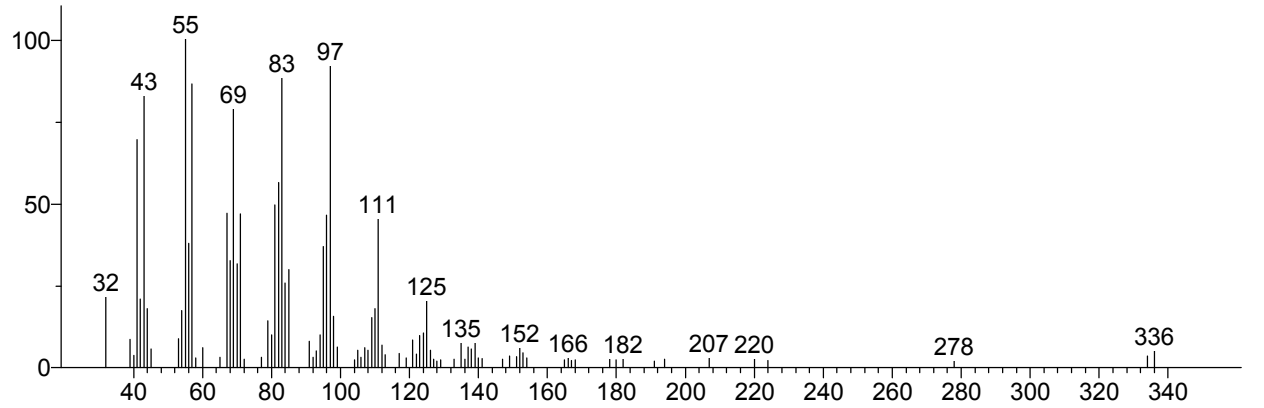
Hit 1 : 1-Eicosanol
C20H42O; MF: 830; RMF: 902; Prob 11.3%; CAS: 629-96-9; Lib: replib; ID: 1938.



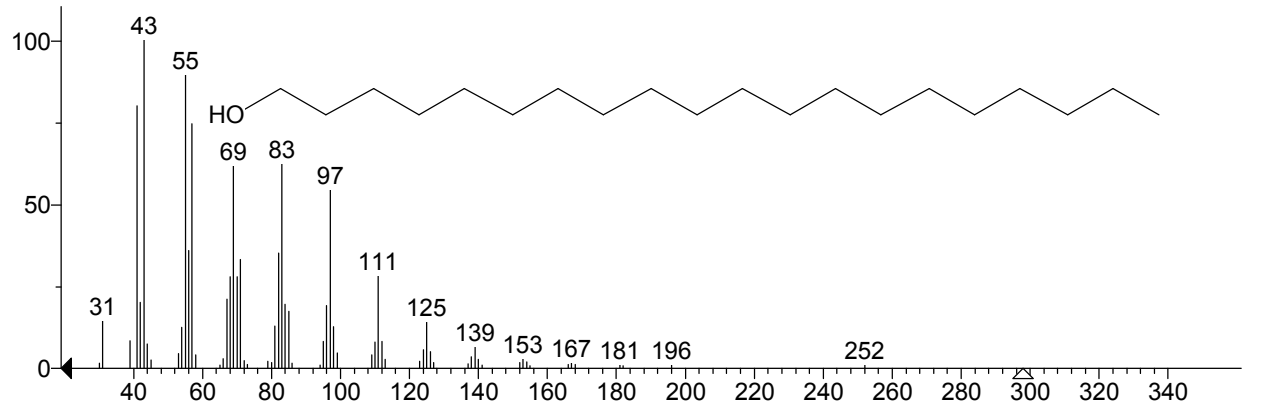
Hit 2 : 1-Docosene
C22H44; MF: 805; RMF: 875; Prob 3.44%; CAS: 1599-67-3; Lib: replib; ID: 4382.



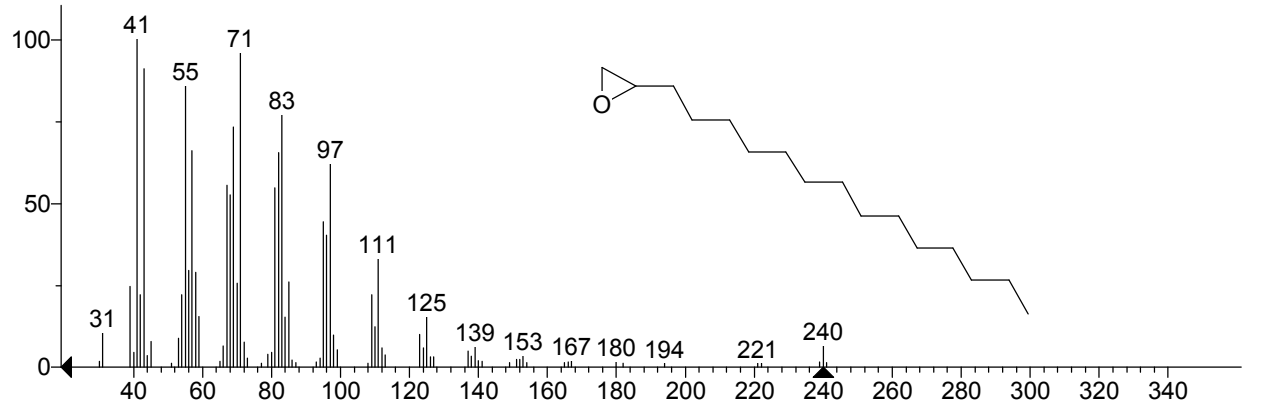
Unknown: Scan 1160 (8.828 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -688



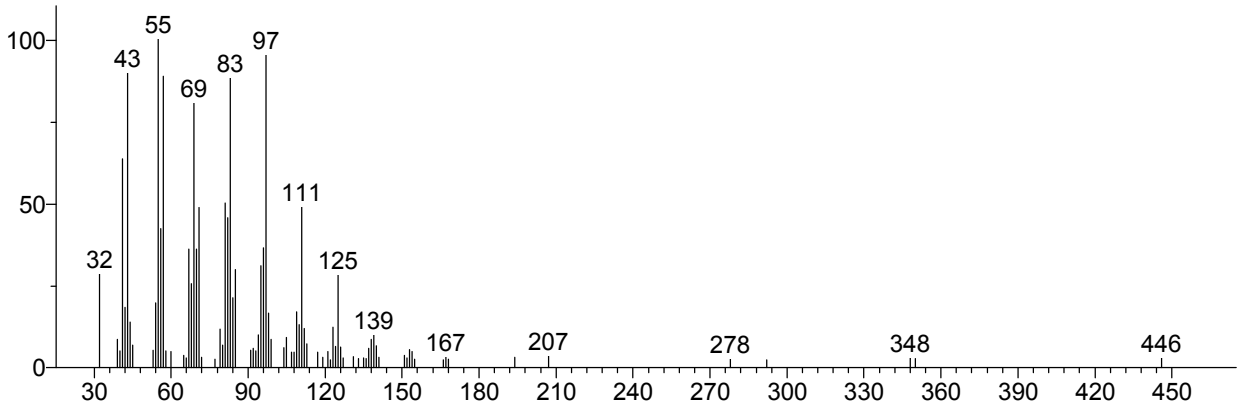
Hit 1 : 1-Eicosanol
C20H42O; MF: 804; RMF: 882; Prob 5.57%; CAS: 629-96-9; Lib: replib; ID: 1938.



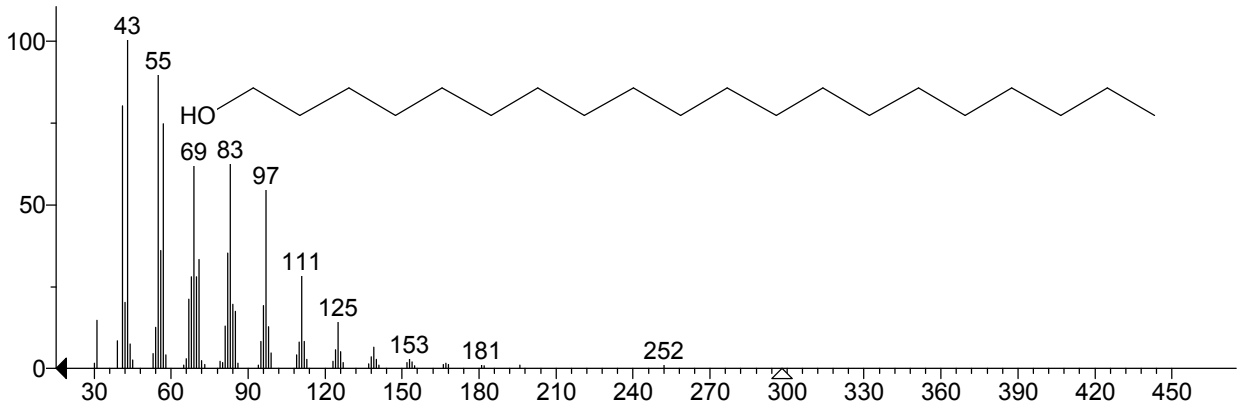
Hit 2 : Oxirane, tetradecyl-
C16H32O; MF: 802; RMF: 863; Prob 5.14%; CAS: 7320-37-8; Lib: replib; ID: 1171.



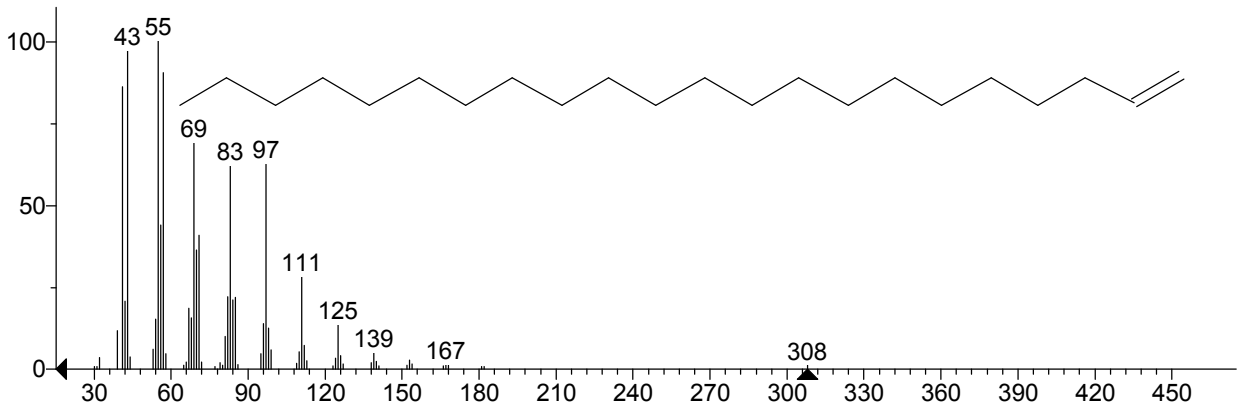
Unknown: Scan 1211 (9.213 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -367



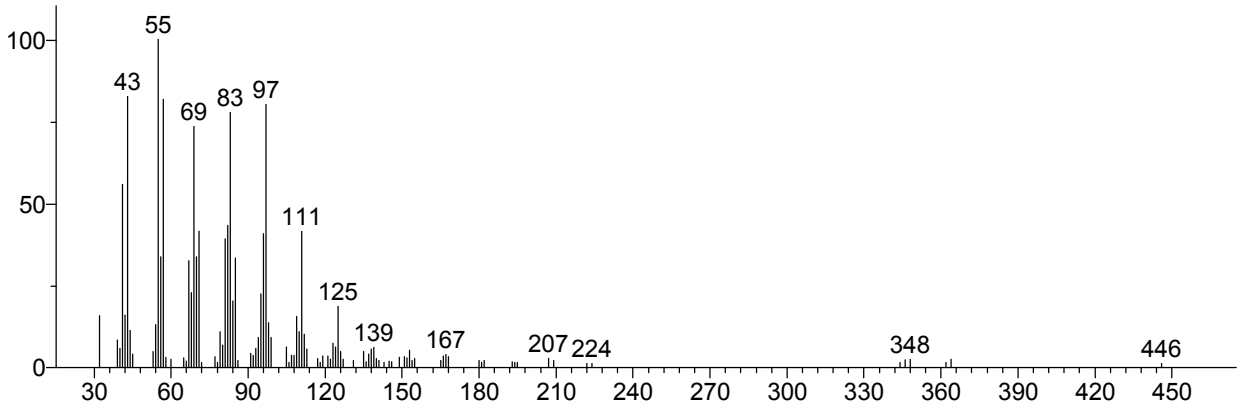
Hit 1 : 1-Eicosanol
C20H42O; MF: 823; RMF: 889; Prob 6.76%; CAS: 629-96-9; Lib: replib; ID: 1938.



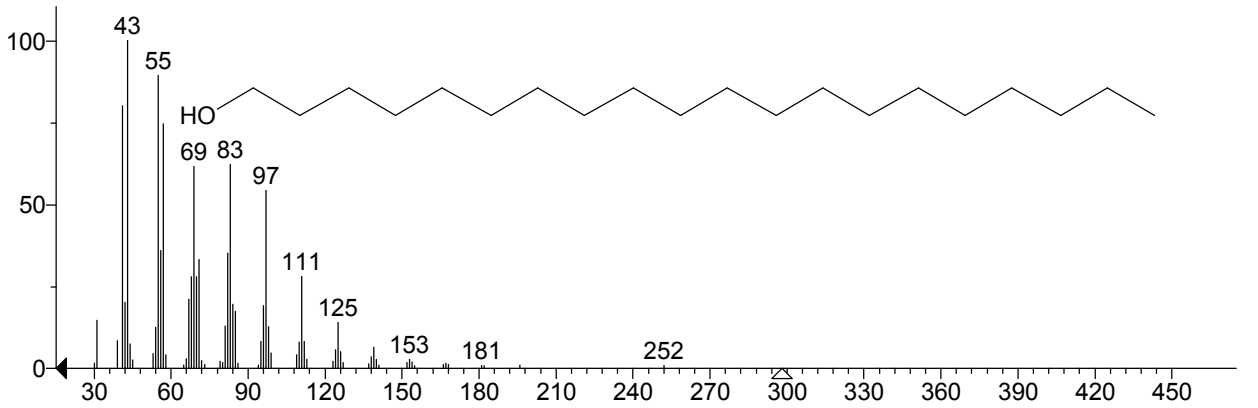
Hit 2 : 1-Docosene
C22H44; MF: 809; RMF: 880; Prob 4.23%; CAS: 1599-67-3; Lib: replib; ID: 4382.



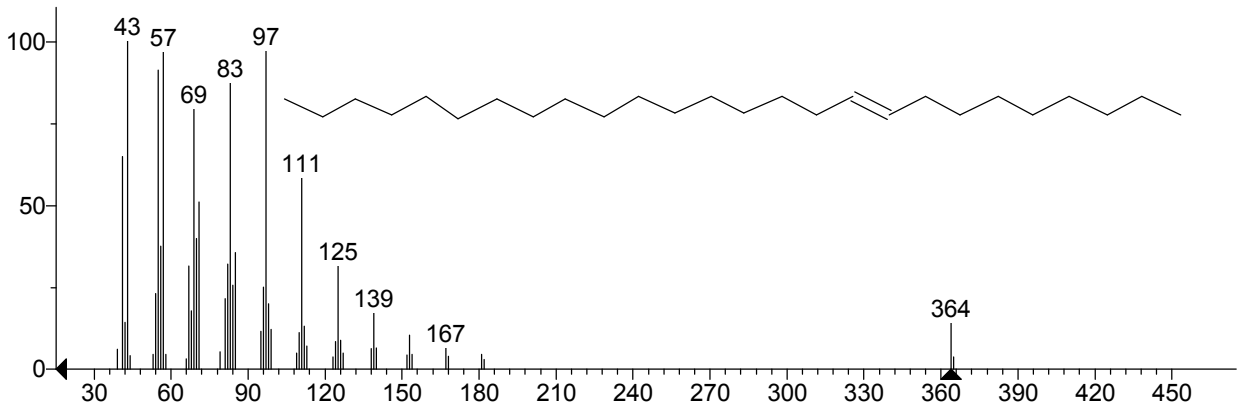
Unknown: Scan 1258 (9.567 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -688



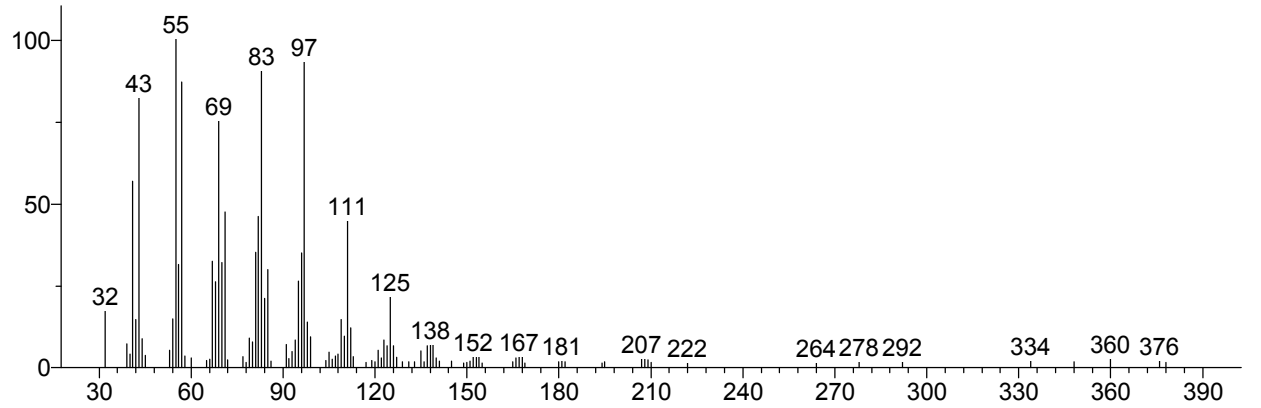
Hit 1 : 1-Eicosanol
C20H42O; MF: 810; RMF: 887; Prob 5.51%; CAS: 629-96-9; Lib: replib; ID: 1938.



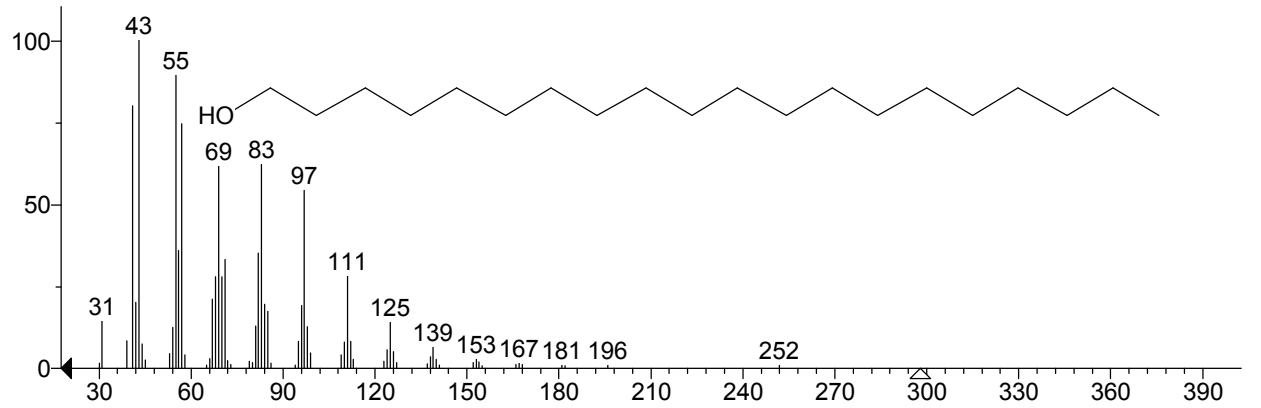
Hit 2 : 9-Hexacosene
C26H52; MF: 808; RMF: 903; Prob 5.08%; CAS: 71502-22-2; Lib: mainlib; ID: 9578.



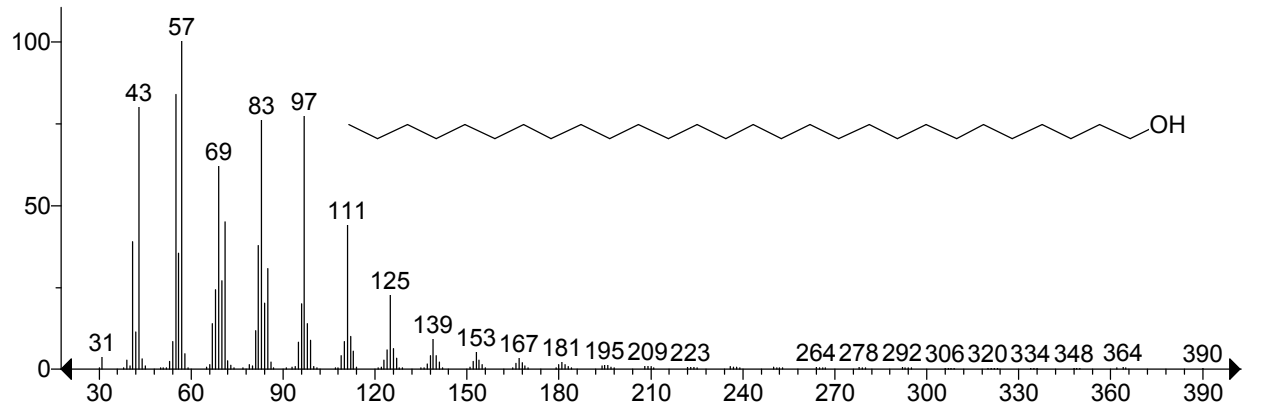
Unknown: Scan 1304 (9.914 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -558



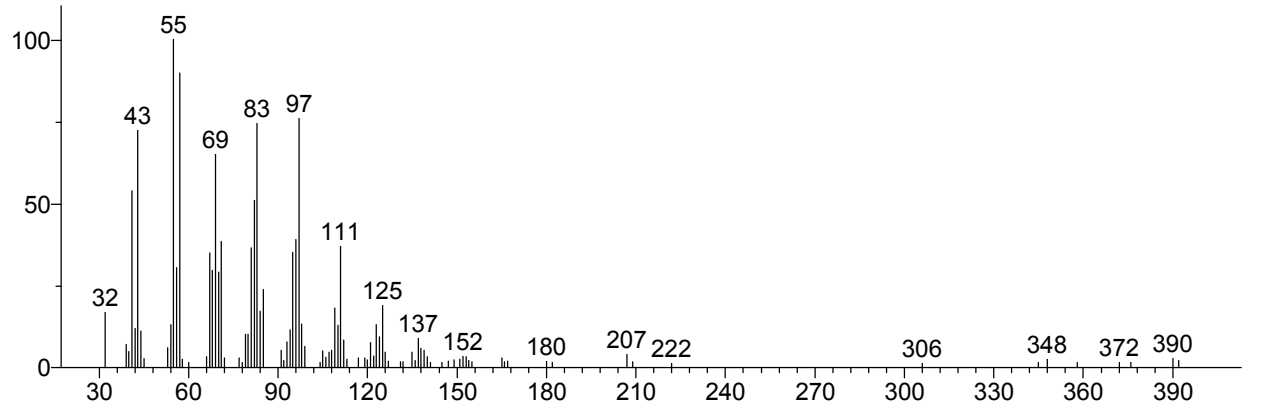
Hit 1 : 1-Eicosanol
C20H42O; MF: 817; RMF: 895; Prob 4.21%; CAS: 629-96-9; Lib: replib; ID: 1938.



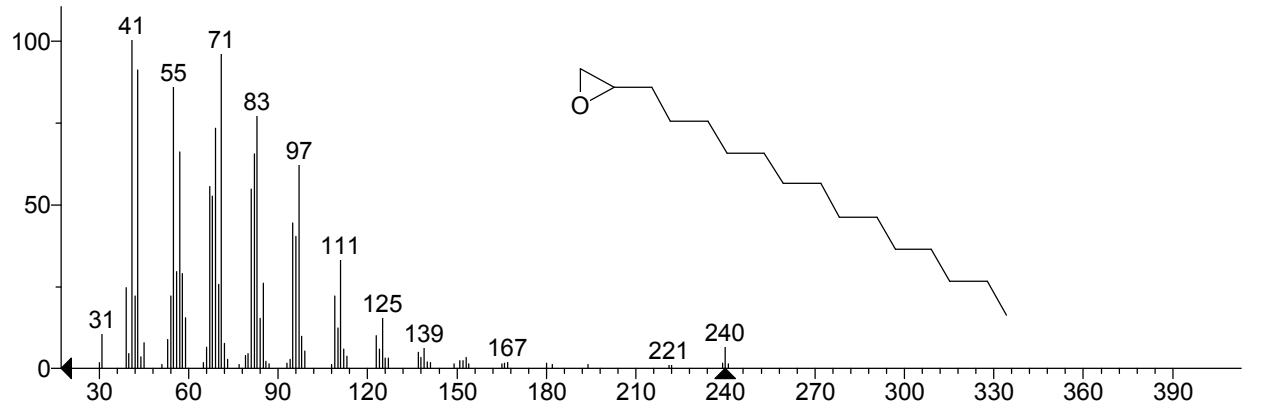
Hit 2 : 1-Octacosanol
C28H58O; MF: 817; RMF: 846; Prob 4.21%; Lib: mainlib; ID: 22288.



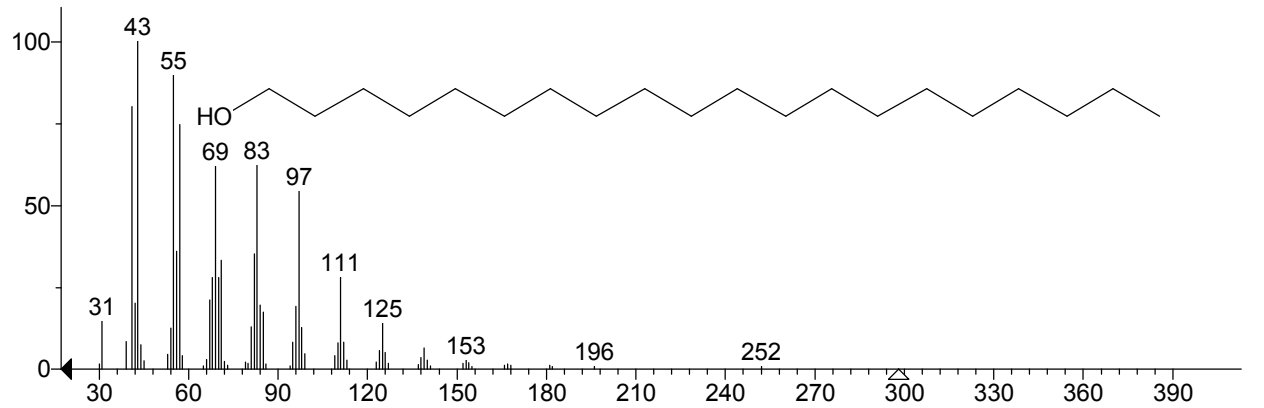
Unknown: Scan 1348 (10.245 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -698



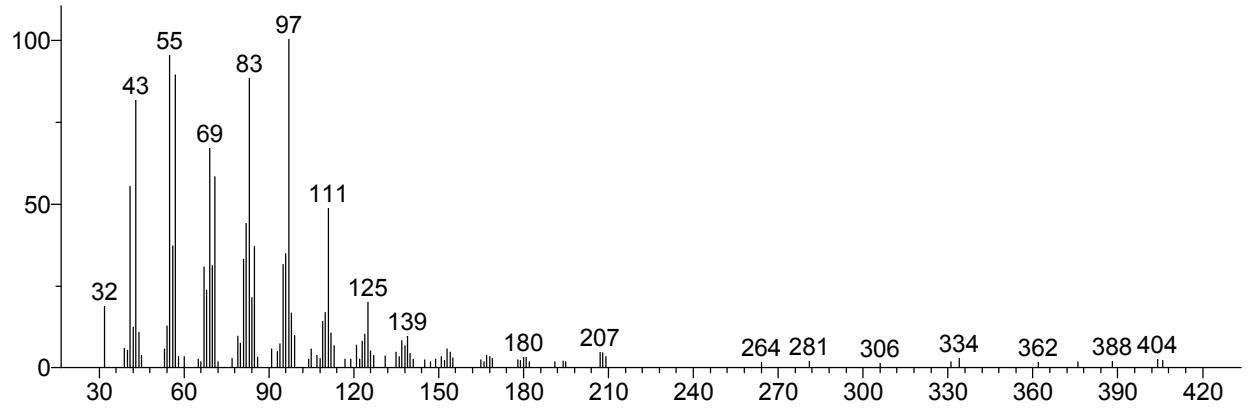
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 800; RMF: 865; Prob 6.14%; CAS: 7320-37-8; Lib: replib; ID: 1171.



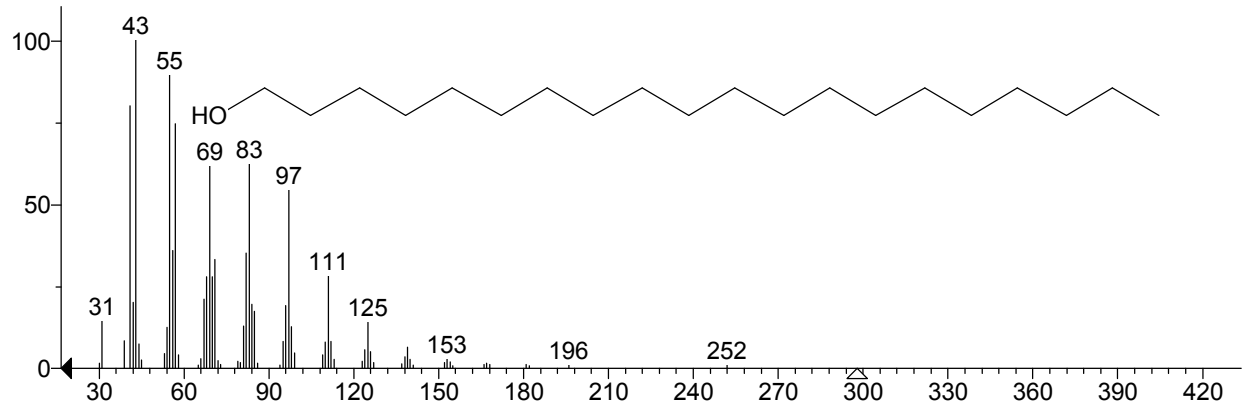
Hit 2 : 1-Eicosanol
C20H42O; MF: 793; RMF: 876; Prob 4.70%; CAS: 629-96-9; Lib: replib; ID: 1938.



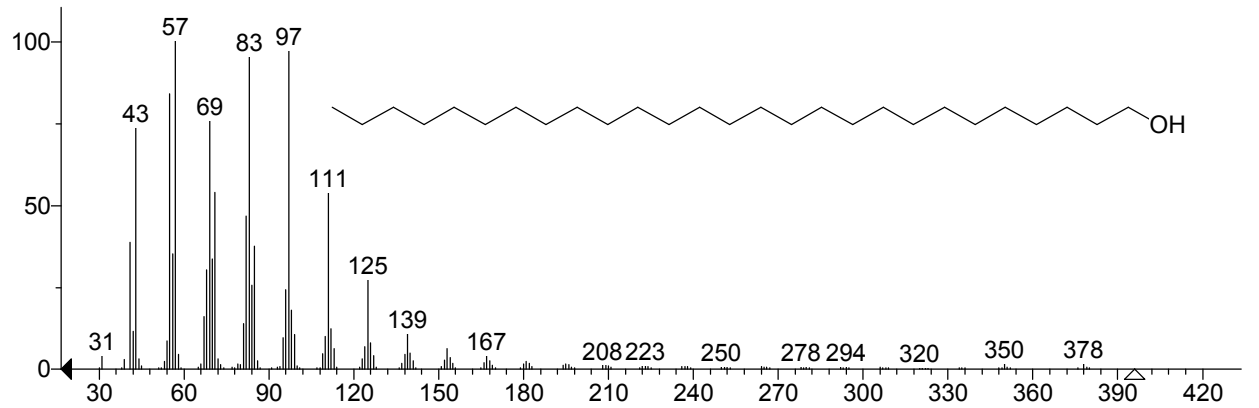
Unknown: Scan 1393 (10.584 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -501



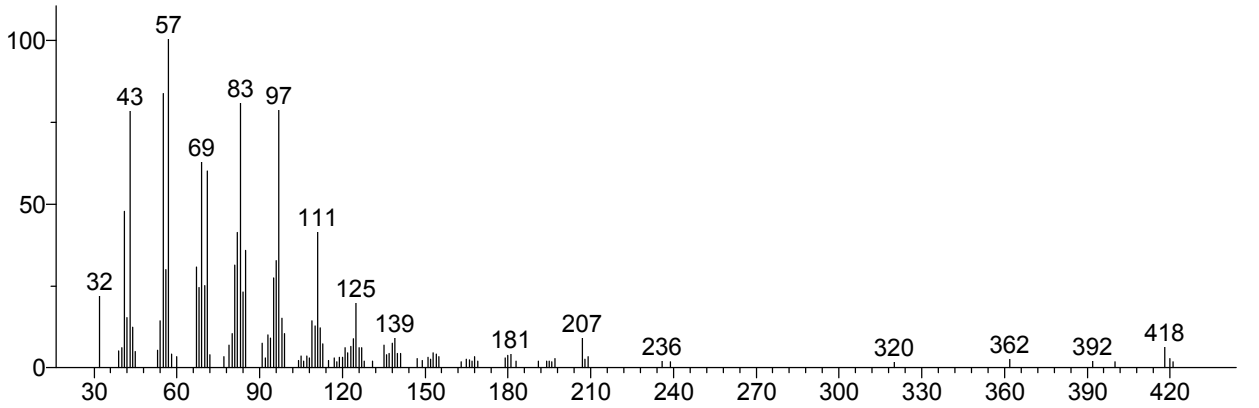
Hit 1 : 1-Eicosanol
C20H42O; MF: 801; RMF: 892; Prob 5.24%; CAS: 629-96-9; Lib: replib; ID: 1938.



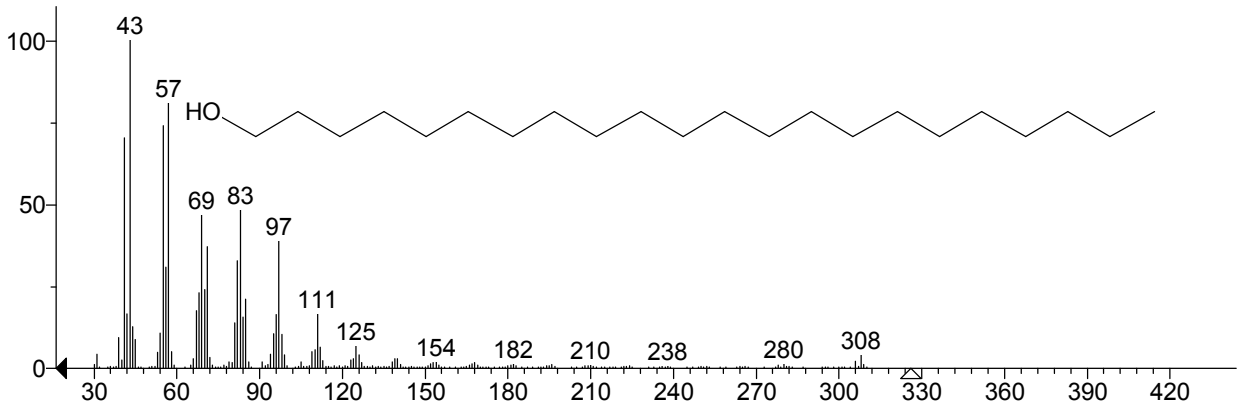
Hit 2 : 1-Heptacosanol
C27H56O; MF: 790; RMF: 834; Prob 3.59%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



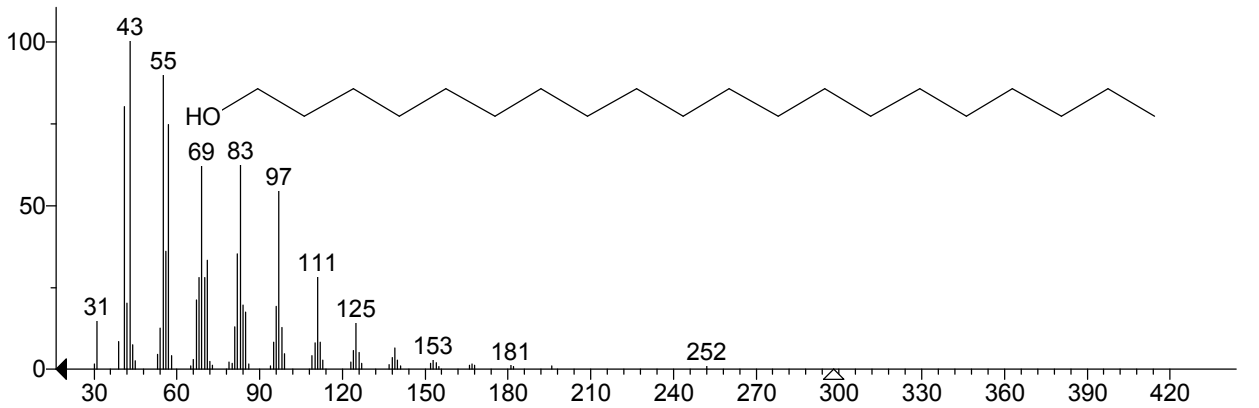
Unknown: Scan 1436 (10.908 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -811



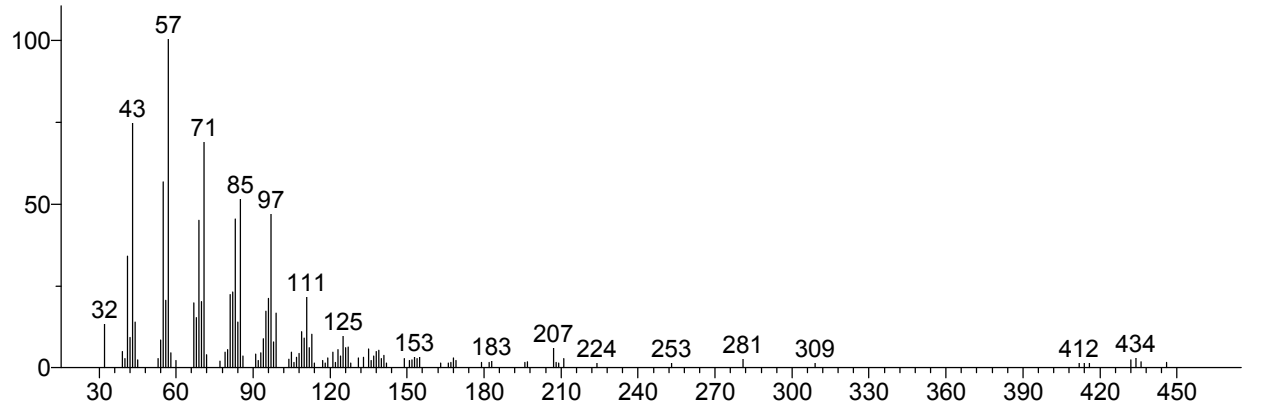
Hit 1 : Behenic alcohol
C22H46O; MF: 774; RMF: 802; Prob 4.30%; CAS: 661-19-8; Lib: replib; ID: 2104.



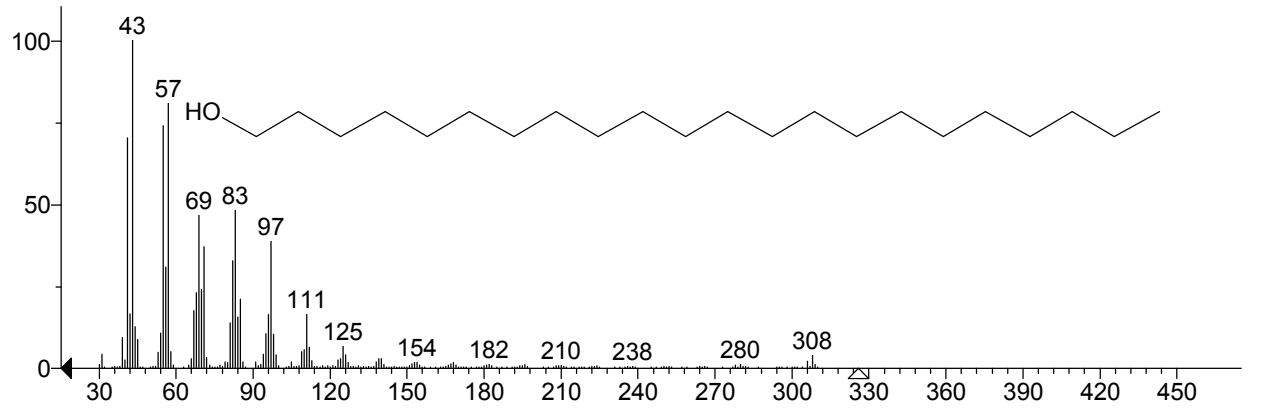
Hit 2 : 1-Eicosanol
C20H42O; MF: 768; RMF: 882; Prob 3.38%; CAS: 629-96-9; Lib: replib; ID: 1938.



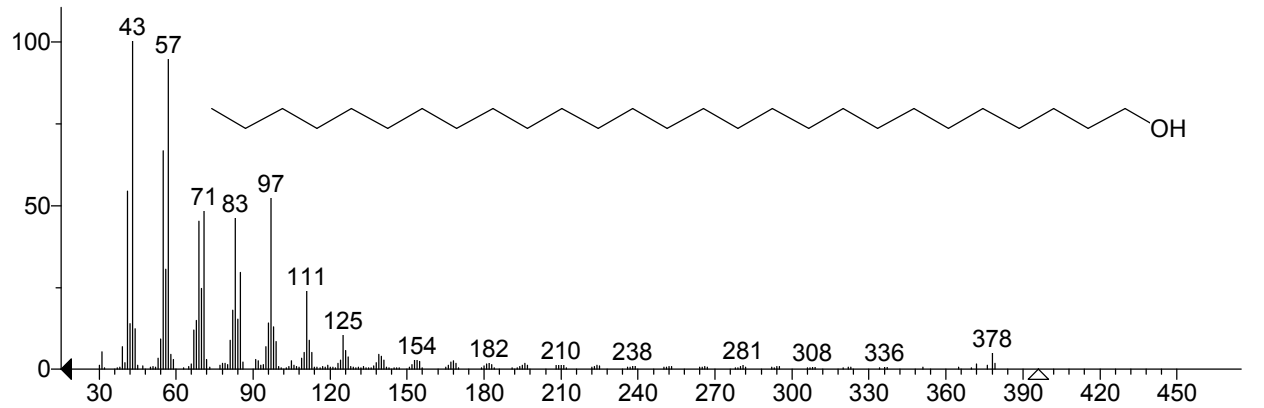
Unknown: Scan 1478 (11.225 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -858



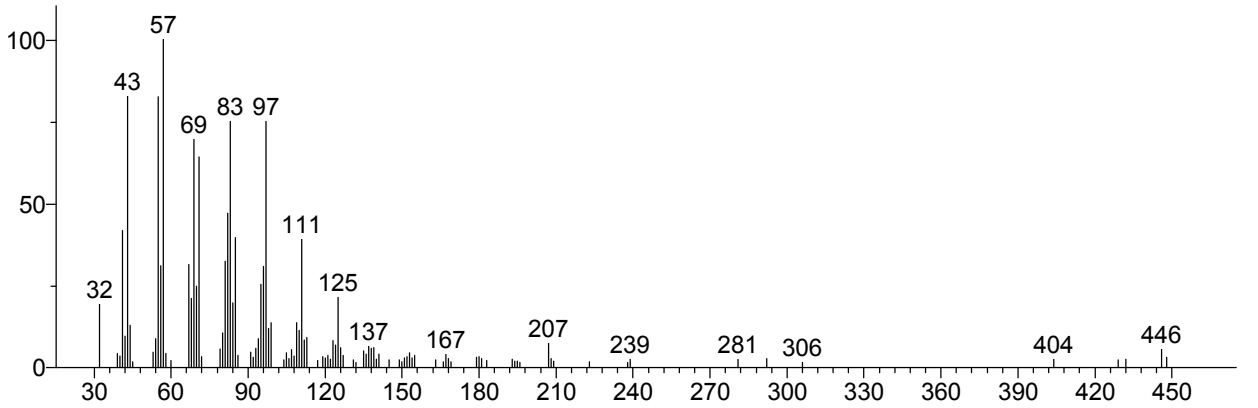
Hit 1 : Behenic alcohol
C22H46O; MF: 767; RMF: 796; Prob 5.64%; CAS: 661-19-8; Lib: replib; ID: 2104.



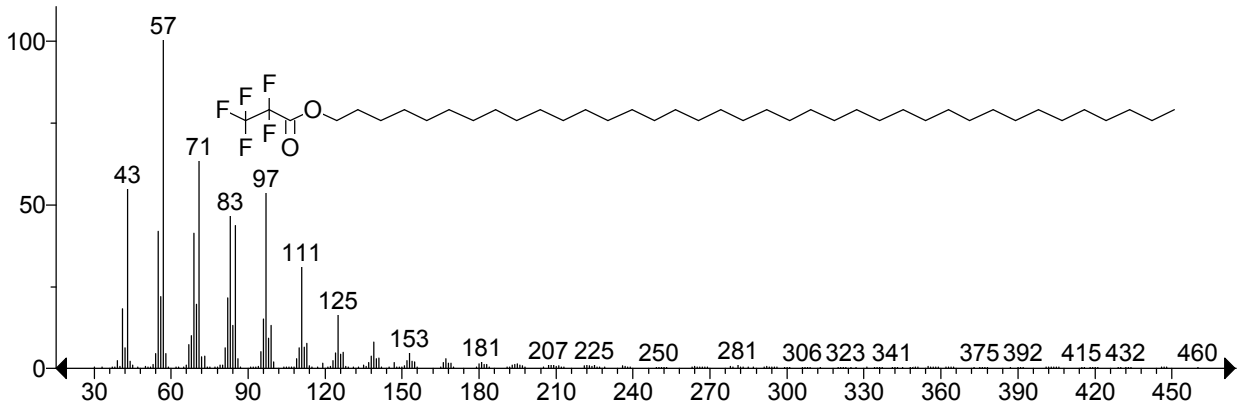
Hit 2 : 1-Heptacosanol
C27H56O; MF: 759; RMF: 797; Prob 4.21%; CAS: 2004-39-9; Lib: replib; ID: 2100.



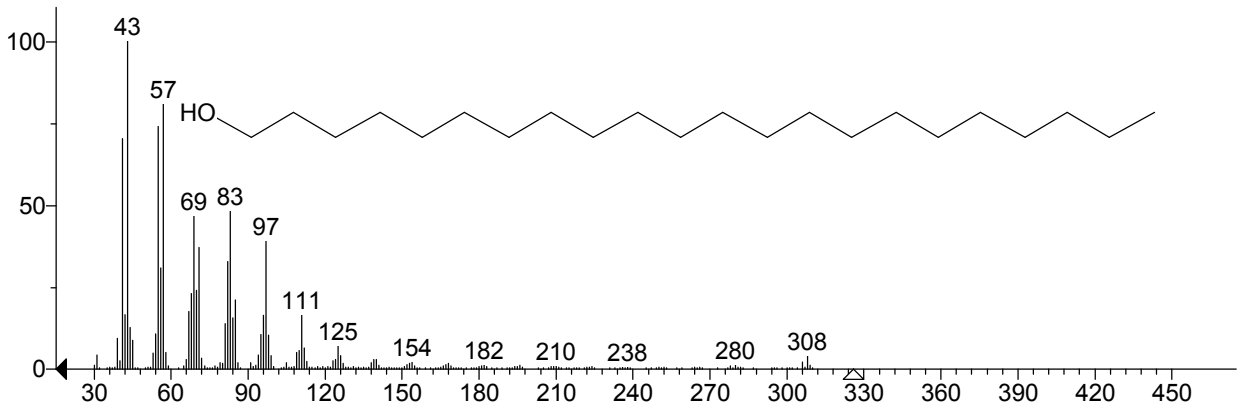
Unknown: Scan 1516 (11.511 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -591



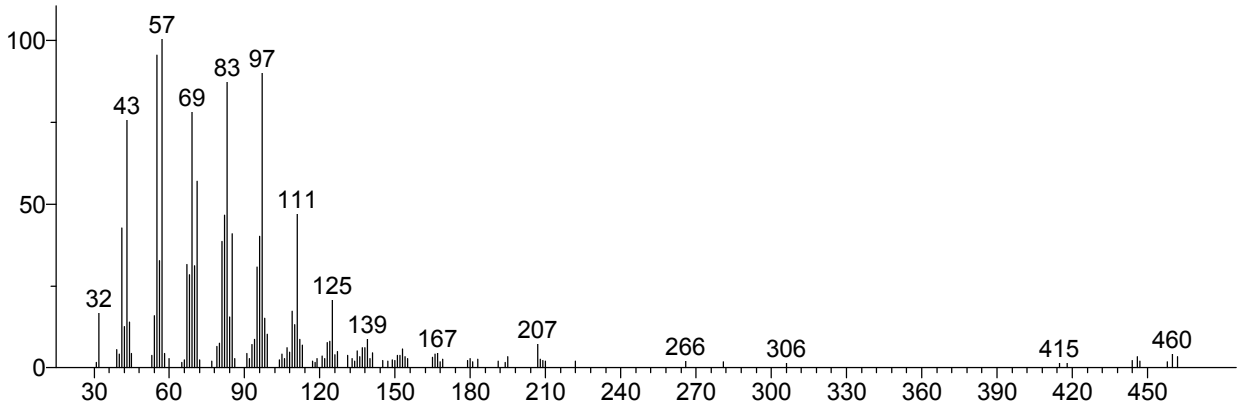
Hit 1 : Octatriacontyl pentafluoropropionate
C41H77F5O2; MF: 771; RMF: 777; Prob 4.56%; Lib: mainlib; ID: 22753.



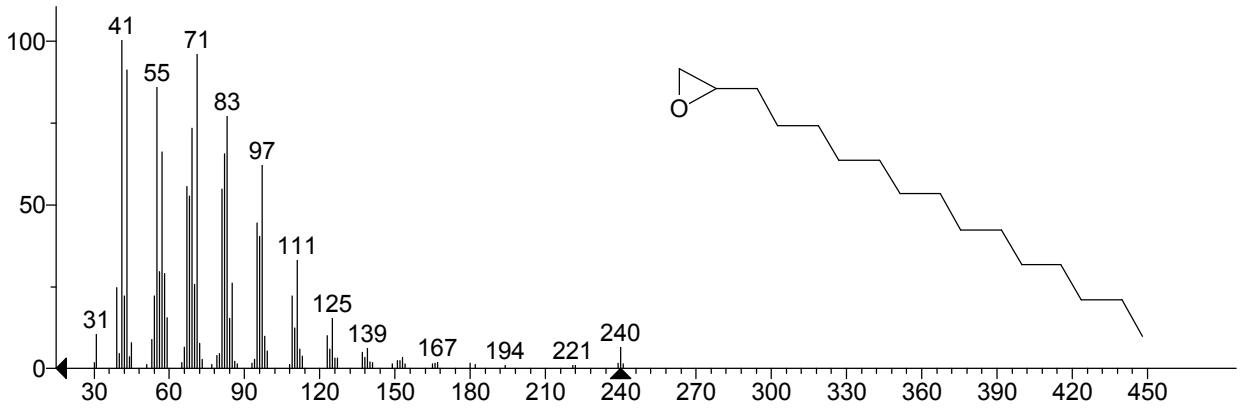
Hit 2 : Behenic alcohol
C22H46O; MF: 760; RMF: 792; Prob 3.13%; CAS: 661-19-8; Lib: replib; ID: 2104.



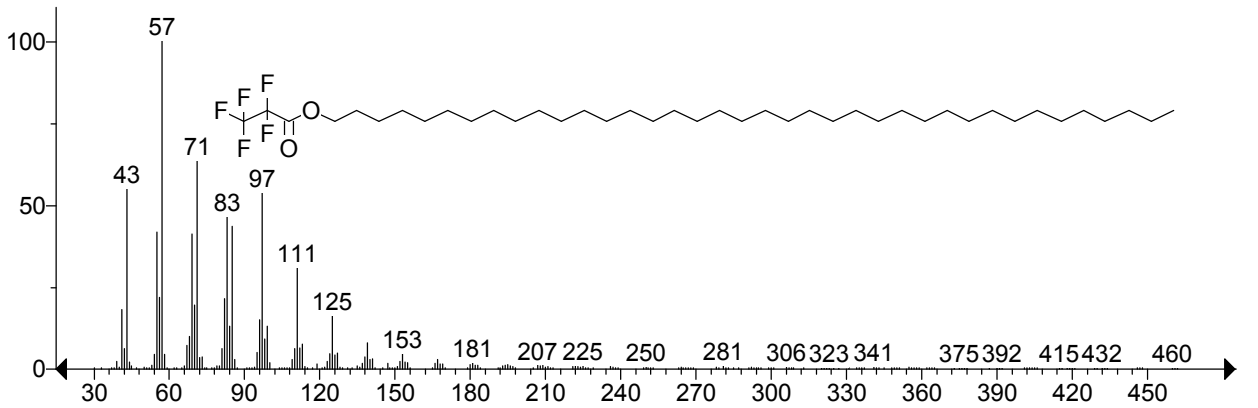
Unknown: Scan 1554 (11.797 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -520



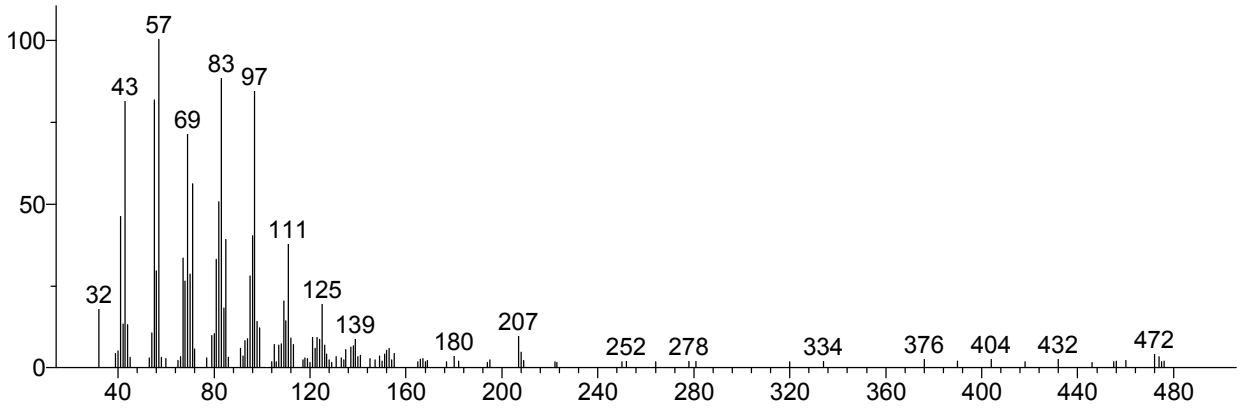
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 782; RMF: 877; Prob 6.11%; CAS: 7320-37-8; Lib: replib; ID: 1171.



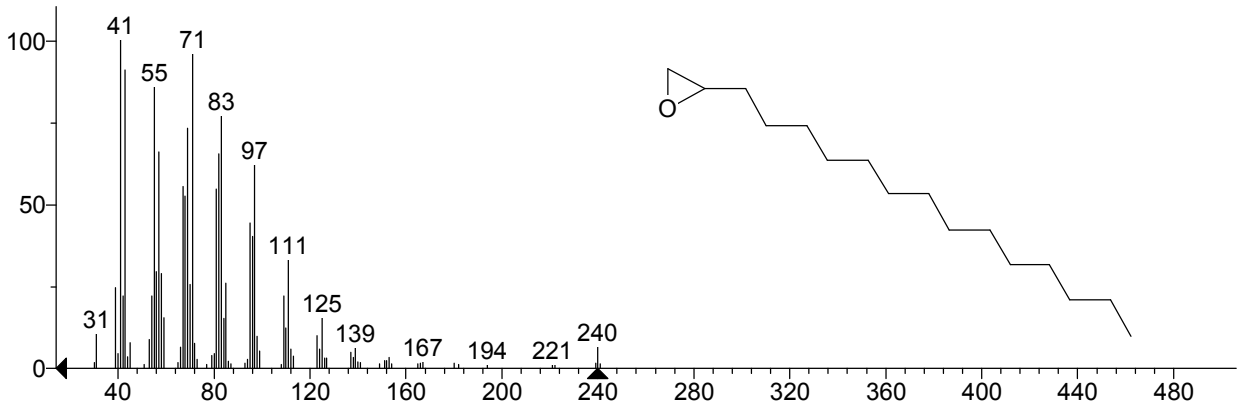
Hit 2 : Octatriacontyl pentafluoropropionate
C41H77F5O2; MF: 767; RMF: 778; Prob 3.70%; Lib: mainlib; ID: 22753.



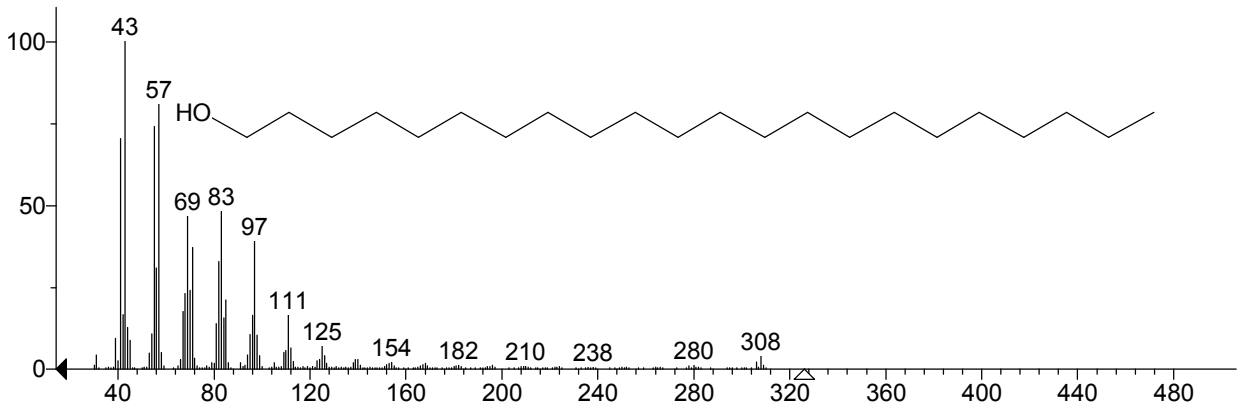
Unknown: Scan 1591 (12.076 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -1067



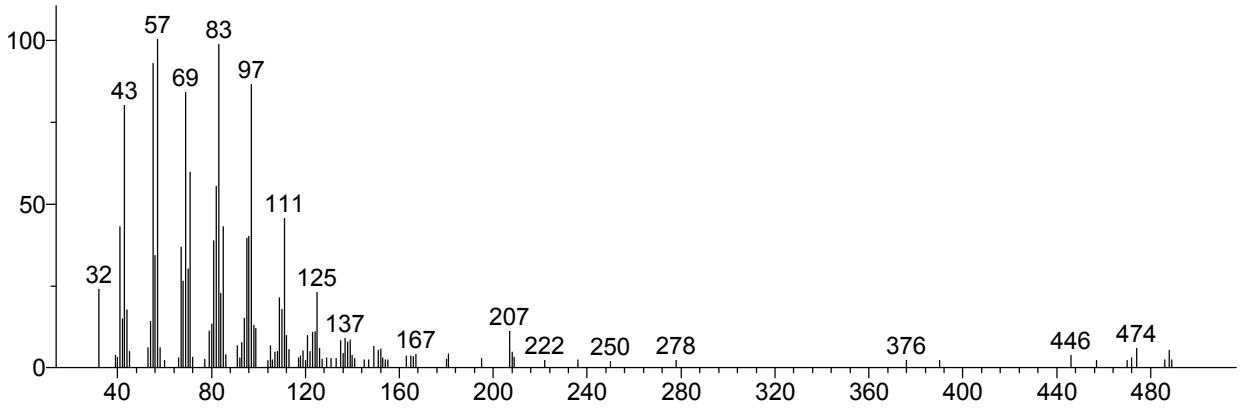
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 751; RMF: 870; Prob 3.85%; CAS: 7320-37-8; Lib: replib; ID: 1171.



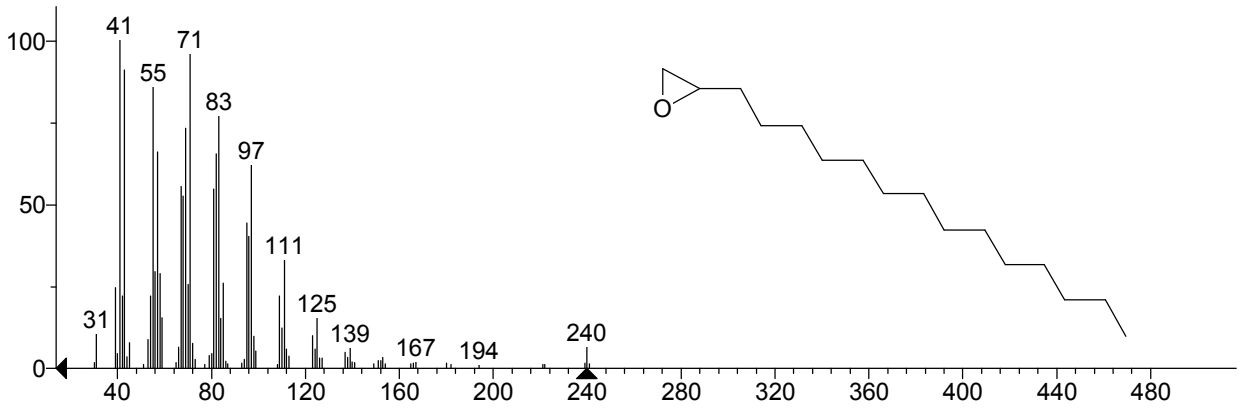
Hit 2 : Behenic alcohol
C22H46O; MF: 745; RMF: 795; Prob 3.02%; CAS: 661-19-8; Lib: replib; ID: 2104.



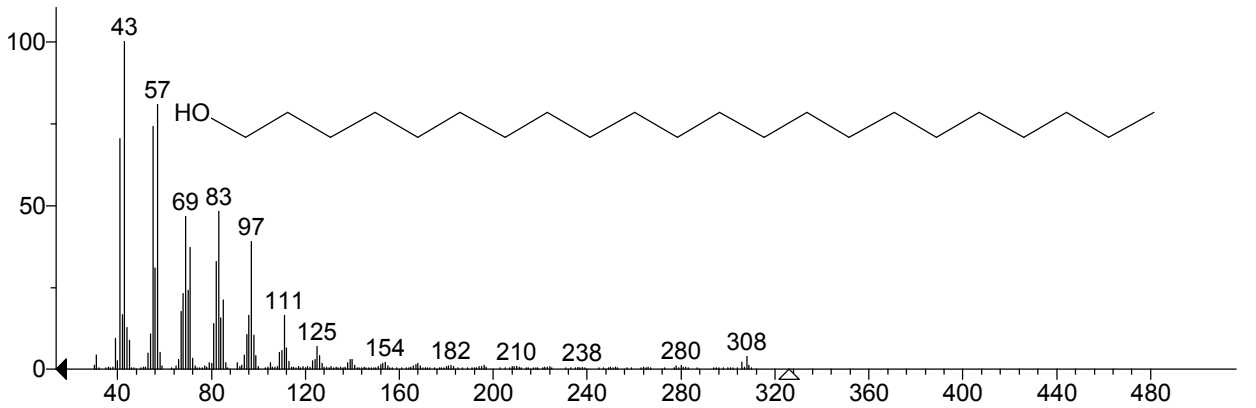
Unknown: Scan 1627 (12.347 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -1103



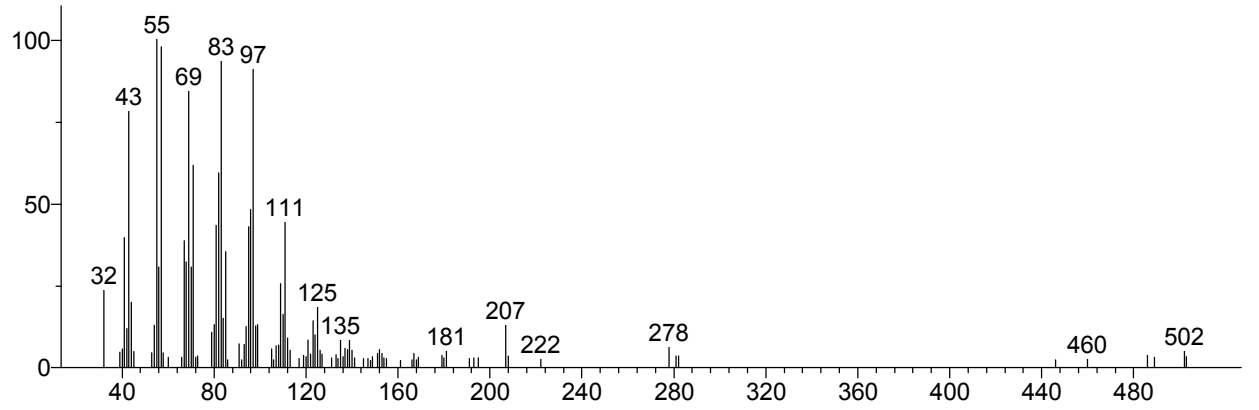
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 750; RMF: 861; Prob 4.72%; CAS: 7320-37-8; Lib: replib; ID: 1171.



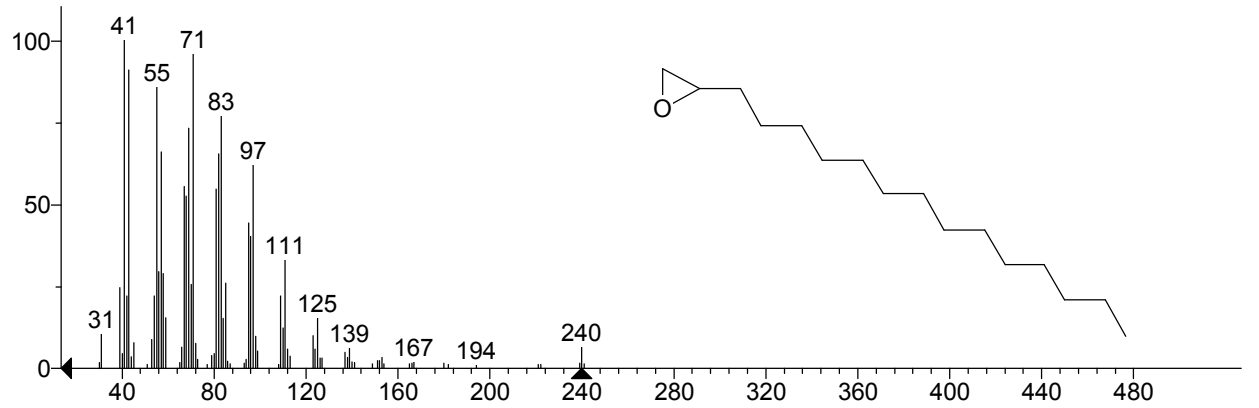
Hit 2 : Behenic alcohol
C22H46O; MF: 743; RMF: 789; Prob 3.62%; CAS: 661-19-8; Lib: replib; ID: 2104.



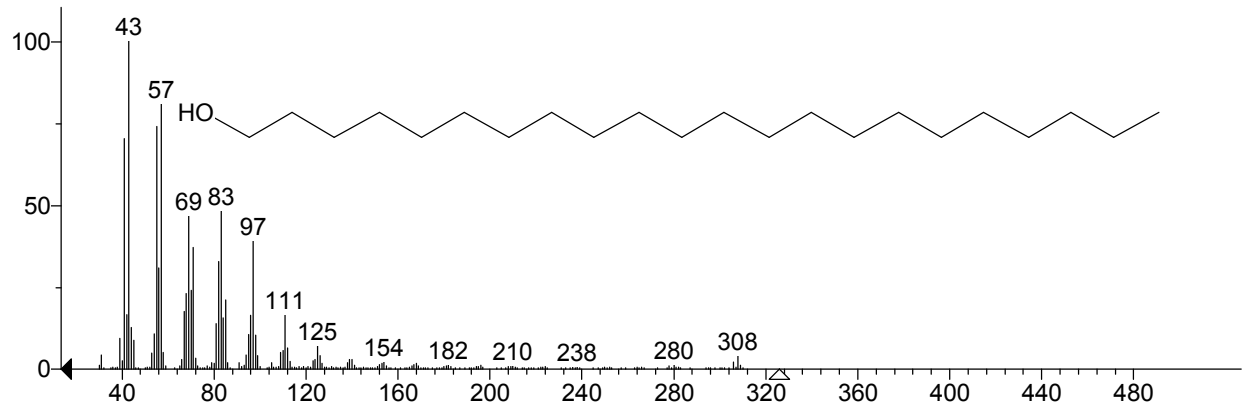
Unknown: Scan 1662 (12.611 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -778



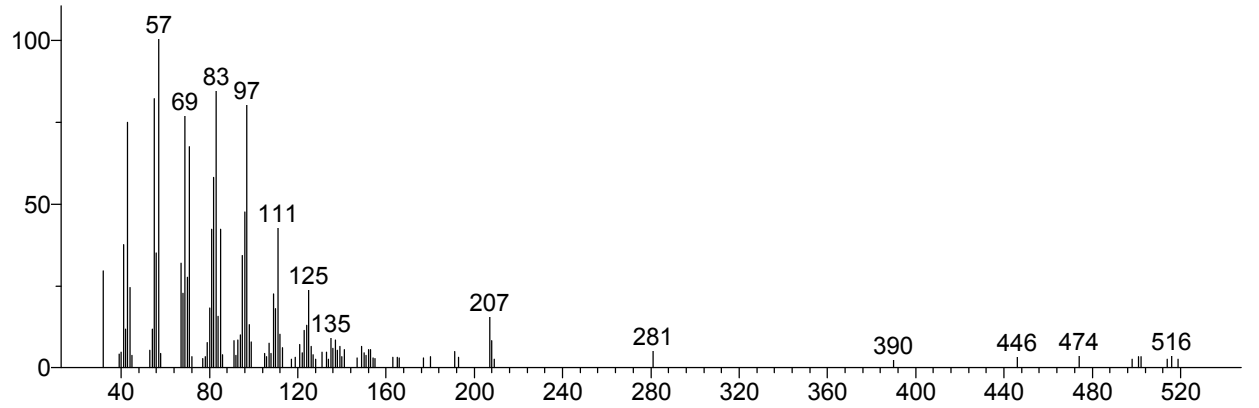
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 751; RMF: 863; Prob 4.27%; CAS: 7320-37-8; Lib: replib; ID: 1171.



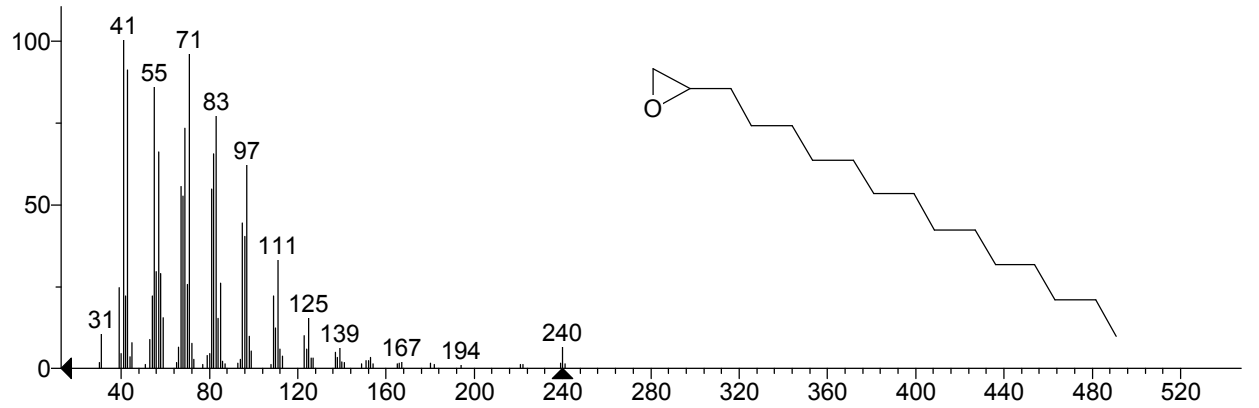
Hit 2 : Behenic alcohol
C22H46O; MF: 751; RMF: 783; Prob 4.27%; CAS: 661-19-8; Lib: replib; ID: 2104.



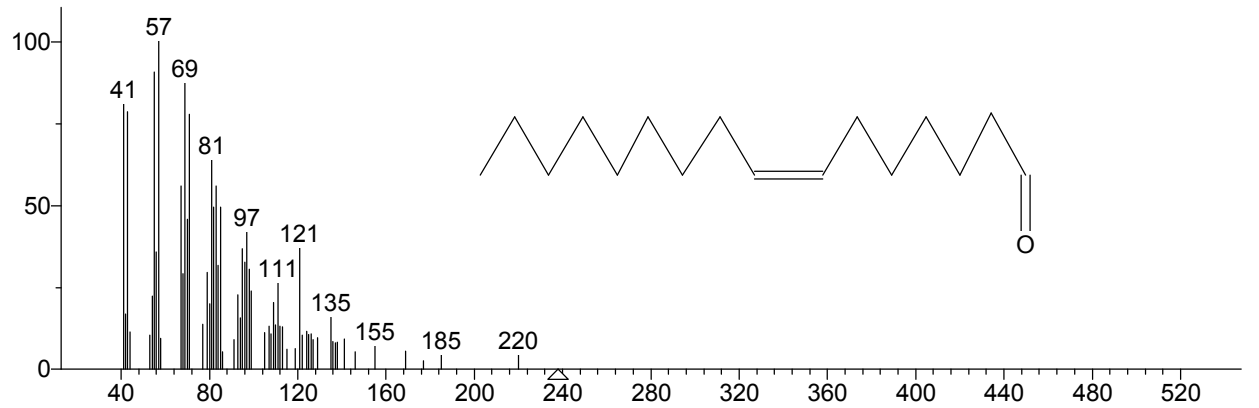
Unknown: Scan 1697 (12.875 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -1131



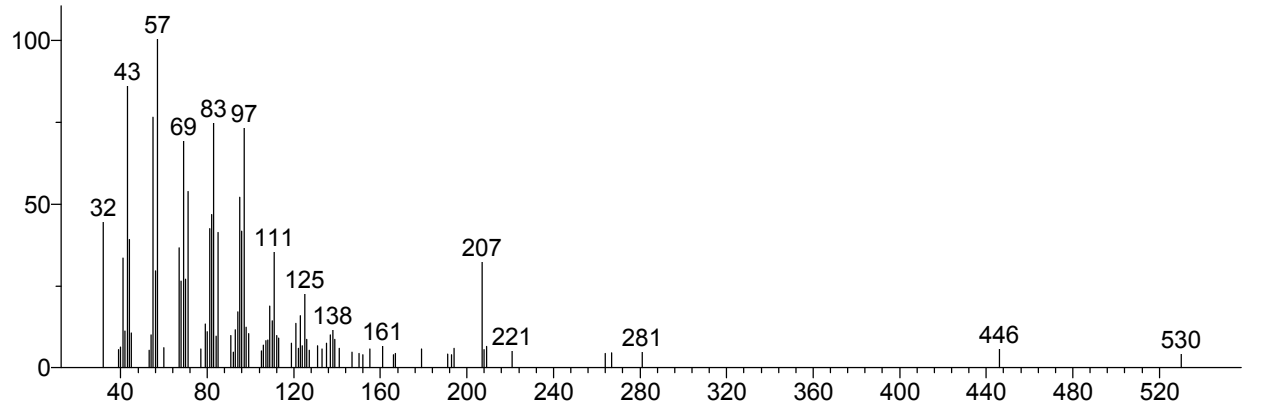
Hit 1 : Oxirane, tetradecyl-
C16H32O; MF: 730; RMF: 851; Prob 4.65%; CAS: 7320-37-8; Lib: replib; ID: 1171.



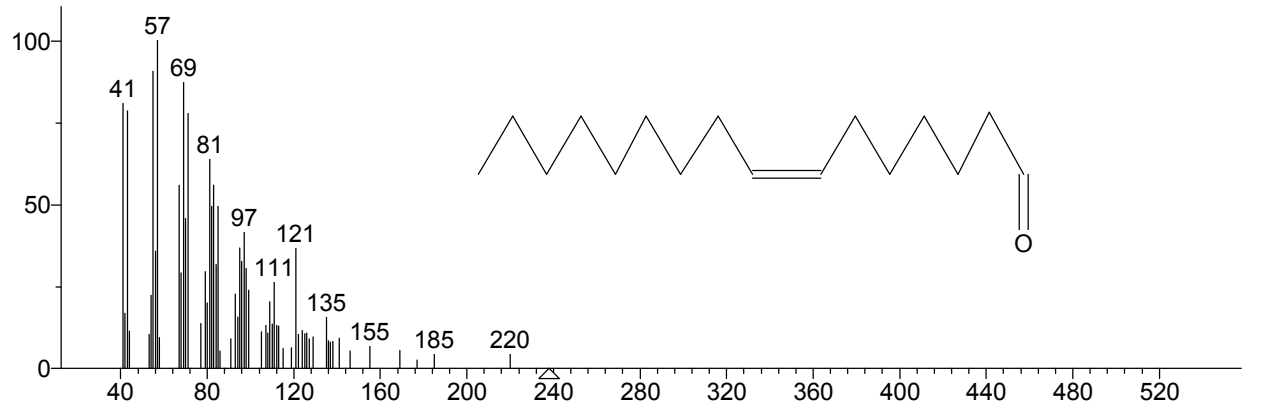
Hit 2 : 7-Hexadecenal, (Z)-
C16H30O; MF: 722; RMF: 847; Prob 3.47%; CAS: 56797-40-1; Lib: replib; ID: 5616.



Unknown: Scan 1734 (13.154 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -632

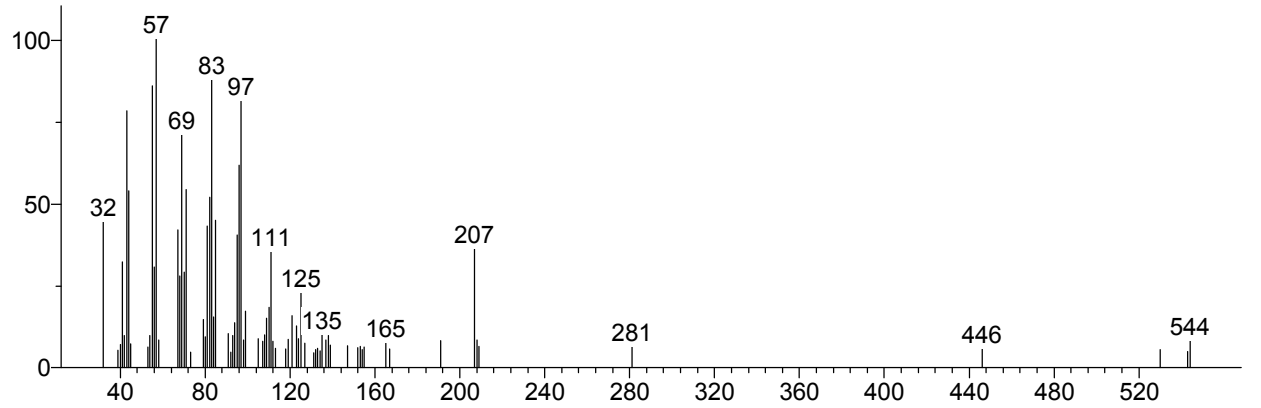


Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 733; RMF: 857; Prob 12.1%; CAS: 56797-40-1; Lib: replib; ID: 5616.

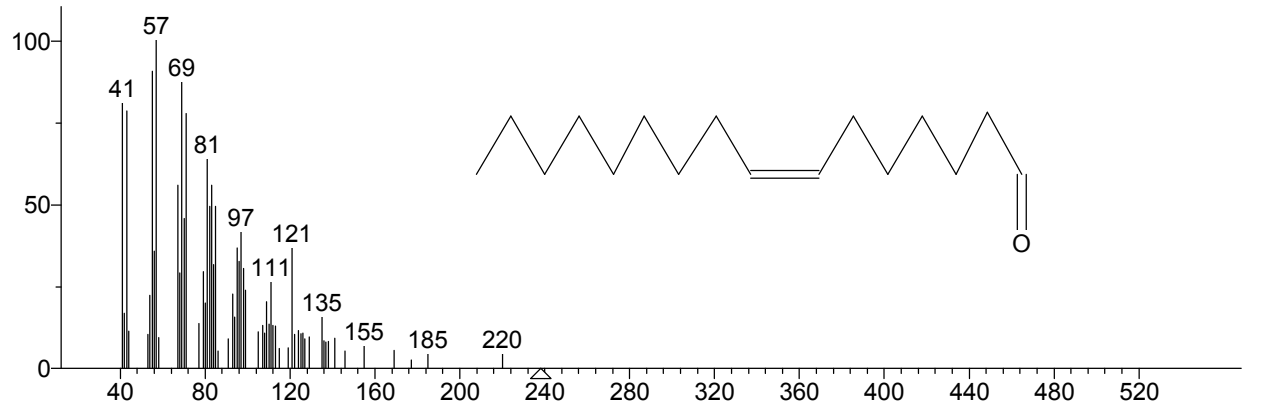


Hit 2 : 13-Octadecenal, (Z)-
C18H34O; MF: 703; RMF: 748; Prob 3.36%; CAS: 58594-45-9; Lib: mainlib; ID: 17493.

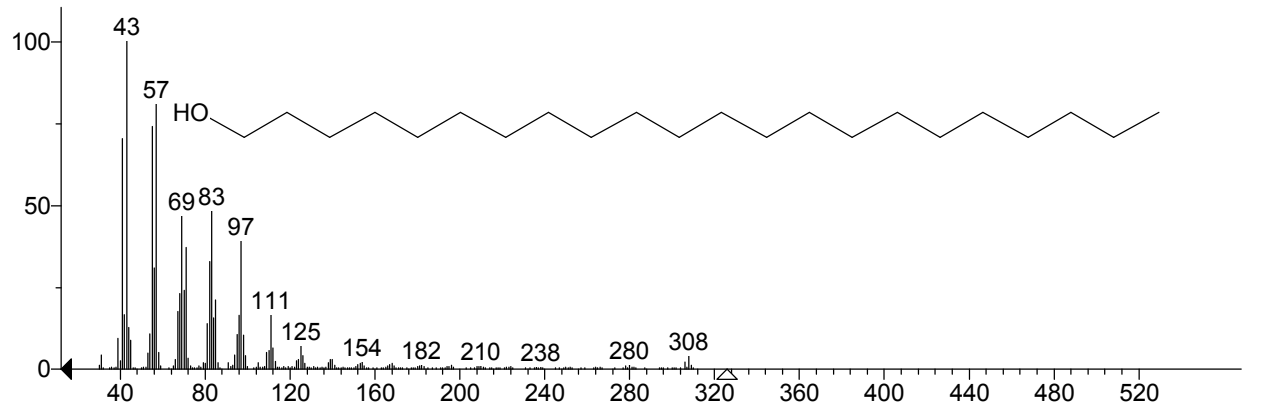
Unknown: Scan 1766 (13.395 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -918



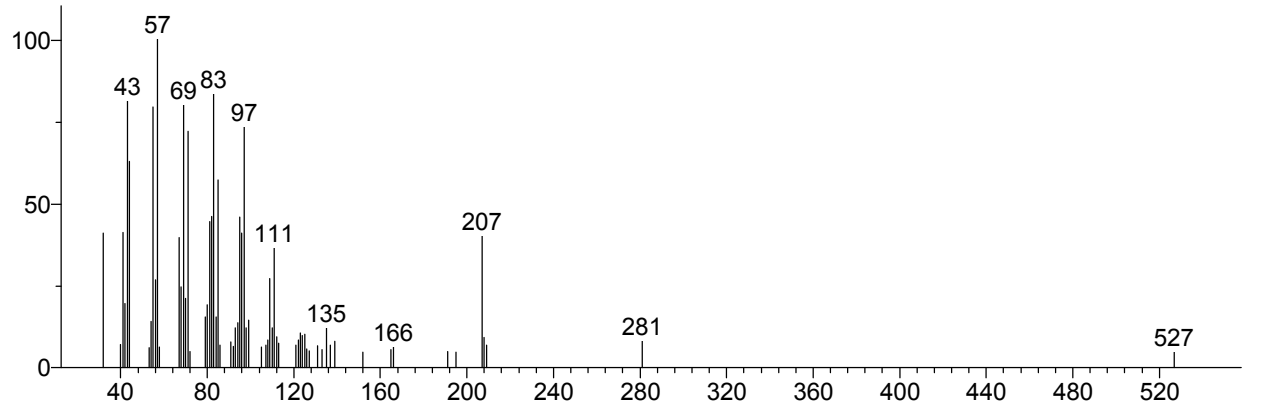
Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 700; RMF: 830; Prob 6.49%; CAS: 56797-40-1; Lib: replib; ID: 5616.



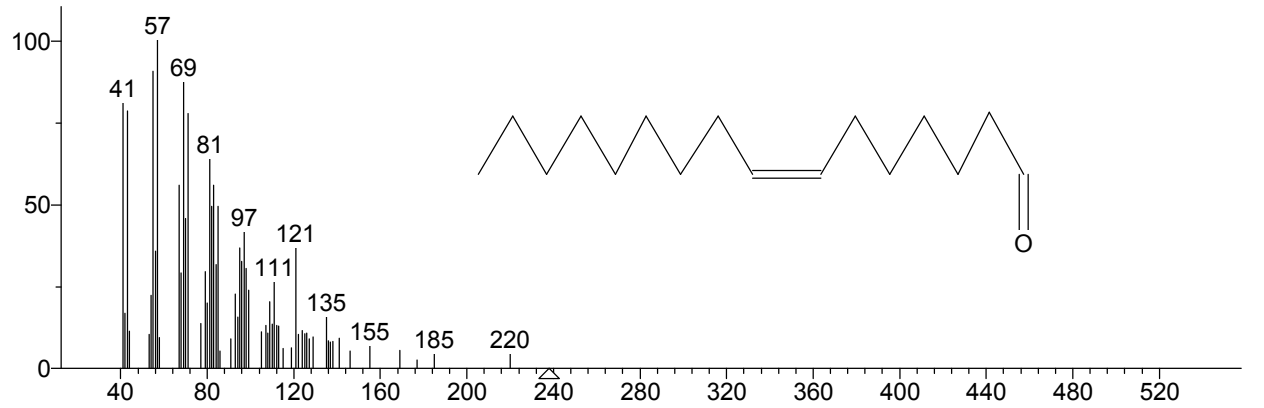
Hit 2 : Behenic alcohol
C22H46O; MF: 679; RMF: 713; Prob 2.76%; CAS: 661-19-8; Lib: replib; ID: 2104.



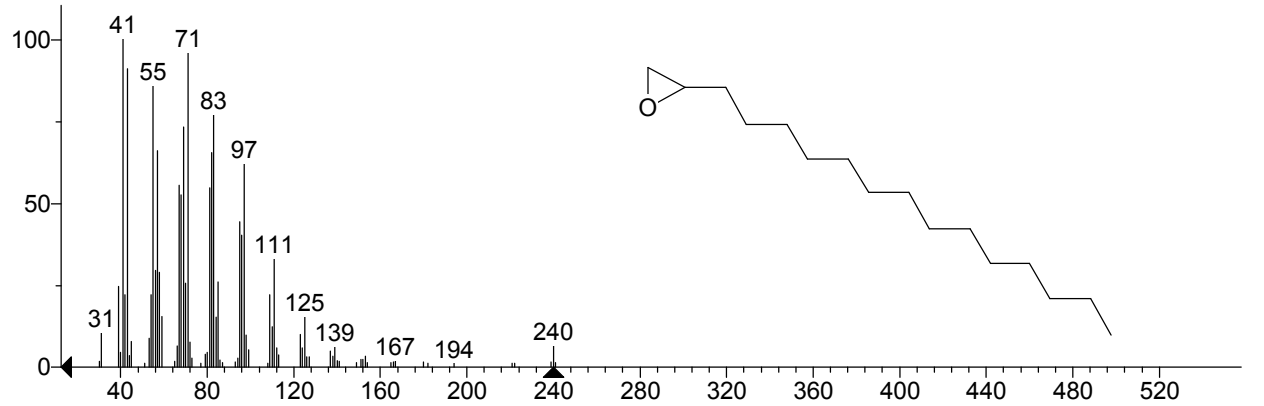
Unknown: Scan 1796 (13.621 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -816



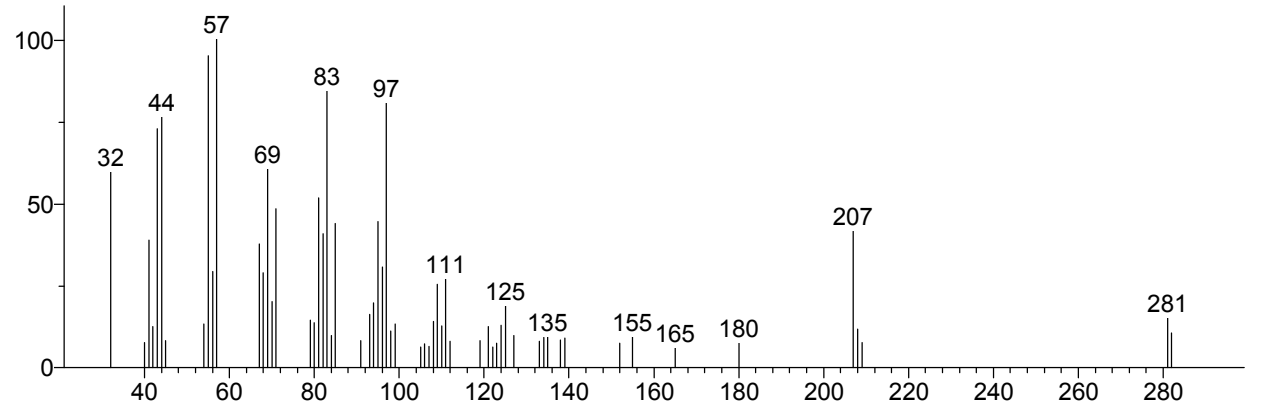
Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 740; RMF: 832; Prob 9.14%; CAS: 56797-40-1; Lib: replib; ID: 5616.



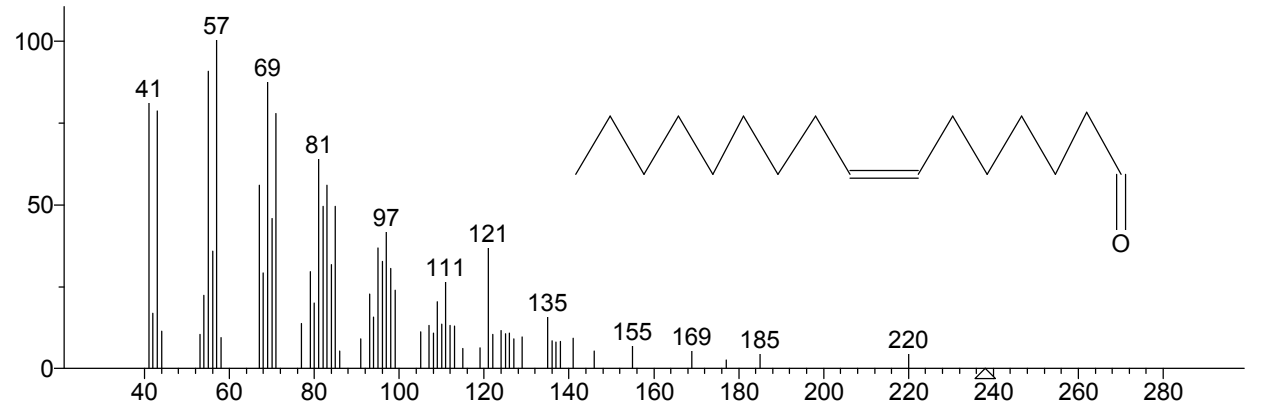
Hit 2 : Oxirane, tetradecyl-
C16H32O; MF: 724; RMF: 823; Prob 5.26%; CAS: 7320-37-8; Lib: replib; ID: 1171.



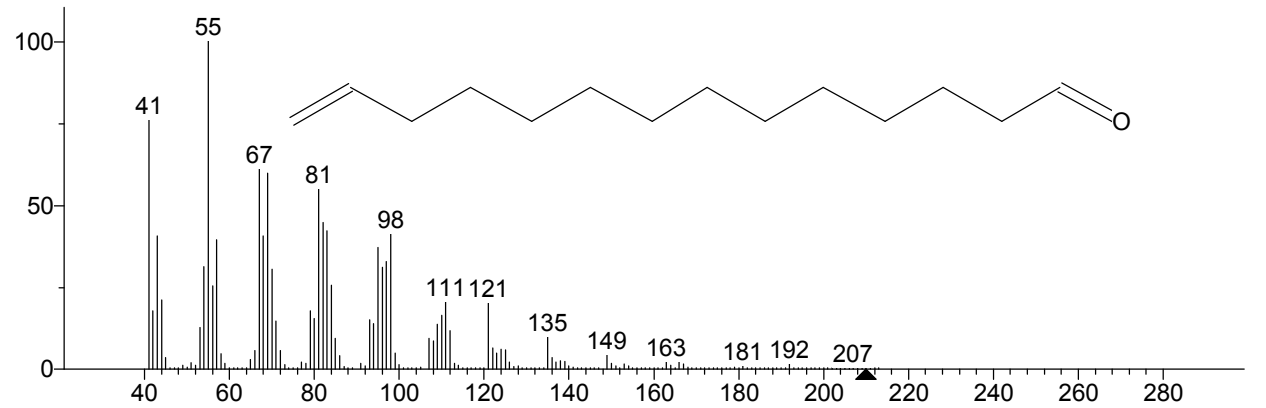
Unknown: Scan 1829 (13.870 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -897



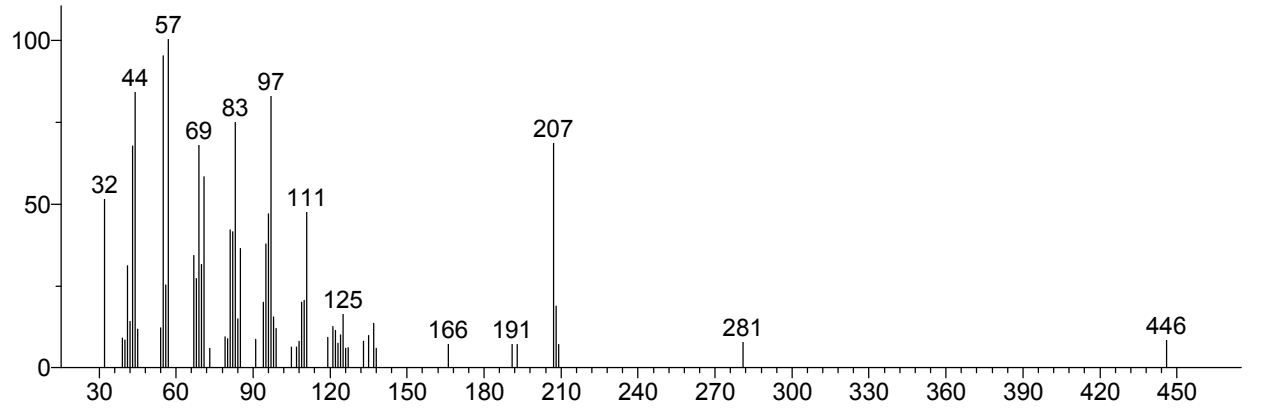
Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 706; RMF: 813; Prob 10.2%; CAS: 56797-40-1; Lib: replib; ID: 5616.



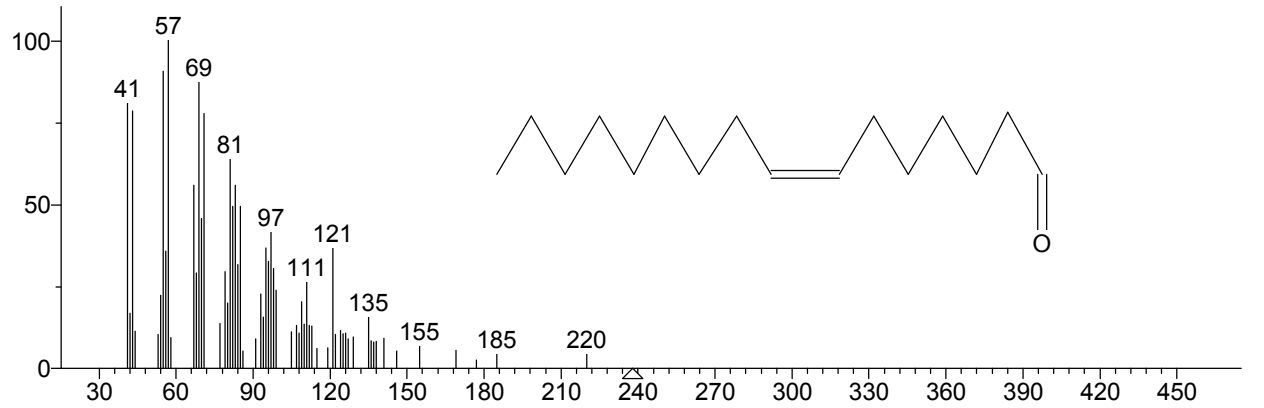
Hit 2 : 13-Tetradecenal
C14H26O; MF: 686; RMF: 712; Prob 4.65%; CAS: 85896-31-7; Lib: mainlib; ID: 17396.



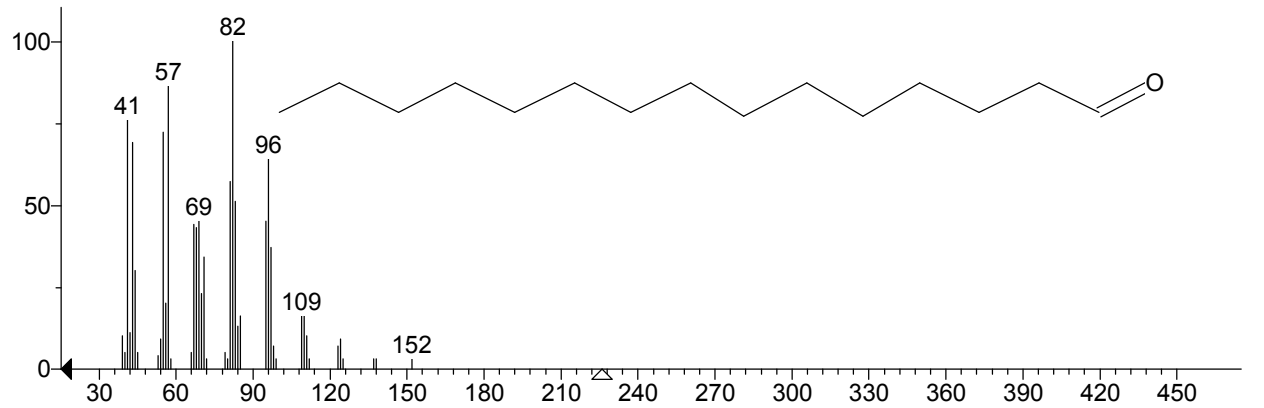
Unknown: Scan 1856 (14.073 min): J9163_Jordi_Inside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -1032



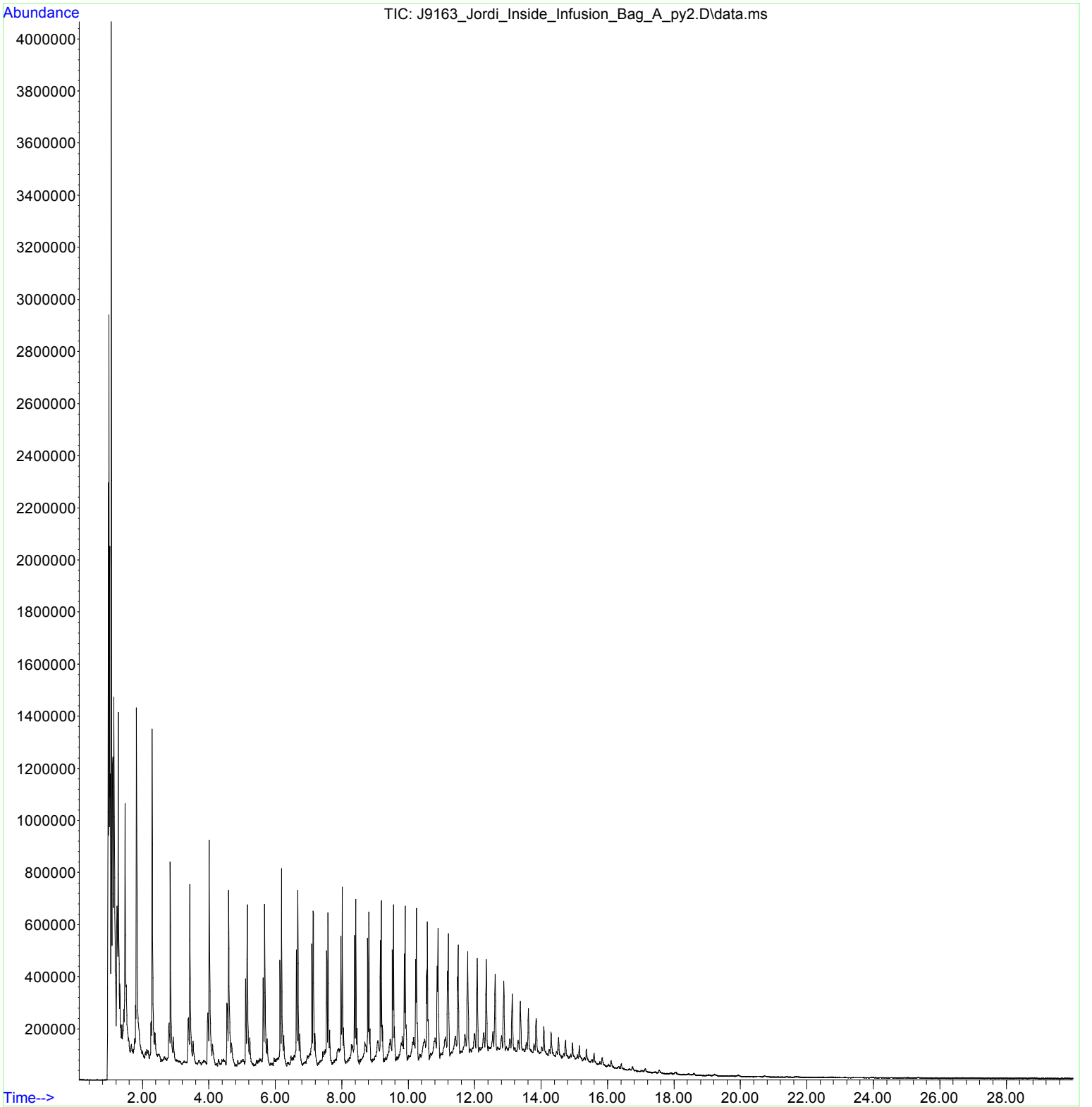
Hit 1 : 7-Hexadecenal, (Z)-
C16H30O; MF: 689; RMF: 800; Prob 7.36%; CAS: 56797-40-1; Lib: replib; ID: 5616.



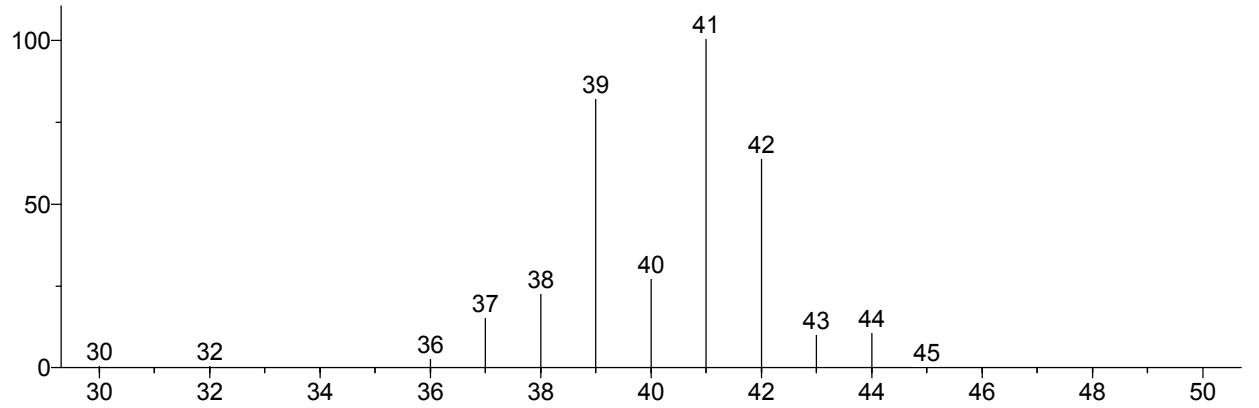
Hit 2 : Pentadecanal-
C15H30O; MF: 673; RMF: 837; Prob 4.24%; CAS: 2765-11-9; Lib: mainlib; ID: 43923.



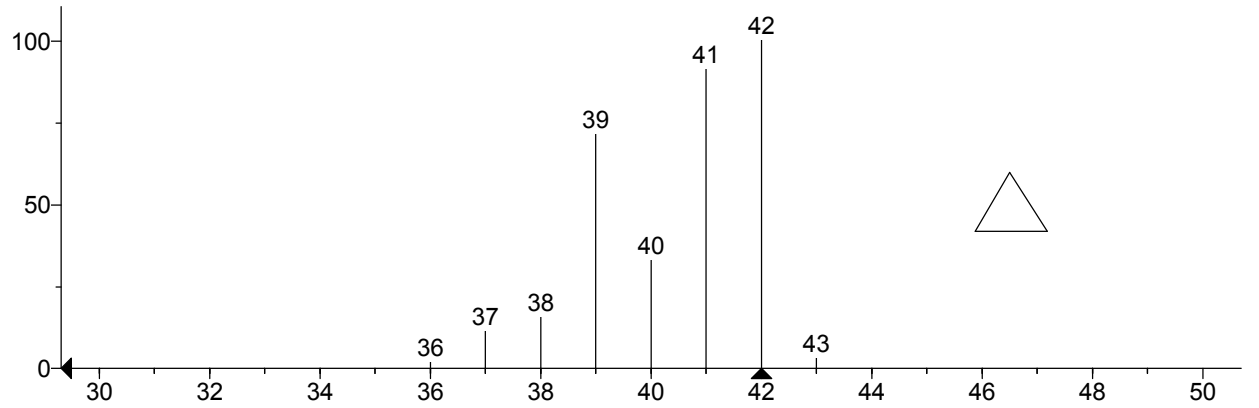
File :C:\msdchem\1\DATA\2014\Temp\102014\J9163_Jordi_Inside_Infusi
... on_Bag_A_py2.D
Operator : Julia Berk
Instrument : Instrument #1
Acquired : 21 Oct 2014 15:47 using AcqMethod PYMSSP30.M
Sample Name: J9163 Jordi Inside Infusion Bag
Misc Info : J9163 Jordi Inside Infusion Bag



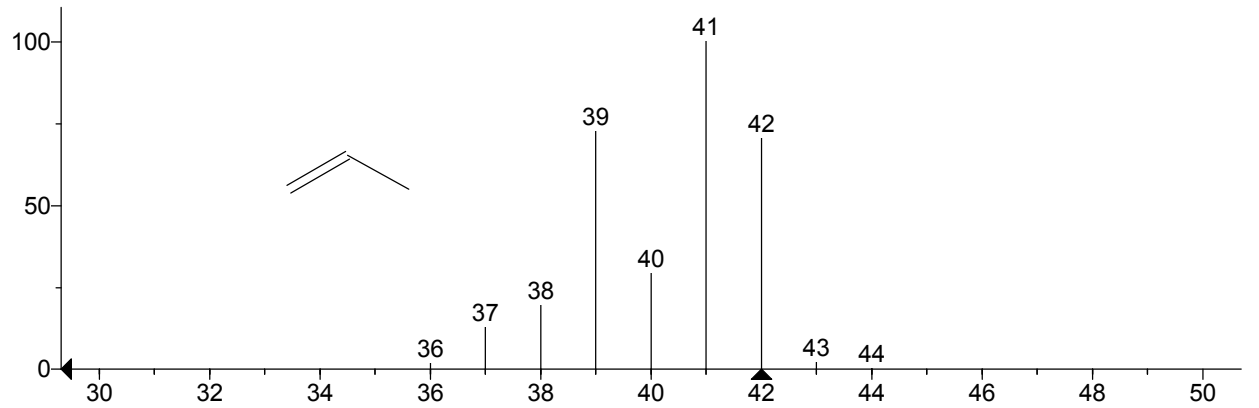
Unknown: Scan 117 (0.969 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = 237



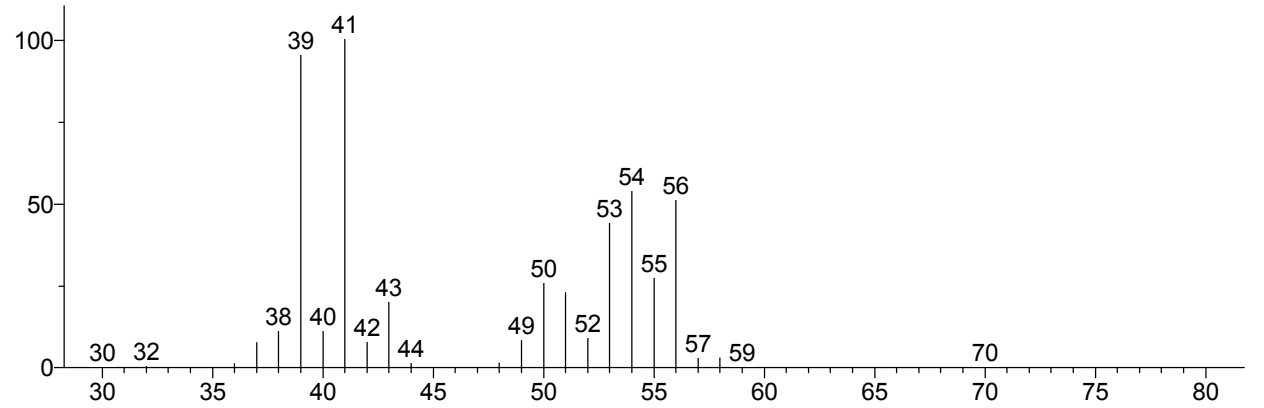
Hit 1 : Cyclopropane
C3H6; MF: 882; RMF: 901; Prob 50.7%; CAS: 75-19-4; Lib: replib; ID: 1331.



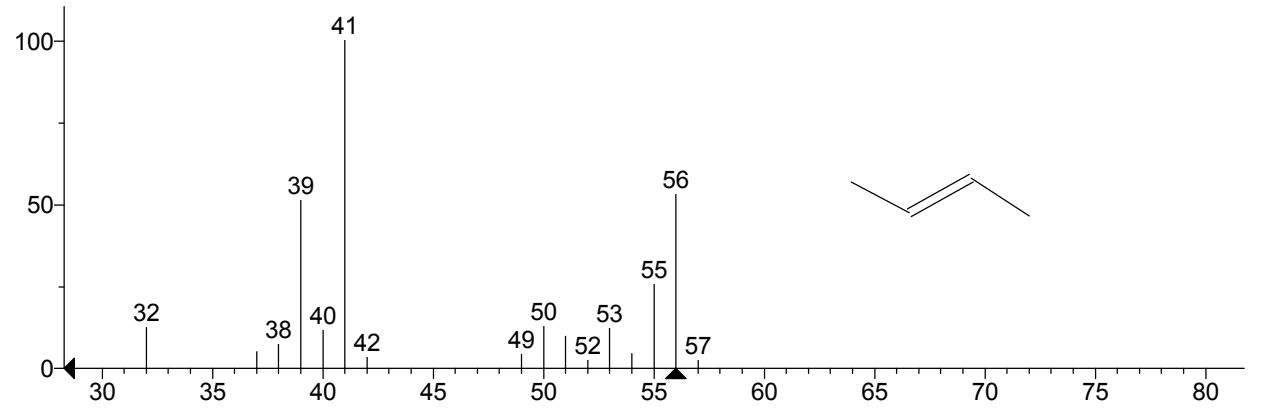
Hit 2 : Propene
C3H6; MF: 875; RMF: 876; Prob 38.8%; CAS: 115-07-1; Lib: mainlib; ID: 1934.



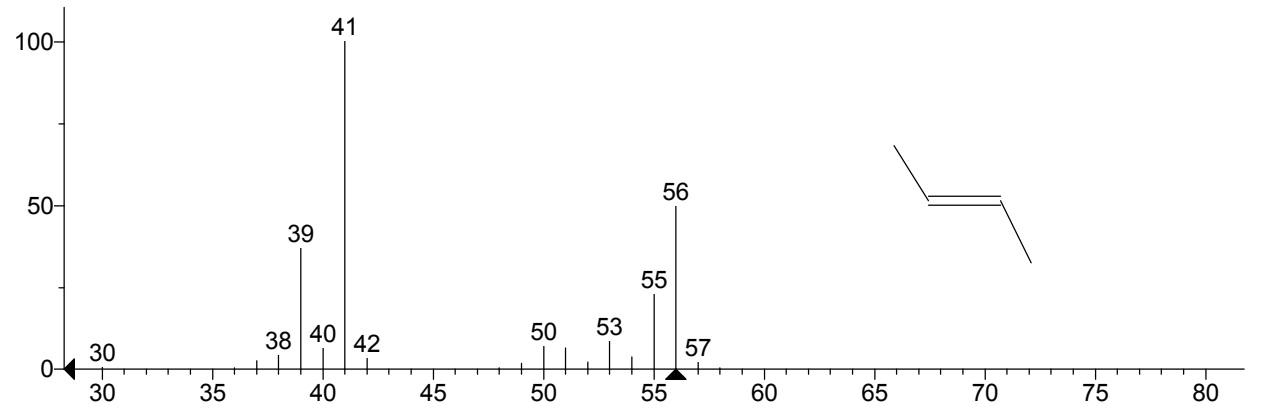
Unknown: Scan 120 (0.992 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -234



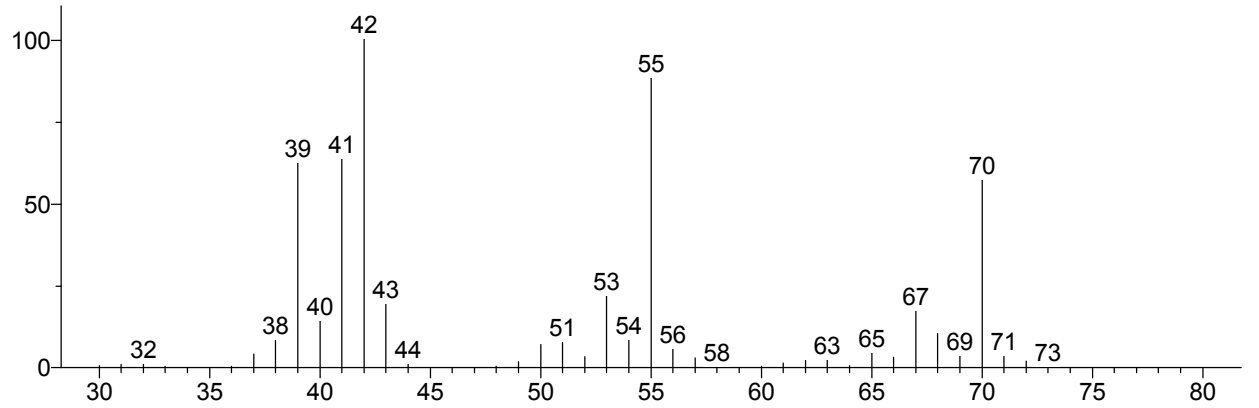
Hit 1 : 2-Butene
C4H8; MF: 830; RMF: 854; Prob 52.8%; CAS: 107-01-7; Lib: mainlib; ID: 1863.



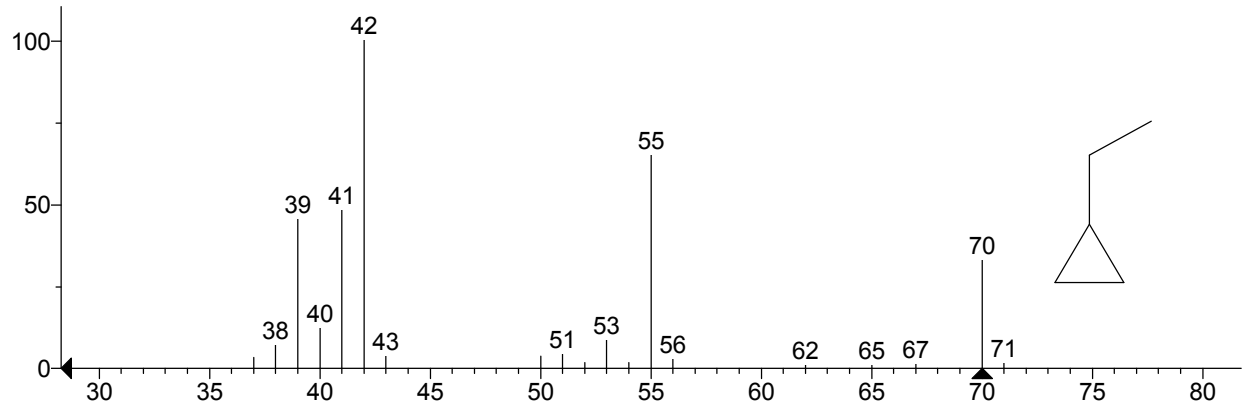
Hit 2 : 2-Butene, (E)-
C4H8; MF: 798; RMF: 817; Prob 14.1%; CAS: 624-64-6; Lib: replib; ID: 964.



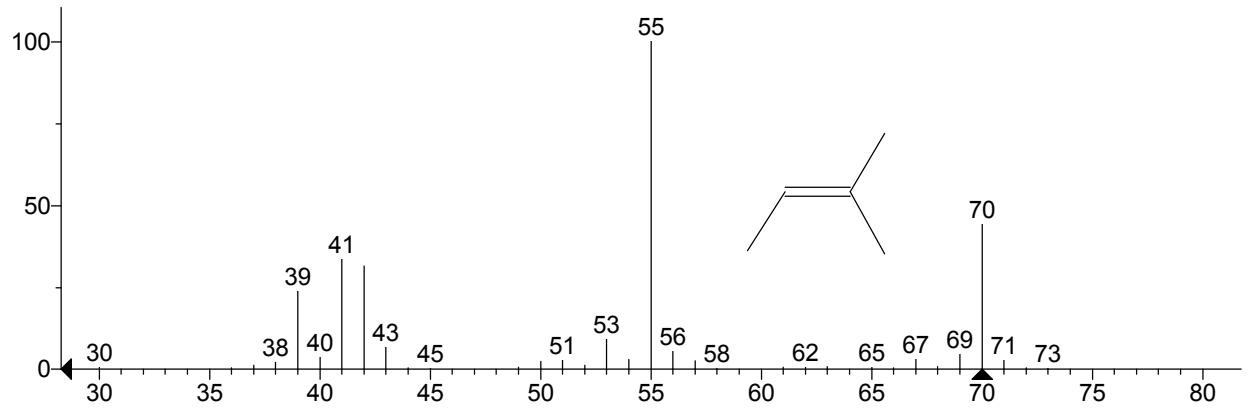
Unknown: Scan 123 (1.014 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -246



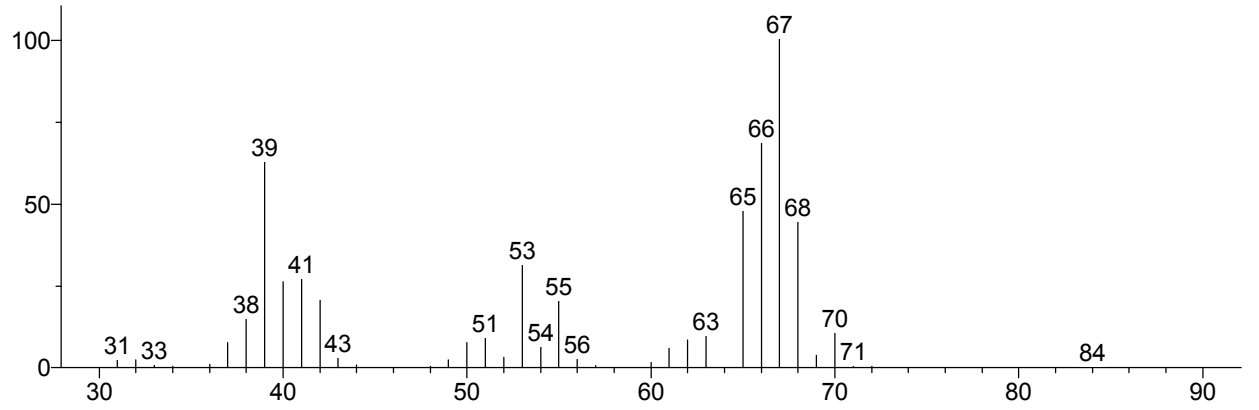
Hit 1 : Cyclopropane, ethyl-
C5H10; MF: 863; RMF: 903; Prob 13.5%; CAS: 1191-96-4; Lib: replib; ID: 1385.



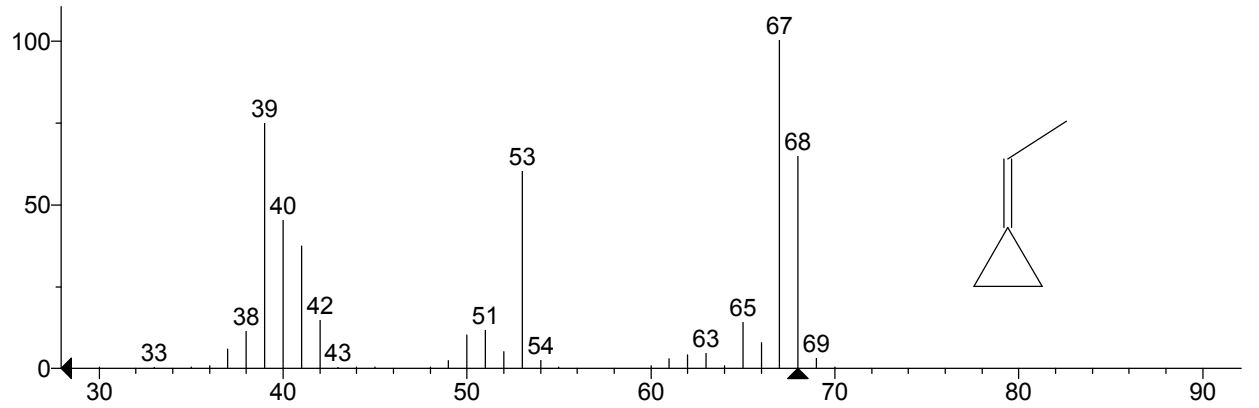
Hit 2 : 2-Butene, 2-methyl-
C5H10; MF: 860; RMF: 862; Prob 11.9%; CAS: 513-35-9; Lib: mainlib; ID: 18422.



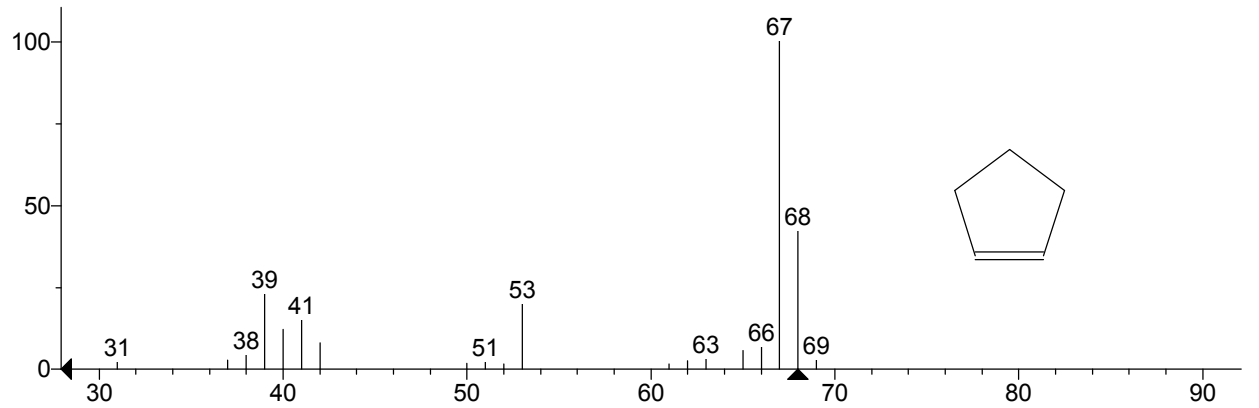
Unknown: Scan 125 (1.030 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -457



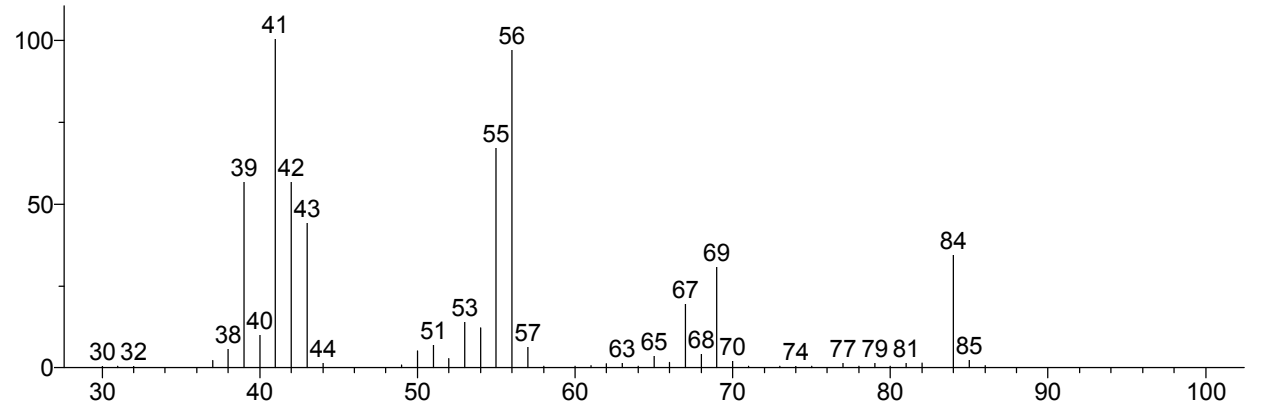
Hit 1 : Cyclopropane, ethylidene-
C5H8; MF: 807; RMF: 842; Prob 13.5%; CAS: 18631-83-9; Lib: mainlib; ID: 28385.



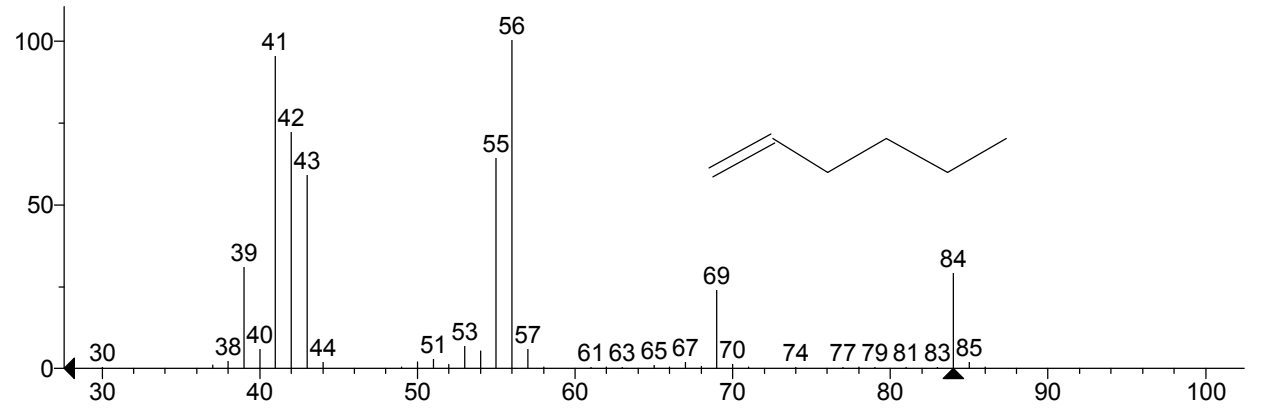
Hit 2 : Cyclopentene
C5H8; MF: 802; RMF: 847; Prob 10.9%; CAS: 142-29-0; Lib: replib; ID: 7176.



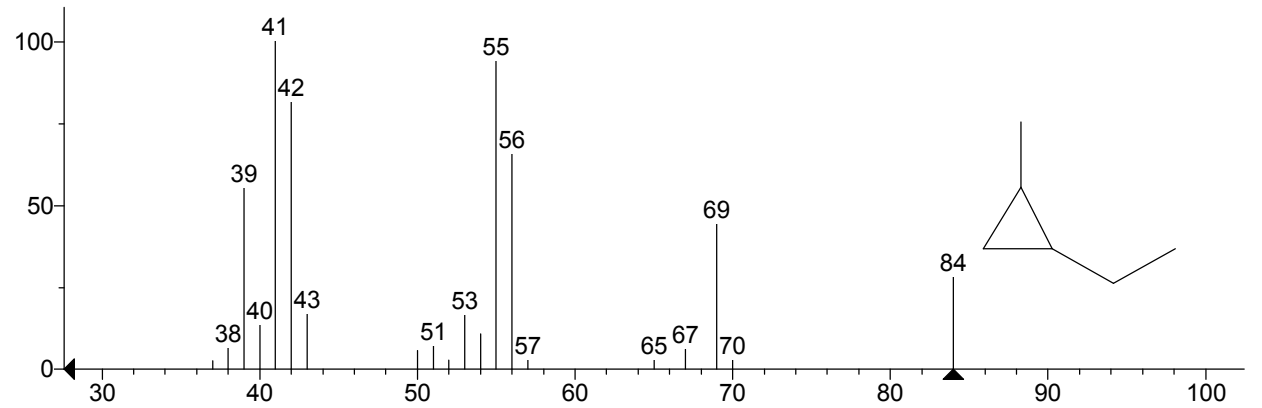
Unknown: Scan 129 (1.060 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -151



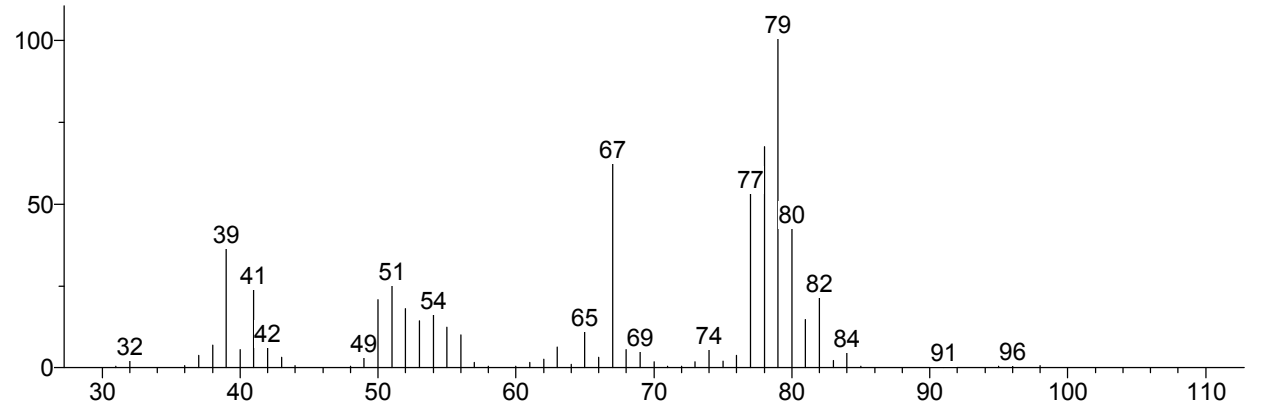
Hit 1 : 1-Hexene
C6H12; MF: 899; RMF: 901; Prob 15.9%; CAS: 592-41-6; Lib: mainlib; ID: 19842.



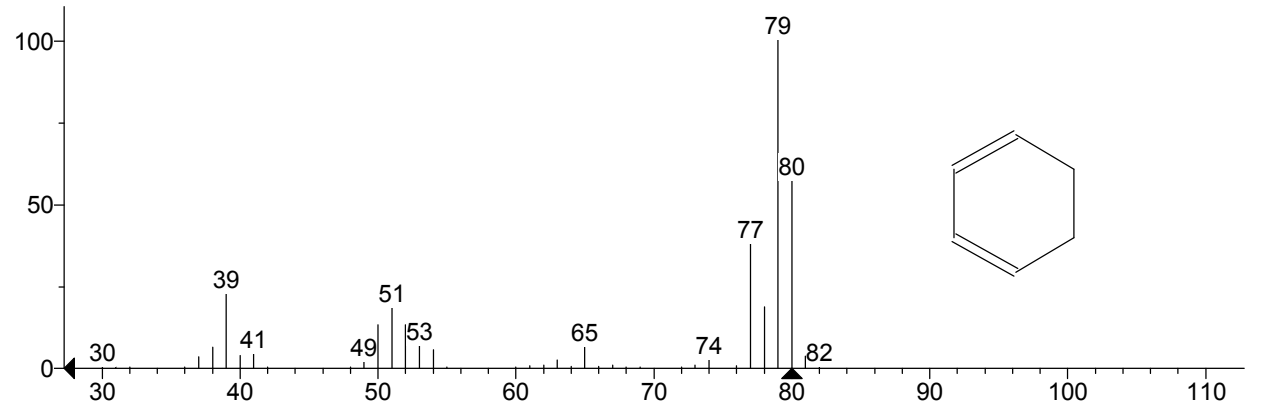
Hit 2 : Cyclopropane, 1-ethyl-2-methyl-, cis-
C6H12; MF: 891; RMF: 917; Prob 11.9%; CAS: 19781-68-1; Lib: mainlib; ID: 2449.



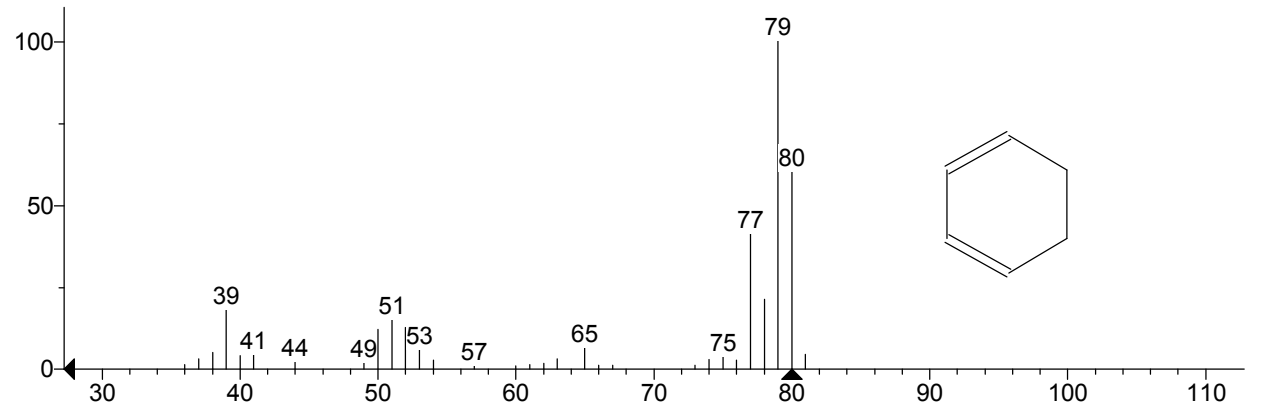
Unknown: Scan 135 (1.105 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -804



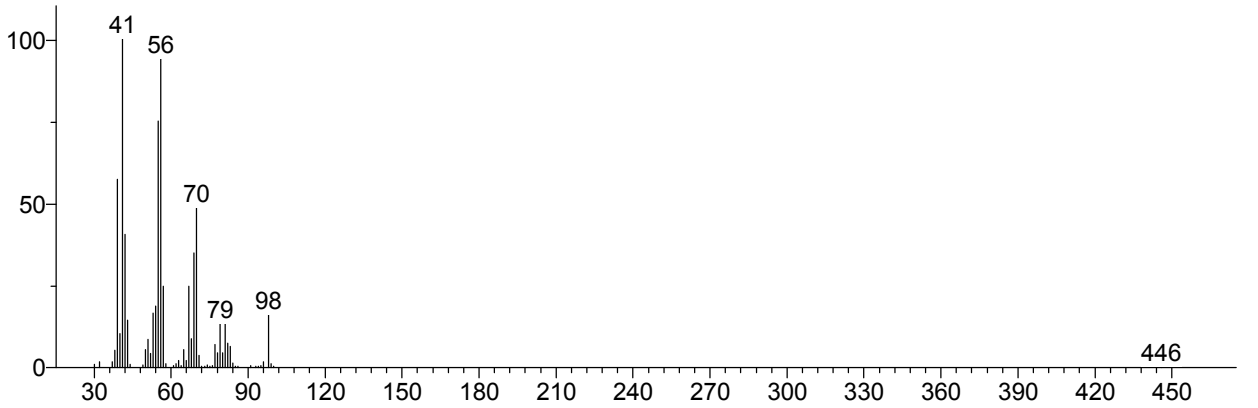
Hit 1 : 1,3-Cyclohexadiene
C6H8; MF: 742; RMF: 760; Prob 14.5%; CAS: 592-57-4; Lib: replib; ID: 9711.



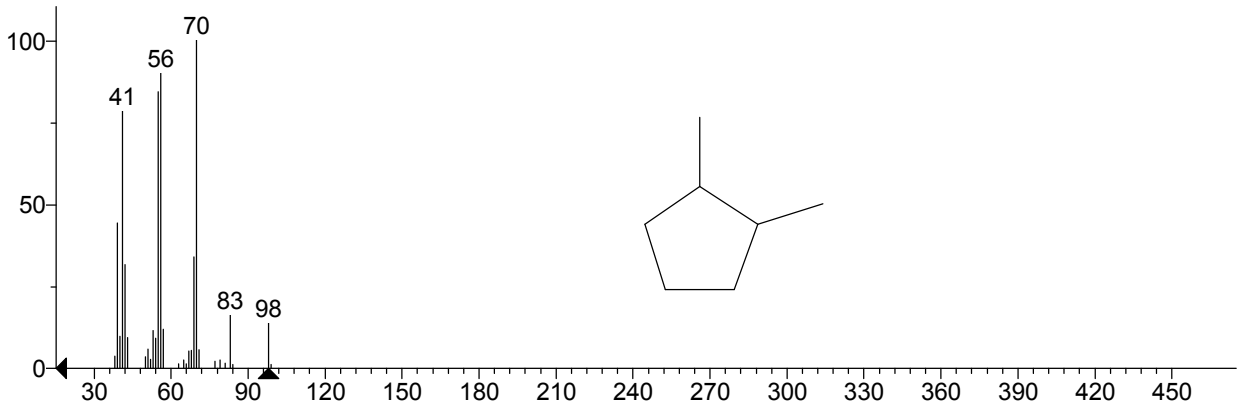
Hit 2 : 1,3-Cyclohexadiene
C6H8; MF: 728; RMF: 785; Prob 14.5%; CAS: 592-57-4; Lib: replib; ID: 9712.



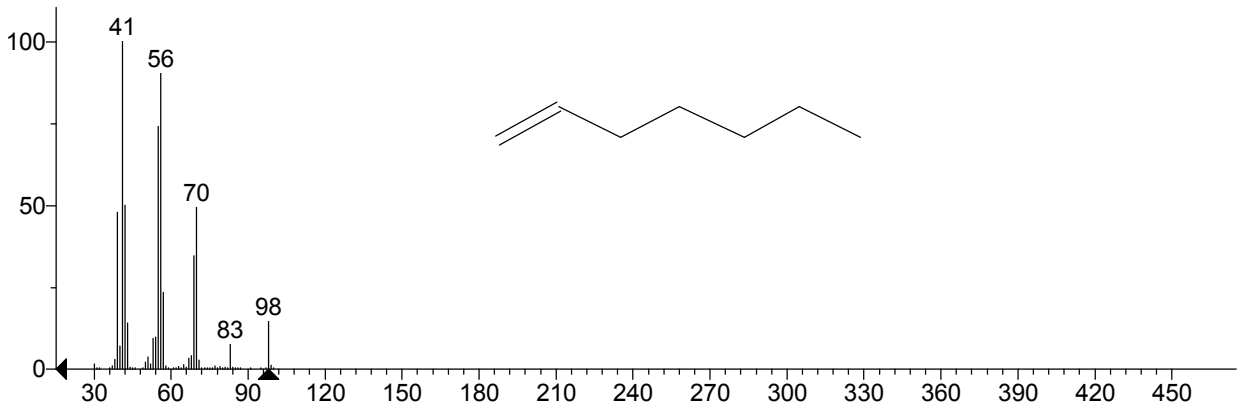
Unknown: Scan 139 (1.135 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -454



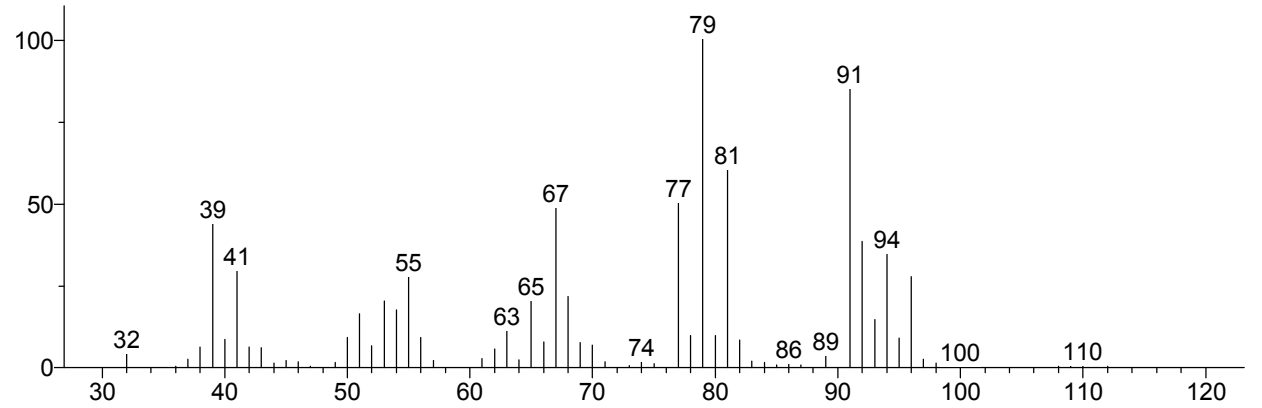
Hit 1 : Cyclopentane, 1,2-dimethyl-, cis-
C7H14; MF: 850; RMF: 880; Prob 10.1%; CAS: 1192-18-3; Lib: mainlib; ID: 32333.



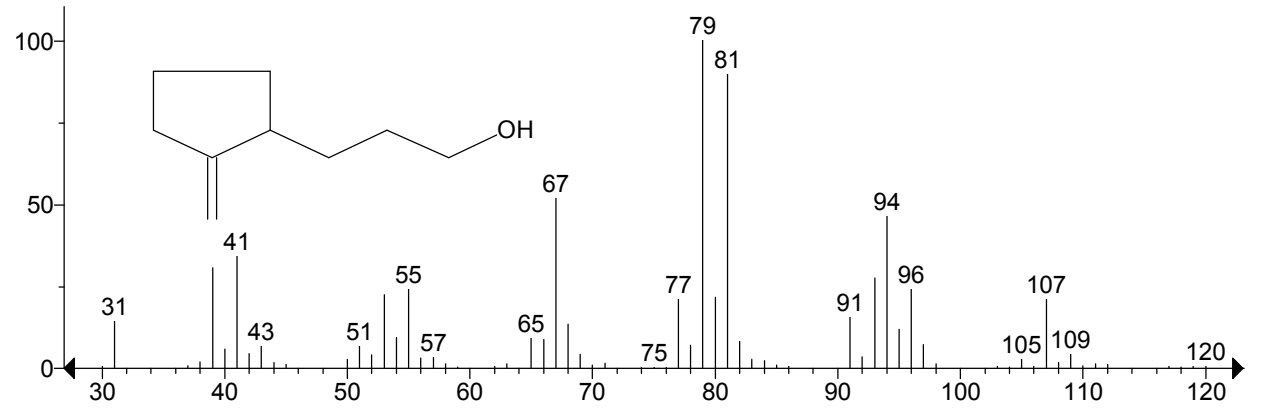
Hit 2 : 1-Heptene
C7H14; MF: 848; RMF: 857; Prob 9.35%; CAS: 592-76-7; Lib: replib; ID: 981.



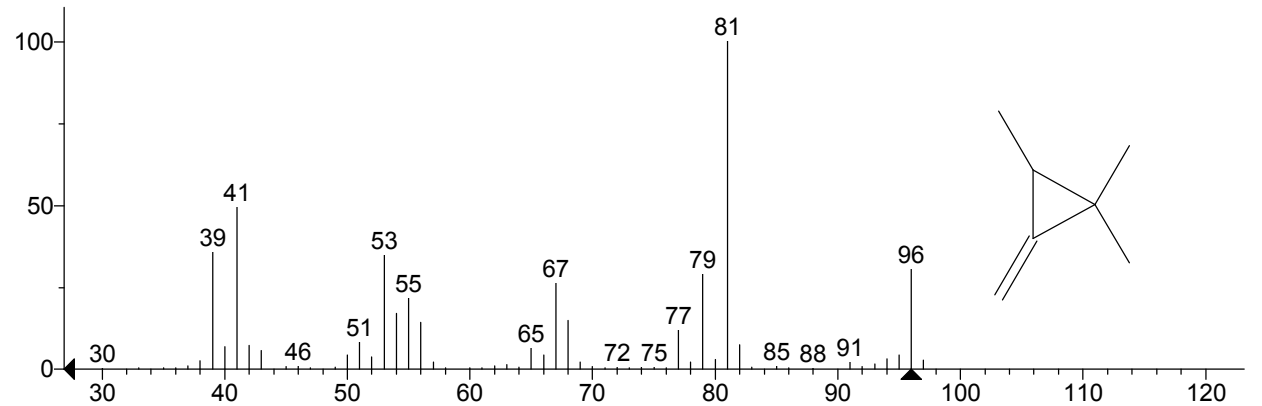
Unknown: Scan 152 (1.233 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -778



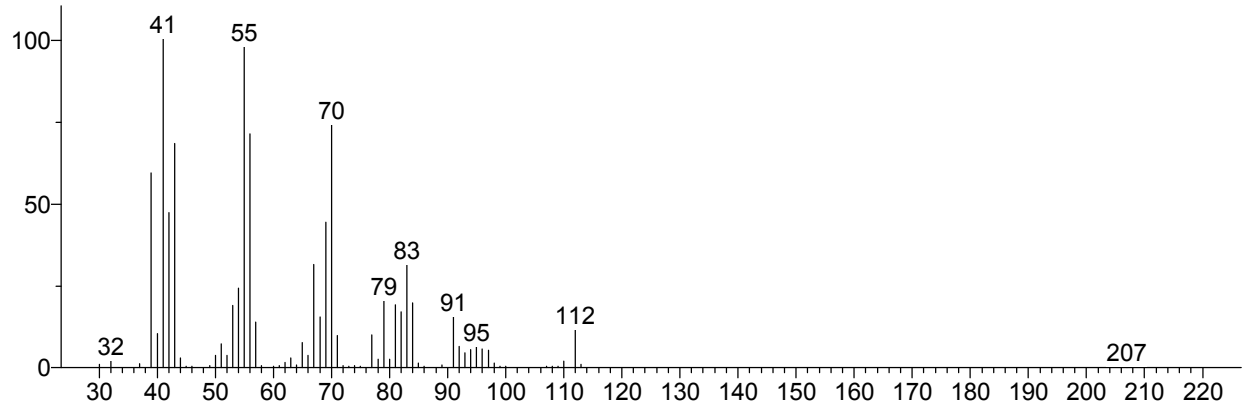
Hit 1 : Cyclopentanepropanol, 2-methylene-
C9H16O; MF: 752; RMF: 760; Prob 8.26%; CAS: 53544-48-2; Lib: mainlib; ID: 41912.



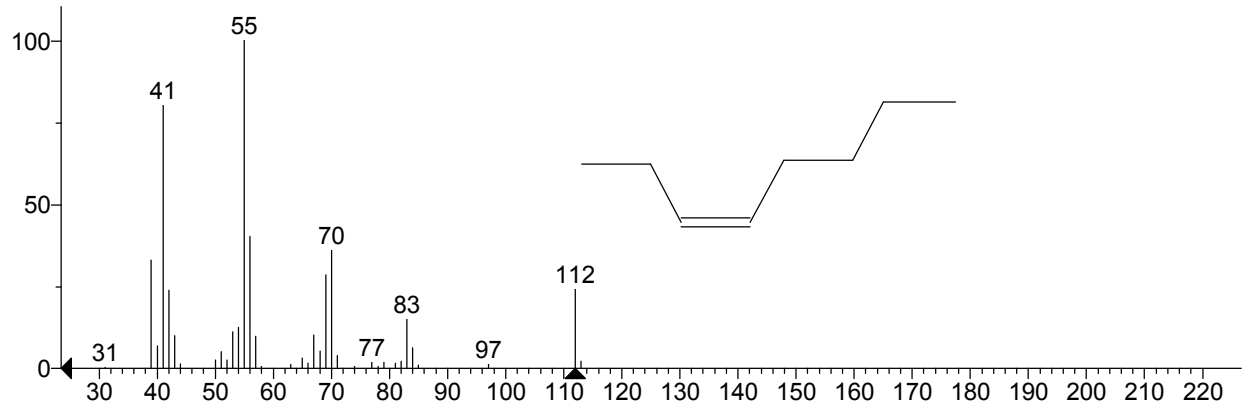
Hit 2 : Cyclopropane, trimethylmethylene-
C7H12; MF: 742; RMF: 748; Prob 5.83%; CAS: 34462-28-7; Lib: mainlib; ID: 42667.



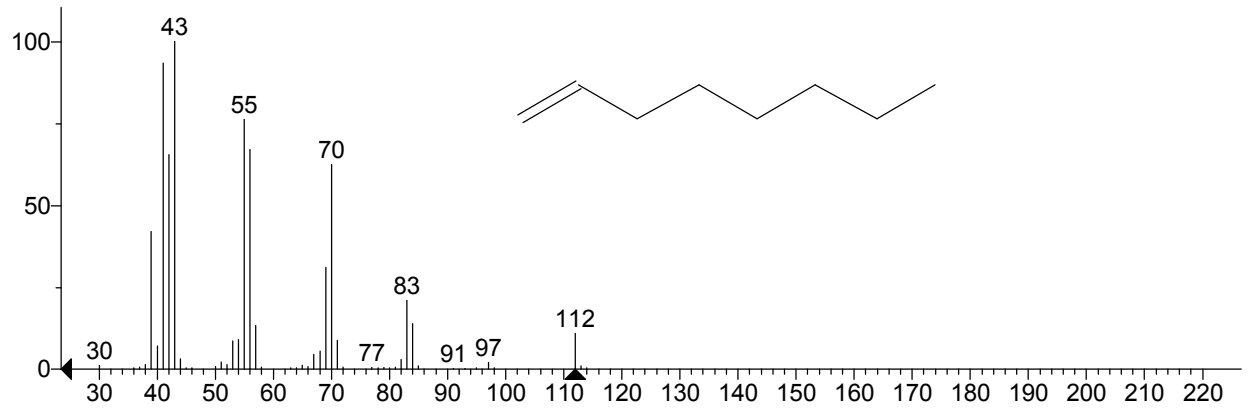
Unknown: Scan 157 (1.271 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -503



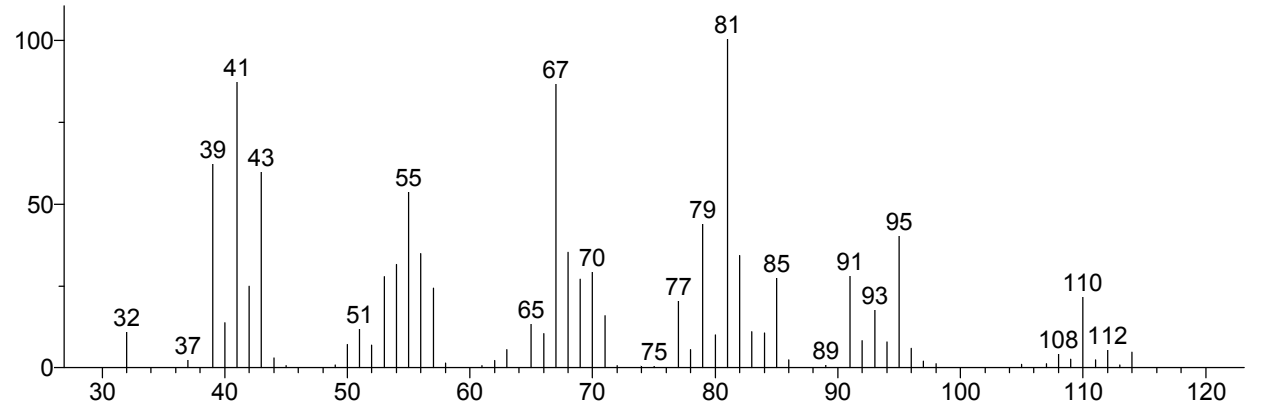
Hit 1 : 3-Octene, (Z)-
C8H16; MF: 827; RMF: 875; Prob 6.75%; CAS: 14850-22-7; Lib: replib; ID: 4204.



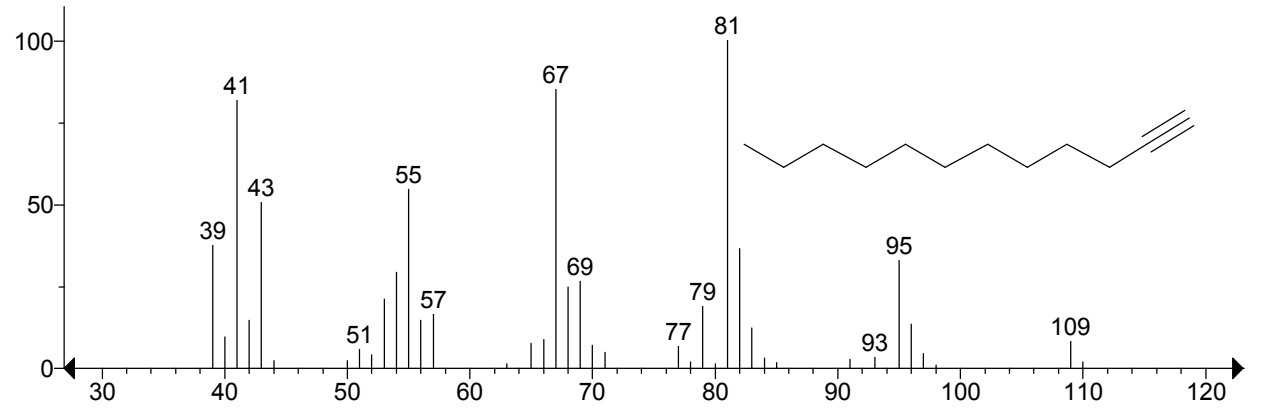
Hit 2 : 1-Octene
C8H16; MF: 821; RMF: 841; Prob 5.30%; CAS: 111-66-0; Lib: replib; ID: 1671.



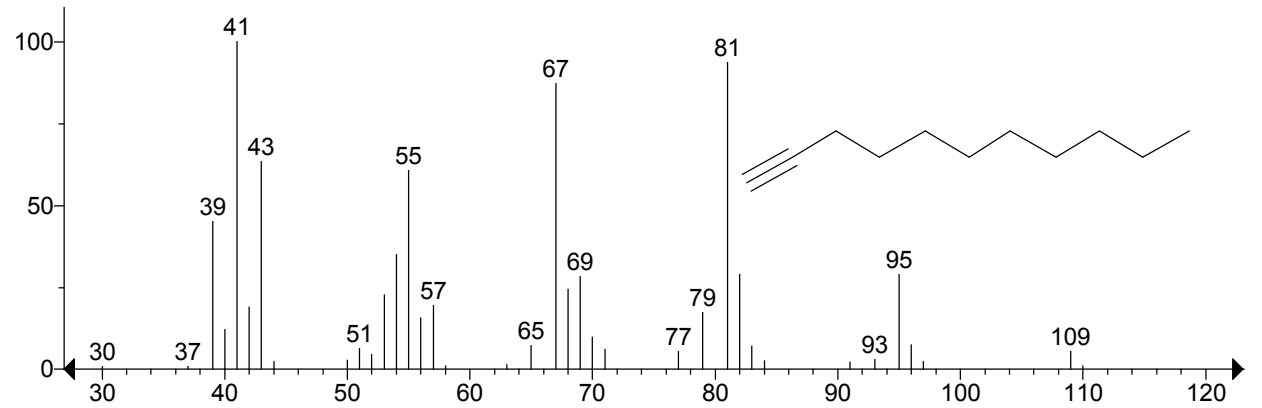
Unknown: Scan 163 (1.316 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -698



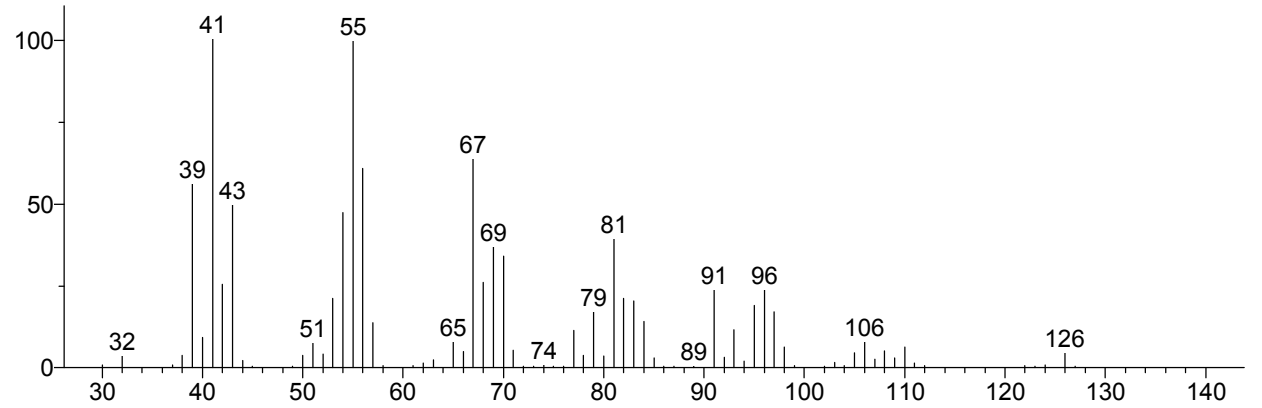
Hit 1 : 1-Dodecyne
C12H22; MF: 795; RMF: 827; Prob 6.85%; CAS: 765-03-7; Lib: replib; ID: 9944.



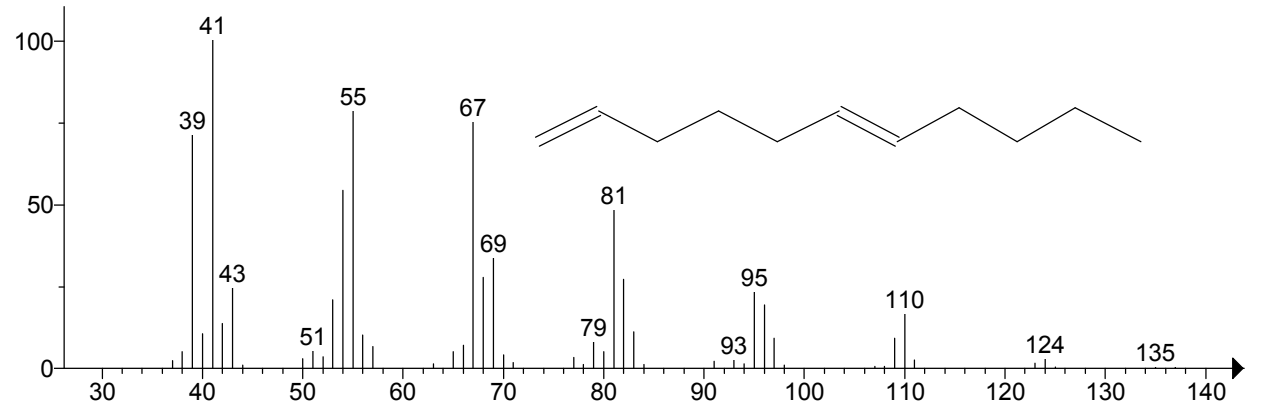
Hit 2 : 1-Undecyne
C11H20; MF: 792; RMF: 857; Prob 6.05%; CAS: 2243-98-3; Lib: replib; ID: 1202.



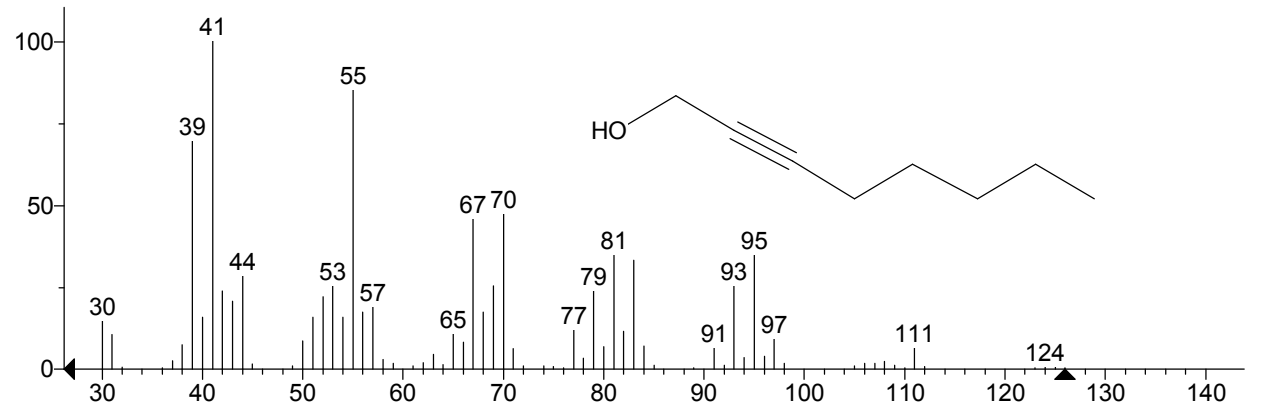
Unknown: Scan 184 (1.474 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -713



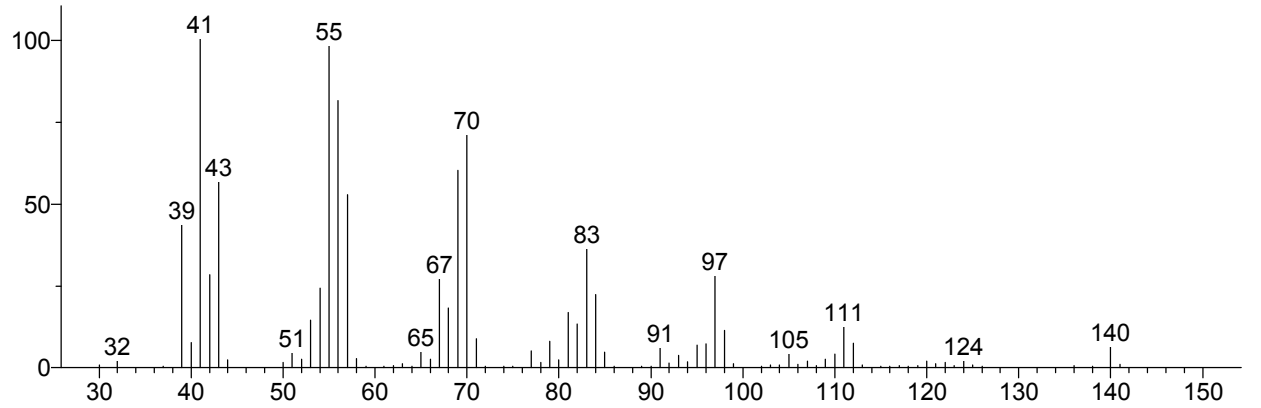
Hit 1 : E-1,6-Undecadiene
C11H20; MF: 786; RMF: 810; Prob 4.06%; Lib: mainlib; ID: 2540.



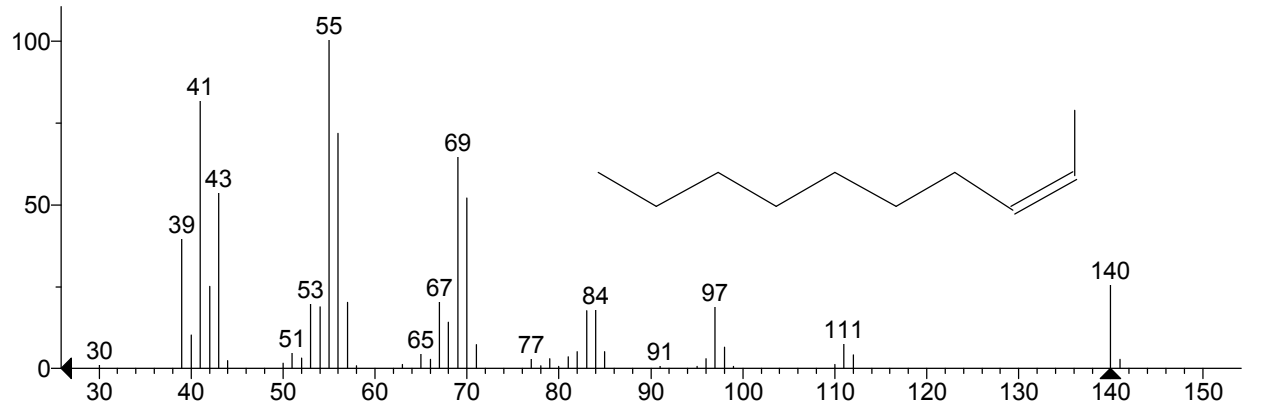
Hit 2 : 2-Octyn-1-ol
C8H14O; MF: 782; RMF: 785; Prob 3.43%; CAS: 20739-58-6; Lib: replib; ID: 871.



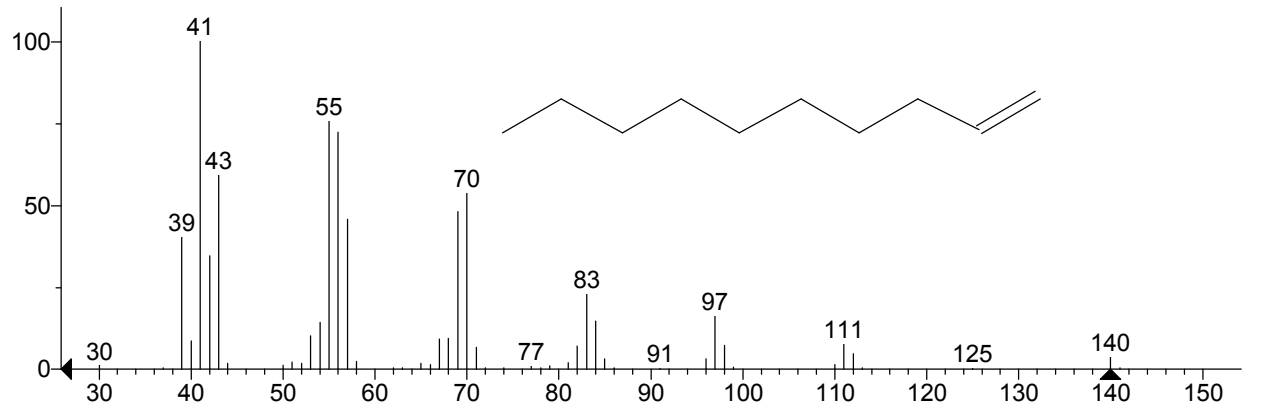
Unknown: Scan 230 (1.821 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -297



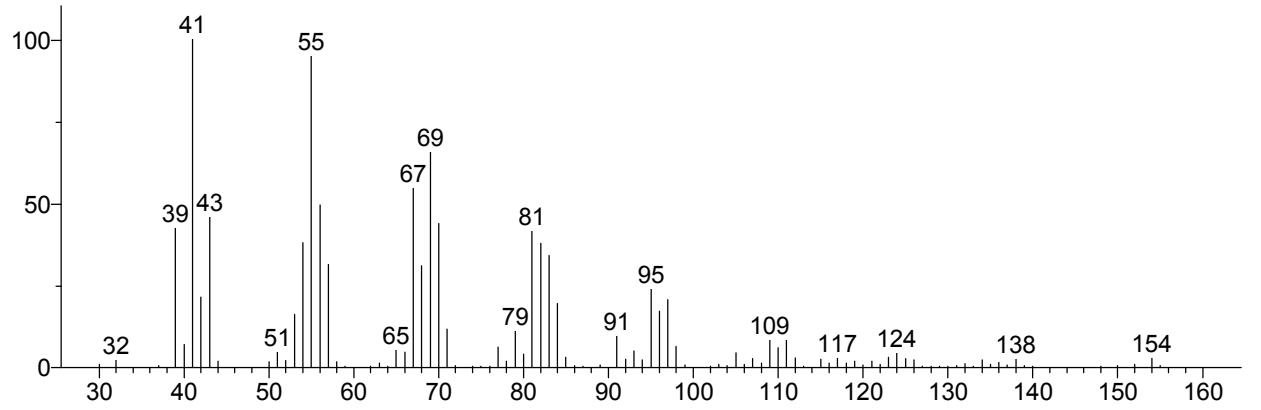
Hit 1 : 2-Decene, (Z)-
C10H20; MF: 871; RMF: 898; Prob 8.23%; CAS: 20348-51-0; Lib: mainlib; ID: 17331.



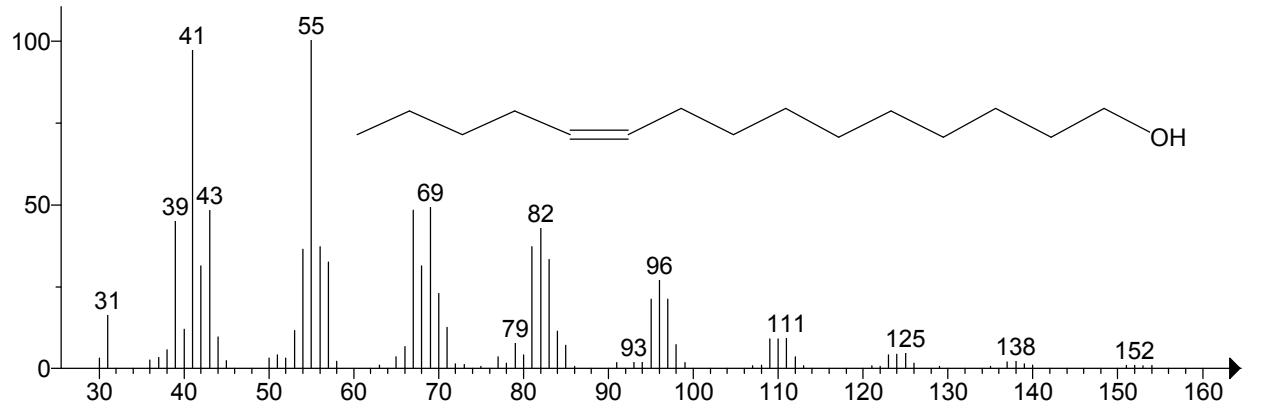
Hit 2 : 1-Decene
C10H20; MF: 869; RMF: 902; Prob 7.59%; CAS: 872-05-9; Lib: replib; ID: 896.



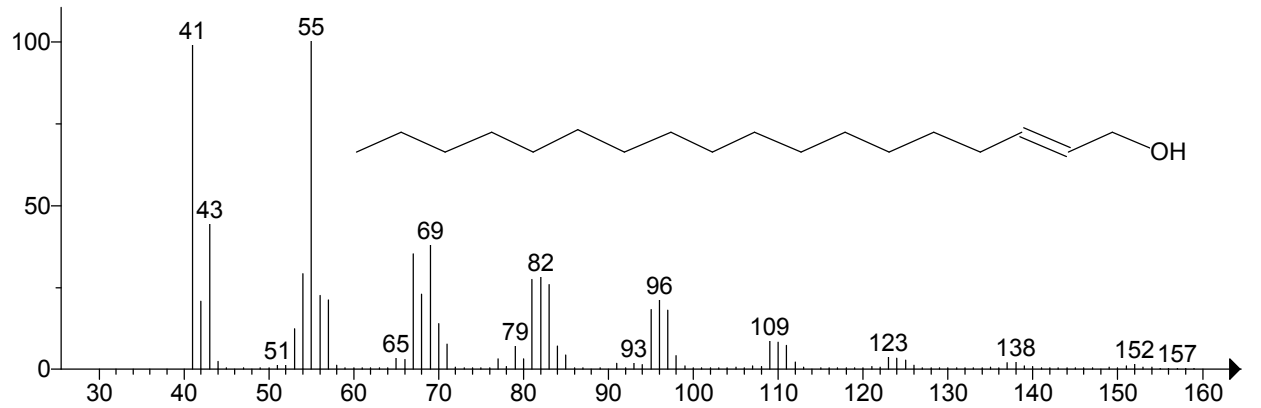
Unknown: Scan 292 (2.288 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -359



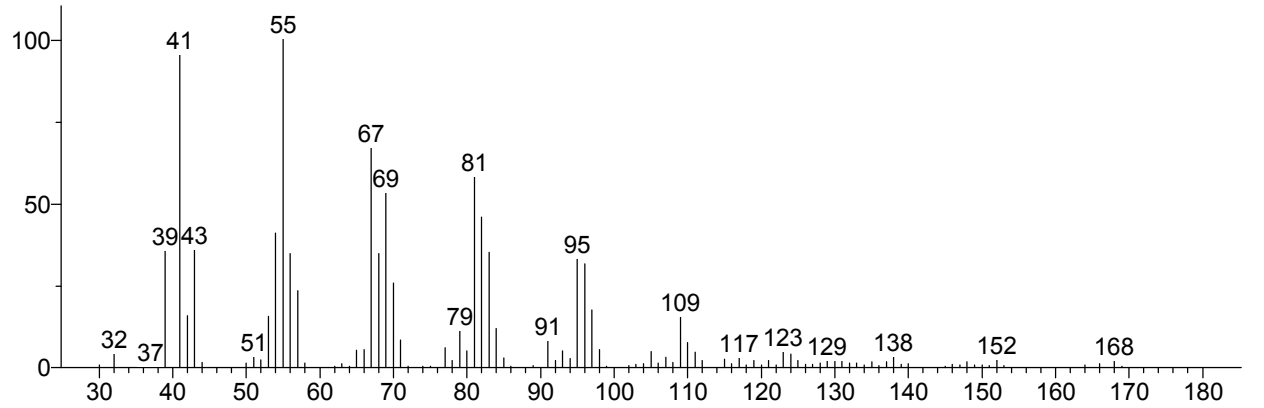
Hit 1 : Z-10-Pentadecen-1-ol
C15H30O; MF: 836; RMF: 862; Prob 8.08%; Lib: mainlib; ID: 17434.



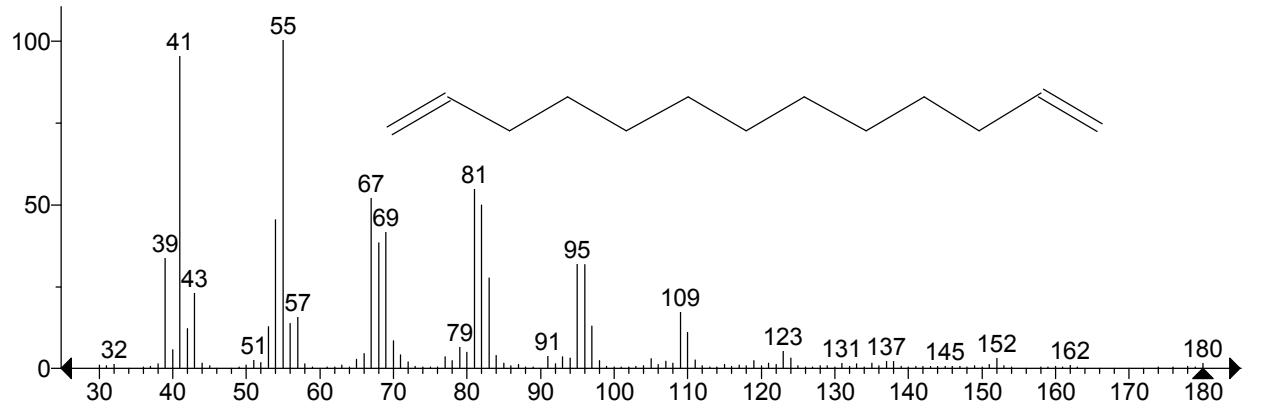
Hit 2 : E-2-Octadecadecen-1-ol
C18H36O; MF: 825; RMF: 829; Prob 5.54%; Lib: mainlib; ID: 17230.



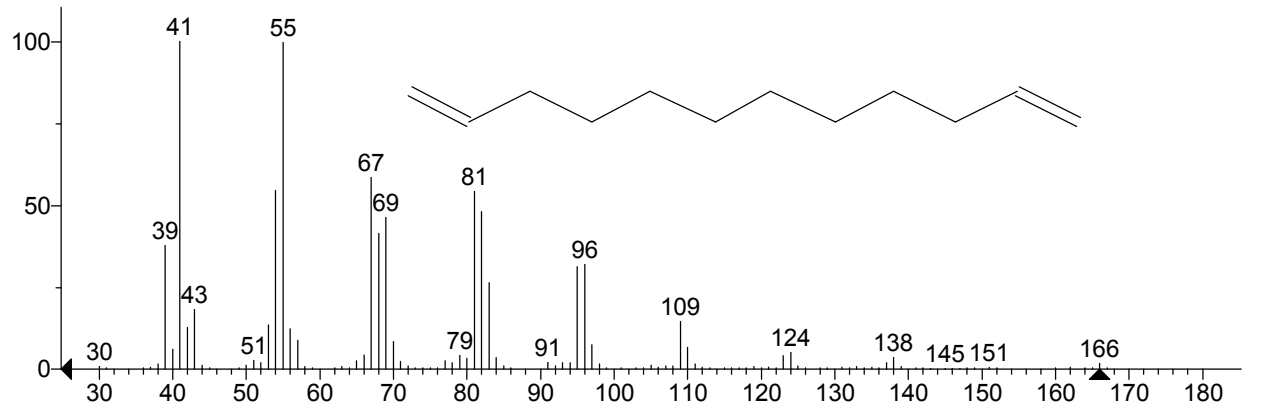
Unknown: Scan 364 (2.830 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -283



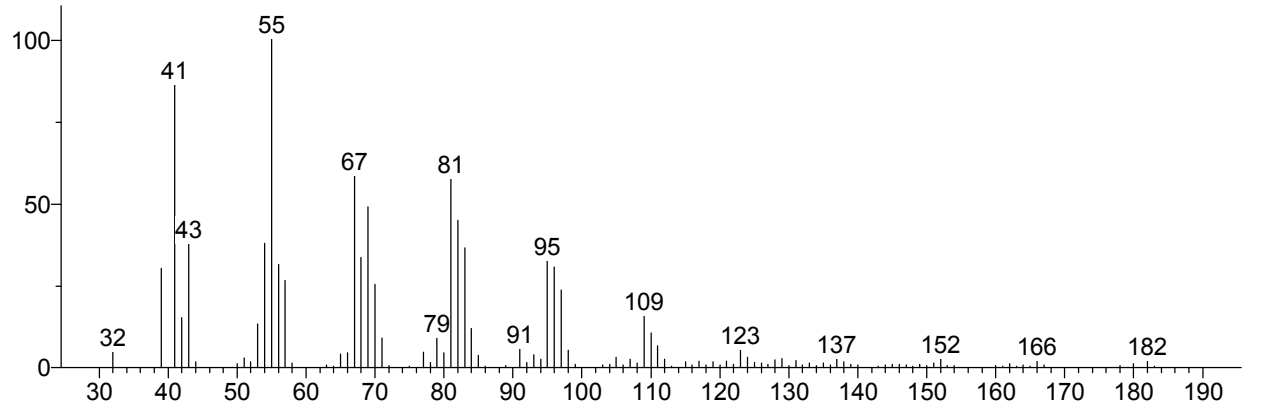
Hit 1 : 1,12-Tridecadiene
C13H24; MF: 859; RMF: 864; Prob 7.82%; CAS: 21964-48-7; Lib: mainlib; ID: 17578.



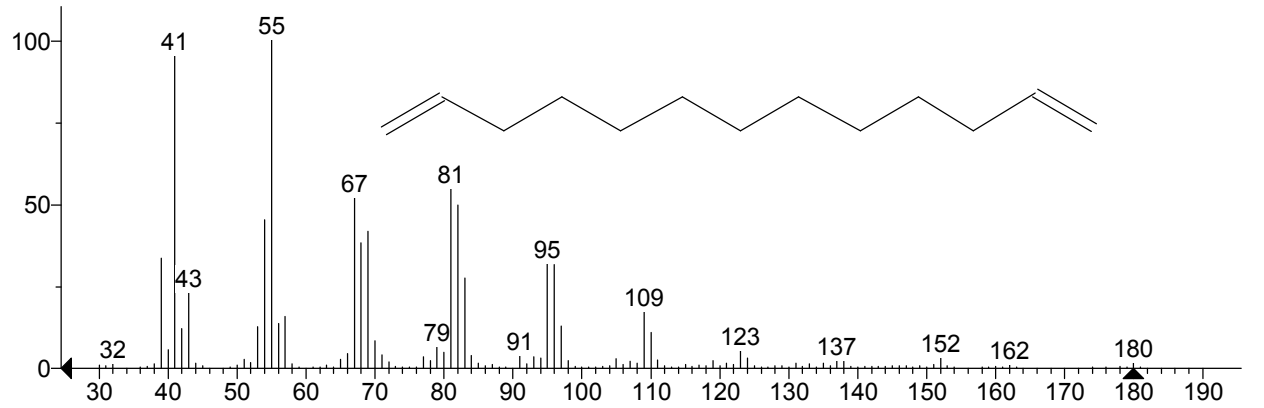
Hit 2 : 1,11-Dodecadiene
C12H22; MF: 845; RMF: 854; Prob 4.89%; CAS: 5876-87-9; Lib: mainlib; ID: 2567.



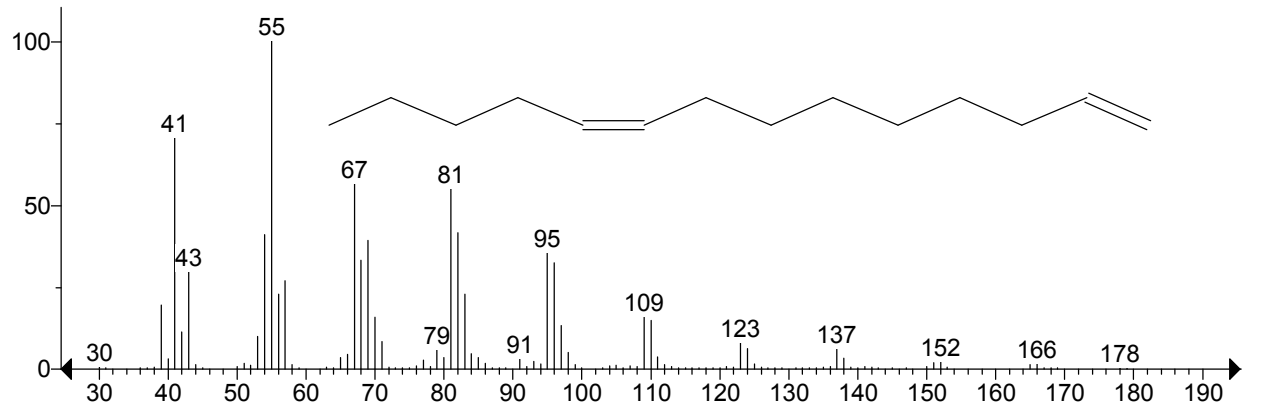
Unknown: Scan 442 (3.418 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -143



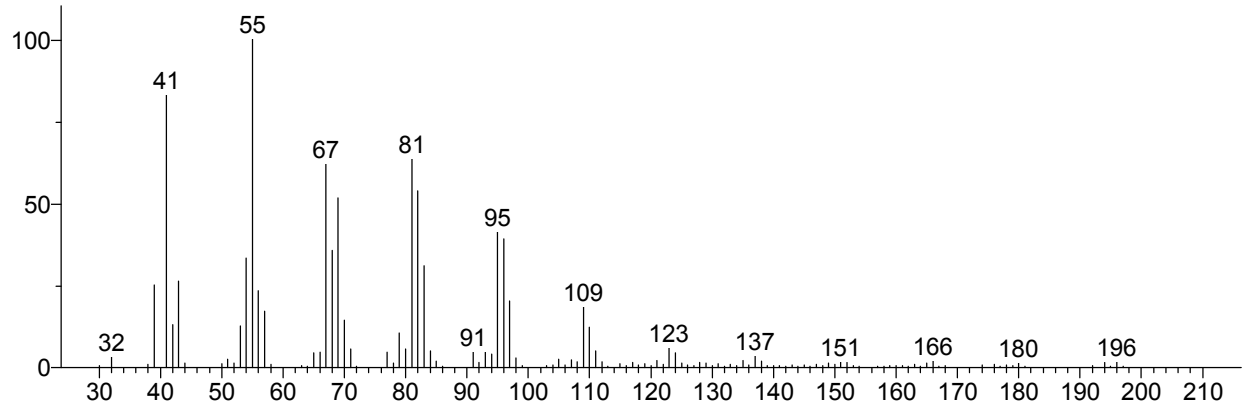
Hit 1 : 1,12-Tridecadiene
C13H24; MF: 883; RMF: 890; Prob 16.6%; CAS: 21964-48-7; Lib: mainlib; ID: 17578.



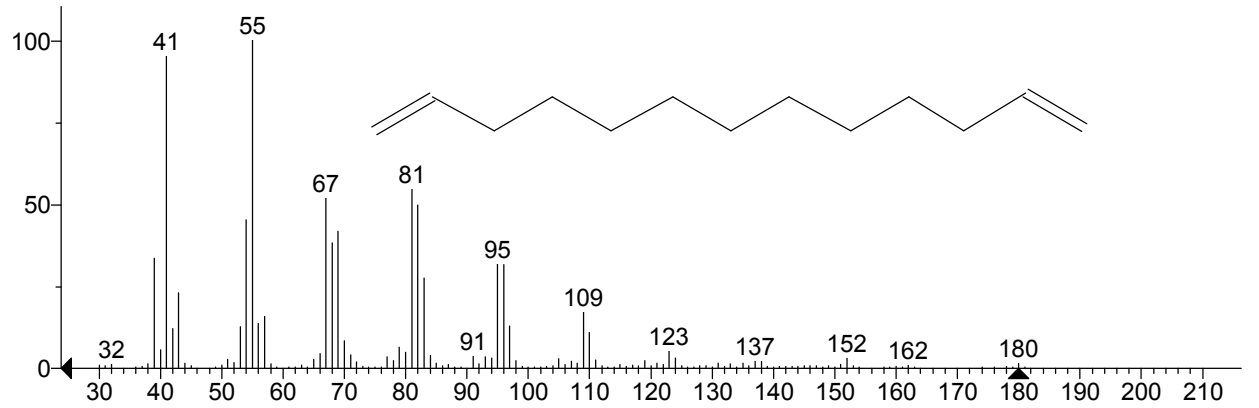
Hit 2 : 1,9-Tetradecadiene
C14H26; MF: 853; RMF: 866; Prob 4.60%; CAS: 112929-06-3; Lib: mainlib; ID: 17388.



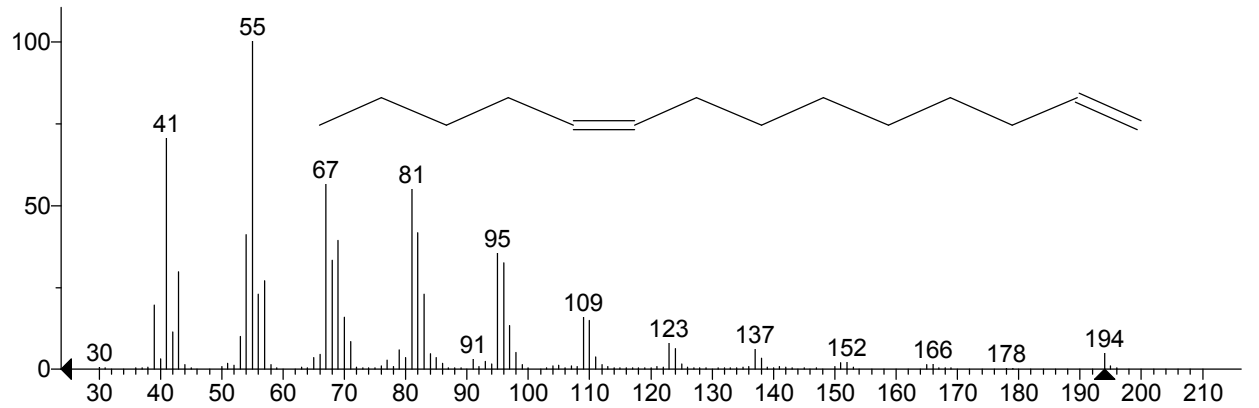
Unknown: Scan 520 (4.006 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -338



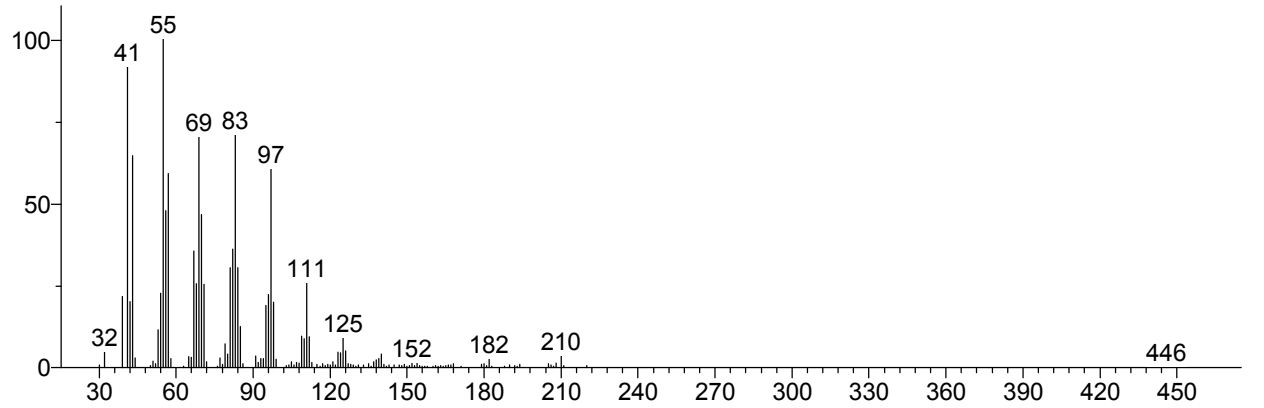
Hit 1 : 1,12-Tridecadiene
C13H24; MF: 864; RMF: 875; Prob 4.62%; CAS: 21964-48-7; Lib: mainlib; ID: 17578.



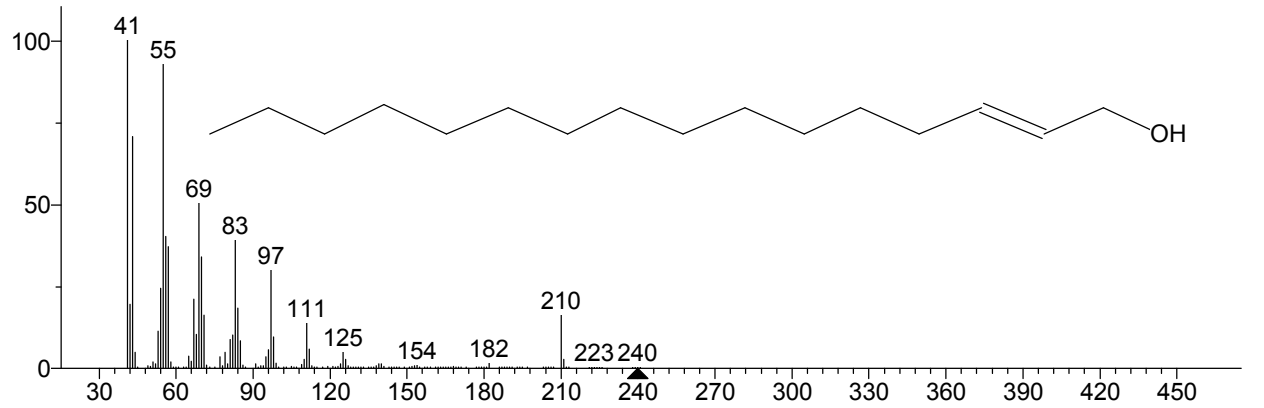
Hit 2 : 1,9-Tetradecadiene
C14H26; MF: 862; RMF: 874; Prob 4.26%; CAS: 112929-06-3; Lib: mainlib; ID: 17388.



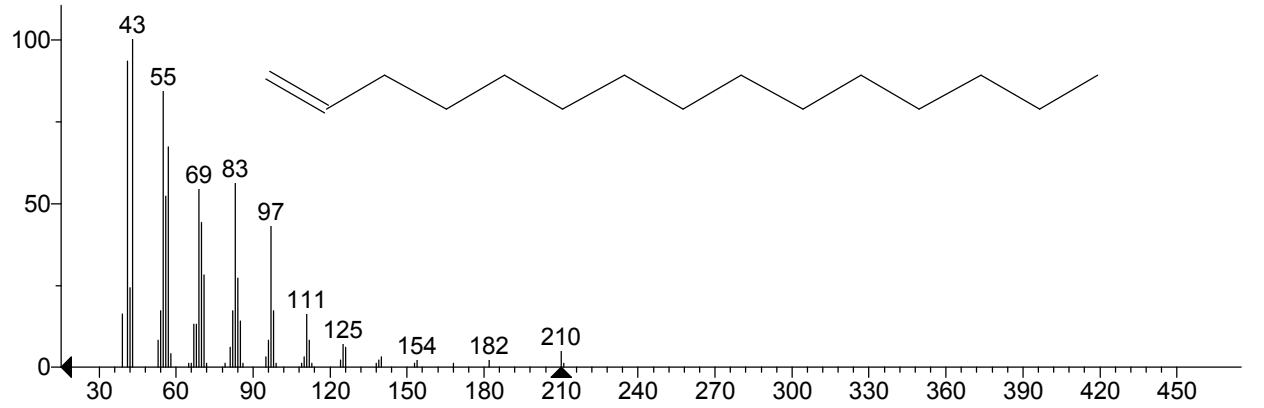
Unknown: Scan 598 (4.594 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -283



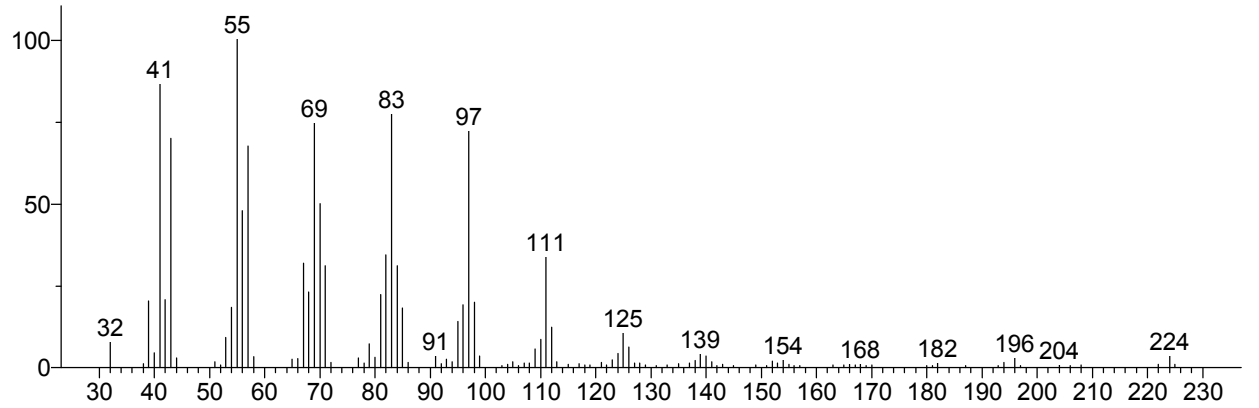
Hit 1 : E-2-Hexadecacen-1-ol
C16H32O; MF: 856; RMF: 870; Prob 6.21%; Lib: mainlib; ID: 2454.



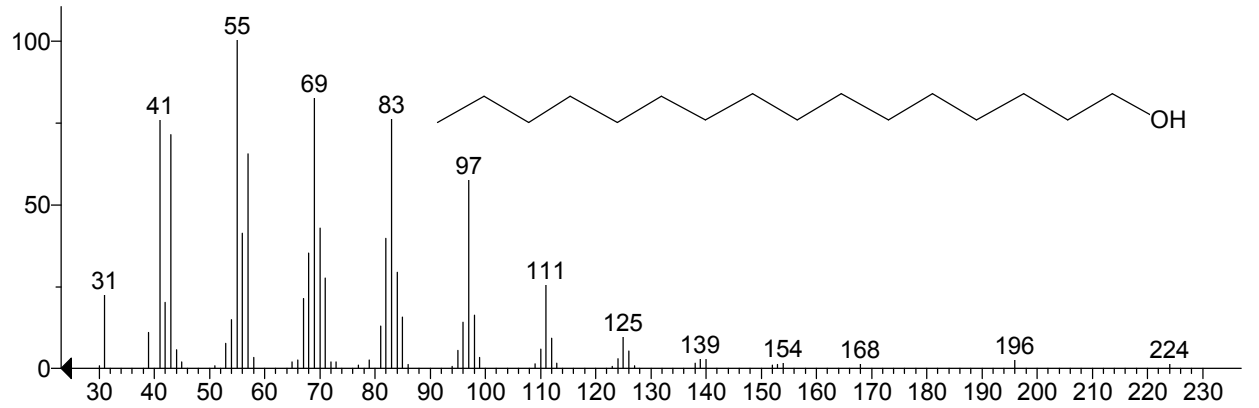
Hit 2 : 1-Pentadecene
C15H30; MF: 843; RMF: 899; Prob 4.01%; CAS: 13360-61-7; Lib: replib; ID: 1695.



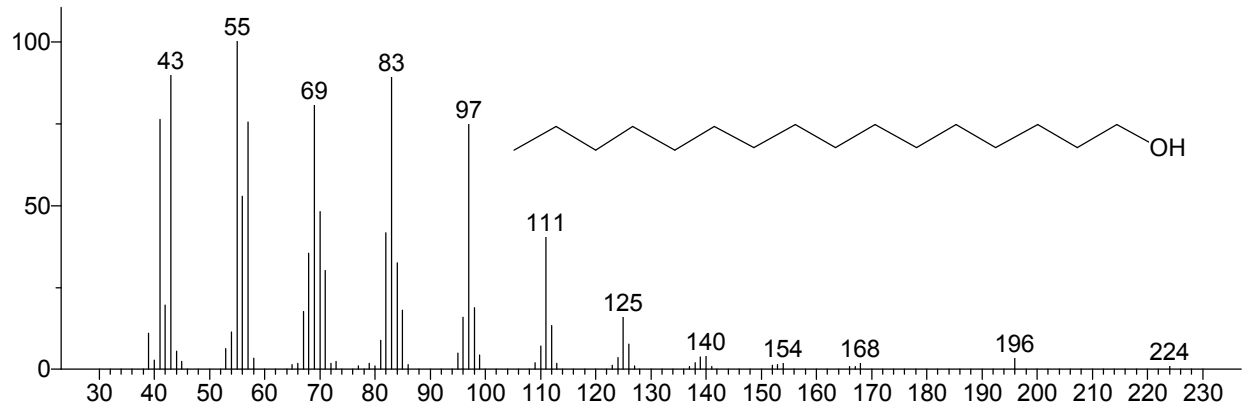
Unknown: Scan 673 (5.159 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -185



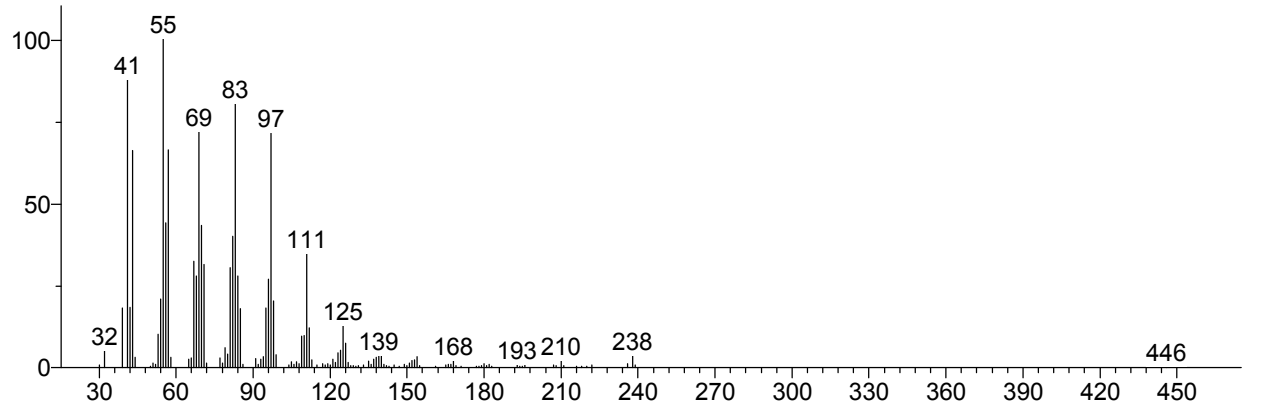
Hit 1 : 1-Hexadecanol
C16H34O; MF: 888; RMF: 932; Prob 6.56%; CAS: 36653-82-4; Lib: mainlib; ID: 18356.



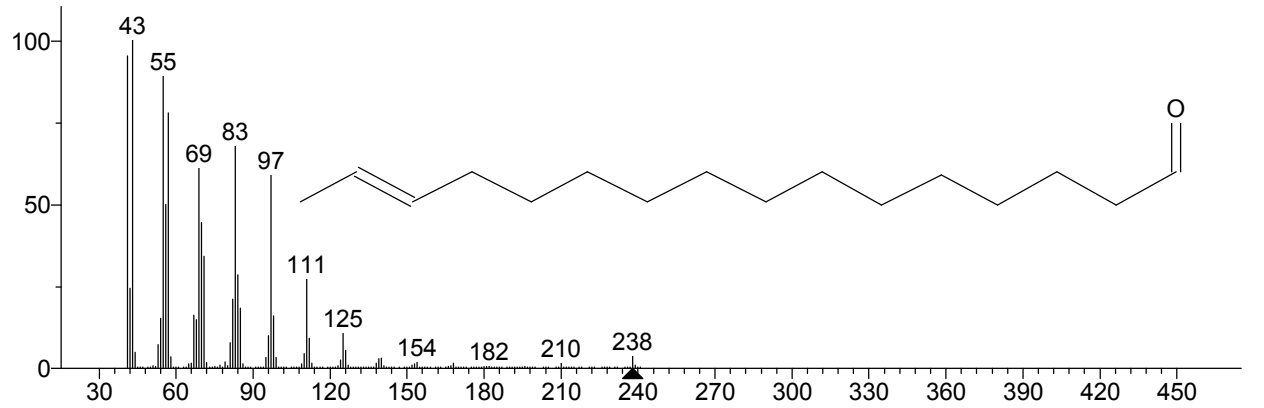
Hit 2 : 1-Hexadecanol
C16H34O; MF: 880; RMF: 915; Prob 6.56%; CAS: 36653-82-4; Lib: replib; ID: 4395.



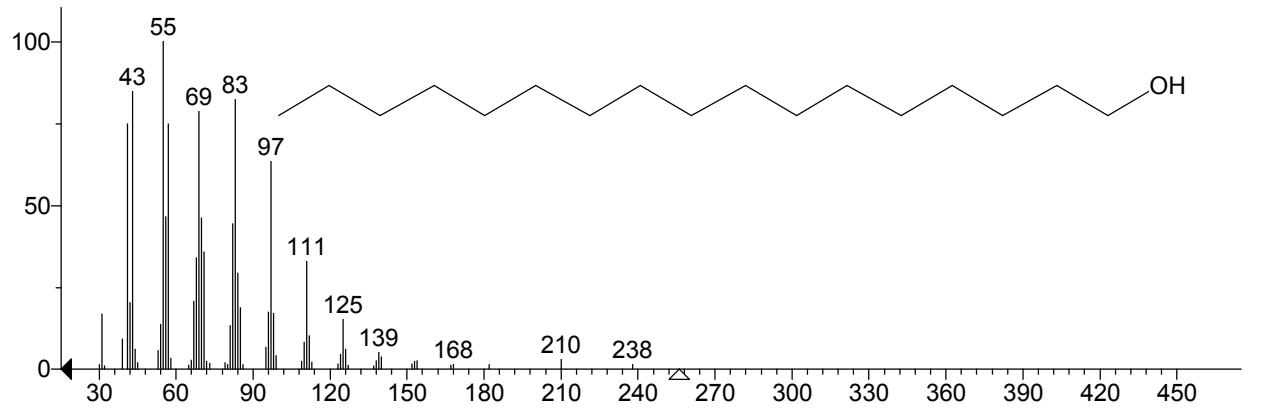
Unknown: Scan 742 (5.679 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -297



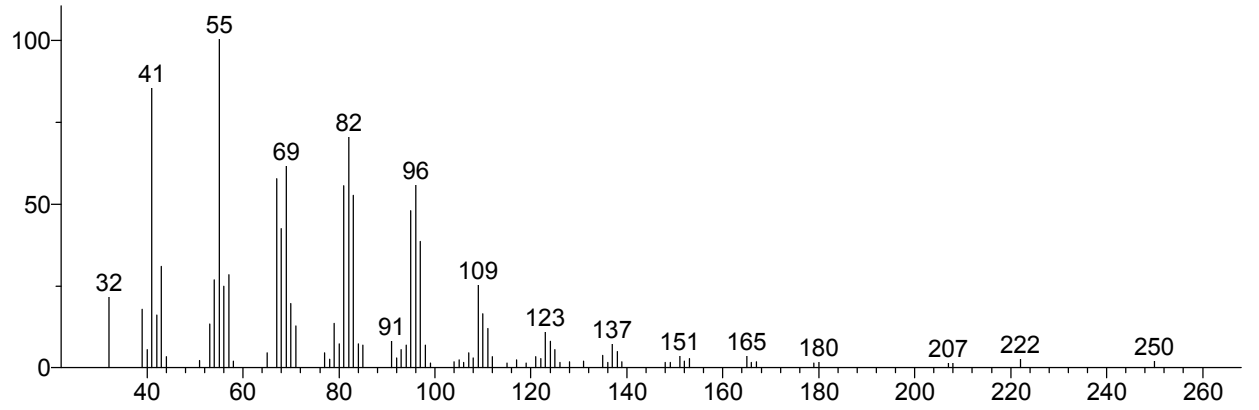
Hit 1 : E-14-Hexadecenal
C16H30O; MF: 874; RMF: 884; Prob 6.15%; CAS: 330207-53-9; Lib: mainlib; ID: 5588.



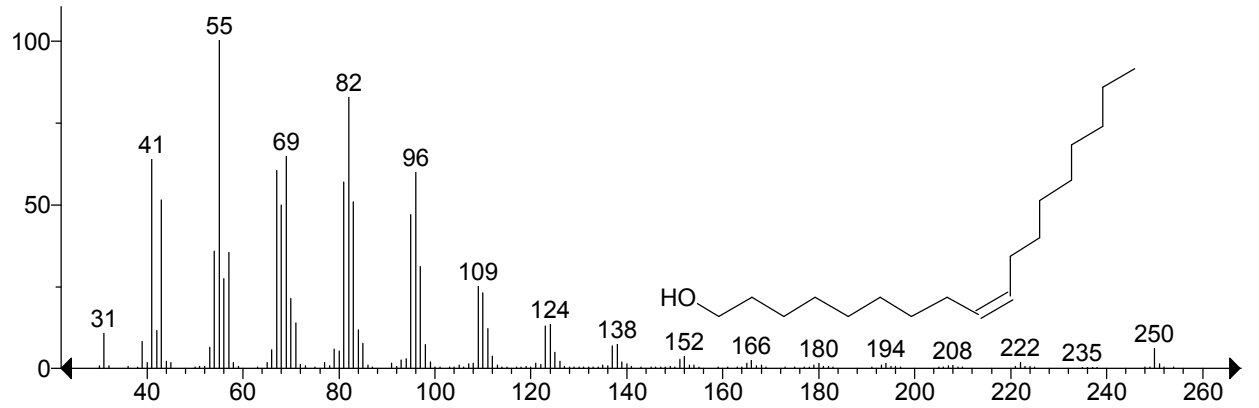
Hit 2 : n-Heptadecanol-1
C17H36O; MF: 867; RMF: 908; Prob 4.71%; CAS: 1454-85-9; Lib: replib; ID: 4396.



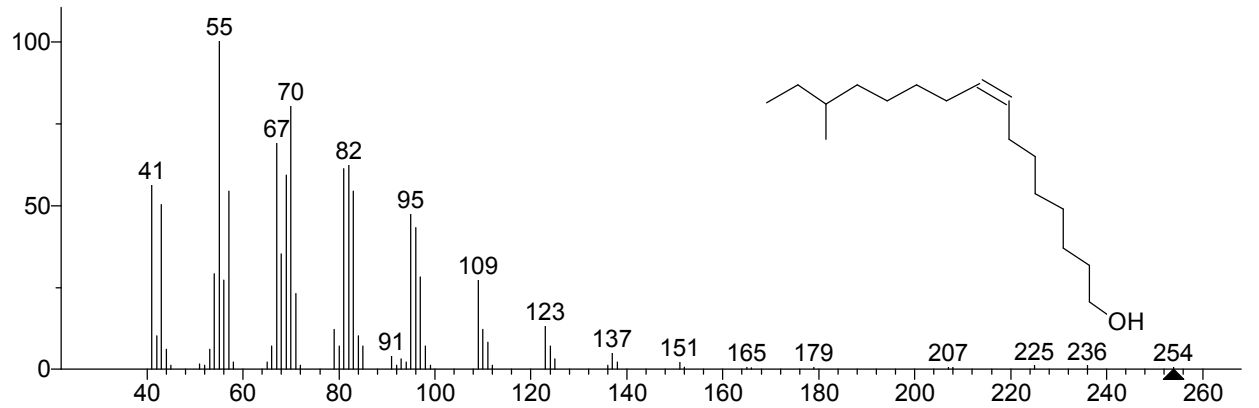
Unknown: Scan 808 (6.176 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -454



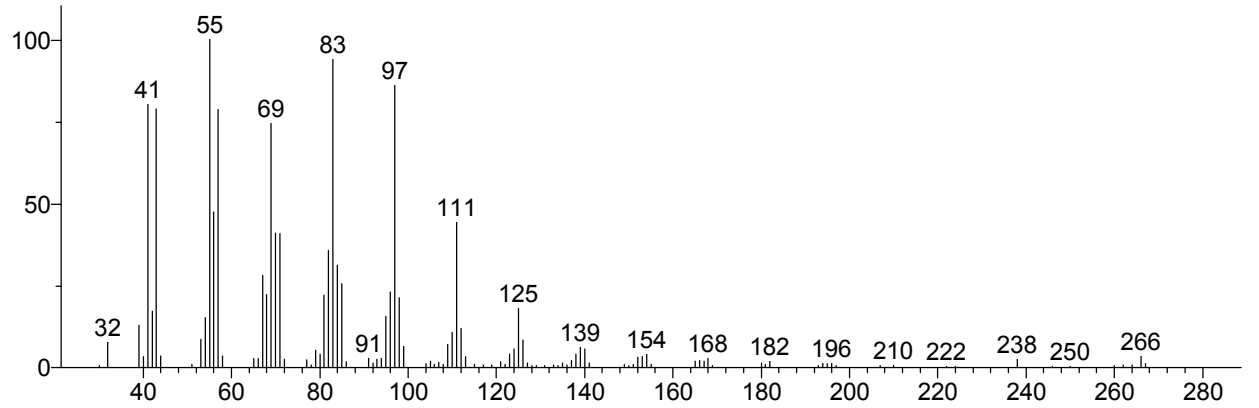
Hit 1 : Oleyl Alcohol
C18H36O; MF: 849; RMF: 849; Prob 4.54%; CAS: 143-28-2; Lib: replib; ID: 4592.



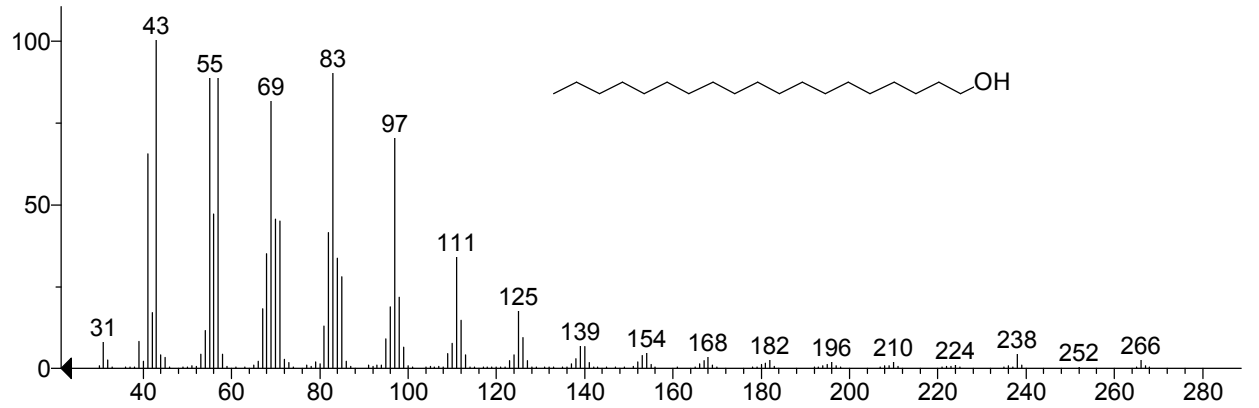
Hit 2 : (R)-(-)-(Z)-14-Methyl-8-hexadecen-1-ol
C17H34O; MF: 846; RMF: 890; Prob 4.01%; CAS: 30689-78-2; Lib: mainlib; ID: 18448.



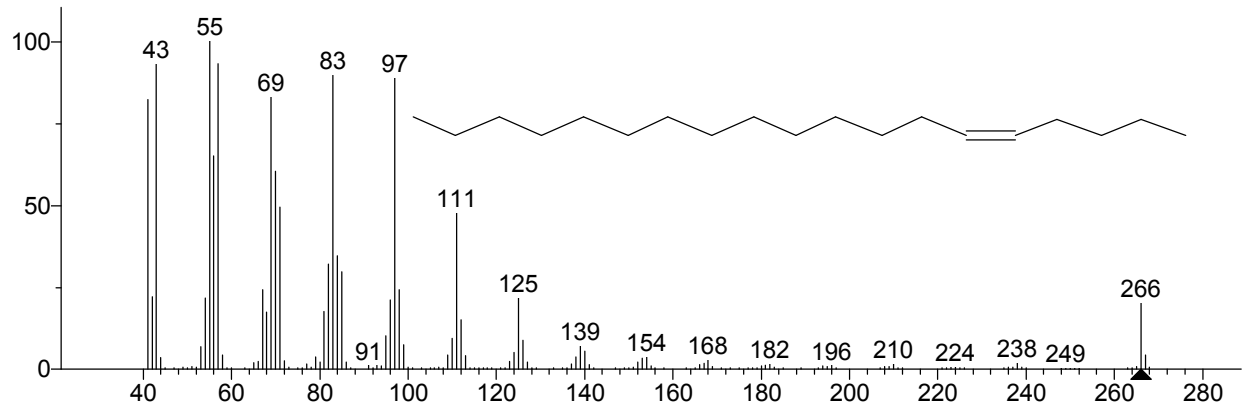
Unknown: Scan 875 (6.681 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -207



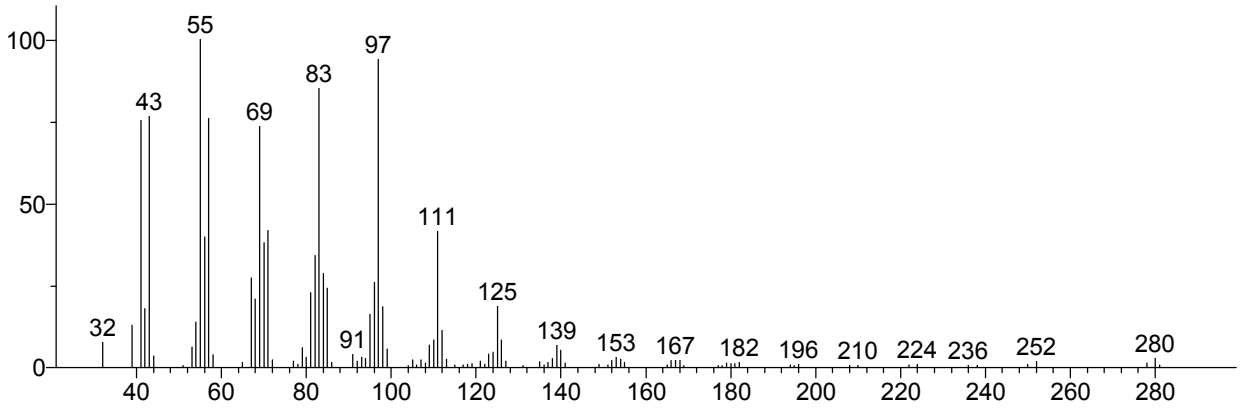
Hit 1 : n-Nonadecanol-1
C19H40O; MF: 895; RMF: 900; Prob 7.90%; CAS: 1454-84-8; Lib: replib; ID: 2624.



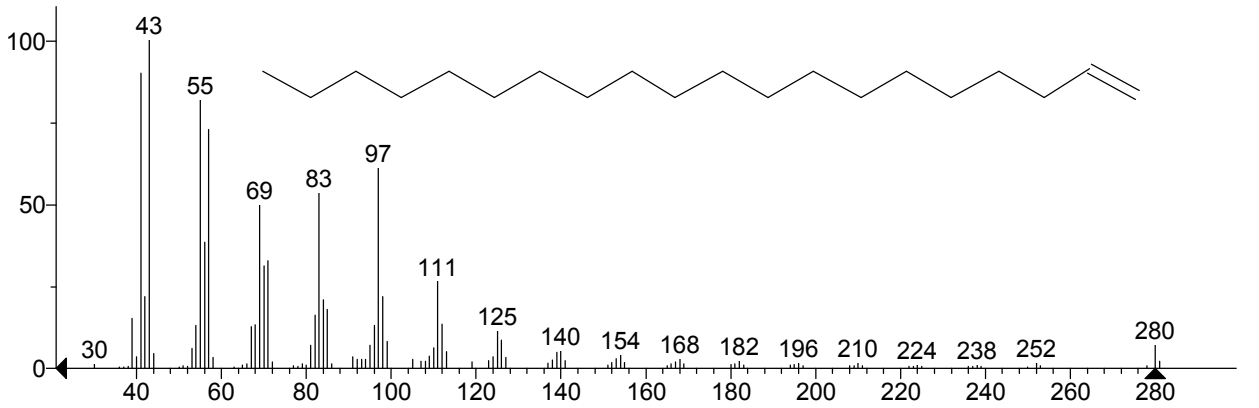
Hit 2 : Z-5-Nonadecene
C19H38; MF: 887; RMF: 894; Prob 5.89%; Lib: mainlib; ID: 17837.



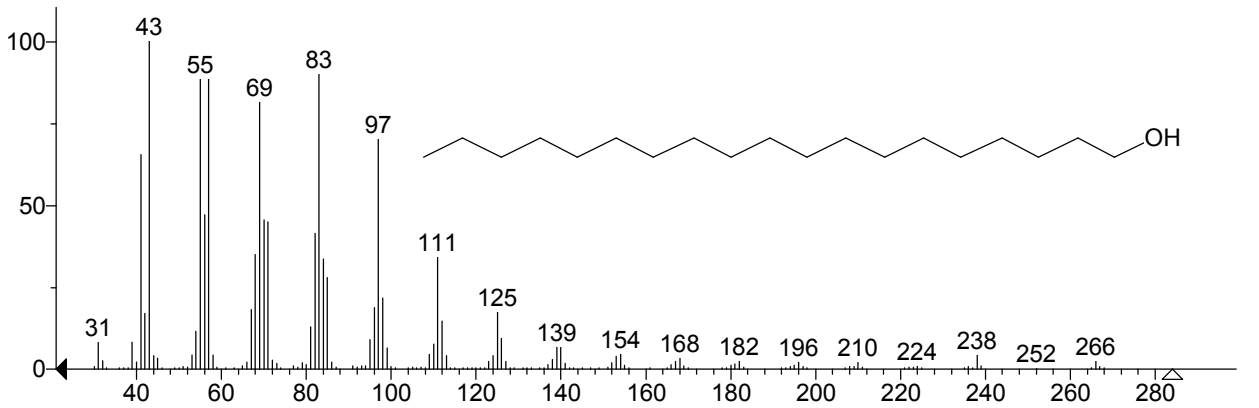
Unknown: Scan 937 (7.148 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -253



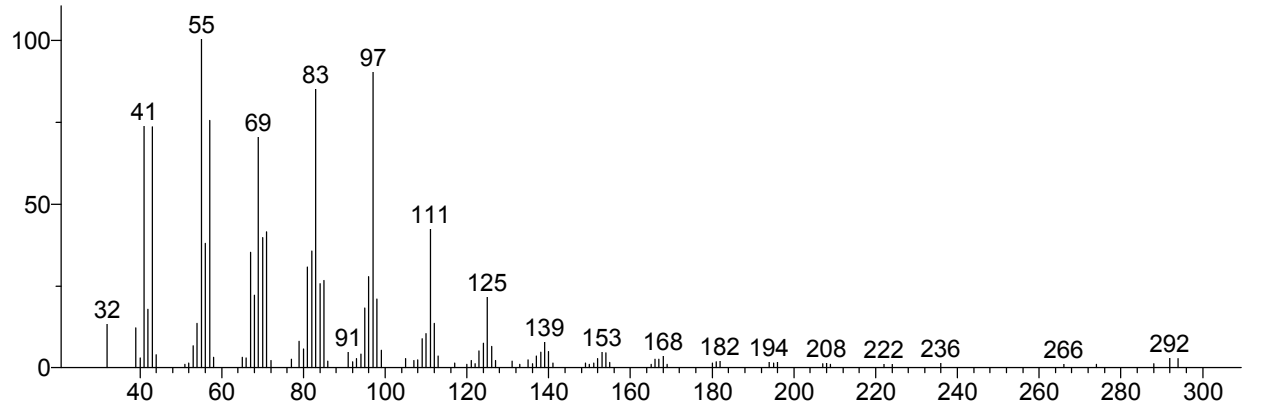
Hit 1 : 1-Eicosene
C20H40; MF: 886; RMF: 897; Prob 4.71%; CAS: 3452-07-1; Lib: replib; ID: 1690.



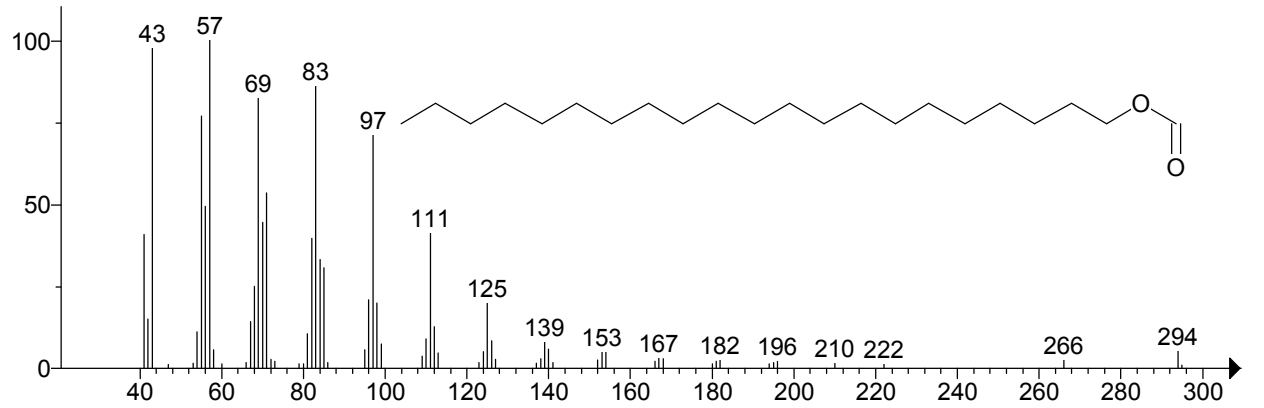
Hit 2 : n-Nonadecanol-1
C19H40O; MF: 884; RMF: 894; Prob 4.34%; CAS: 1454-84-8; Lib: replib; ID: 2624.



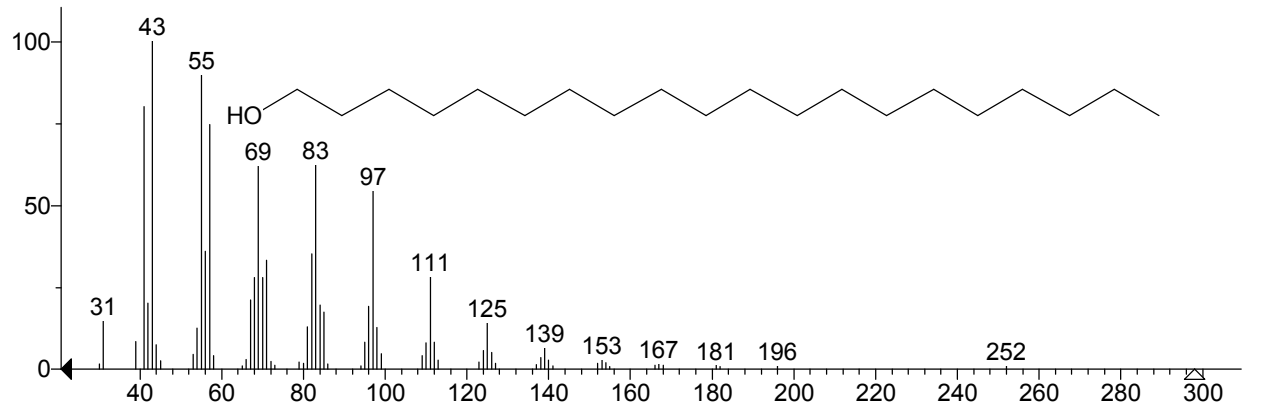
Unknown: Scan 997 (7.600 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -297



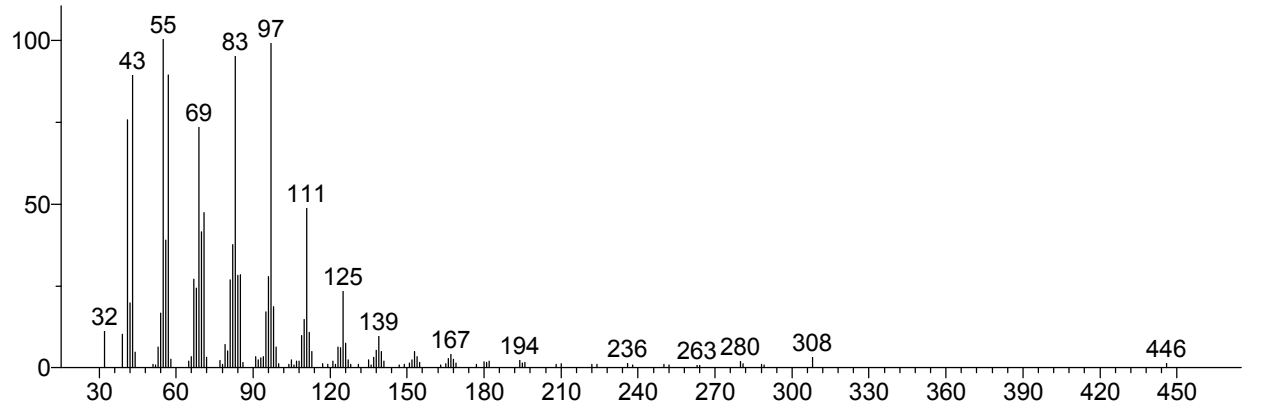
Hit 1 : 1-Heneicosyl formate
C22H44O2; MF: 871; RMF: 912; Prob 4.94%; CAS: 77899-03-7; Lib: mainlib; ID: 22067.



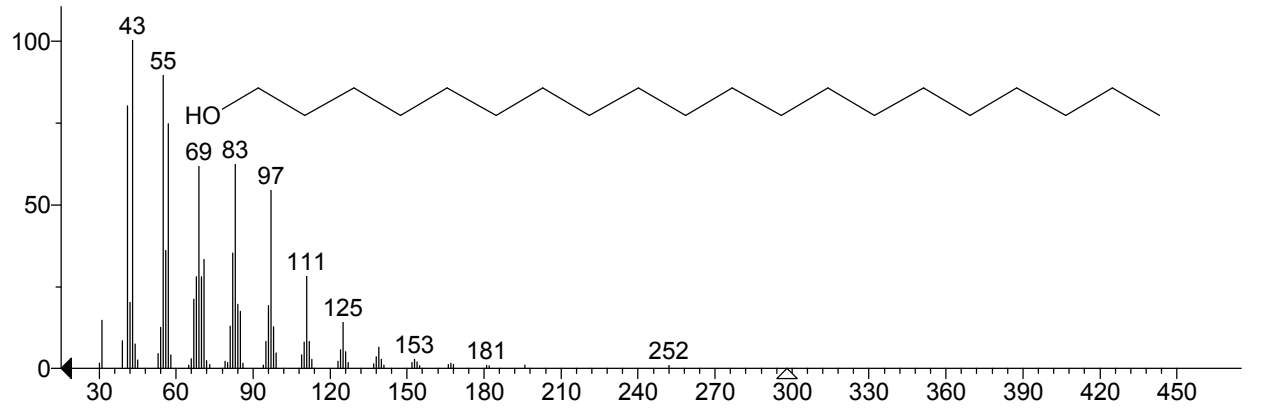
Hit 2 : 1-Eicosanol
C20H42O; MF: 869; RMF: 919; Prob 4.55%; CAS: 629-96-9; Lib: replib; ID: 1938.



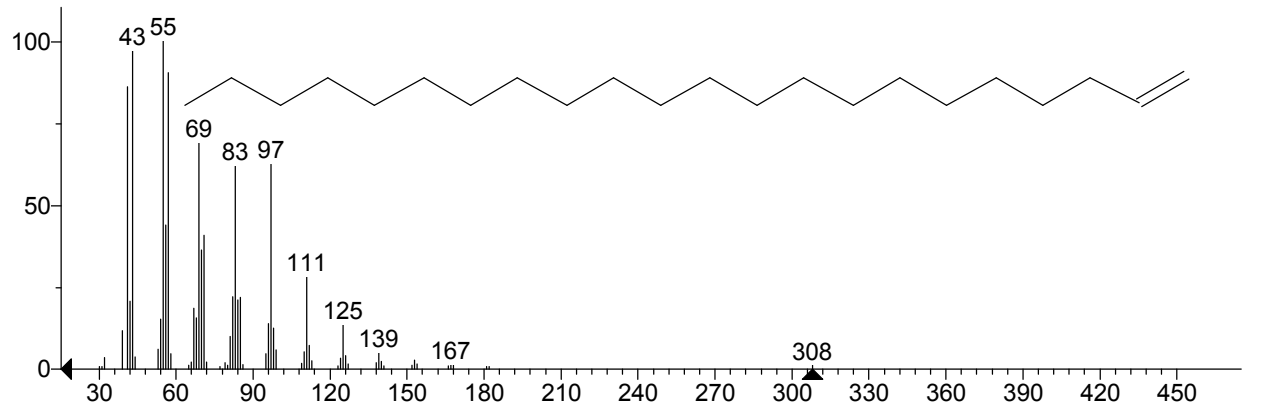
Unknown: Scan 1053 (8.022 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -297



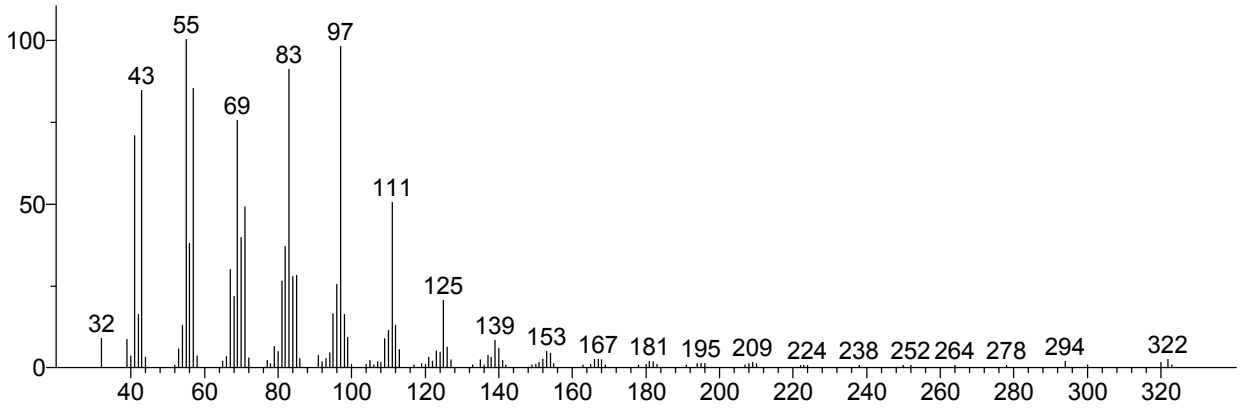
Hit 1 : 1-Eicosanol
C20H42O; MF: 880; RMF: 932; Prob 6.05%; CAS: 629-96-9; Lib: replib; ID: 1938.



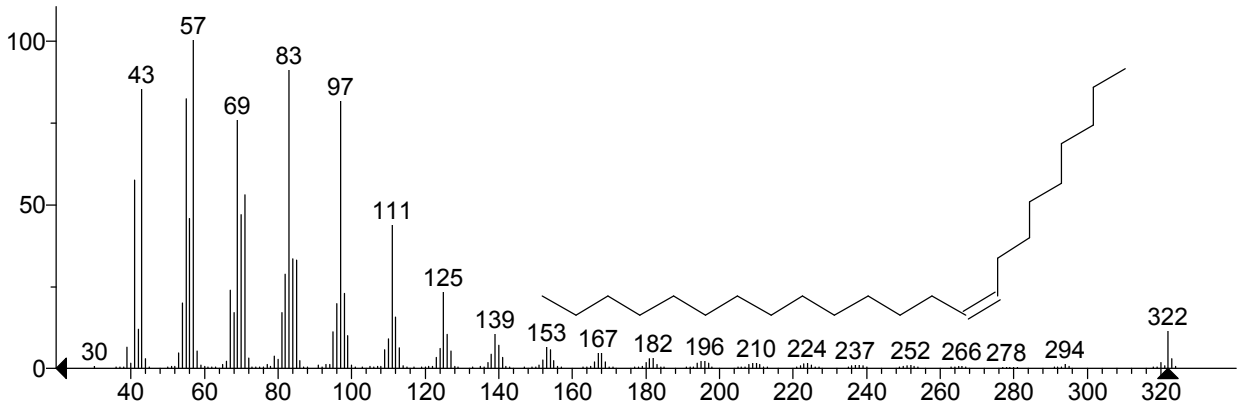
Hit 2 : 1-Docosene
C22H44; MF: 878; RMF: 929; Prob 5.58%; CAS: 1599-67-3; Lib: replib; ID: 4382.



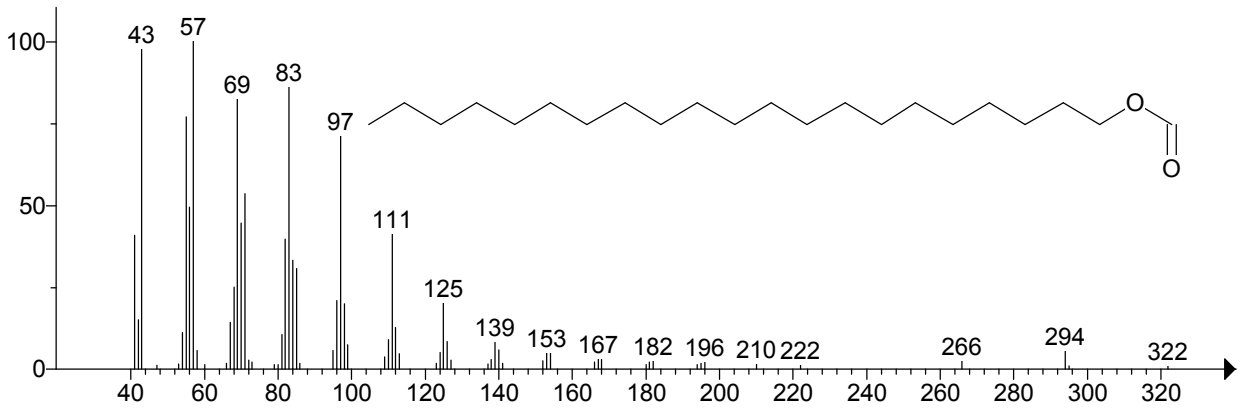
Unknown: Scan 1107 (8.429 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -253



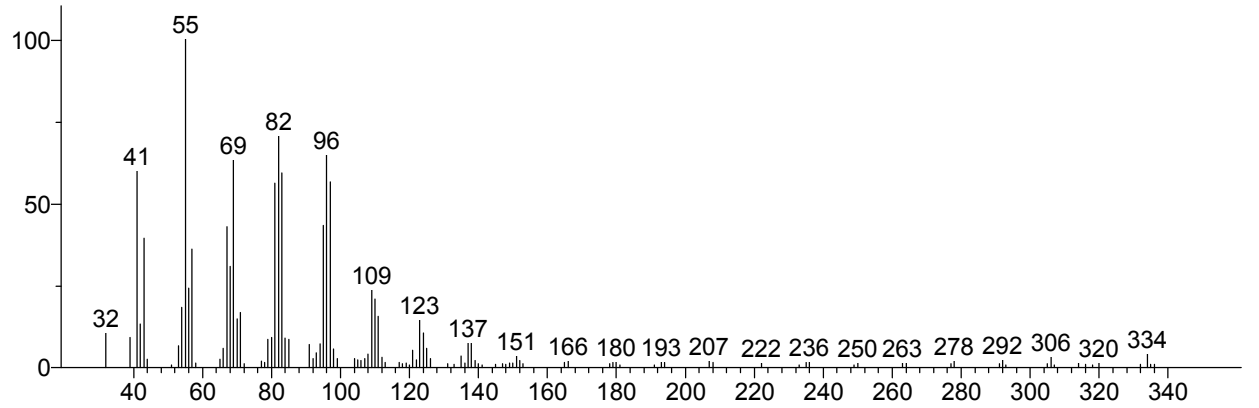
Hit 1 : 9-Tricosene, (Z)-
C23H46; MF: 886; RMF: 889; Prob 6.29%; CAS: 27519-02-4; Lib: replib; ID: 5831.



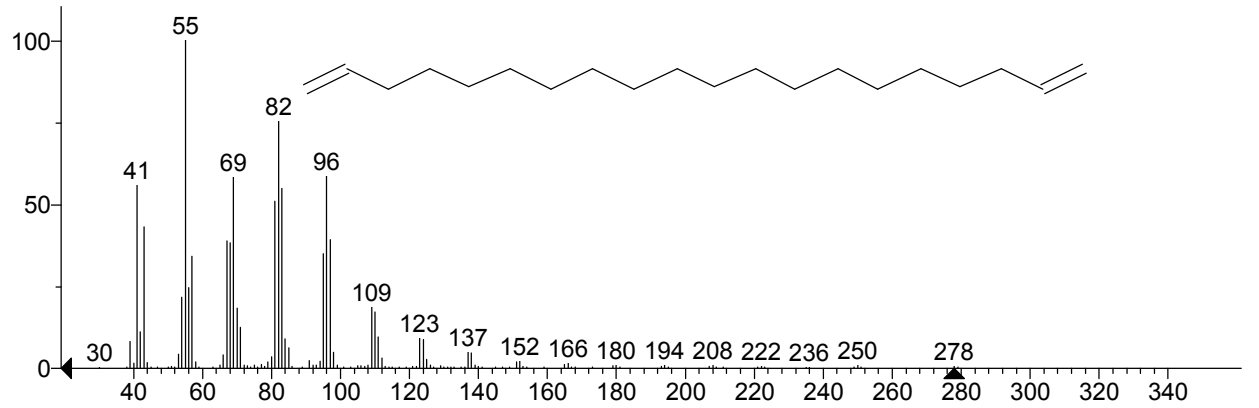
Hit 2 : 1-Heneicosyl formate
C22H44O2; MF: 878; RMF: 922; Prob 4.69%; CAS: 77899-03-7; Lib: mainlib; ID: 22067.



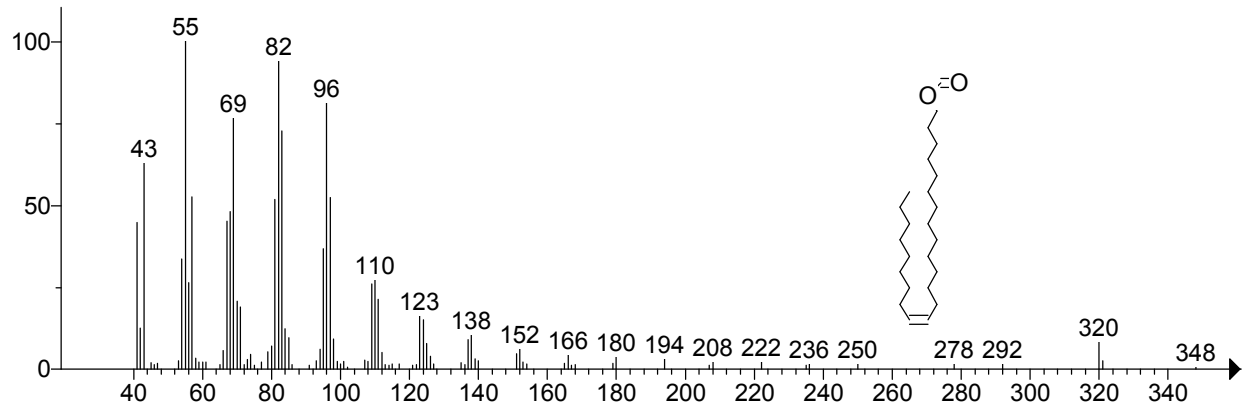
Unknown: Scan 1155 (8.791 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -359



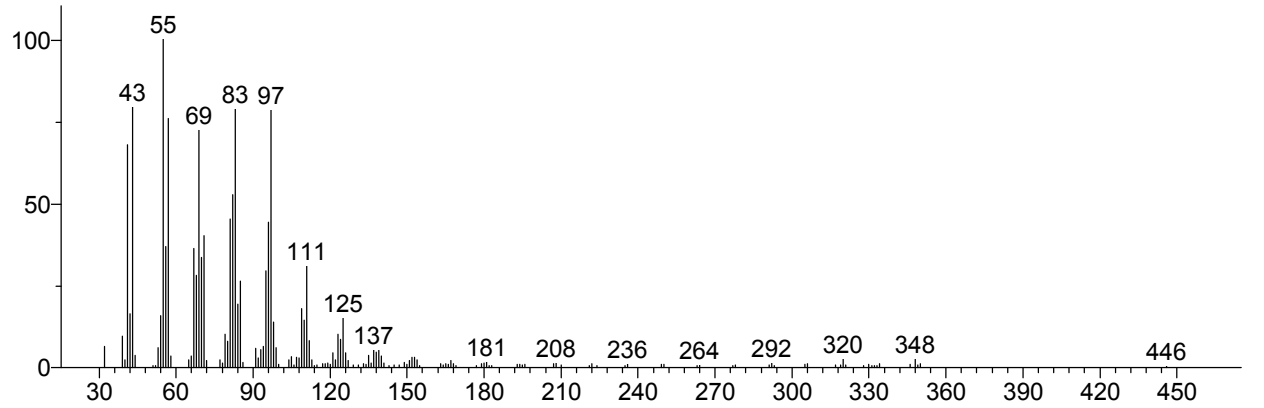
Hit 1 : 1,19-Eicosadiene
C20H38; MF: 831; RMF: 880; Prob 9.30%; CAS: 14811-95-1; Lib: mainlib; ID: 18670.



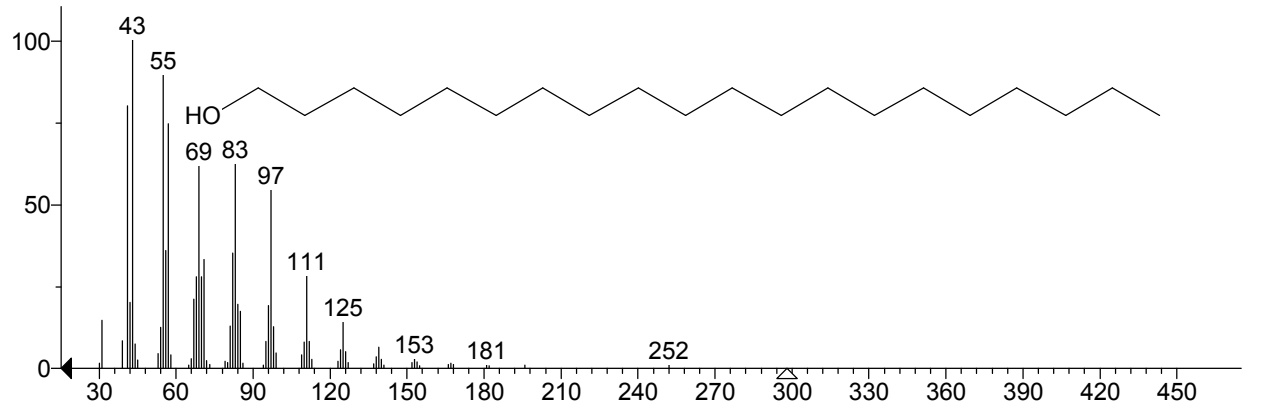
Hit 2 : (Z)-14-Tricosenyl formate
C24H46O2; MF: 827; RMF: 883; Prob 7.86%; CAS: 77899-10-6; Lib: mainlib; ID: 18672.



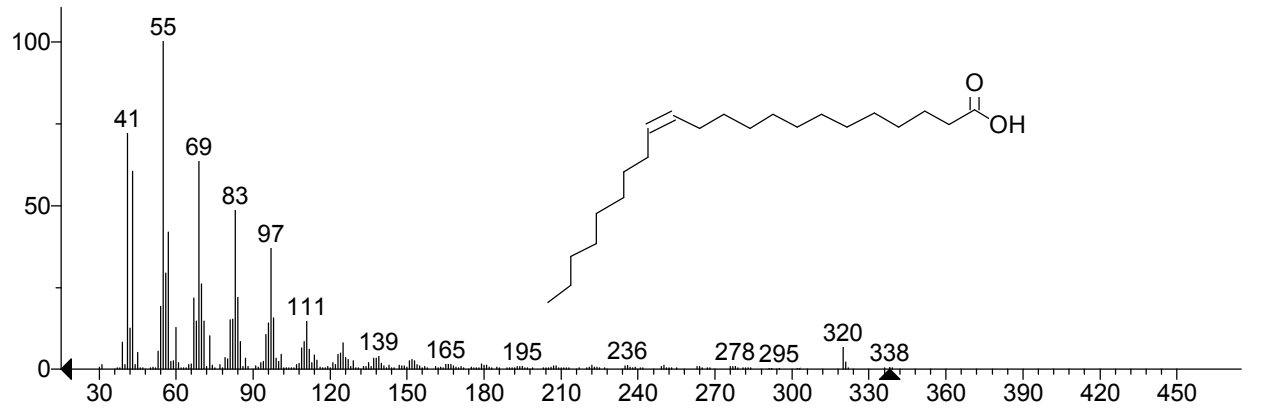
Unknown: Scan 1207 (9.183 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -407



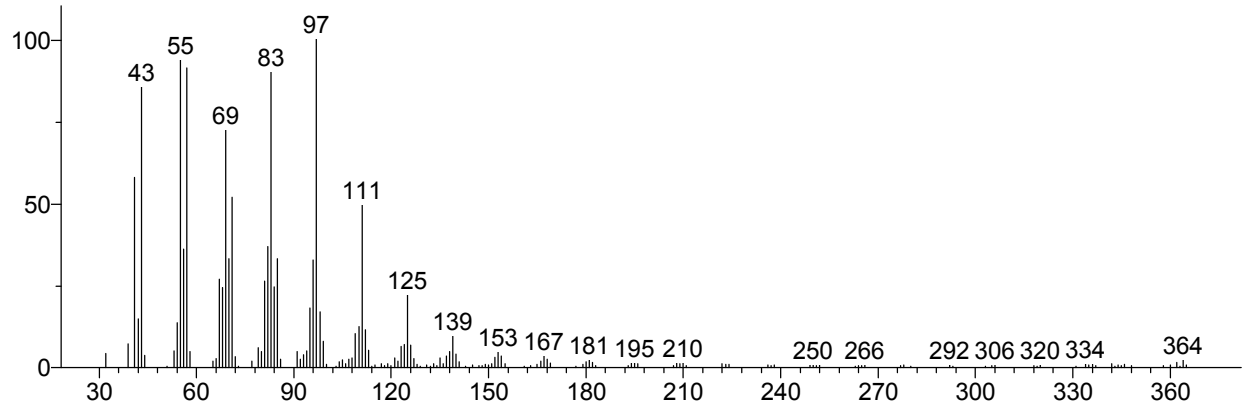
Hit 1 : 1-Eicosanol
C20H42O; MF: 815; RMF: 895; Prob 4.57%; CAS: 629-96-9; Lib: replib; ID: 1938.



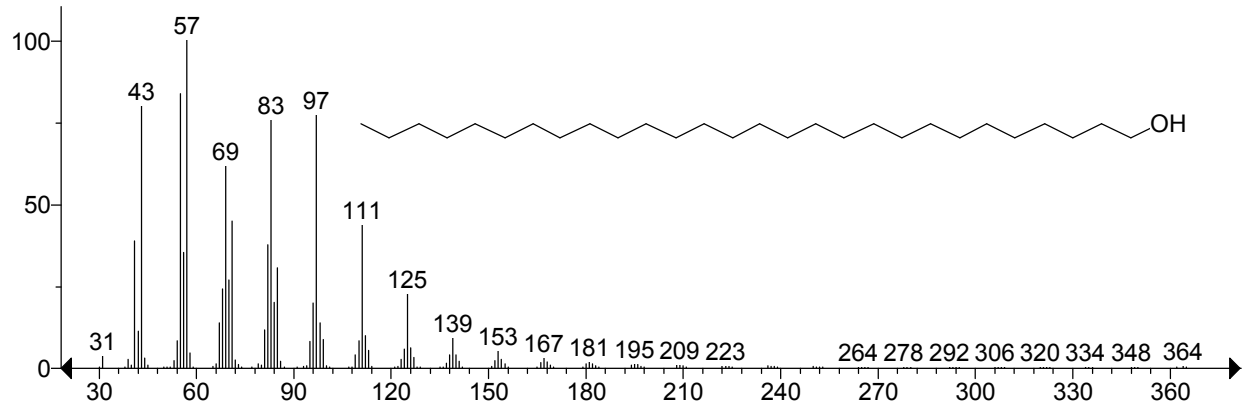
Hit 2 : Erucic acid
C22H42O2; MF: 815; RMF: 835; Prob 4.57%; CAS: 112-86-7; Lib: replib; ID: 4279.



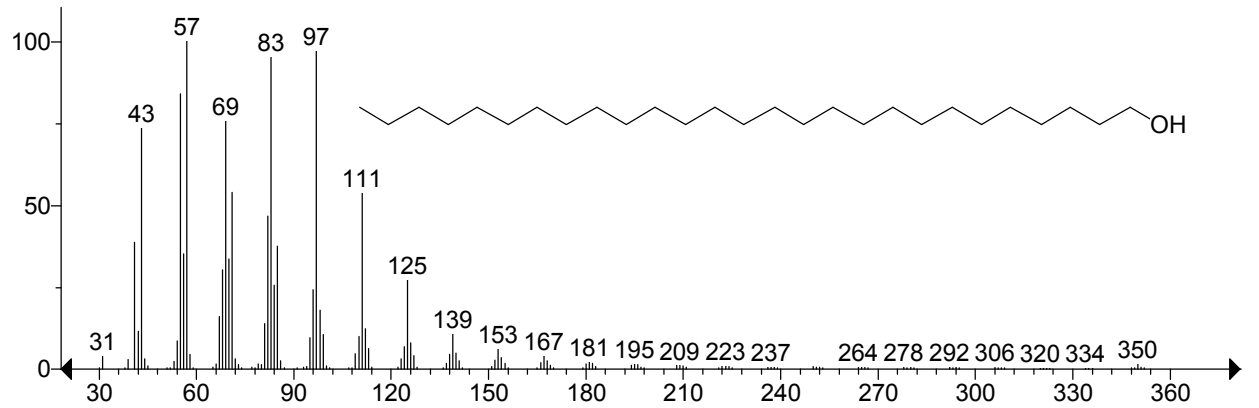
Unknown: Scan 1256 (9.552 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -217



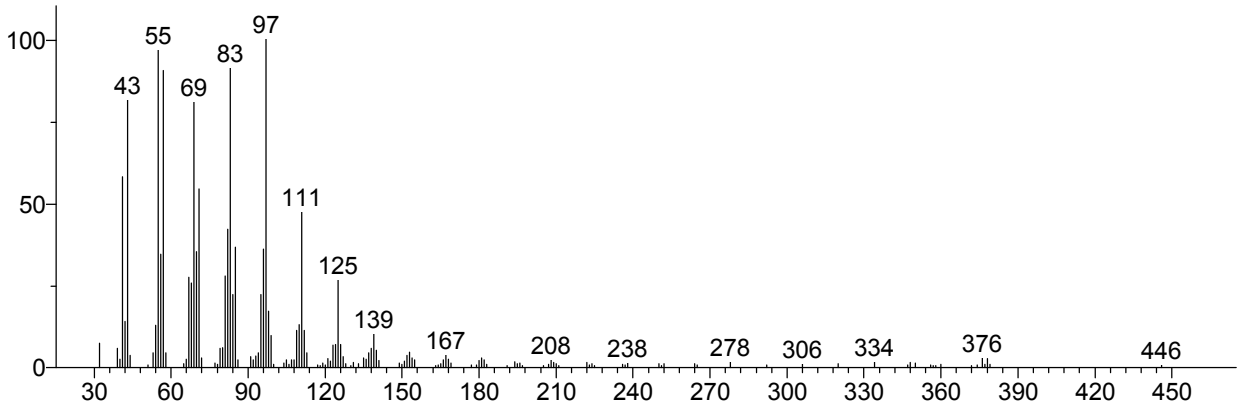
Hit 1 : 1-Octacosanol
C28H58O; MF: 877; RMF: 901; Prob 7.79%; Lib: mainlib; ID: 22288.



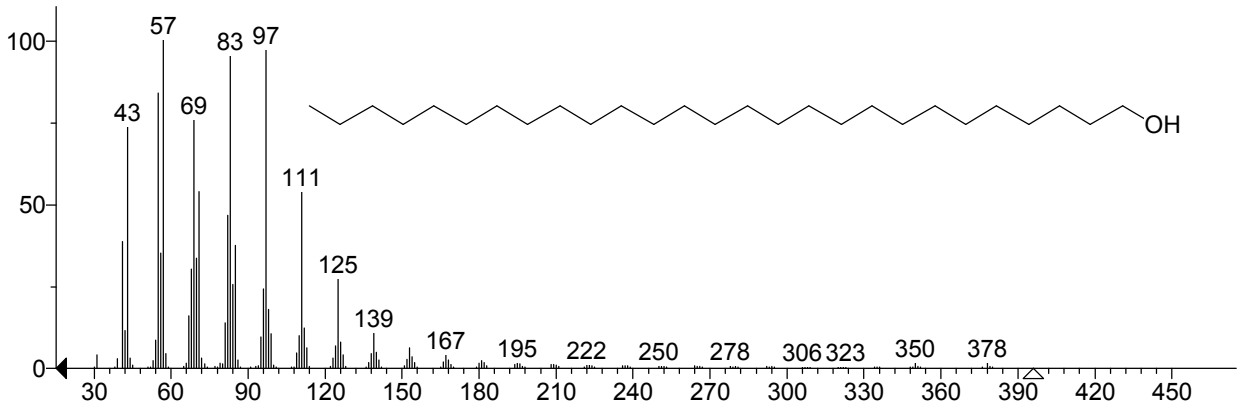
Hit 2 : 1-Heptacosanol
C27H56O; MF: 863; RMF: 898; Prob 4.88%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



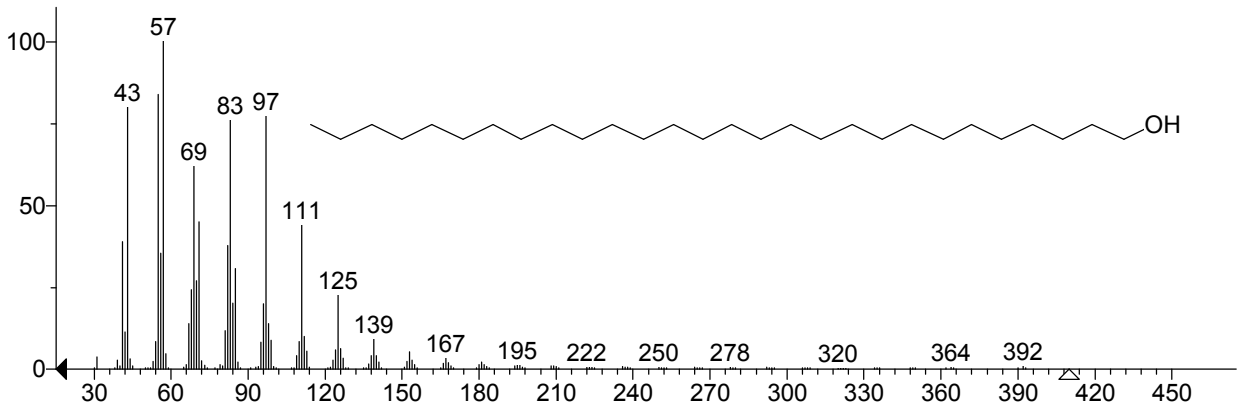
Unknown: Scan 1304 (9.914 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -246



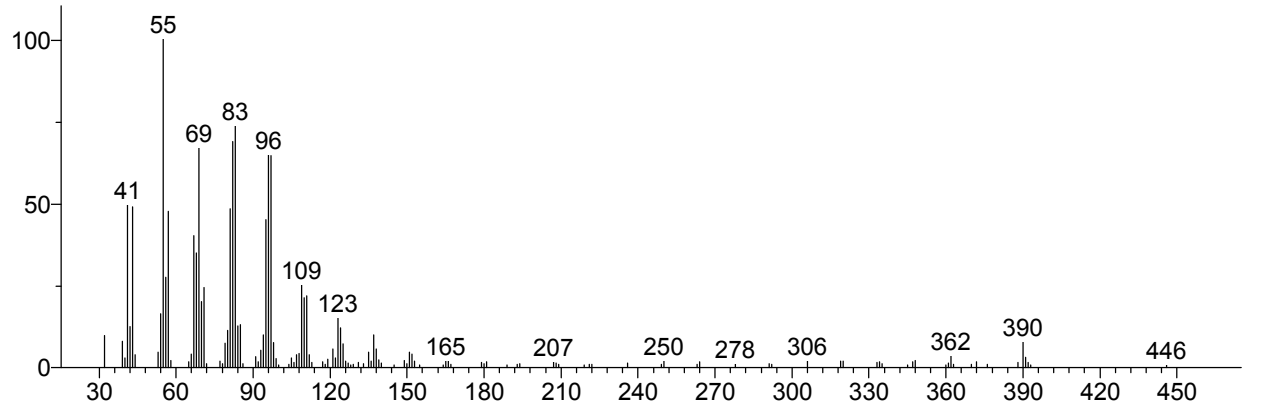
Hit 1 : 1-Heptacosanol
C27H56O; MF: 870; RMF: 896; Prob 8.61%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



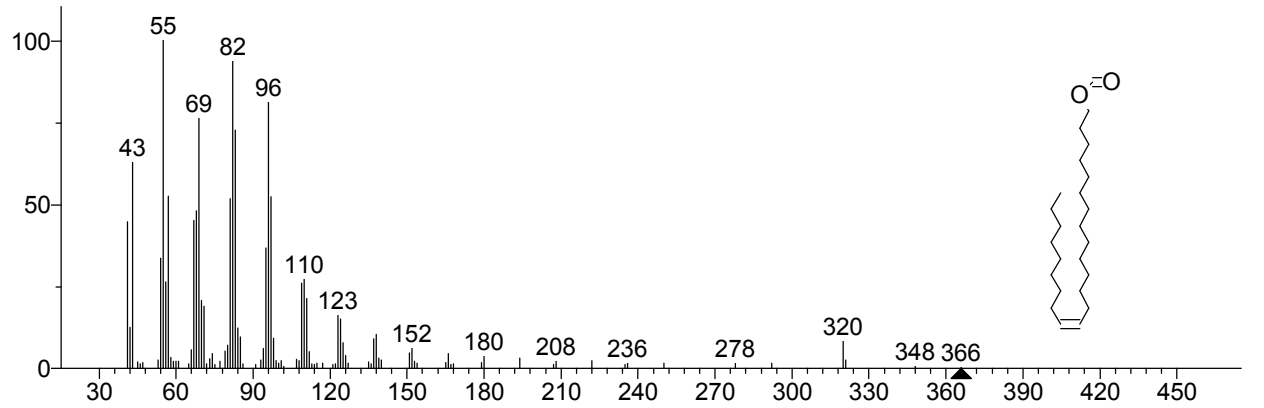
Hit 2 : 1-Octacosanol
C28H58O; MF: 858; RMF: 890; Prob 5.73%; Lib: mainlib; ID: 22288.



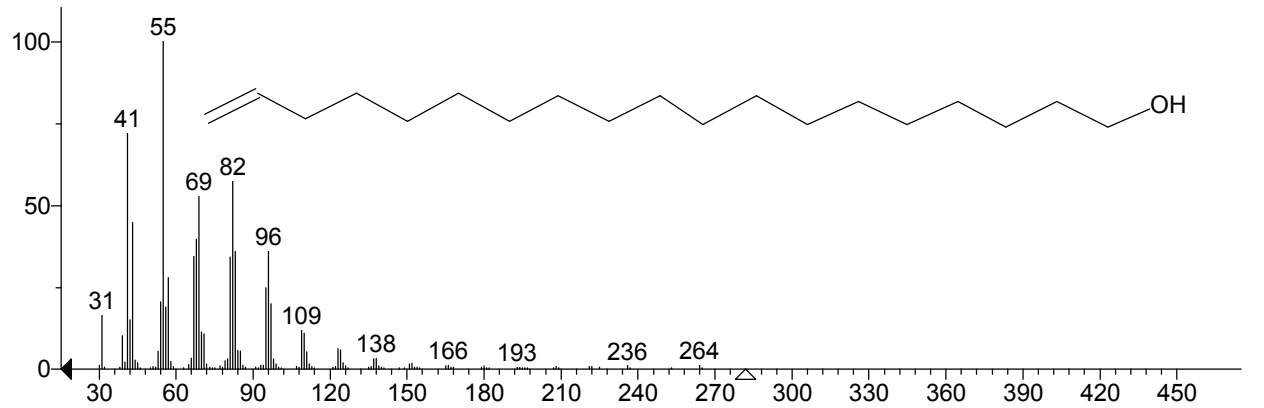
Unknown: Scan 1346 (10.230 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -520



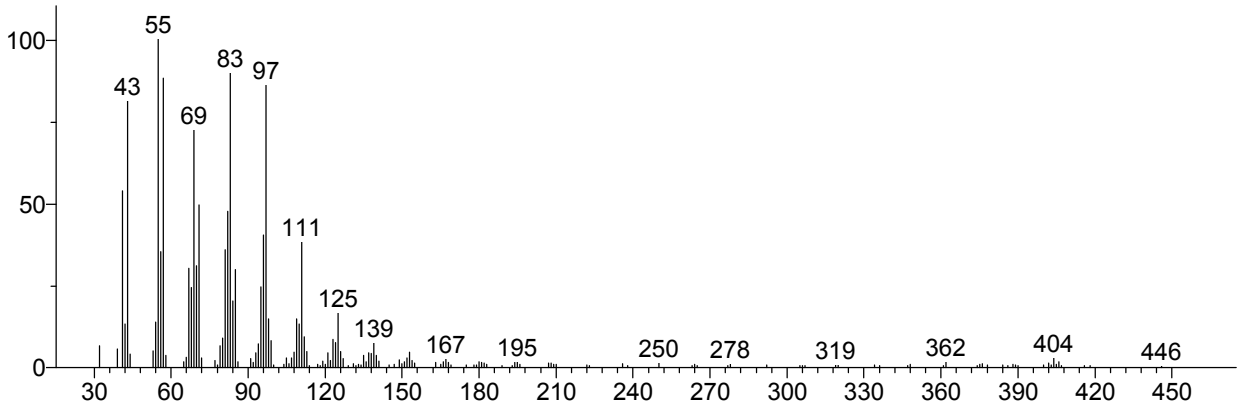
Hit 1 : (Z)-14-Tricosenyl formate
C24H46O2; MF: 784; RMF: 872; Prob 5.86%; CAS: 77899-10-6; Lib: mainlib; ID: 18672.



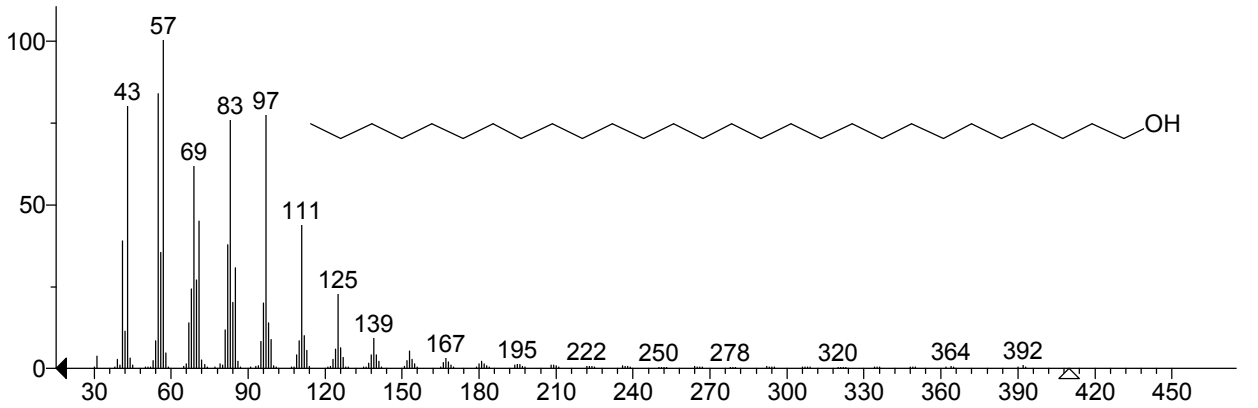
Hit 2 : 18-Nonadecen-1-ol
C19H38O; MF: 774; RMF: 859; Prob 4.14%; Lib: mainlib; ID: 17586.



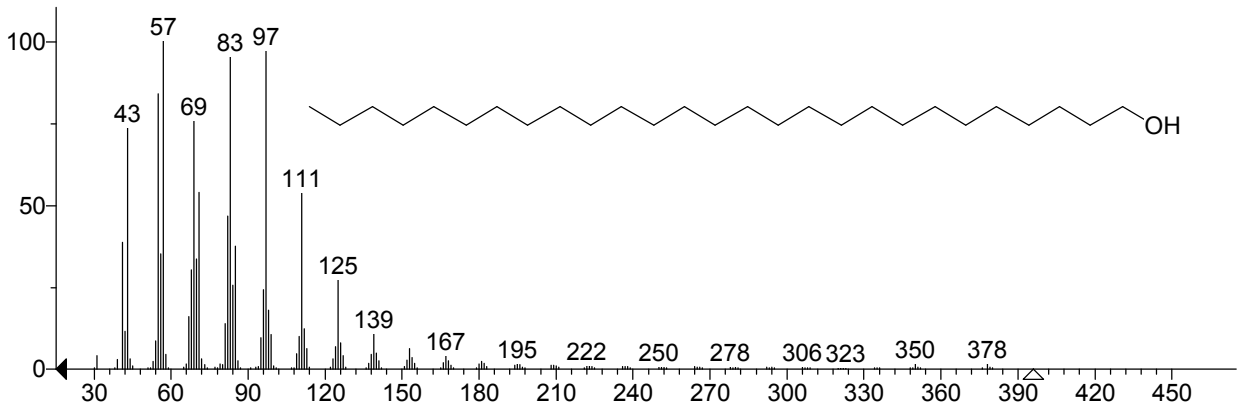
Unknown: Scan 1391 (10.569 min): J9163_Jordi_Inside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -503



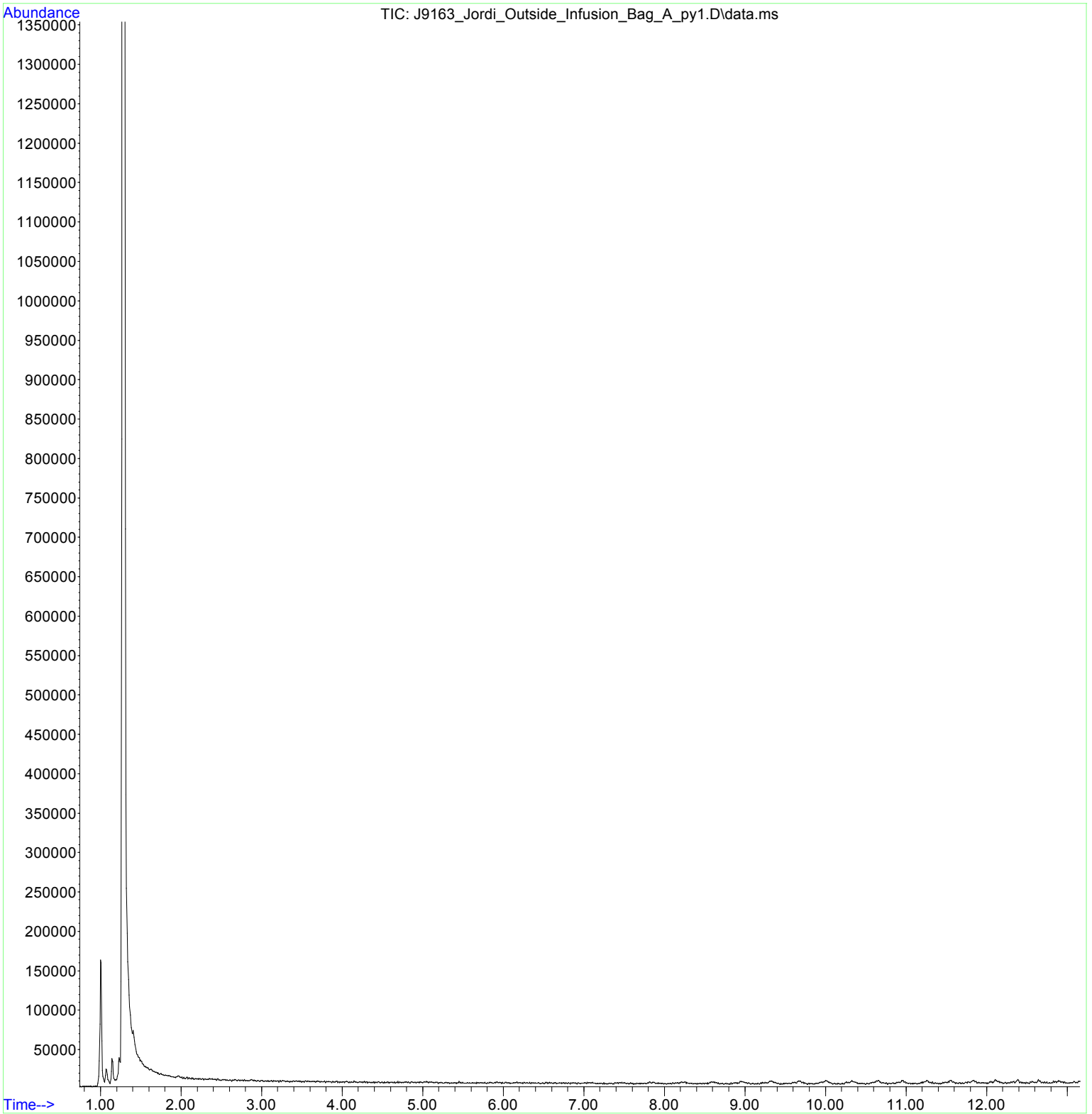
Hit 1 : 1-Octacosanol
C28H58O; MF: 825; RMF: 875; Prob 6.00%; Lib: mainlib; ID: 22288.



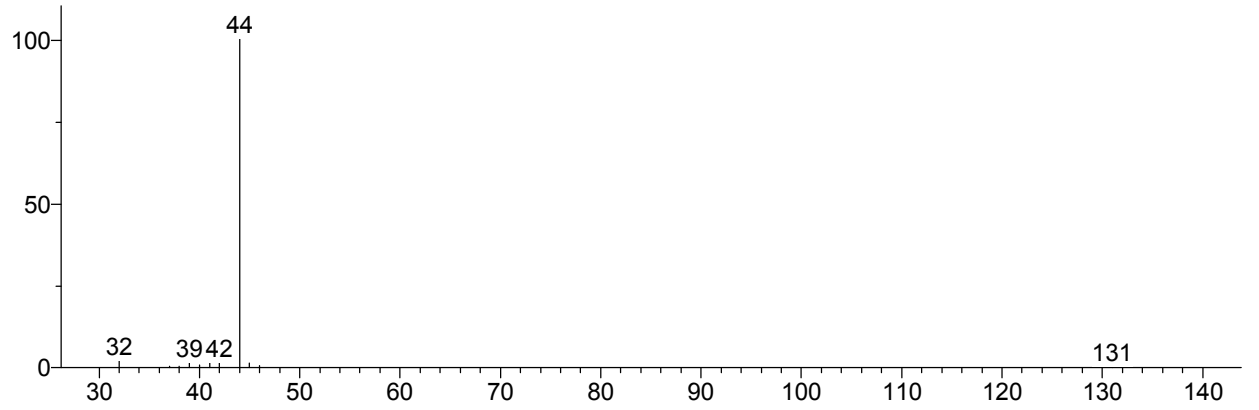
Hit 2 : 1-Heptacosanol
C27H56O; MF: 821; RMF: 876; Prob 5.07%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



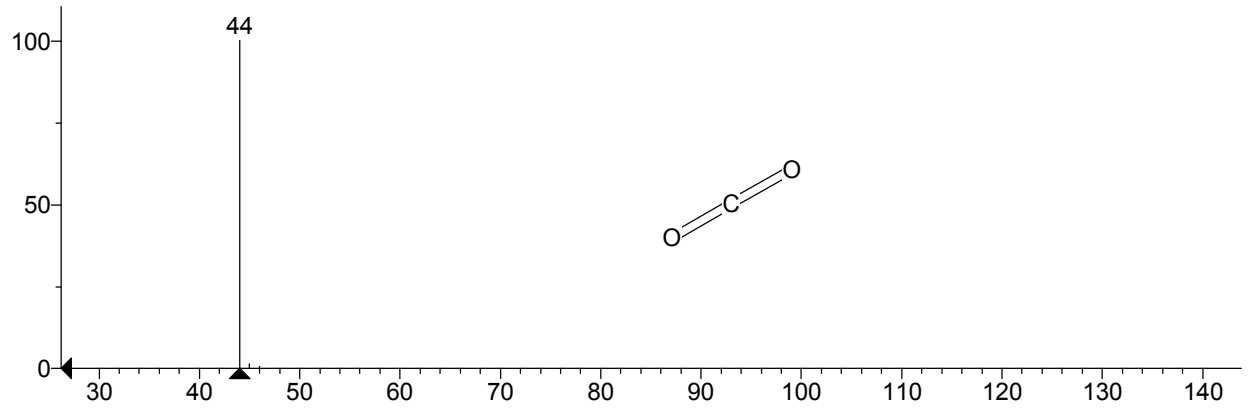
File :C:\msdchem\1\DATA\2014\Temp\102014\J9163_Jordi_Outside_Infus
... ion_Bag_A_py1.D
Operator : Julia Berk
Instrument : Instrument #1
Acquired : 21 Oct 2014 7:20 using AcqMethod PYMSSP30.M
Sample Name: J9163 Jordi Outside Infusion Bag
Misc Info : J9163 Jordi Outside Infusion Bag



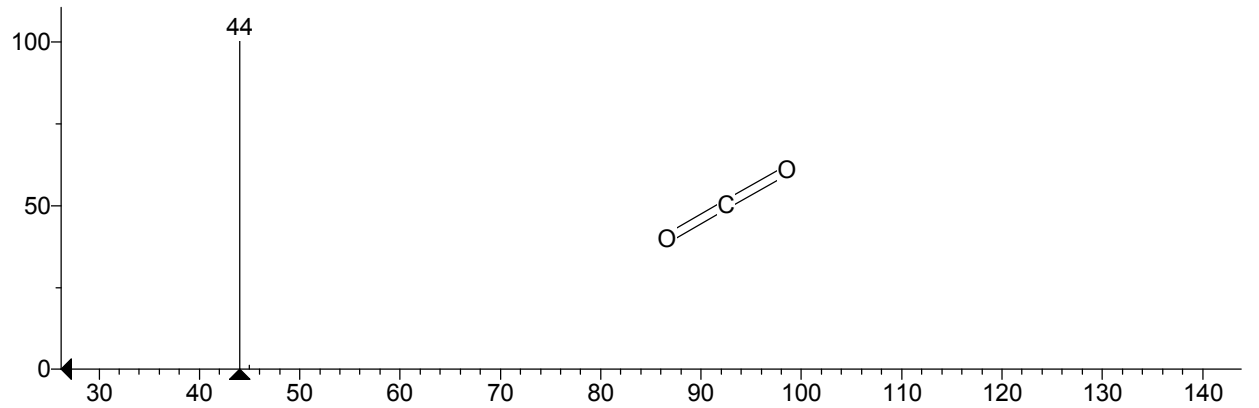
Unknown: Scan 121 (0.999 min): J9163_Jordi_Outside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = 251



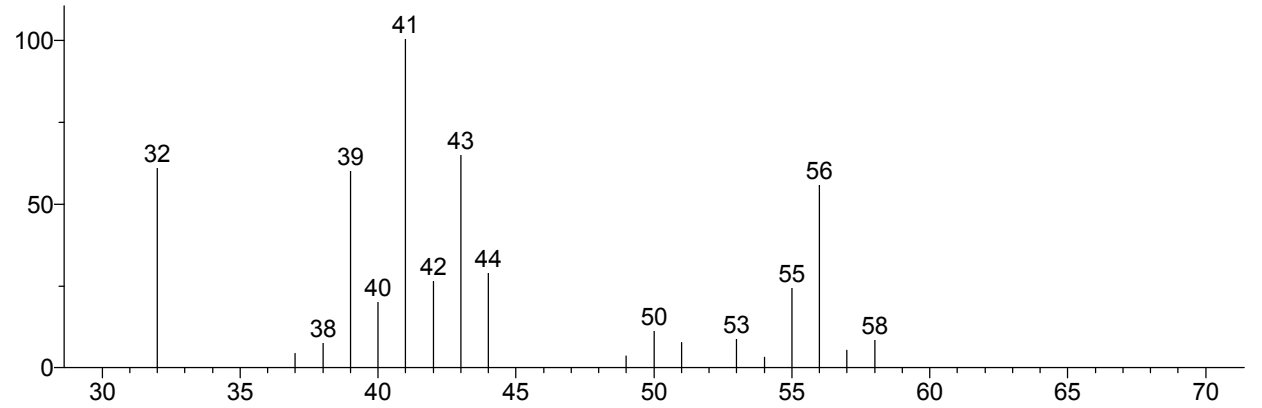
Hit 1 : Carbon dioxide
CO2; MF: 967; RMF: 999; Prob 82.1%; CAS: 124-38-9; Lib: mainlib; ID: 13702.



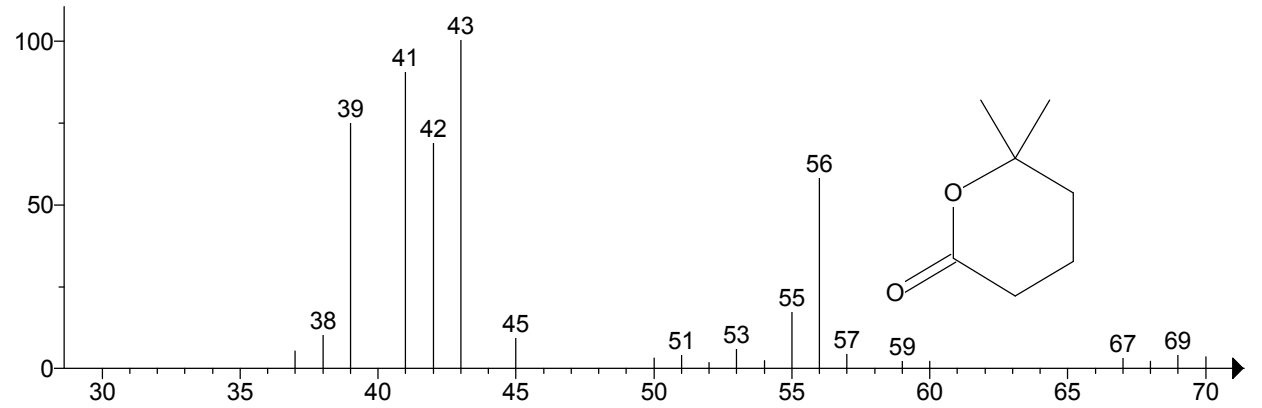
Hit 2 : Carbon dioxide
CO2; MF: 947; RMF: 985; Prob 82.1%; CAS: 124-38-9; Lib: replib; ID: 3160.



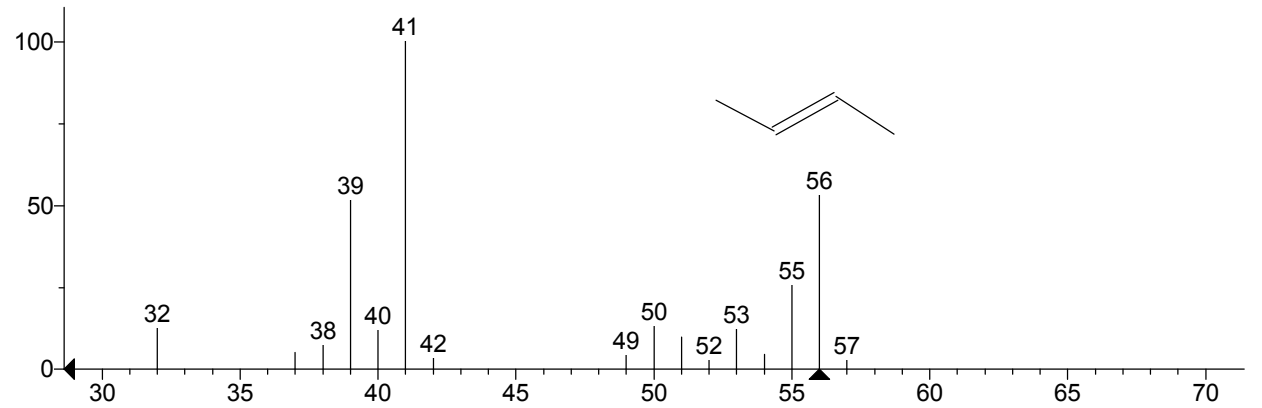
Unknown: Scan 131 (1.075 min): J9163_Jordi_Outside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -474



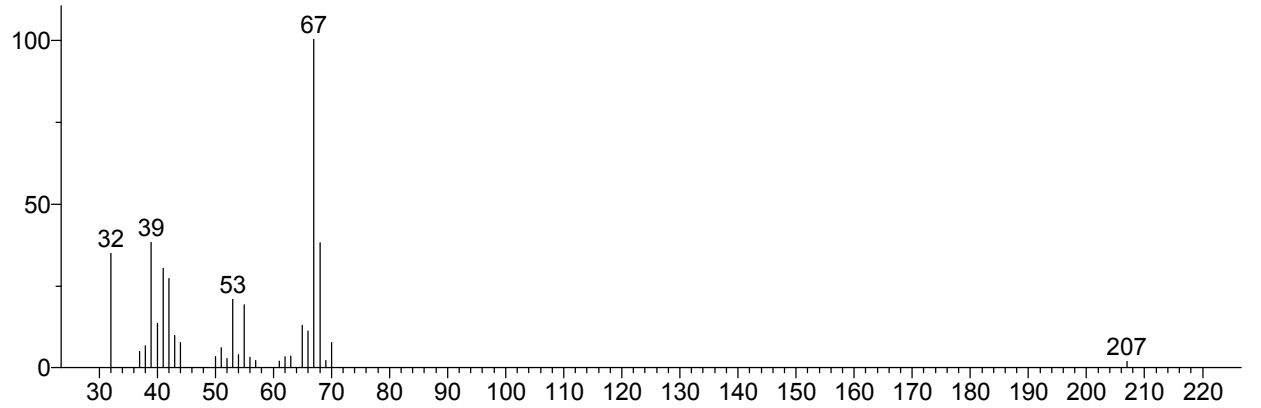
Hit 1 : 2H-Pyran-2-one, tetrahydro-6,6-dimethyl-
C7H12O2; MF: 789; RMF: 858; Prob 36.0%; CAS: 2610-95-9; Lib: mainlib; ID: 5443.



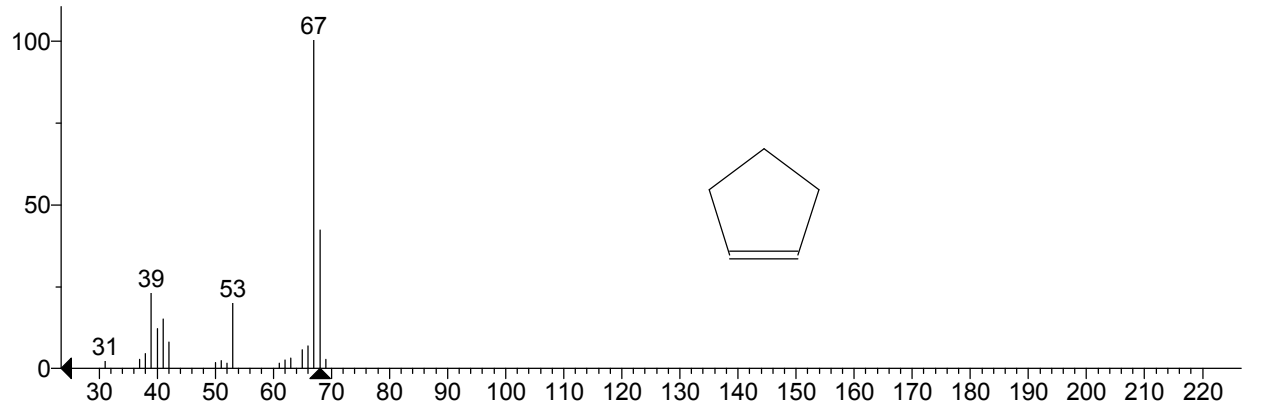
Hit 2 : 2-Butene
C4H8; MF: 773; RMF: 880; Prob 20.7%; CAS: 107-01-7; Lib: mainlib; ID: 1863.



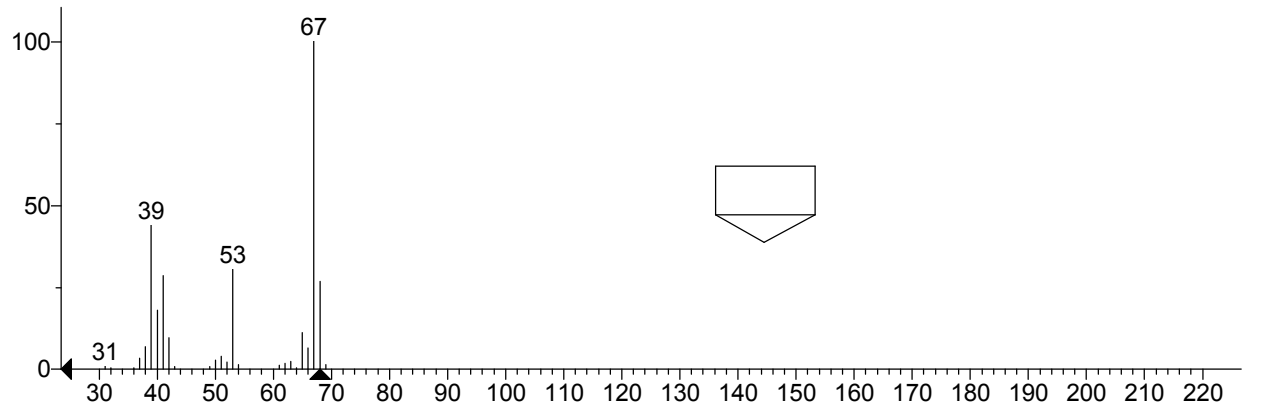
Unknown: Scan 140 (1.143 min): J9163_Jordi_Outside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = -407



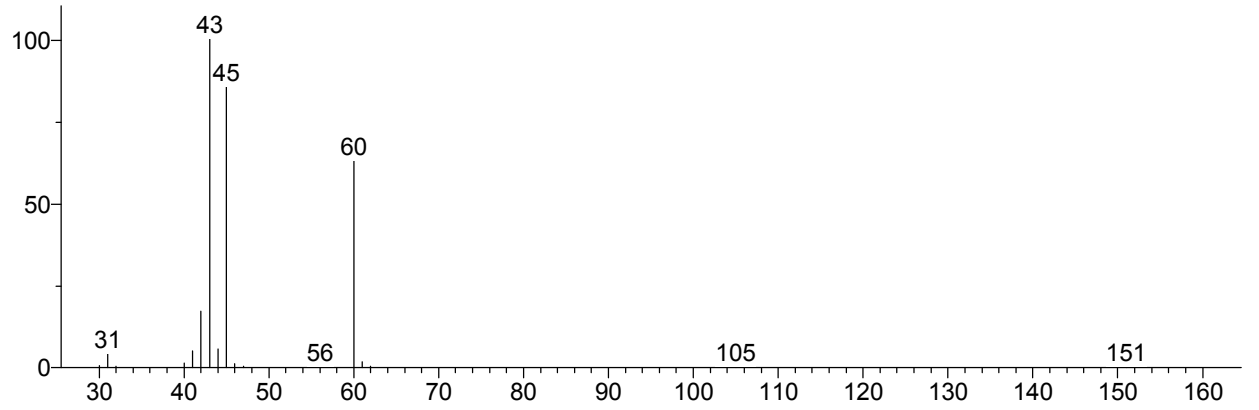
Hit 1 : Cyclopentene
C5H8; MF: 812; RMF: 915; Prob 16.9%; CAS: 142-29-0; Lib: replib; ID: 7176.



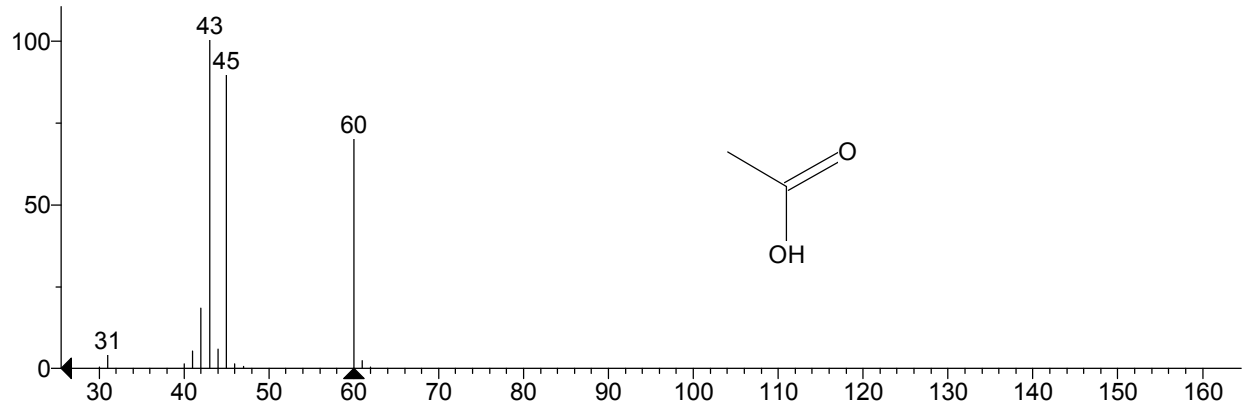
Hit 2 : Bicyclo[2.1.0]pentane
C5H8; MF: 805; RMF: 866; Prob 12.9%; CAS: 185-94-4; Lib: mainlib; ID: 28376.



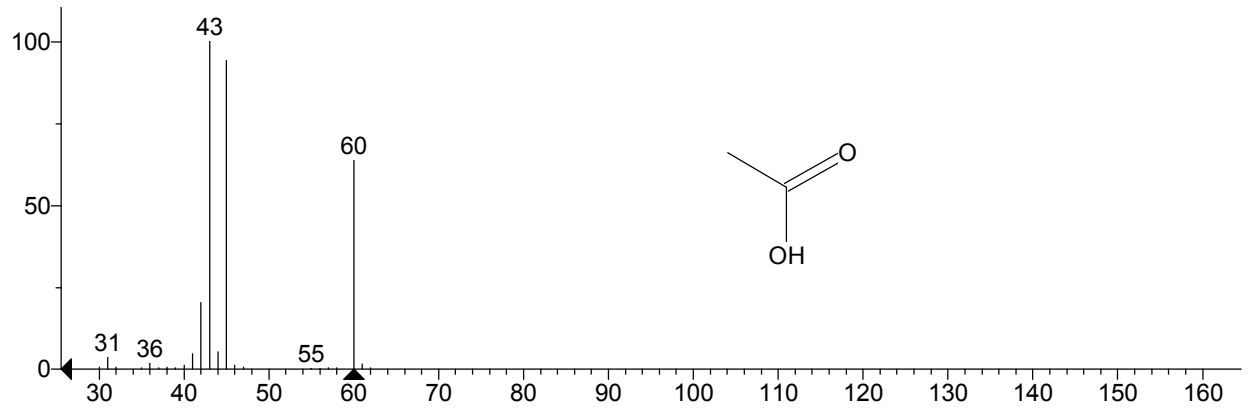
Unknown: Scan 161 (1.301 min): J9163_Jordi_Outside_Infusion_Bag_A_py1.D\data.ms
Compound in Library Factor = 676



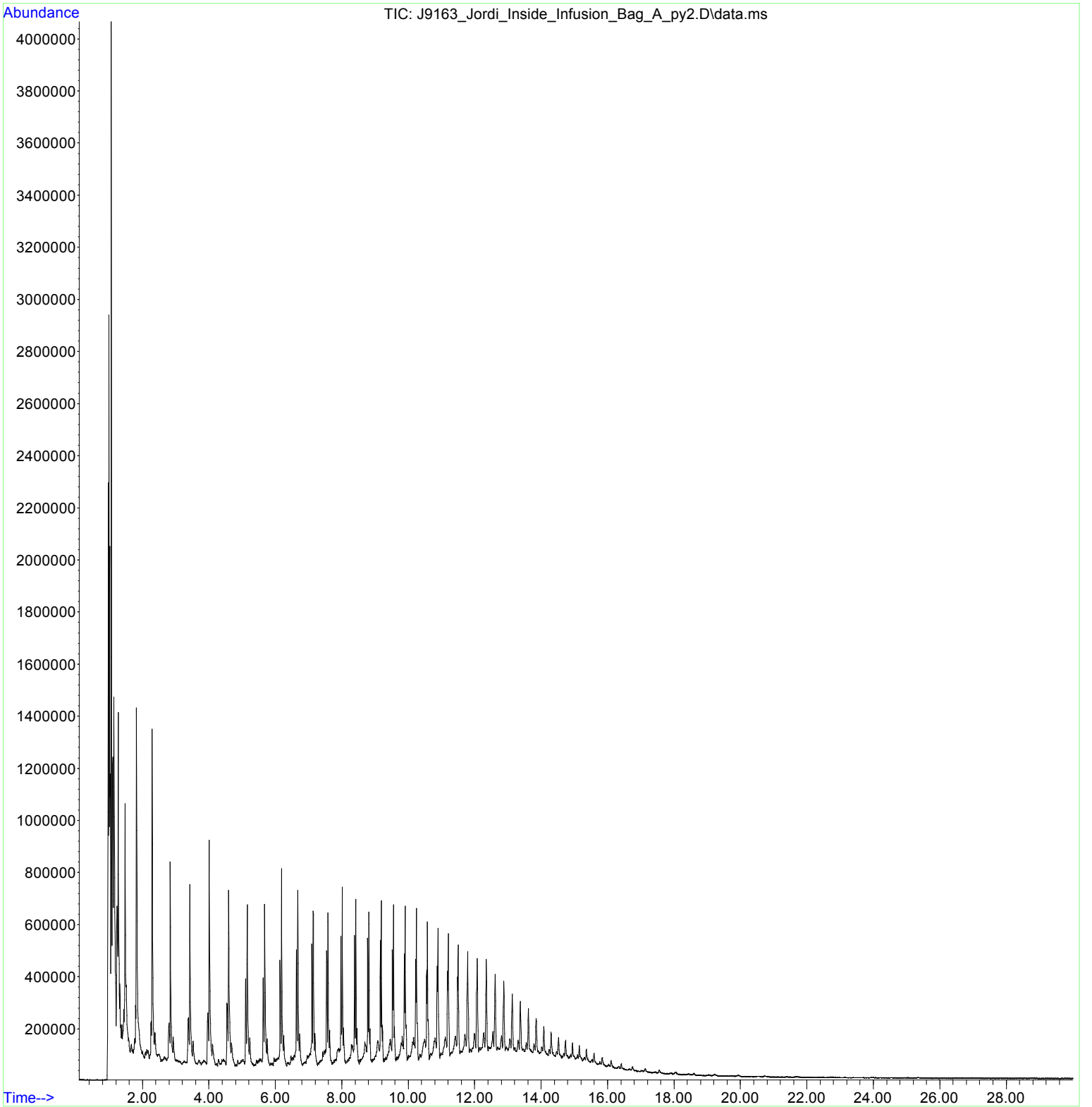
Hit 1 : Acetic acid
C2H4O2; MF: 966; RMF: 966; Prob 97.7%; CAS: 64-19-7; Lib: replib; ID: 1870.



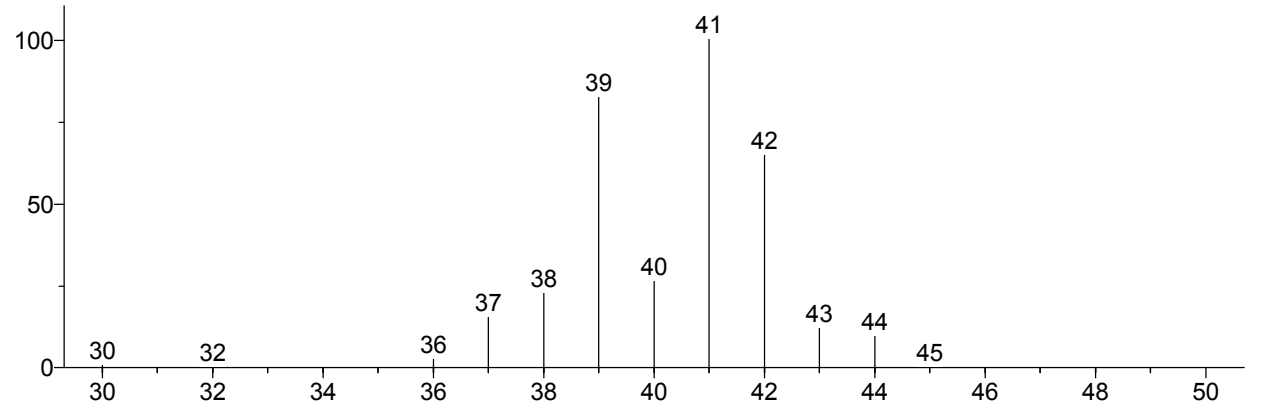
Hit 2 : Acetic acid
C2H4O2; MF: 957; RMF: 957; Prob 97.7%; CAS: 64-19-7; Lib: replib; ID: 1869.



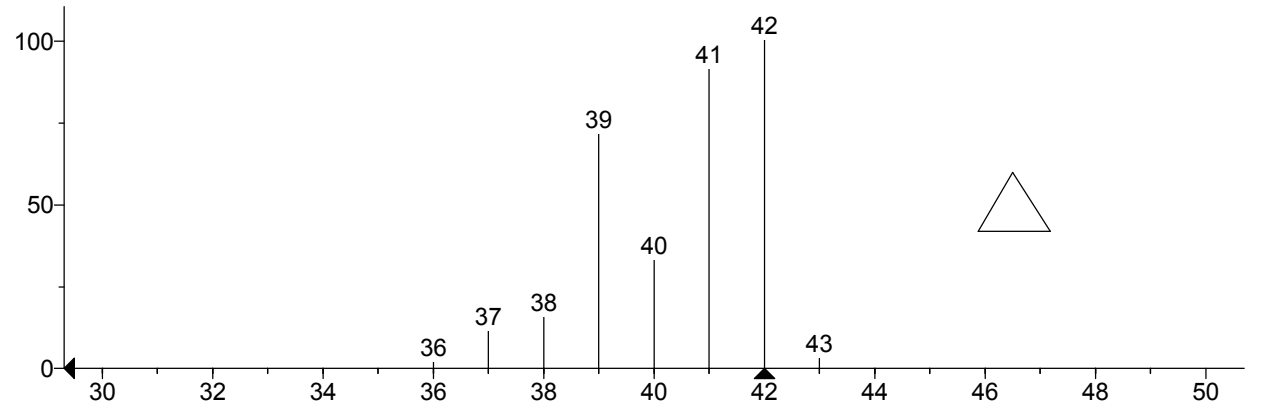
File :C:\msdchem\1\DATA\2014\Temp\102014\J9163_Jordi_Inside_Infusi
... on_Bag_A_py2.D
Operator : Julia Berk
Instrument : Instrument #1
Acquired : 21 Oct 2014 15:47 using AcqMethod PYMSSP30.M
Sample Name: J9163 Jordi Inside Infusion Bag
Misc Info : J9163 Jordi Inside Infusion Bag



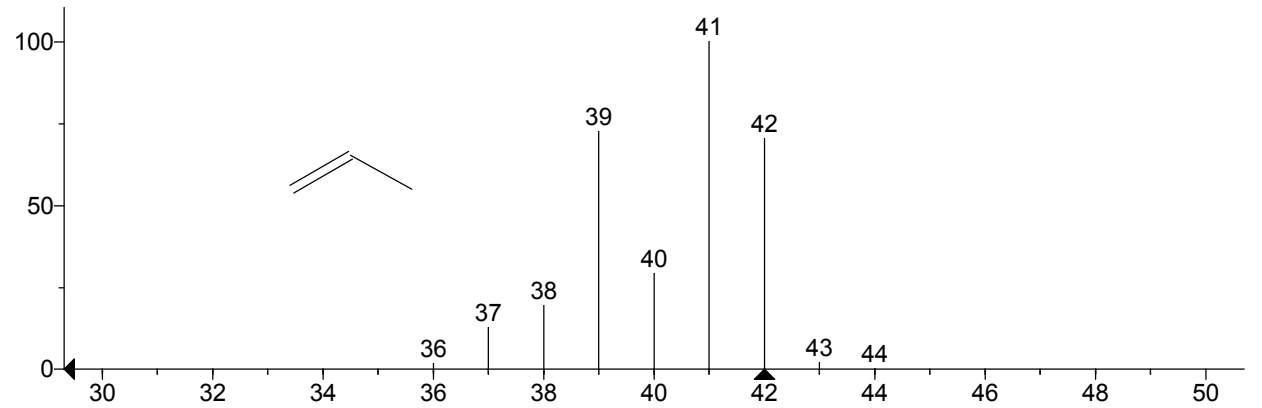
Unknown: Scan 114 (0.947 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = 171



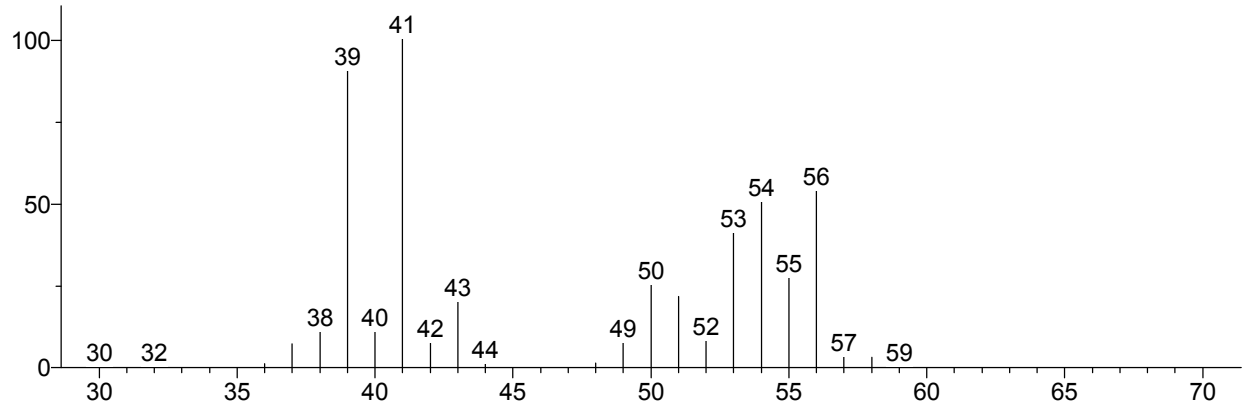
Hit 1 : Cyclopropane
C3H6; MF: 877; RMF: 895; Prob 45.8%; CAS: 75-19-4; Lib: replib; ID: 1331.



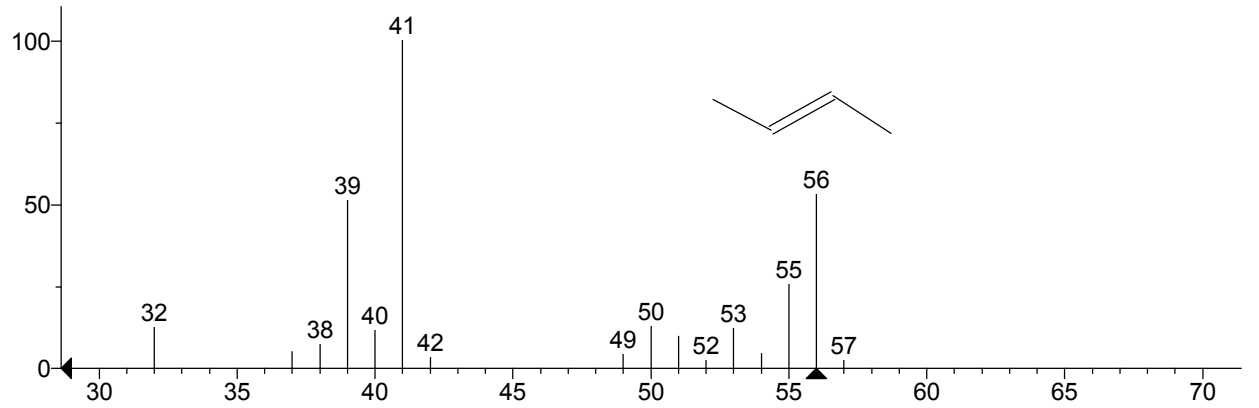
Hit 2 : Propene
C3H6; MF: 875; RMF: 876; Prob 42.2%; CAS: 115-07-1; Lib: mainlib; ID: 1934.



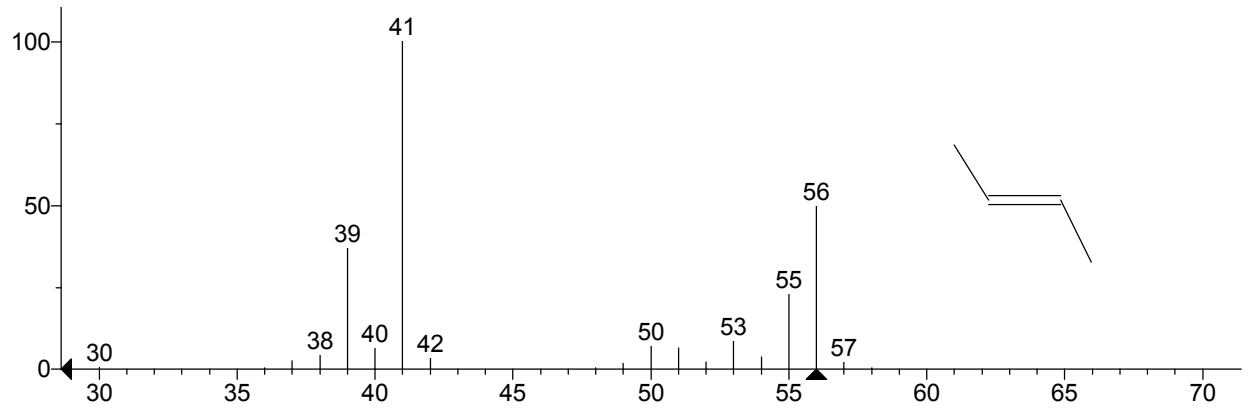
Unknown: Scan 117 (0.969 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -229



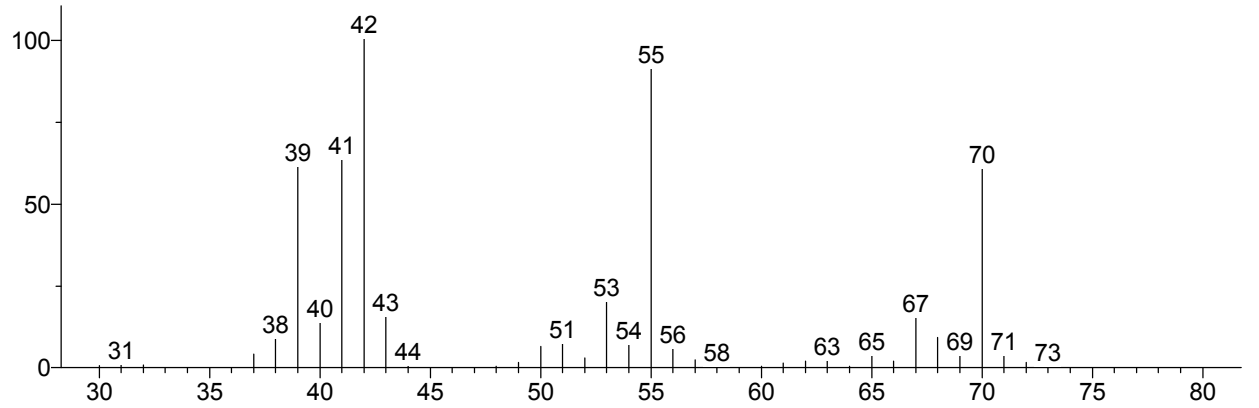
Hit 1 : 2-Butene
C4H8; MF: 833; RMF: 859; Prob 51.4%; CAS: 107-01-7; Lib: mainlib; ID: 1863.



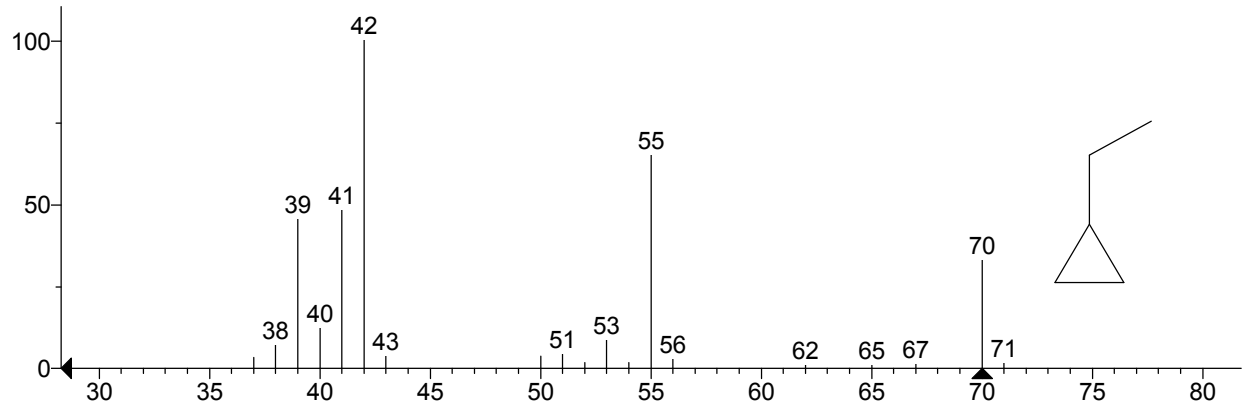
Hit 2 : 2-Butene, (E)-
C4H8; MF: 805; RMF: 824; Prob 14.9%; CAS: 624-64-6; Lib: replib; ID: 964.



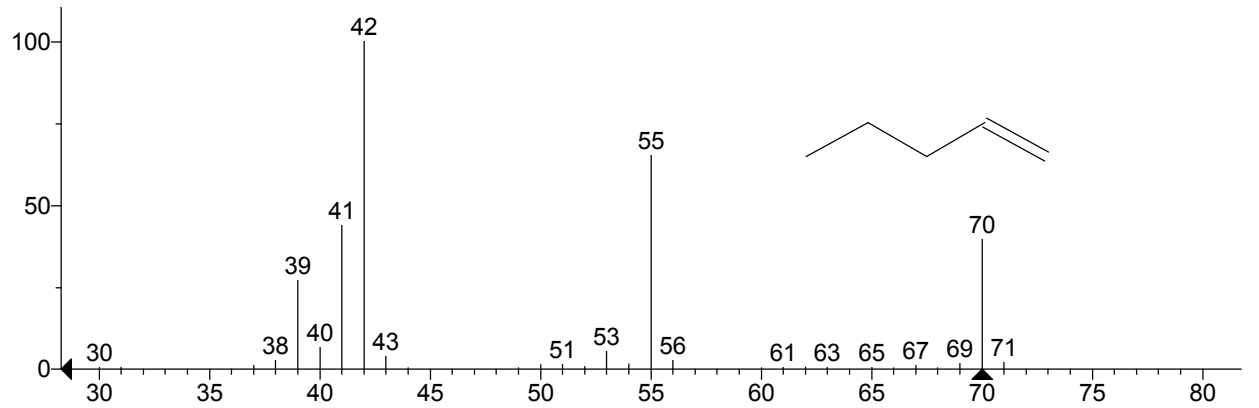
Unknown: Scan 121 (0.999 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -168



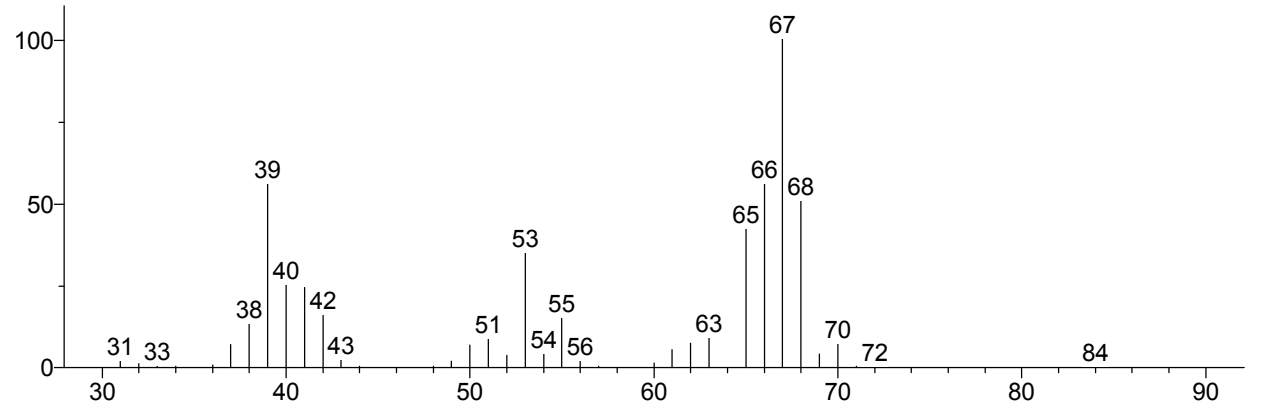
Hit 1 : Cyclopropane, ethyl-
C5H10; MF: 881; RMF: 917; Prob 15.9%; CAS: 1191-96-4; Lib: replib; ID: 1385.



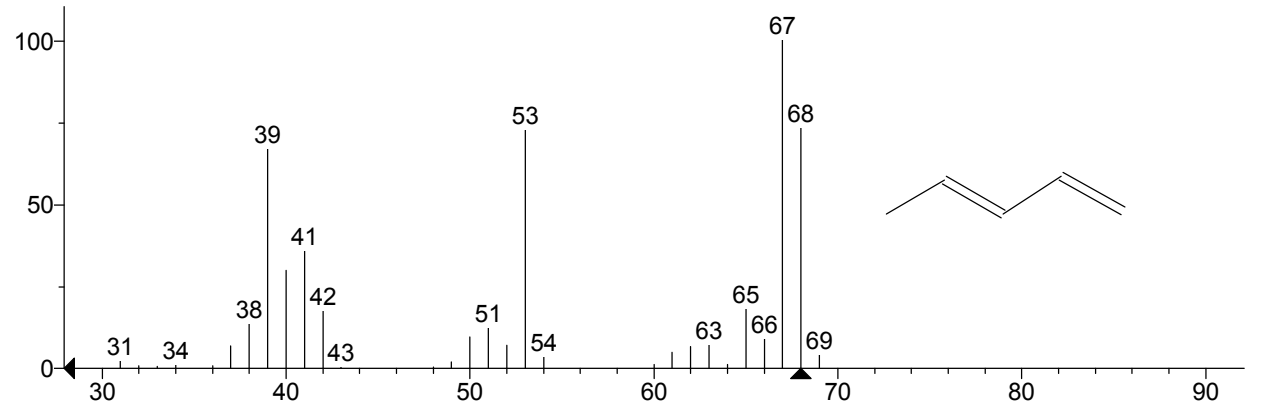
Hit 2 : 1-Pentene
C5H10; MF: 876; RMF: 881; Prob 12.8%; CAS: 109-67-1; Lib: mainlib; ID: 4375.



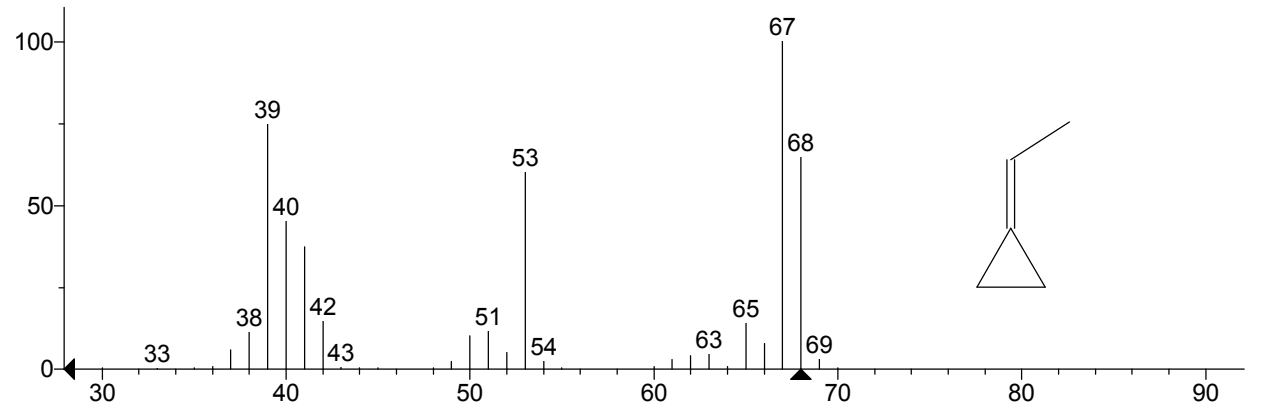
Unknown: Scan 124 (1.022 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -328



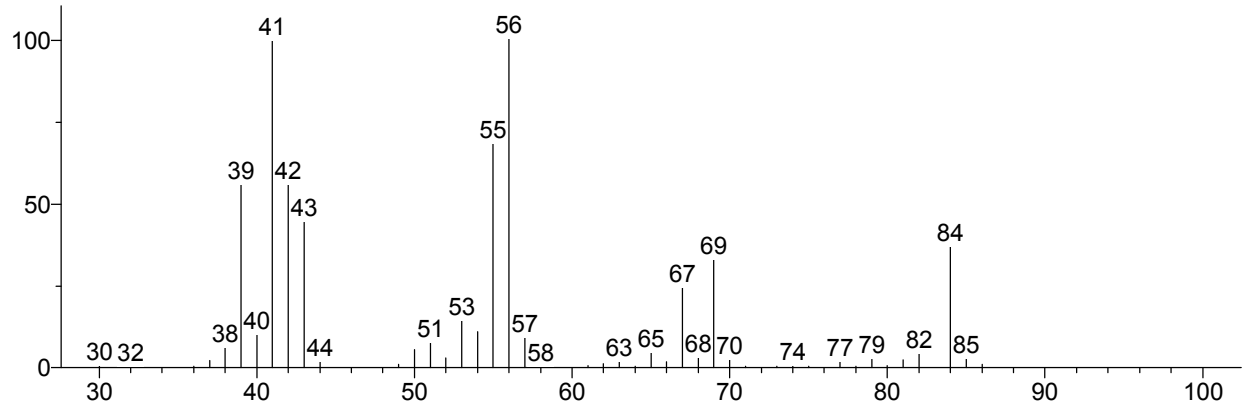
Hit 1 : 1,3-Pentadiene
C5H8; MF: 840; RMF: 865; Prob 14.3%; CAS: 504-60-9; Lib: replib; ID: 7184.



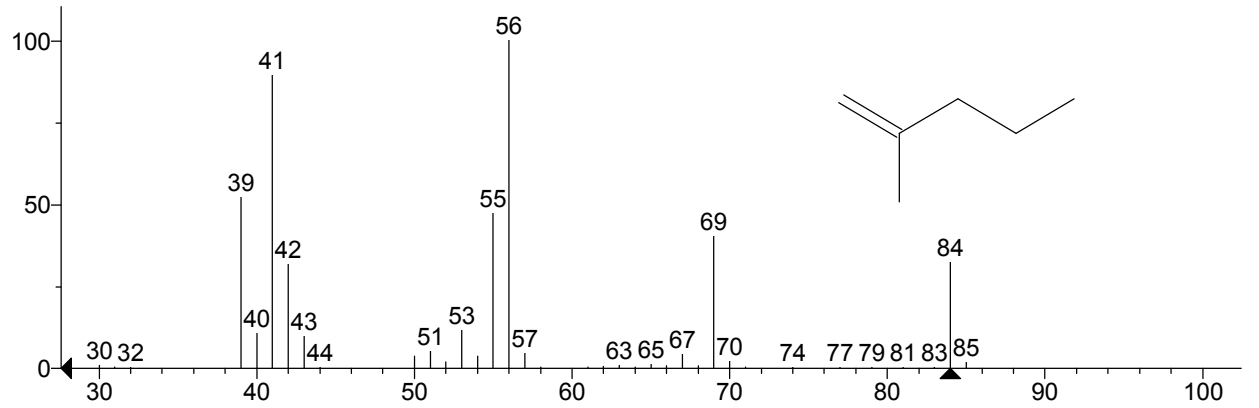
Hit 2 : Cyclopropane, ethylidene-
C5H8; MF: 837; RMF: 865; Prob 12.6%; CAS: 18631-83-9; Lib: mainlib; ID: 28385.



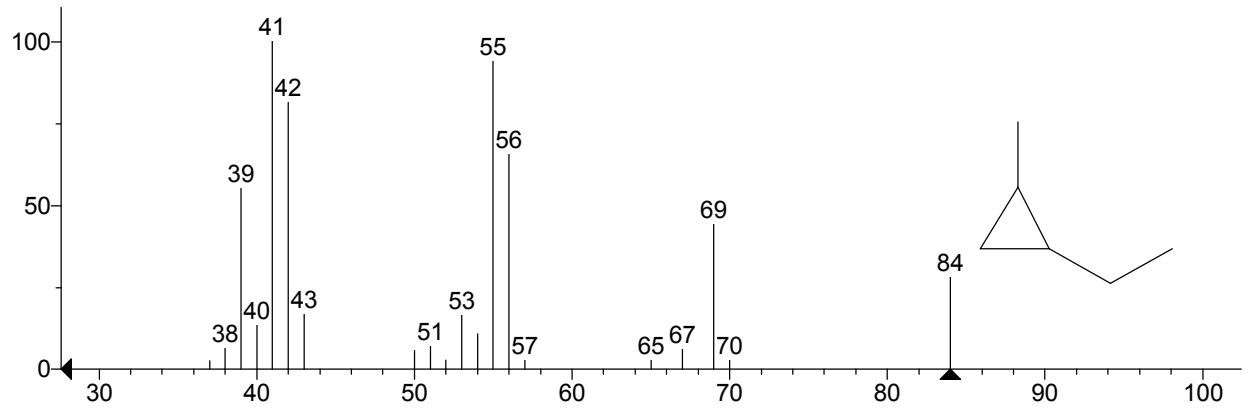
Unknown: Scan 130 (1.067 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -217



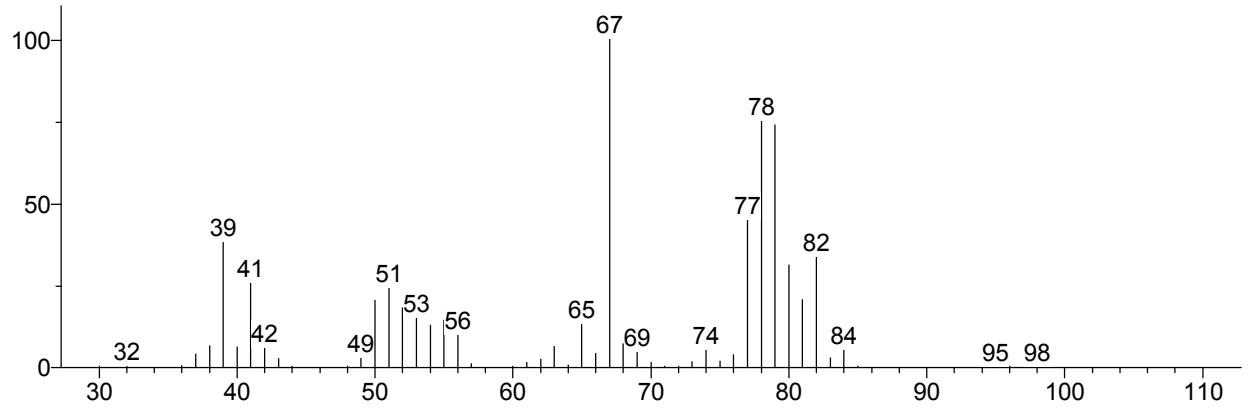
Hit 1 : 1-Pentene, 2-methyl-
C6H12; MF: 879; RMF: 892; Prob 11.5%; CAS: 763-29-1; Lib: mainlib; ID: 19838.



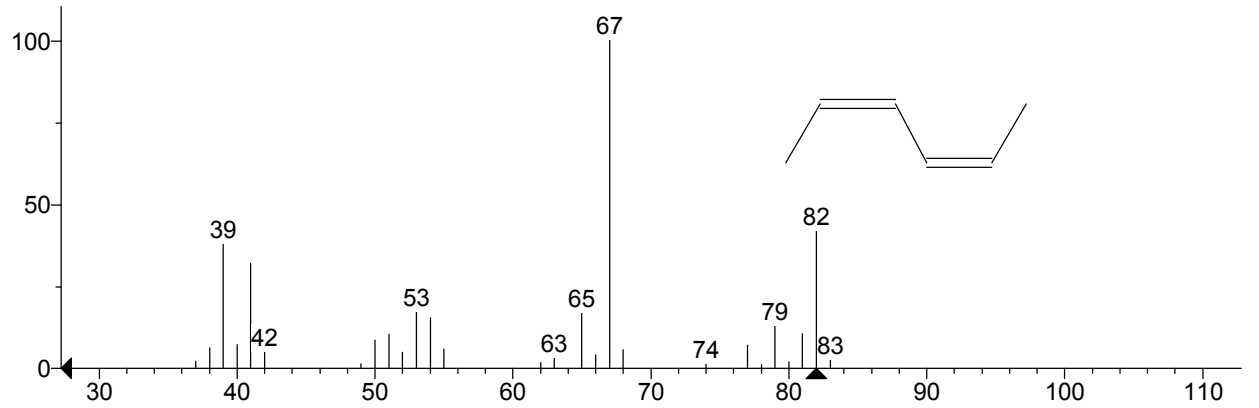
Hit 2 : Cyclopropane, 1-ethyl-2-methyl-, cis-
C6H12; MF: 878; RMF: 911; Prob 11.1%; CAS: 19781-68-1; Lib: mainlib; ID: 2449.



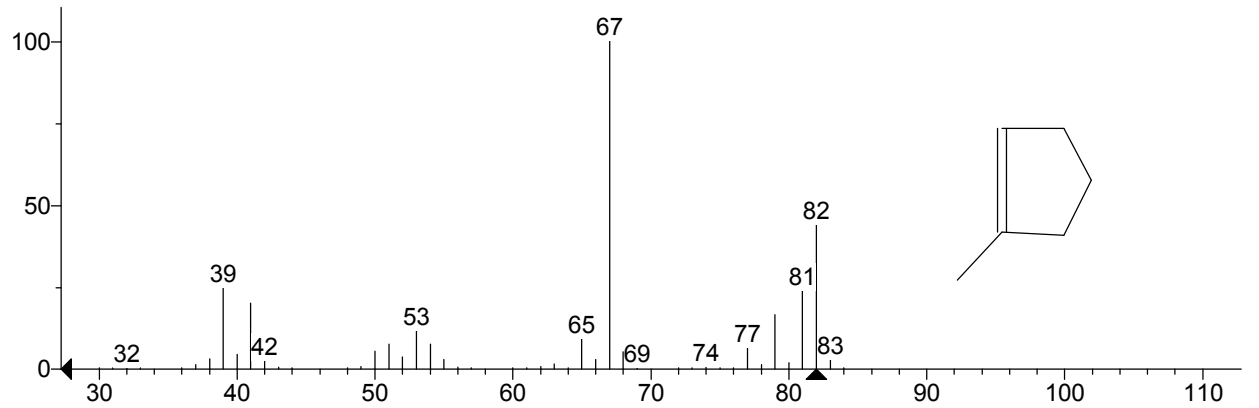
Unknown: Scan 135 (1.105 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -1131



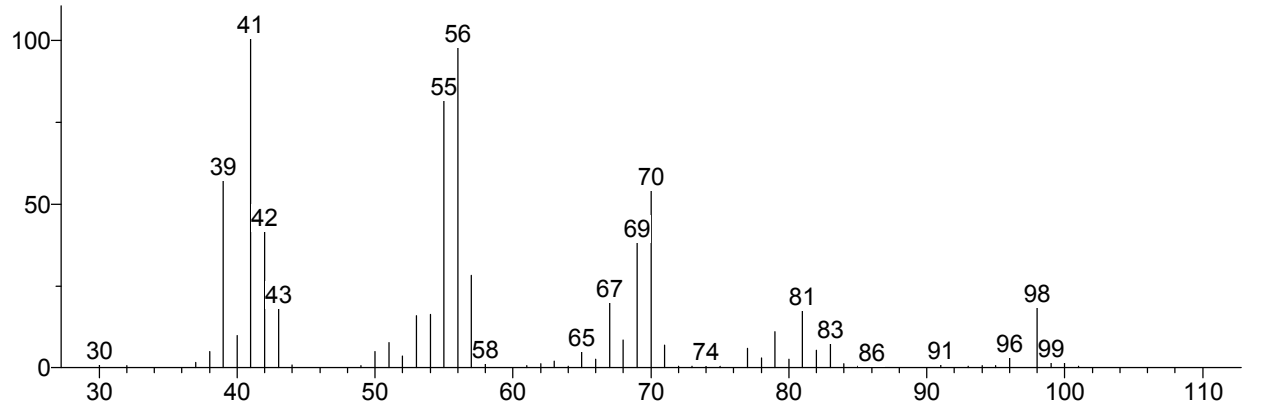
Hit 1 : 2,4-Hexadiene, (Z,Z)-
C6H10; MF: 723; RMF: 747; Prob 7.01%; CAS: 6108-61-8; Lib: mainlib; ID: 28907.



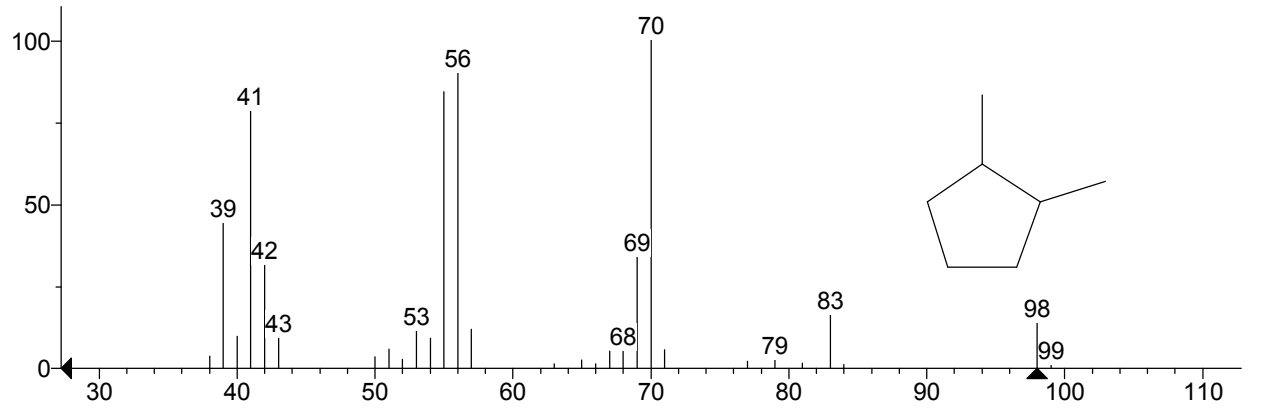
Hit 2 : Cyclopentene, 1-methyl-
C6H10; MF: 722; RMF: 729; Prob 6.74%; CAS: 693-89-0; Lib: replib; ID: 7234.



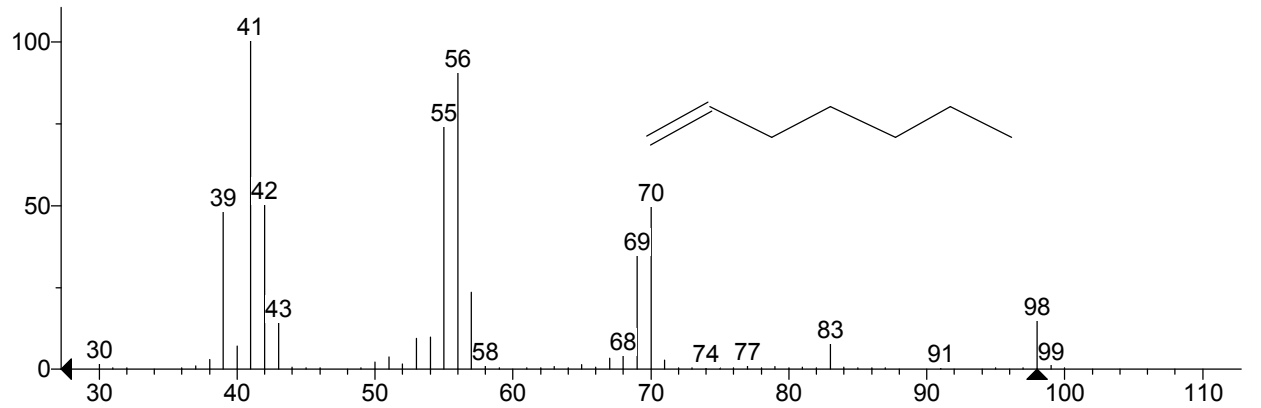
Unknown: Scan 140 (1.143 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -338



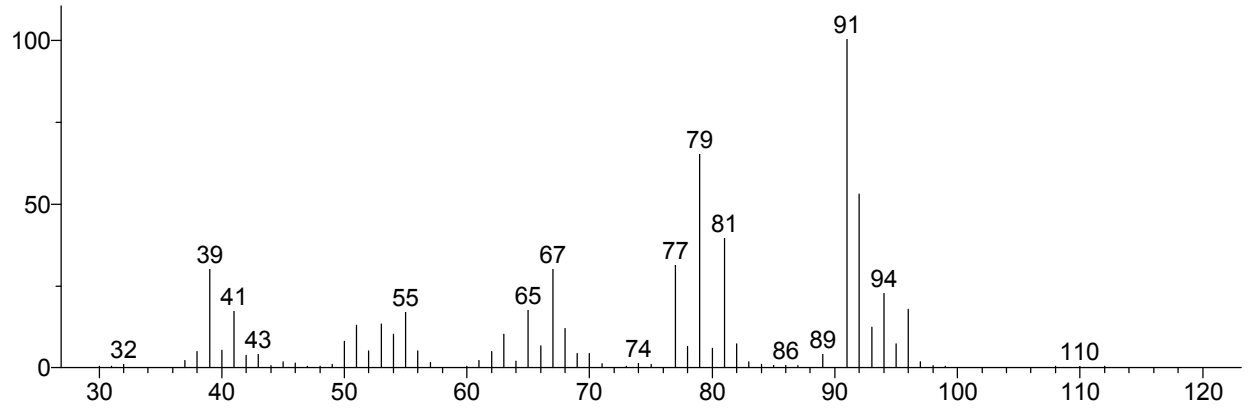
Hit 1 : Cyclopentane, 1,2-dimethyl-, cis-
C7H14; MF: 868; RMF: 894; Prob 11.7%; CAS: 1192-18-3; Lib: mainlib; ID: 32333.



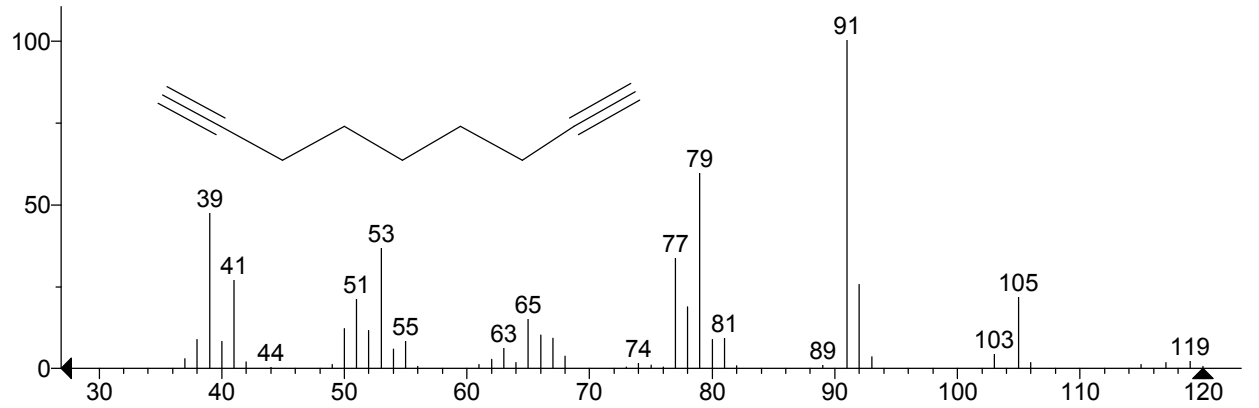
Hit 2 : 1-Heptene
C7H14; MF: 863; RMF: 873; Prob 9.43%; CAS: 592-76-7; Lib: replib; ID: 981.



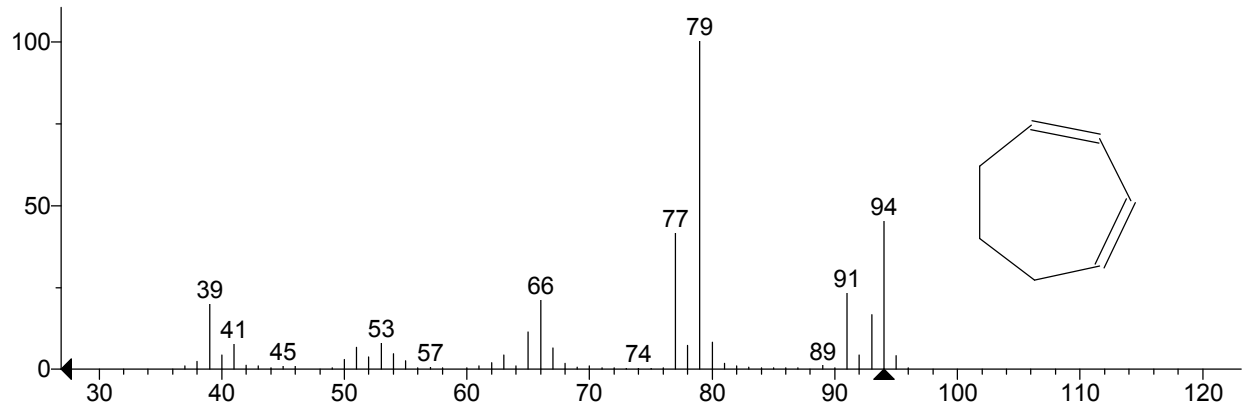
Unknown: Scan 152 (1.233 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -1131



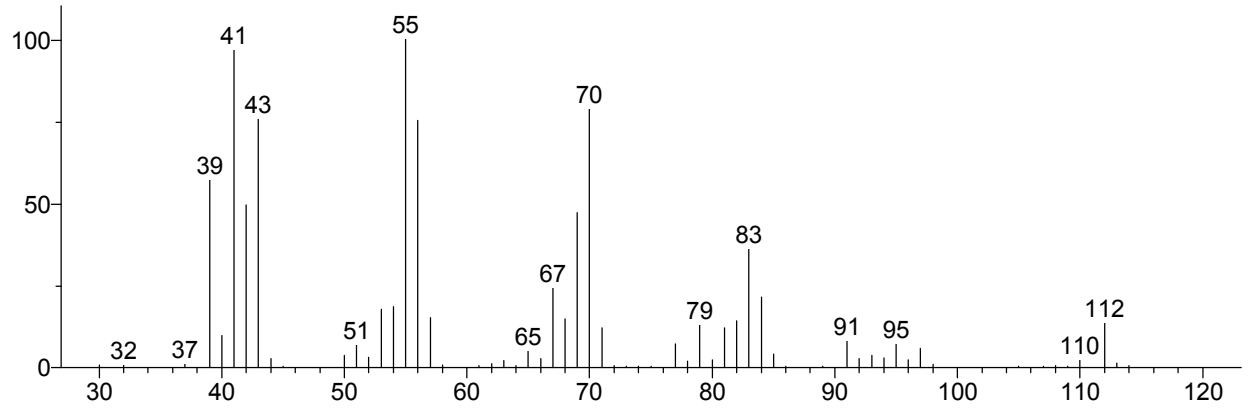
Hit 1 : 1,8-Nonadiyne
C9H12; MF: 730; RMF: 792; Prob 9.35%; CAS: 2396-65-8; Lib: mainlib; ID: 51427.



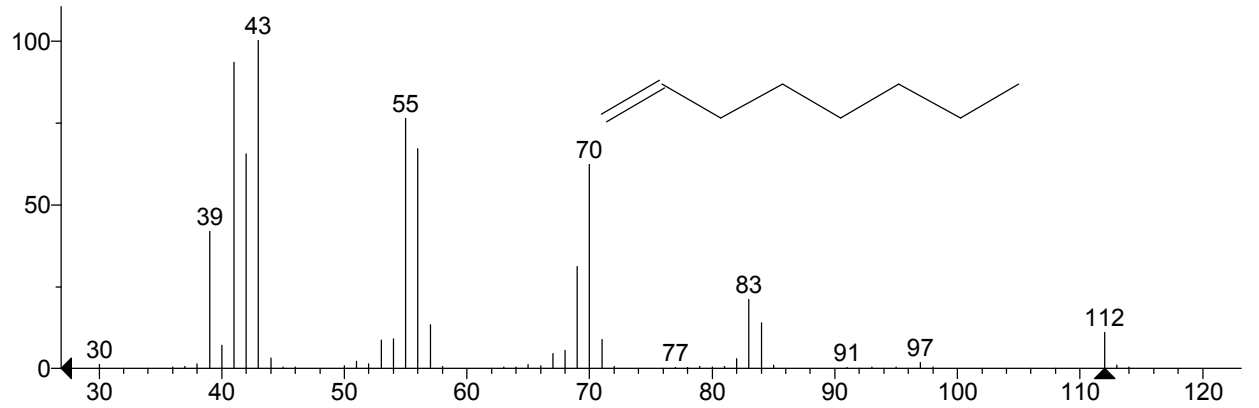
Hit 2 : 1,3-Cycloheptadiene
C7H10; MF: 728; RMF: 730; Prob 8.63%; CAS: 4054-38-0; Lib: replib; ID: 9747.



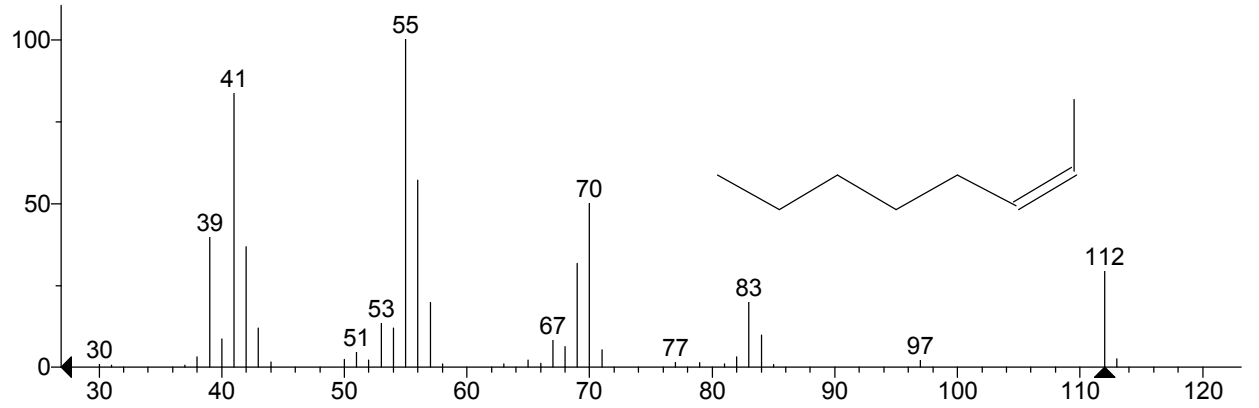
Unknown: Scan 159 (1.286 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -454



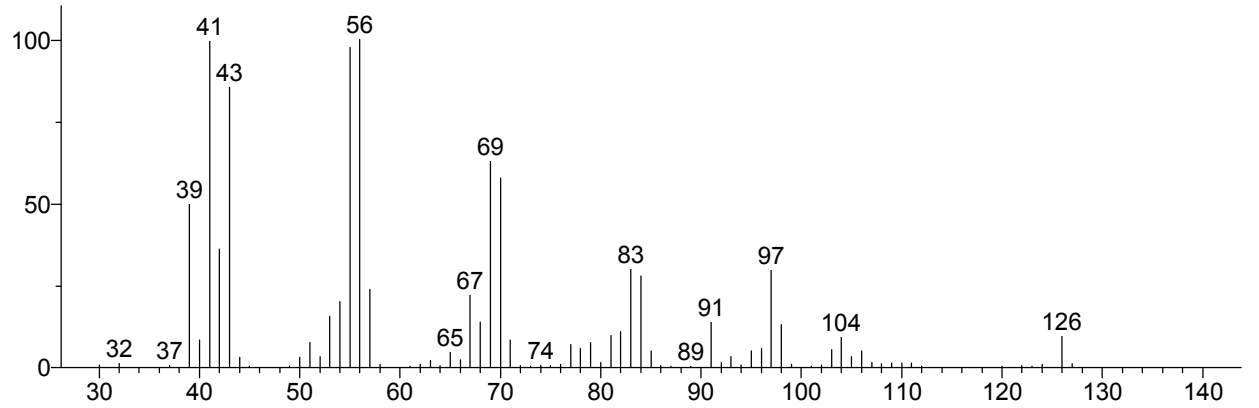
Hit 1 : 1-Octene
C8H16; MF: 850; RMF: 862; Prob 5.93%; CAS: 111-66-0; Lib: replib; ID: 1671.



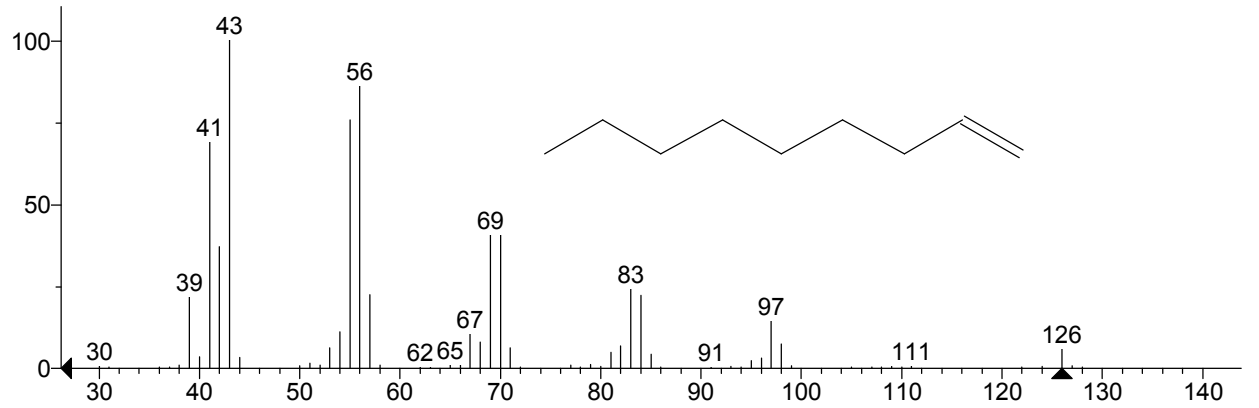
Hit 2 : 2-Octene, (Z)-
C8H16; MF: 847; RMF: 883; Prob 5.24%; CAS: 7642-04-8; Lib: replib; ID: 4208.



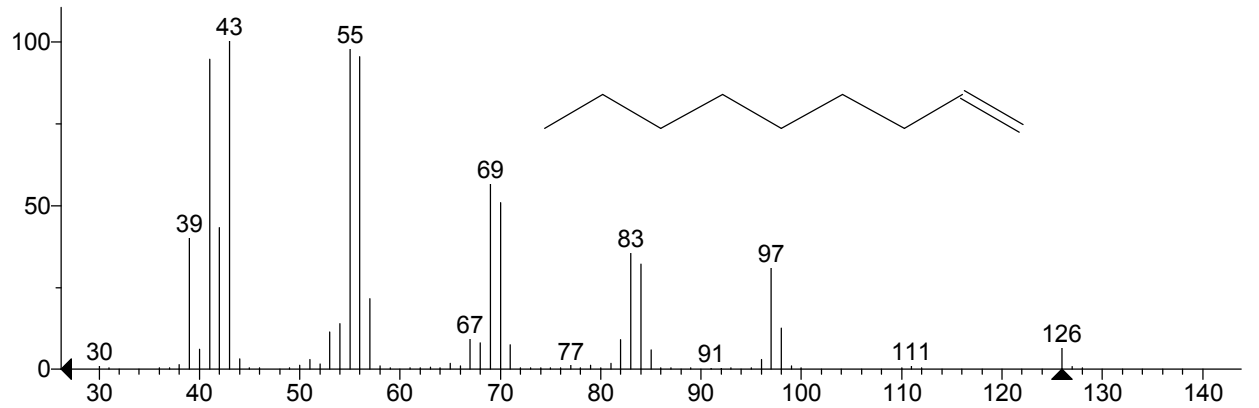
Unknown: Scan 186 (1.489 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -246



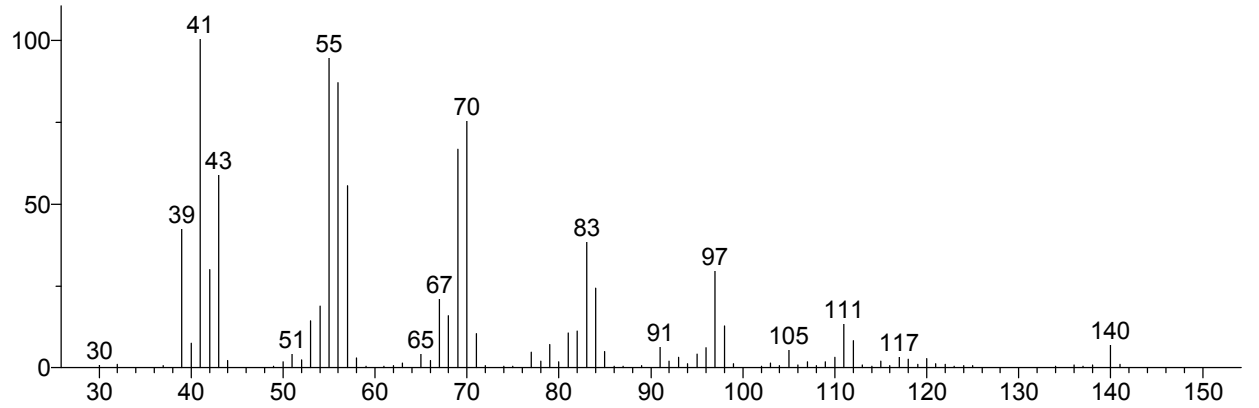
Hit 1 : 1-Nonene
C9H18; MF: 865; RMF: 888; Prob 11.0%; CAS: 124-11-8; Lib: mainlib; ID: 7048.



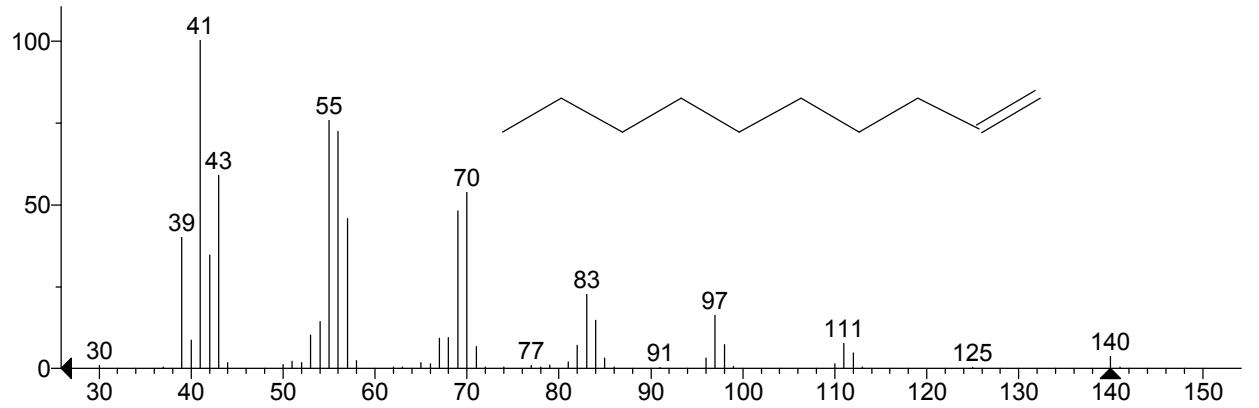
Hit 2 : 1-Nonene
C9H18; MF: 857; RMF: 893; Prob 11.0%; CAS: 124-11-8; Lib: replib; ID: 1943.



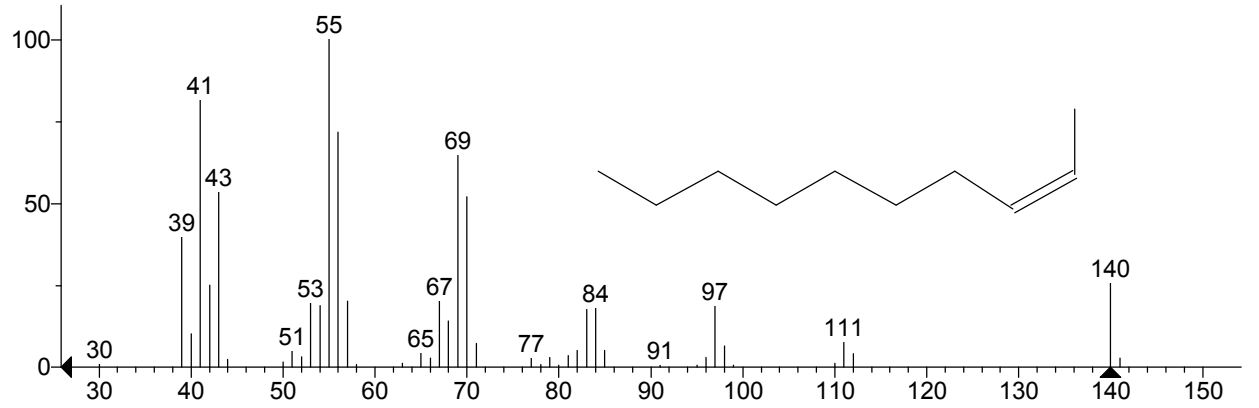
Unknown: Scan 234 (1.851 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -122



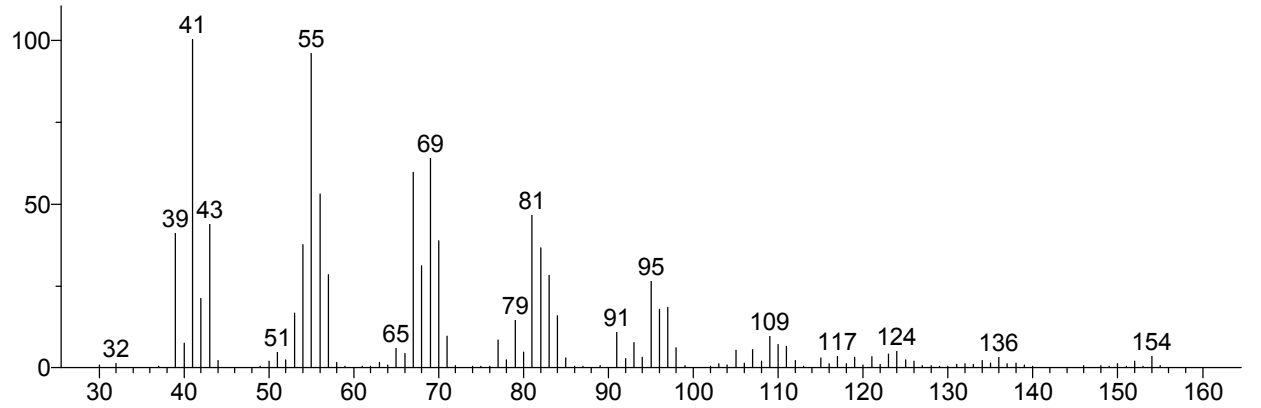
Hit 1 : 1-Decene
C10H20; MF: 902; RMF: 939; Prob 14.4%; CAS: 872-05-9; Lib: replib; ID: 896.



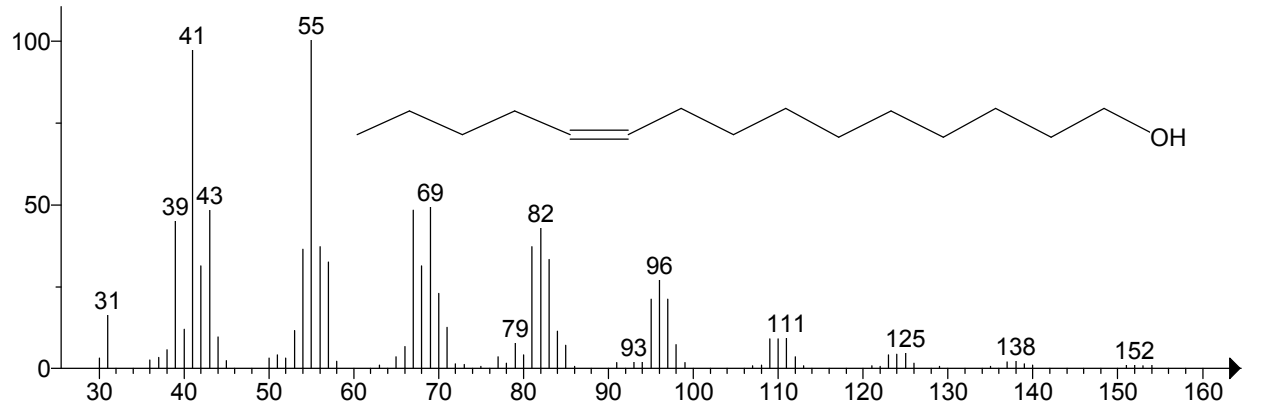
Hit 2 : 2-Decene, (Z)-
C10H20; MF: 881; RMF: 914; Prob 6.13%; CAS: 20348-51-0; Lib: mainlib; ID: 17331.



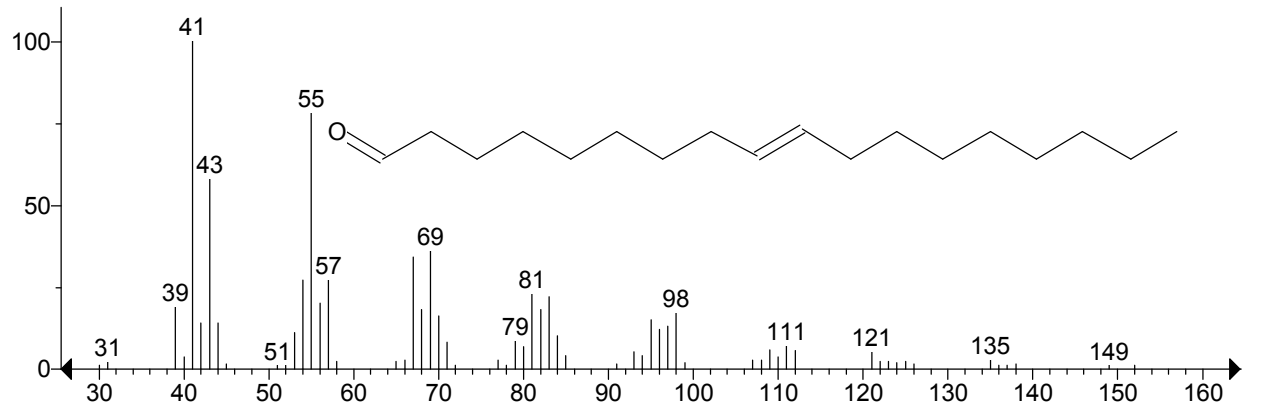
Unknown: Scan 294 (2.303 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -688



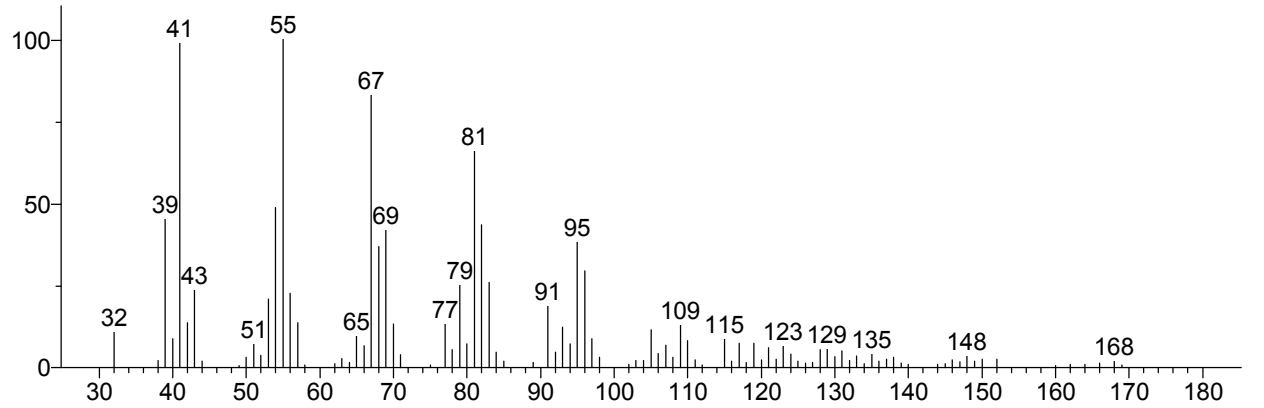
Hit 1 : Z-10-Pentadecen-1-ol
C15H30O; MF: 808; RMF: 840; Prob 4.66%; Lib: mainlib; ID: 17434.



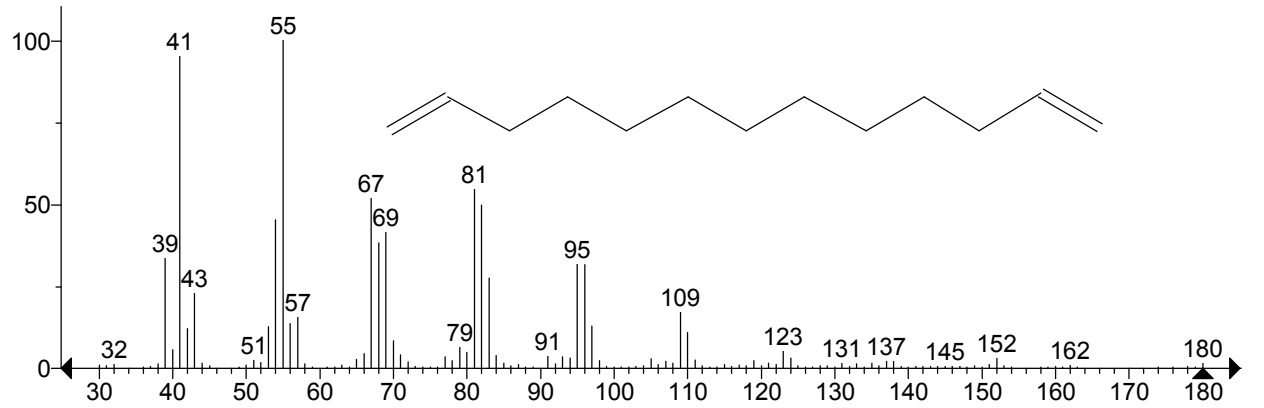
Hit 2 : 9-Octadecenal
C18H34O; MF: 803; RMF: 838; Prob 3.75%; CAS: 5090-41-5; Lib: mainlib; ID: 2481.



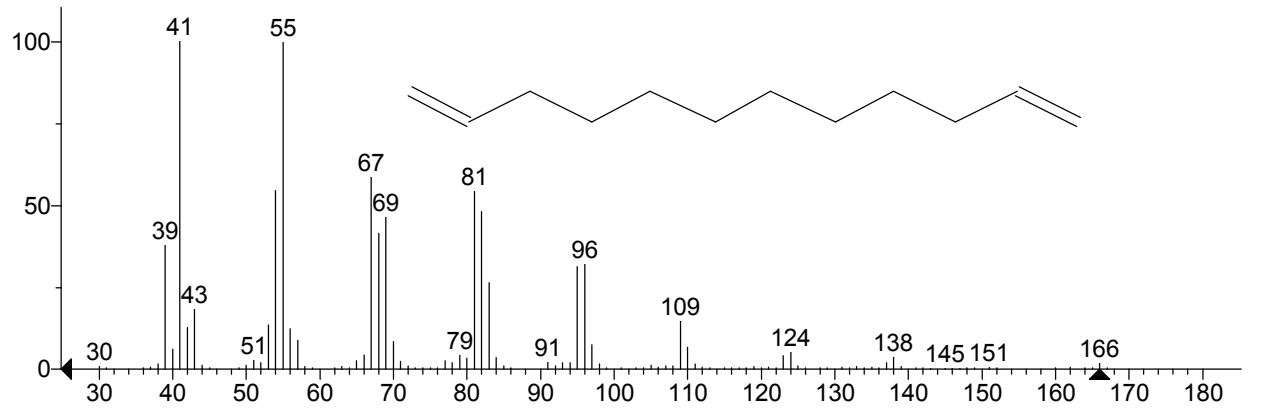
Unknown: Scan 365 (2.838 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -181



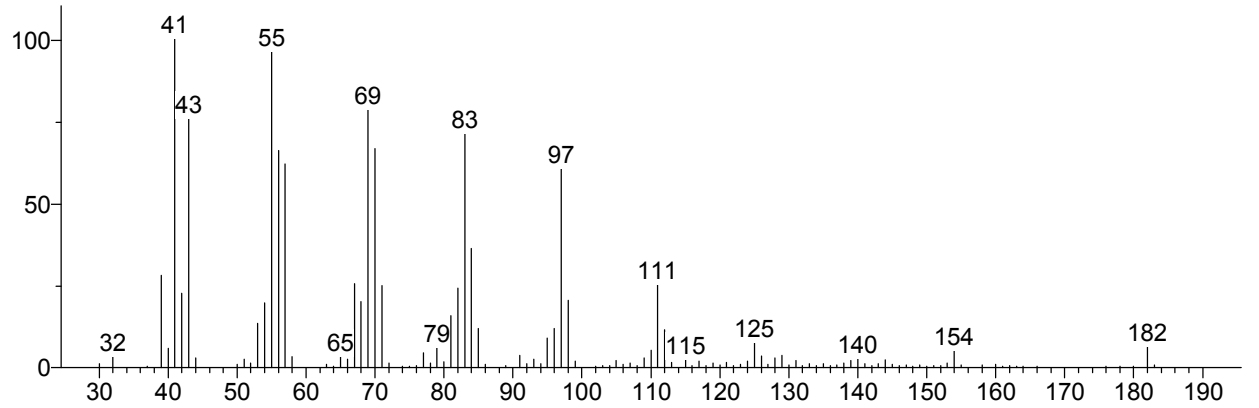
Hit 1 : 1,12-Tridecadiene
C13H24; MF: 854; RMF: 859; Prob 18.3%; CAS: 21964-48-7; Lib: mainlib; ID: 17578.



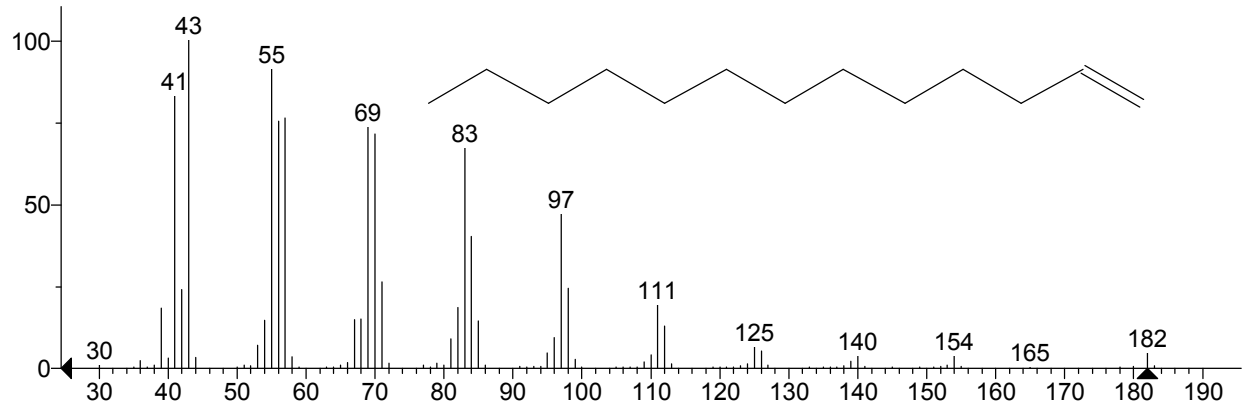
Hit 2 : 1,11-Dodecadiene
C12H22; MF: 806; RMF: 819; Prob 3.78%; CAS: 5876-87-9; Lib: mainlib; ID: 2567.



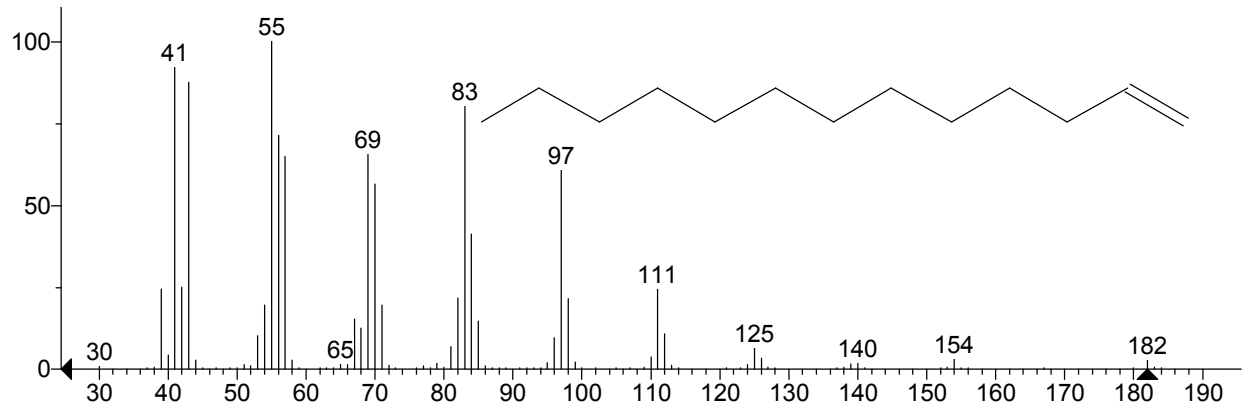
Unknown: Scan 445 (3.441 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -185



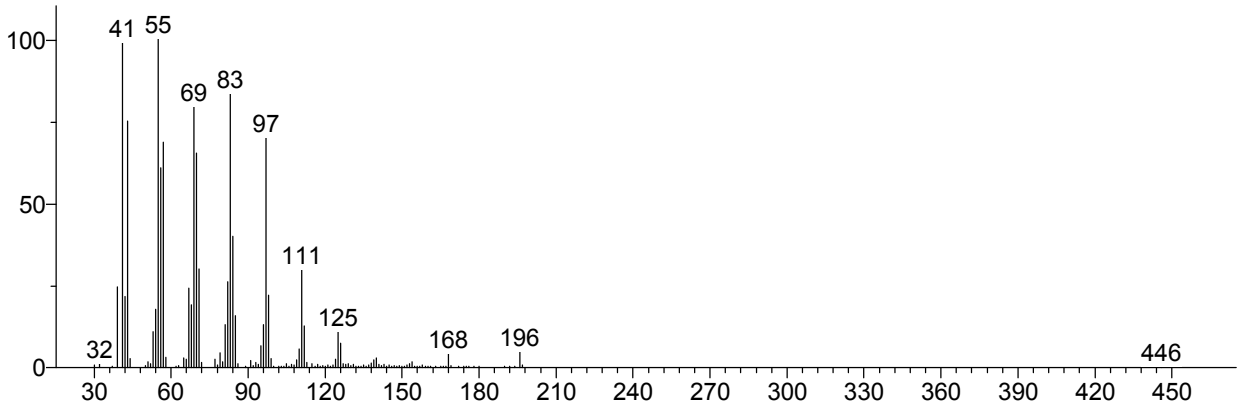
Hit 1 : 1-Tridecene
C13H26; MF: 884; RMF: 907; Prob 6.31%; CAS: 2437-56-1; Lib: mainlib; ID: 6680.



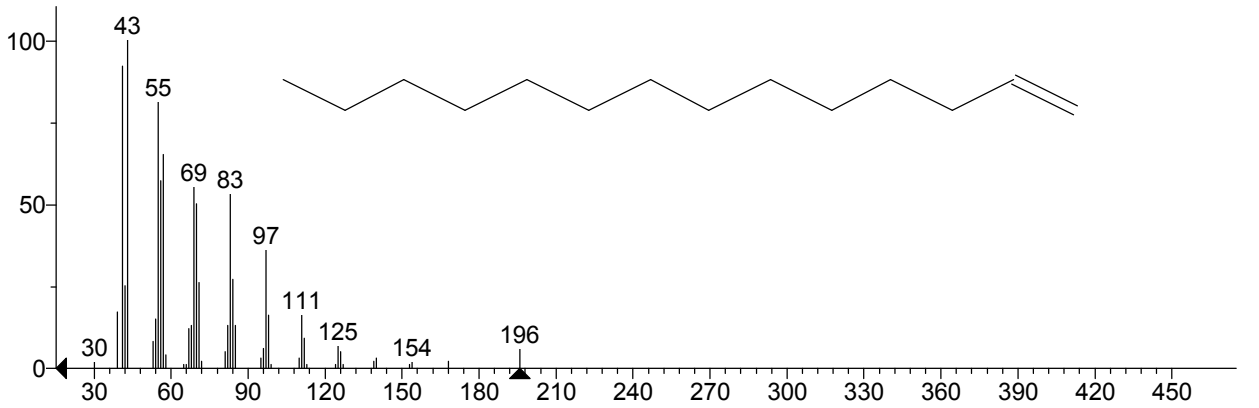
Hit 2 : 1-Tridecene
C13H26; MF: 879; RMF: 917; Prob 6.31%; CAS: 2437-56-1; Lib: replib; ID: 4180.



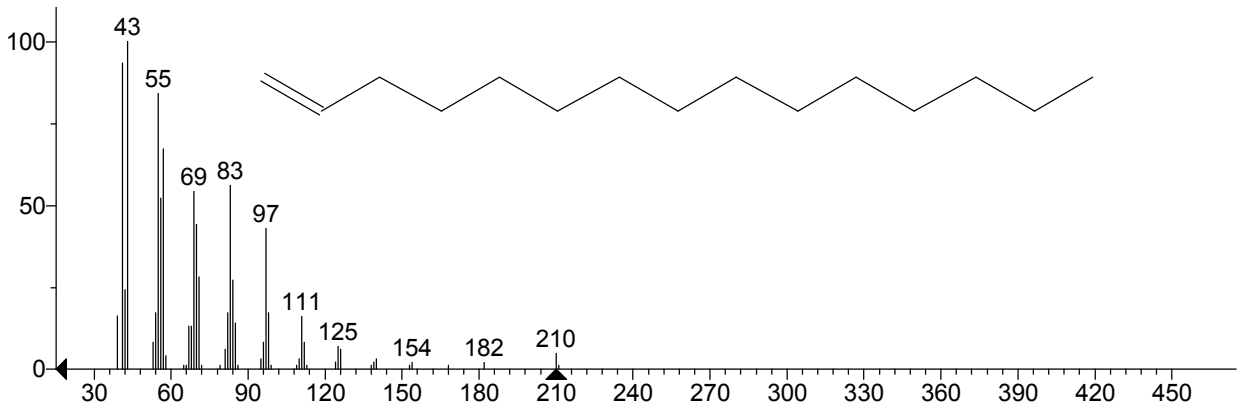
Unknown: Scan 522 (4.021 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -124



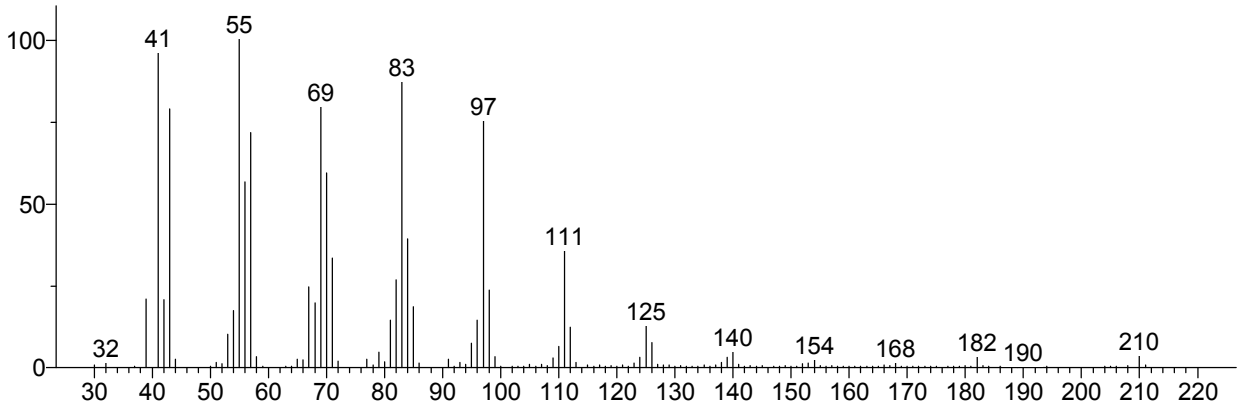
Hit 1 : 1-Tetradecene
C14H28; MF: 912; RMF: 948; Prob 7.01%; CAS: 1120-36-1; Lib: replib; ID: 1681.



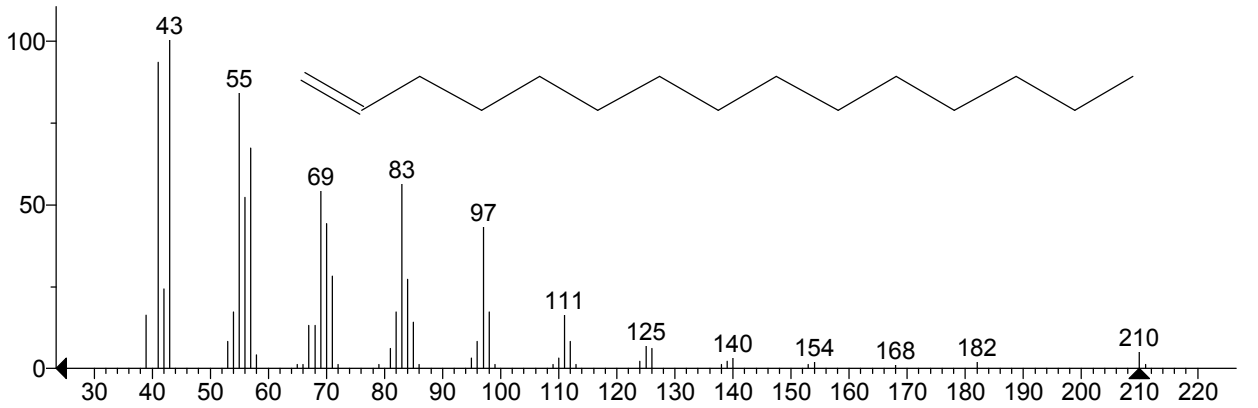
Hit 2 : 1-Pentadecene
C15H30; MF: 901; RMF: 936; Prob 4.81%; CAS: 13360-61-7; Lib: replib; ID: 1695.



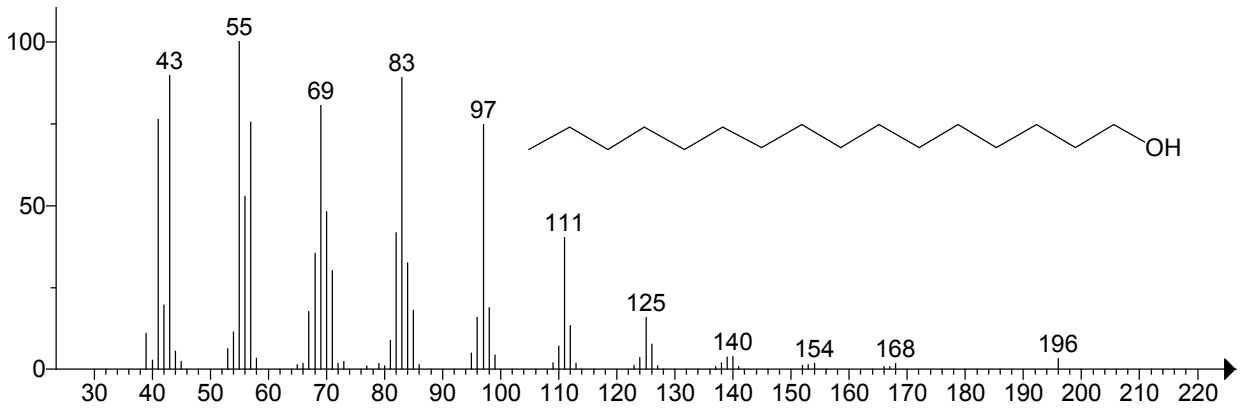
Unknown: Scan 598 (4.594 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -117



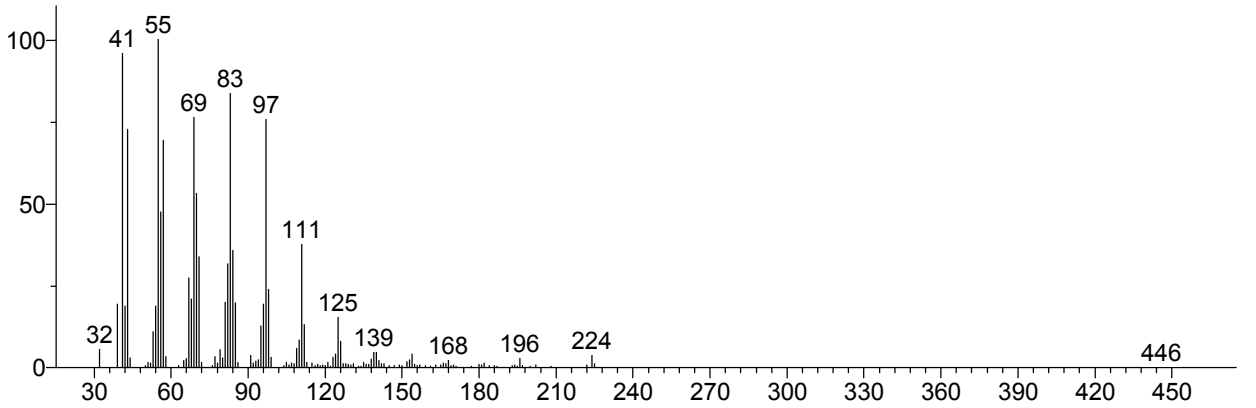
Hit 1 : 1-Pentadecene
C15H30; MF: 925; RMF: 953; Prob 11.4%; CAS: 13360-61-7; Lib: replib; ID: 1695.



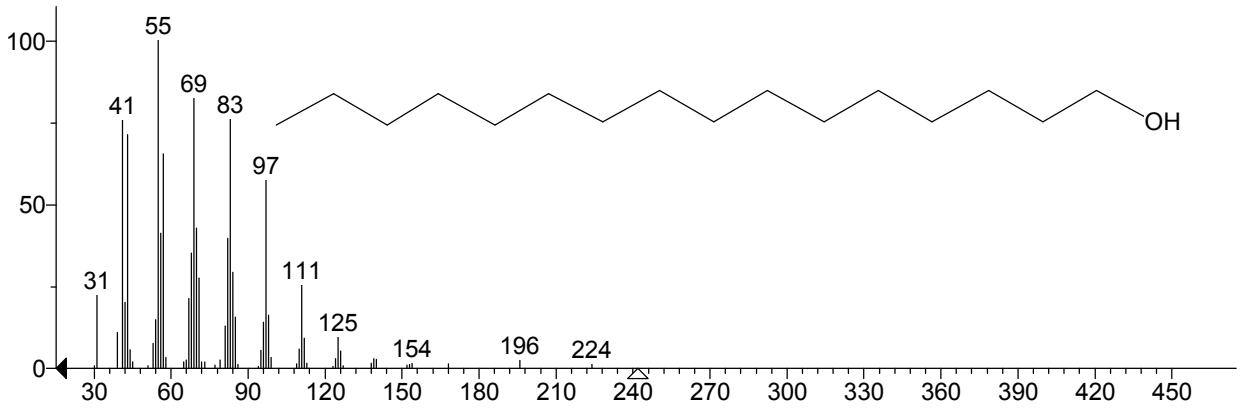
Hit 2 : 1-Hexadecanol
C16H34O; MF: 911; RMF: 939; Prob 7.14%; CAS: 36653-82-4; Lib: replib; ID: 4395.



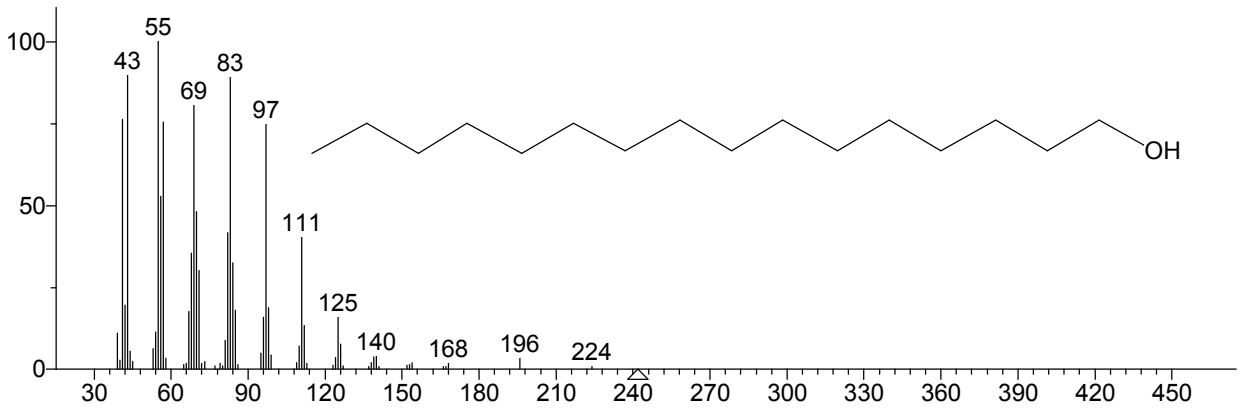
Unknown: Scan 673 (5.159 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -151



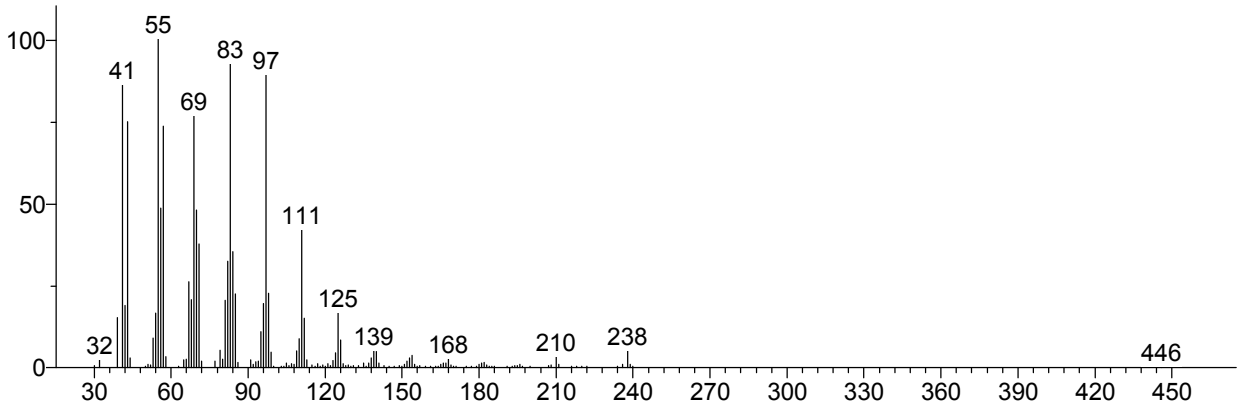
Hit 1 : 1-Hexadecanol
C16H34O; MF: 891; RMF: 937; Prob 7.99%; CAS: 36653-82-4; Lib: mainlib; ID: 18356.



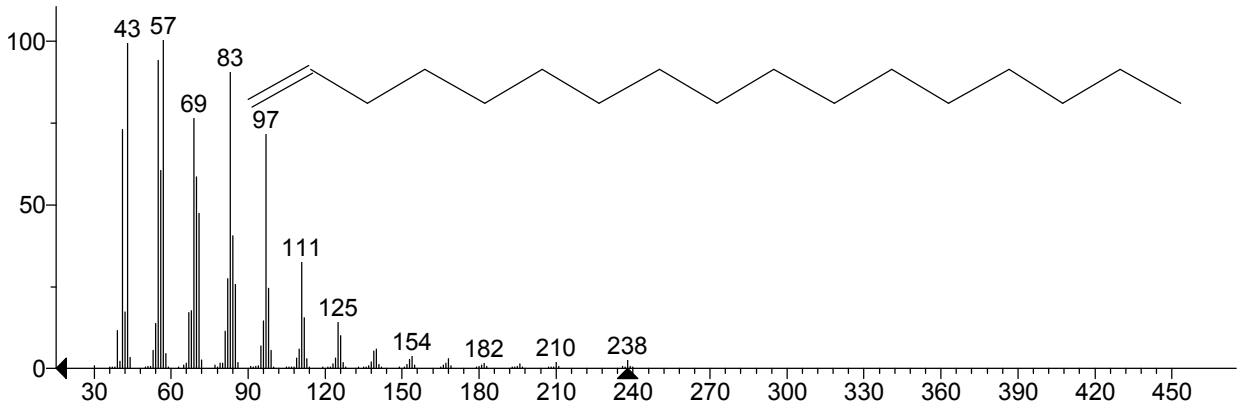
Hit 2 : 1-Hexadecanol
C16H34O; MF: 890; RMF: 931; Prob 7.99%; CAS: 36653-82-4; Lib: replib; ID: 4395.



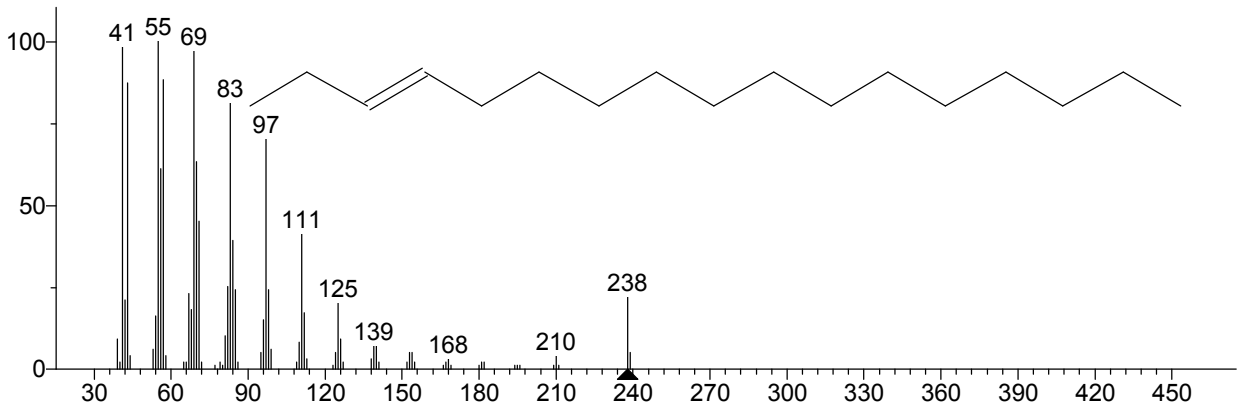
Unknown: Scan 743 (5.686 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -184



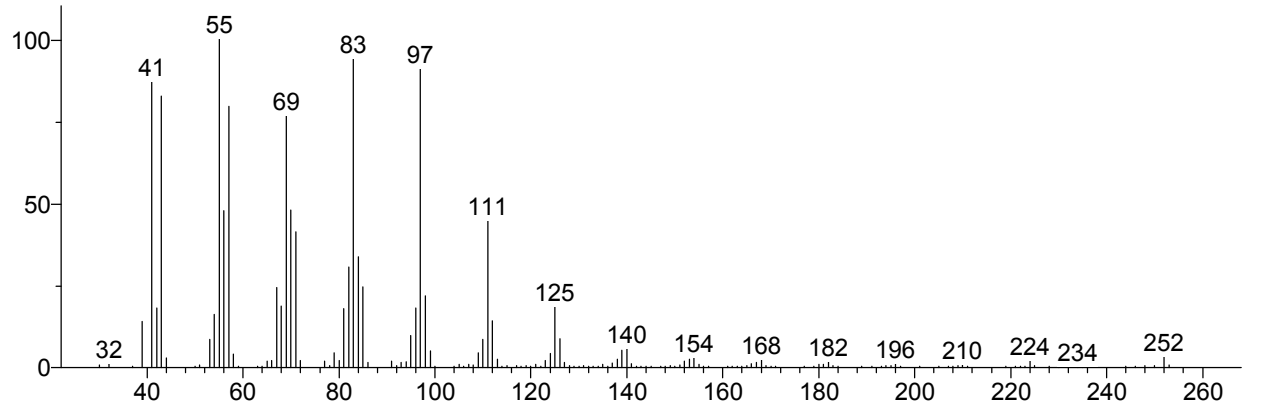
Hit 1 : 1-Heptadecene
C17H34; MF: 902; RMF: 910; Prob 5.85%; CAS: 6765-39-5; Lib: replib; ID: 5445.



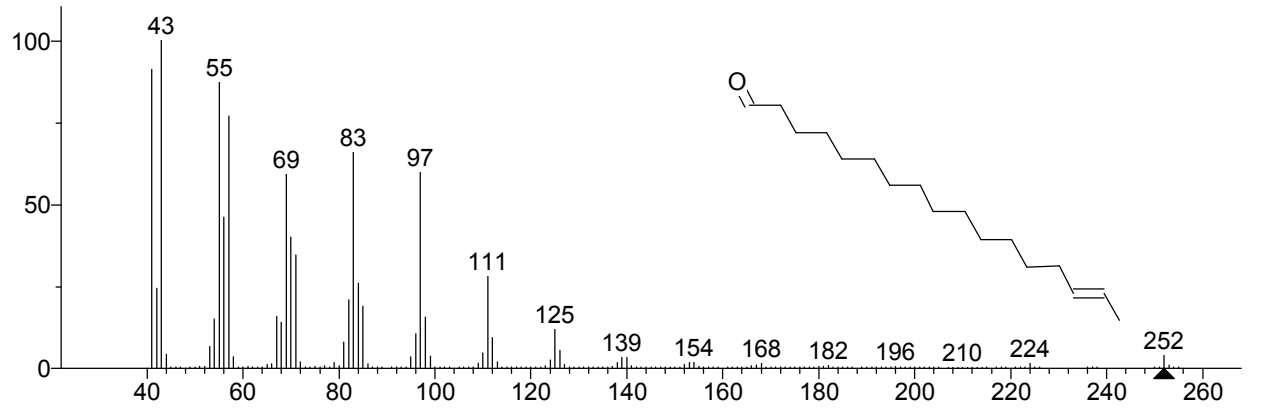
Hit 2 : 3-Heptadecene, (Z)-
C17H34; MF: 901; RMF: 925; Prob 5.63%; Lib: mainlib; ID: 17426.



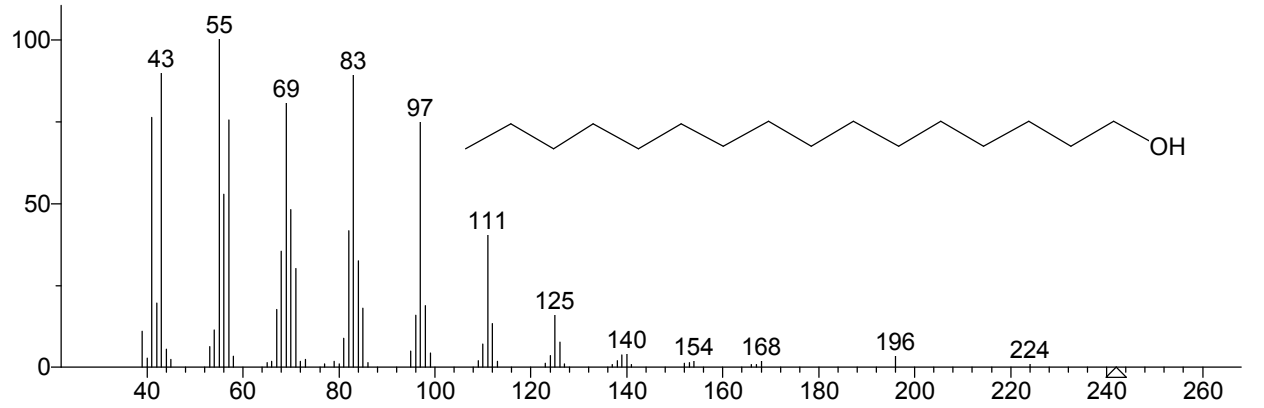
Unknown: Scan 810 (6.191 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -117



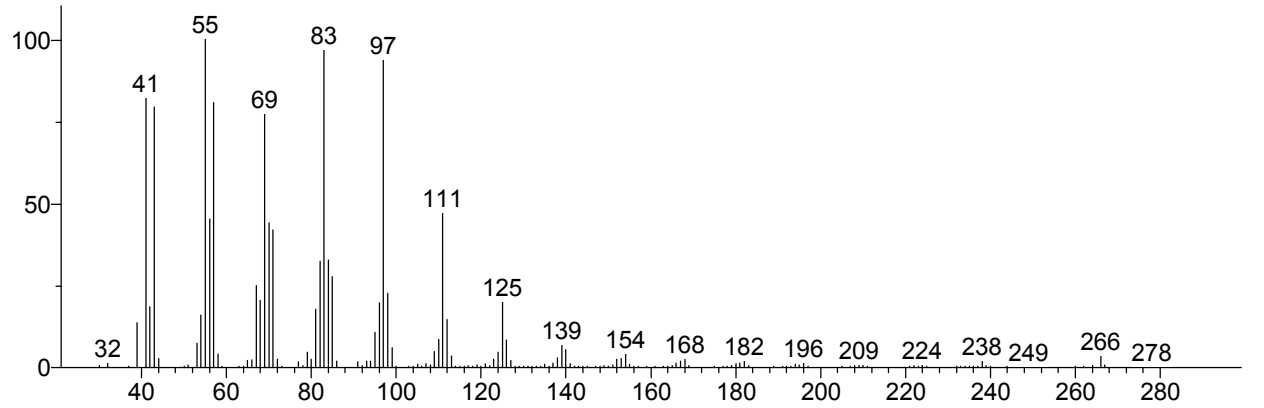
Hit 1 : E-15-Heptadecenal
C17H32O; MF: 925; RMF: 931; Prob 8.58%; Lib: mainlib; ID: 5518.



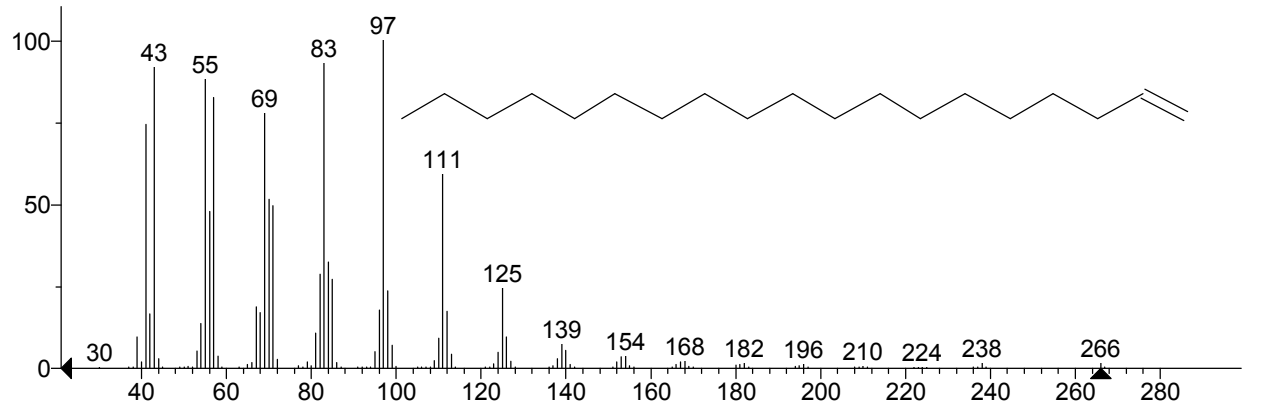
Hit 2 : 1-Hexadecanol
C16H34O; MF: 909; RMF: 940; Prob 4.94%; CAS: 36653-82-4; Lib: replib; ID: 4395.



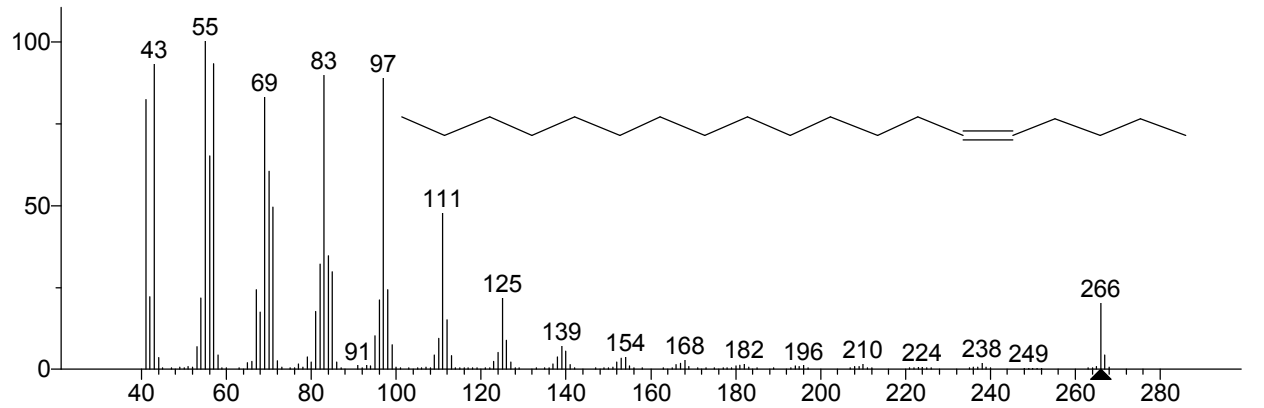
Unknown: Scan 875 (6.681 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -117



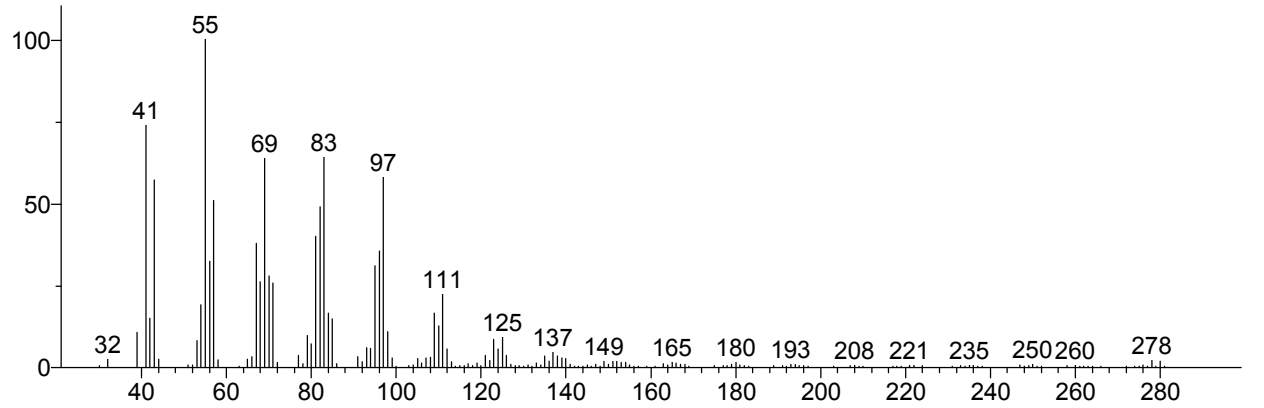
Hit 1 : 1-Nonadecene
C19H38; MF: 924; RMF: 934; Prob 8.78%; CAS: 18435-45-5; Lib: replib; ID: 12742.



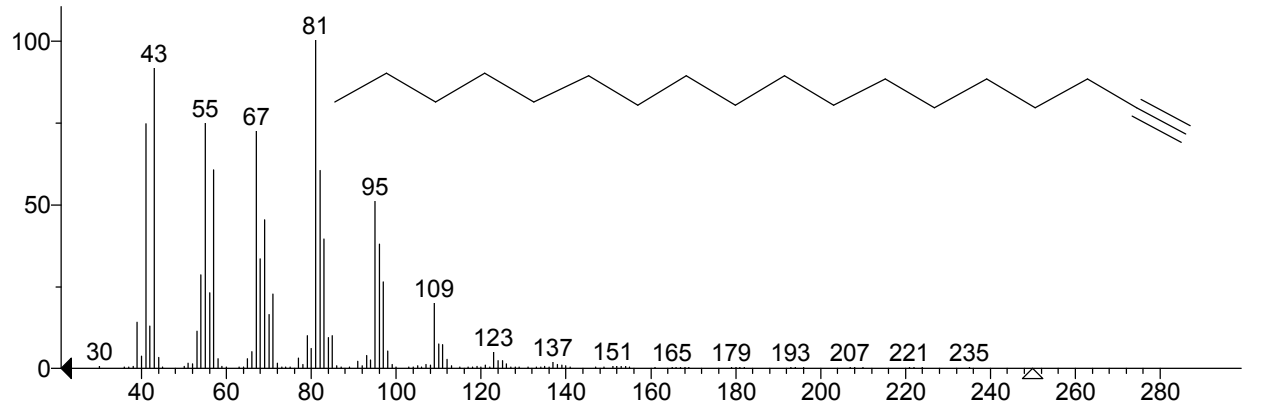
Hit 2 : Z-5-Nonadecene
C19H38; MF: 916; RMF: 919; Prob 6.55%; Lib: mainlib; ID: 17837.



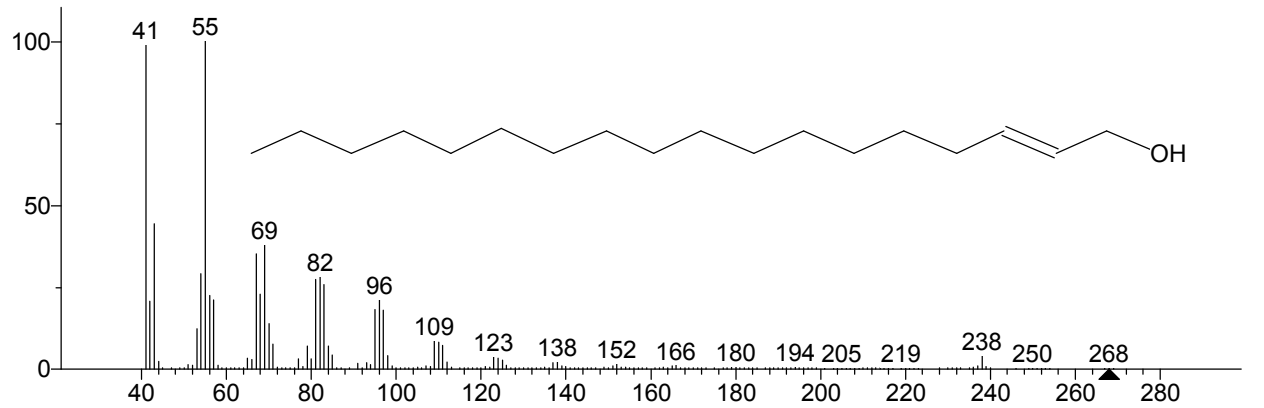
Unknown: Scan 935 (7.133 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -331



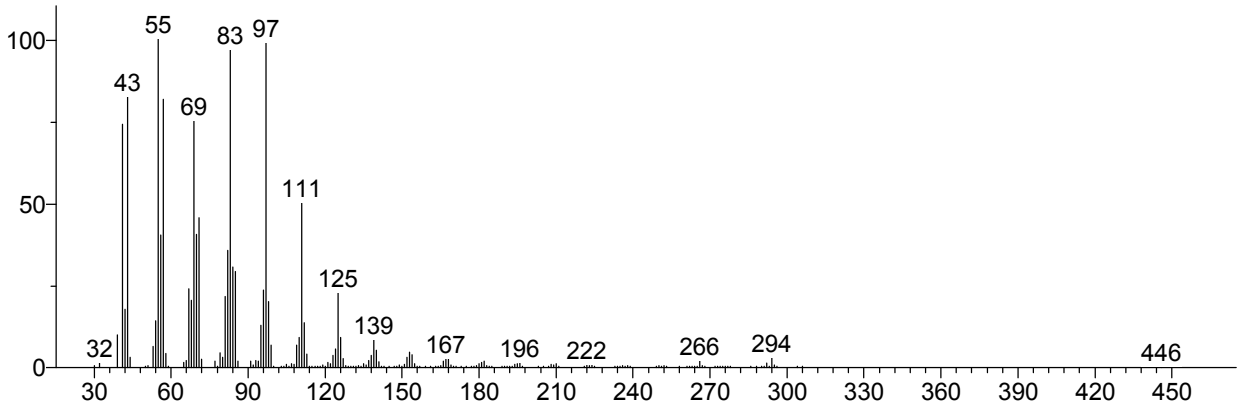
Hit 1 : 1-Octadecyne
C18H34; MF: 846; RMF: 876; Prob 8.53%; CAS: 629-89-0; Lib: replib; ID: 9902.



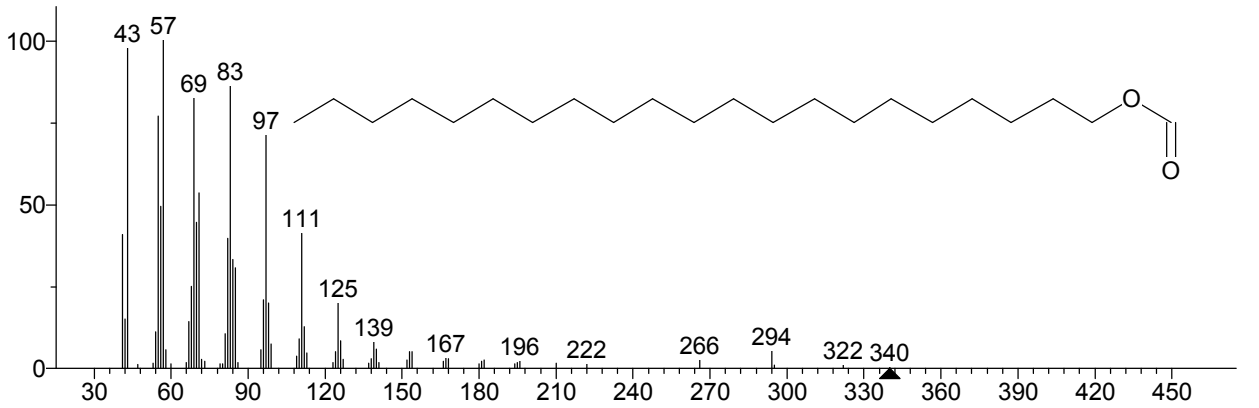
Hit 2 : E-2-Octadecadecen-1-ol
C18H36O; MF: 828; RMF: 849; Prob 4.39%; Lib: mainlib; ID: 17230.



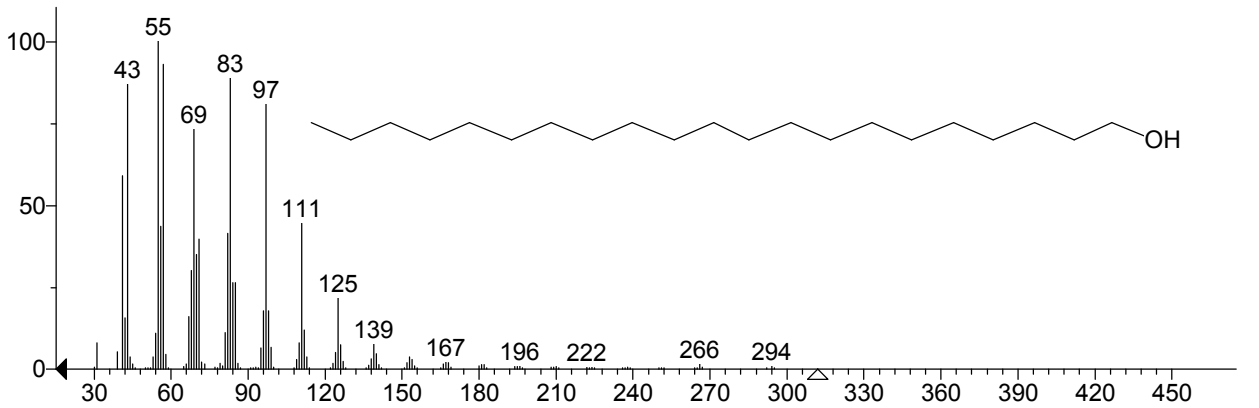
Unknown: Scan 996 (7.593 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -170



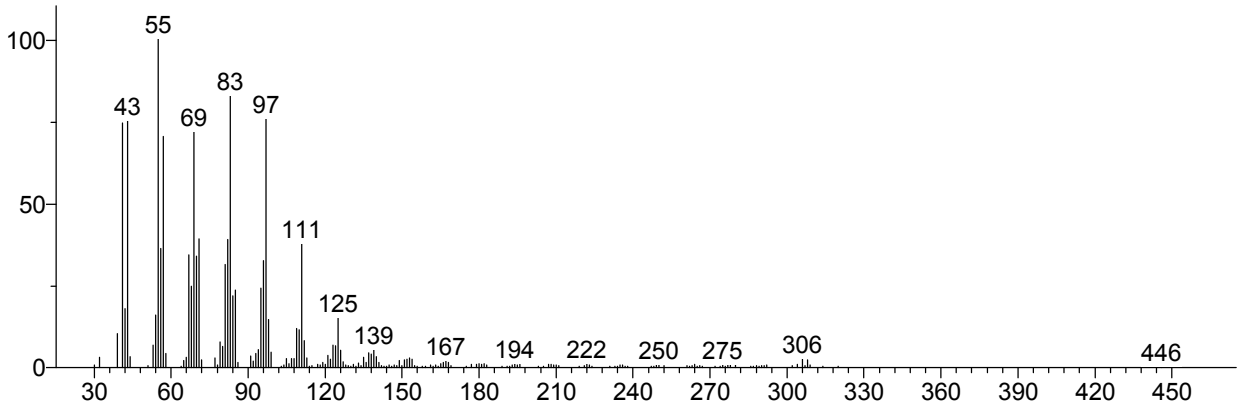
Hit 1 : 1-Heneicosyl formate
C22H44O2; MF: 911; RMF: 943; Prob 7.67%; CAS: 77899-03-7; Lib: mainlib; ID: 22067.



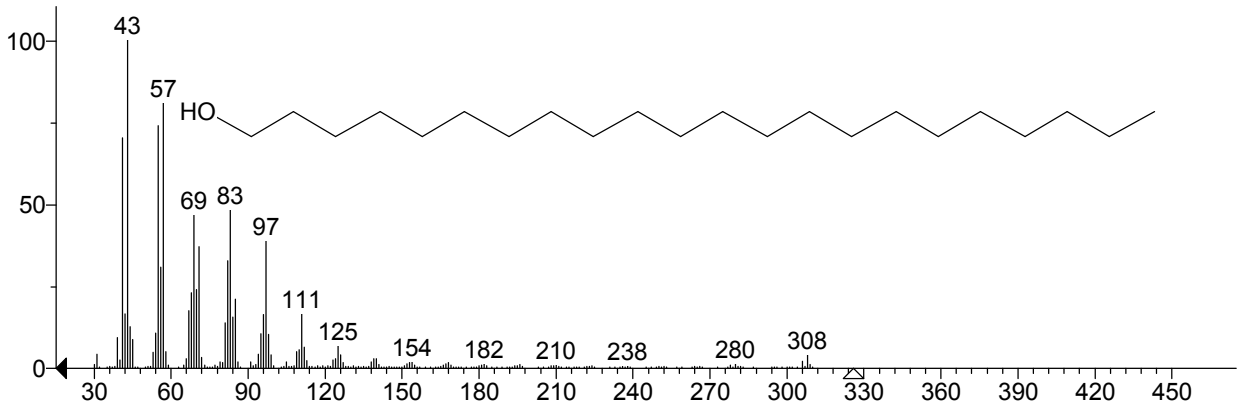
Hit 2 : 1-Heneicosanol
C21H44O; MF: 909; RMF: 920; Prob 7.07%; CAS: 15594-90-8; Lib: mainlib; ID: 18102.



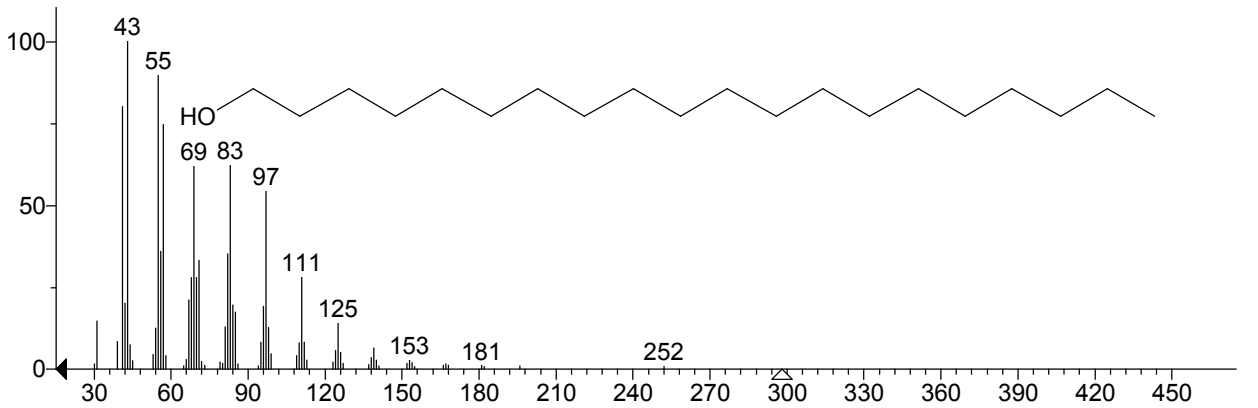
Unknown: Scan 1051 (8.007 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -258



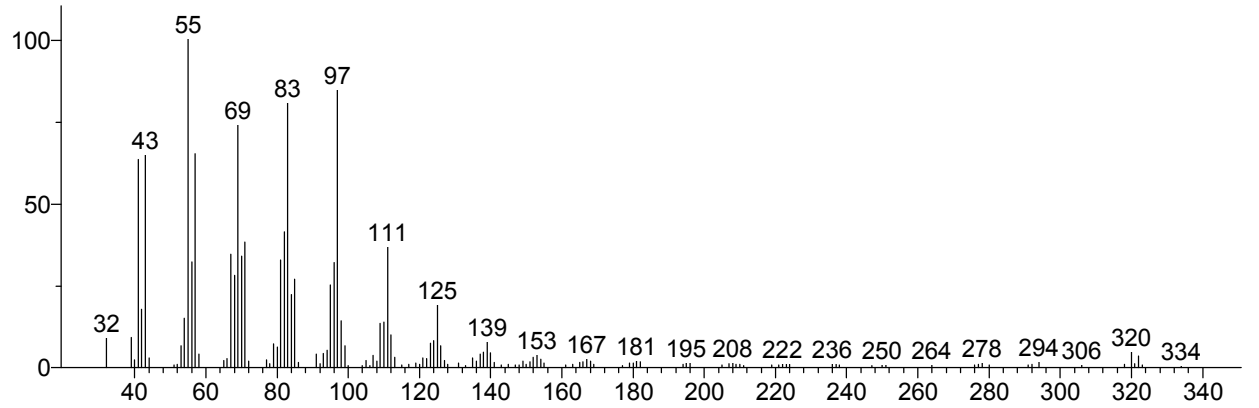
Hit 1 : Behenic alcohol
C22H46O; MF: 856; RMF: 865; Prob 12.6%; CAS: 661-19-8; Lib: replib; ID: 2104.



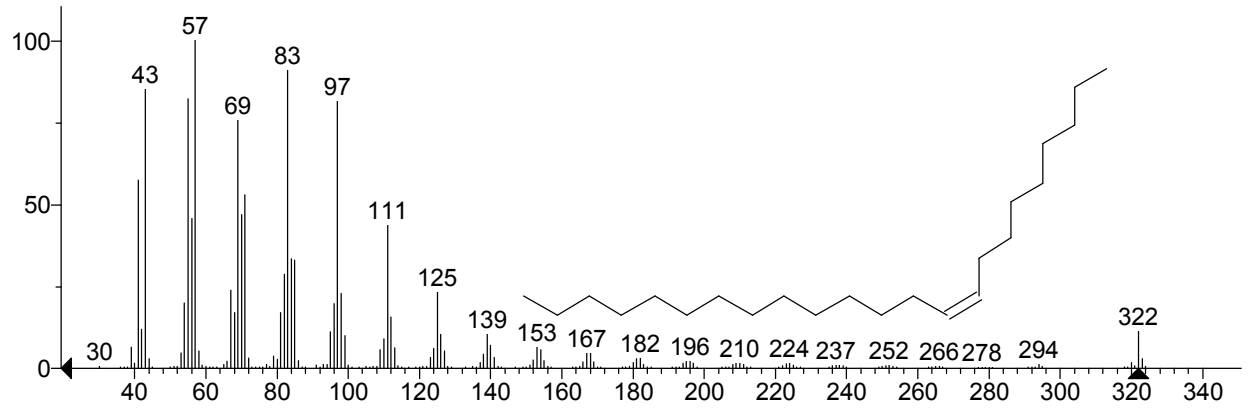
Hit 2 : 1-Eicosanol
C20H42O; MF: 835; RMF: 917; Prob 5.37%; CAS: 629-96-9; Lib: replib; ID: 1938.



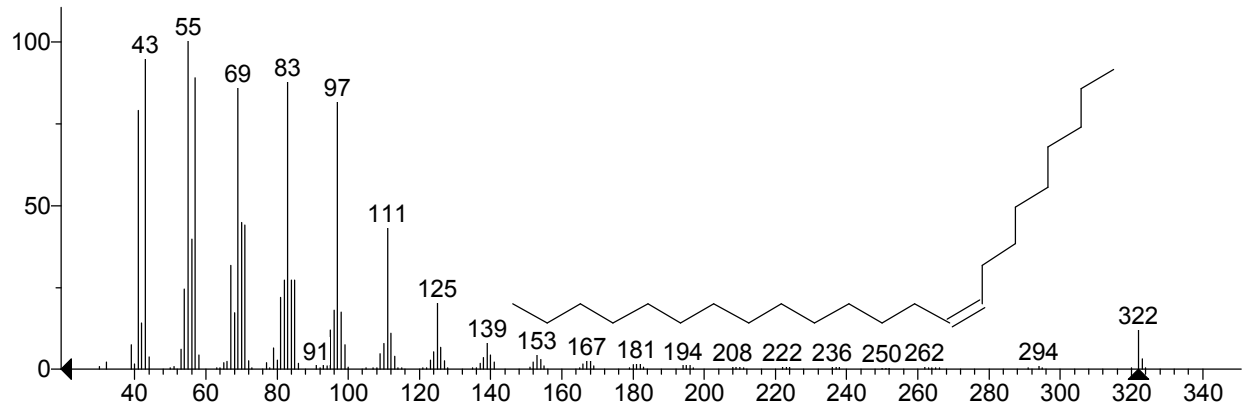
Unknown: Scan 1109 (8.444 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -283



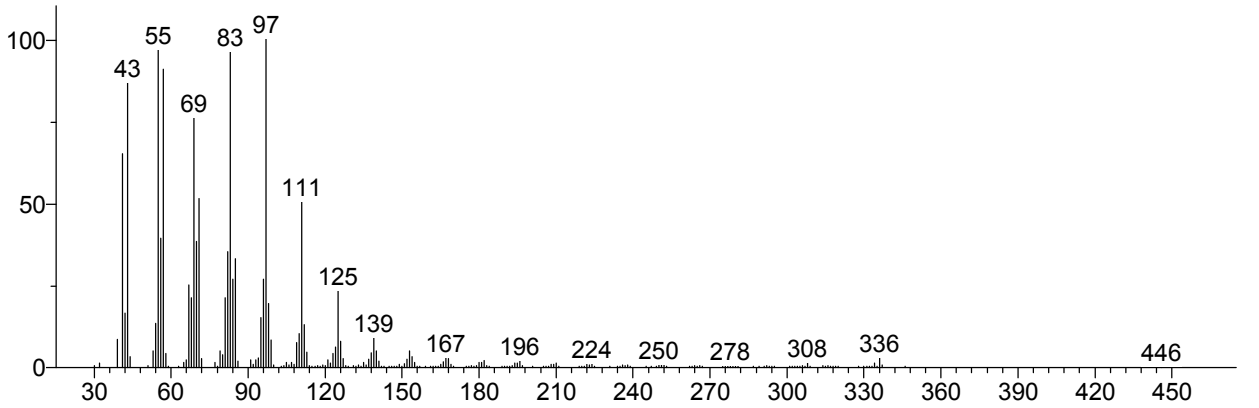
Hit 1 : 9-Tricosene, (Z)-
C23H46; MF: 853; RMF: 861; Prob 8.24%; CAS: 27519-02-4; Lib: replib; ID: 5831.



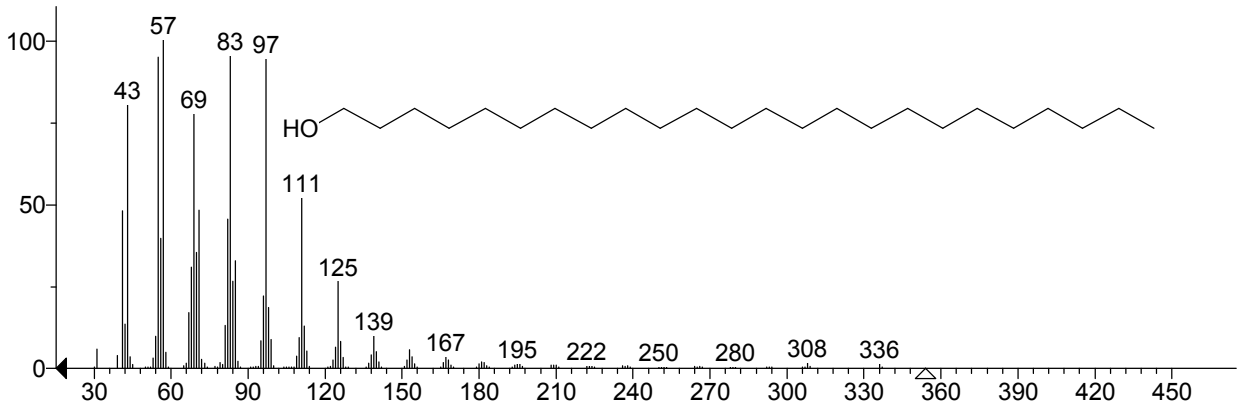
Hit 2 : 9-Tricosene, (Z)-
C23H46; MF: 850; RMF: 874; Prob 8.24%; CAS: 27519-02-4; Lib: replib; ID: 4381.



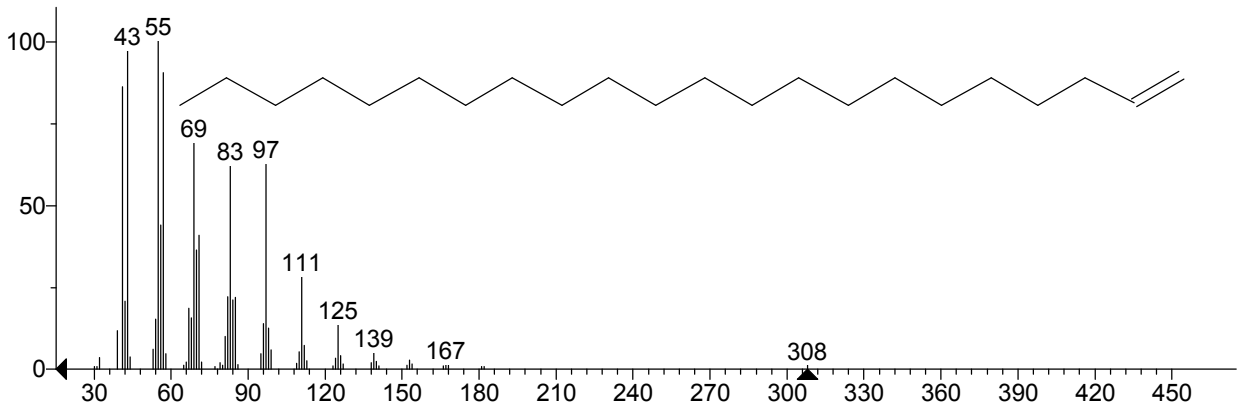
Unknown: Scan 1159 (8.821 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -253



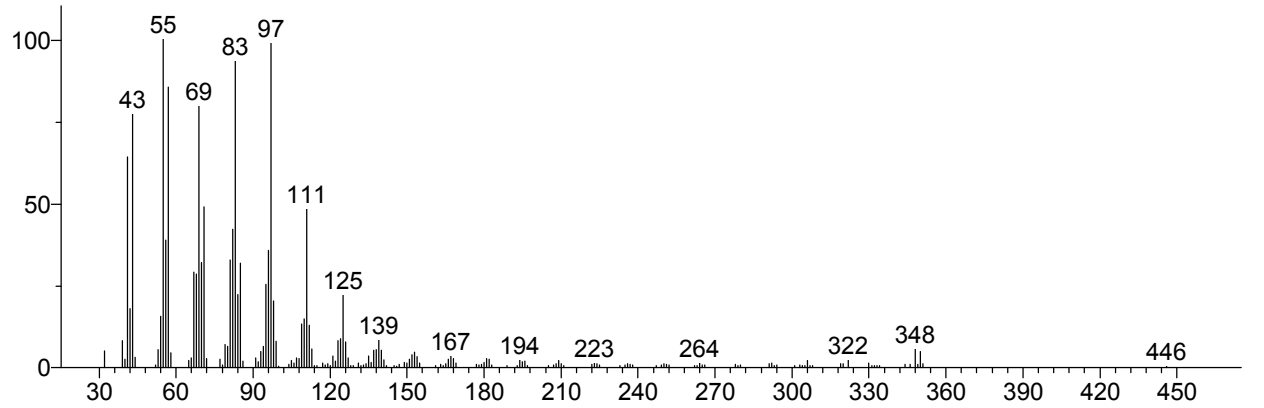
Hit 1 : n-Tetracosanol-1
C24H50O; MF: 889; RMF: 904; Prob 6.15%; CAS: 506-51-4; Lib: mainlib; ID: 23058.



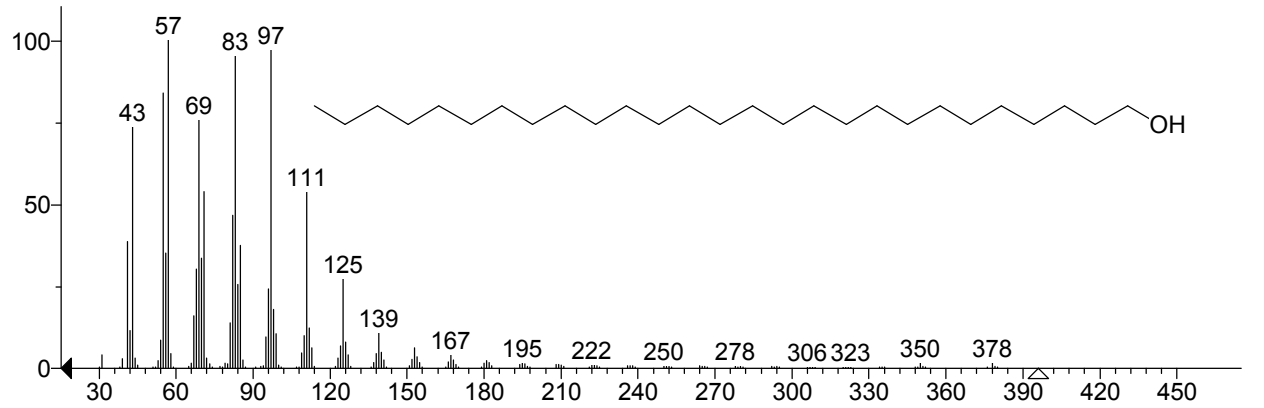
Hit 2 : 1-Docosene
C22H44; MF: 885; RMF: 945; Prob 5.19%; CAS: 1599-67-3; Lib: replib; ID: 4382.



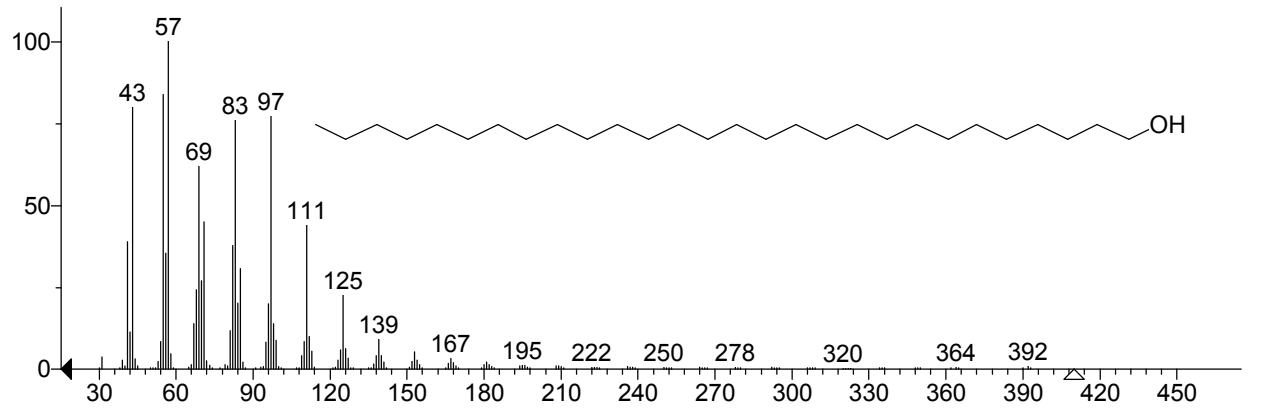
Unknown: Scan 1211 (9.213 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -331



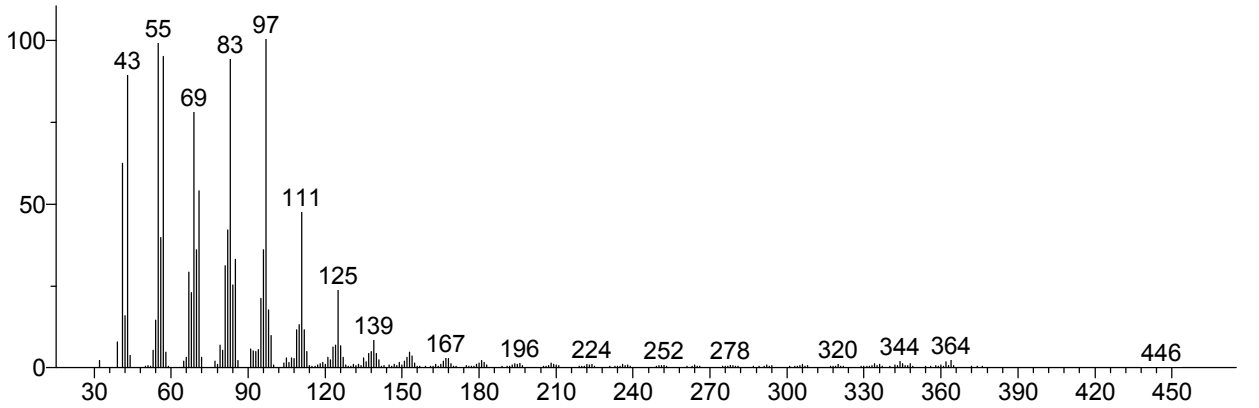
Hit 1 : 1-Heptacosanol
C27H56O; MF: 846; RMF: 879; Prob 8.65%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



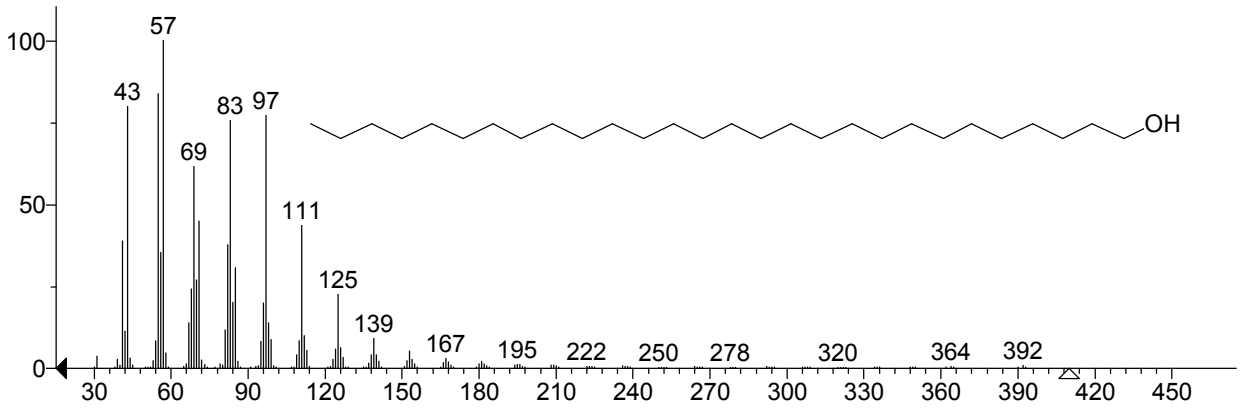
Hit 2 : 1-Octacosanol
C28H58O; MF: 829; RMF: 859; Prob 4.72%; Lib: mainlib; ID: 22288.



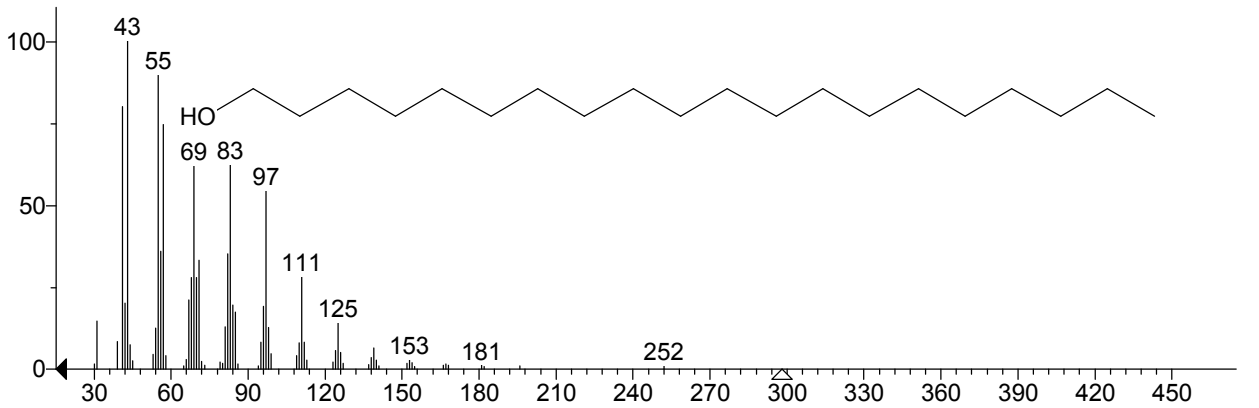
Unknown: Scan 1257 (9.560 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -454



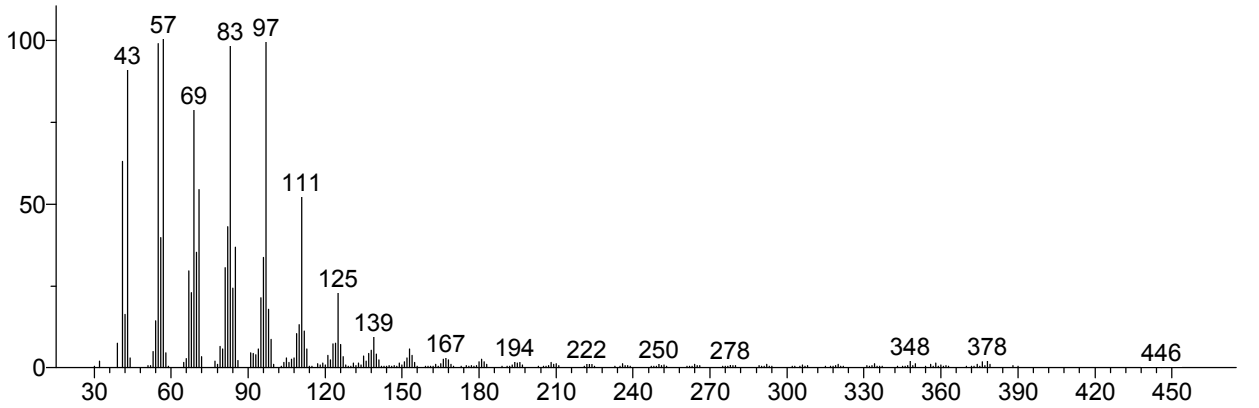
Hit 1 : 1-Octacosanol
C28H58O; MF: 845; RMF: 882; Prob 5.06%; Lib: mainlib; ID: 22288.



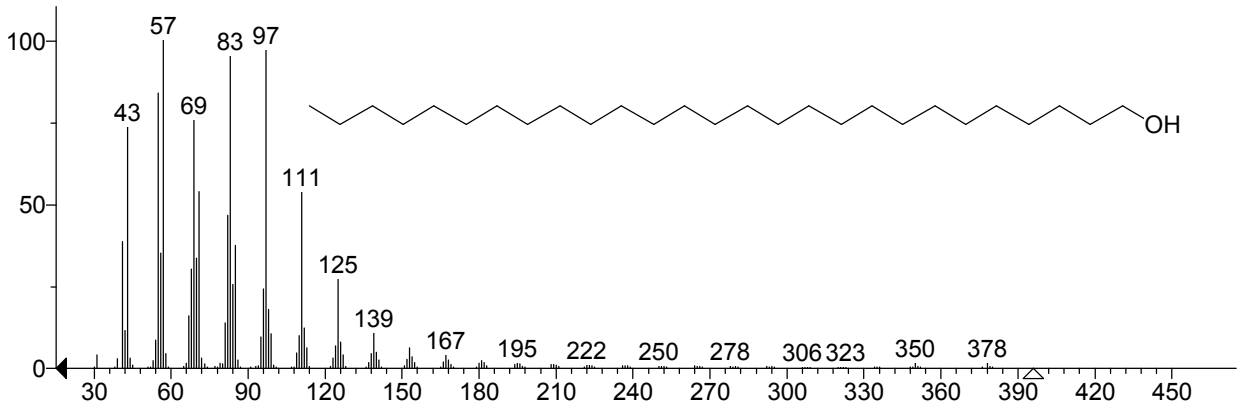
Hit 2 : 1-Eicosanol
C20H42O; MF: 836; RMF: 929; Prob 3.68%; CAS: 629-96-9; Lib: replib; ID: 1938.



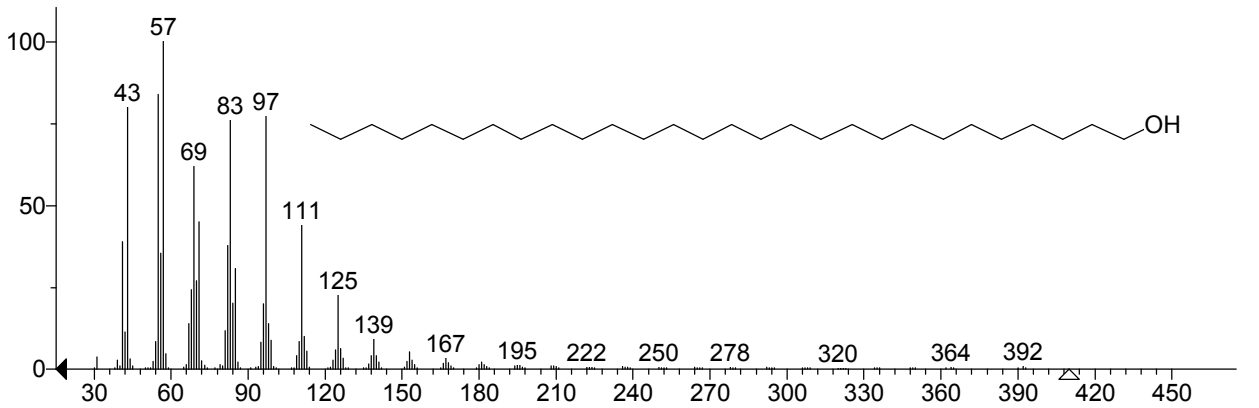
Unknown: Scan 1304 (9.914 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -283



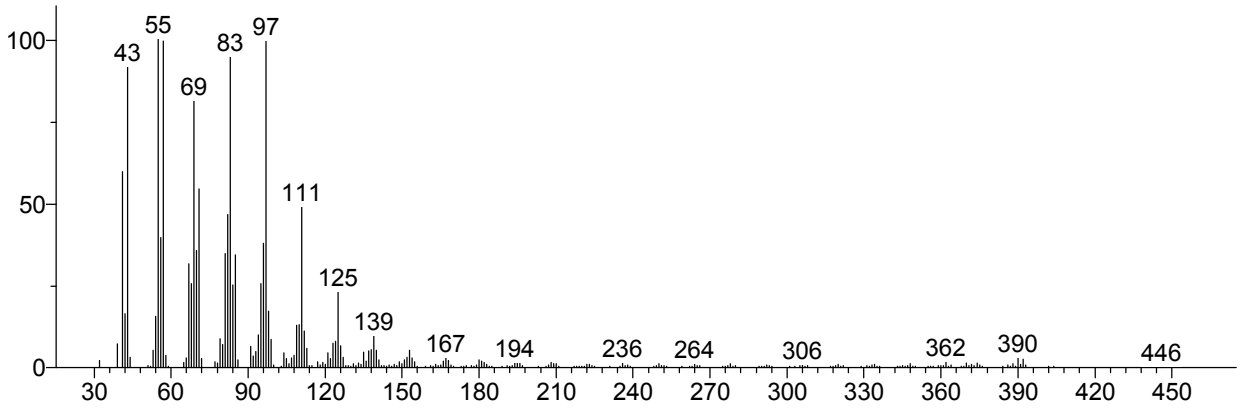
Hit 1 : 1-Heptacosanol
C27H56O; MF: 854; RMF: 894; Prob 6.78%; CAS: 2004-39-9; Lib: mainlib; ID: 23358.



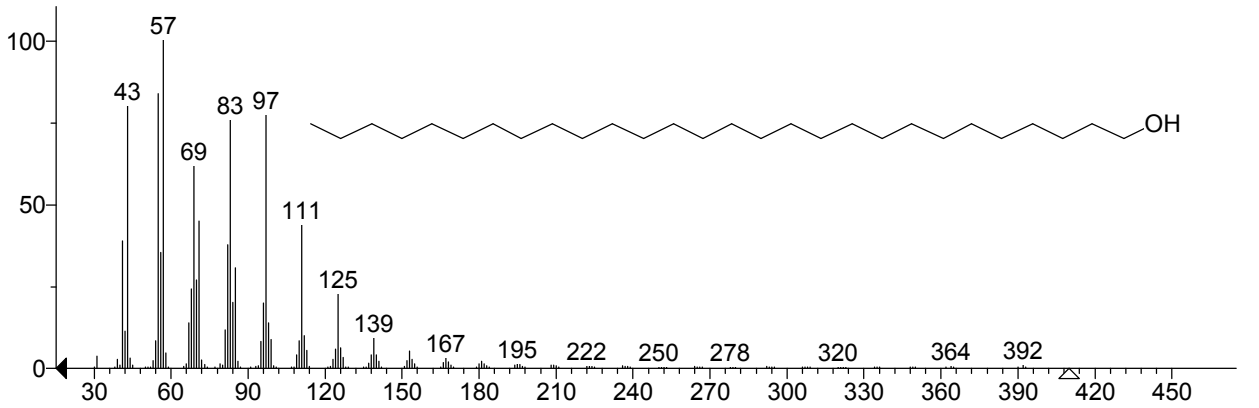
Hit 2 : 1-Octacosanol
C28H58O; MF: 843; RMF: 886; Prob 4.65%; Lib: mainlib; ID: 22288.



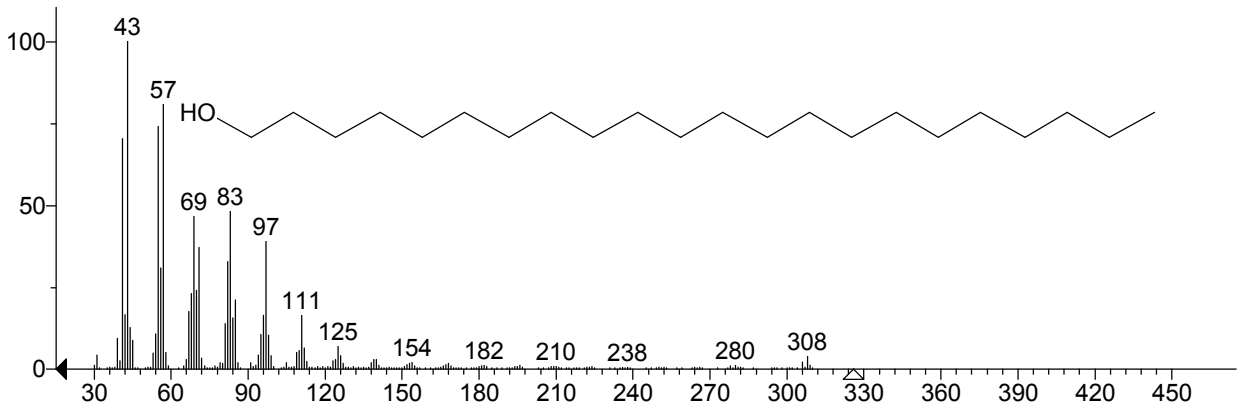
Unknown: Scan 1349 (10.253 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -503



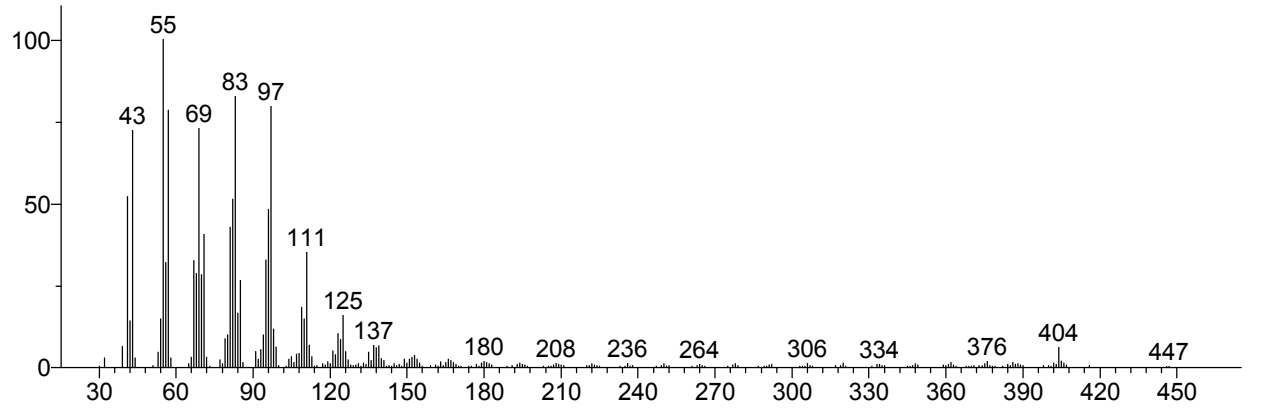
Hit 1 : 1-Octacosanol
C28H58O; MF: 826; RMF: 873; Prob 6.41%; Lib: mainlib; ID: 22288.



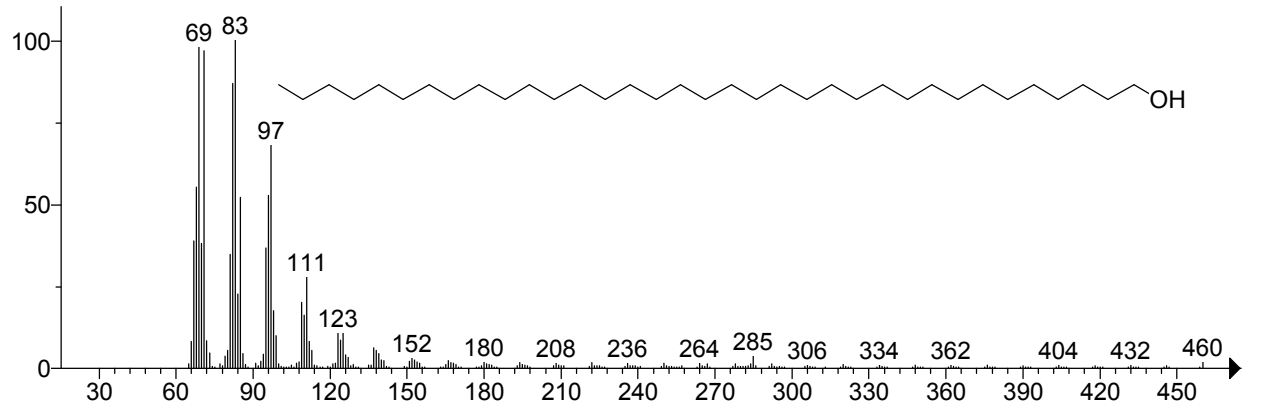
Hit 2 : Behenic alcohol
C22H46O; MF: 817; RMF: 861; Prob 4.65%; CAS: 661-19-8; Lib: replib; ID: 2104.



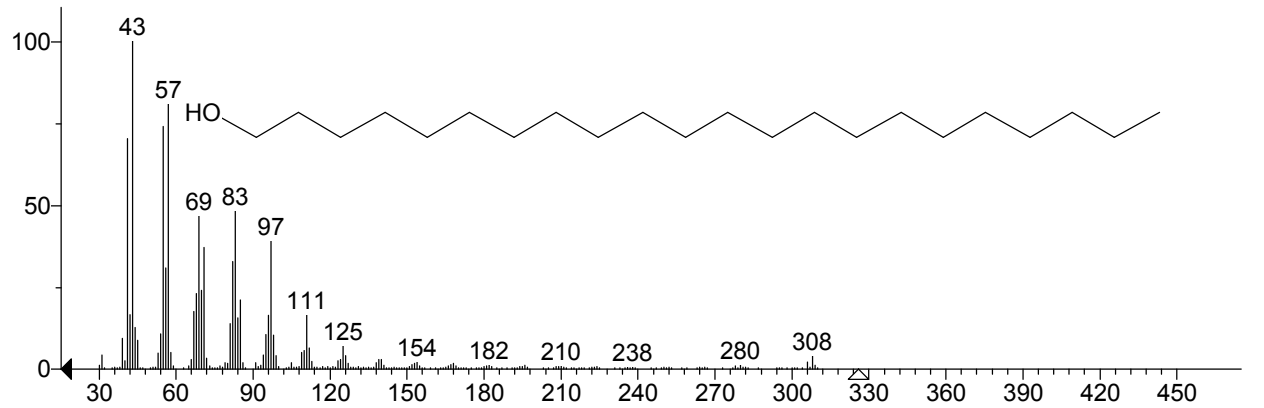
Unknown: Scan 1392 (10.577 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -520



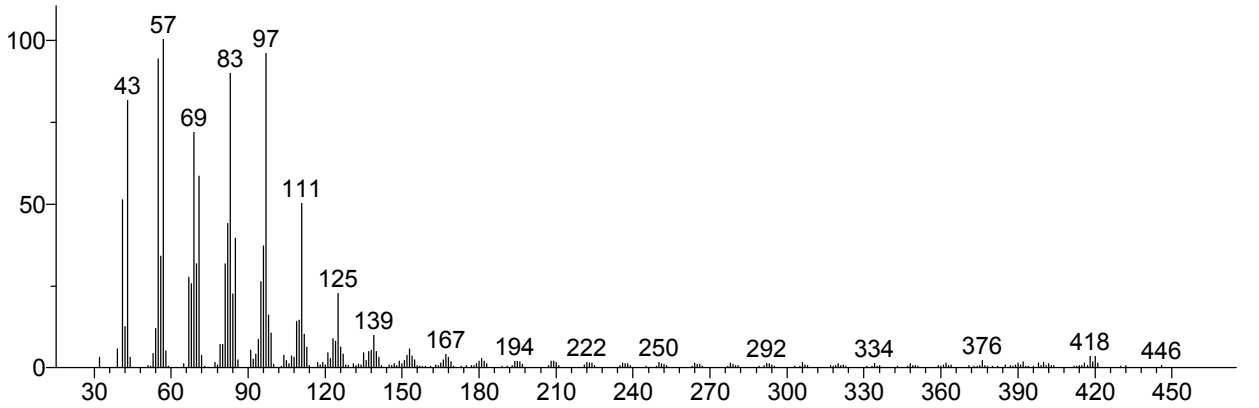
Hit 1 : 1-Pentatriacontanol
C35H72O; MF: 786; RMF: 816; Prob 6.61%; CAS: 55517-90-3; Lib: mainlib; ID: 44985.



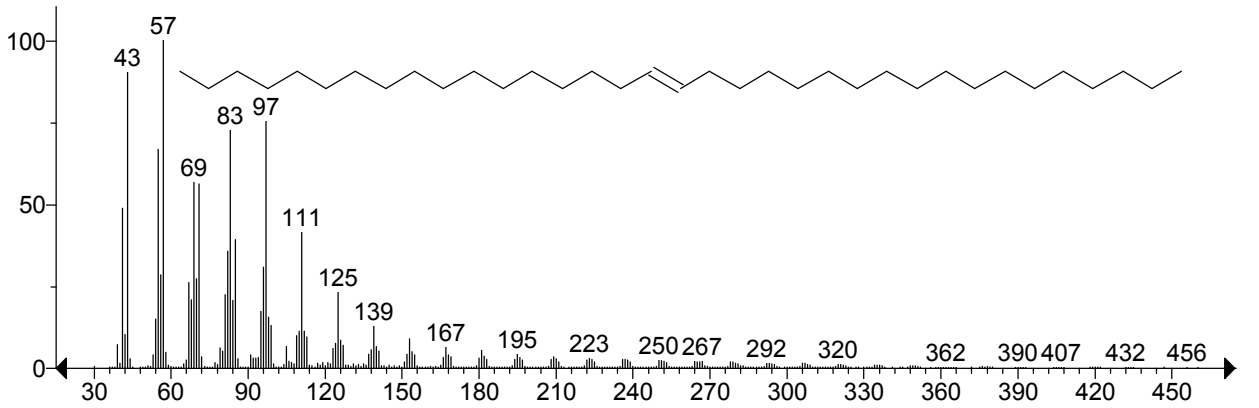
Hit 2 : Behenic alcohol
C22H46O; MF: 776; RMF: 838; Prob 4.67%; CAS: 661-19-8; Lib: replib; ID: 2104.



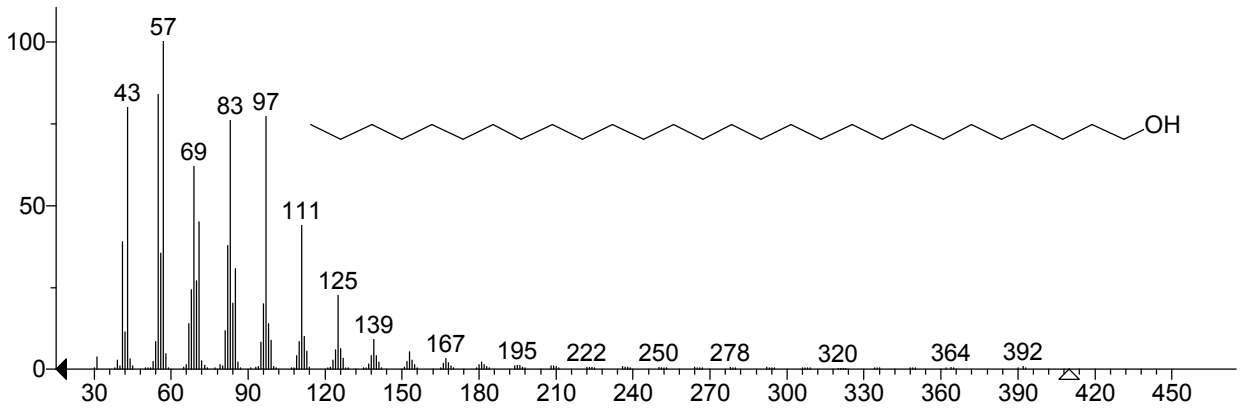
Unknown: Scan 1437 (10.916 min): J9163_Jordi_Outside_Infusion_Bag_A_py2.D\data.ms
Compound in Library Factor = -359



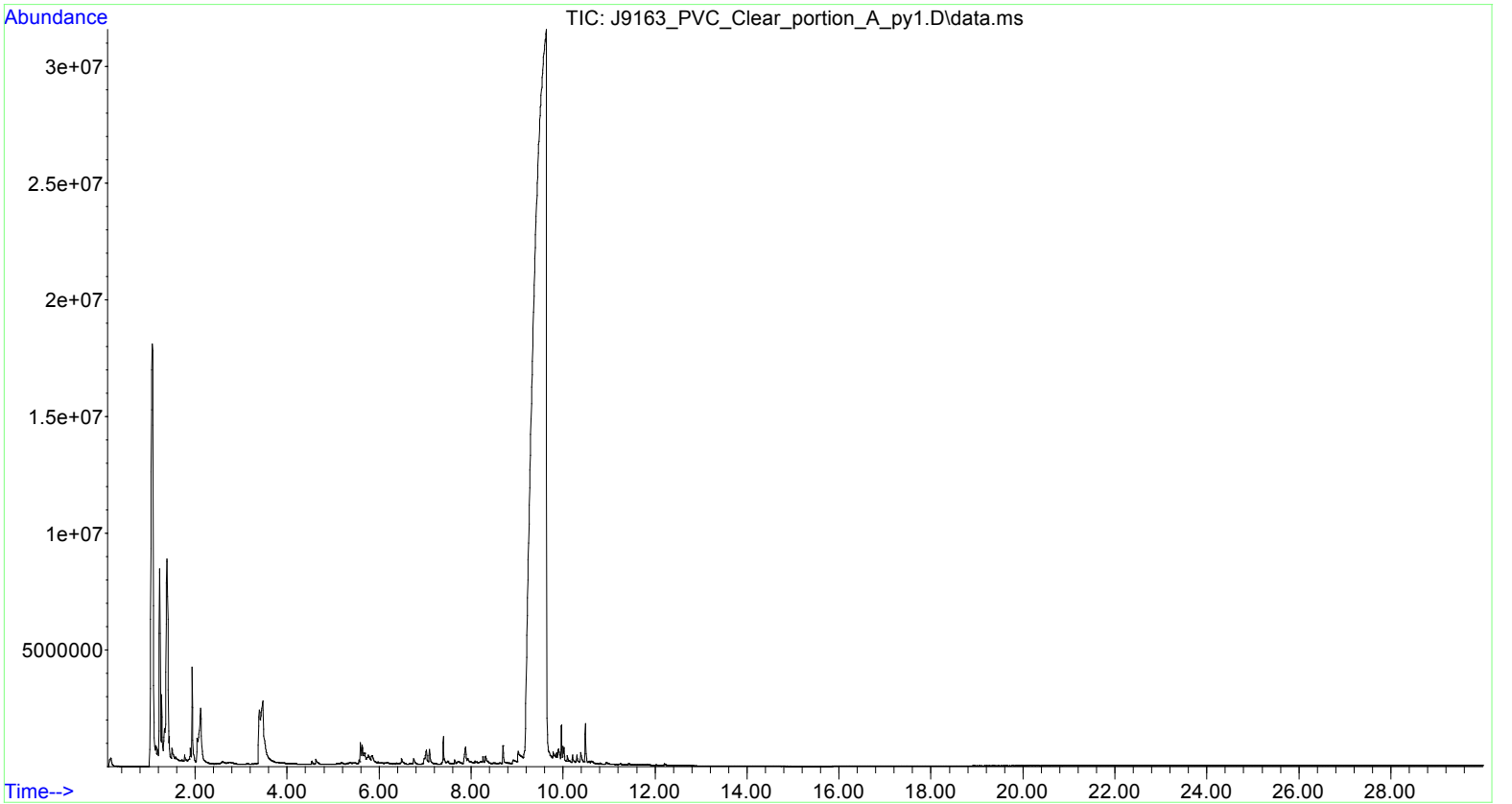
Hit 1 : 17-Pentatriacontene
C35H70; MF: 833; RMF: 852; Prob 7.71%; CAS: 6971-40-0; Lib: mainlib; ID: 22111.



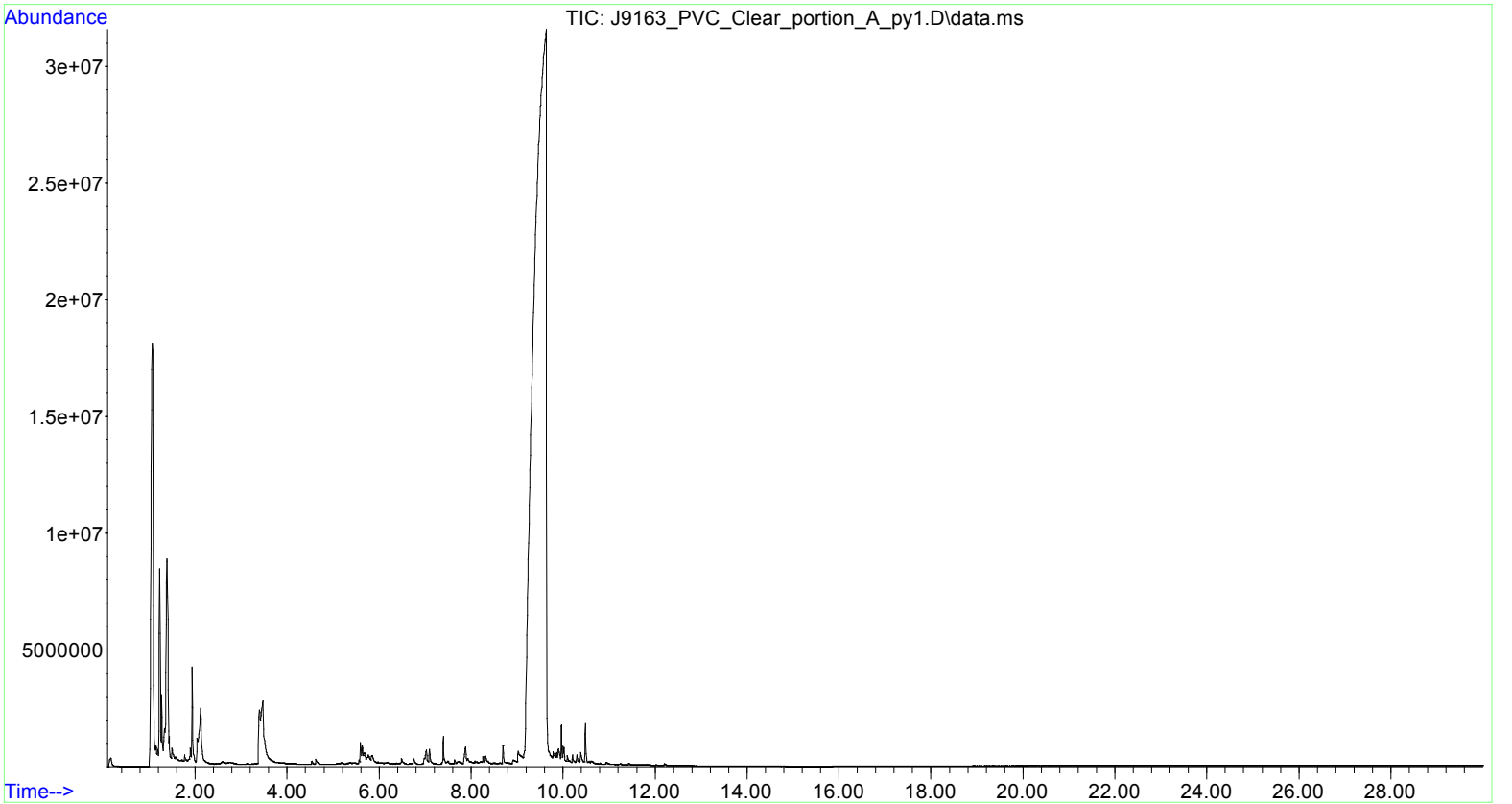
Hit 2 : 1-Octacosanol
C28H58O; MF: 817; RMF: 886; Prob 4.44%; Lib: mainlib; ID: 22288.



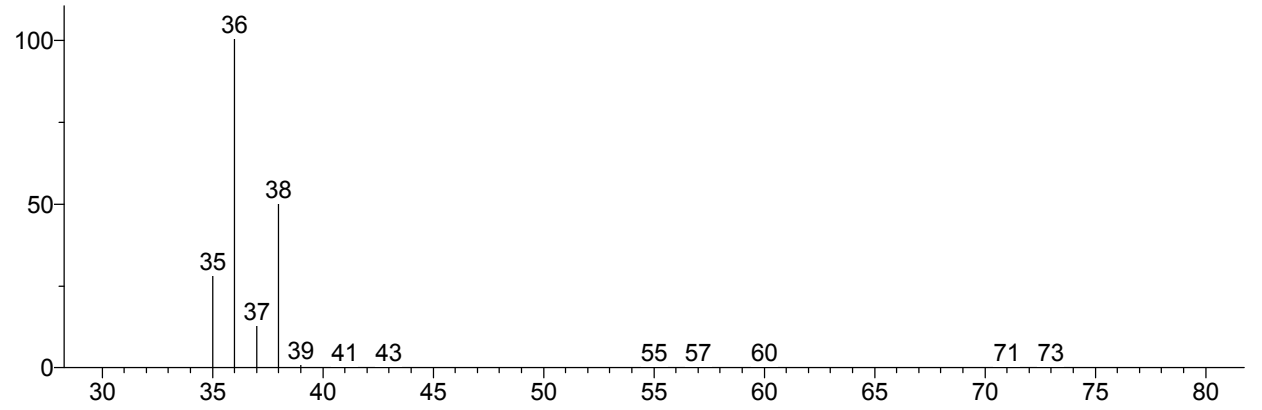
File :C:\msdchem\1\DATA\2014\J9163 Jordi\111114\J9163_PVC_Clear_po
... rtion_A_py1.D
Operator : Courtney McGowan
Instrument : Instrument #1
Acquired : 12 Nov 2014 3:05 using AcqMethod PYMSSP30.M
Sample Name: J9163 PVC Clear portion
Misc Info : J9163 PVC Clear portion



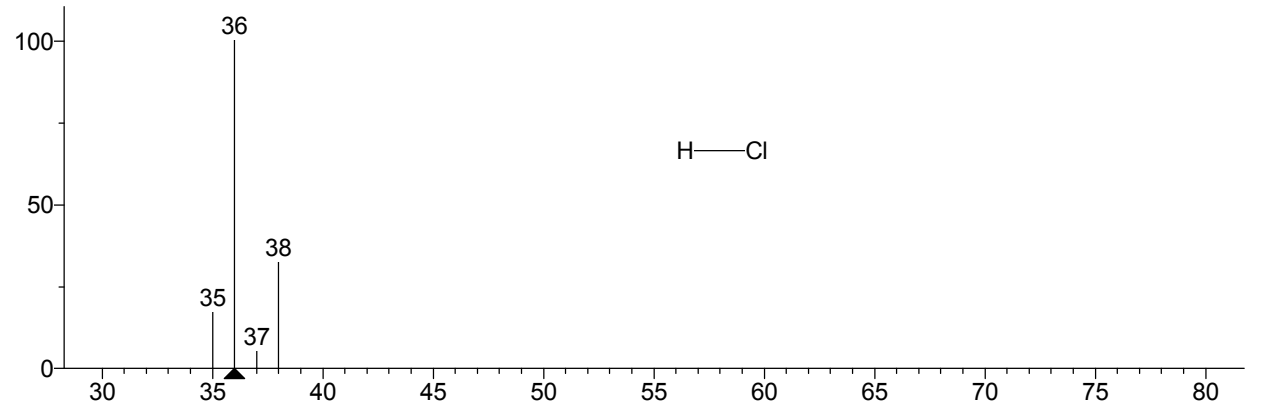
File :C:\msdchem\1\DATA\2014\J9163 Jordi\111114\J9163_PVC_Clear_po
... rtion_A_py1.D
Operator : Courtney McGowan
Instrument : Instrument #1
Acquired : 12 Nov 2014 3:05 using AcqMethod PYMSSP30.M
Sample Name: J9163 PVC Clear portion
Misc Info : J9163 PVC Clear portion



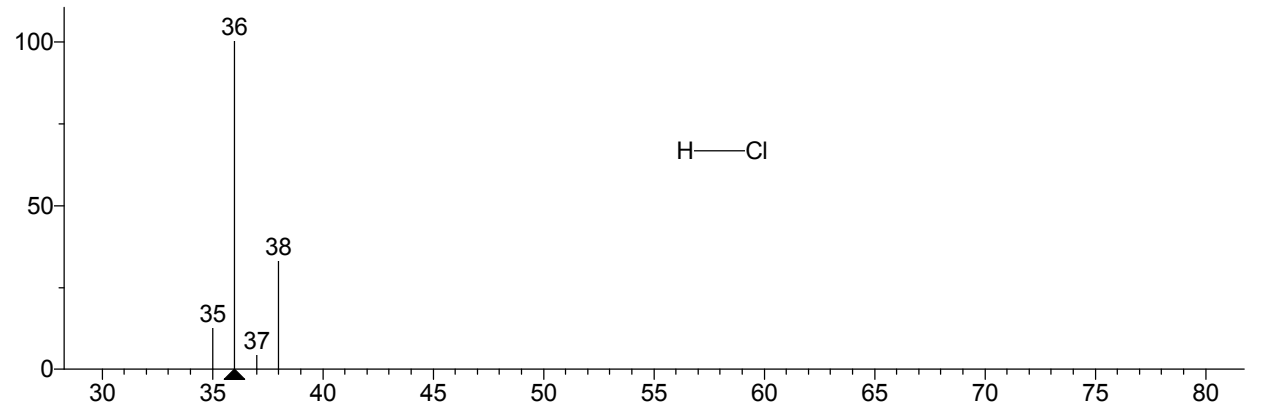
Unknown: Scan 130 (1.067 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 333



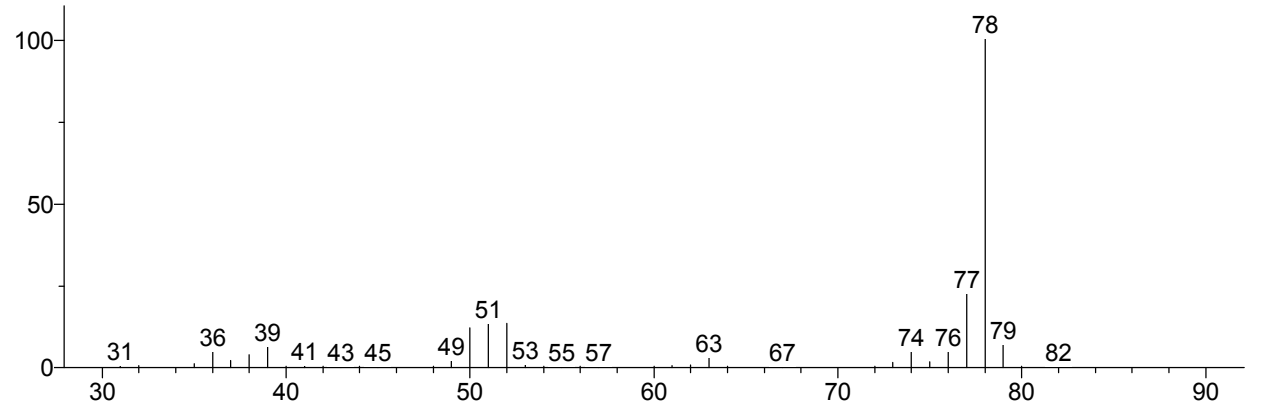
Hit 1 : Hydrogen chloride
ClH; MF: 876; RMF: 880; Prob 98.9%; CAS: 7647-01-0; Lib: mainlib; ID: 1496.



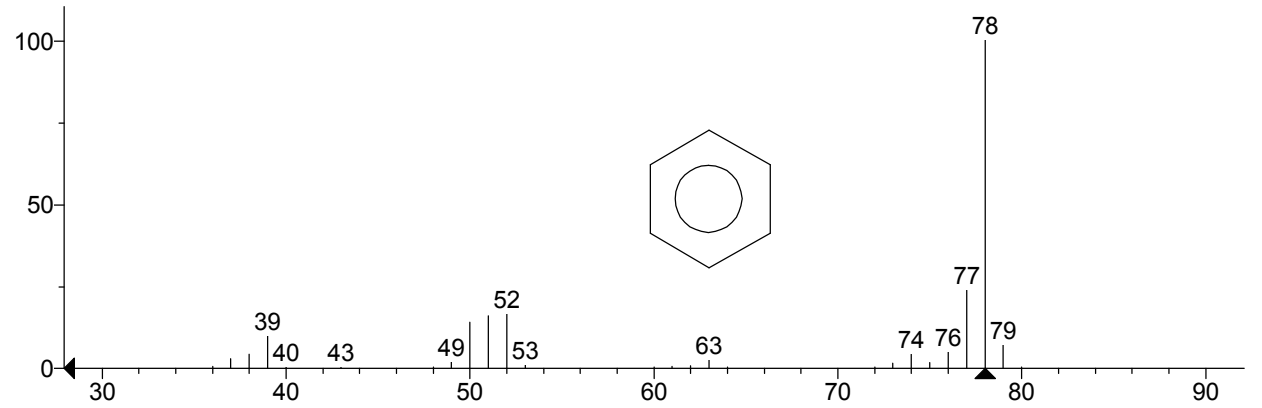
Hit 2 : Hydrogen chloride
ClH; MF: 826; RMF: 830; Prob 98.9%; CAS: 7647-01-0; Lib: replib; ID: 634.



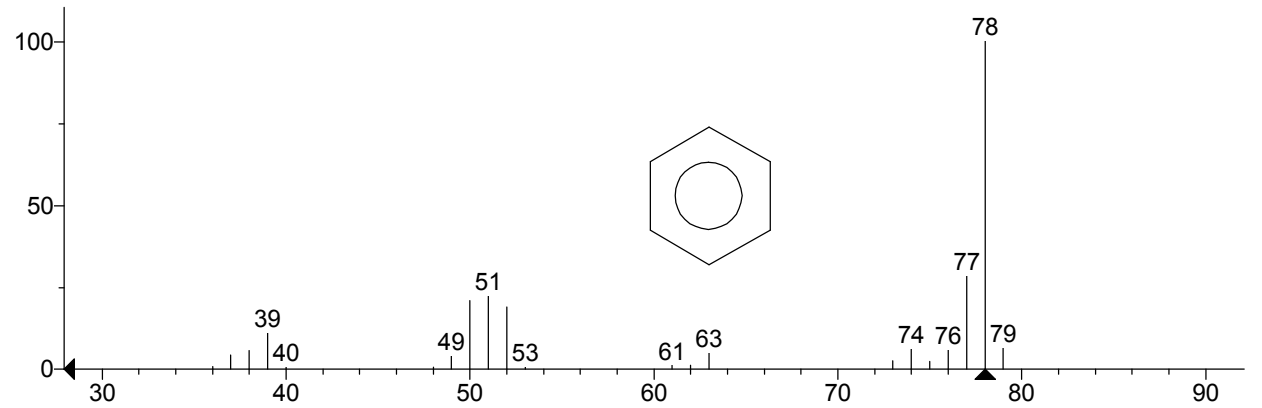
Unknown: Scan 153 (1.241 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 201



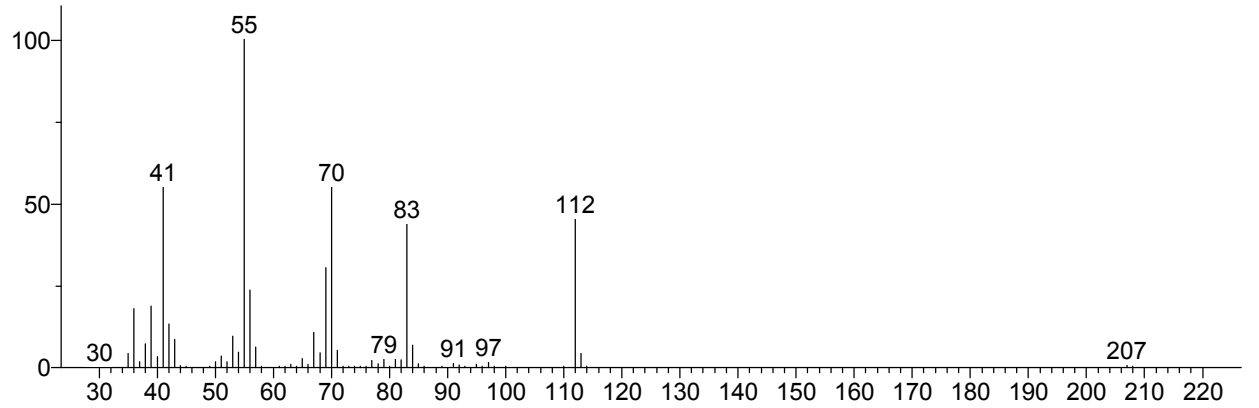
Hit 1 : Benzene
C6H6; MF: 942; RMF: 947; Prob 74.4%; CAS: 71-43-2; Lib: replib; ID: 9593.



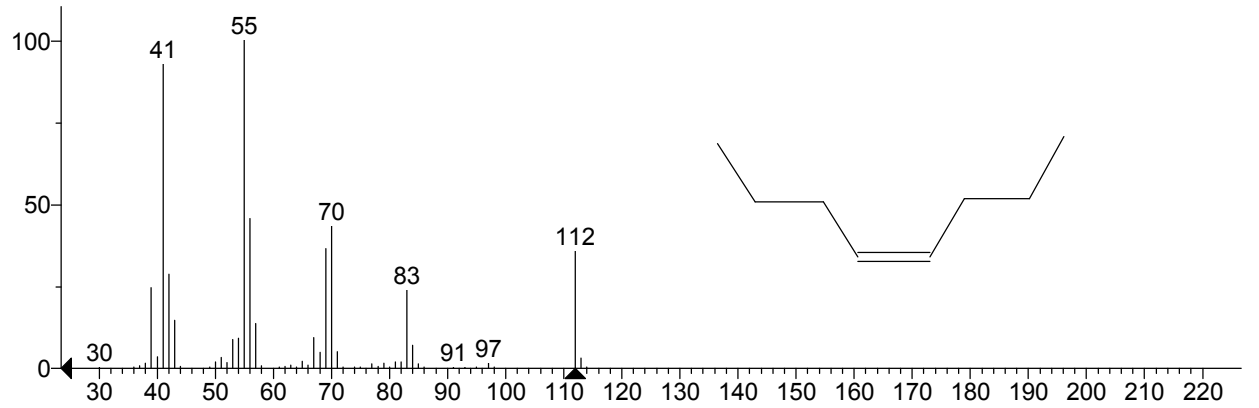
Hit 2 : Benzene
C6H6; MF: 937; RMF: 944; Prob 74.4%; CAS: 71-43-2; Lib: mainlib; ID: 41198.



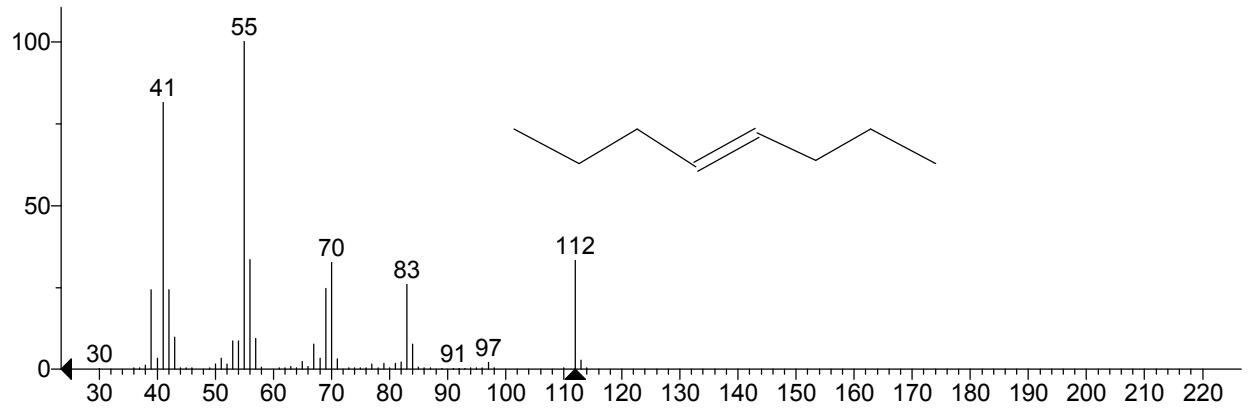
Unknown: Scan 173 (1.391 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -185



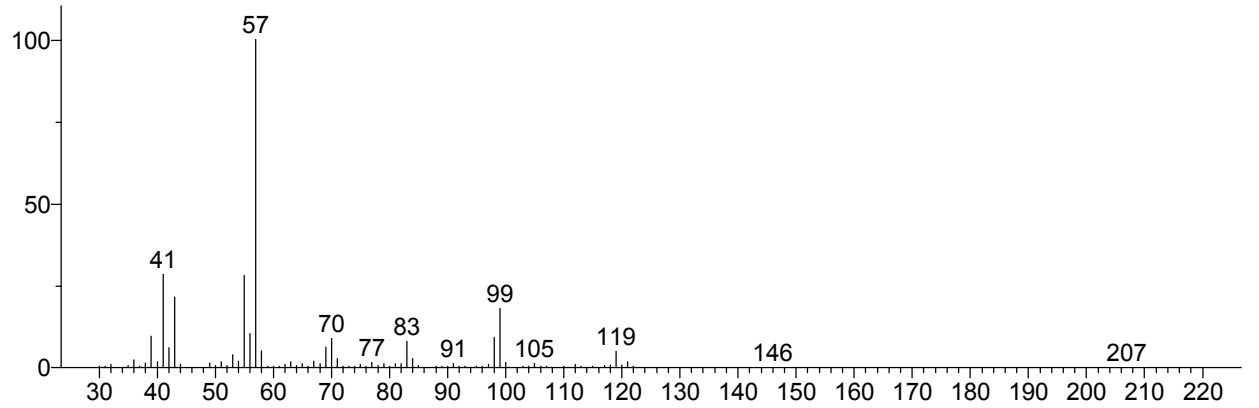
Hit 1 : 4-Octene, (Z)-
C8H16; MF: 883; RMF: 889; Prob 15.8%; CAS: 7642-15-1; Lib: mainlib; ID: 17325.



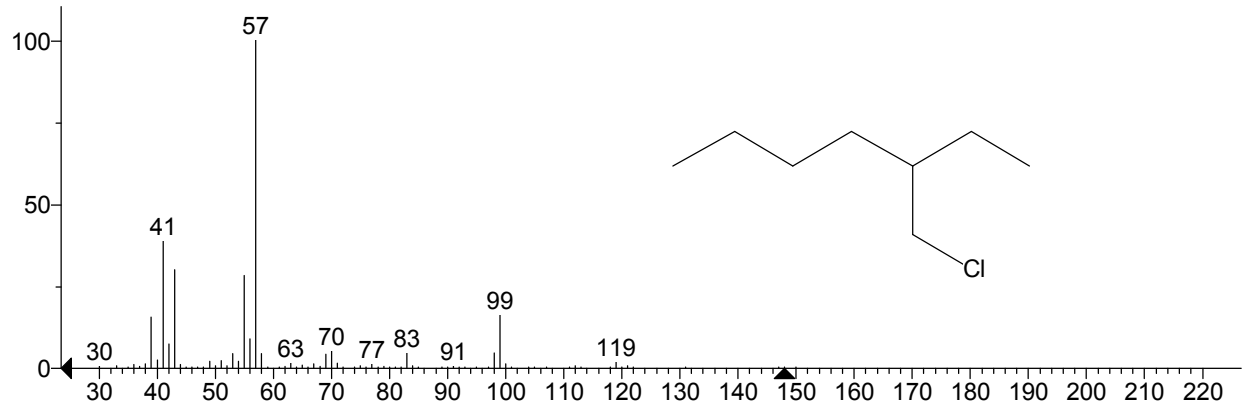
Hit 2 : 4-Octene, (E)-
C8H16; MF: 878; RMF: 895; Prob 12.8%; CAS: 14850-23-8; Lib: replib; ID: 4206.



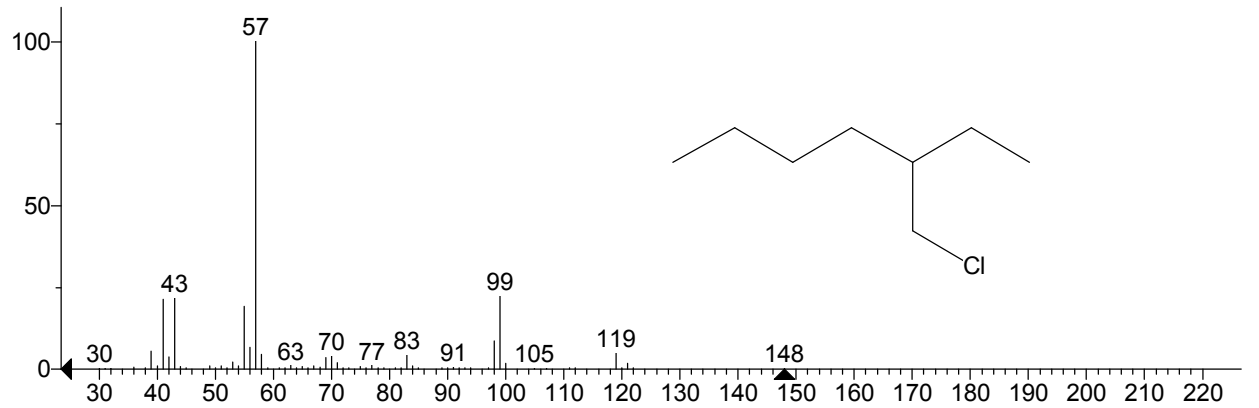
Unknown: Scan 246 (1.941 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 145



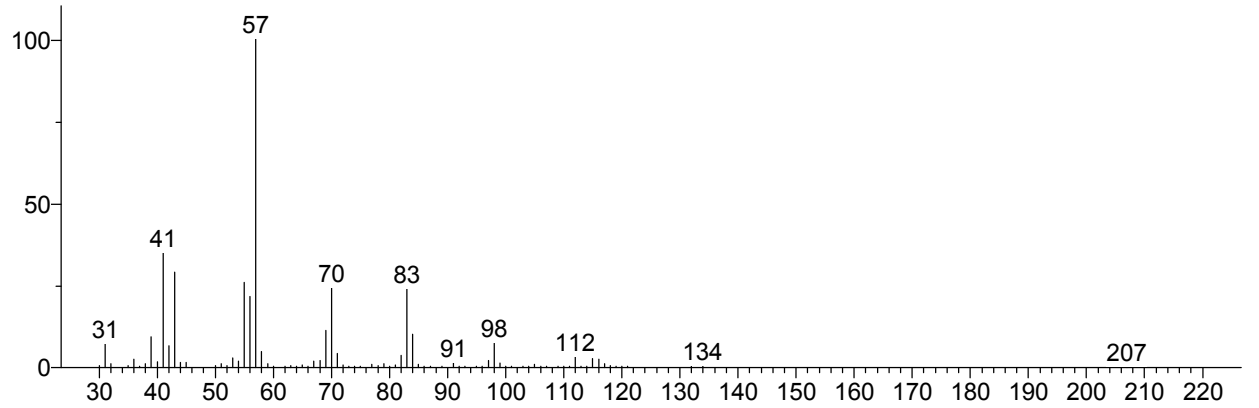
Hit 1 : Heptane, 3-(chloromethyl)-
C8H17Cl; MF: 890; RMF: 900; Prob 58.5%; CAS: 123-04-6; Lib: mainlib; ID: 21205.



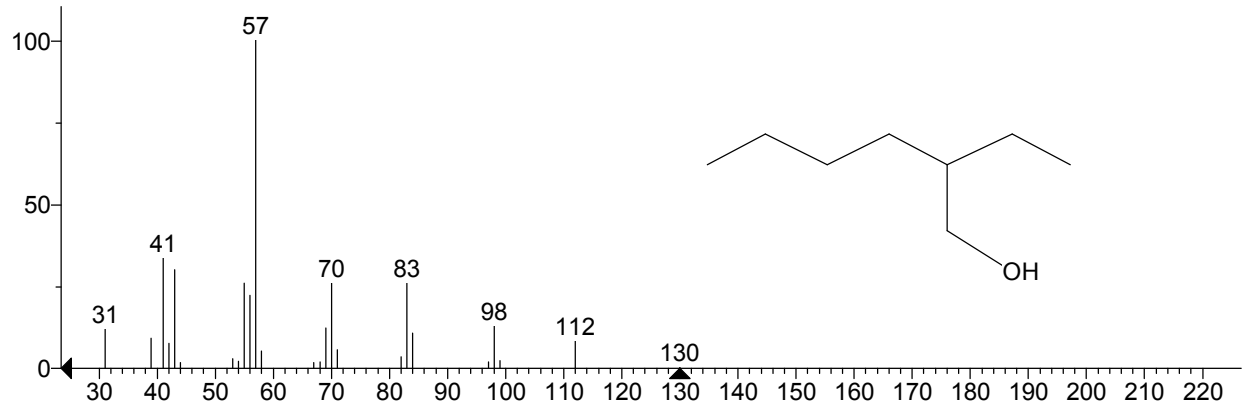
Hit 2 : Heptane, 3-(chloromethyl)-
C8H17Cl; MF: 883; RMF: 890; Prob 58.5%; CAS: 123-04-6; Lib: replib; ID: 5898.



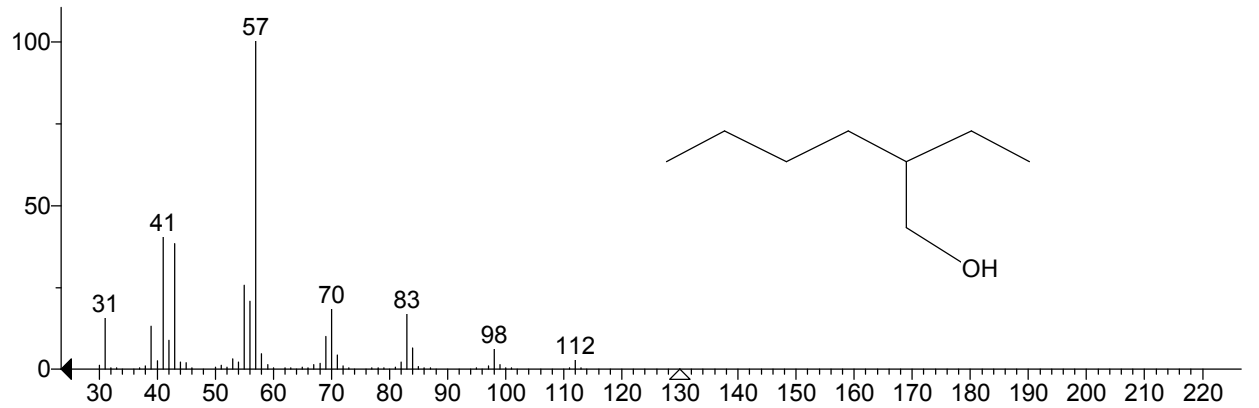
Unknown: Scan 270 (2.122 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 146



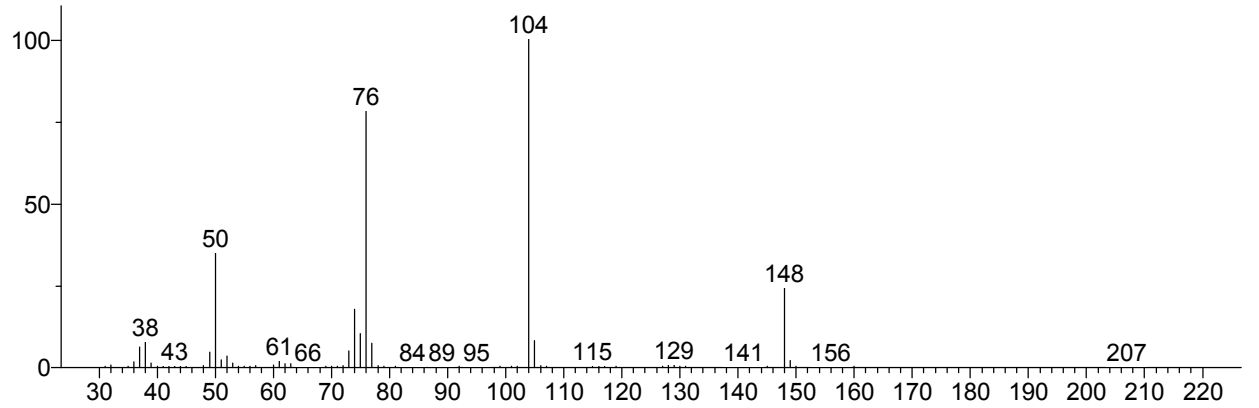
Hit 1 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 912; RMF: 969; Prob 58.8%; CAS: 104-76-7; Lib: replib; ID: 5259.



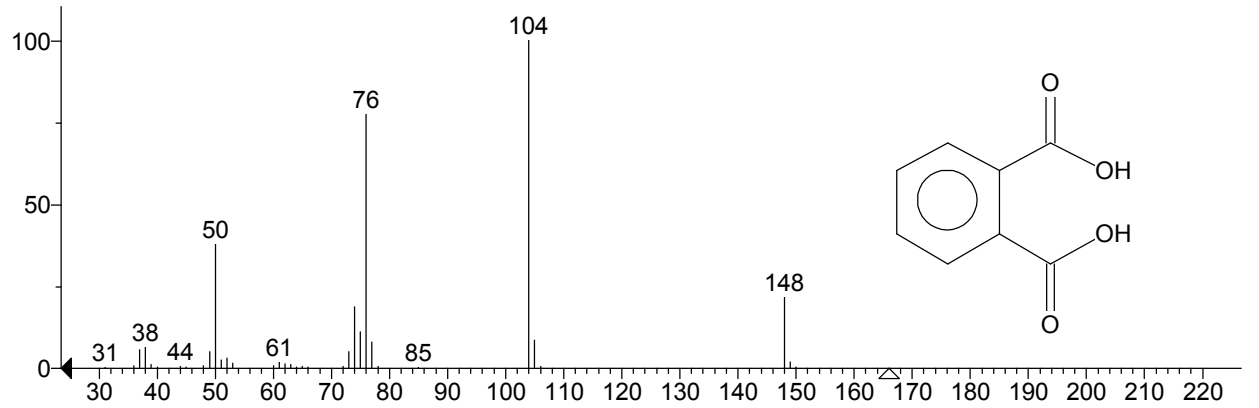
Hit 2 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 910; RMF: 939; Prob 58.8%; CAS: 104-76-7; Lib: mainlib; ID: 21179.



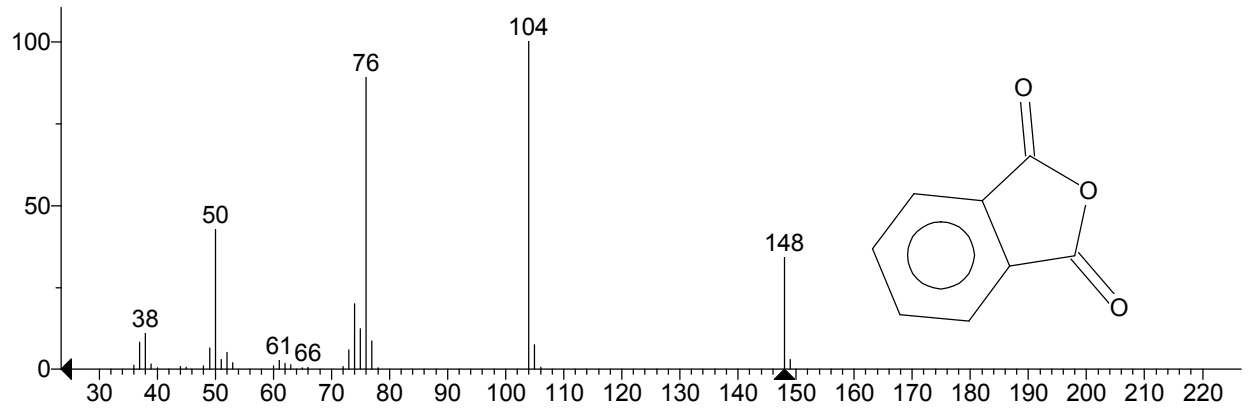
Unknown: Scan 449 (3.471 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 248



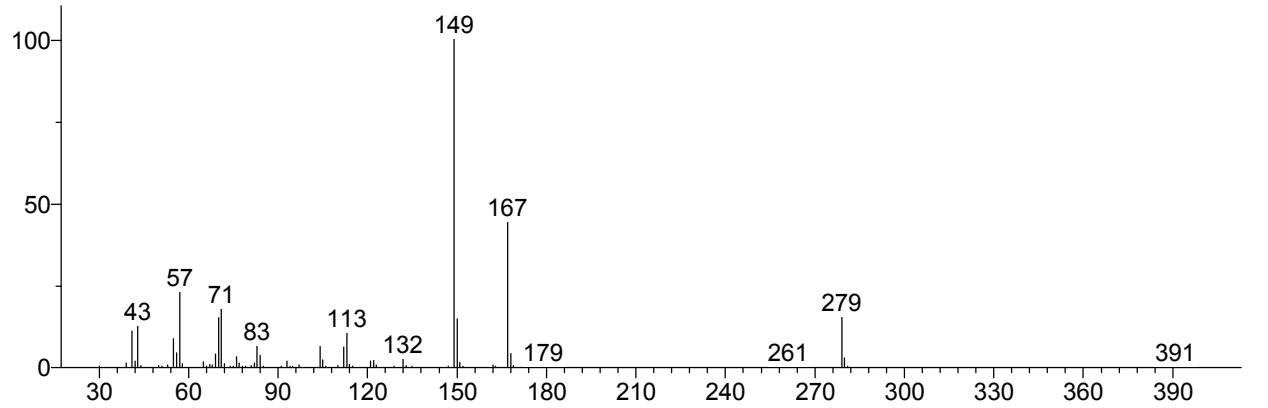
Hit 1 : 1,2-Benzenedicarboxylic acid
C8H6O4; MF: 957; RMF: 971; Prob 53.6%; CAS: 88-99-3; Lib: replib; ID: 13464.



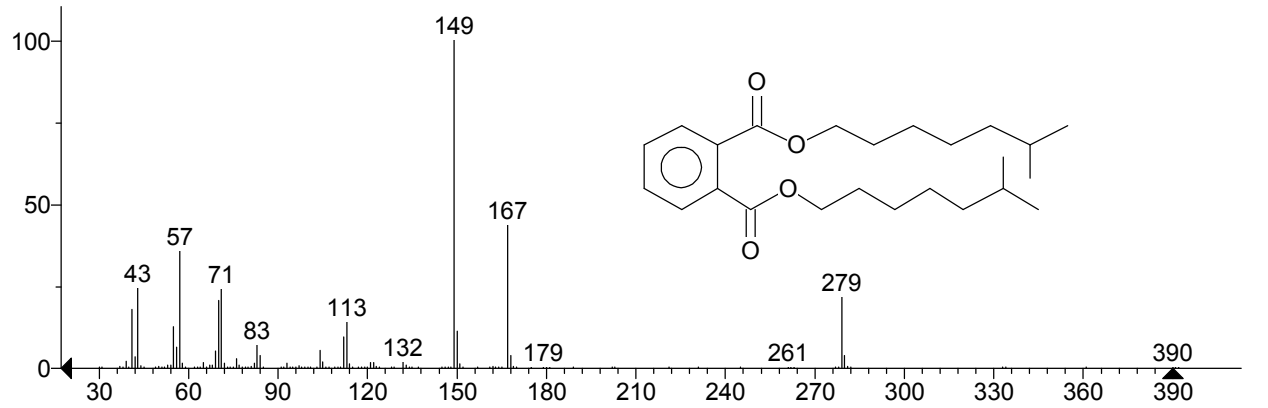
Hit 2 : Phthalic anhydride
C8H4O3; MF: 949; RMF: 964; Prob 40.0%; CAS: 85-44-9; Lib: mainlib; ID: 65271.



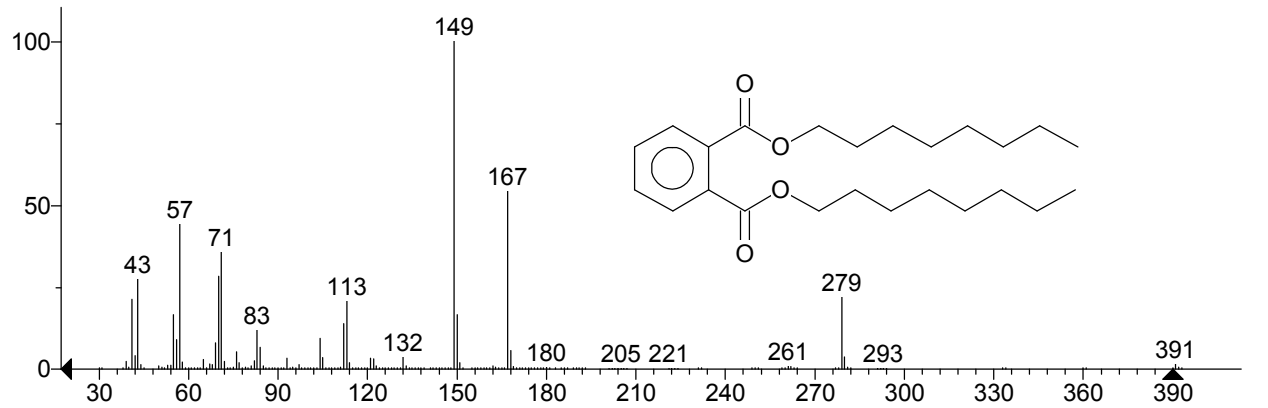
Unknown: Scan 1262 (9.597 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = 201



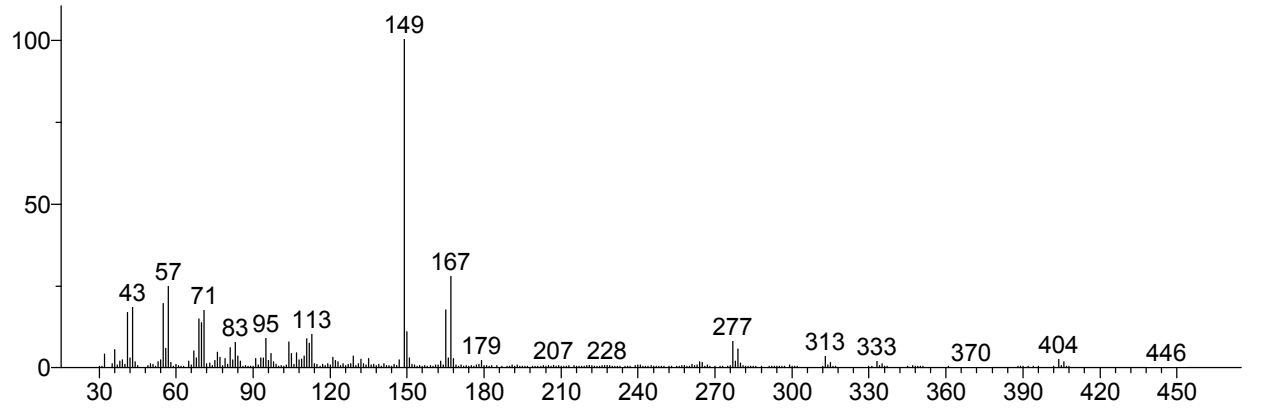
Hit 1 : 1,2-Benzenedicarboxylic acid, diisooctyl ester
C24H38O4; MF: 945; RMF: 945; Prob 30.4%; CAS: 27554-26-3; Lib: mainlib; ID: 110649.



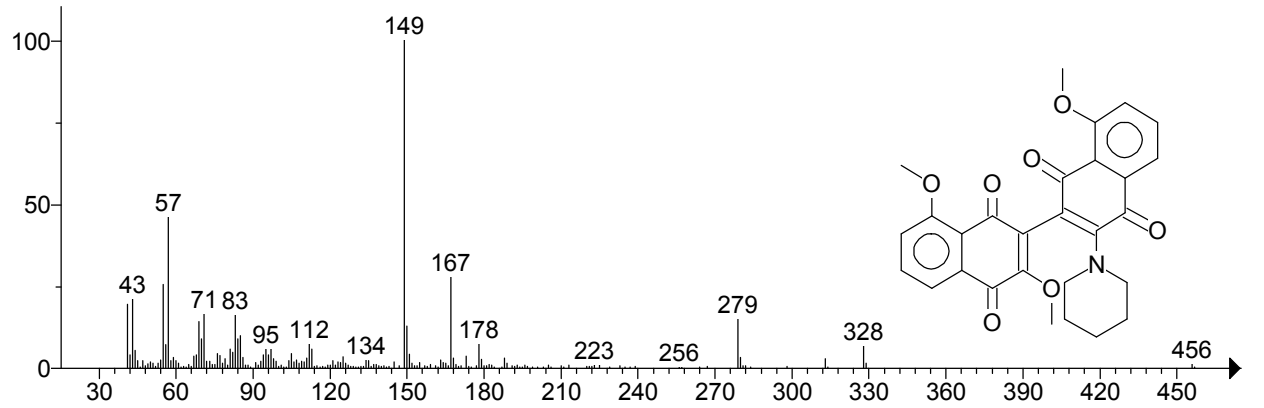
Hit 2 : Di-n-octyl phthalate
C24H38O4; MF: 936; RMF: 936; Prob 22.1%; CAS: 117-84-0; Lib: replib; ID: 20060.



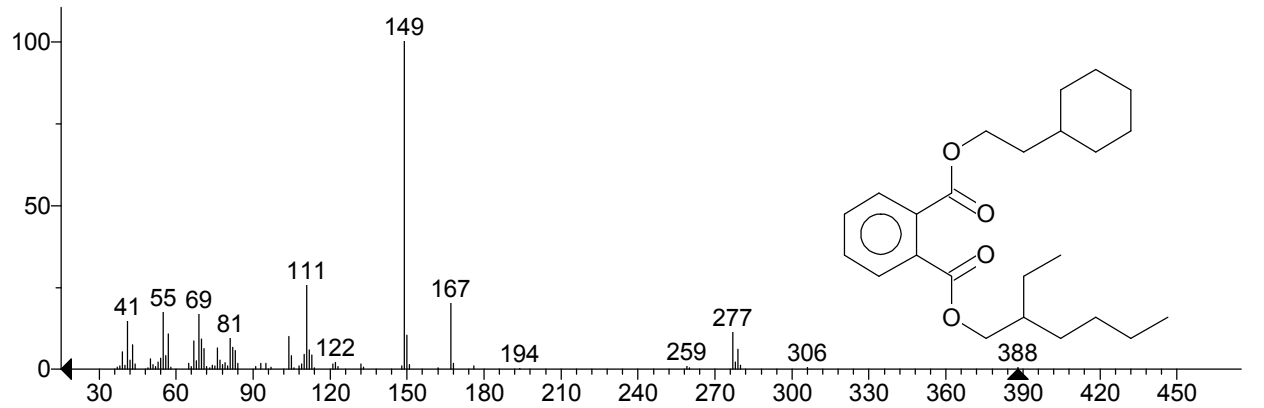
Unknown: Scan 1302 (9.899 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -1032



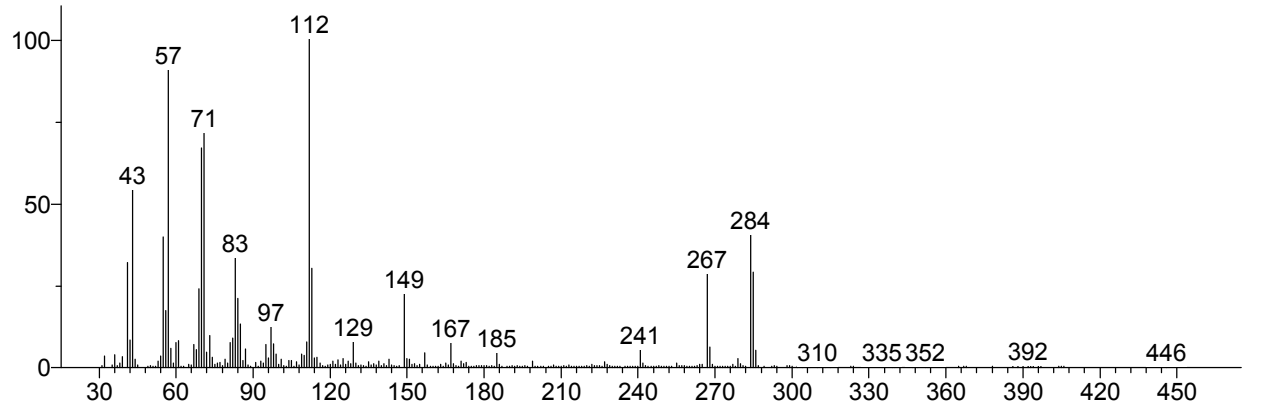
Hit 1 : 3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone
C28H25NO7; MF: 686; RMF: 758; Prob 19.8%; CAS: 127611-84-1; Lib: mainlib; ID: 109695.



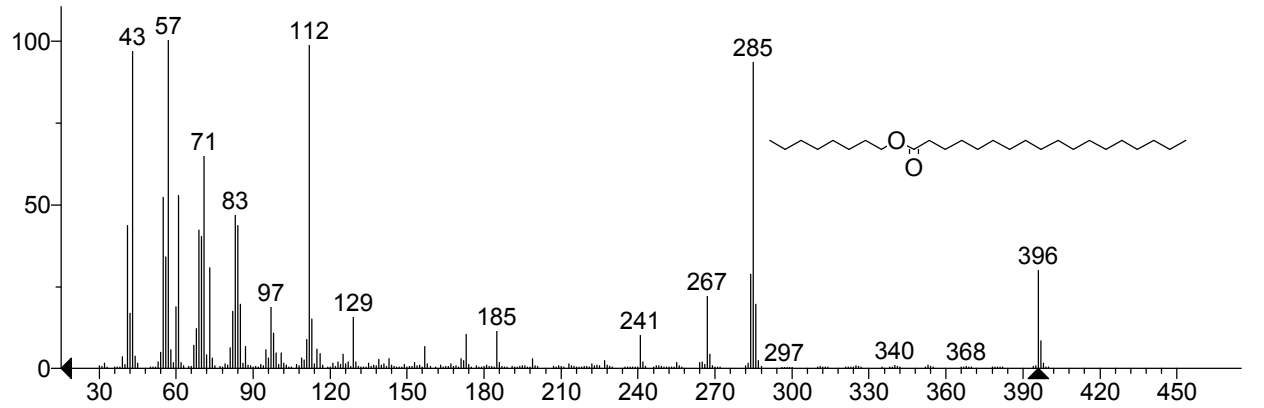
Hit 2 : Phthalic acid, 2-cyclohexylethyl 2-ethylhexyl ester
C24H36O4; MF: 680; RMF: 861; Prob 15.6%; Lib: mainlib; ID: 110126.



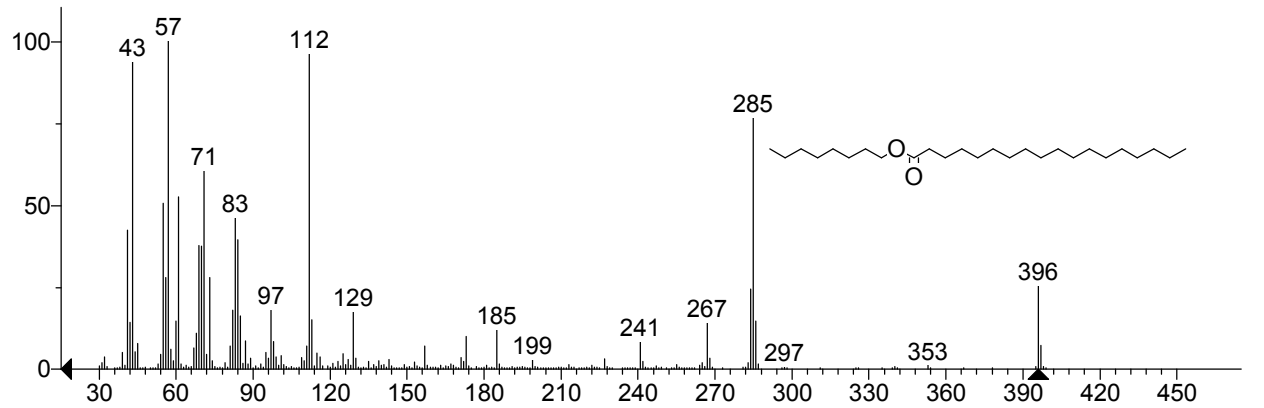
Unknown: Scan 1311 (9.966 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -285



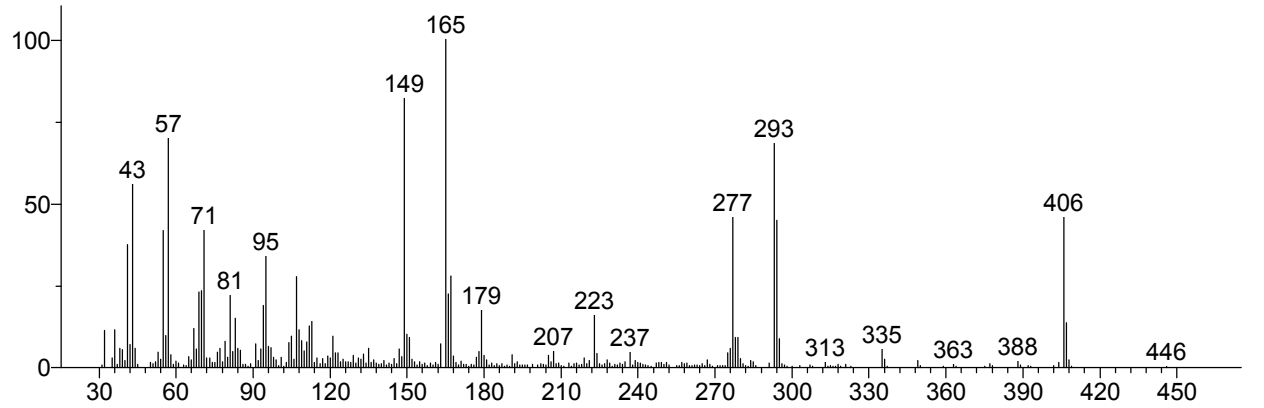
Hit 1 : Octadecanoic acid, octyl ester
C26H52O2; MF: 783; RMF: 795; Prob 50.7%; CAS: 109-36-4; Lib: mainlib; ID: 23536.



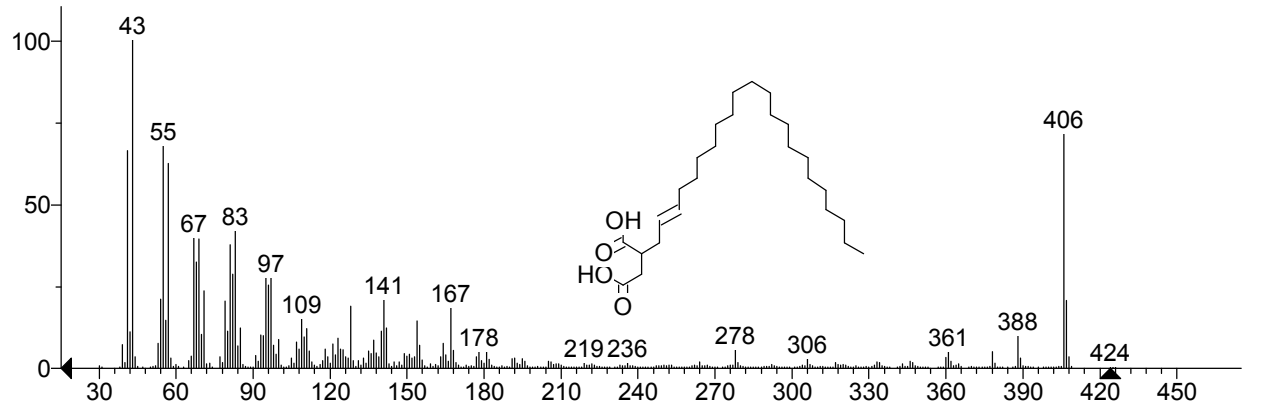
Hit 2 : Octadecanoic acid, octyl ester
C26H52O2; MF: 765; RMF: 779; Prob 50.7%; CAS: 109-36-4; Lib: replib; ID: 5914.



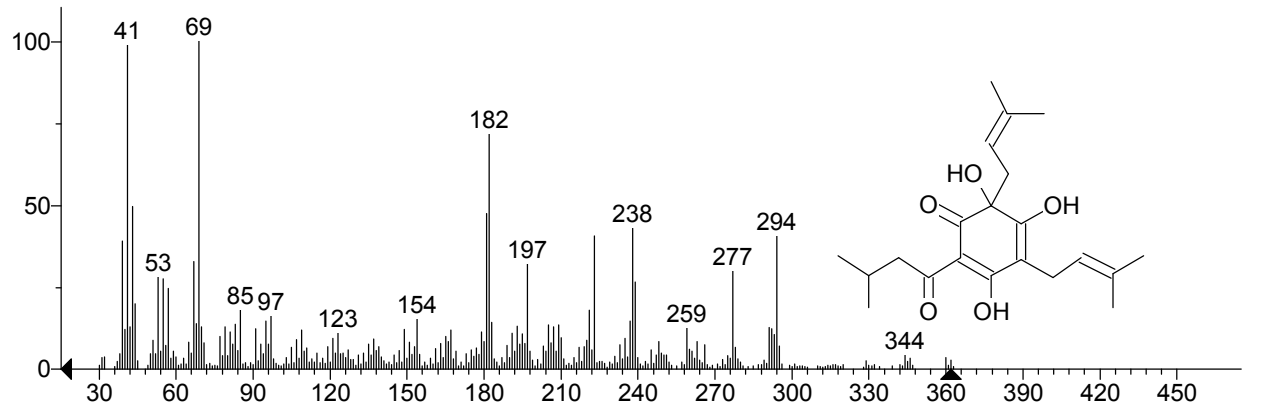
Unknown: Scan 1316 (10.004 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -1302



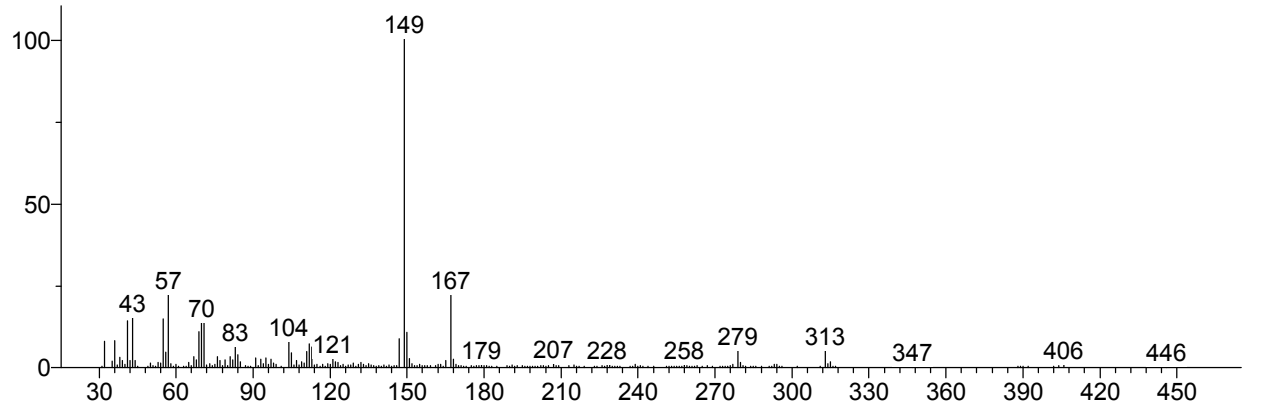
Hit 1 : trans-(2-Docosenyl)succinic acid
C26H48O4; MF: 608; RMF: 610; Prob 22.1%; Lib: mainlib; ID: 13587.



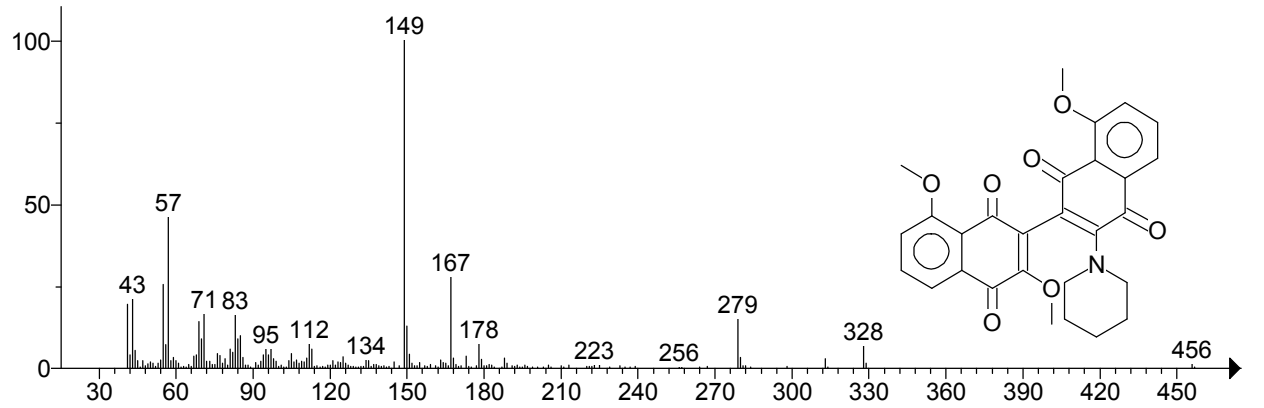
Hit 2 : 2,4-Cyclohexadien-1-one, 3,5,6-trihydroxy-2-isovaleryl-4,6-bis(3-methyl-2-butenyl)-, (R)-(-)-
C21H30O5; MF: 590; RMF: 634; Prob 11.4%; CAS: 26472-41-3; Lib: replib; ID: 7601.



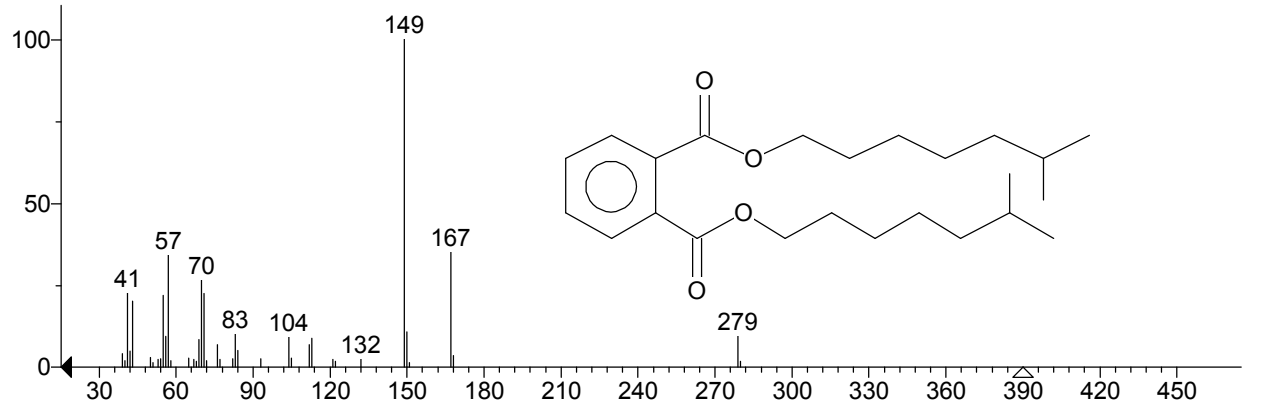
Unknown: Scan 1329 (10.102 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -898



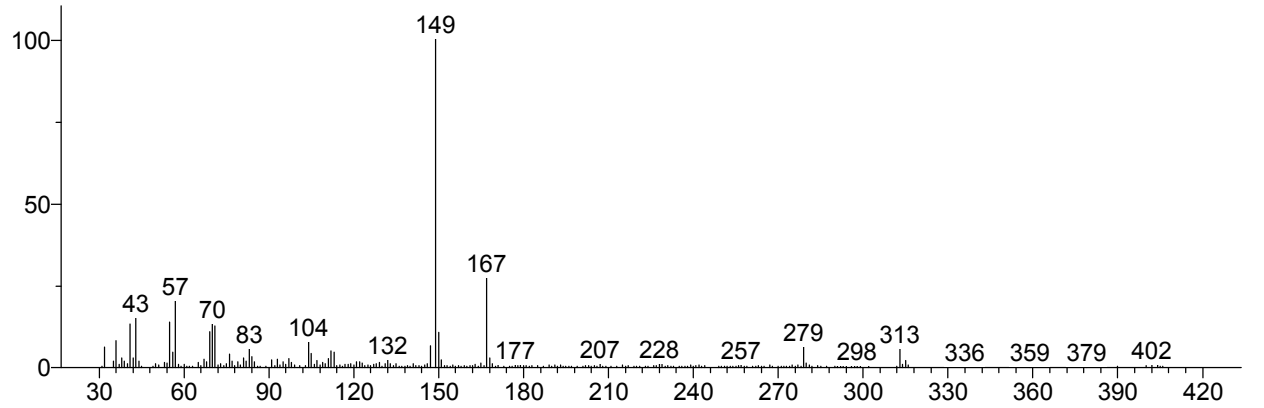
Hit 1 : 3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone
C28H25NO7; MF: 712; RMF: 764; Prob 16.1%; CAS: 127611-84-1; Lib: mainlib; ID: 109695.



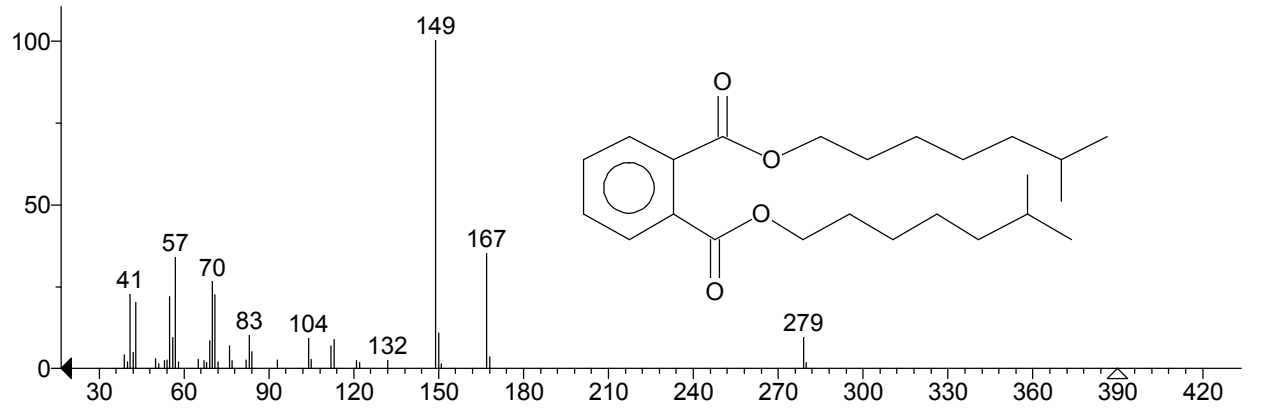
Hit 2 : 1,2-Benzenedicarboxylic acid, diisooctyl ester
C24H38O4; MF: 706; RMF: 929; Prob 12.6%; CAS: 27554-26-3; Lib: replib; ID: 20061.



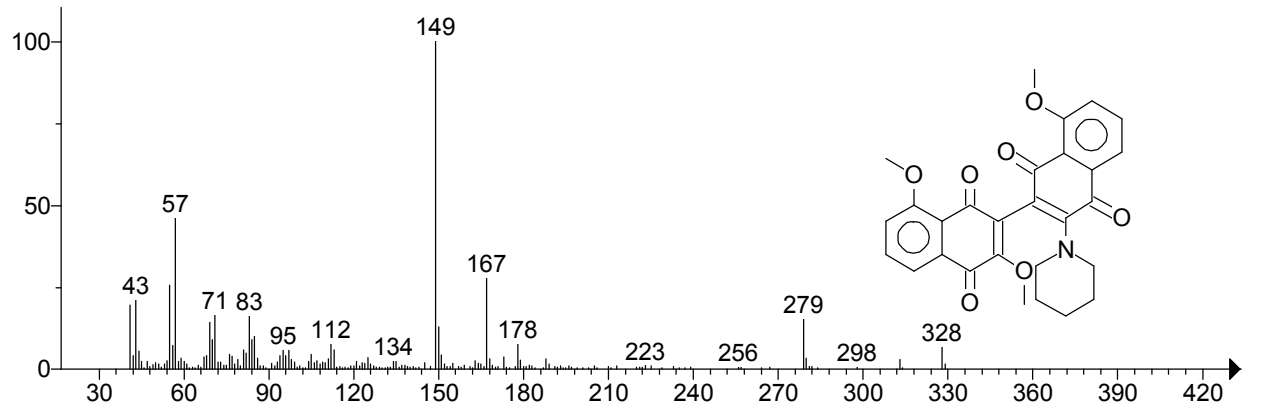
Unknown: Scan 1344 (10.215 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -752



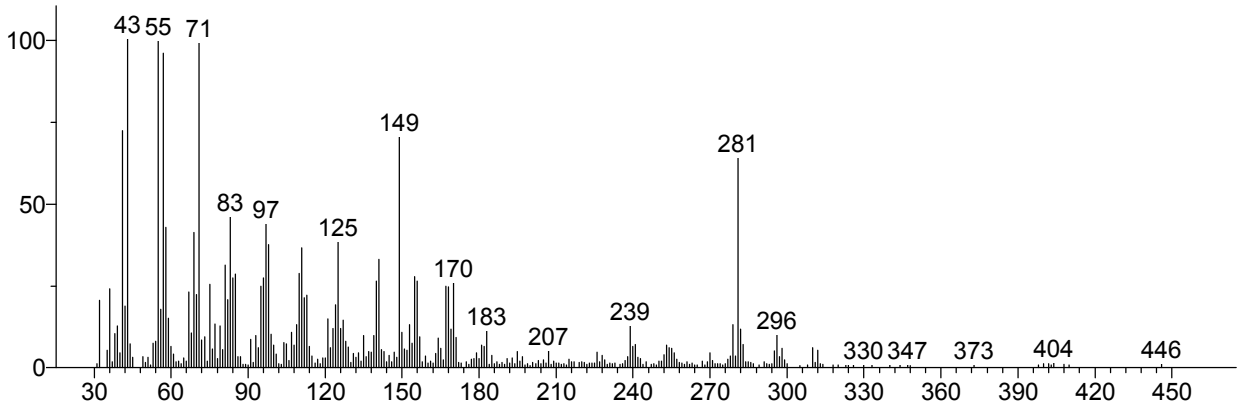
Hit 1 : 1,2-Benzenedicarboxylic acid, diisooctyl ester
C24H38O4; MF: 726; RMF: 943; Prob 20.1%; CAS: 27554-26-3; Lib: replib; ID: 20061.



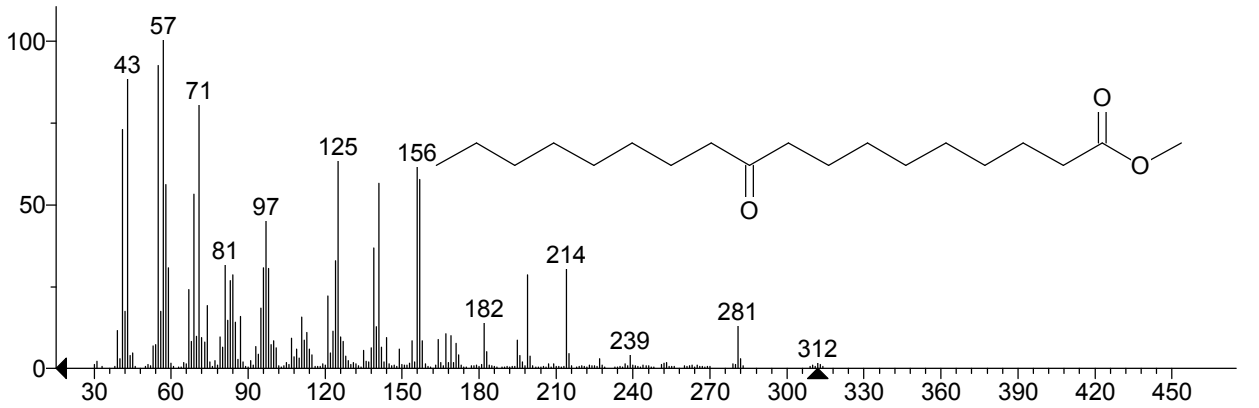
Hit 2 : 3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone
C28H25NO7; MF: 711; RMF: 765; Prob 12.2%; CAS: 127611-84-1; Lib: mainlib; ID: 109695.



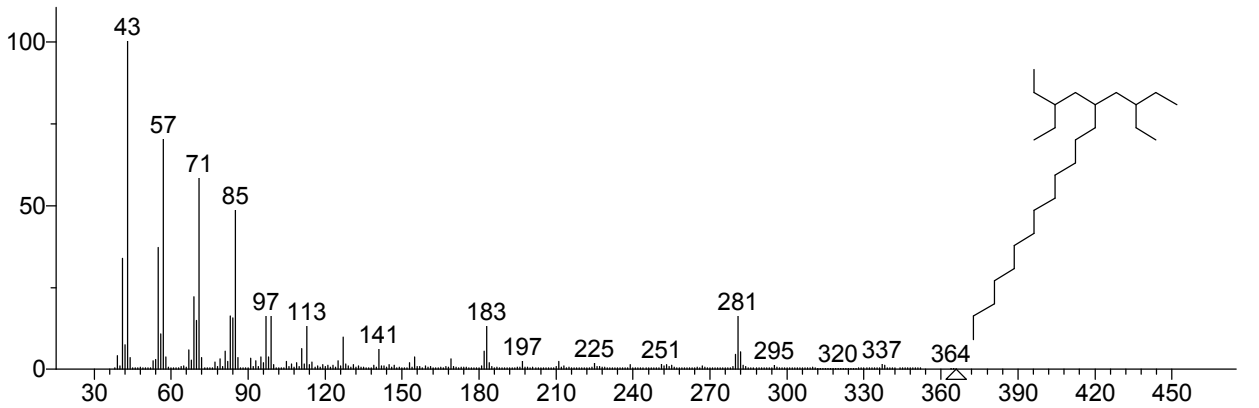
Unknown: Scan 1367 (10.388 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -941



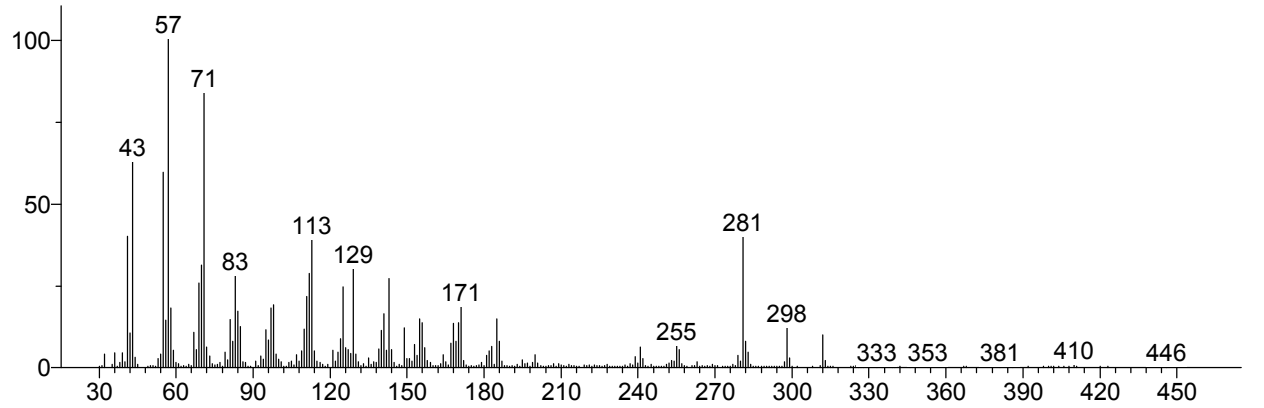
Hit 1 : Octadecanoic acid, 10-oxo-, methyl ester
C19H36O3; MF: 687; RMF: 723; Prob 16.1%; CAS: 870-10-0; Lib: replib; ID: 5613.



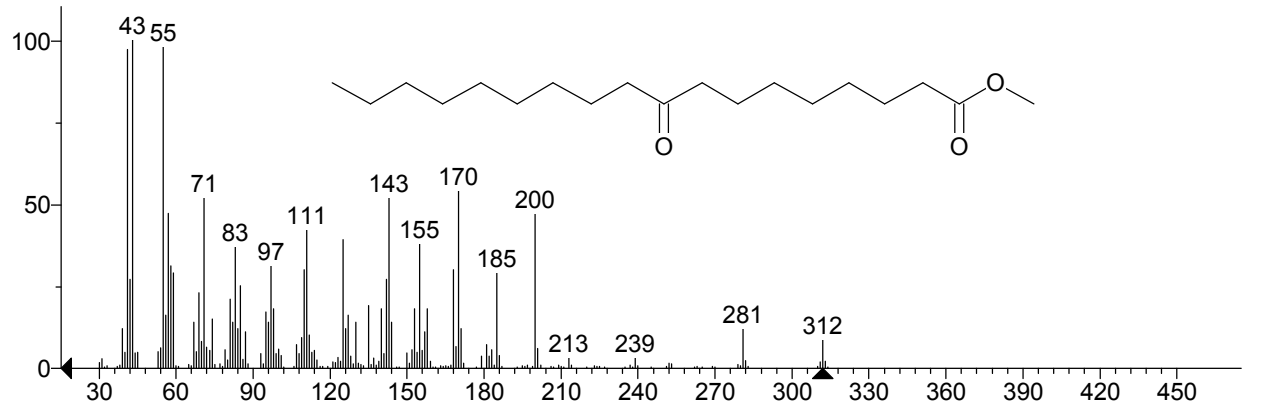
Hit 2 : Octadecane, 3-ethyl-5-(2-ethylbutyl)-
C26H54; MF: 683; RMF: 710; Prob 13.6%; CAS: 55282-12-7; Lib: replib; ID: 2152.



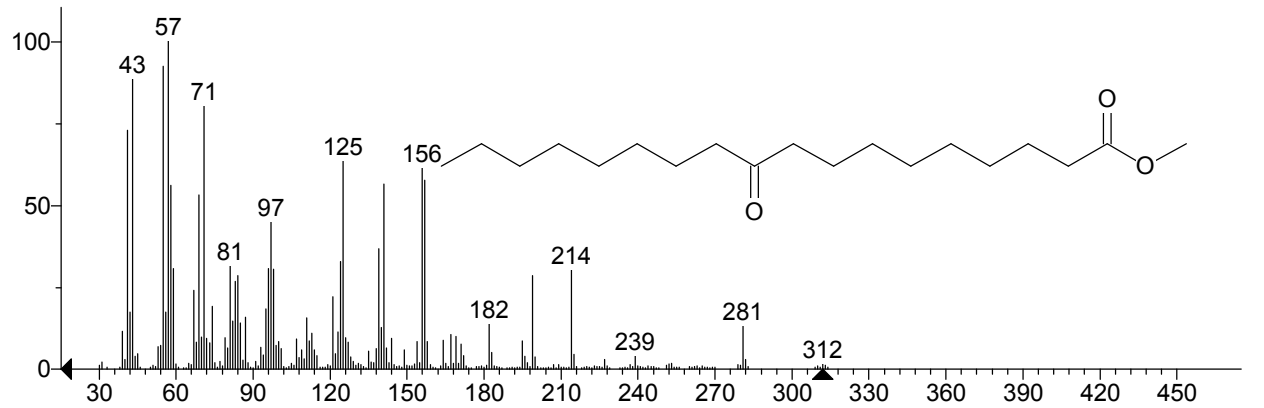
Unknown: Scan 1380 (10.486 min): J9163_PVC_Clear_portion_A_py1.D\data.ms
Compound in Library Factor = -1006



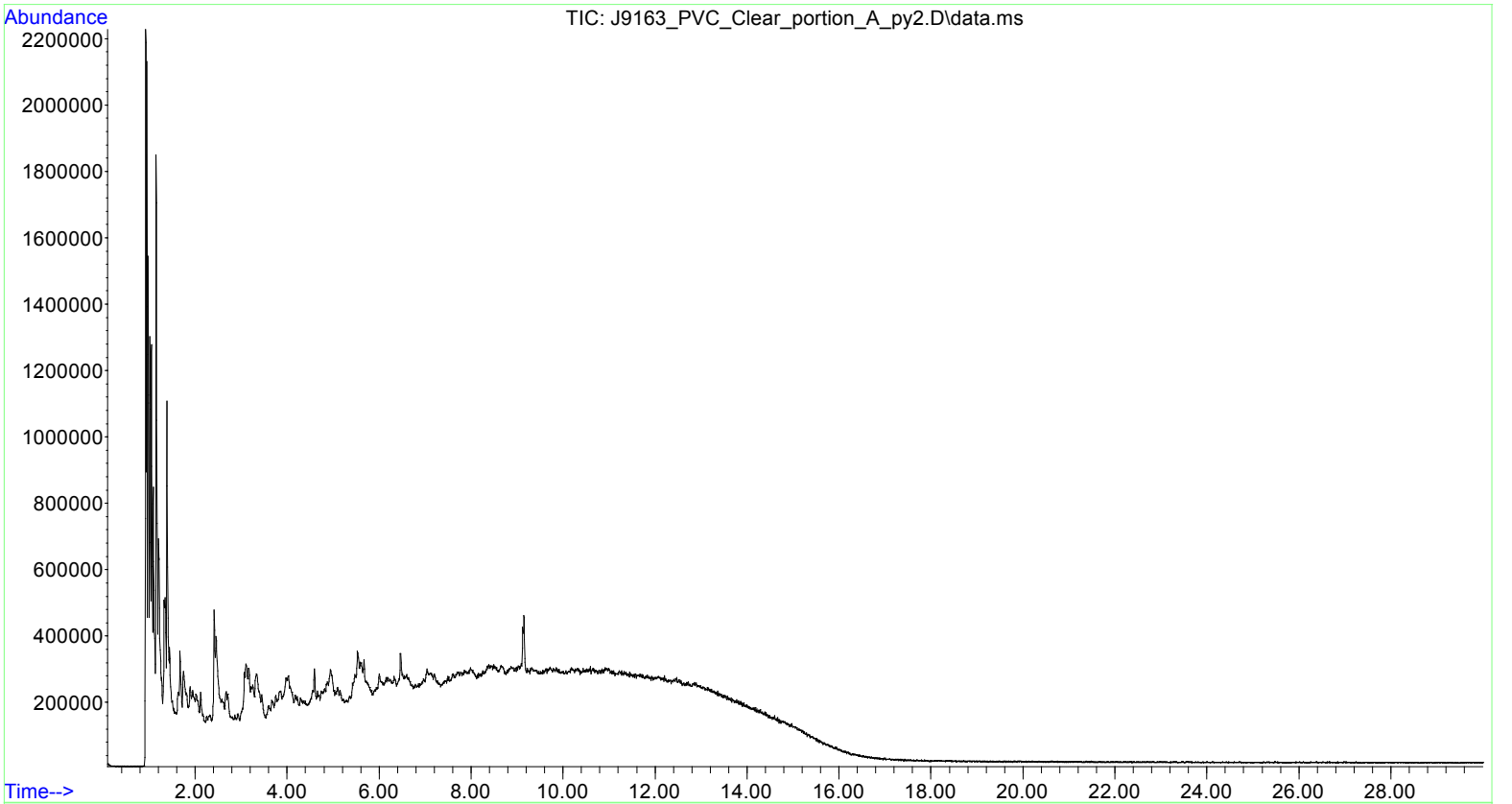
Hit 1 : Octadecanoic acid, 9-oxo-, methyl ester
C19H36O3; MF: 695; RMF: 751; Prob 22.9%; CAS: 1842-70-2; Lib: mainlib; ID: 6620.

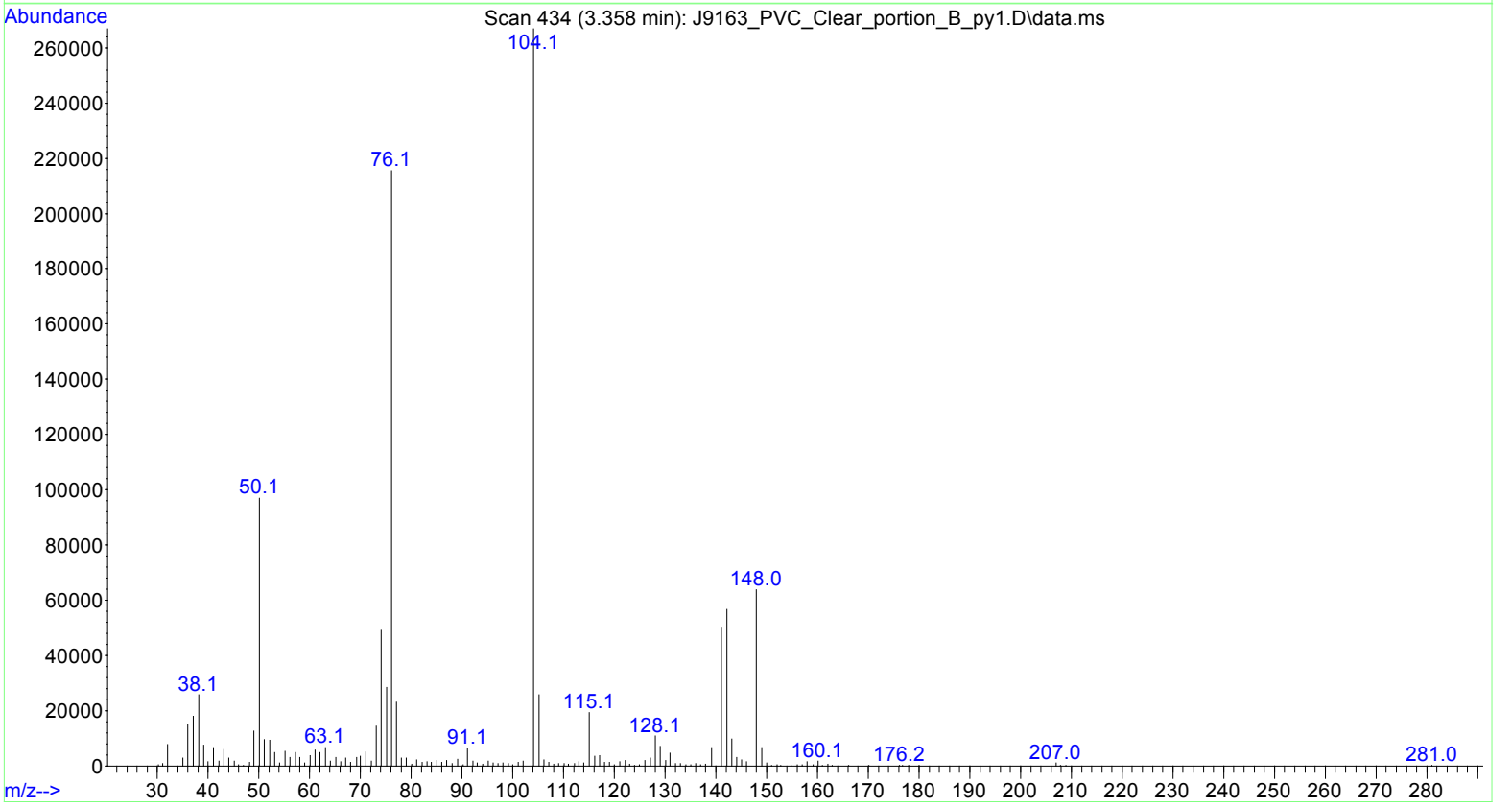


Hit 2 : Octadecanoic acid, 10-oxo-, methyl ester
C19H36O3; MF: 681; RMF: 701; Prob 14.4%; CAS: 870-10-0; Lib: replib; ID: 5613.

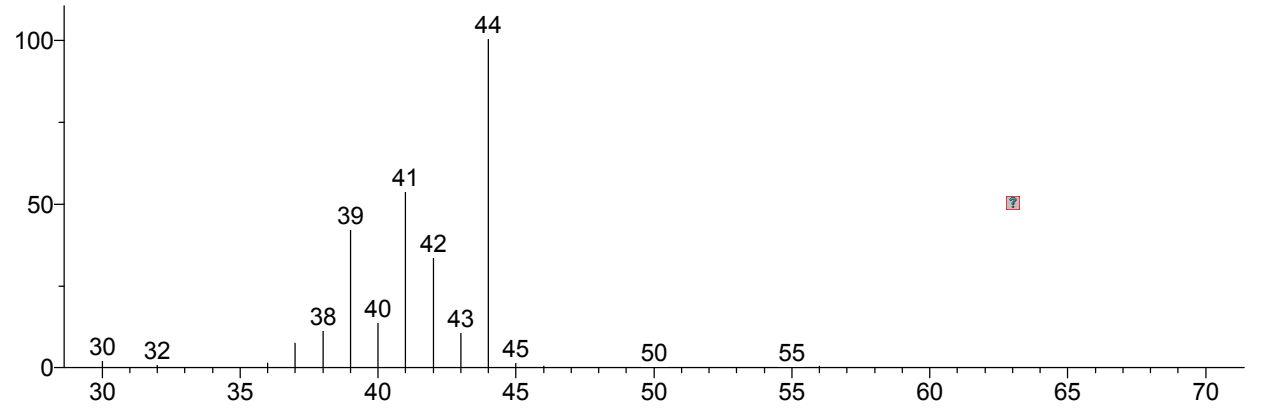


File :C:\msdchem\1\DATA\2014\J9163 Jordi\111114\J9163_PVC_Clear_po
... rtion_A_py2.D
Operator : Courtney McGowan
Instrument : Instrument #1
Acquired : 12 Nov 2014 3:49 using AcqMethod PYMS.M
Sample Name: J9163 PVC Clear portion
Misc Info : J9163 PVC Clear portion

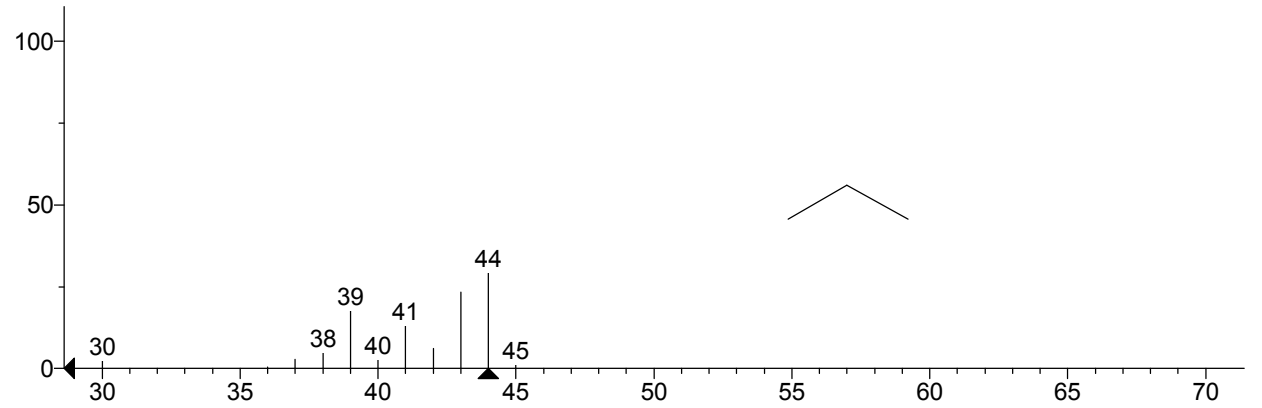




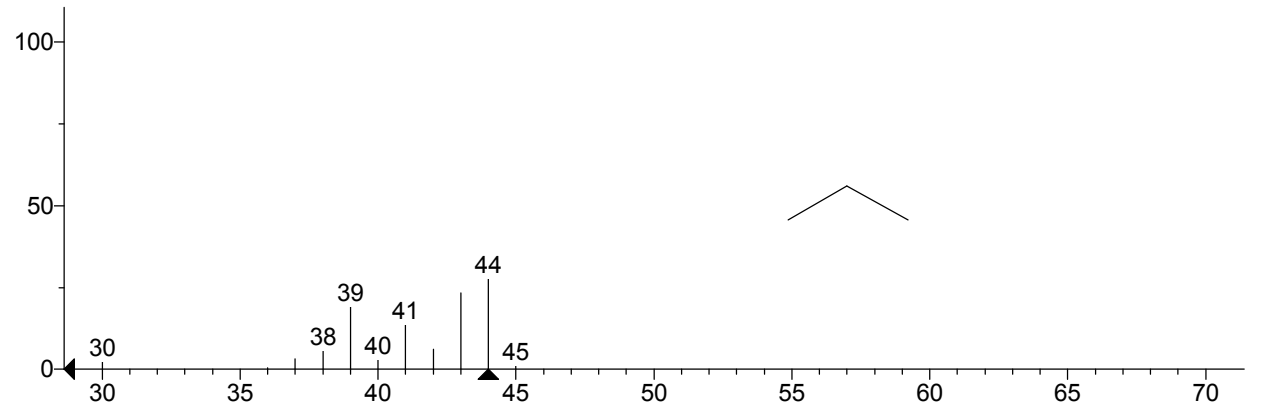
Unknown: Scan 111 (0.924 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -275



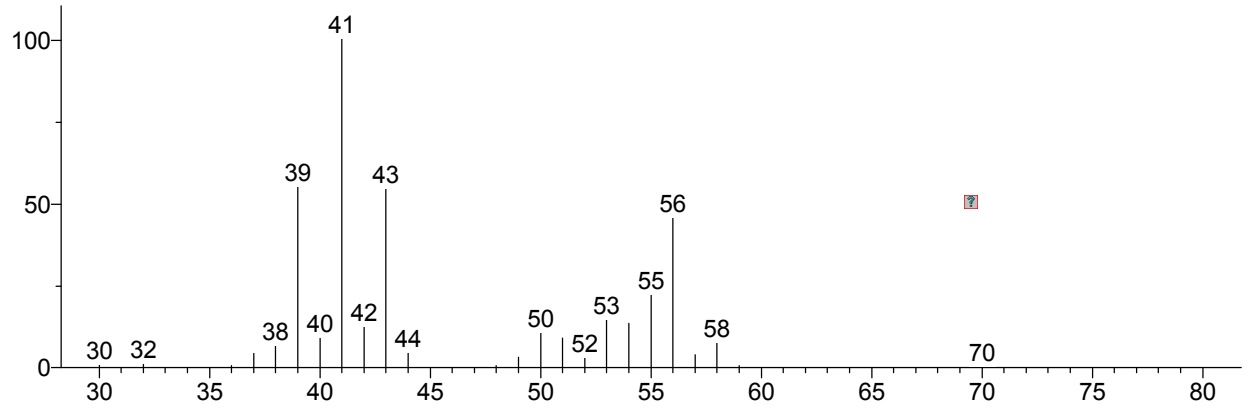
Hit 1 : Propane
C3H8; MF: 807; RMF: 810; Prob 36.0%; CAS: 74-98-6; Lib: replib; ID: 139.



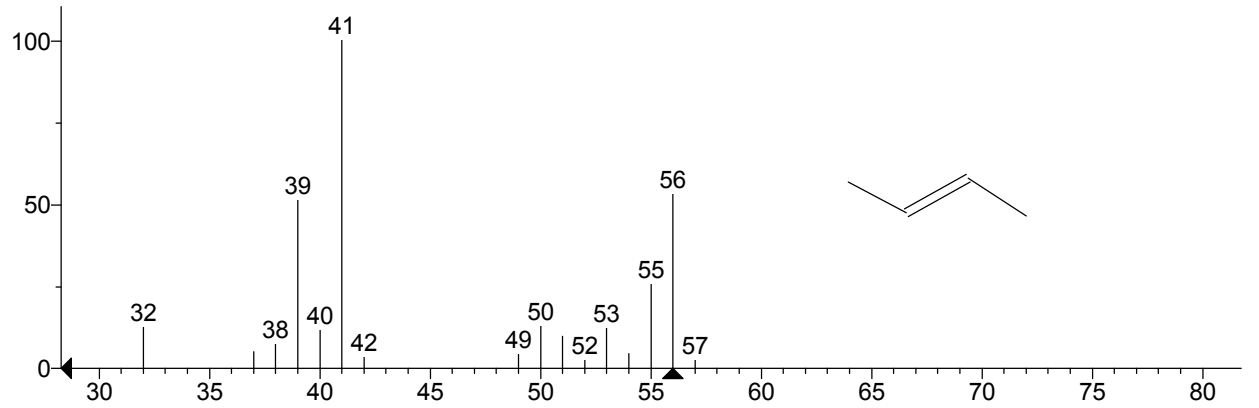
Hit 2 : Propane
C3H8; MF: 802; RMF: 805; Prob 36.0%; CAS: 74-98-6; Lib: mainlib; ID: 399.



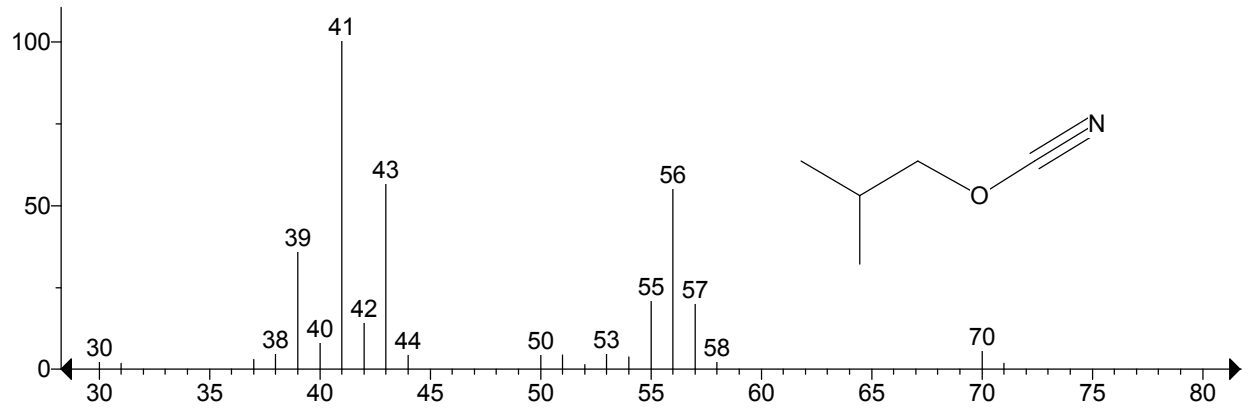
Unknown: Scan 114 (0.947 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -501



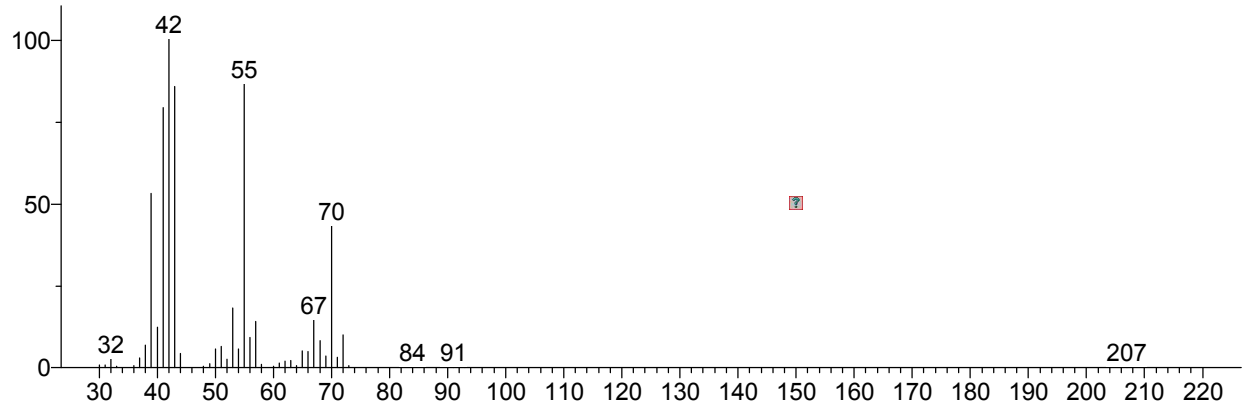
Hit 1 : 2-Butene
C4H8; MF: 809; RMF: 902; Prob 17.3%; CAS: 107-01-7; Lib: mainlib; ID: 1863.



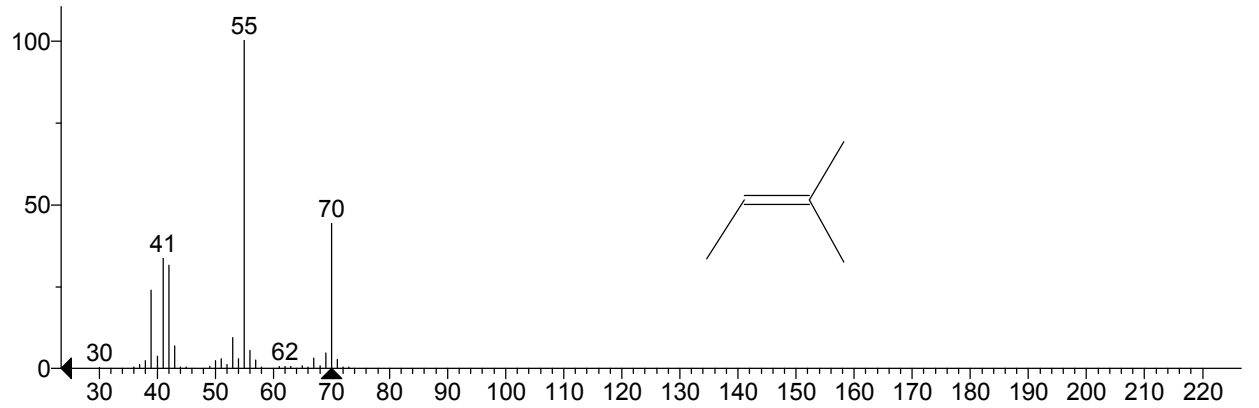
Hit 2 : Cyanic acid, 2-methylpropyl ester
C5H9NO; MF: 797; RMF: 803; Prob 11.5%; CAS: 1768-25-8; Lib: mainlib; ID: 2242.



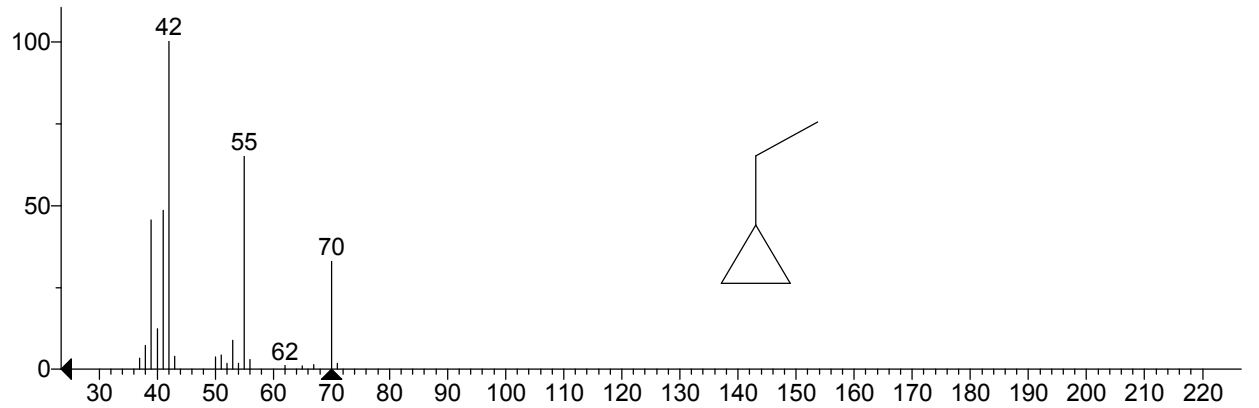
Unknown: Scan 118 (0.977 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -520



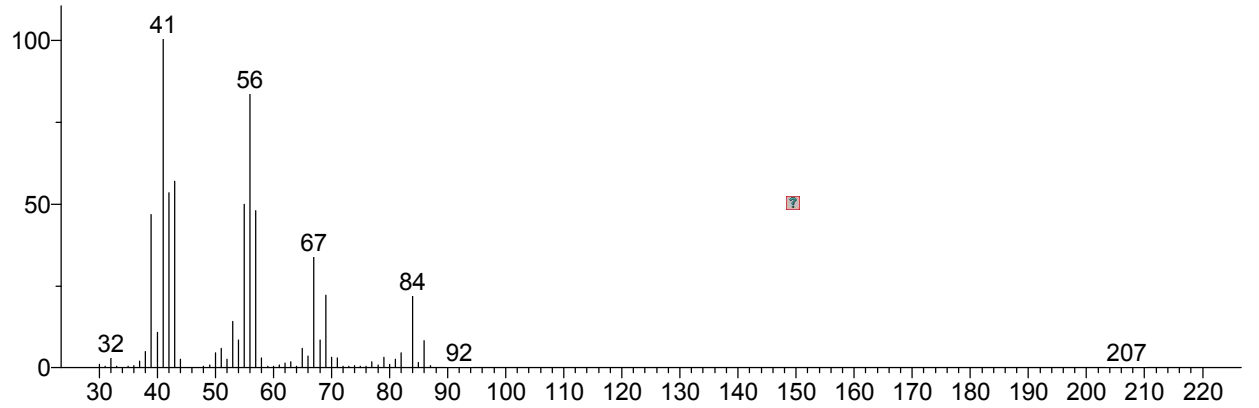
Hit 1 : 2-Butene, 2-methyl-
C5H10; MF: 790; RMF: 792; Prob 8.35%; CAS: 513-35-9; Lib: mainlib; ID: 18422.



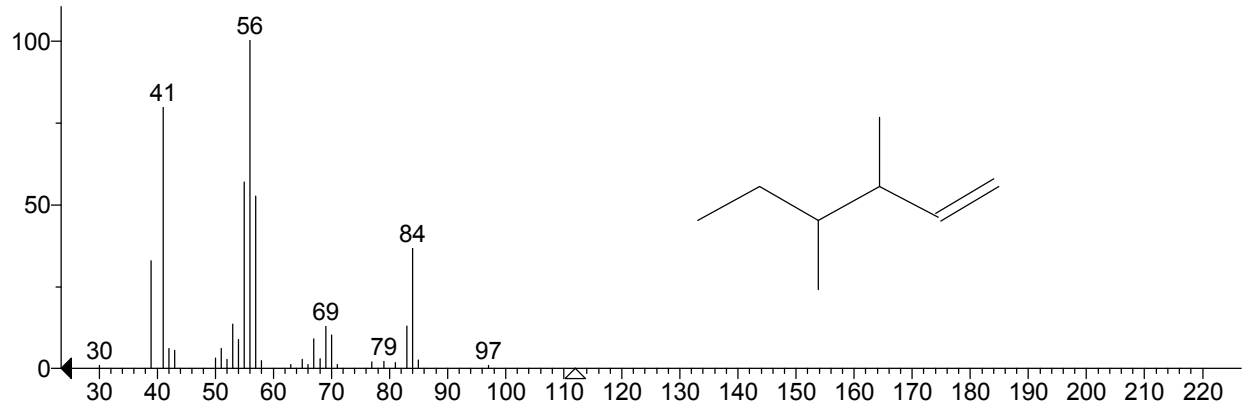
Hit 2 : Cyclopropane, ethyl-
C5H10; MF: 788; RMF: 848; Prob 7.70%; CAS: 1191-96-4; Lib: replib; ID: 1385.



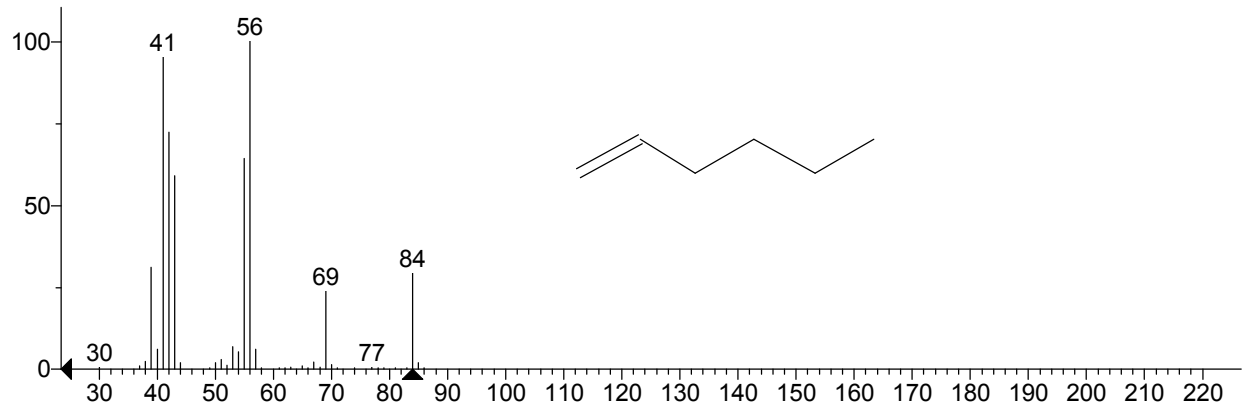
Unknown: Scan 123 (1.014 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -698



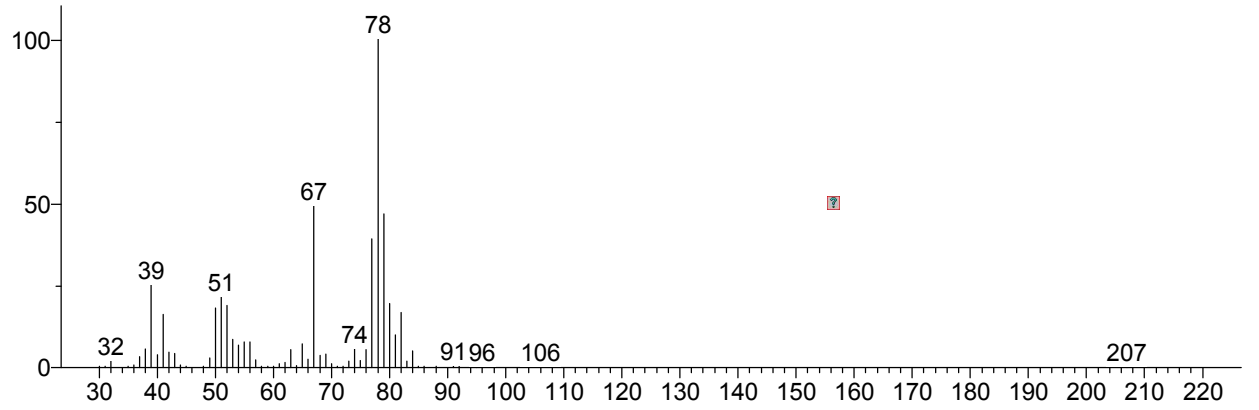
Hit 1 : 1-Hexene, 3,4-dimethyl-
C8H16; MF: 797; RMF: 834; Prob 8.73%; CAS: 16745-94-1; Lib: mainlib; ID: 19899.



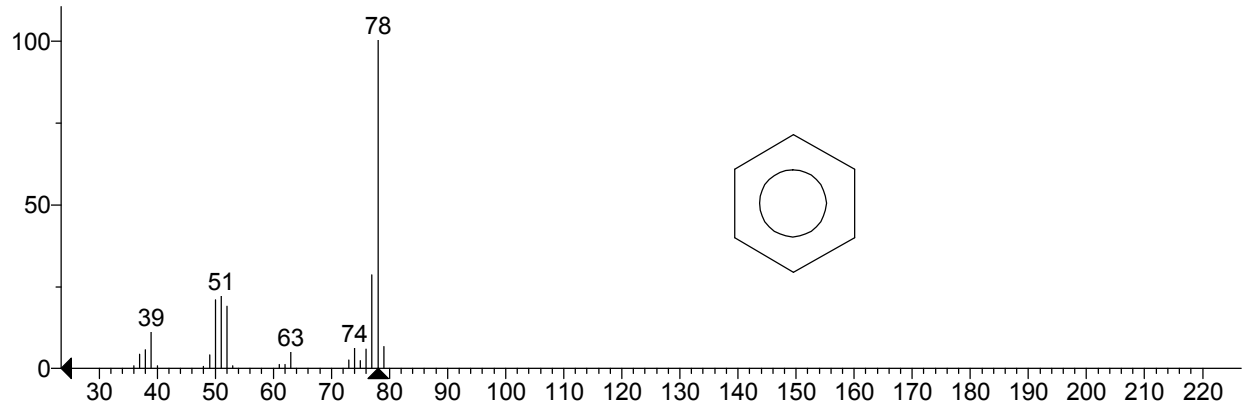
Hit 2 : 1-Hexene
C6H12; MF: 791; RMF: 801; Prob 6.86%; CAS: 592-41-6; Lib: mainlib; ID: 19842.



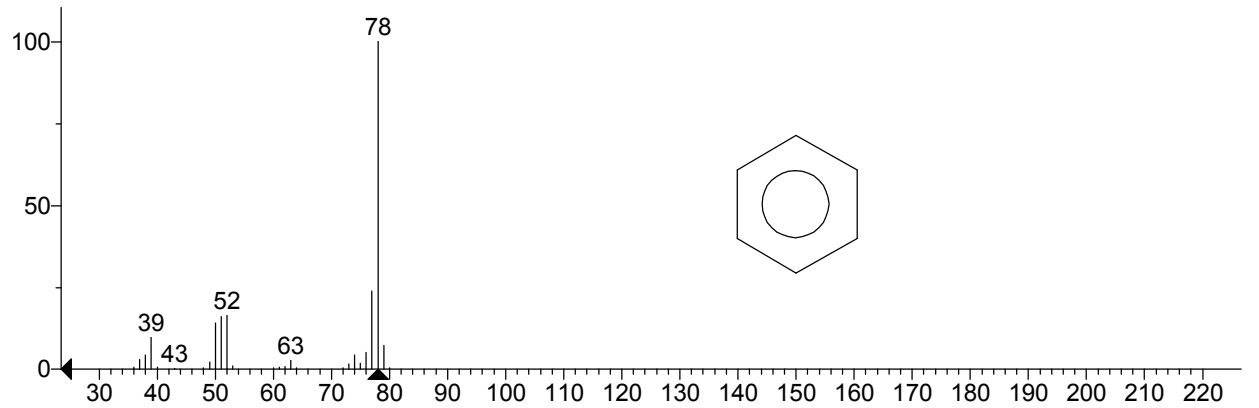
Unknown: Scan 128 (1.052 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -918



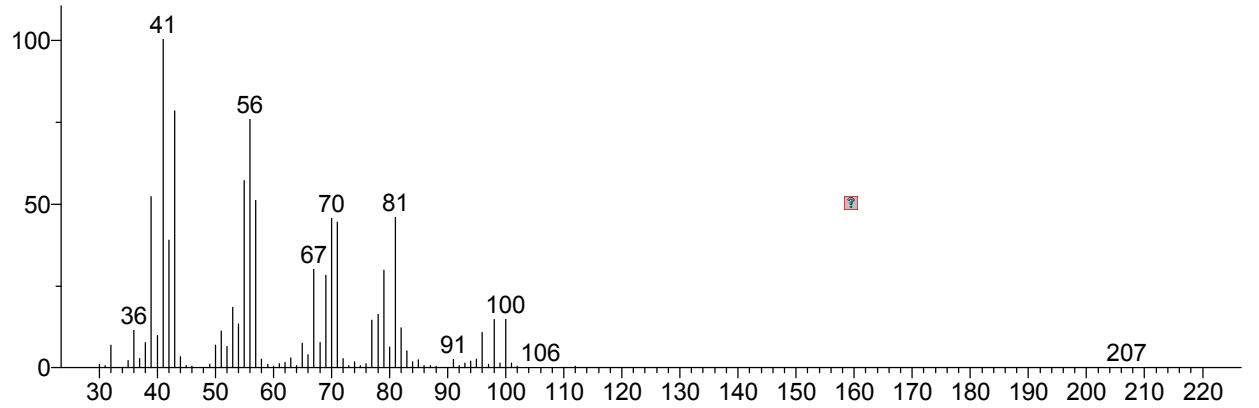
Hit 1 : Benzene
C6H6; MF: 692; RMF: 871; Prob 22.7%; CAS: 71-43-2; Lib: mainlib; ID: 41198.



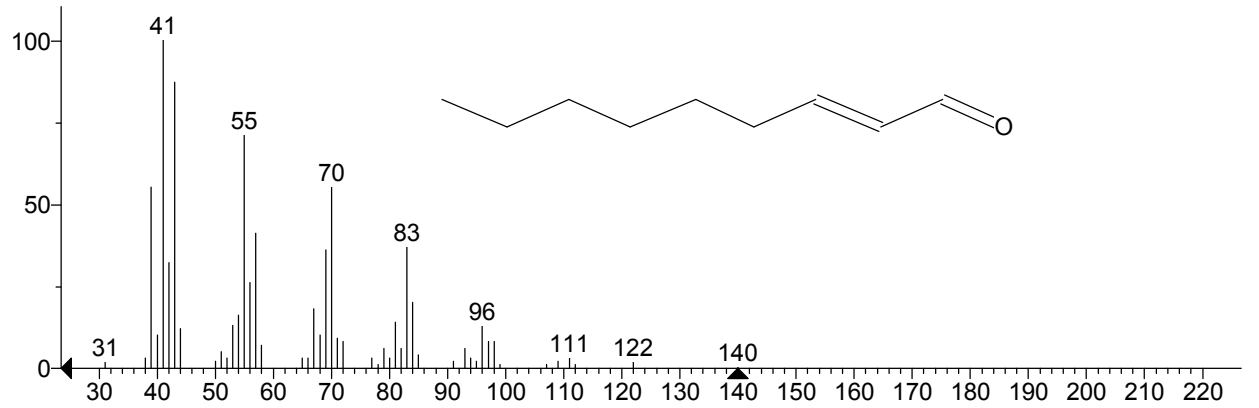
Hit 2 : Benzene
C6H6; MF: 676; RMF: 820; Prob 22.7%; CAS: 71-43-2; Lib: replib; ID: 9593.



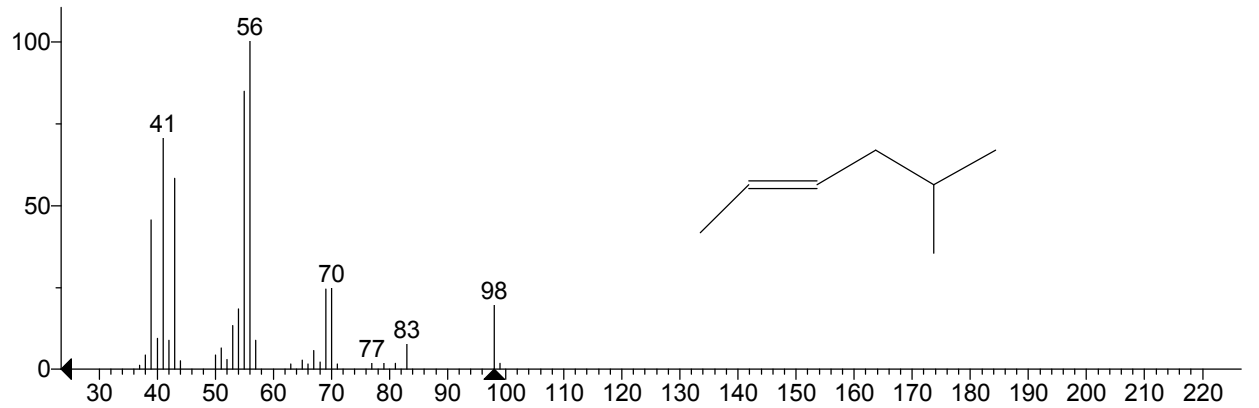
Unknown: Scan 133 (1.090 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -1131



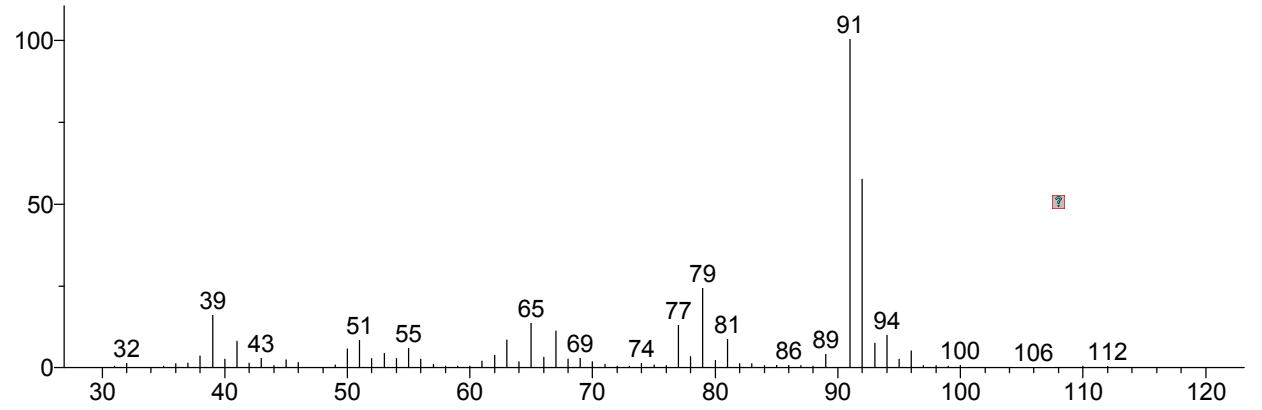
Hit 1 : 2-Nonenal, (E)-
C9H16O; MF: 724; RMF: 753; Prob 5.97%; CAS: 18829-56-6; Lib: replib; ID: 711.



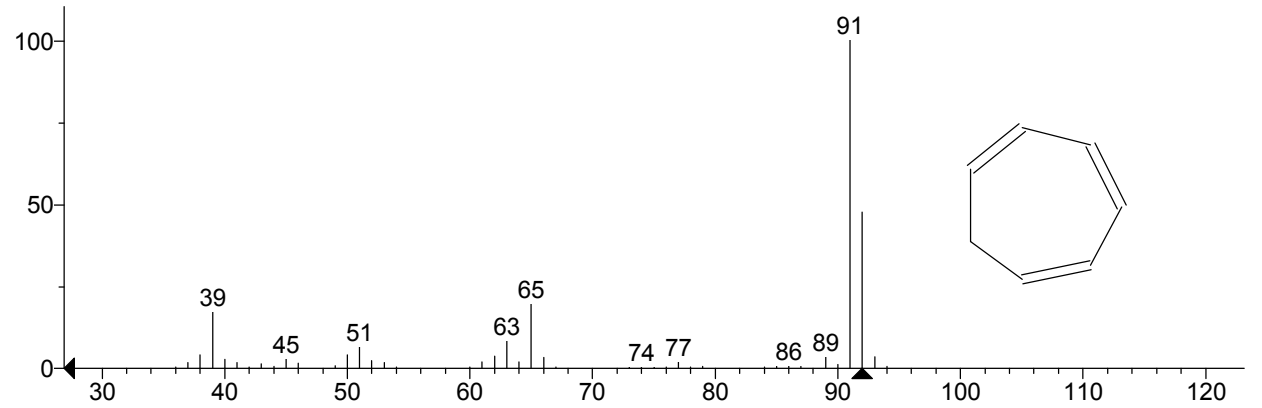
Hit 2 : 2-Hexene, 5-methyl-, (E)-
C7H14; MF: 715; RMF: 788; Prob 4.33%; CAS: 7385-82-2; Lib: replib; ID: 4947.



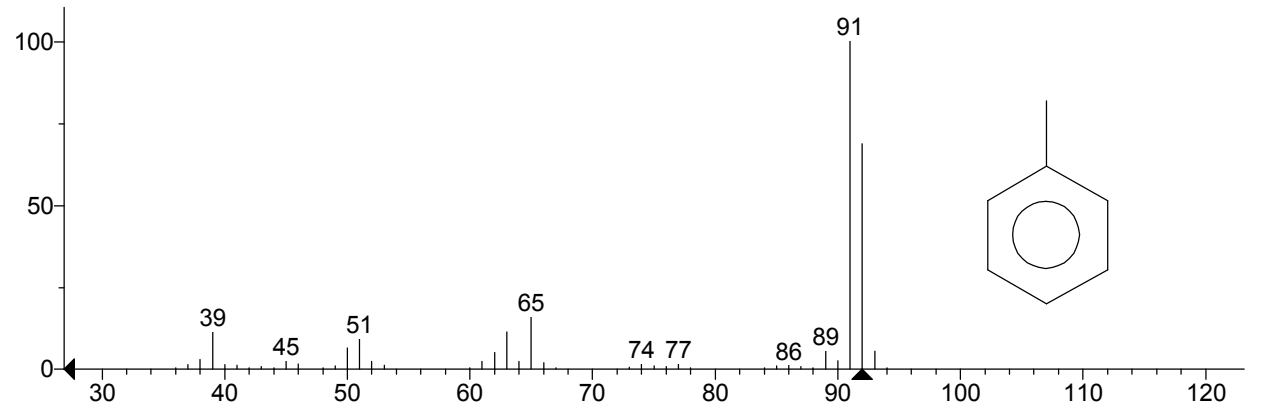
Unknown: Scan 141 (1.150 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -625



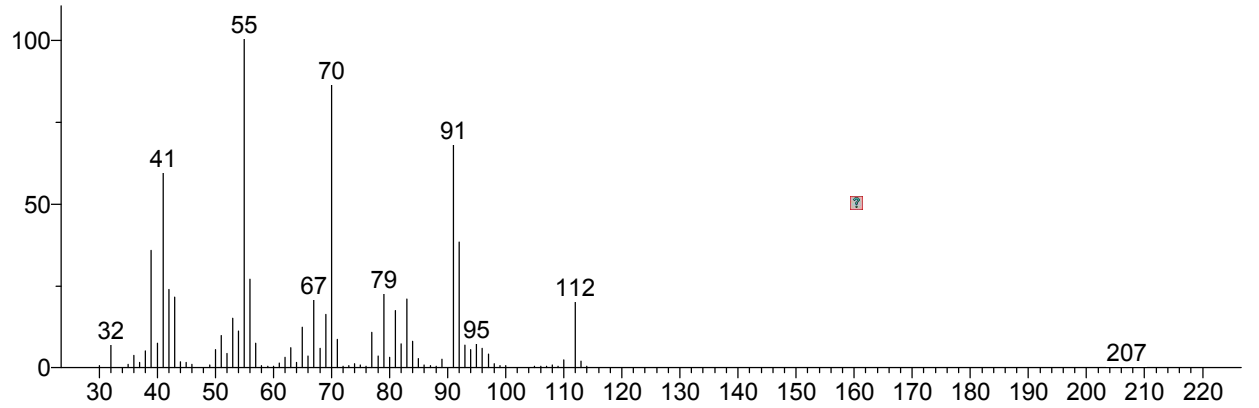
Hit 1 : 1,3,5-Cycloheptatriene
C7H8; MF: 763; RMF: 812; Prob 15.5%; CAS: 544-25-2; Lib: mainlib; ID: 51695.



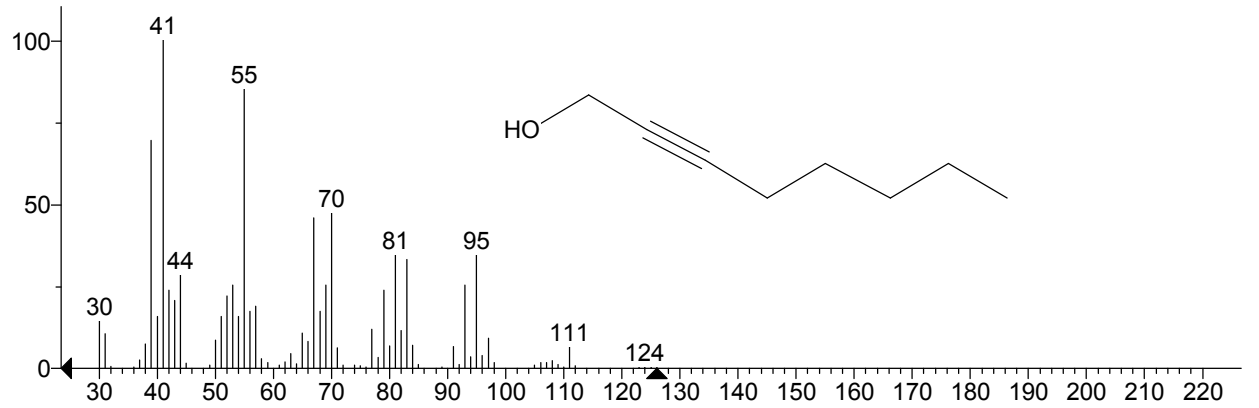
Hit 2 : Toluene
C7H8; MF: 751; RMF: 837; Prob 10.3%; CAS: 108-88-3; Lib: replib; ID: 11404.



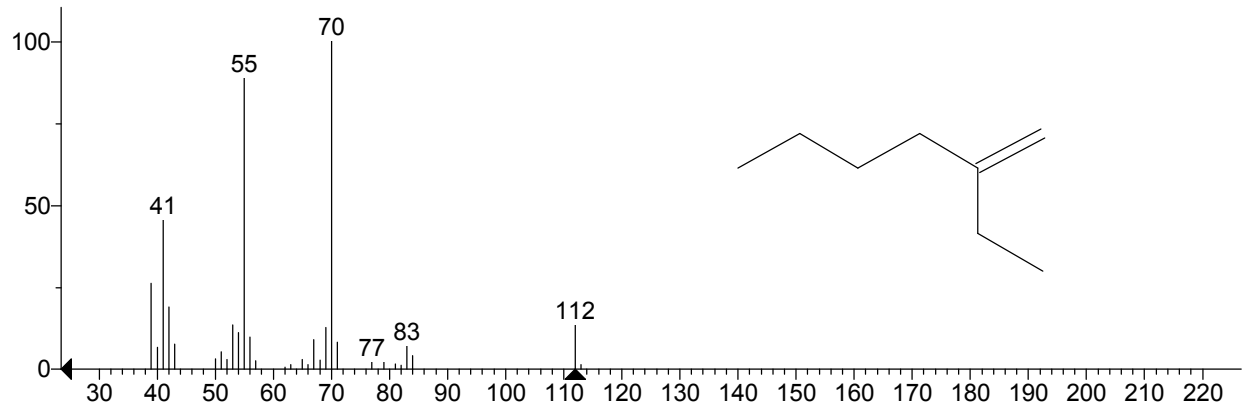
Unknown: Scan 148 (1.203 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -816



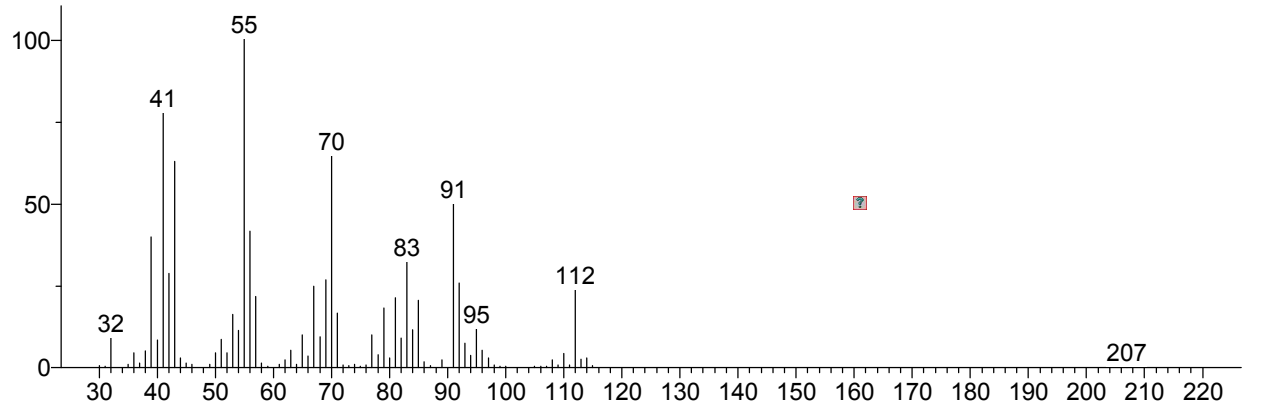
Hit 1 : 2-Octyn-1-ol
C8H14O; MF: 736; RMF: 740; Prob 8.05%; CAS: 20739-58-6; Lib: replib; ID: 871.



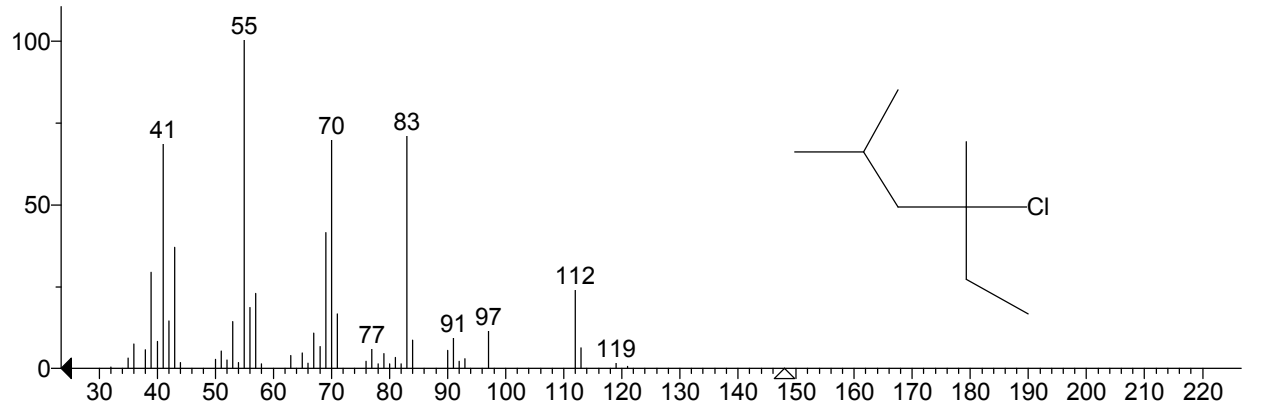
Hit 2 : Heptane, 3-methylene-
C8H16; MF: 734; RMF: 891; Prob 7.43%; CAS: 1632-16-2; Lib: replib; ID: 7908.



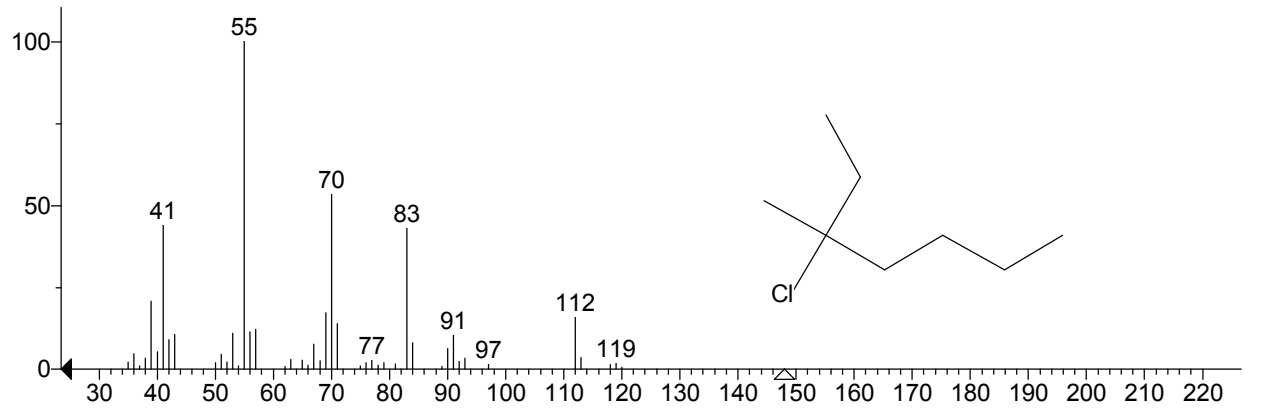
Unknown: Scan 150 (1.218 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -1103



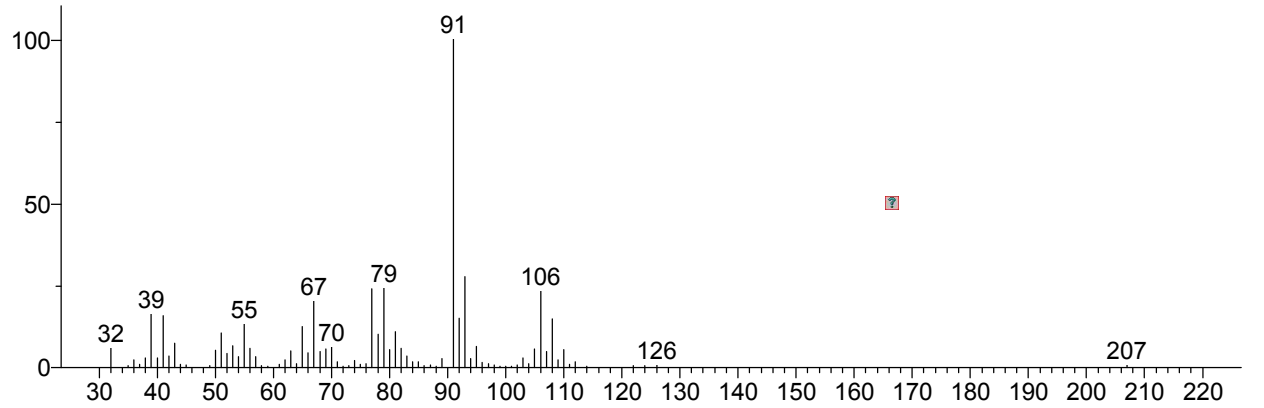
Hit 1 : 4-Chloro-2,4-dimethylhexane
C8H17Cl; MF: 748; RMF: 801; Prob 7.44%; CAS: 54059-76-6; Lib: mainlib; ID: 18865.



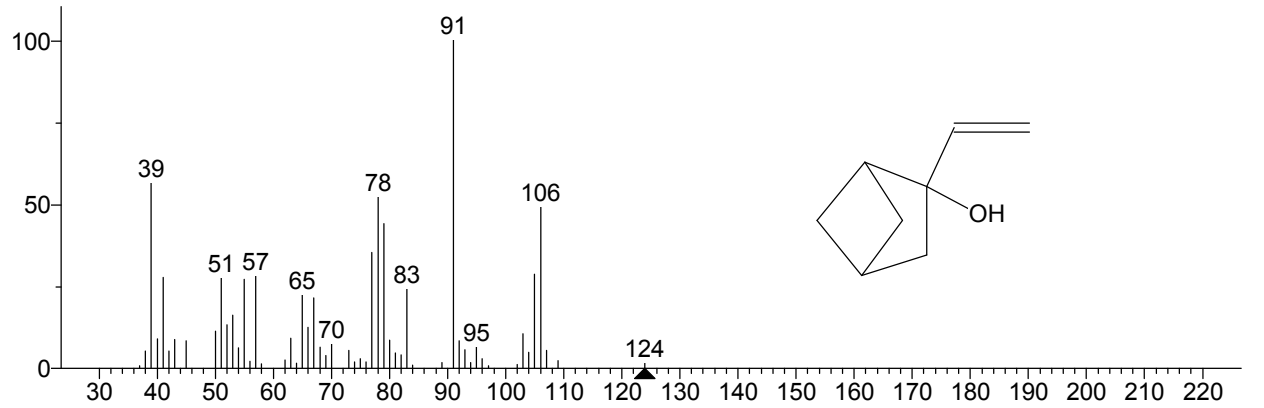
Hit 2 : Heptane, 3-chloro-3-methyl-
C8H17Cl; MF: 746; RMF: 806; Prob 6.86%; CAS: 5272-02-6; Lib: mainlib; ID: 18427.



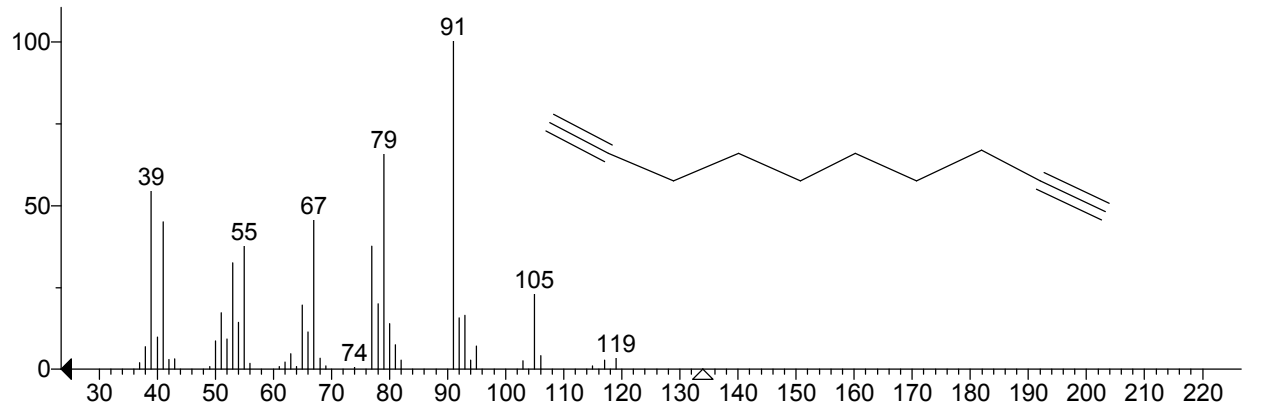
Unknown: Scan 164 (1.323 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -804



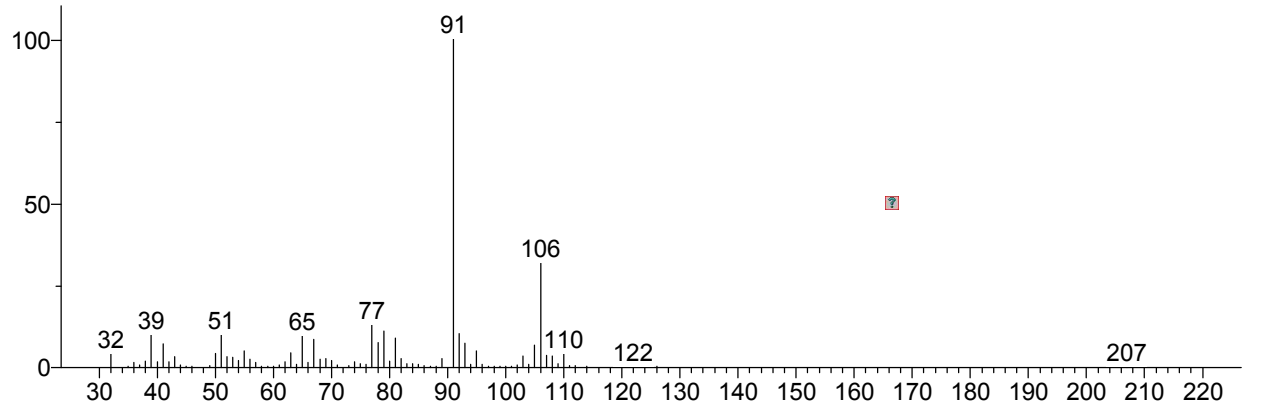
Hit 1 : Bicyclo[2.1.1]hexan-2-ol, 2-ethenyl-
C8H12O; MF: 749; RMF: 791; Prob 11.4%; Lib: mainlib; ID: 50226.



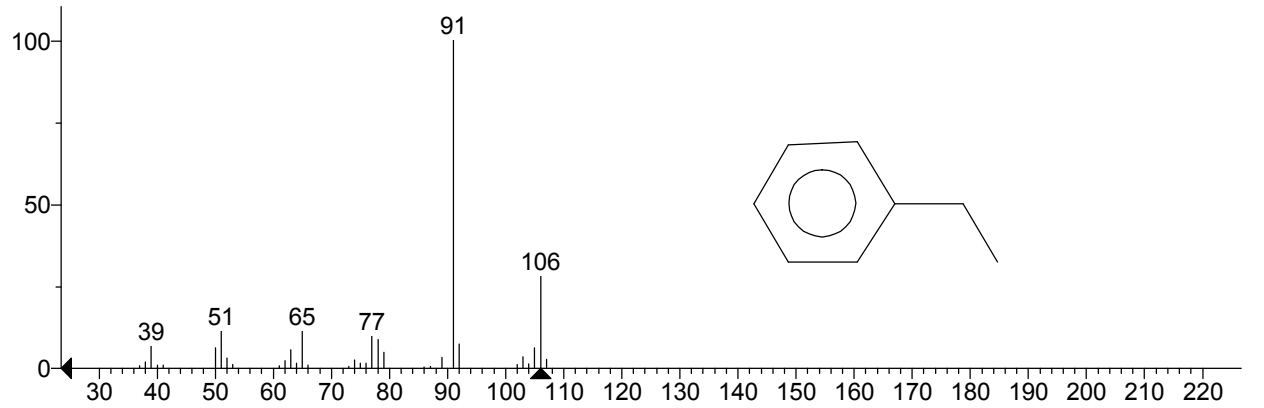
Hit 2 : 1,9-Decadiyne
C10H14; MF: 742; RMF: 821; Prob 8.73%; CAS: 1720-38-3; Lib: mainlib; ID: 51425.



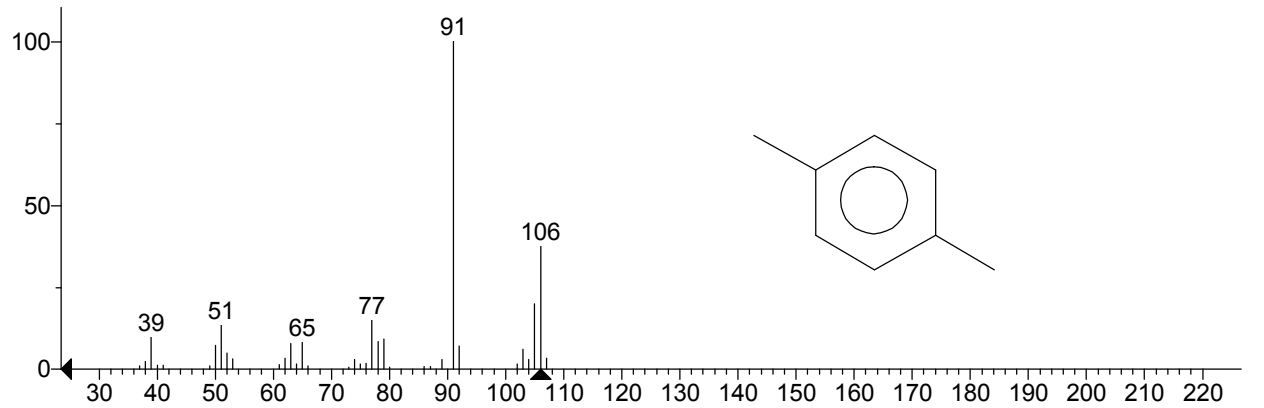
Unknown: Scan 167 (1.346 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -509



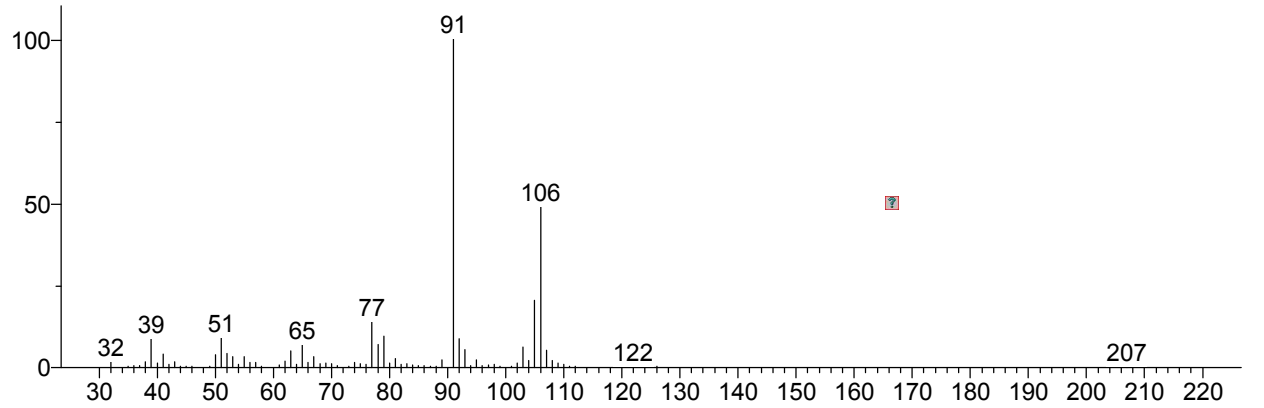
Hit 1 : Ethylbenzene
C8H10; MF: 793; RMF: 913; Prob 17.6%; CAS: 100-41-4; Lib: mainlib; ID: 52160.



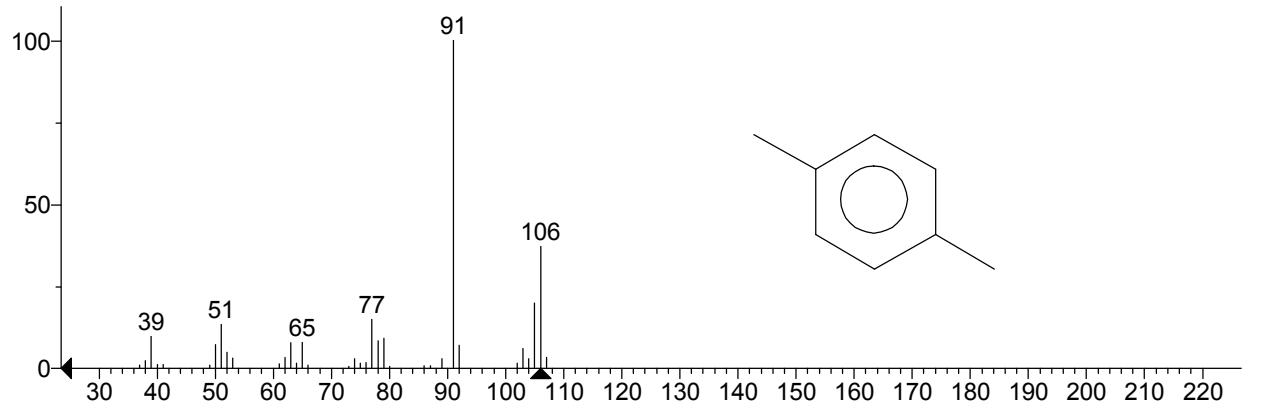
Hit 2 : p-Xylene
C8H10; MF: 792; RMF: 907; Prob 16.9%; CAS: 106-42-3; Lib: replib; ID: 11521.



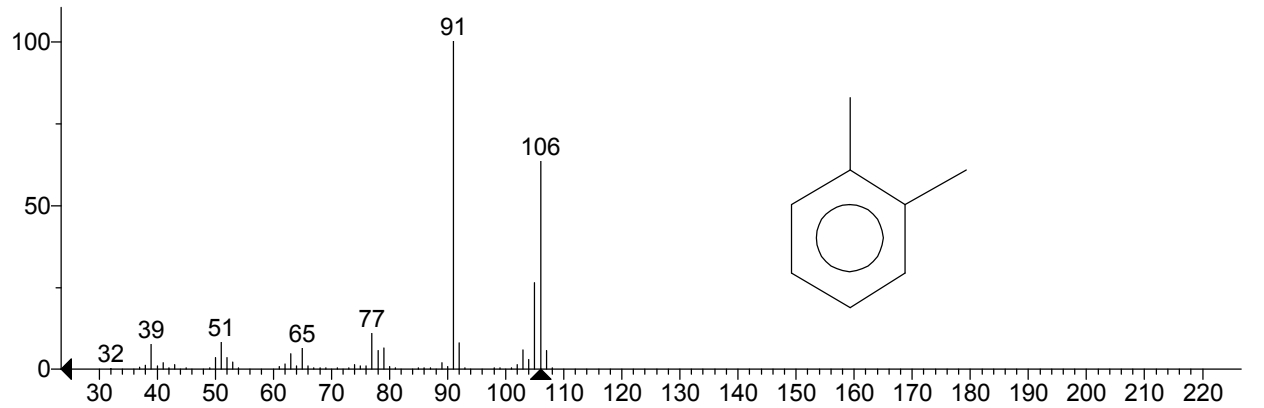
Unknown: Scan 172 (1.384 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -224



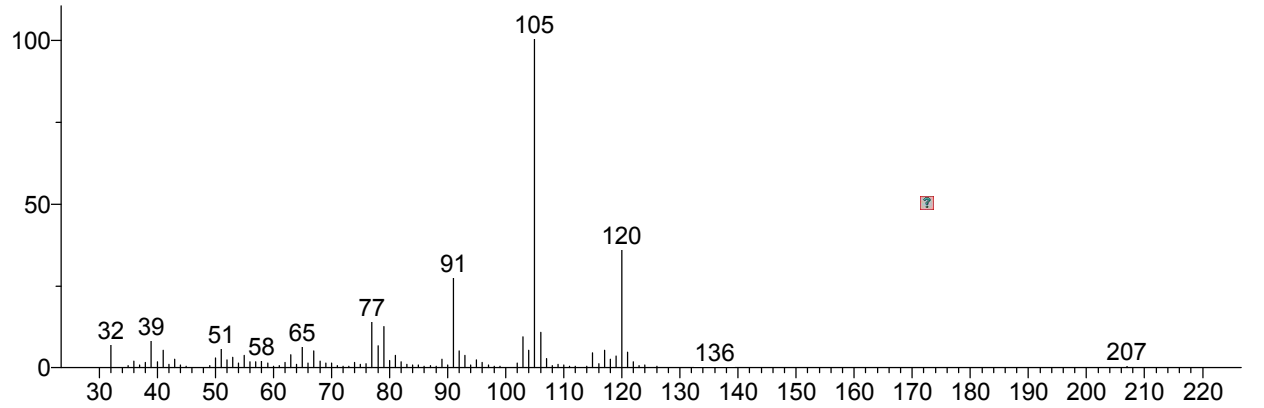
Hit 1 : p-Xylene
C8H10; MF: 870; RMF: 929; Prob 26.9%; CAS: 106-42-3; Lib: replib; ID: 11521.



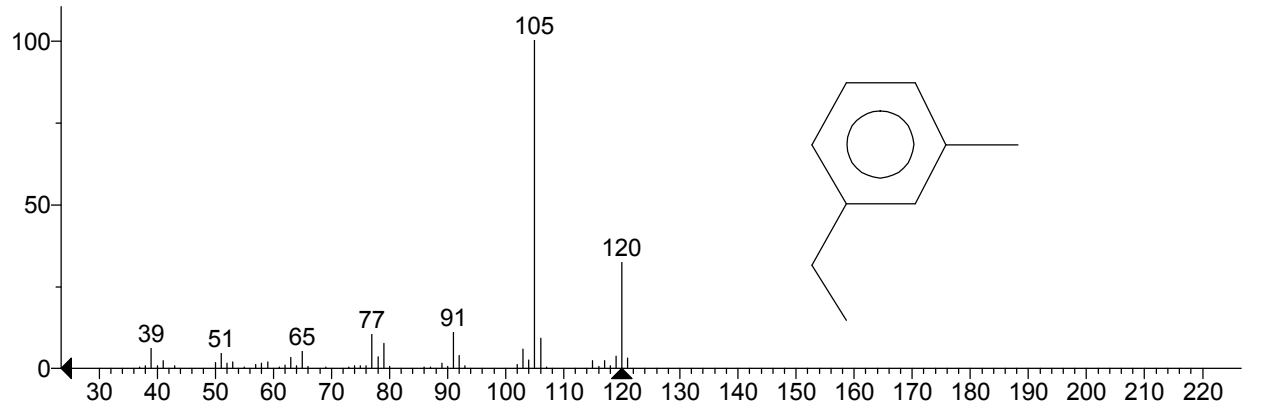
Hit 2 : o-Xylene
C8H10; MF: 862; RMF: 888; Prob 20.1%; CAS: 95-47-6; Lib: replib; ID: 11528.



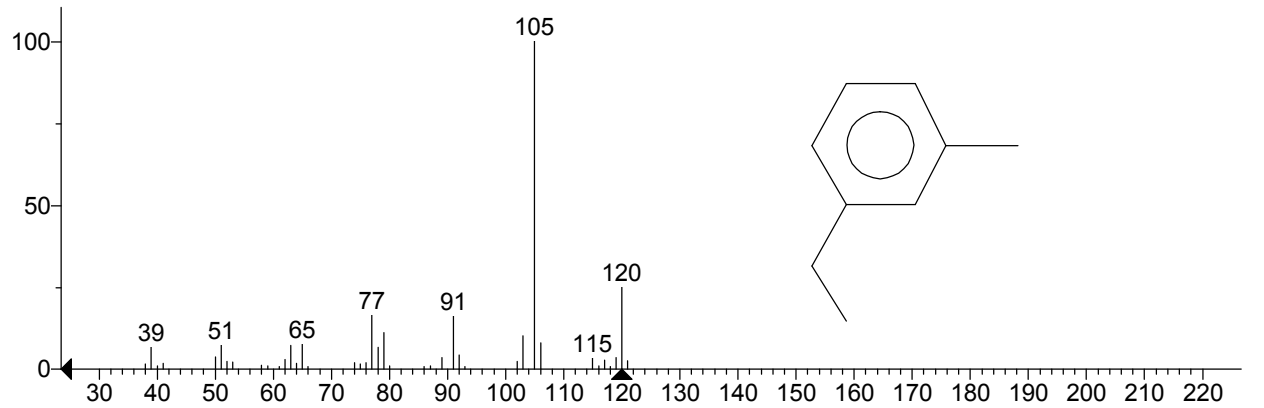
Unknown: Scan 211 (1.677 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -301



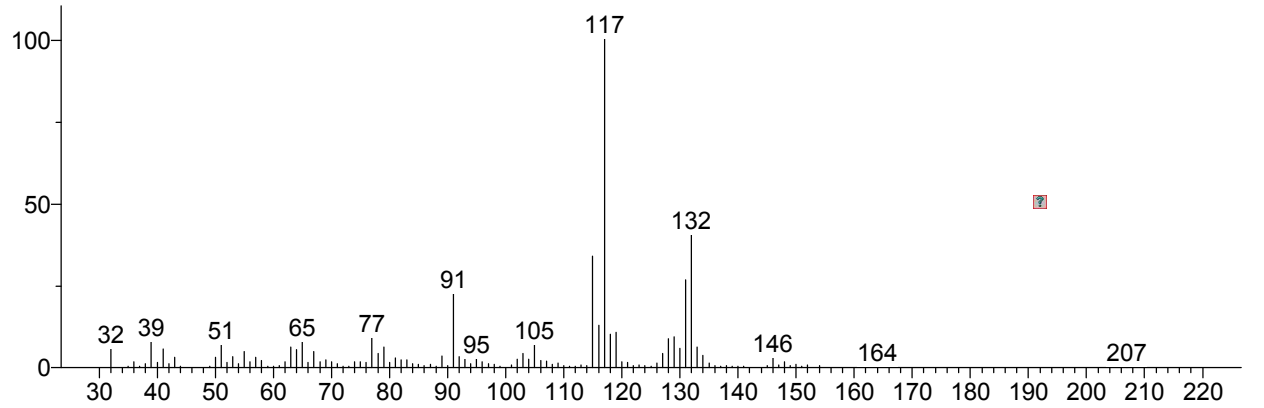
Hit 1 : Benzene, 1-ethyl-3-methyl-
C9H12; MF: 842; RMF: 893; Prob 19.2%; CAS: 620-14-4; Lib: mainlib; ID: 68592.



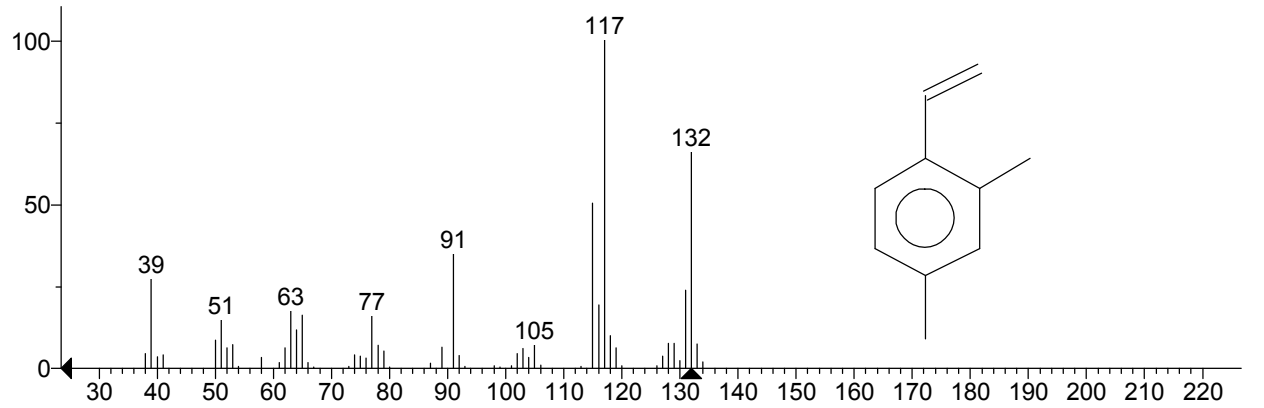
Hit 2 : Benzene, 1-ethyl-3-methyl-
C9H12; MF: 833; RMF: 910; Prob 19.2%; CAS: 620-14-4; Lib: replib; ID: 14016.



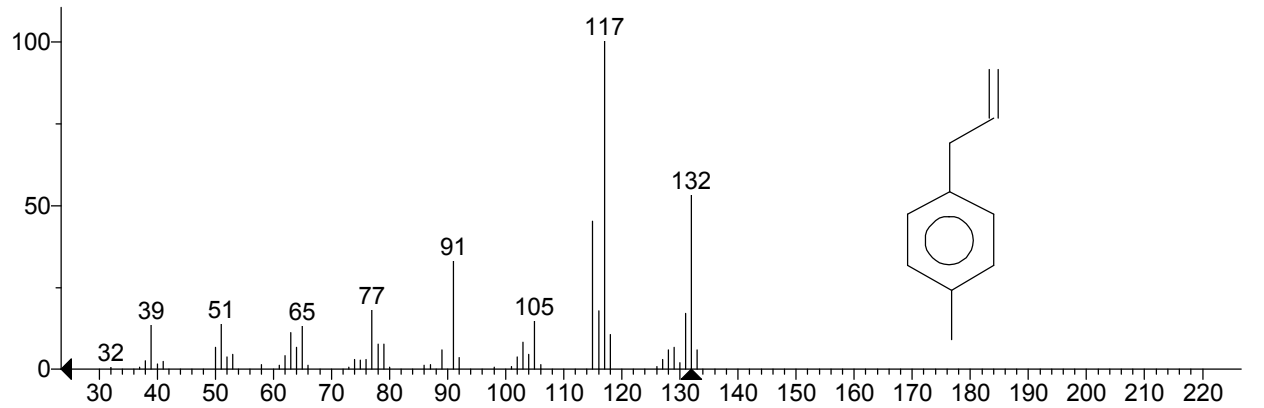
Unknown: Scan 309 (2.416 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -367



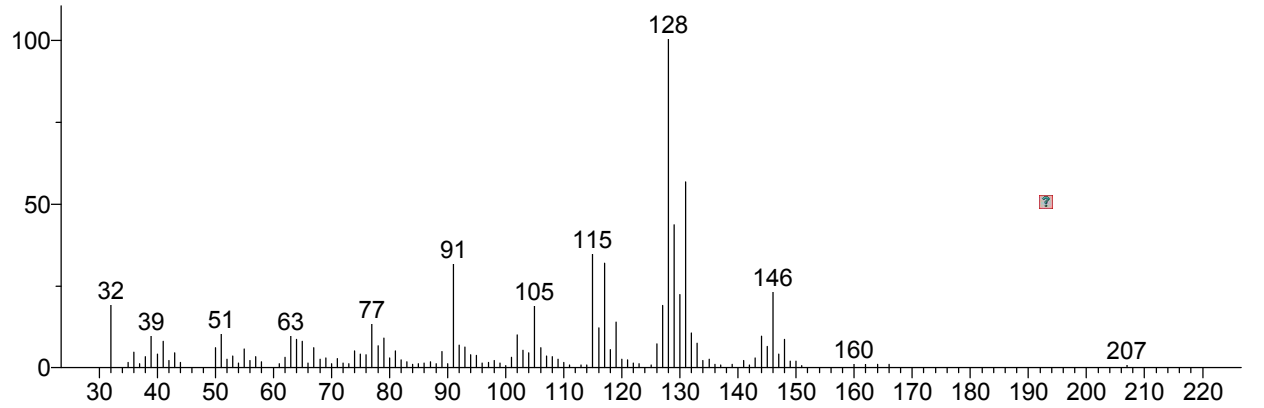
Hit 1 : 2,4-Dimethylstyrene
C10H12; MF: 828; RMF: 889; Prob 11.3%; CAS: 2234-20-0; Lib: mainlib; ID: 79184.



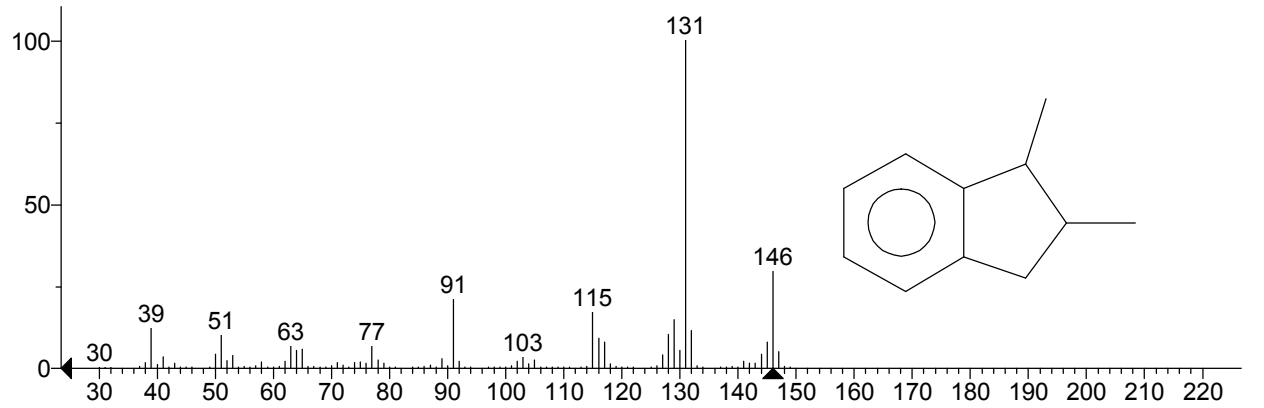
Hit 2 : Benzene, 1-methyl-4-(2-propenyl)-
C10H12; MF: 825; RMF: 915; Prob 10.0%; CAS: 3333-13-9; Lib: mainlib; ID: 79179.



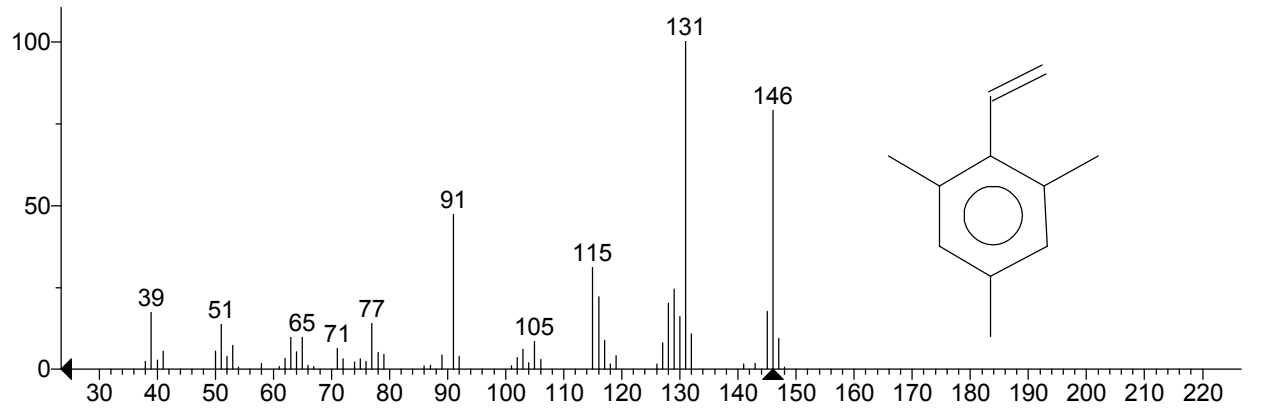
Unknown: Scan 347 (2.702 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -825



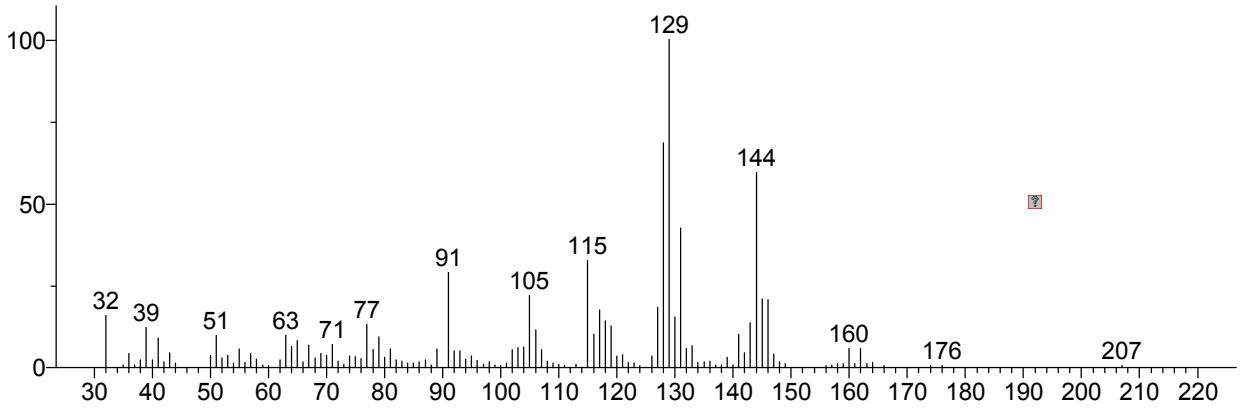
Hit 1 : 1H-Indene, 2,3-dihydro-1,2-dimethyl-
C11H14; MF: 730; RMF: 743; Prob 13.0%; CAS: 17057-82-8; Lib: mainlib; ID: 93604.



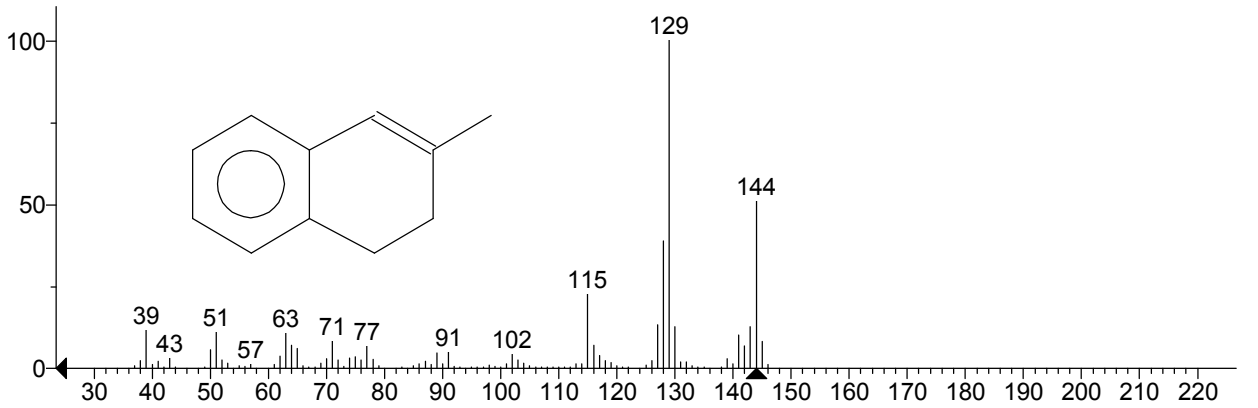
Hit 2 : Benzene, 2-ethenyl-1,3,5-trimethyl-
C11H14; MF: 716; RMF: 789; Prob 8.10%; CAS: 769-25-5; Lib: mainlib; ID: 93610.



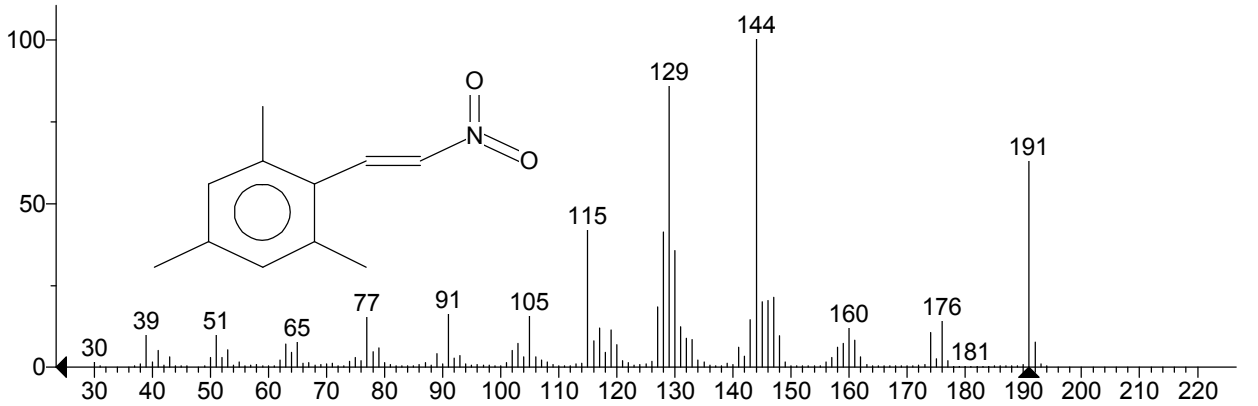
Unknown: Scan 402 (3.117 min): J9163_PVC_Clear_portion_A_py2.D\data.ms
Compound in Library Factor = -804



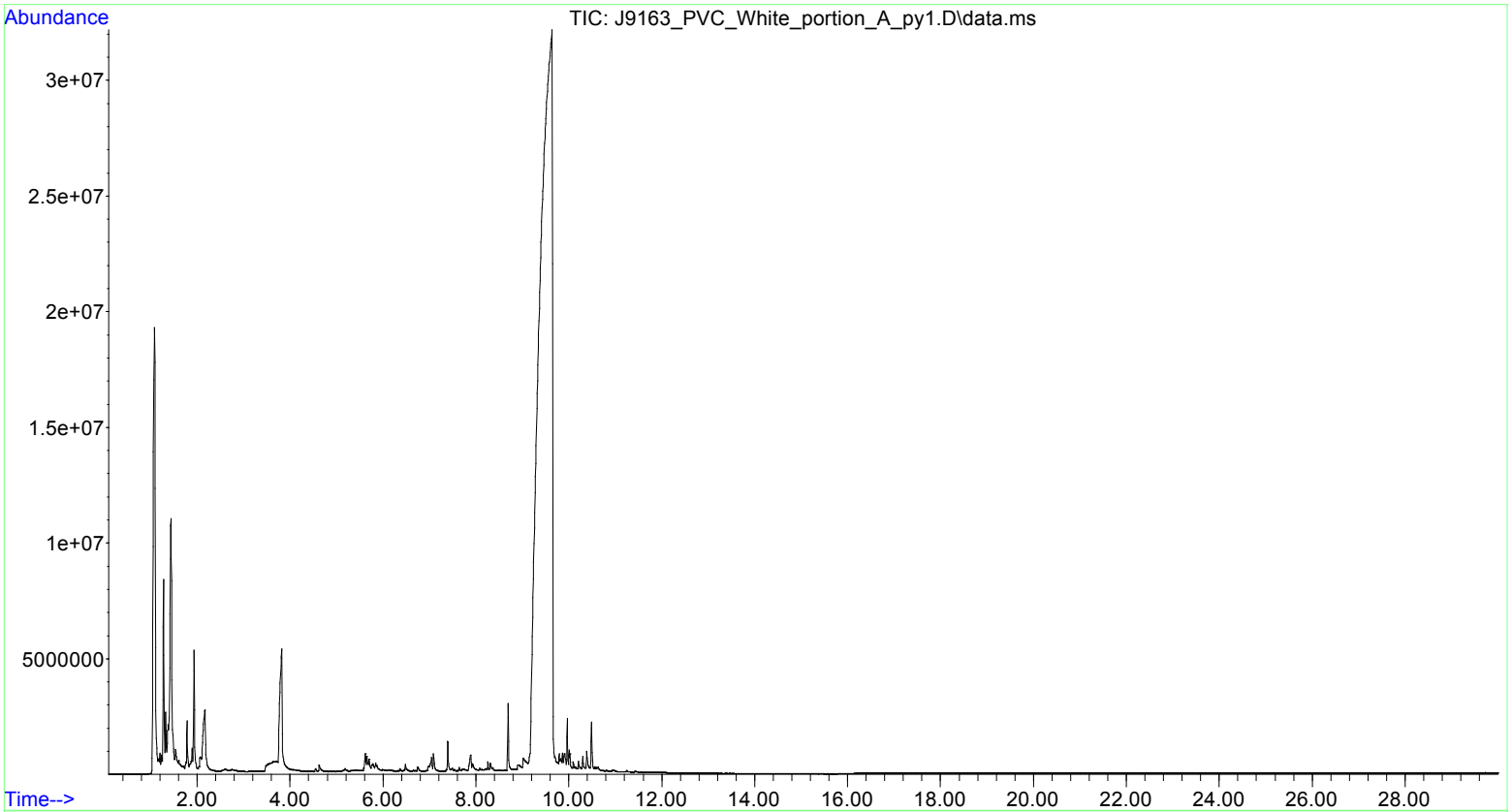
Hit 1 : Naphthalene, 1,2-dihydro-3-methyl-
C11H12; MF: 746; RMF: 784; Prob 13.2%; CAS: 2717-44-4; Lib: mainlib; ID: 91866.

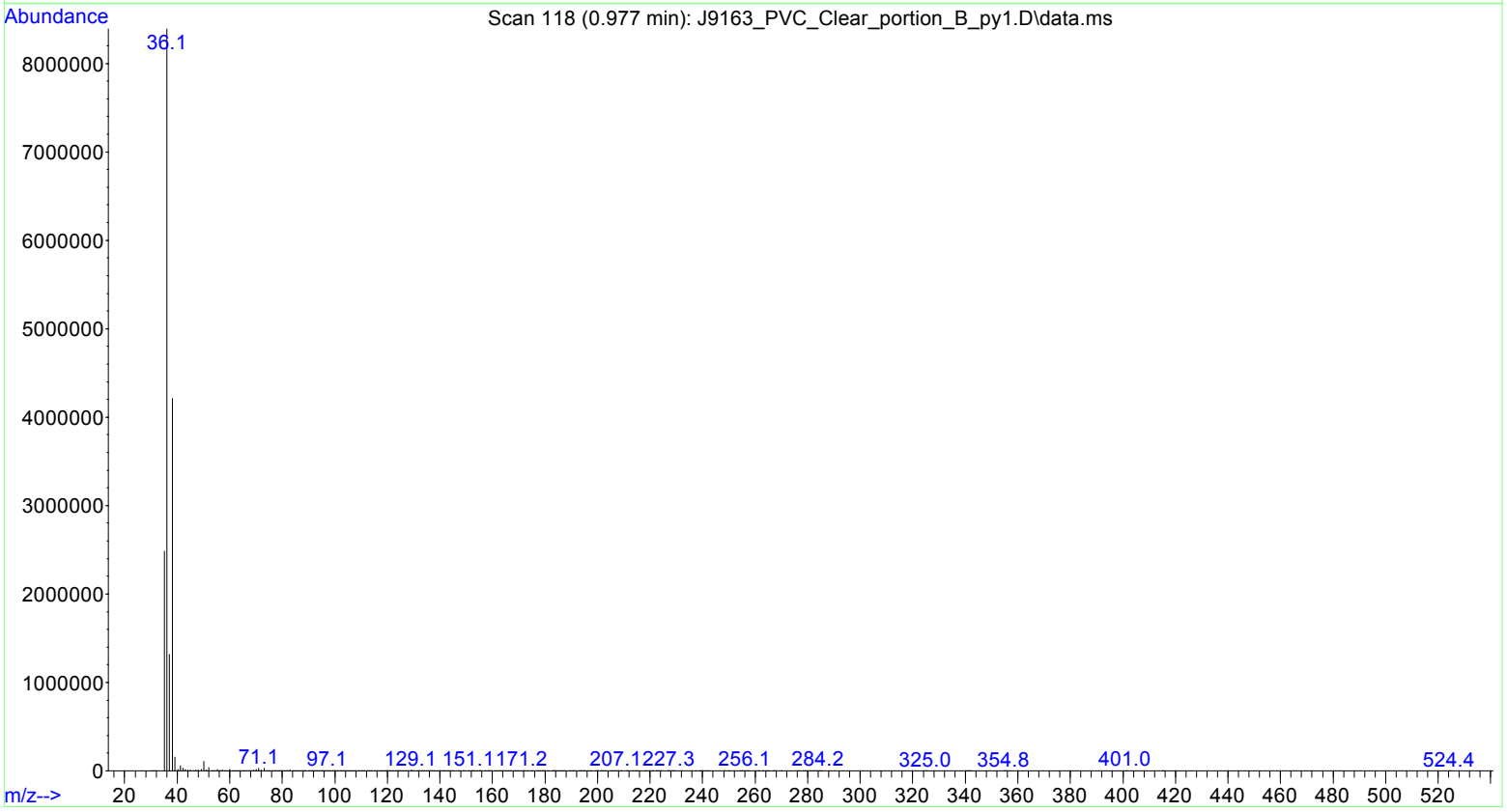


Hit 2 : 1,3,5-Trimethyl-2-(2-nitrovinyl)benzene
C11H13NO2; MF: 742; RMF: 746; Prob 11.1%; Lib: mainlib; ID: 106101.

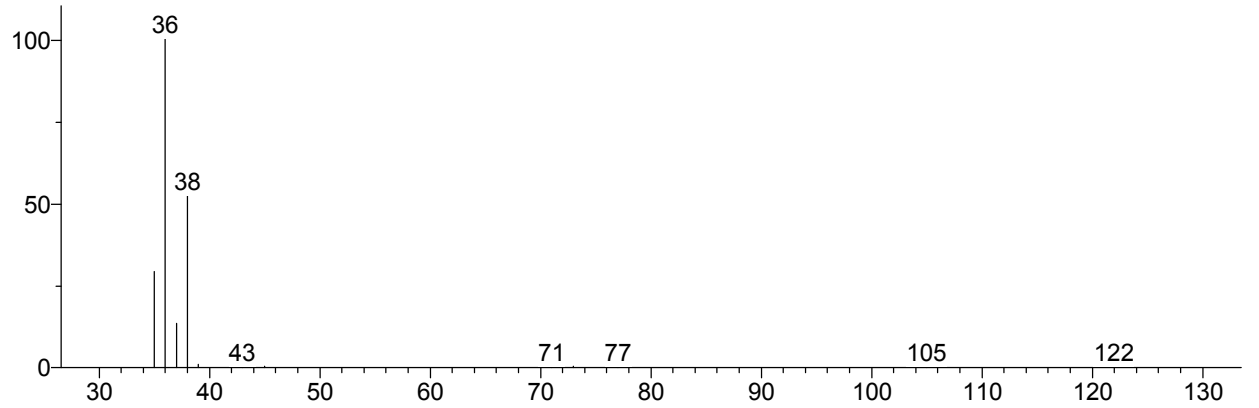


File :C:\msdchem\1\DATA\2014\J9163 Jordi\111114\J9163_PVC_White_po
... rtion_A_py1.D
Operator : Courtney McGowan
Instrument : Instrument #1
Acquired : 11 Nov 2014 21:26 using AcqMethod PYMSSP30.M
Sample Name: J9163 PVC White portion
Misc Info : J9163 PVC White portion

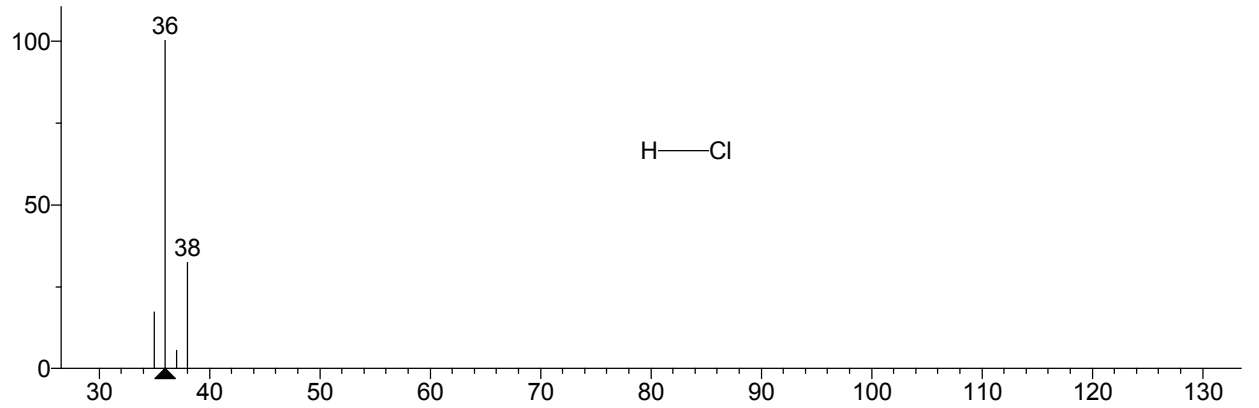




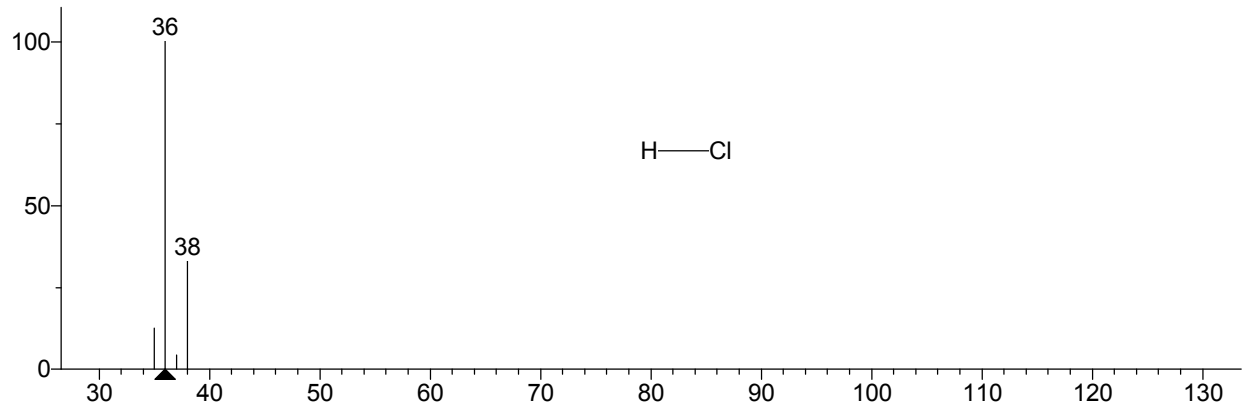
Unknown: Scan 131 (1.075 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 280



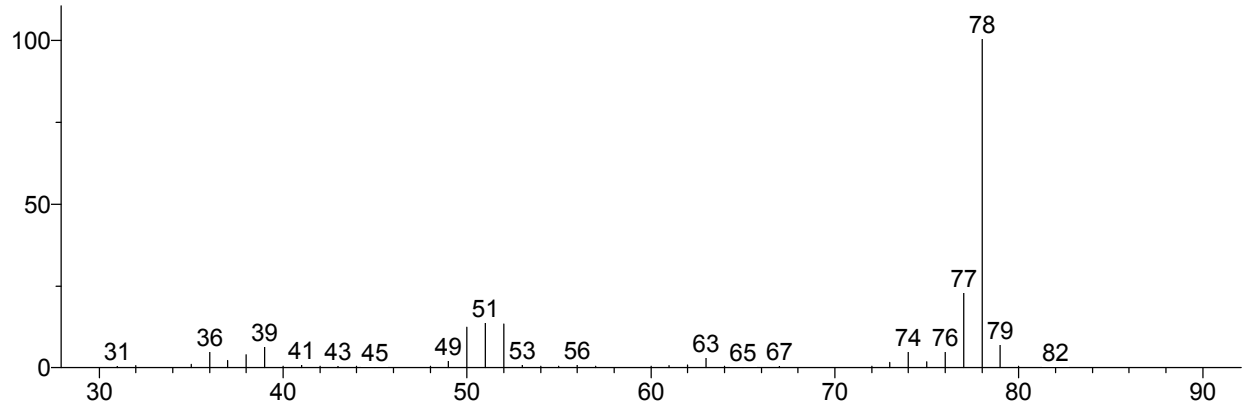
Hit 1 : Hydrogen chloride
ClH; MF: 869; RMF: 875; Prob 99.0%; CAS: 7647-01-0; Lib: mainlib; ID: 1496.



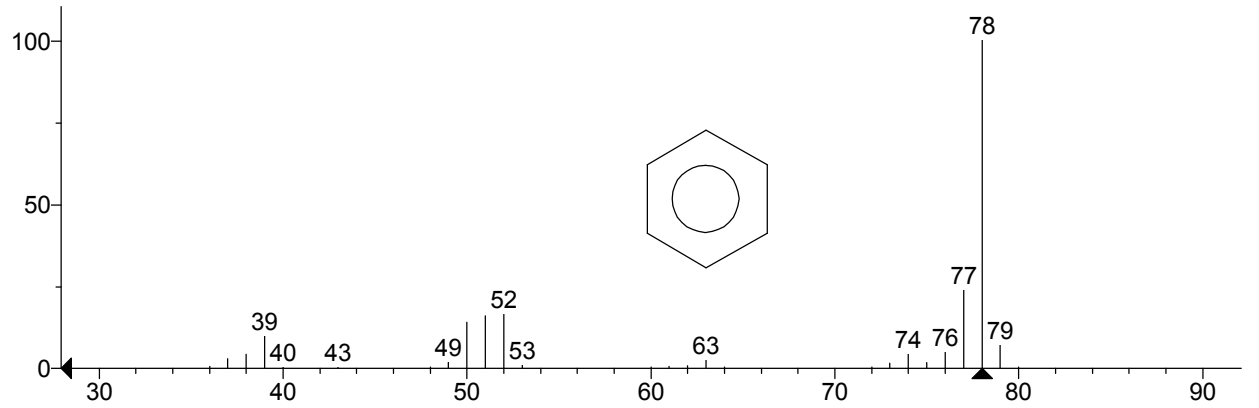
Hit 2 : Hydrogen chloride
ClH; MF: 819; RMF: 824; Prob 99.0%; CAS: 7647-01-0; Lib: replib; ID: 634.



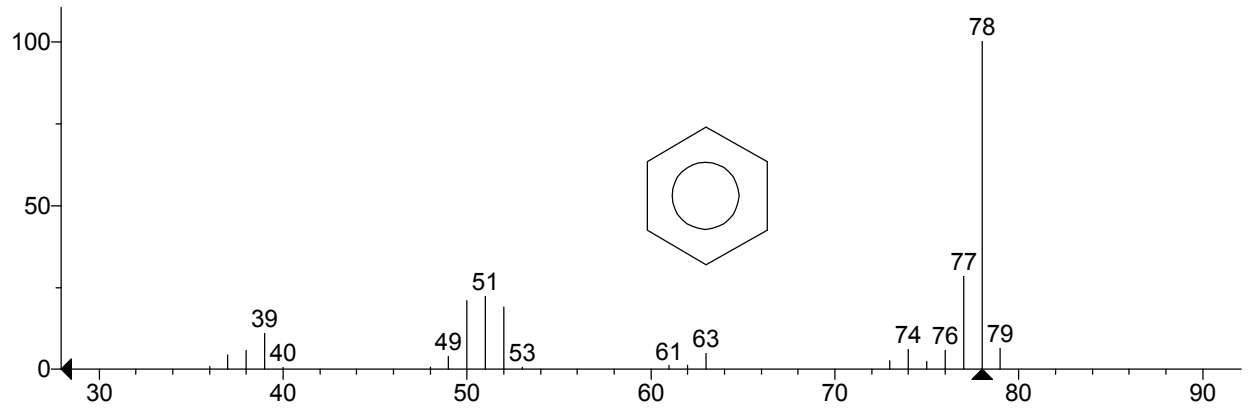
Unknown: Scan 159 (1.286 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 189



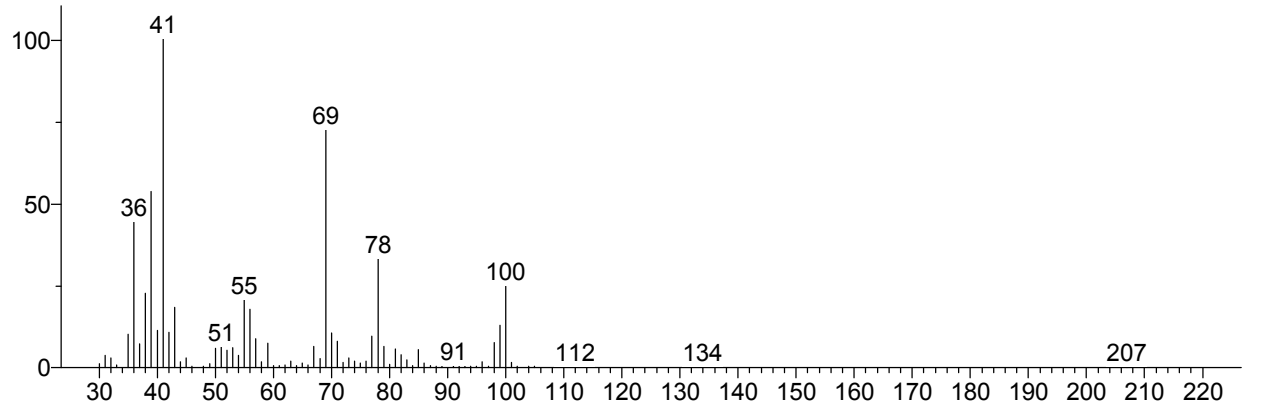
Hit 1 : Benzene
C6H6; MF: 946; RMF: 953; Prob 75.8%; CAS: 71-43-2; Lib: replib; ID: 9593.



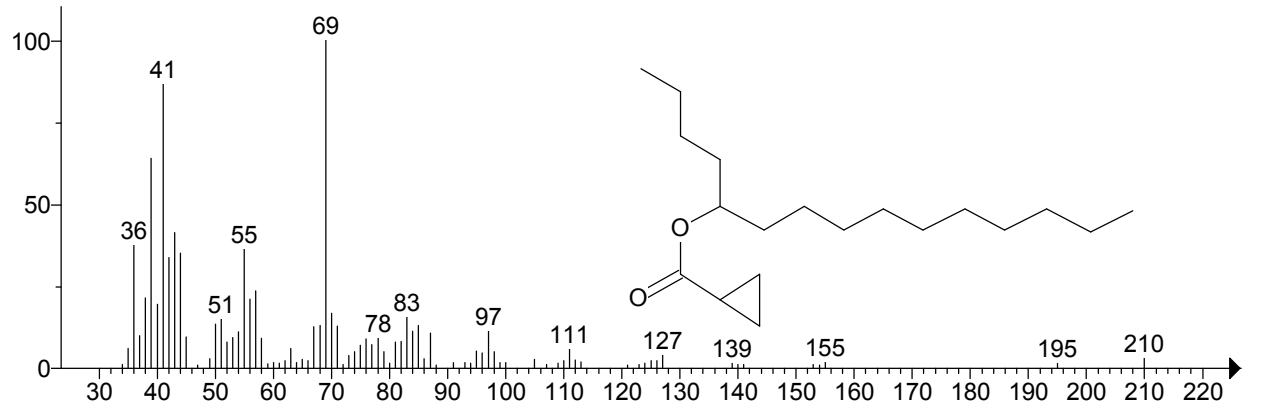
Hit 2 : Benzene
C6H6; MF: 941; RMF: 950; Prob 75.8%; CAS: 71-43-2; Lib: mainlib; ID: 41198.



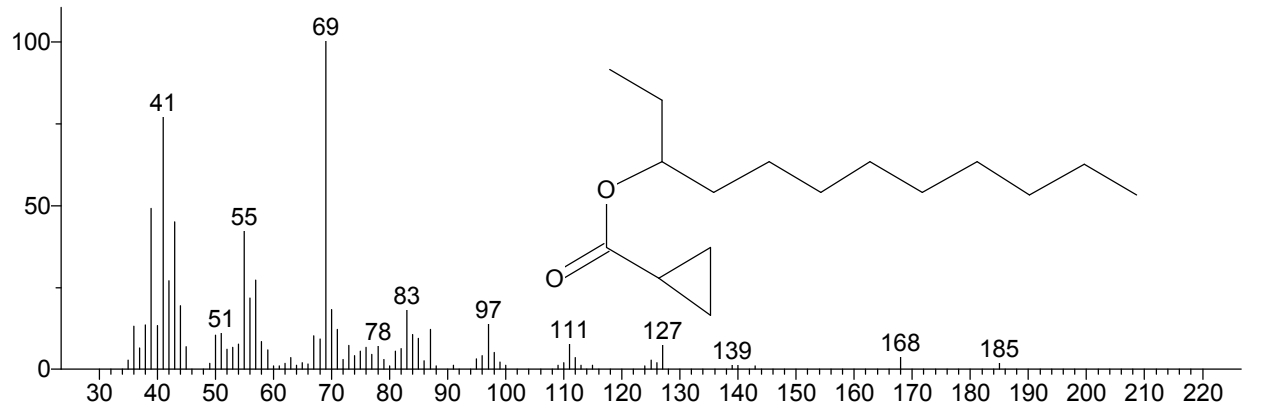
Unknown: Scan 163 (1.316 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = -1381



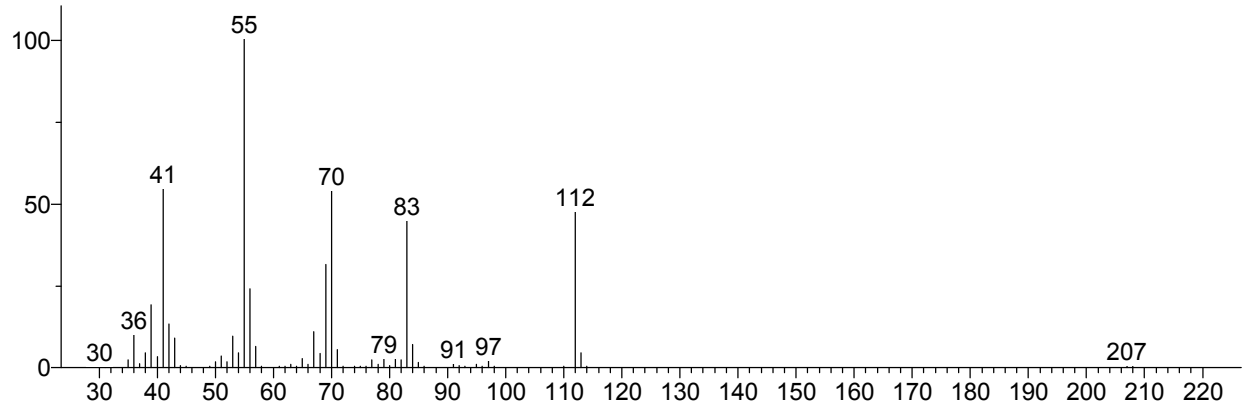
Hit 1 : 5-Cyclopropylcarbonyloxypentadecane
C19H36O2; MF: 692; RMF: 695; Prob 8.62%; Lib: mainlib; ID: 29786.



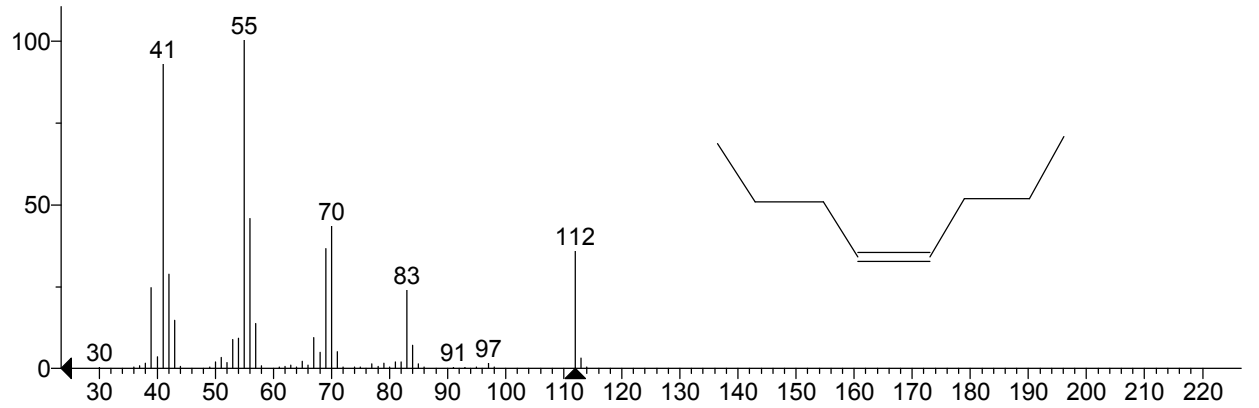
Hit 2 : 3-Cyclopropylcarbonyloxydodecane
C16H30O2; MF: 690; RMF: 692; Prob 7.95%; Lib: mainlib; ID: 29777.



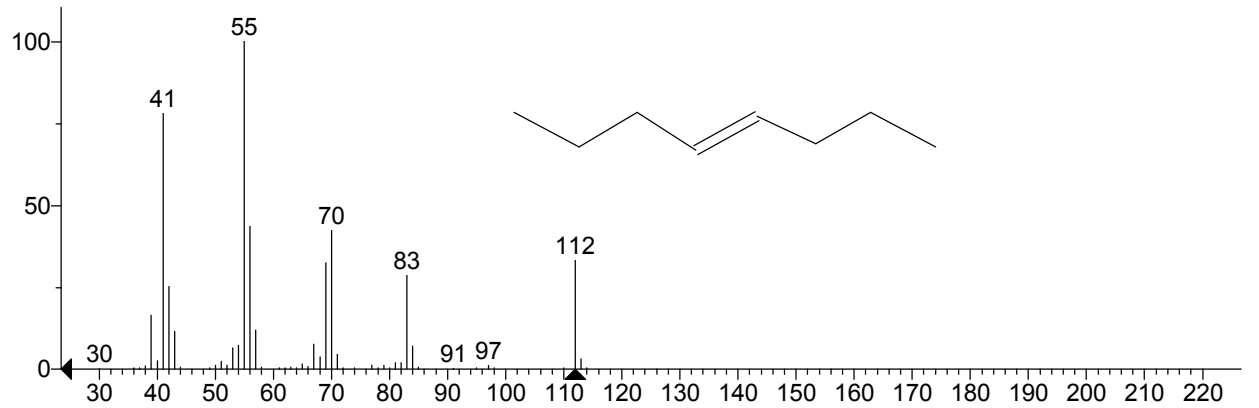
Unknown: Scan 179 (1.436 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = -151



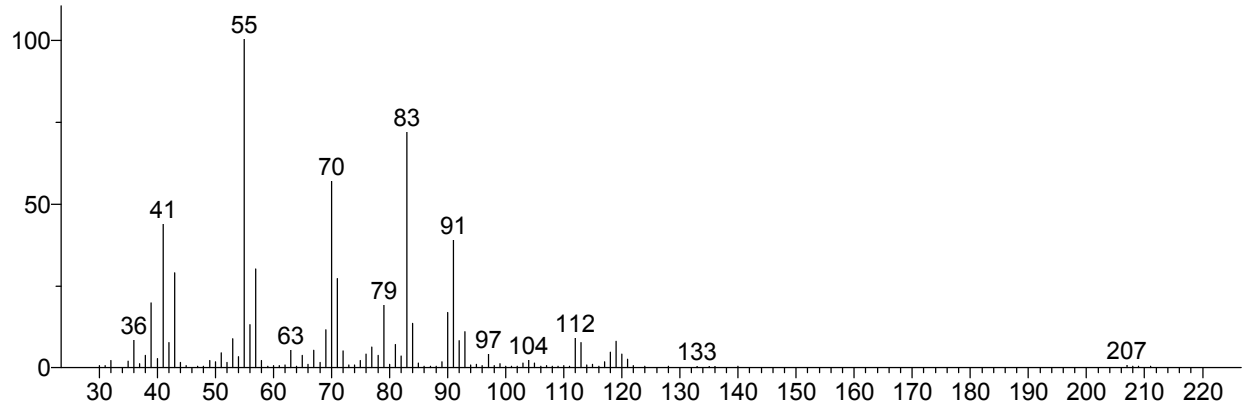
Hit 1 : 4-Octene, (Z)-
C8H16; MF: 893; RMF: 897; Prob 17.2%; CAS: 7642-15-1; Lib: mainlib; ID: 17325.



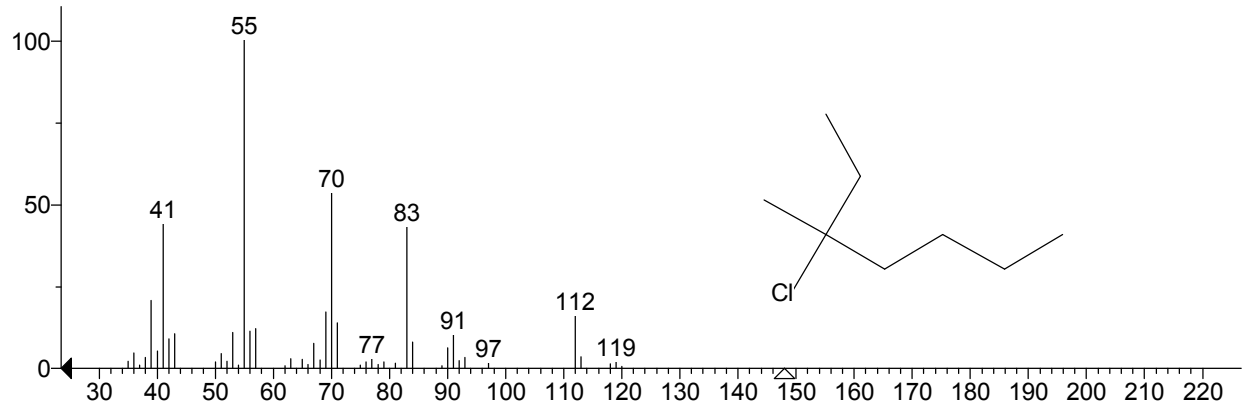
Hit 2 : 4-Octene, (E)-
C8H16; MF: 890; RMF: 893; Prob 15.2%; CAS: 14850-23-8; Lib: mainlib; ID: 17340.



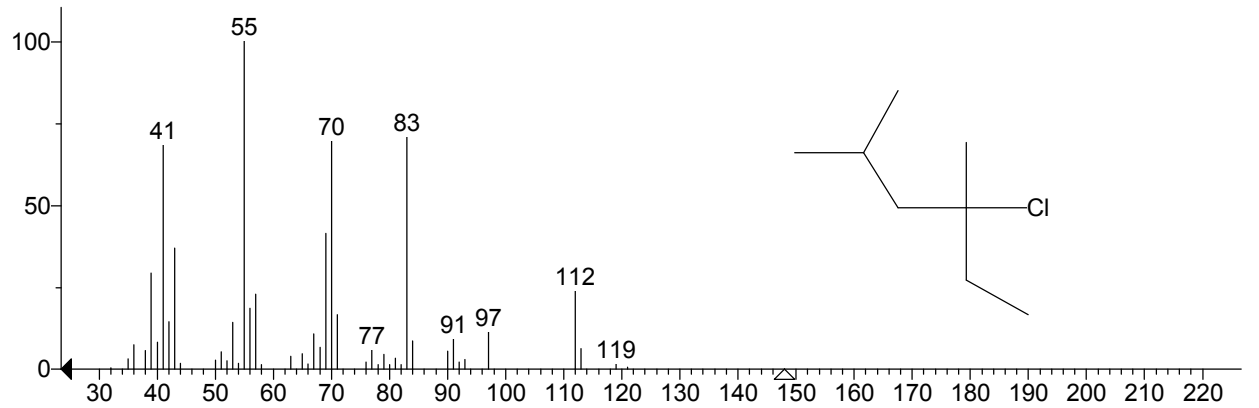
Unknown: Scan 225 (1.783 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = -172



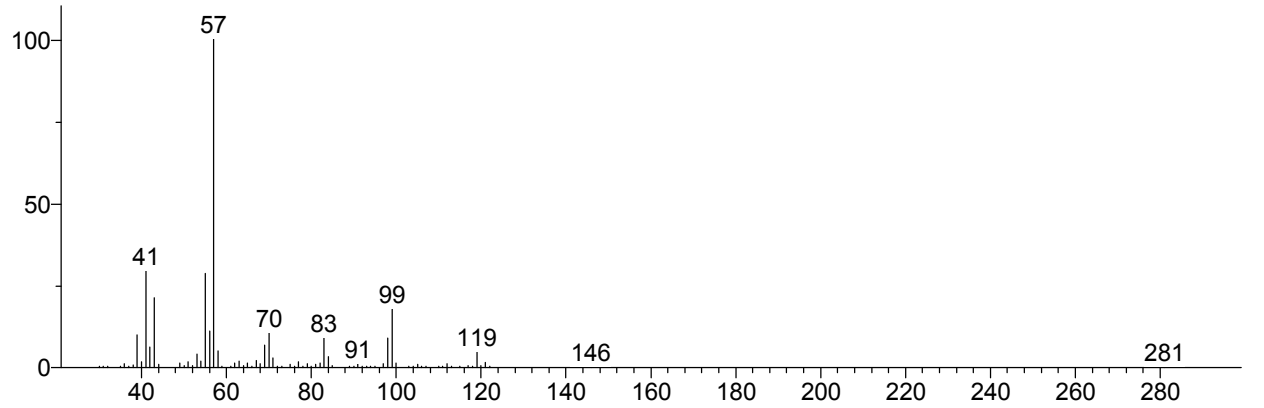
Hit 1 : Heptane, 3-chloro-3-methyl-
C8H17Cl; MF: 835; RMF: 874; Prob 73.1%; CAS: 5272-02-6; Lib: mainlib; ID: 18427.



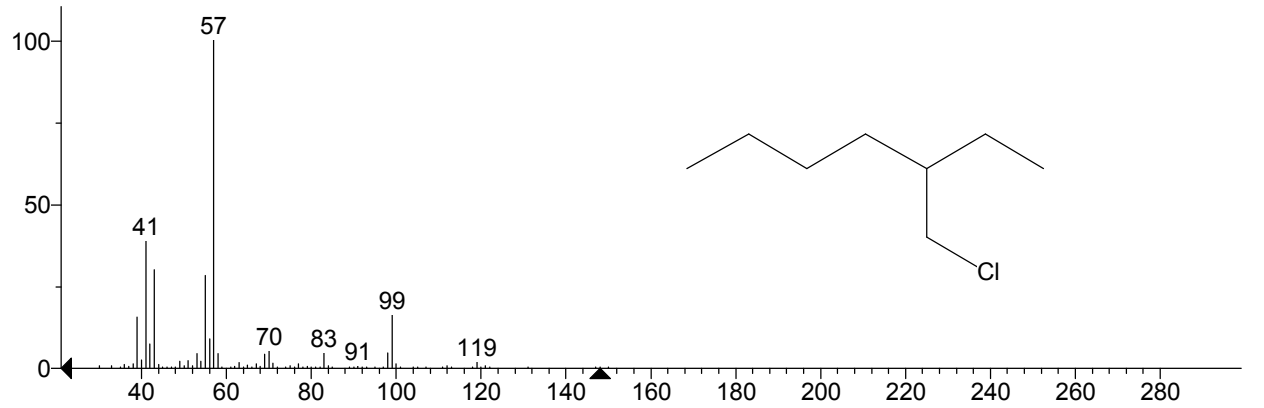
Hit 2 : 4-Chloro-2,4-dimethylhexane
C8H17Cl; MF: 794; RMF: 838; Prob 16.7%; CAS: 54059-76-6; Lib: mainlib; ID: 18865.



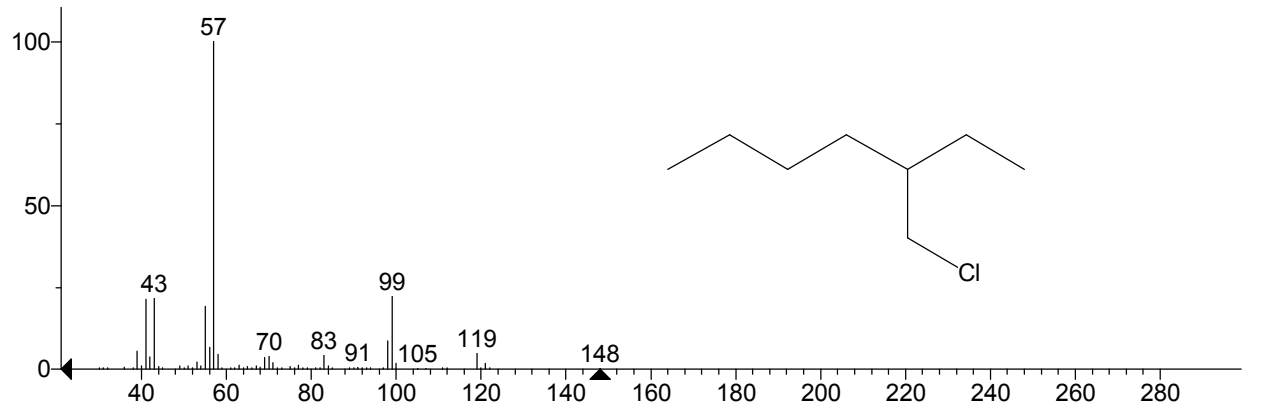
Unknown: Scan 245 (1.934 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 177



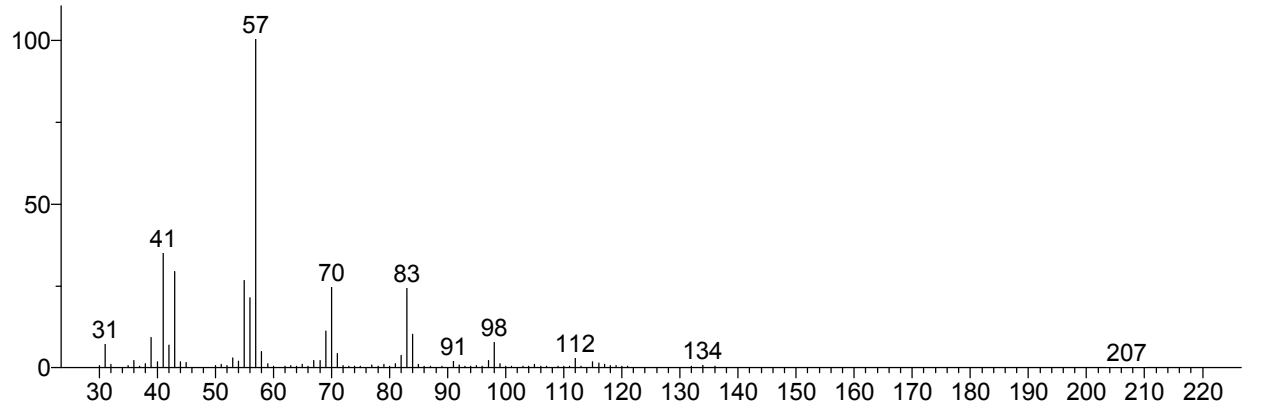
Hit 1 : Heptane, 3-(chloromethyl)-
C8H17Cl; MF: 891; RMF: 897; Prob 55.0%; CAS: 123-04-6; Lib: mainlib; ID: 21205.



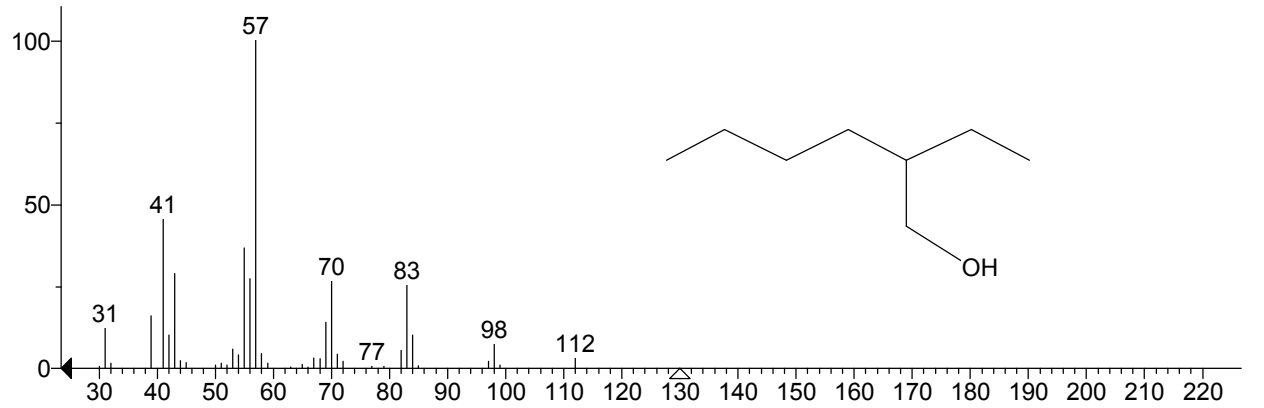
Hit 2 : Heptane, 3-(chloromethyl)-
C8H17Cl; MF: 878; RMF: 883; Prob 55.0%; CAS: 123-04-6; Lib: replib; ID: 5898.



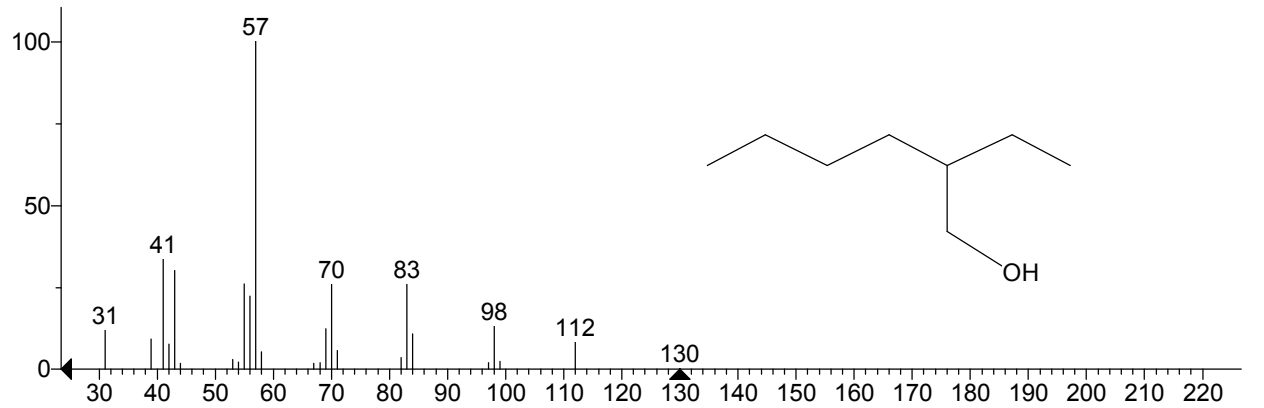
Unknown: Scan 275 (2.160 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 146



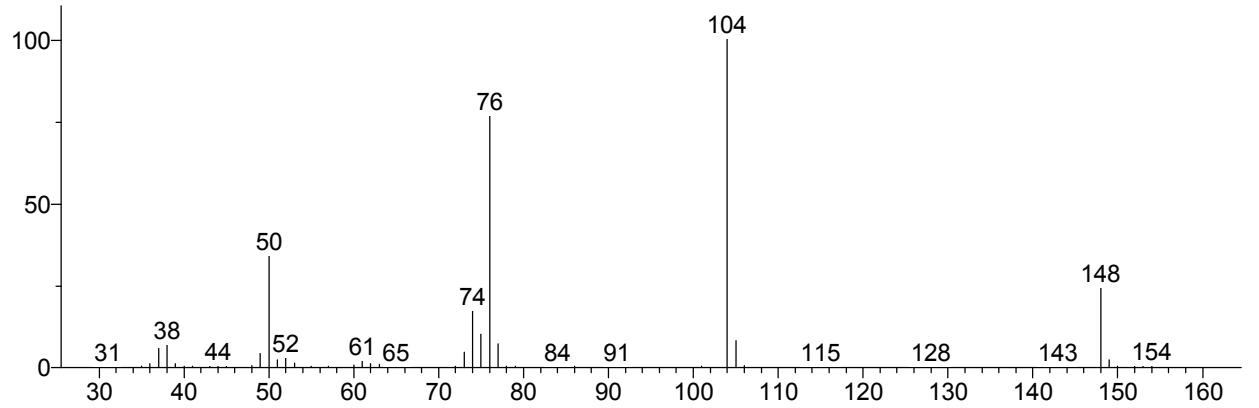
Hit 1 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 912; RMF: 949; Prob 58.1%; CAS: 104-76-7; Lib: replib; ID: 5289.



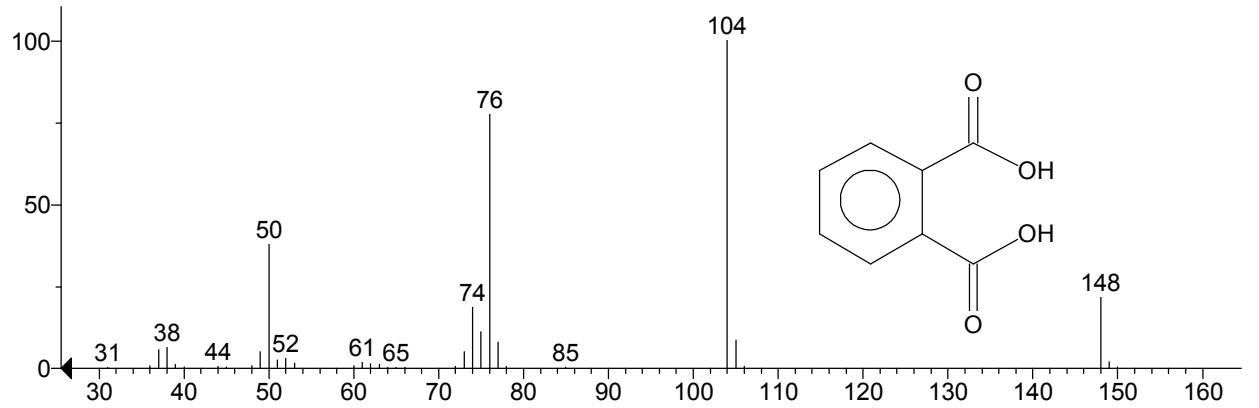
Hit 2 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 911; RMF: 965; Prob 58.1%; CAS: 104-76-7; Lib: replib; ID: 5259.



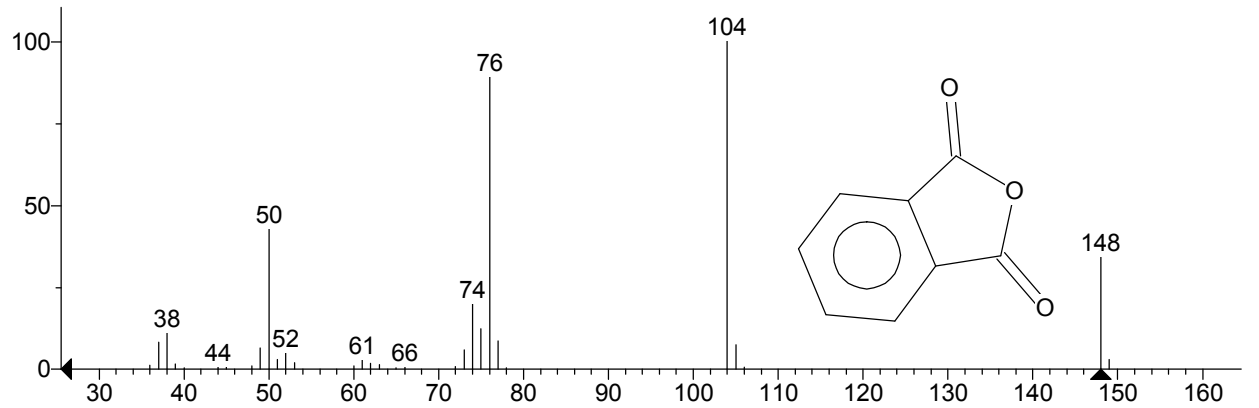
Unknown: Scan 495 (3.817 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 207



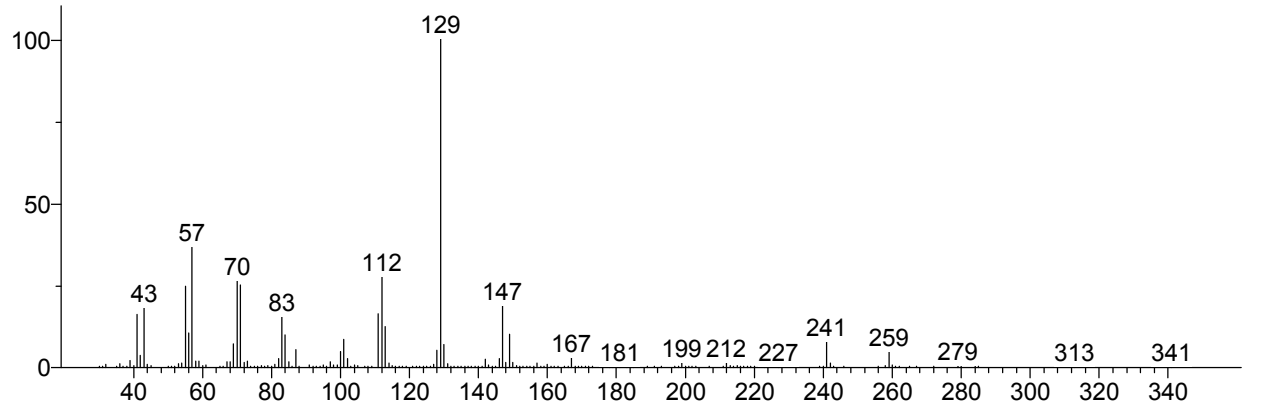
Hit 1 : 1,2-Benzenedicarboxylic acid
C8H6O4; MF: 967; RMF: 969; Prob 60.6%; CAS: 88-99-3; Lib: replib; ID: 13464.



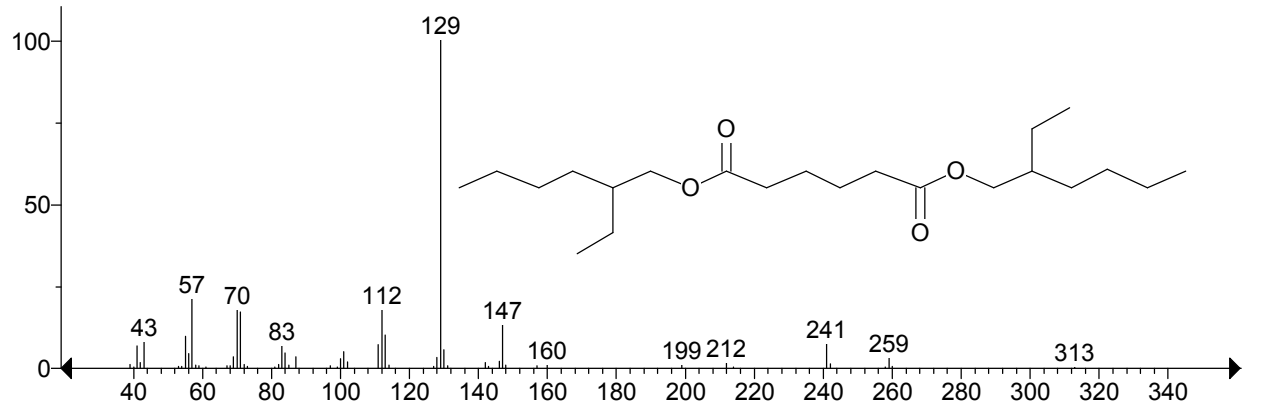
Hit 2 : Phthalic anhydride
C8H4O3; MF: 950; RMF: 954; Prob 33.1%; CAS: 85-44-9; Lib: mainlib; ID: 65271.



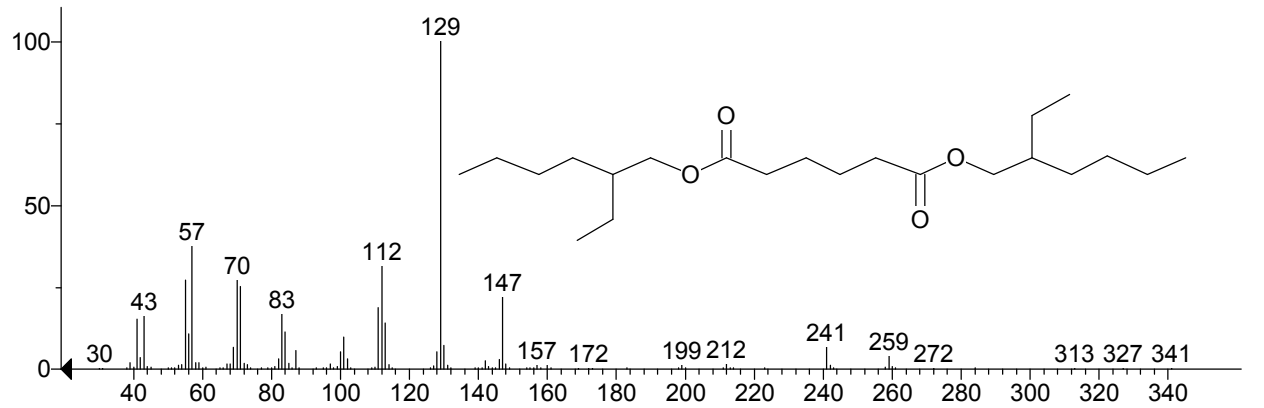
Unknown: Scan 1142 (8.693 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = 155



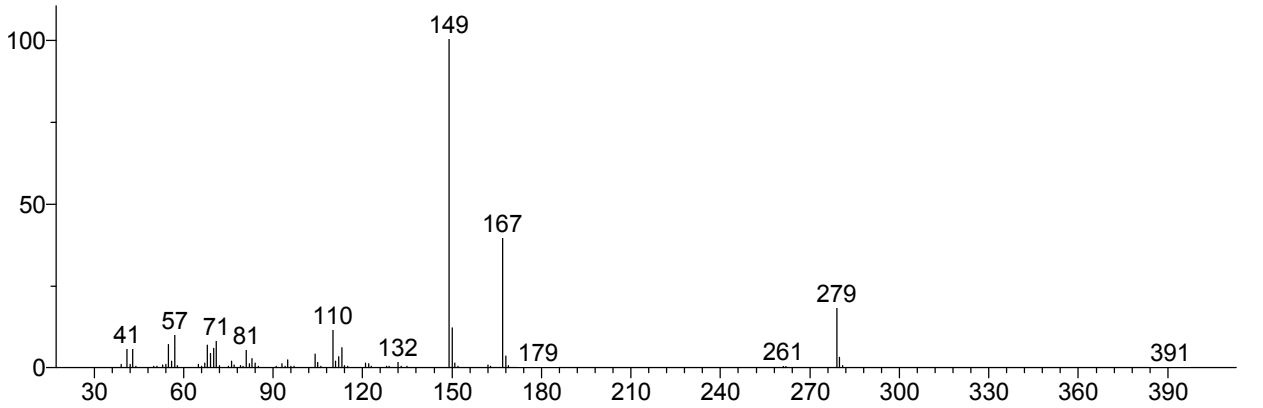
Hit 1 : Hexanedioic acid, bis(2-ethylhexyl) ester
C22H42O4; MF: 901; RMF: 953; Prob 58.4%; CAS: 103-23-1; Lib: replib; ID: 17605.



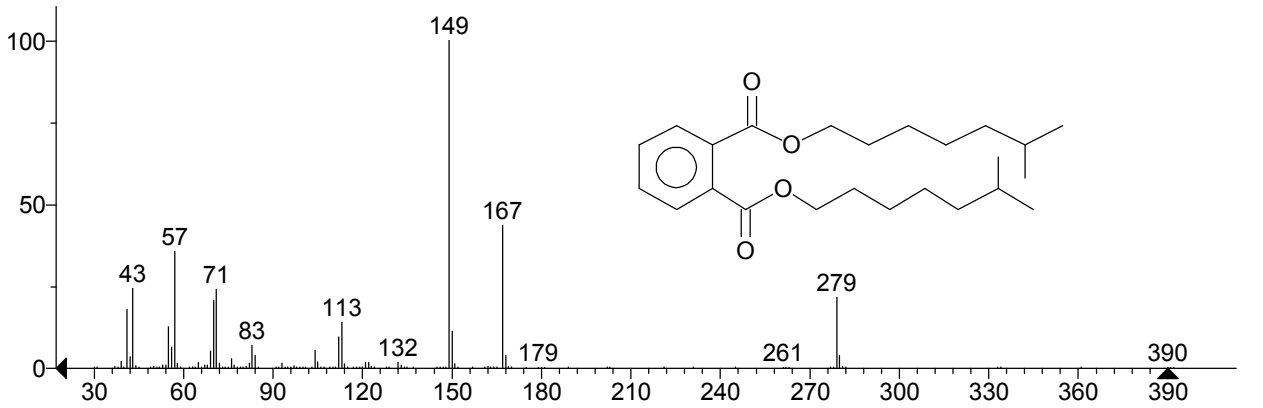
Hit 2 : Hexanedioic acid, bis(2-ethylhexyl) ester
C22H42O4; MF: 891; RMF: 910; Prob 58.4%; CAS: 103-23-1; Lib: mainlib; ID: 91324.



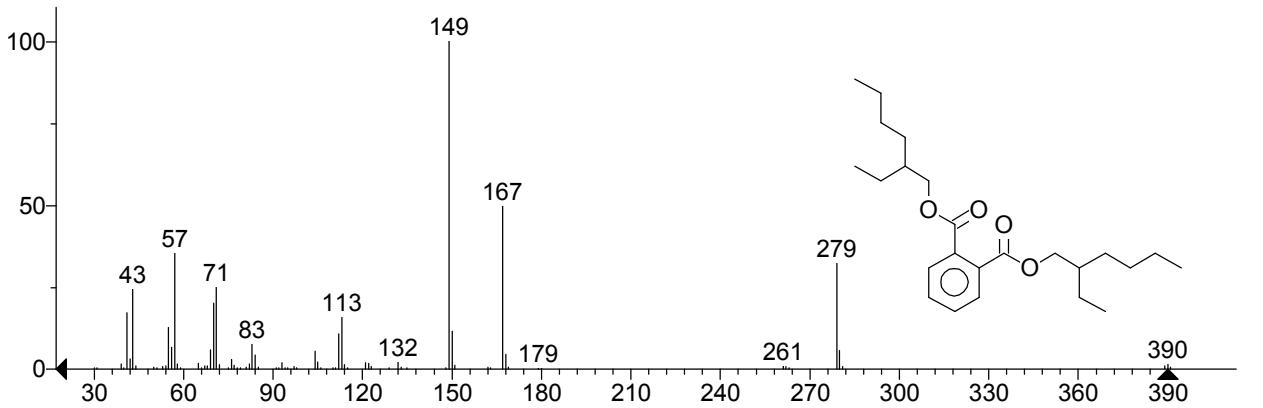
Unknown: Scan 1269 (9.650 min): J9163_PVC_White_portion_A_py1.D\data.ms
Compound in Library Factor = -155



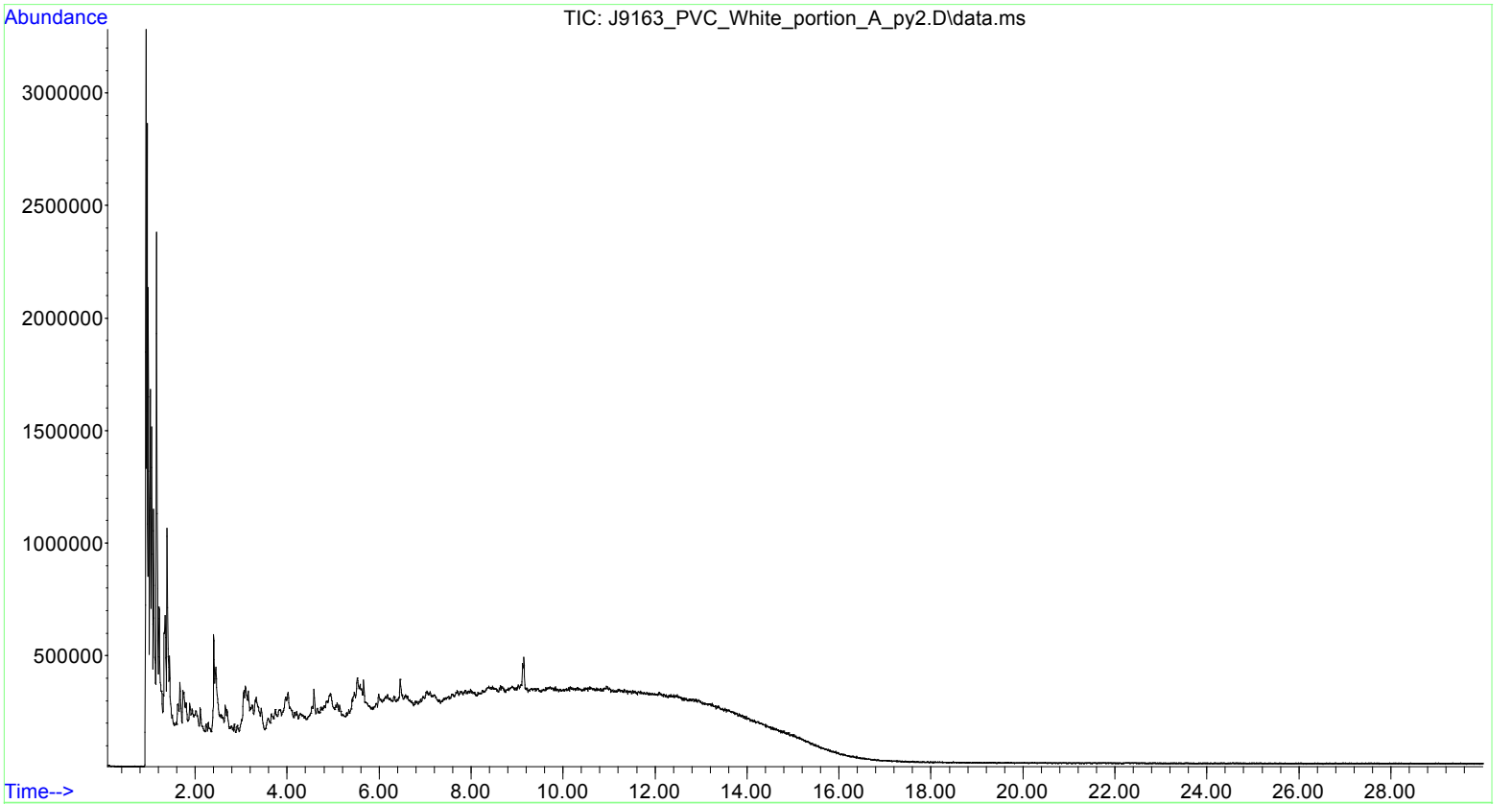
Hit 1 : 1,2-Benzenedicarboxylic acid, diisooctyl ester
C24H38O4; MF: 858; RMF: 858; Prob 23.2%; CAS: 27554-26-3; Lib: mainlib; ID: 110649.

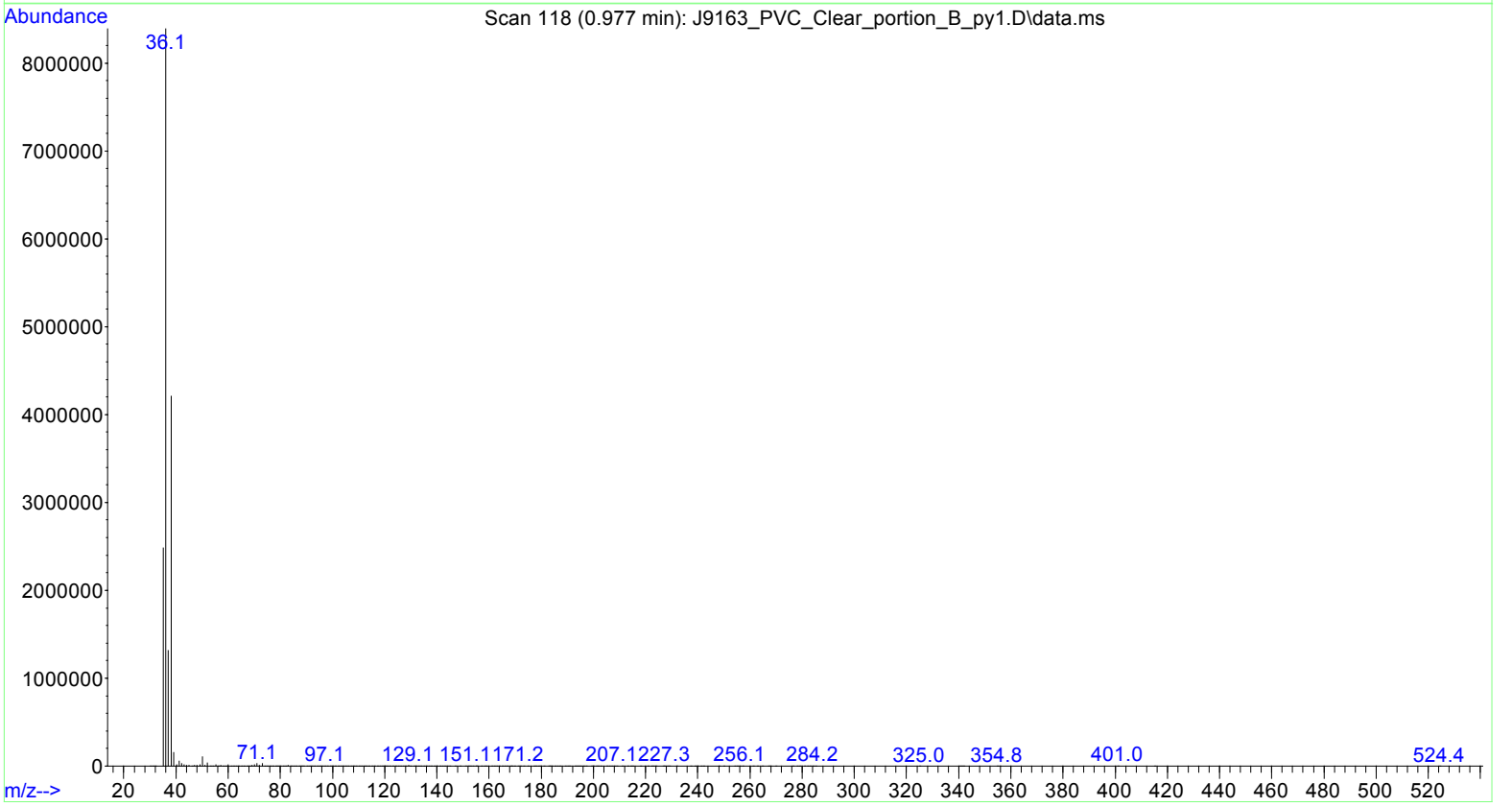


Hit 2 : Bis(2-ethylhexyl) phthalate
C24H38O4; MF: 855; RMF: 855; Prob 20.5%; CAS: 117-81-7; Lib: mainlib; ID: 110646.

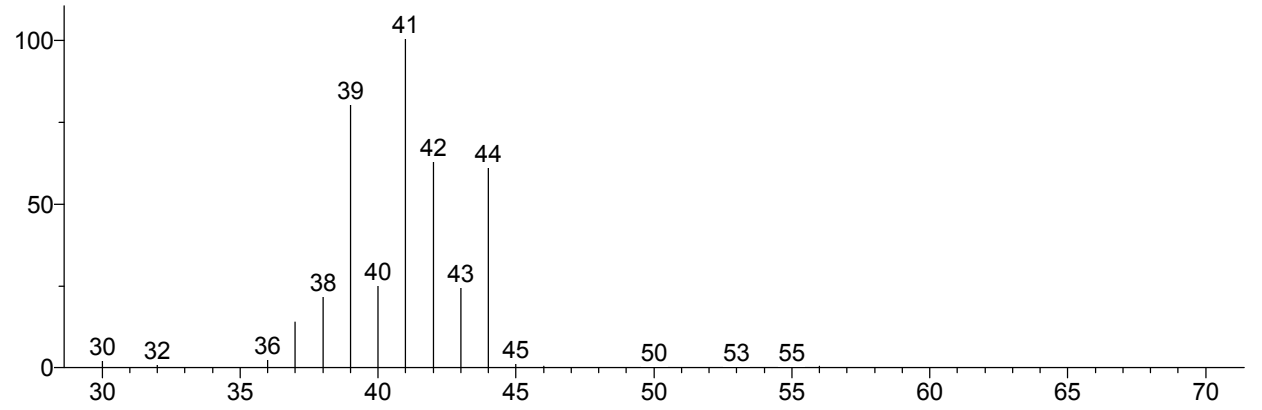


File :C:\msdchem\1\DATA\2014\J9163 Jordi\111114\J9163_PVC_White_po
... rtion_A_py2.D
Operator : Courtney McGowan
Instrument : Instrument #1
Acquired : 11 Nov 2014 22:10 using AcqMethod PYMS.M
Sample Name: J9163 PVC White portion
Misc Info : J9163 PVC White portion

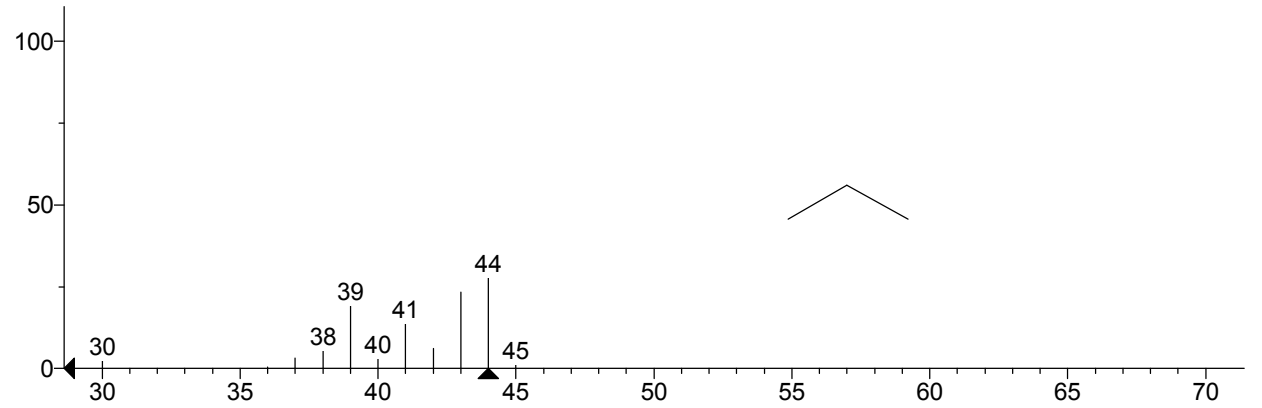




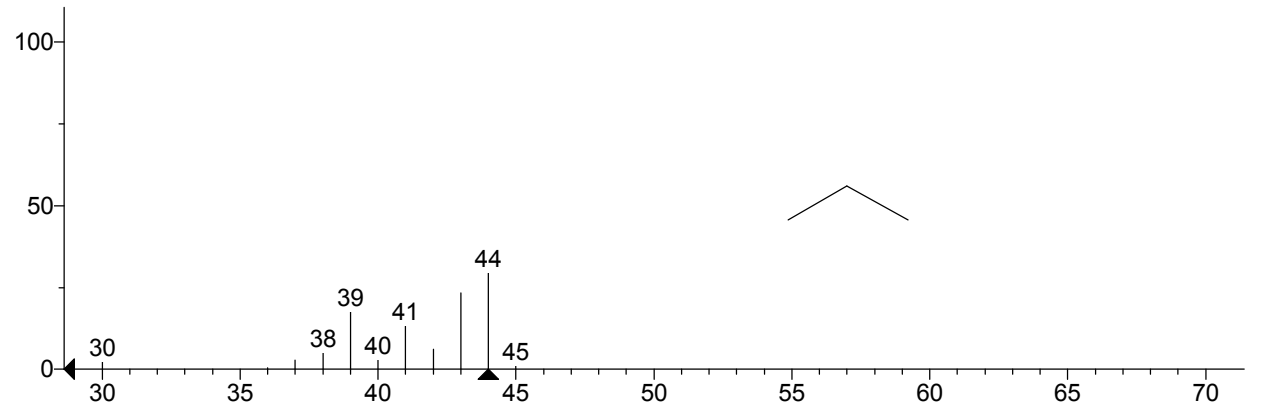
Unknown: Scan 112 (0.932 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -234



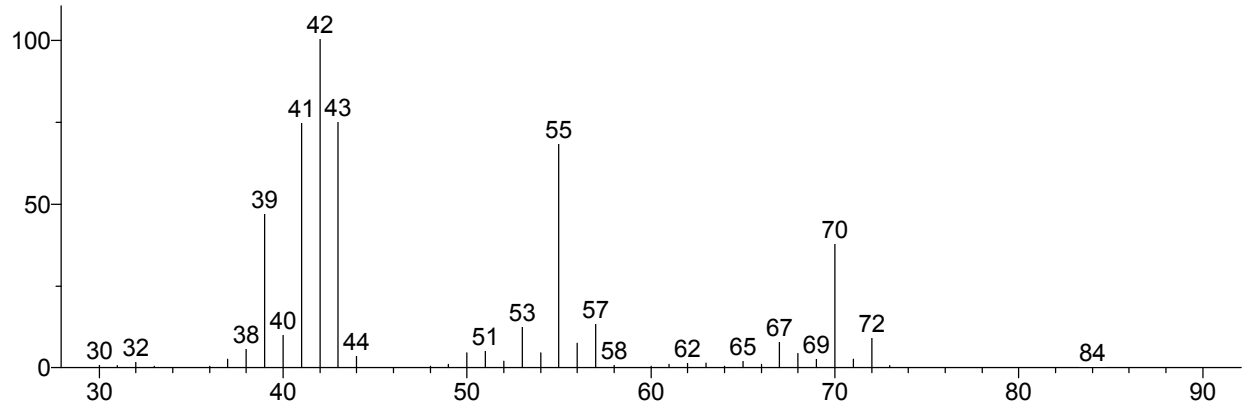
Hit 1 : Propane
C3H8; MF: 821; RMF: 823; Prob 60.4%; CAS: 74-98-6; Lib: mainlib; ID: 399.



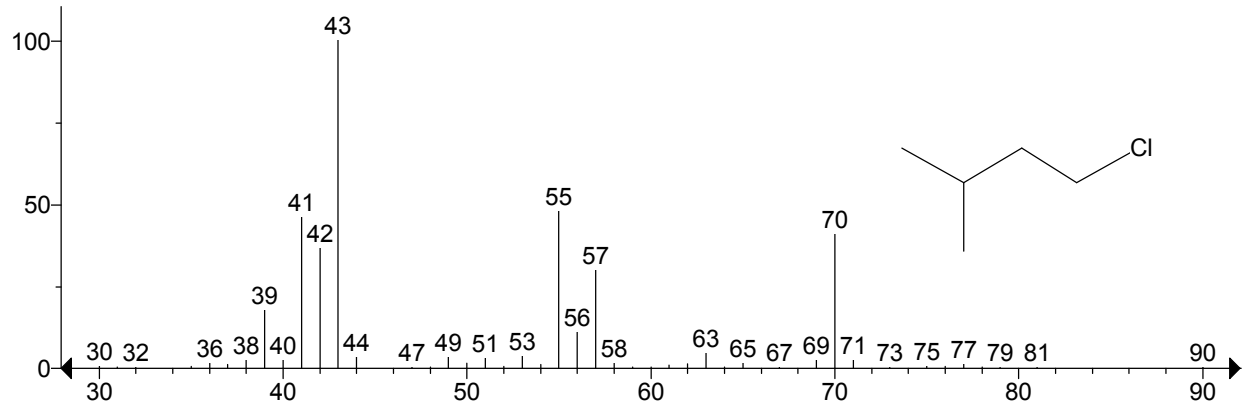
Hit 2 : Propane
C3H8; MF: 821; RMF: 822; Prob 60.4%; CAS: 74-98-6; Lib: replib; ID: 139.



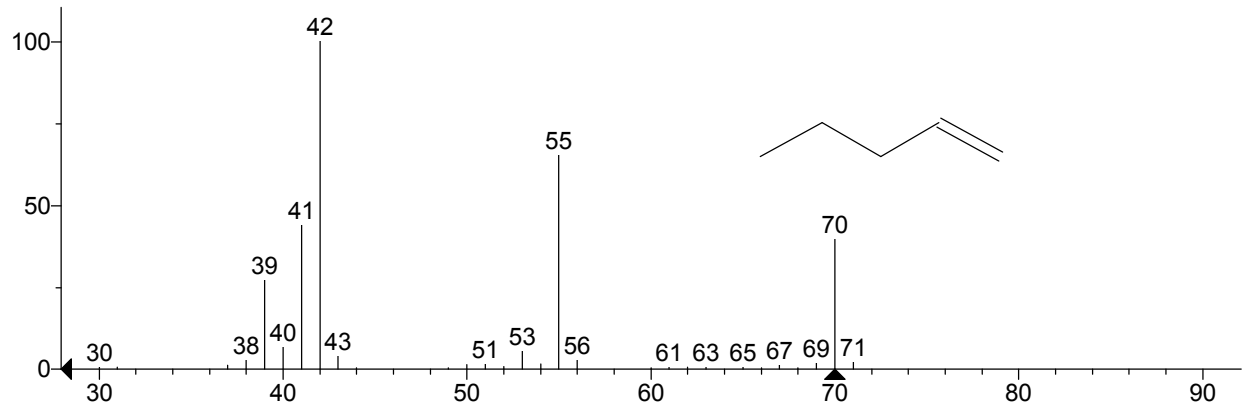
Unknown: Scan 118 (0.977 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -688



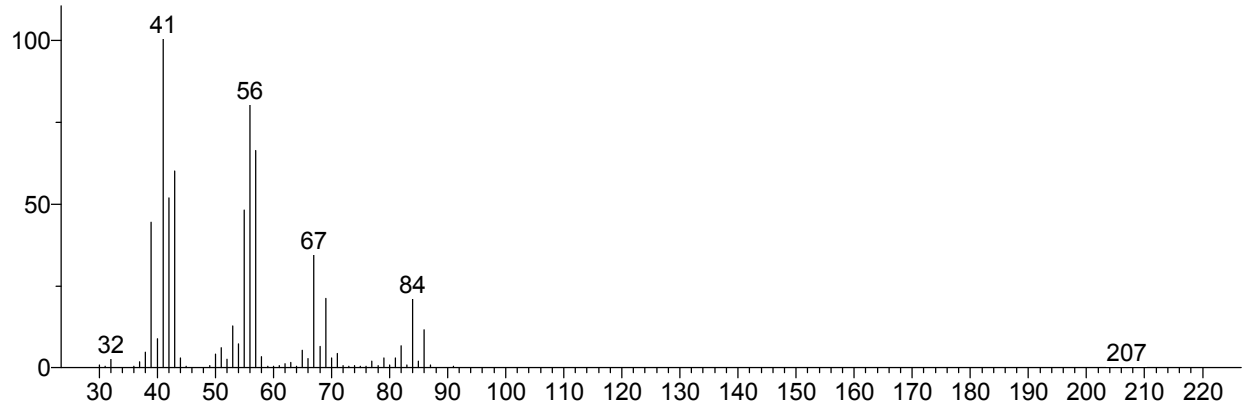
Hit 1 : Butane, 1-chloro-3-methyl-
C5H11Cl; MF: 807; RMF: 827; Prob 9.03%; CAS: 107-84-6; Lib: replib; ID: 1925.



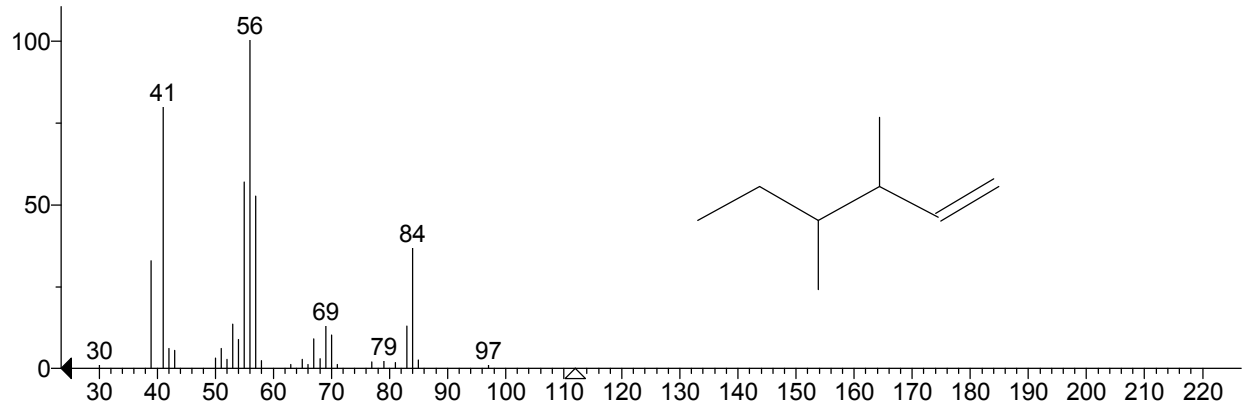
Hit 2 : 1-Pentene
C5H10; MF: 803; RMF: 833; Prob 7.63%; CAS: 109-67-1; Lib: mainlib; ID: 4375.



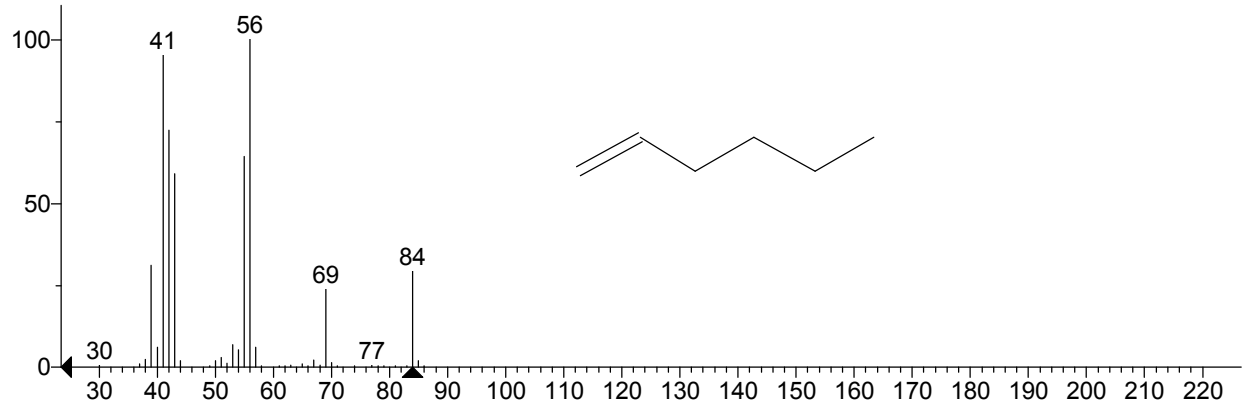
Unknown: Scan 124 (1.022 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -811



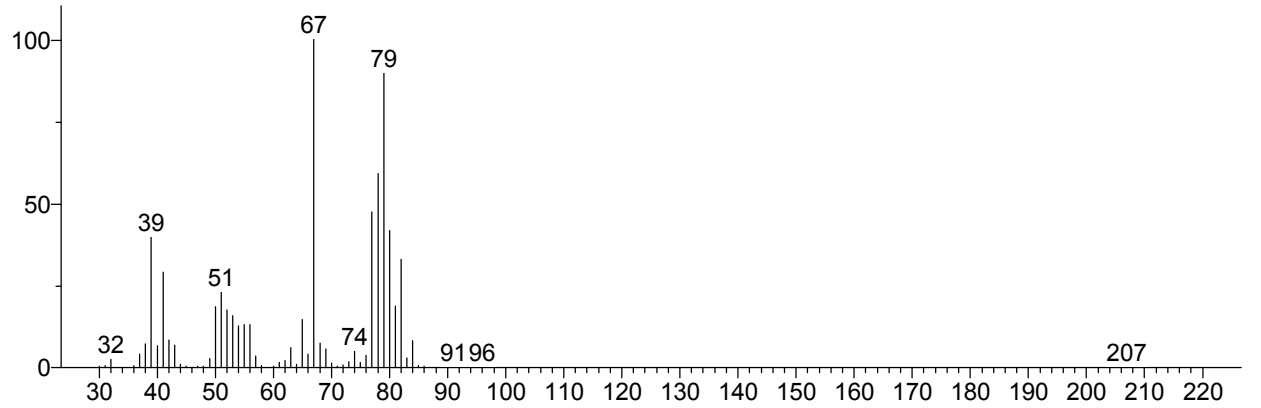
Hit 1 : 1-Hexene, 3,4-dimethyl-
C8H16; MF: 778; RMF: 819; Prob 11.4%; CAS: 16745-94-1; Lib: mainlib; ID: 19899.



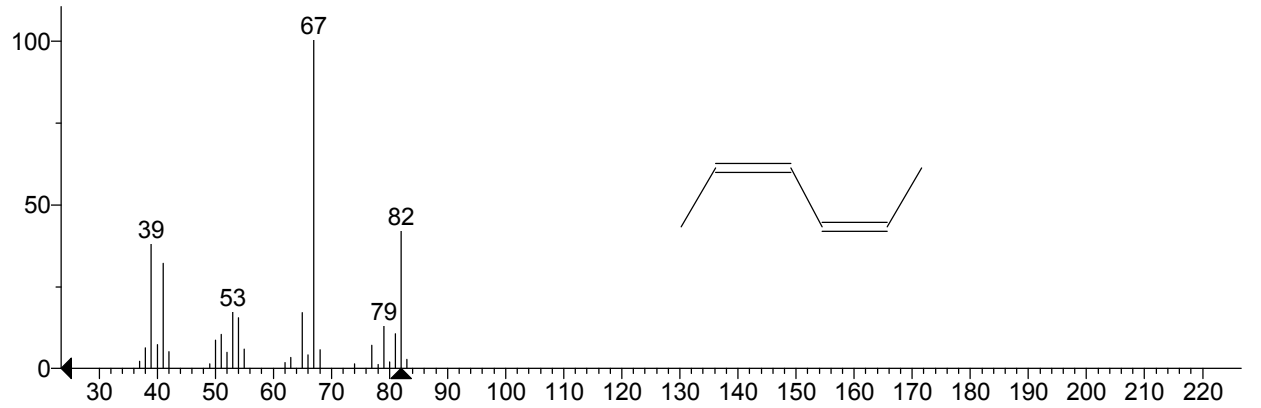
Hit 2 : 1-Hexene
C6H12; MF: 771; RMF: 781; Prob 8.76%; CAS: 592-41-6; Lib: mainlib; ID: 19842.



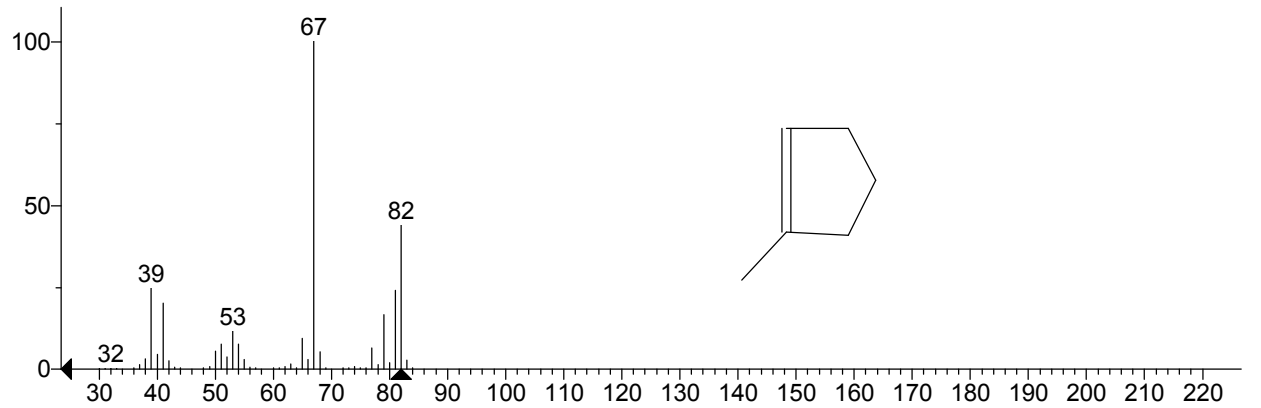
Unknown: Scan 128 (1.052 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -1231



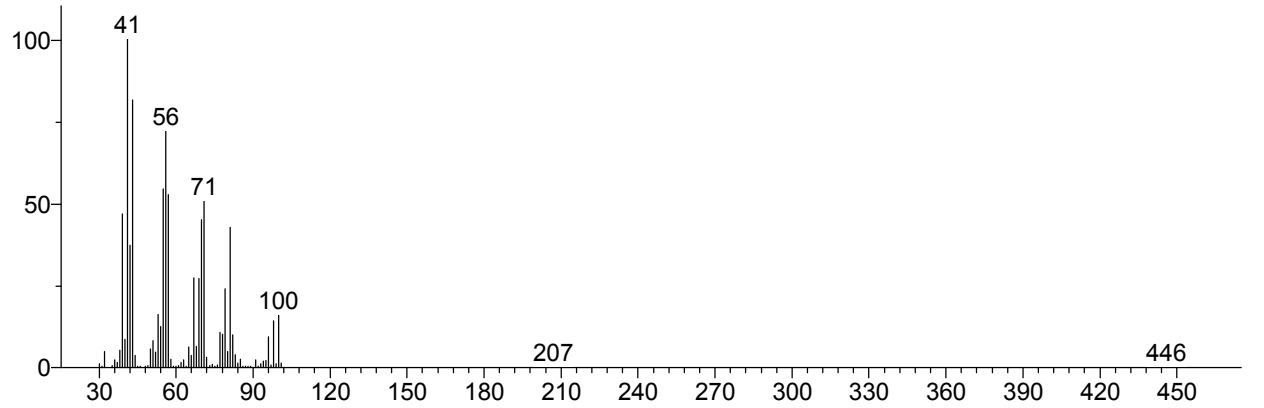
Hit 1 : 2,4-Hexadiene, (Z,Z)-
C6H10; MF: 717; RMF: 750; Prob 7.11%; CAS: 6108-61-8; Lib: mainlib; ID: 28907.



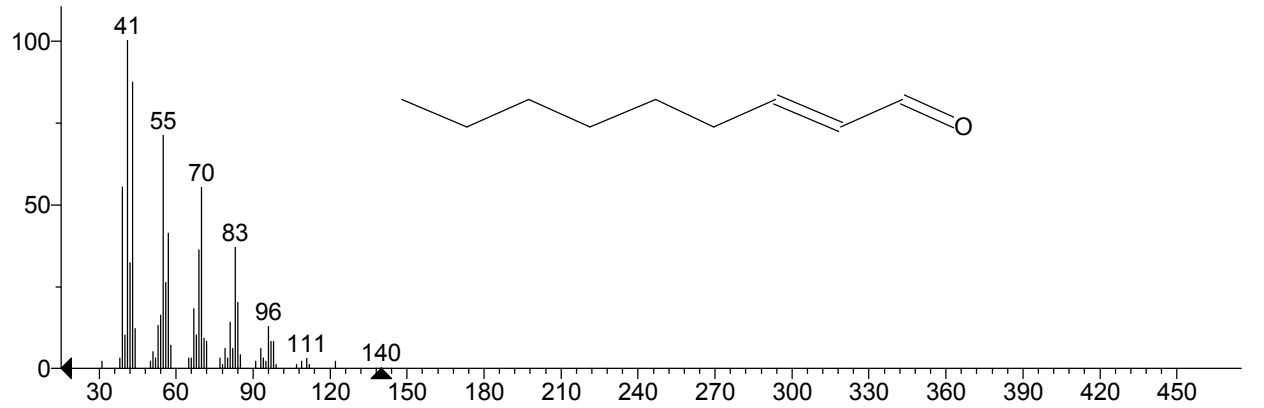
Hit 2 : Cyclopentene, 1-methyl-
C6H10; MF: 714; RMF: 725; Prob 6.28%; CAS: 693-89-0; Lib: replib; ID: 7234.



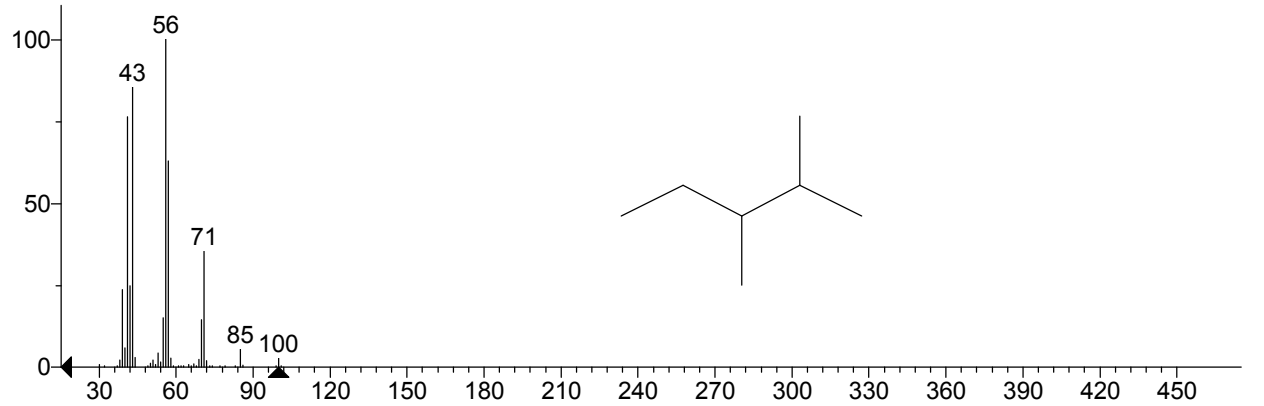
Unknown: Scan 134 (1.097 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -825



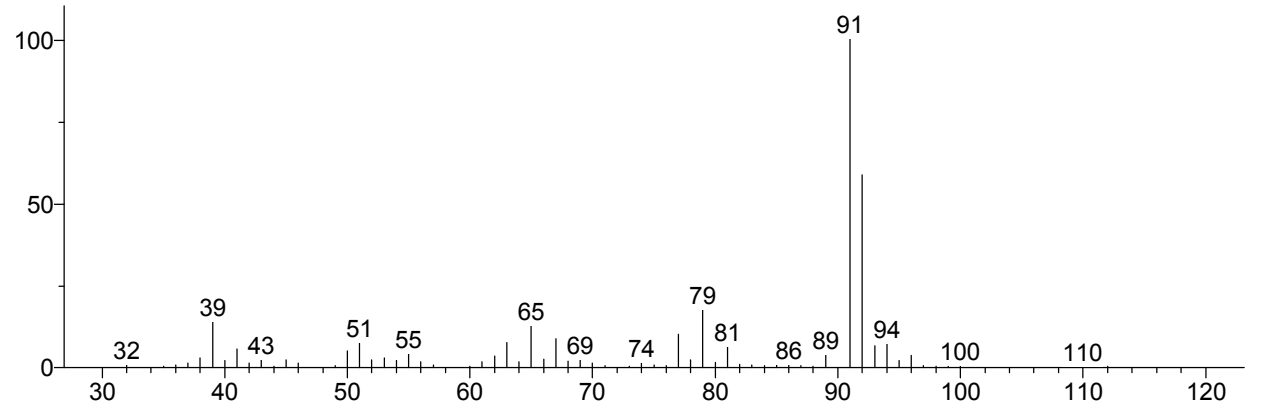
Hit 1 : 2-Nonenal, (E)-
C9H16O; MF: 727; RMF: 751; Prob 6.62%; CAS: 18829-56-6; Lib: replib; ID: 711.



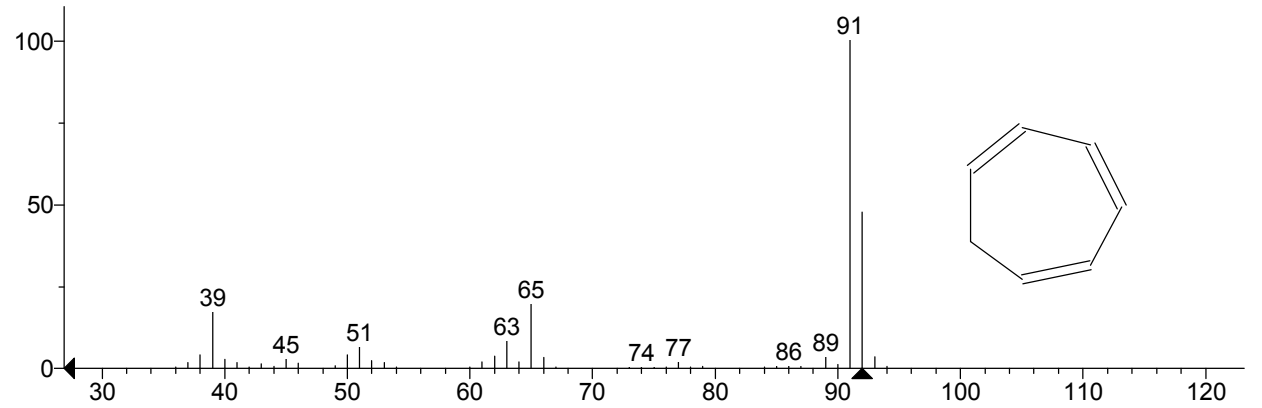
Hit 2 : Pentane, 2,3-dimethyl-
C7H16; MF: 716; RMF: 801; Prob 4.54%; CAS: 565-59-3; Lib: replib; ID: 4916.



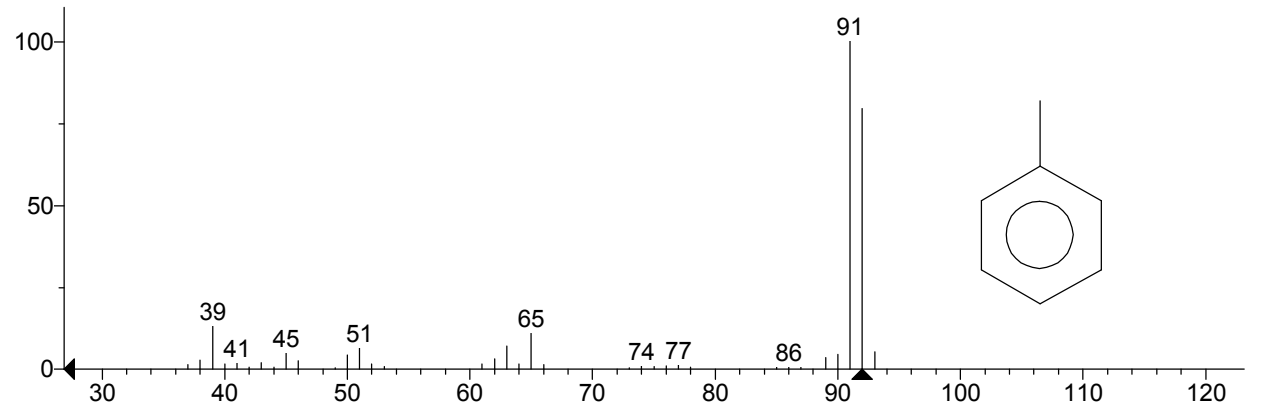
Unknown: Scan 142 (1.158 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -509



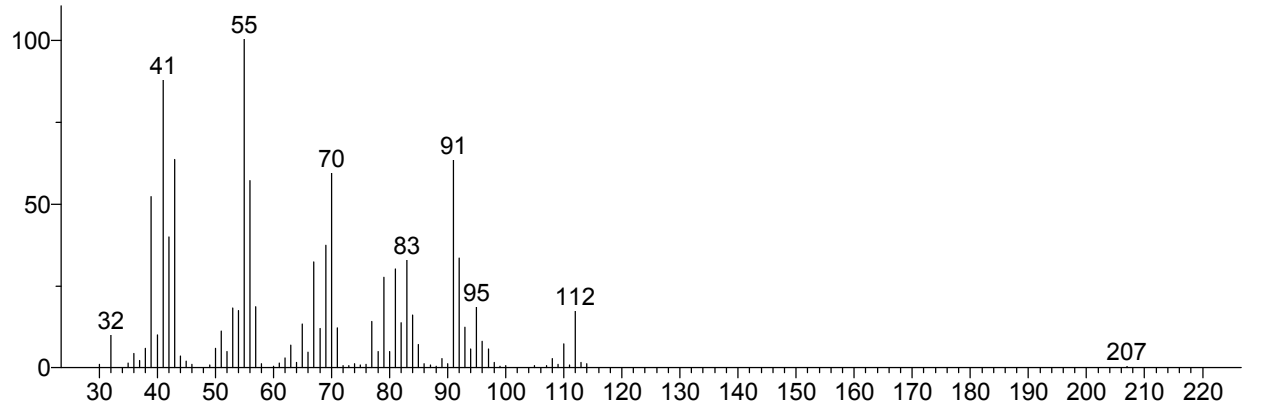
Hit 1 : 1,3,5-Cycloheptatriene
C7H8; MF: 796; RMF: 836; Prob 19.7%; CAS: 544-25-2; Lib: mainlib; ID: 51695.



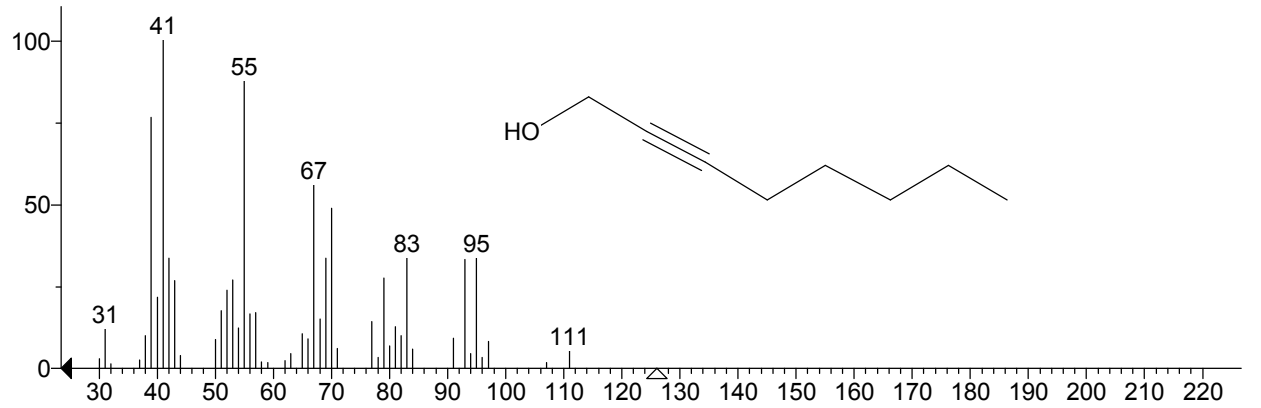
Hit 2 : Toluene
C7H8; MF: 789; RMF: 889; Prob 15.1%; CAS: 108-88-3; Lib: replib; ID: 11393.



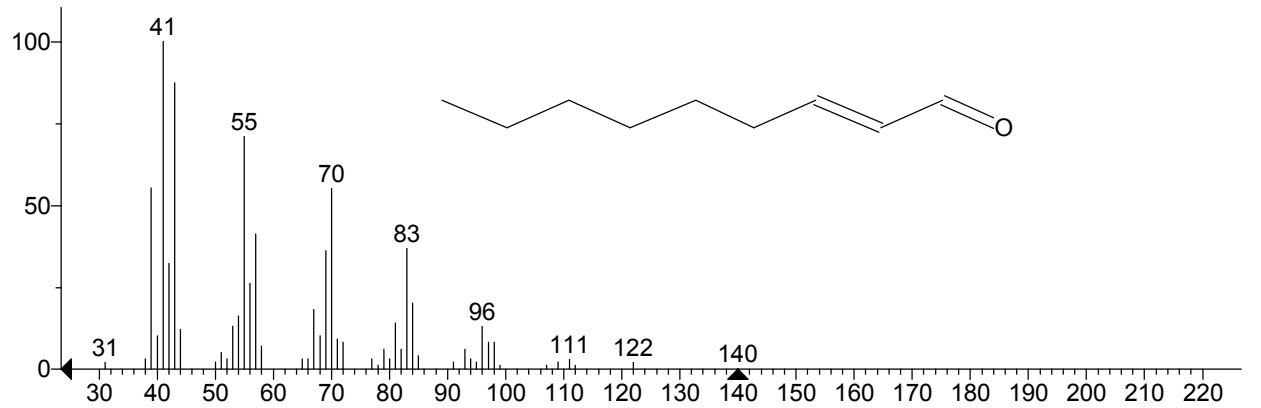
Unknown: Scan 150 (1.218 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -778



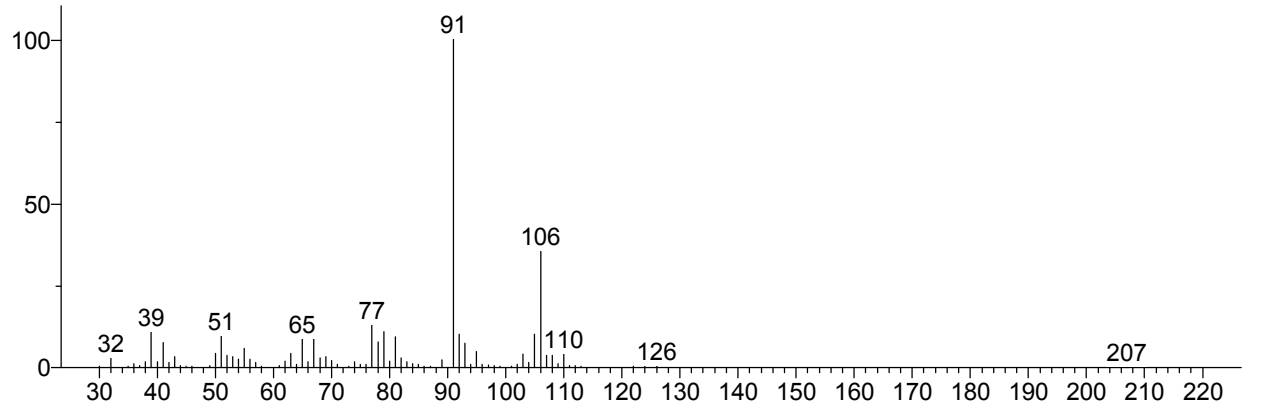
Hit 1 : 2-Octyn-1-ol
C8H14O; MF: 751; RMF: 816; Prob 7.93%; CAS: 20739-58-6; Lib: mainlib; ID: 2436.



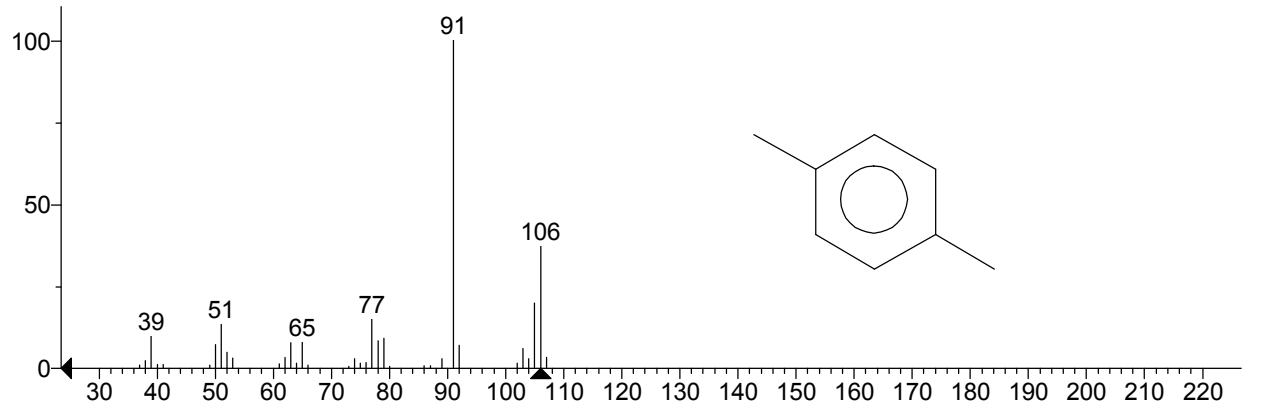
Hit 2 : 2-Nonenal, (E)-
C9H16O; MF: 739; RMF: 787; Prob 5.28%; CAS: 18829-56-6; Lib: replib; ID: 711.



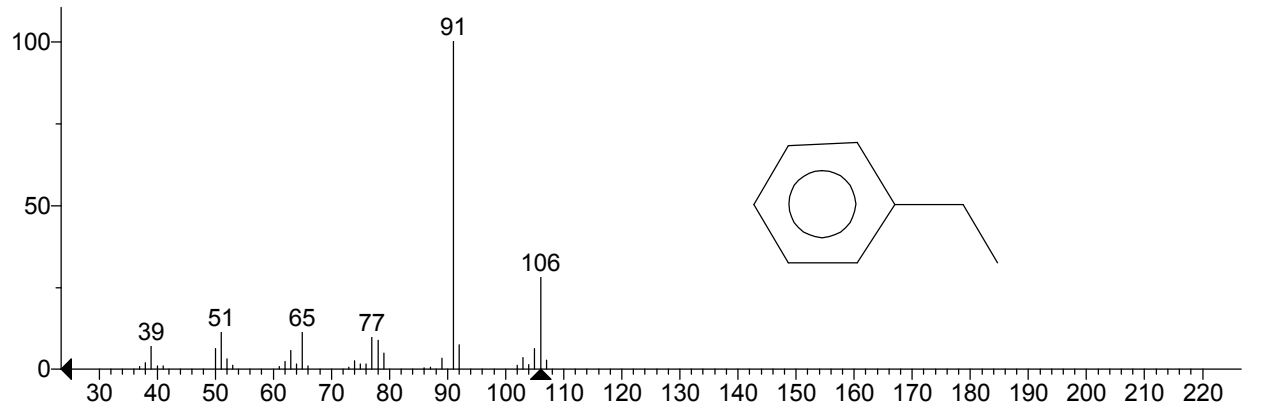
Unknown: Scan 167 (1.346 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -501



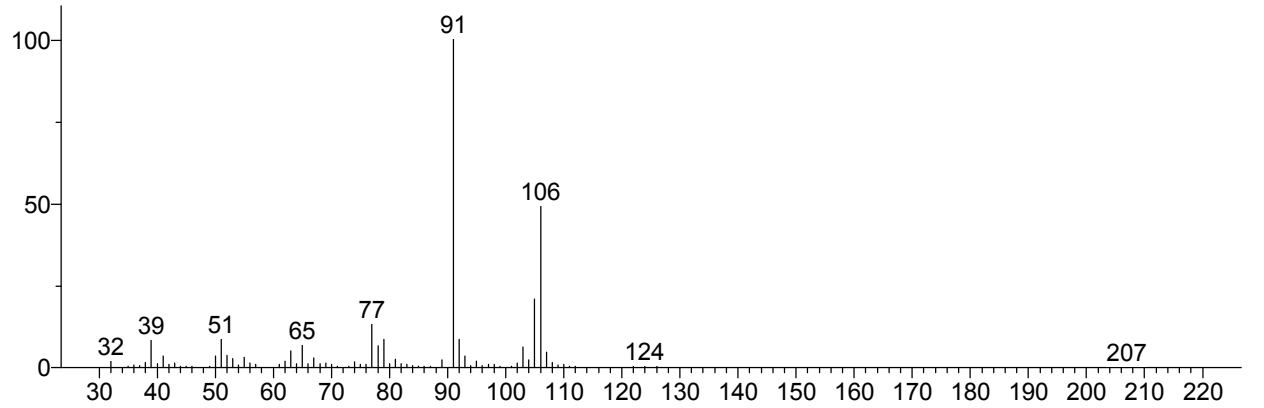
Hit 1 : p-Xylene
C8H10; MF: 809; RMF: 925; Prob 23.9%; CAS: 106-42-3; Lib: replib; ID: 11521.



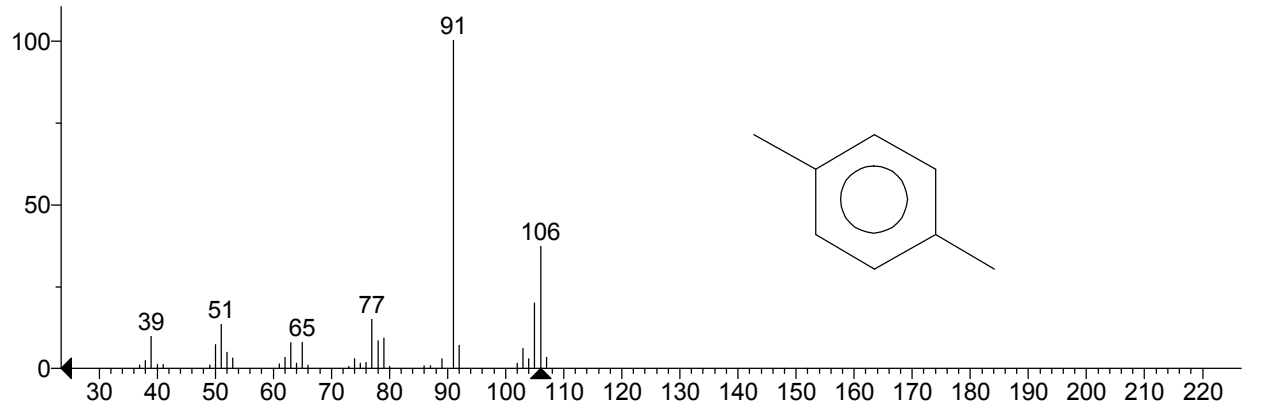
Hit 2 : Ethylbenzene
C8H10; MF: 797; RMF: 918; Prob 15.9%; CAS: 100-41-4; Lib: mainlib; ID: 52160.



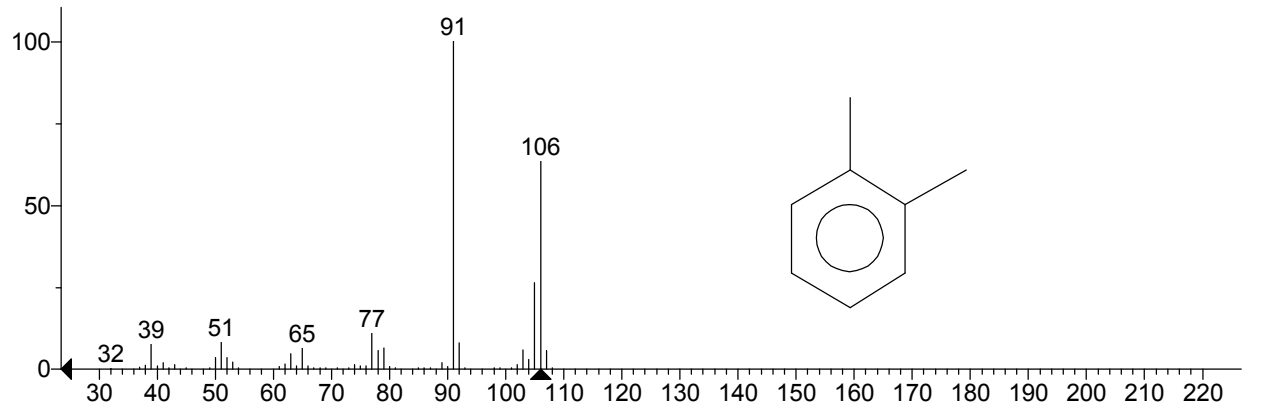
Unknown: Scan 173 (1.391 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -151



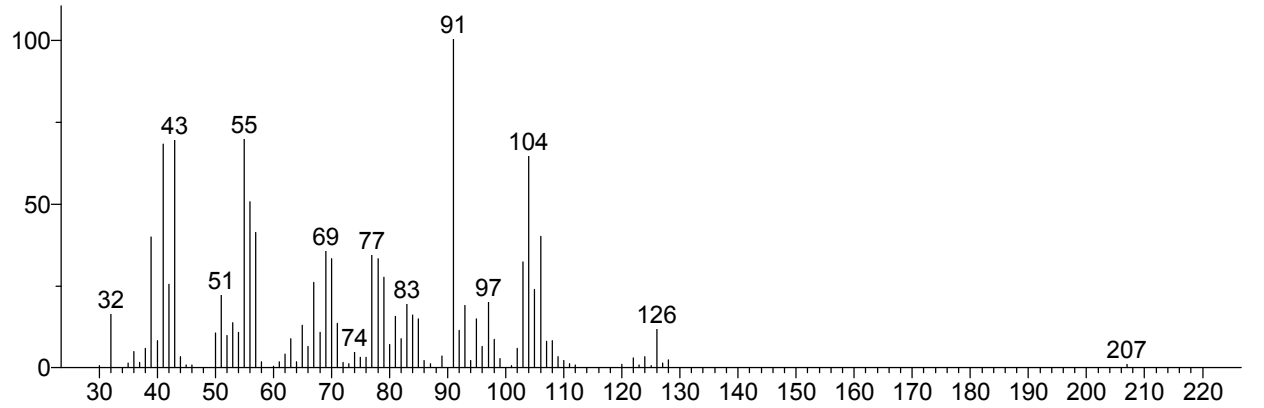
Hit 1 : p-Xylene
C8H10; MF: 891; RMF: 943; Prob 35.1%; CAS: 106-42-3; Lib: replib; ID: 11521.



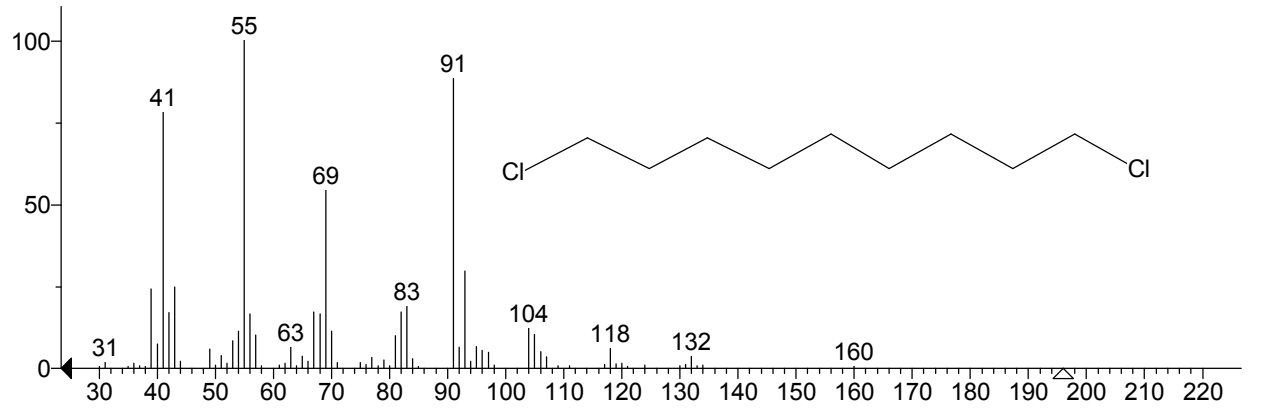
Hit 2 : o-Xylene
C8H10; MF: 874; RMF: 898; Prob 19.1%; CAS: 95-47-6; Lib: replib; ID: 11528.



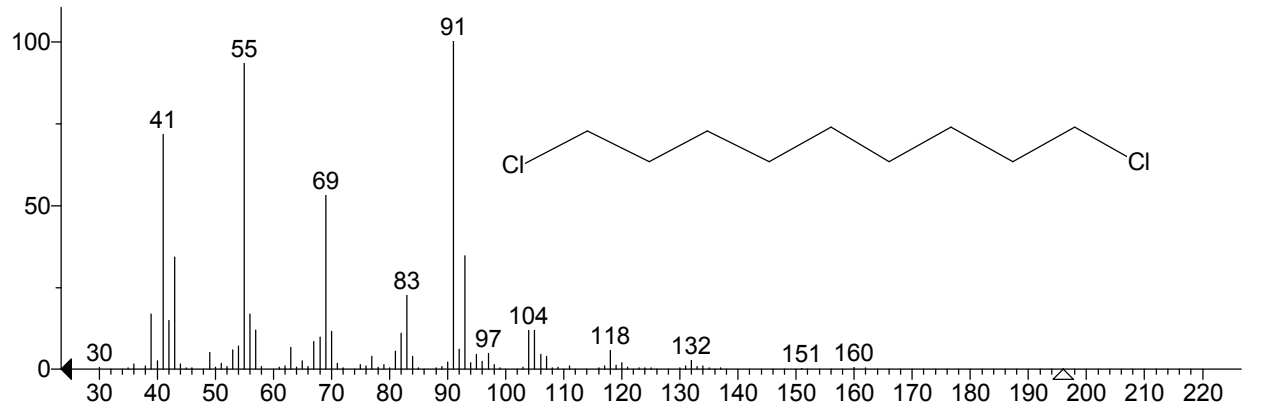
Unknown: Scan 180 (1.444 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -941



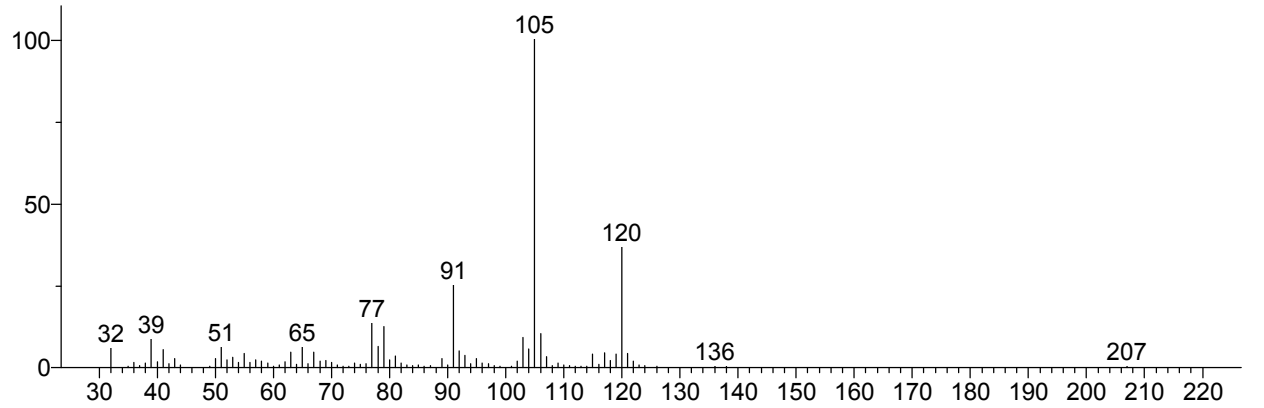
Hit 1 : 1,9-Dichlorononane
C9H18Cl2; MF: 681; RMF: 728; Prob 14.6%; CAS: 821-99-8; Lib: replib; ID: 4694.



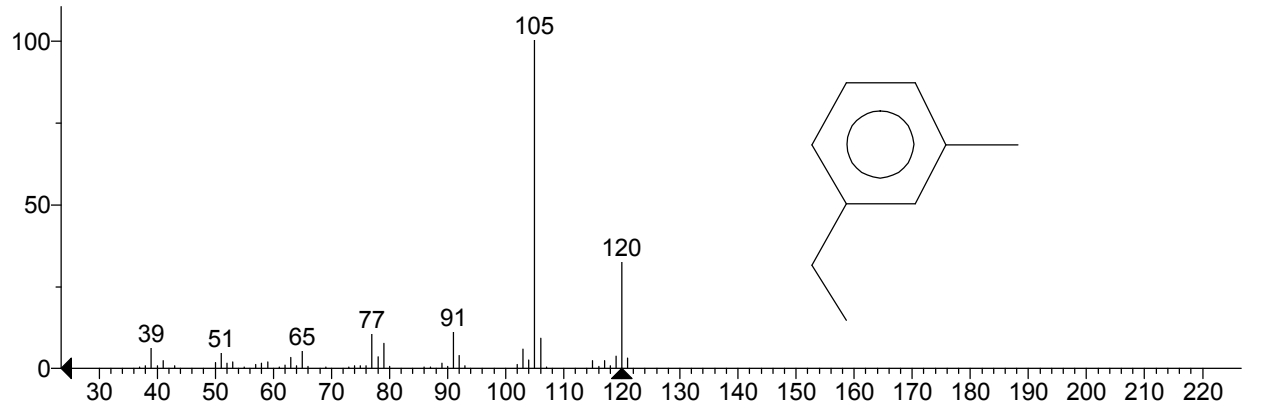
Hit 2 : 1,9-Dichlorononane
C9H18Cl2; MF: 663; RMF: 685; Prob 14.6%; CAS: 821-99-8; Lib: mainlib; ID: 50555.



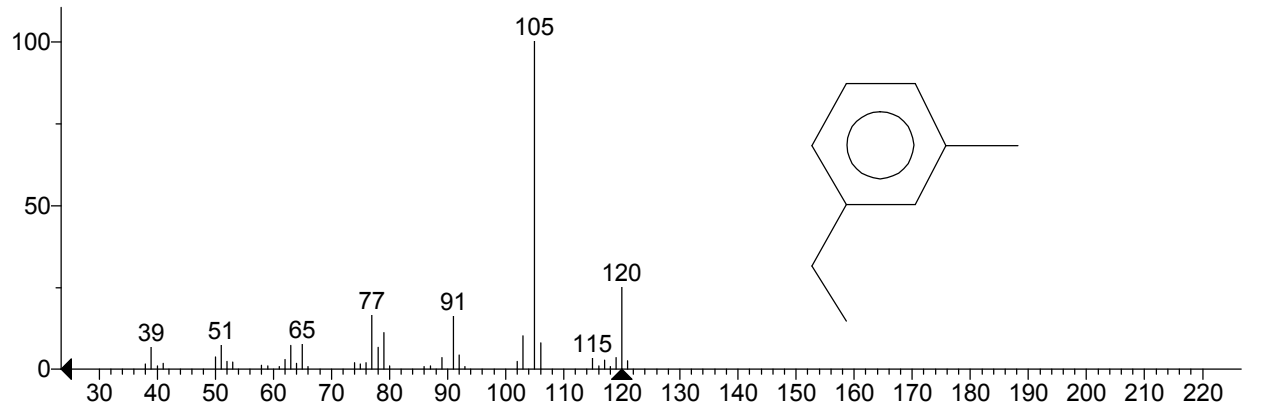
Unknown: Scan 210 (1.670 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -301



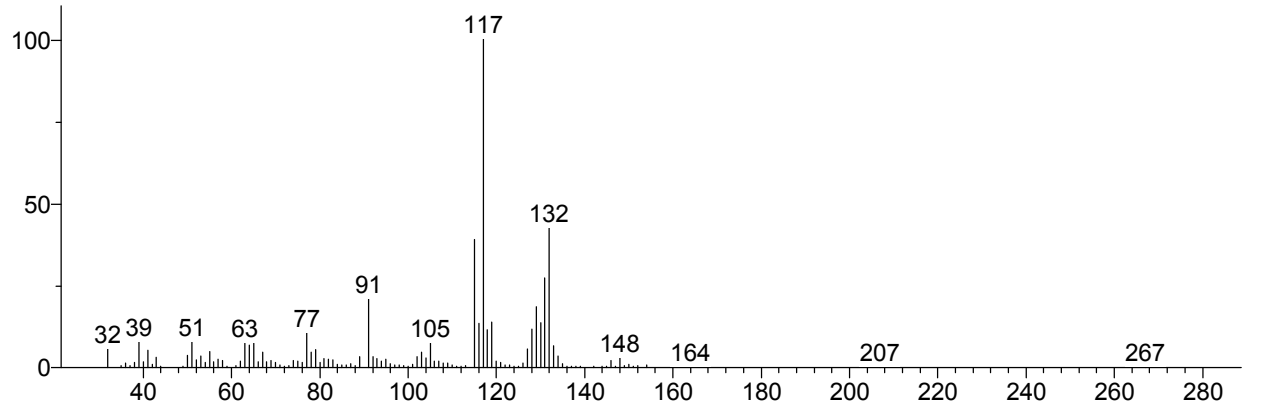
Hit 1 : Benzene, 1-ethyl-3-methyl-
C9H12; MF: 846; RMF: 898; Prob 20.4%; CAS: 620-14-4; Lib: mainlib; ID: 68592.



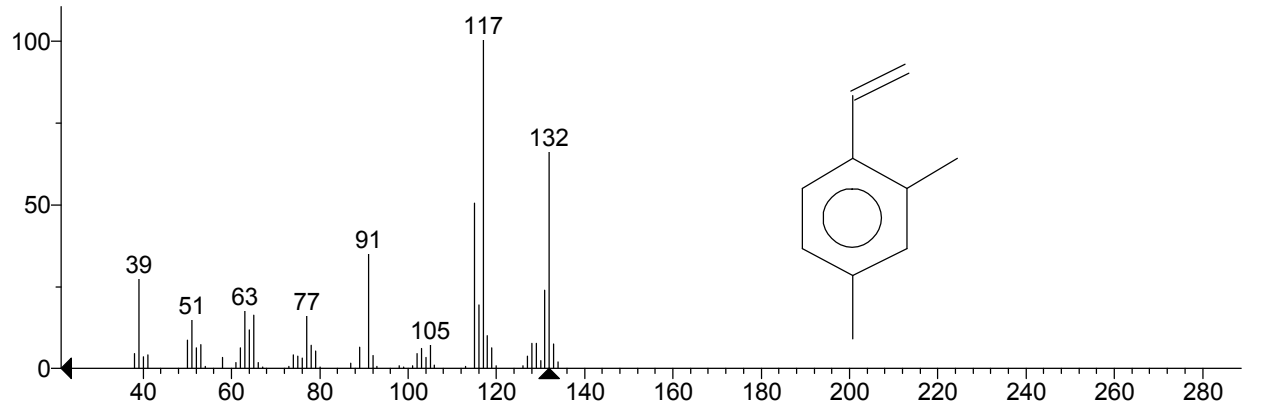
Hit 2 : Benzene, 1-ethyl-3-methyl-
C9H12; MF: 836; RMF: 917; Prob 20.4%; CAS: 620-14-4; Lib: replib; ID: 14016.



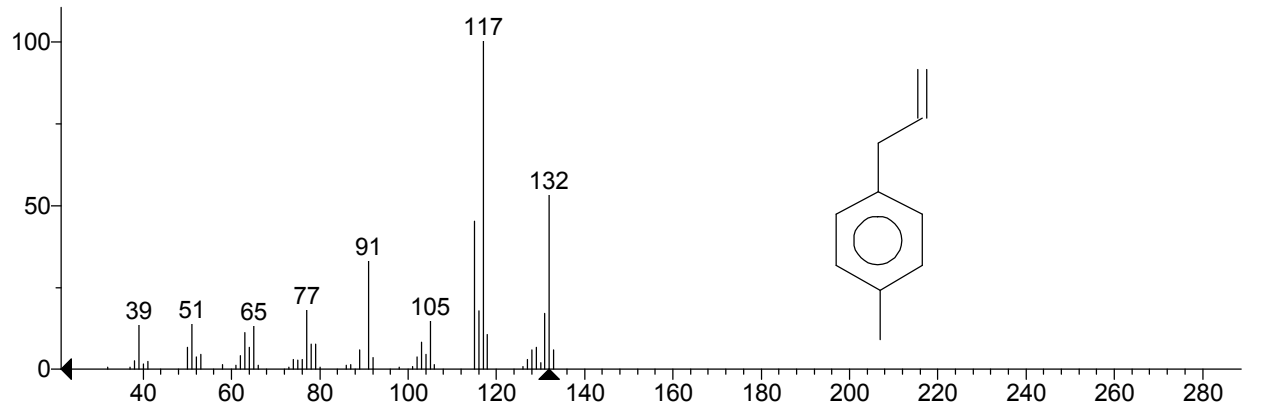
Unknown: Scan 308 (2.409 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -367



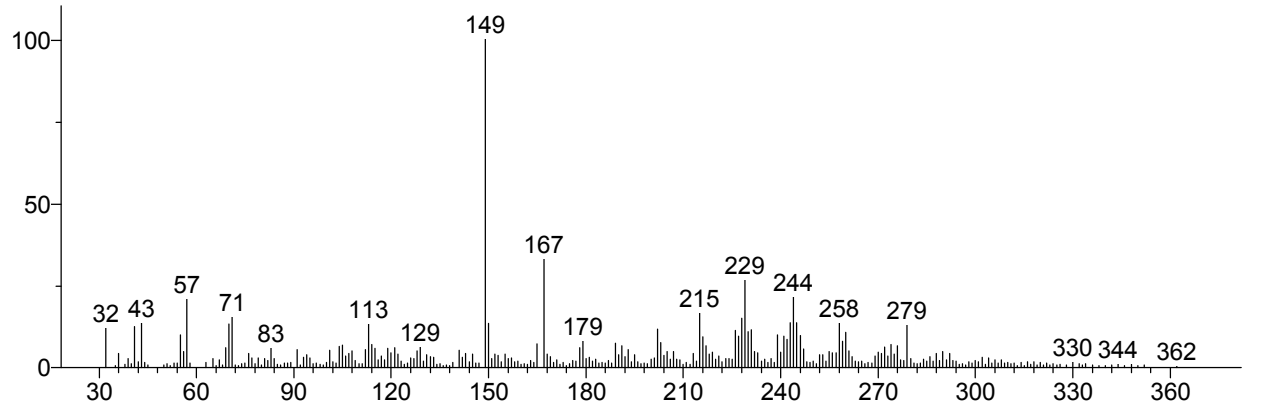
Hit 1 : 2,4-Dimethylstyrene
C10H12; MF: 823; RMF: 873; Prob 13.1%; CAS: 2234-20-0; Lib: mainlib; ID: 79184.



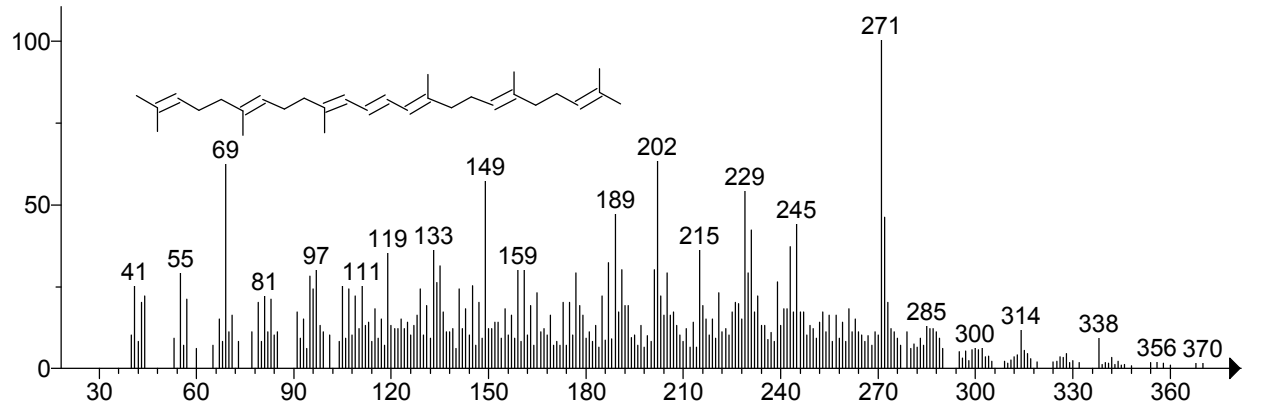
Hit 2 : Benzene, 1-methyl-4-(2-propenyl)-
C10H12; MF: 816; RMF: 896; Prob 10.0%; CAS: 3333-13-9; Lib: mainlib; ID: 79179.



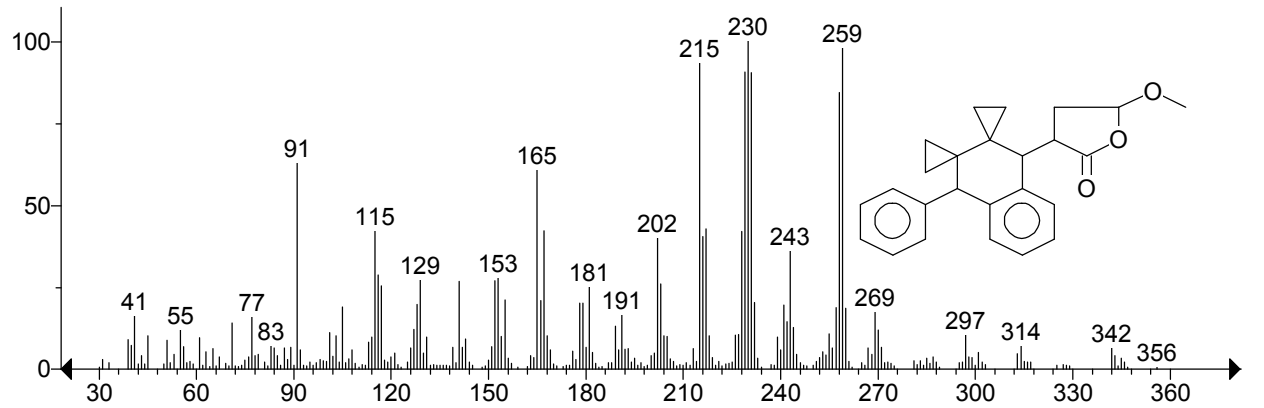
Unknown: Scan 1203 (9.153 min): J9163_PVC_White_portion_A_py2.D\data.ms
Compound in Library Factor = -176



Hit 1 : 2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-, didehydro deriv.
C30H48; MF: 765; RMF: 786; Prob 71.2%; CAS: 11051-27-7; Lib: mainlib; ID: 171612.

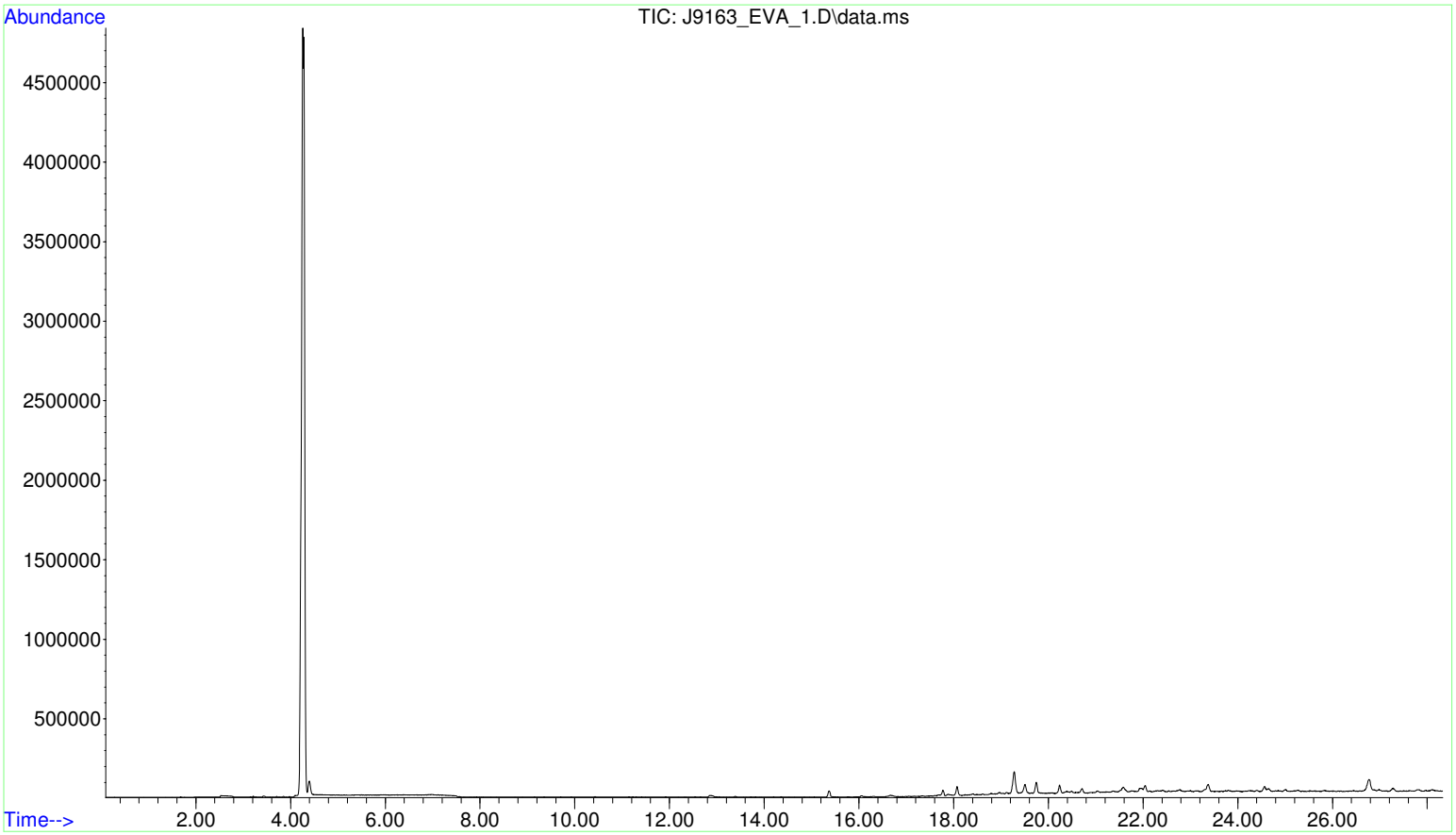


Hit 2 : 8,9-Benzodispiro[2.0.2.4]decane, 7-(3-methoxy-2-oxa-1-oxocyclopent-5-yl)-10-phenyl-
C25H26O3; MF: 661; RMF: 708; Prob 4.93%; Lib: mainlib; ID: 158517.

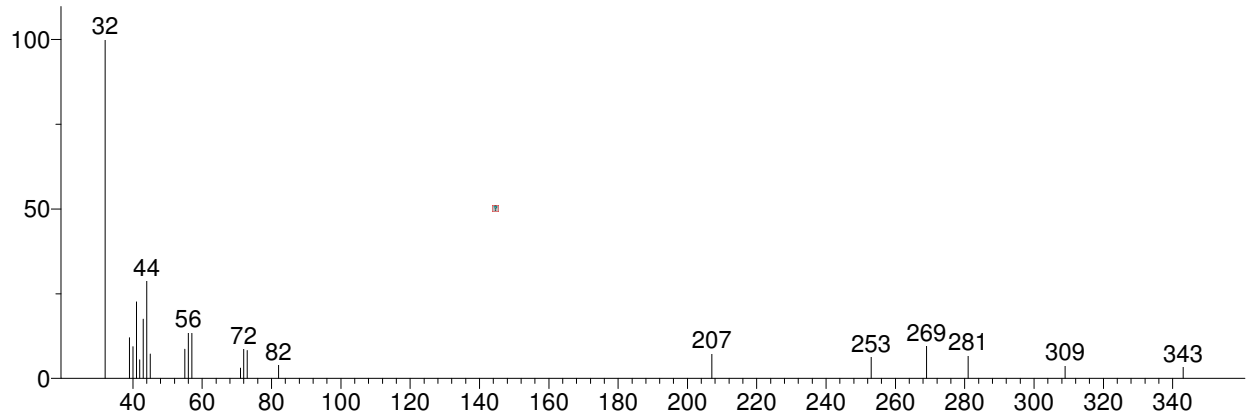


DHGCMS Data

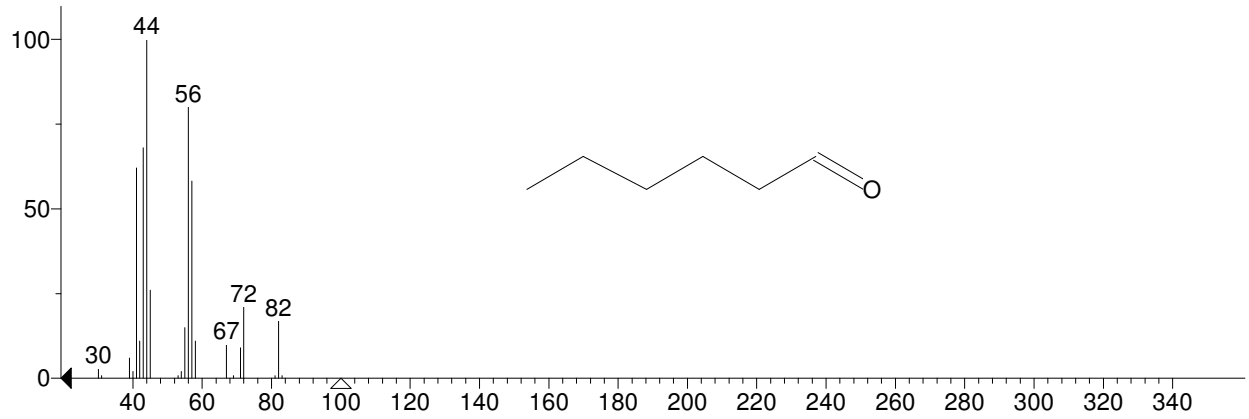
File :D:\msdchem\1\data\2014\J9163 Jordi\dhs\J9163_EVA_1.D
Operator : Oliver Palardy
Acquired : 5 Nov 2014 20:12 using AcqMethod J9163_EVA.M
Instrument : 7890
Sample Name: EVA 1
Misc Info :
Vial Number: 2



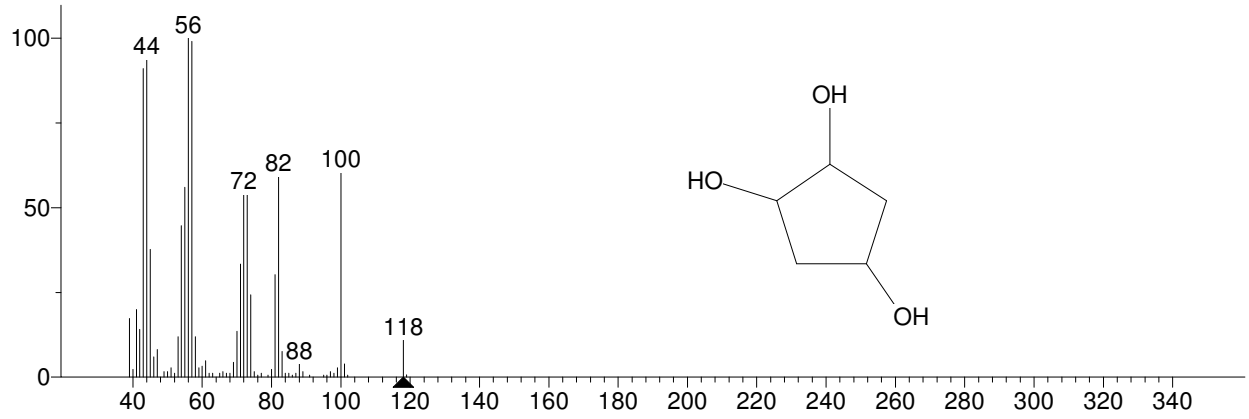
Unknown: Scan 2686 (16.058 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -1709



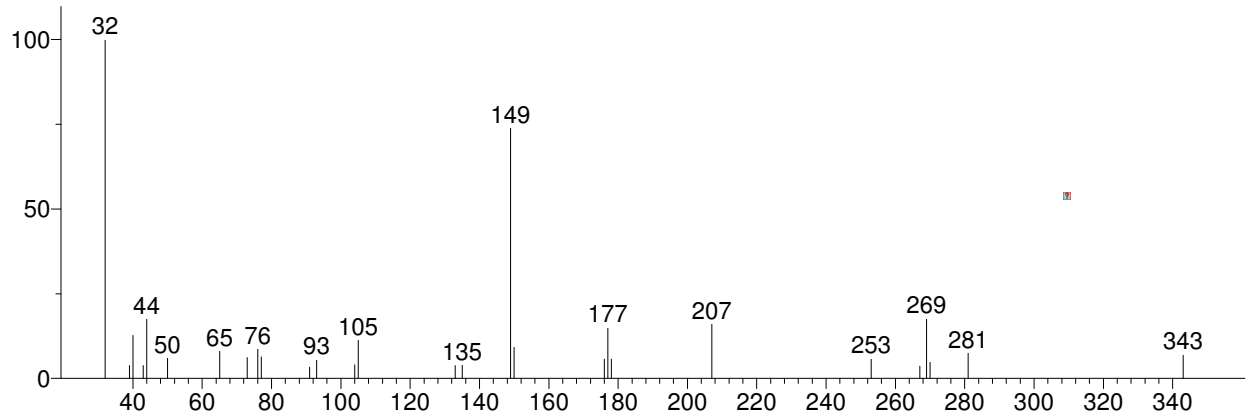
Hit 1 : Hexanal
C6H12O; MF: 490; RMF: 822; Prob 14.2%; CAS: 66-25-1; Lib: replib; ID: 3284.



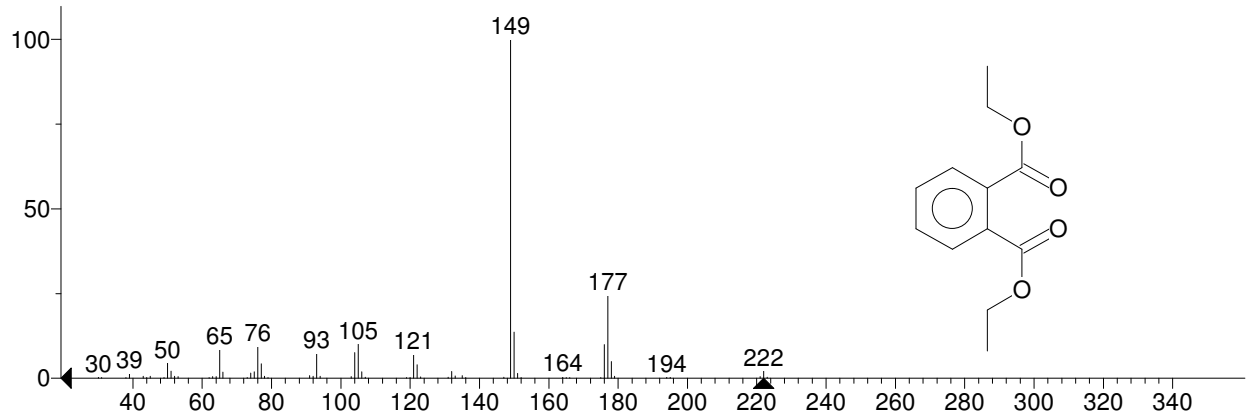
Hit 2 : 1,2,4-Cyclopentanetriol
C5H10O3; MF: 473; RMF: 657; Prob 7.75%; CAS: 56772-26-0; Lib: mainlib; ID: 20241.



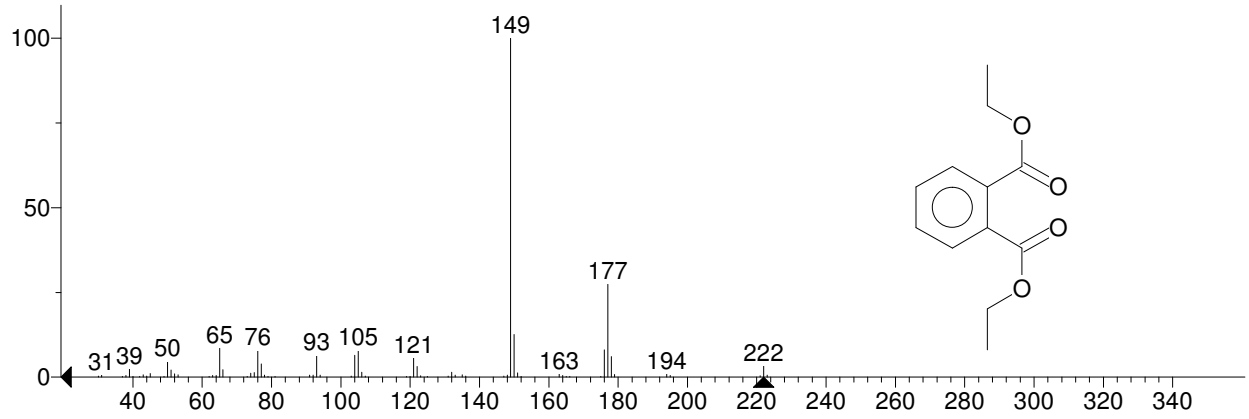
Unknown: Scan 2786 (16.653 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -903



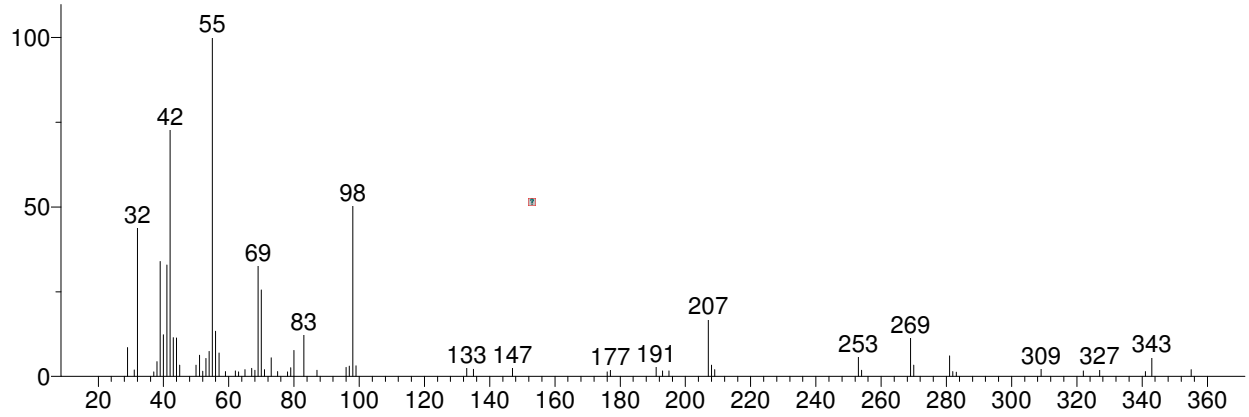
Hit 1 : Diethyl Phthalate
C12H14O4; MF: 547; RMF: 818; Prob 33.2%; CAS: 84-66-2; Lib: mainlib; ID: 110716.



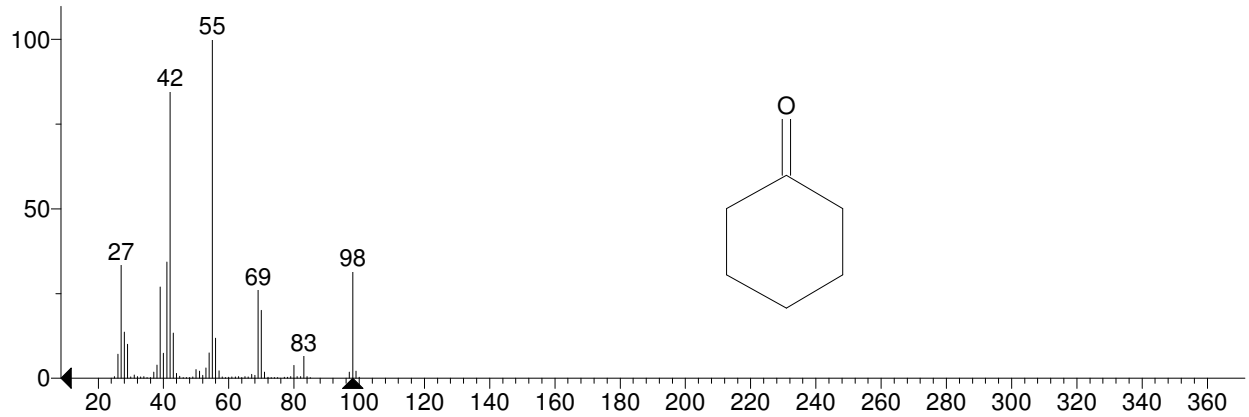
Hit 2 : Diethyl Phthalate
C12H14O4; MF: 541; RMF: 783; Prob 33.2%; CAS: 84-66-2; Lib: replib; ID: 20069.



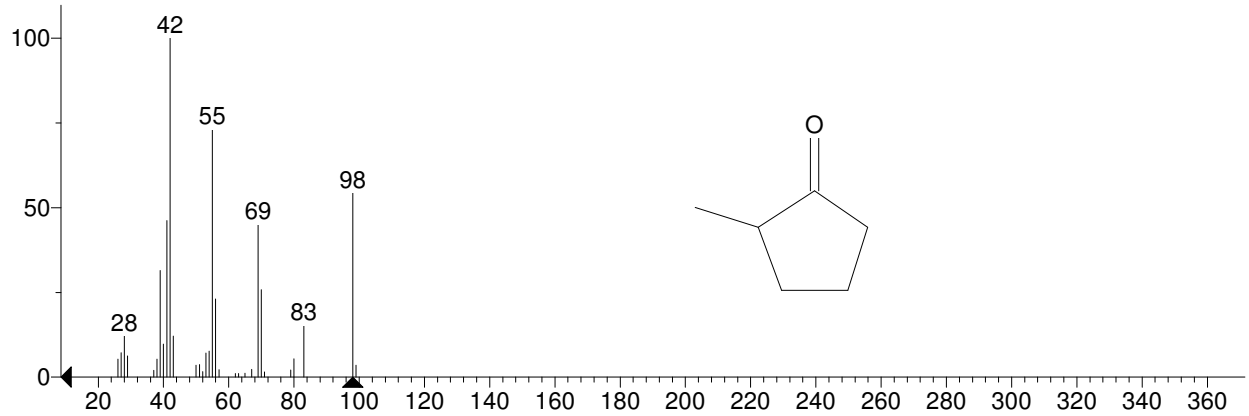
Unknown: Scan 3025 (18.074 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -449



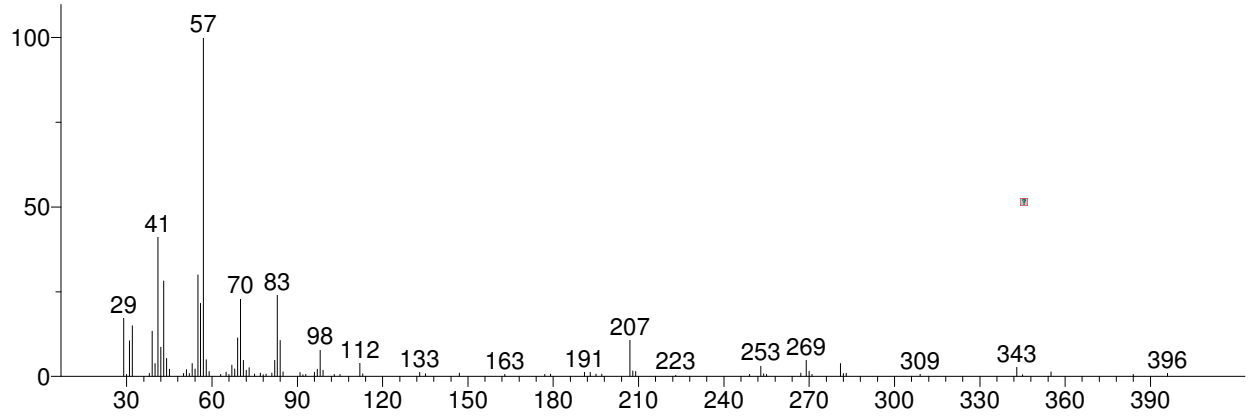
Hit 1 : Cyclohexanone
C6H10O; MF: 654; RMF: 871; Prob 29.2%; CAS: 108-94-1; Lib: replib; ID: 4338.



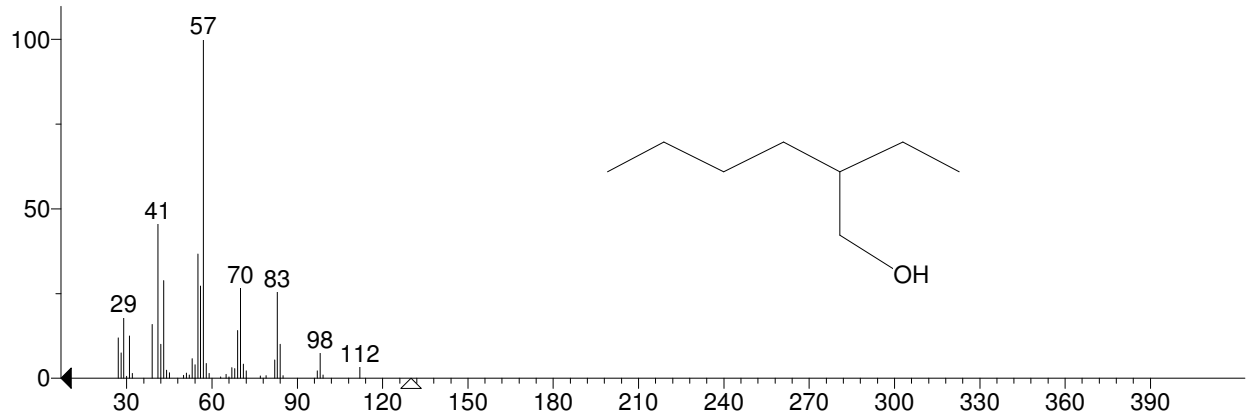
Hit 2 : Cyclopentanone, 2-methyl-
C6H10O; MF: 653; RMF: 917; Prob 28.1%; CAS: 1120-72-5; Lib: mainlib; ID: 4394.



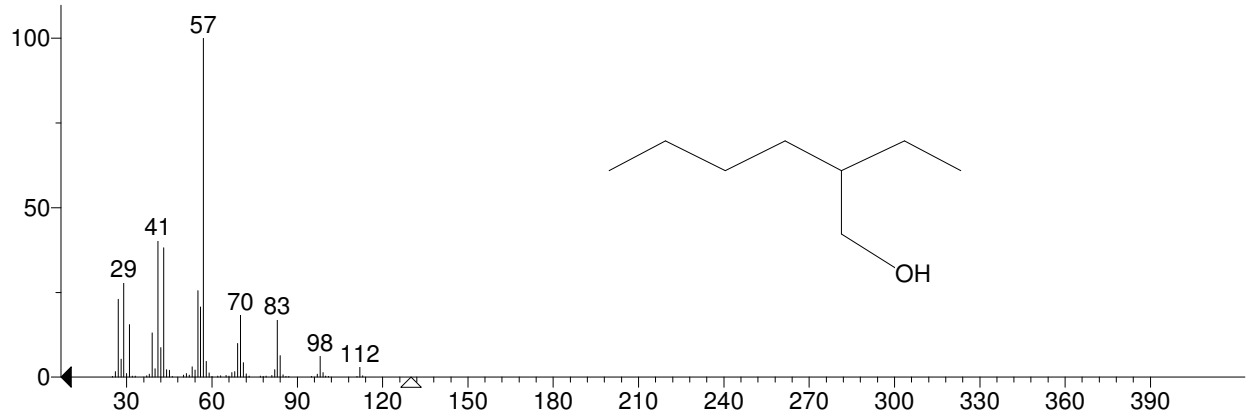
Unknown: Scan 3229 (19.287 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -447



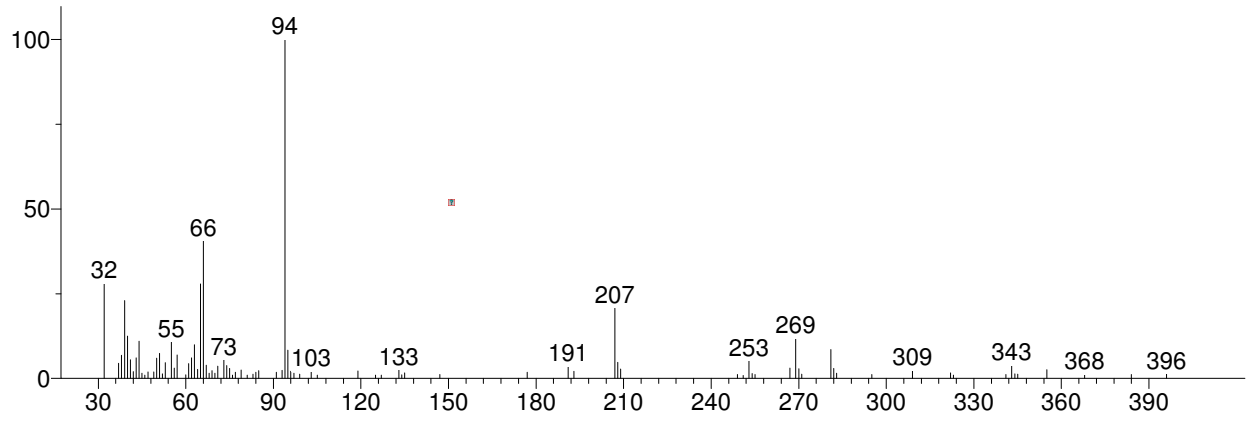
Hit 1 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 737; RMF: 929; Prob 37.5%; CAS: 104-76-7; Lib: replib; ID: 5289.



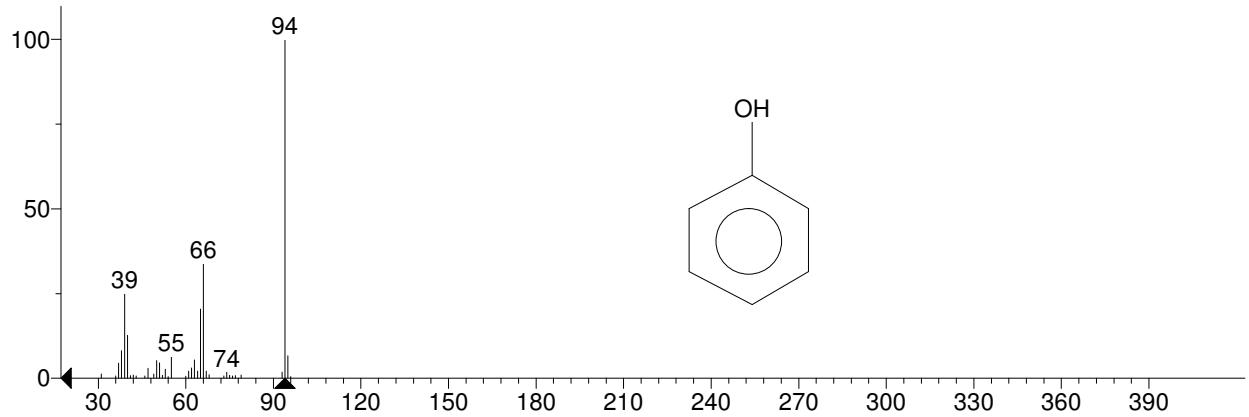
Hit 2 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 737; RMF: 909; Prob 37.5%; CAS: 104-76-7; Lib: mainlib; ID: 21179.



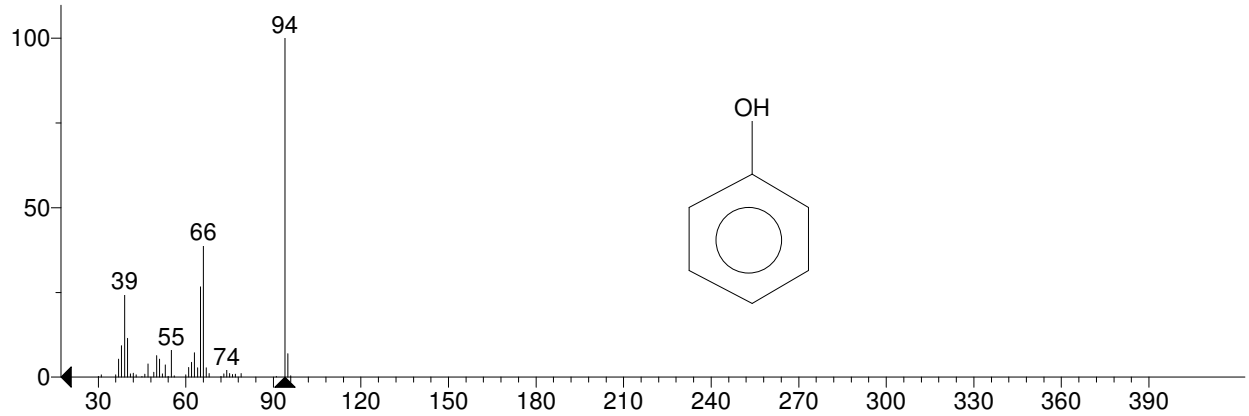
Unknown: Scan 3267 (19.513 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -1424



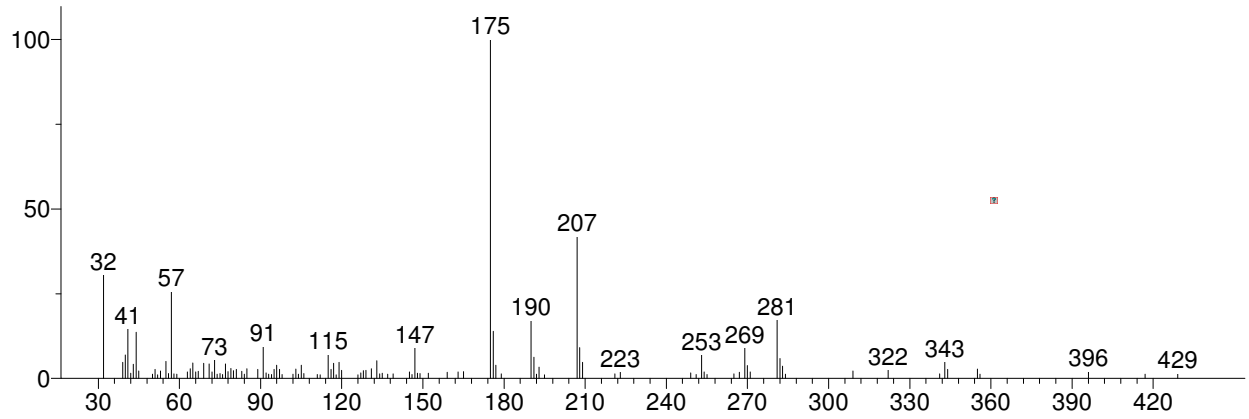
Hit 1 : Phenol
C6H6O; MF: 588; RMF: 890; Prob 30.3%; CAS: 108-95-2; Lib: replib; ID: 12309.



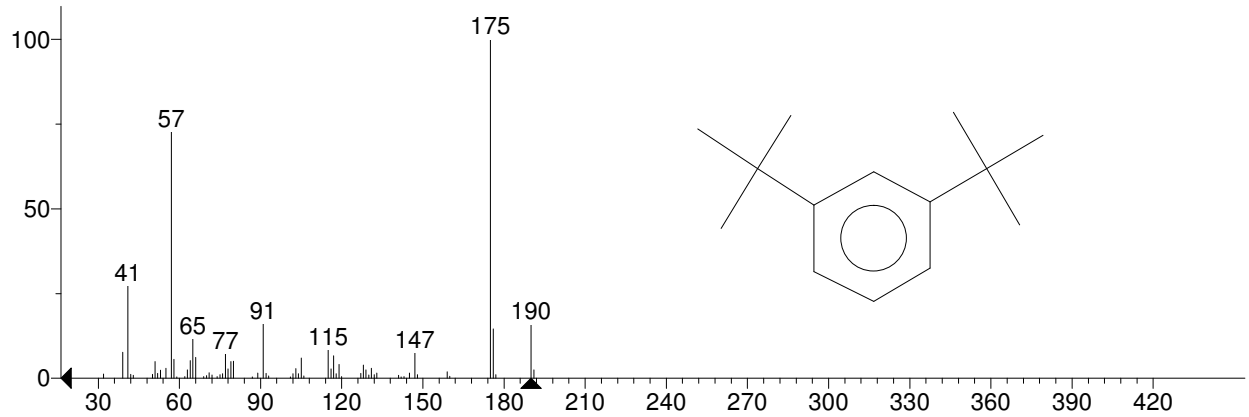
Hit 2 : Phenol
C6H6O; MF: 581; RMF: 880; Prob 30.3%; CAS: 108-95-2; Lib: mainlib; ID: 57401.



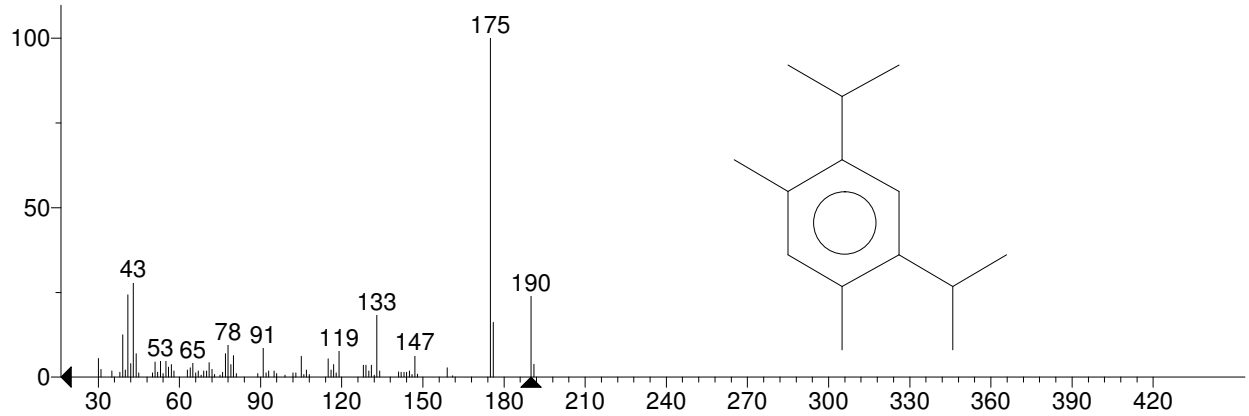
Unknown: Scan 3693 (22.046 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -2179



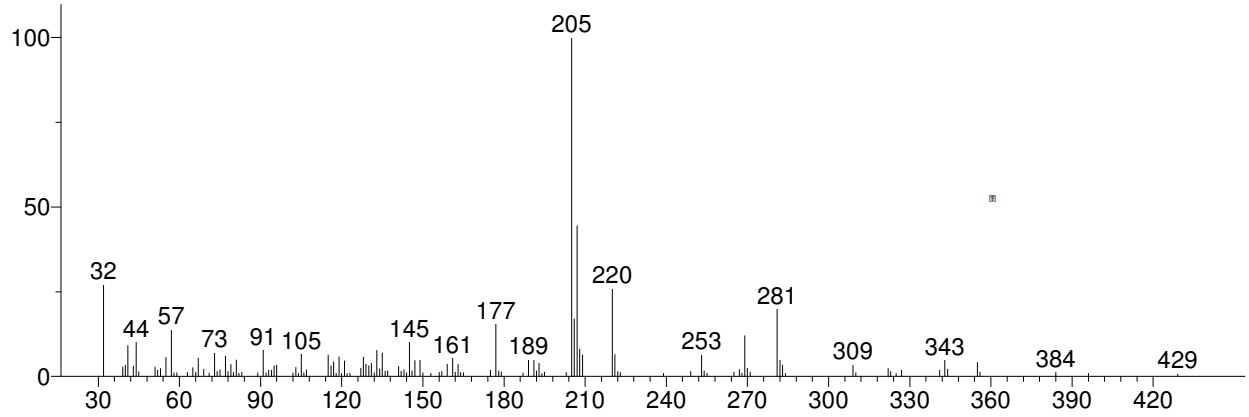
Hit 1 : Benzene, 1,3-bis(1,1-dimethylethyl)-
C14H22; MF: 574; RMF: 856; Prob 15.0%; CAS: 1014-60-4; Lib: replib; ID: 22503.



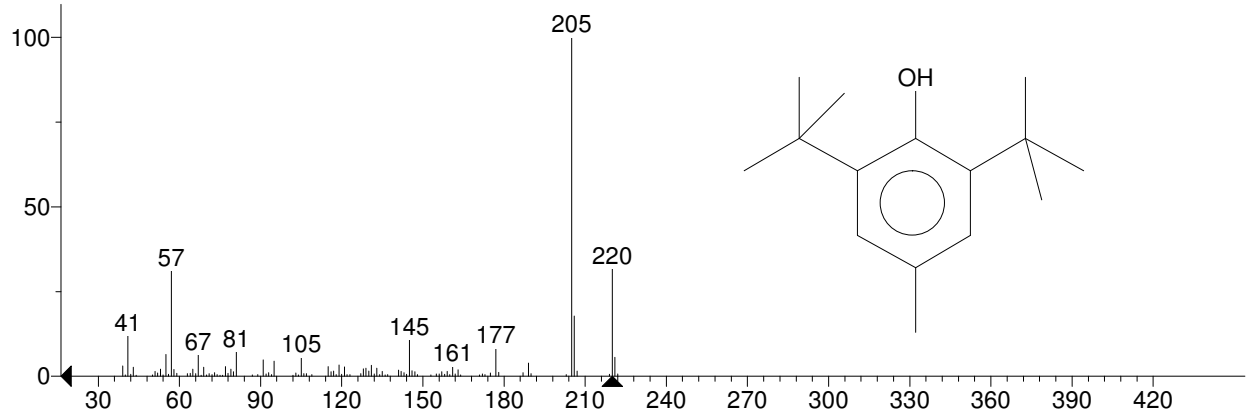
Hit 2 : Benzene, 1,5-dimethyl-2,4-bis(1-methylethyl)-
C14H22; MF: 565; RMF: 831; Prob 10.9%; CAS: 5186-68-5; Lib: mainlib; ID: 130010.



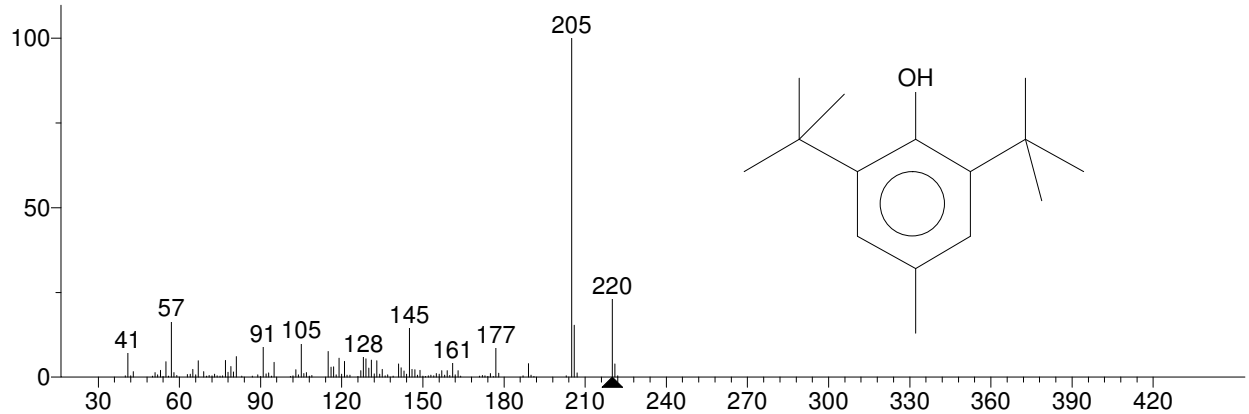
Unknown: Scan 4489 (26.779 min): J9163_EVA_1.D\data.ms
Compound in Library Factor = -1066



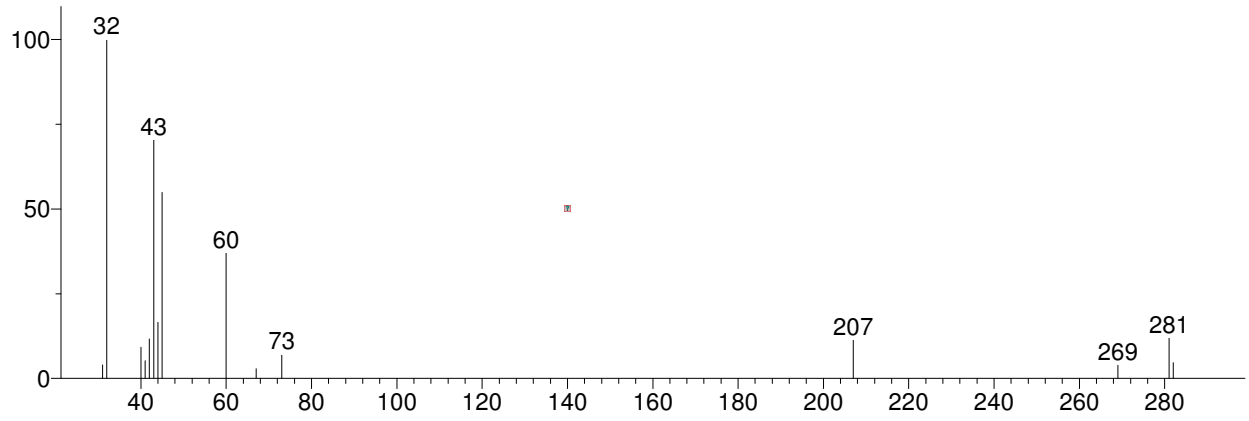
Hit 1 : Butylated Hydroxytoluene
C15H24O; MF: 670; RMF: 830; Prob 47.0%; CAS: 128-37-0; Lib: replib; ID: 24595.



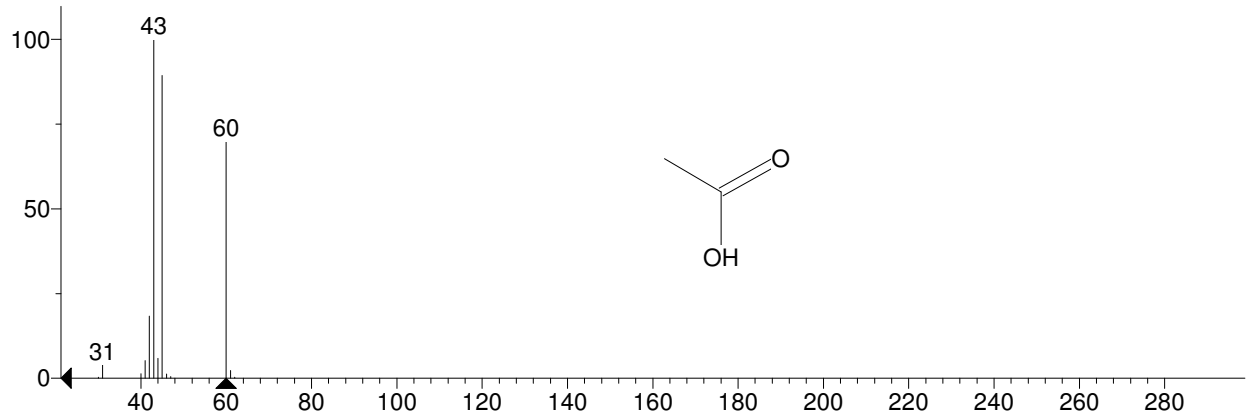
Hit 2 : Butylated Hydroxytoluene
C15H24O; MF: 670; RMF: 823; Prob 47.0%; CAS: 128-37-0; Lib: replib; ID: 24596.



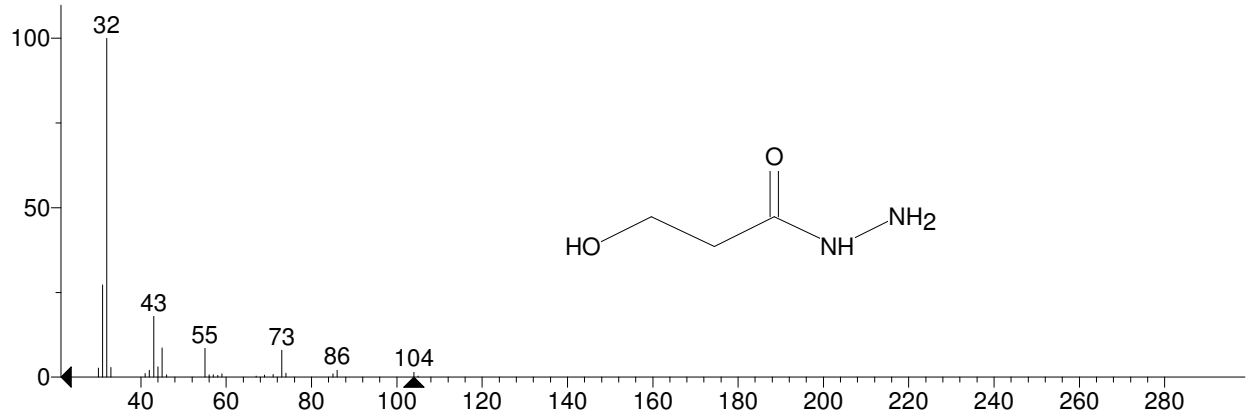
Unknown: Scan 2146 (12.847 min): J9163_EVA_2.D\data.ms
Compound in Library Factor = -1558



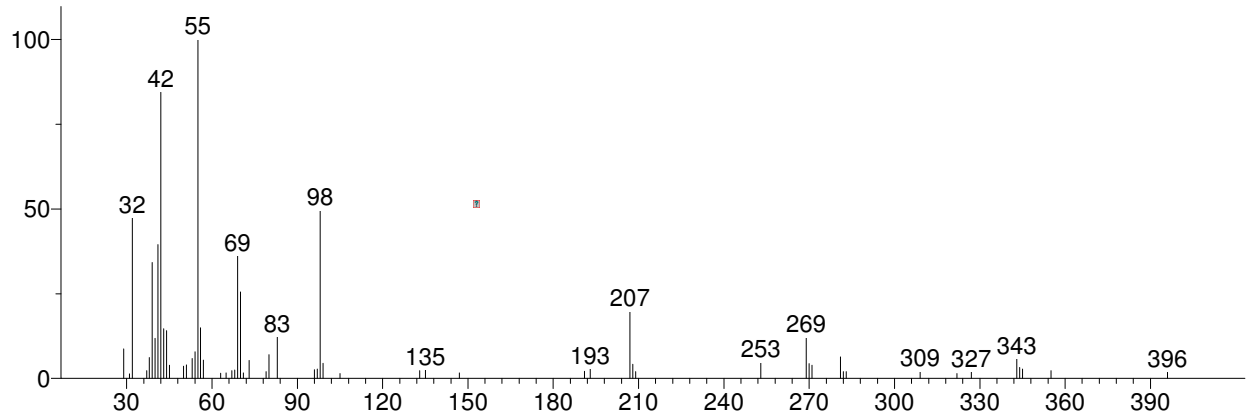
Hit 1 : Acetic acid
C2H4O2; MF: 496; RMF: 816; Prob 11.8%; CAS: 64-19-7; Lib: replib; ID: 1870.



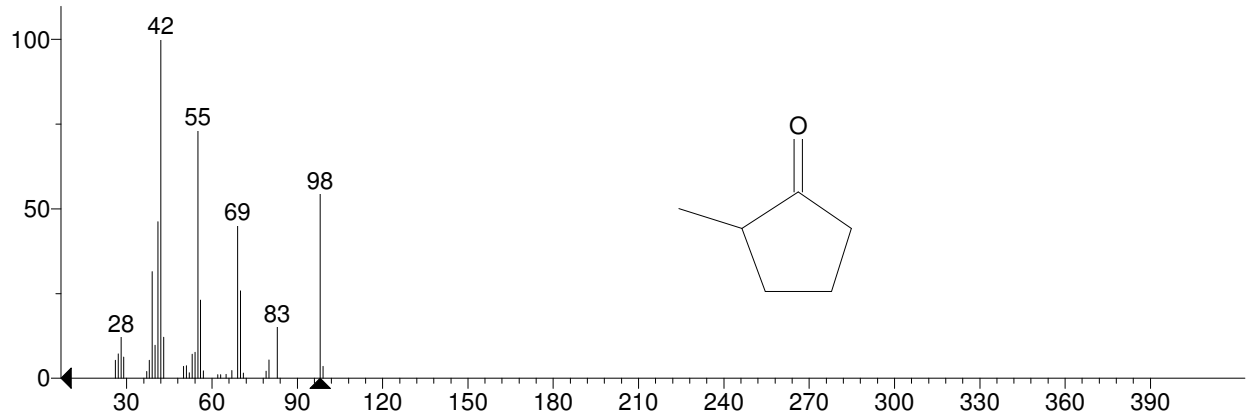
Hit 2 : Propanoic acid, 3-hydroxy-, hydrazide
C3H8N2O2; MF: 494; RMF: 697; Prob 10.9%; CAS: 24535-11-3; Lib: mainlib; ID: 1455.



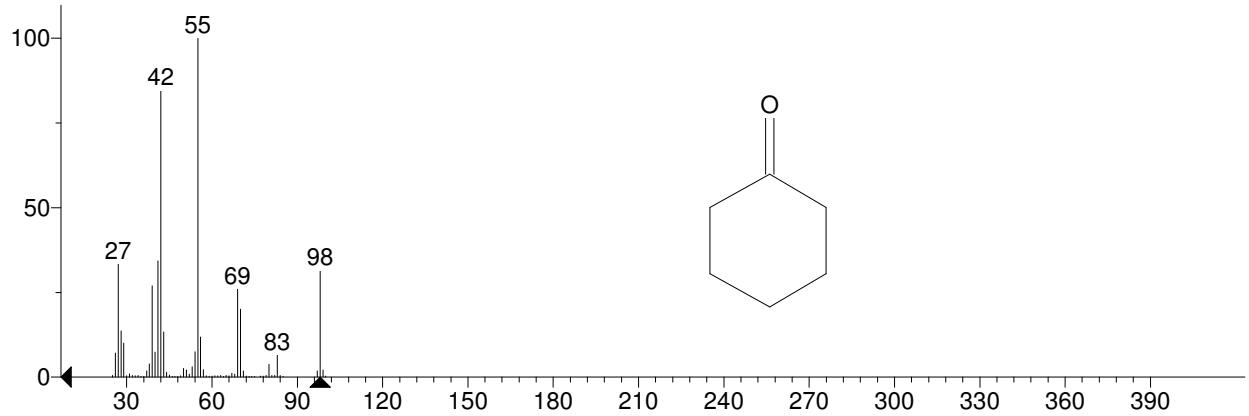
Unknown: Scan 3023 (18.062 min): J9163_EVA_2.D\data.ms
Compound in Library Factor = -454



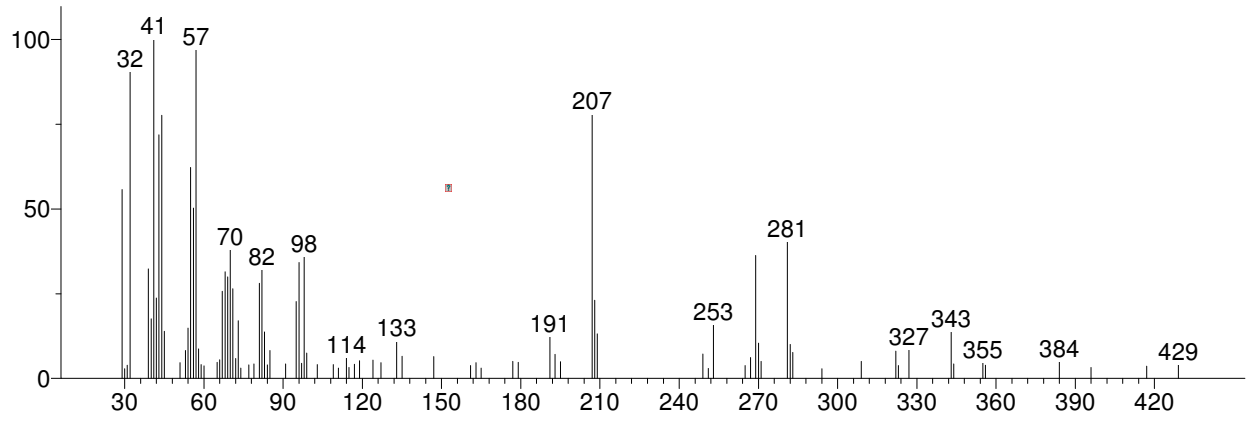
Hit 1 : Cyclopentanone, 2-methyl-
C6H10O; MF: 645; RMF: 933; Prob 33.1%; CAS: 1120-72-5; Lib: mainlib; ID: 4394.



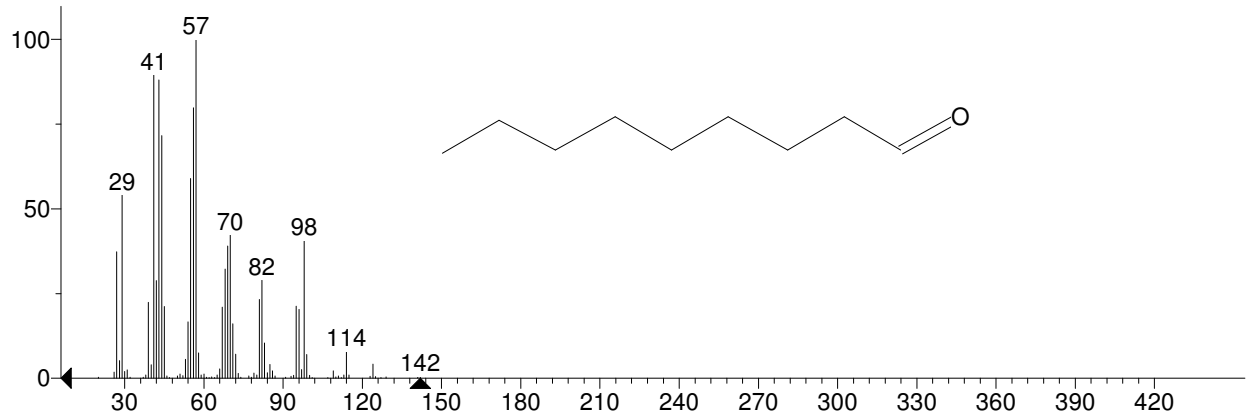
Hit 2 : Cyclohexanone
C6H10O; MF: 635; RMF: 874; Prob 23.4%; CAS: 108-94-1; Lib: replib; ID: 4338.



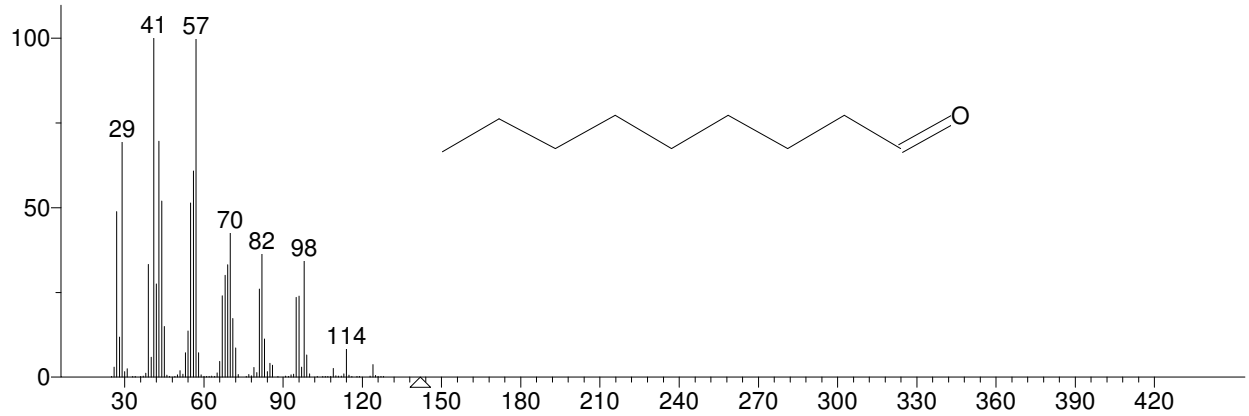
Unknown: Scan 3391 (20.250 min): J9163_EVA_2.D\data.ms
Compound in Library Factor = -1051



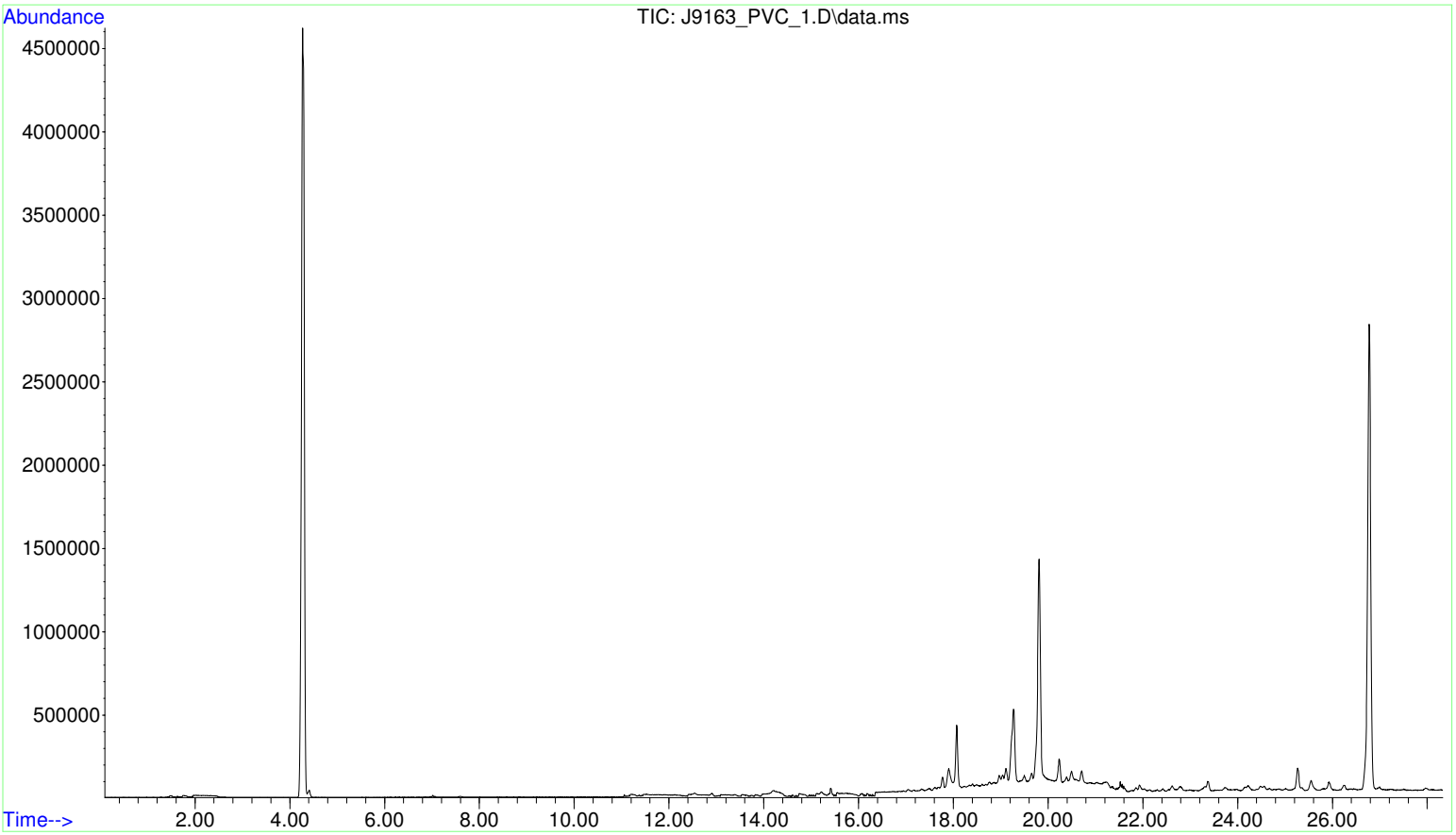
Hit 1 : Nonanal
C9H18O; MF: 530; RMF: 843; Prob 29.3%; CAS: 124-19-6; Lib: mainlib; ID: 21171.



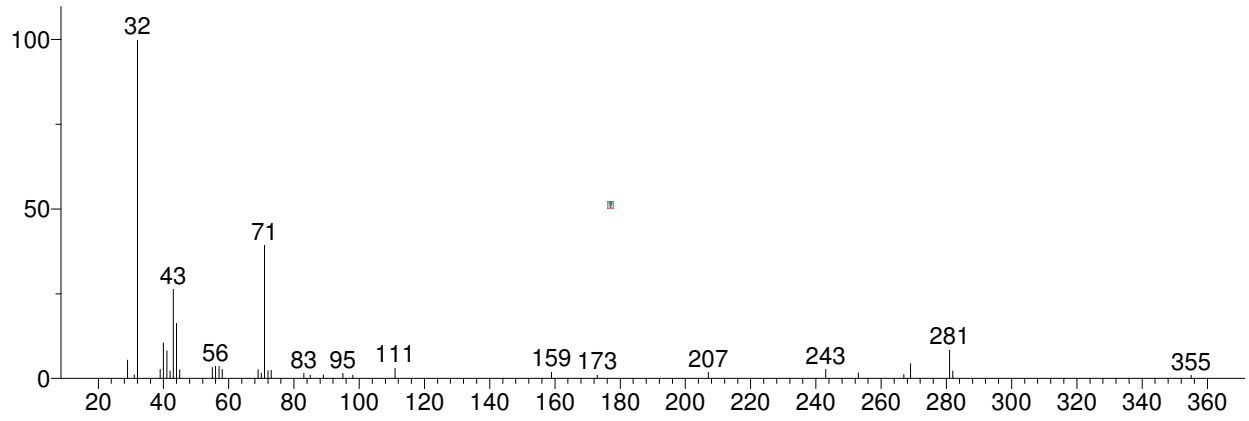
Hit 2 : Nonanal
C9H18O; MF: 522; RMF: 865; Prob 29.3%; CAS: 124-19-6; Lib: replib; ID: 1003.



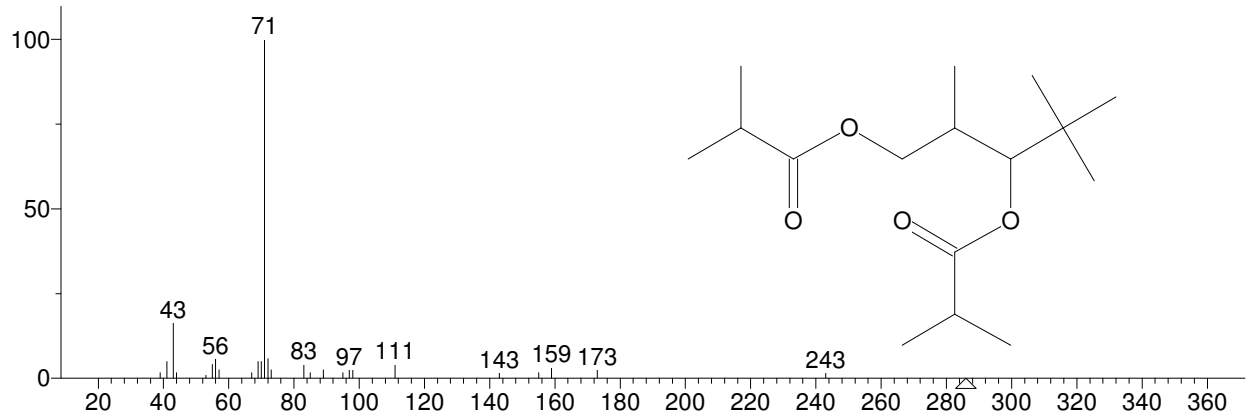
File :D:\msdchem\1\data\2014\J9163 Jordi\dhs\J9163_PVC_1.D
Operator : Oliver Palardy
Acquired : 5 Nov 2014 22:27 using AcqMethod J9163_PVC.M
Instrument : 7890
Sample Name: PVC 1
Misc Info :
Vial Number: 5



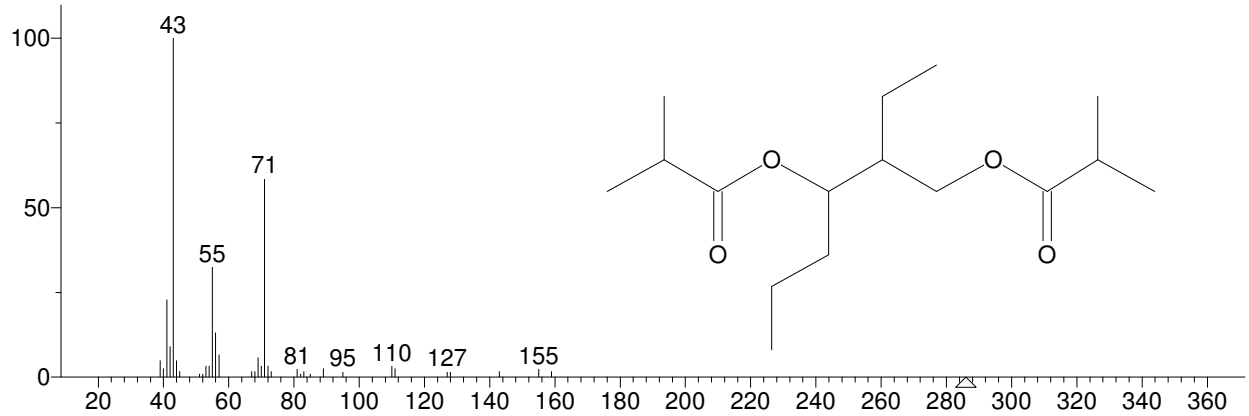
Unknown: Scan 2379 (14.233 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = -997



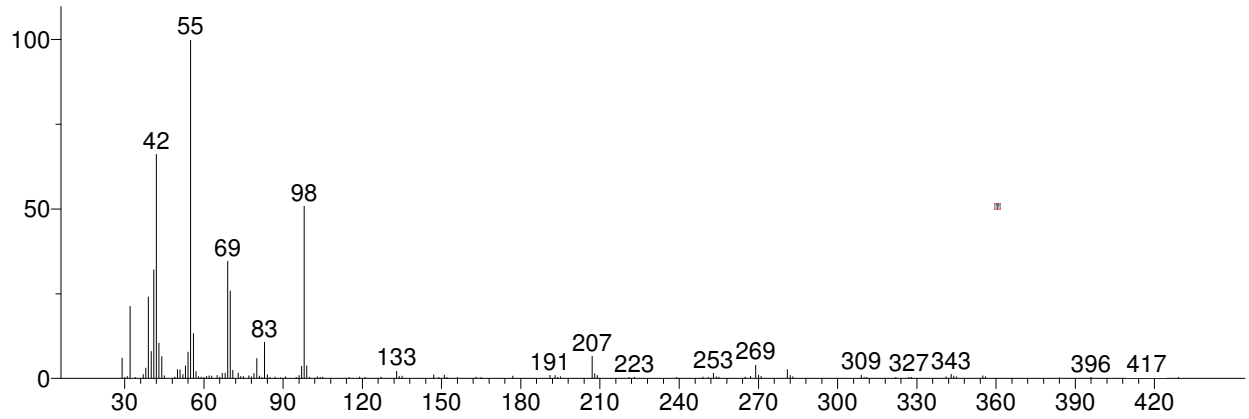
Hit 1 : Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester
C16H30O4; MF: 583; RMF: 802; Prob 56.8%; CAS: 74381-40-1; Lib: mainlib; ID: 33211.



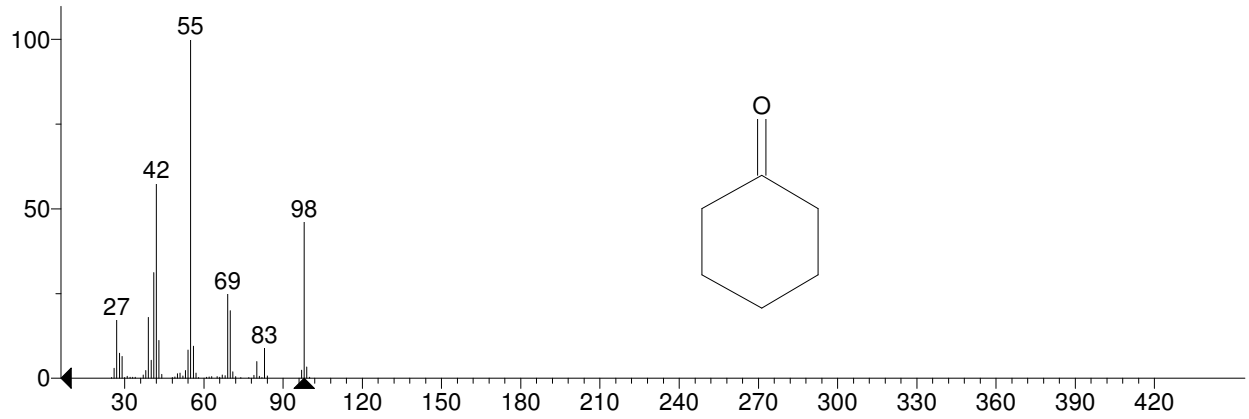
Hit 2 : Propanoic acid, 2-methyl-, 2-ethyl-1-propyl-1,3-propanediyl ester
C16H30O4; MF: 537; RMF: 734; Prob 12.0%; CAS: 74367-30-9; Lib: mainlib; ID: 8180.



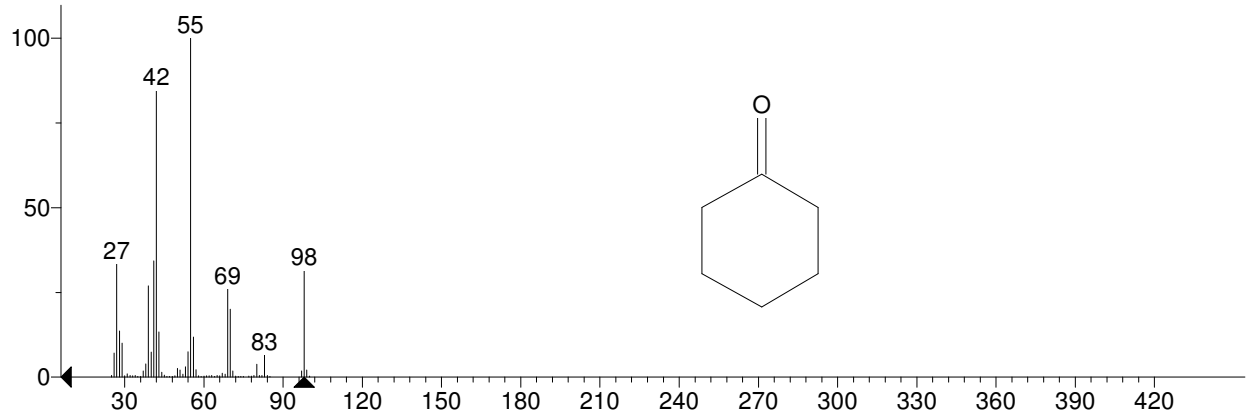
Unknown: Scan 3026 (18.080 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = -282



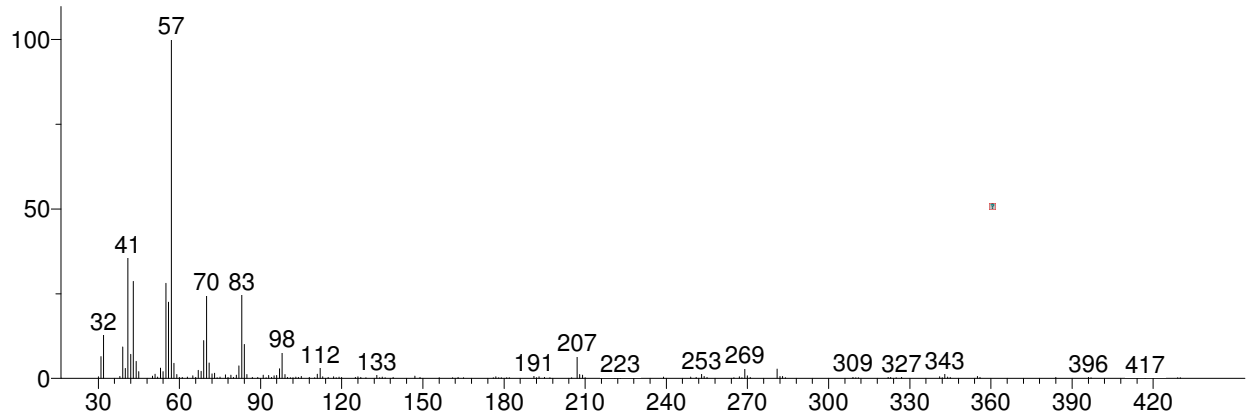
Hit 1 : Cyclohexanone
C6H10O; MF: 773; RMF: 918; Prob 58.3%; CAS: 108-94-1; Lib: replib; ID: 4347.



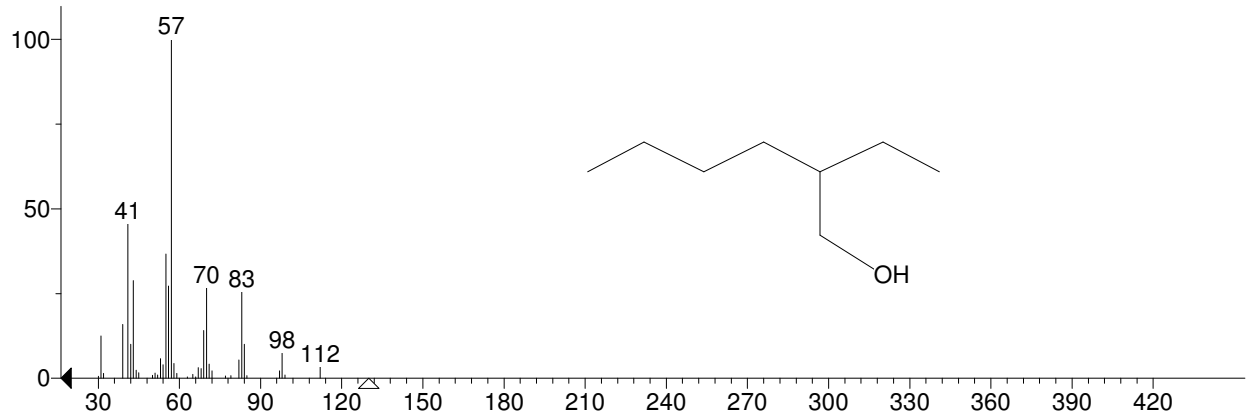
Hit 2 : Cyclohexanone
C6H10O; MF: 757; RMF: 889; Prob 58.3%; CAS: 108-94-1; Lib: replib; ID: 4338.



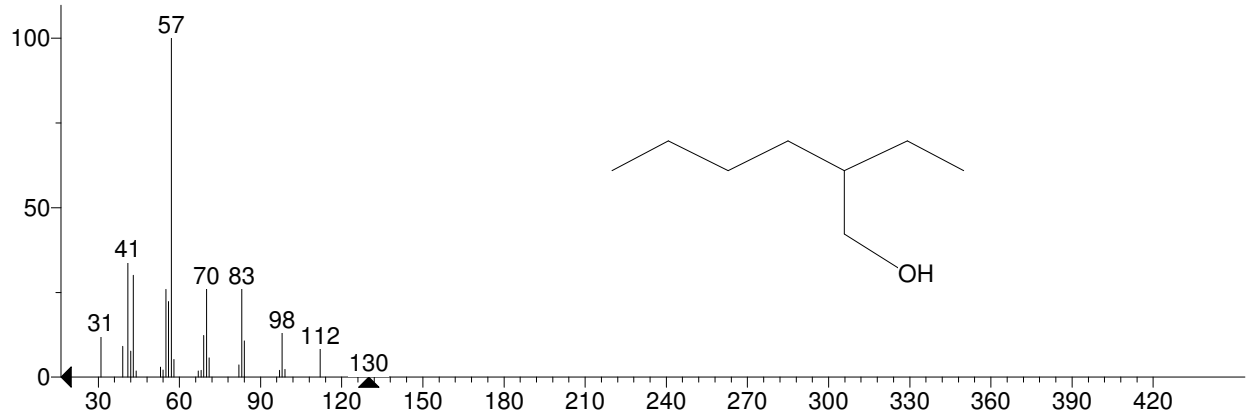
Unknown: Scan 3227 (19.275 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = -377



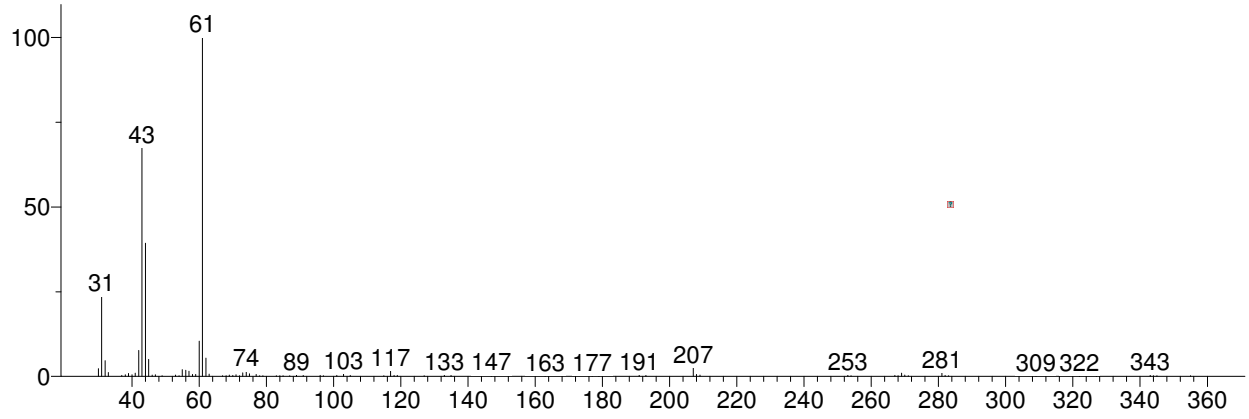
Hit 1 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 777; RMF: 931; Prob 39.0%; CAS: 104-76-7; Lib: replib; ID: 5289.



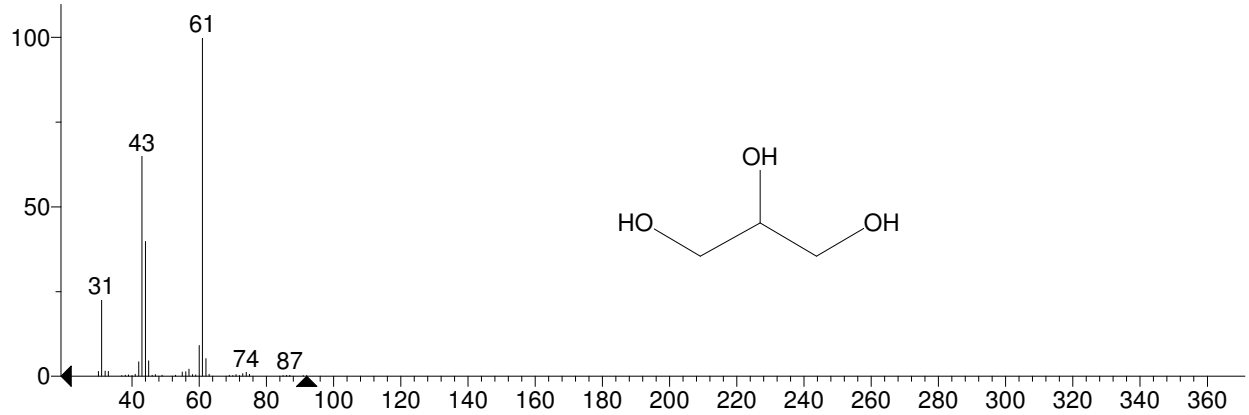
Hit 2 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 767; RMF: 953; Prob 39.0%; CAS: 104-76-7; Lib: replib; ID: 5259.



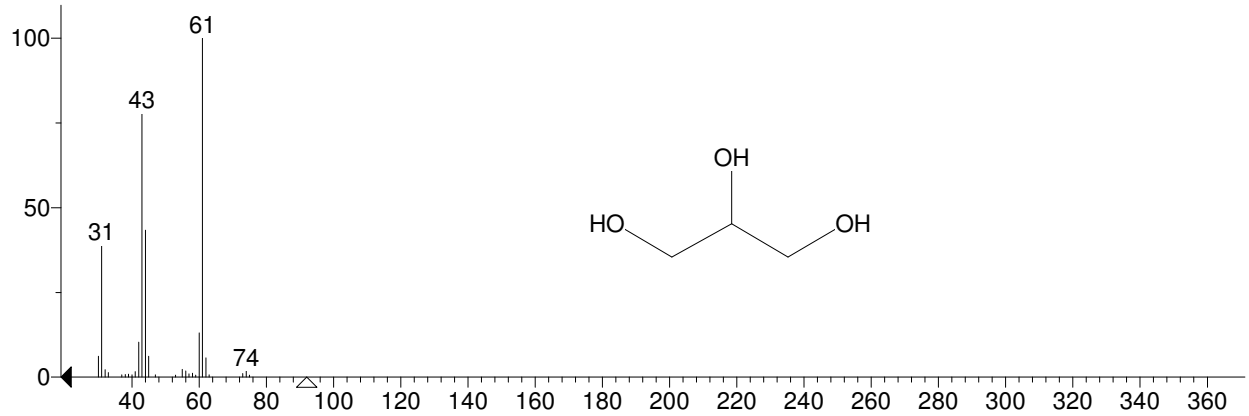
Unknown: Scan 3316 (19.804 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = 106



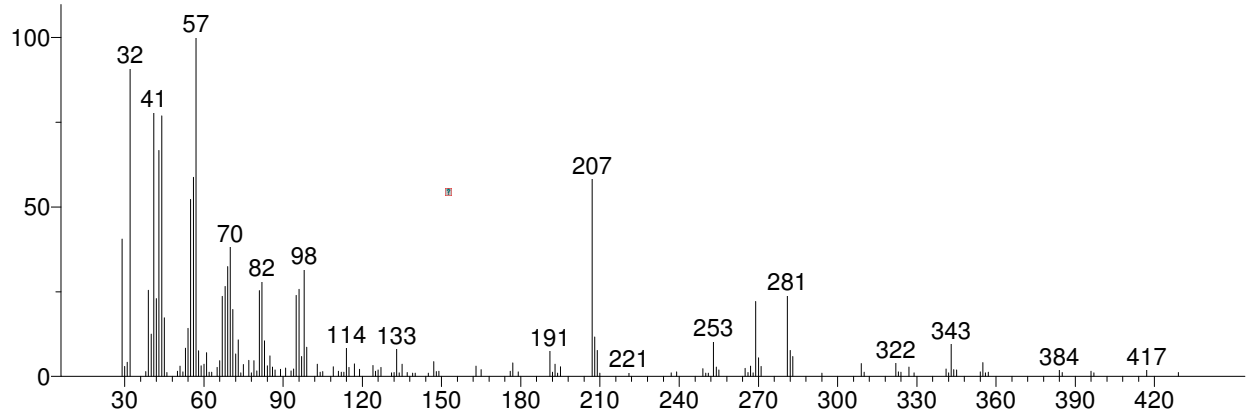
Hit 1 : Glycerin
C3H8O3; MF: 844; RMF: 916; Prob 87.5%; CAS: 56-81-5; Lib: replib; ID: 6753.



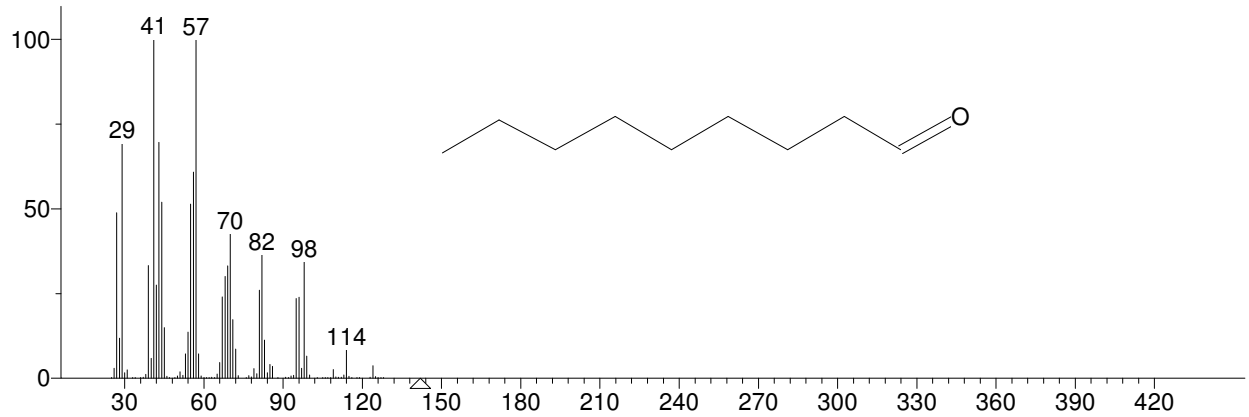
Hit 2 : Glycerin
C3H8O3; MF: 838; RMF: 914; Prob 87.5%; CAS: 56-81-5; Lib: mainlib; ID: 27364.



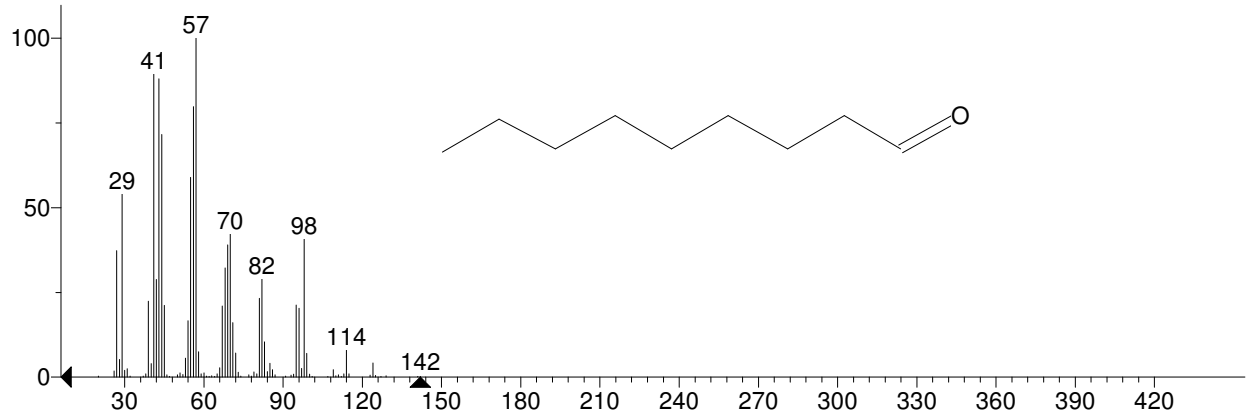
Unknown: Scan 3389 (20.238 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = -1210



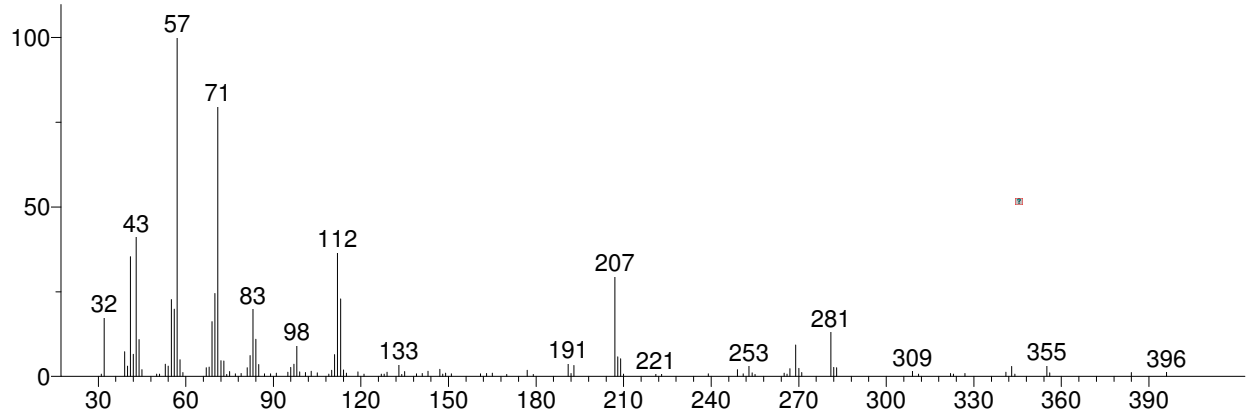
Hit 1 : Nonanal
C9H18O; MF: 584; RMF: 870; Prob 21.6%; CAS: 124-19-6; Lib: replib; ID: 1003.



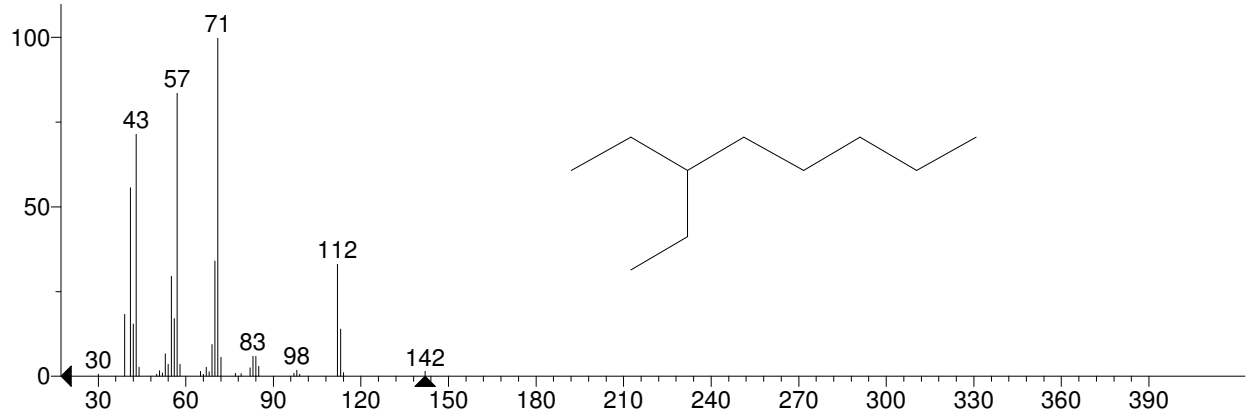
Hit 2 : Nonanal
C9H18O; MF: 581; RMF: 837; Prob 21.6%; CAS: 124-19-6; Lib: mainlib; ID: 21171.



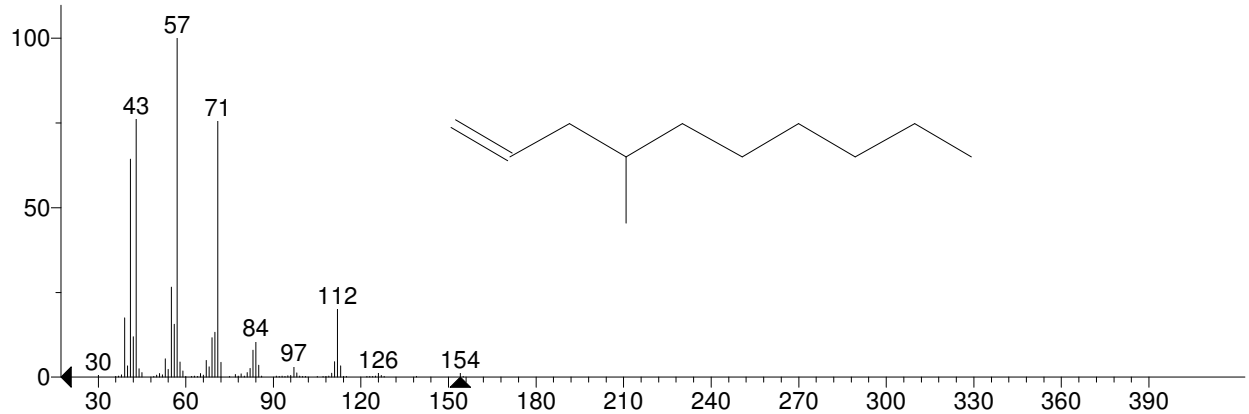
Unknown: Scan 4235 (25.269 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = -1302



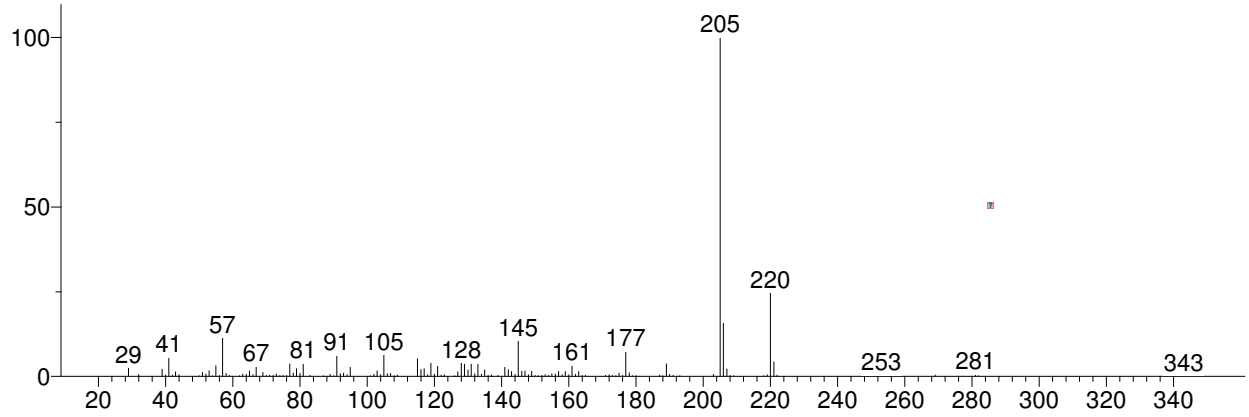
Hit 1 : Octane, 3-ethyl-
C10H22; MF: 617; RMF: 889; Prob 8.41%; CAS: 5881-17-4; Lib: replib; ID: 8109.



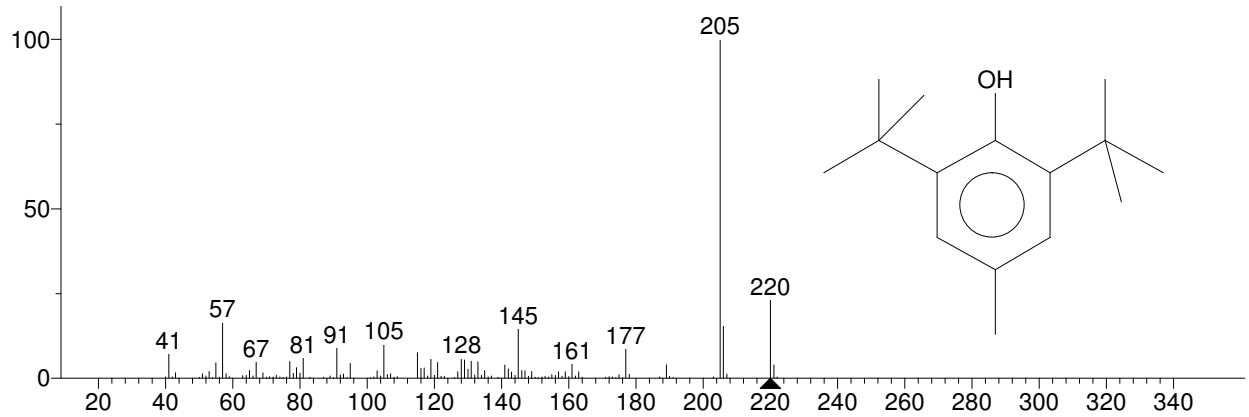
Hit 2 : 1-Decene, 4-methyl-
C11H22; MF: 600; RMF: 839; Prob 4.59%; CAS: 13151-29-6; Lib: mainlib; ID: 21913.



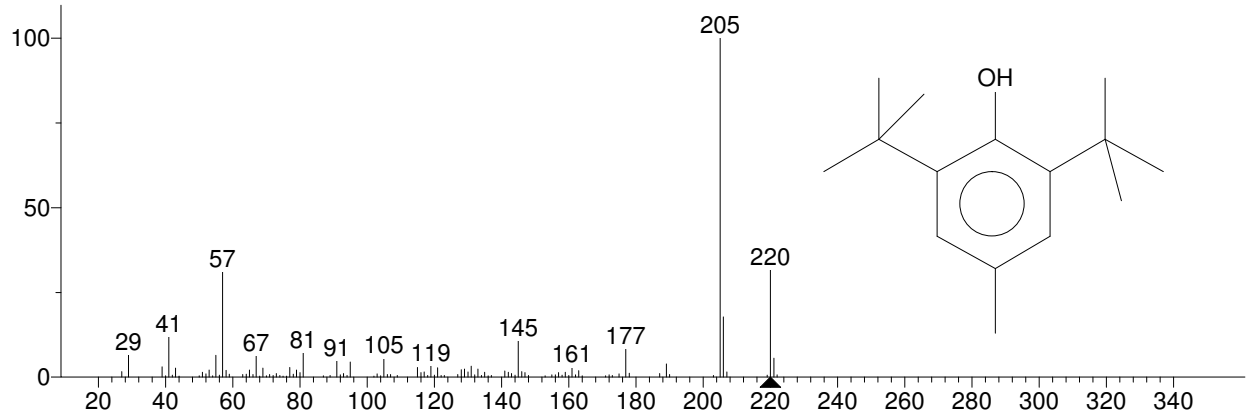
Unknown: Scan 4487 (26.767 min): J9163_PVC_1.D\data.ms
Compound in Library Factor = 165



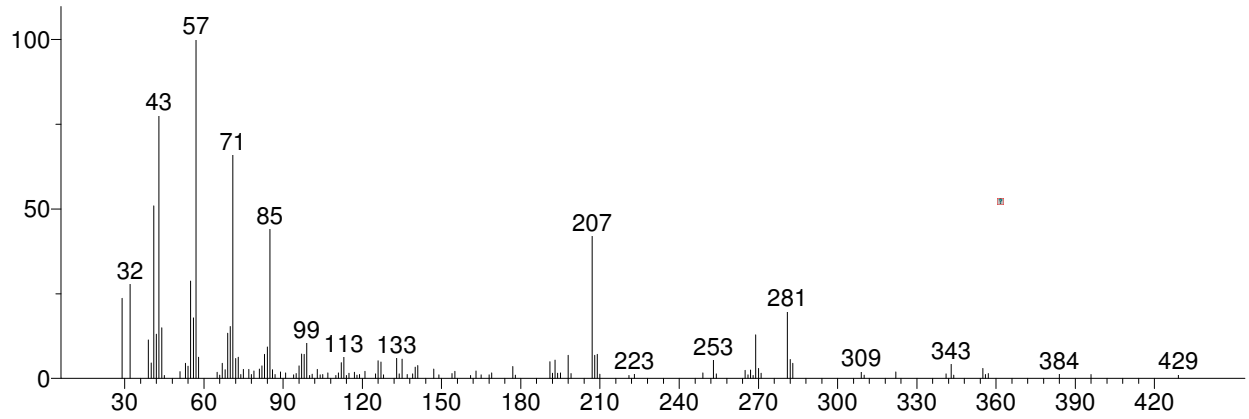
Hit 1 : Butylated Hydroxytoluene
C15H24O; MF: 942; RMF: 947; Prob 76.0%; CAS: 128-37-0; Lib: replib; ID: 24596.



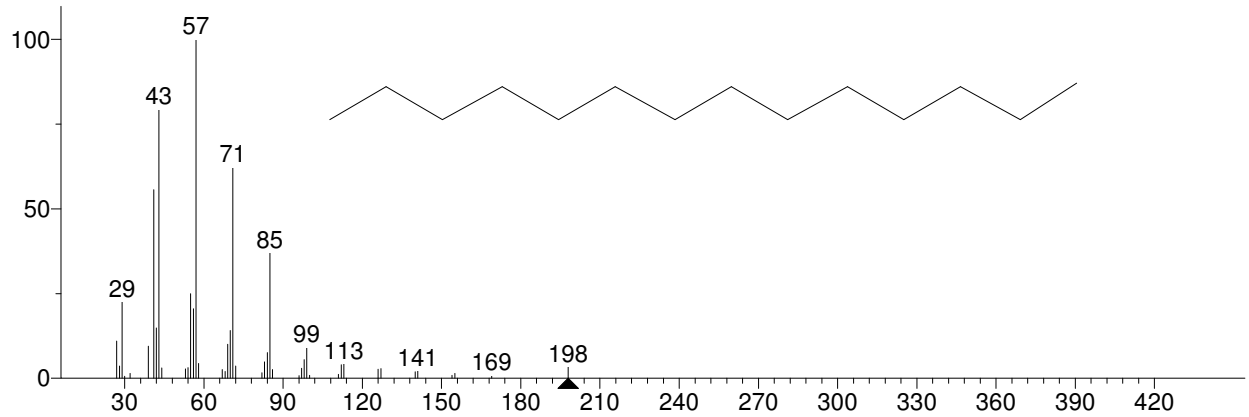
Hit 2 : Butylated Hydroxytoluene
C15H24O; MF: 919; RMF: 928; Prob 76.0%; CAS: 128-37-0; Lib: replib; ID: 24595.



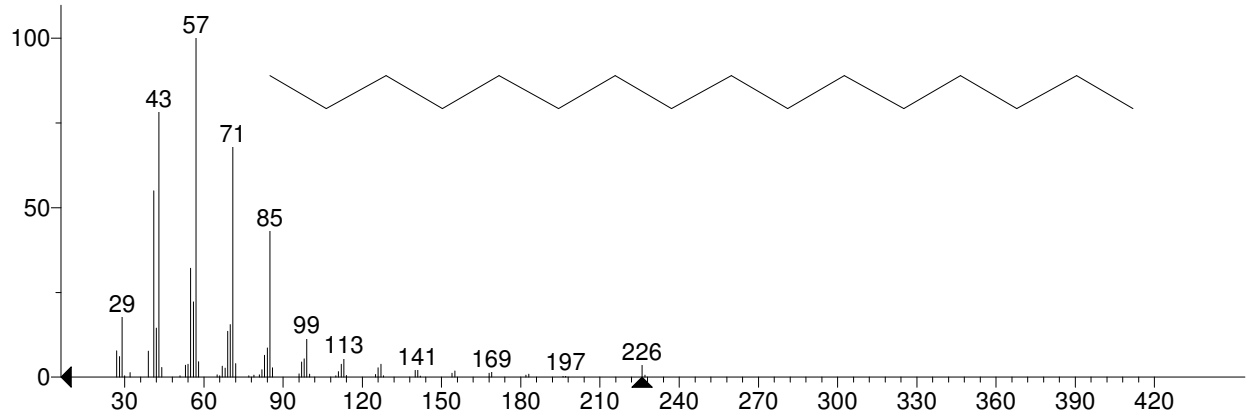
Unknown: Scan 3915 (23.366 min): J9163_PVC_2.D\data.ms
Compound in Library Factor = -1302



Hit 1 : Tetradecane
C14H30; MF: 614; RMF: 931; Prob 8.09%; CAS: 629-59-4; Lib: replib; ID: 5511.



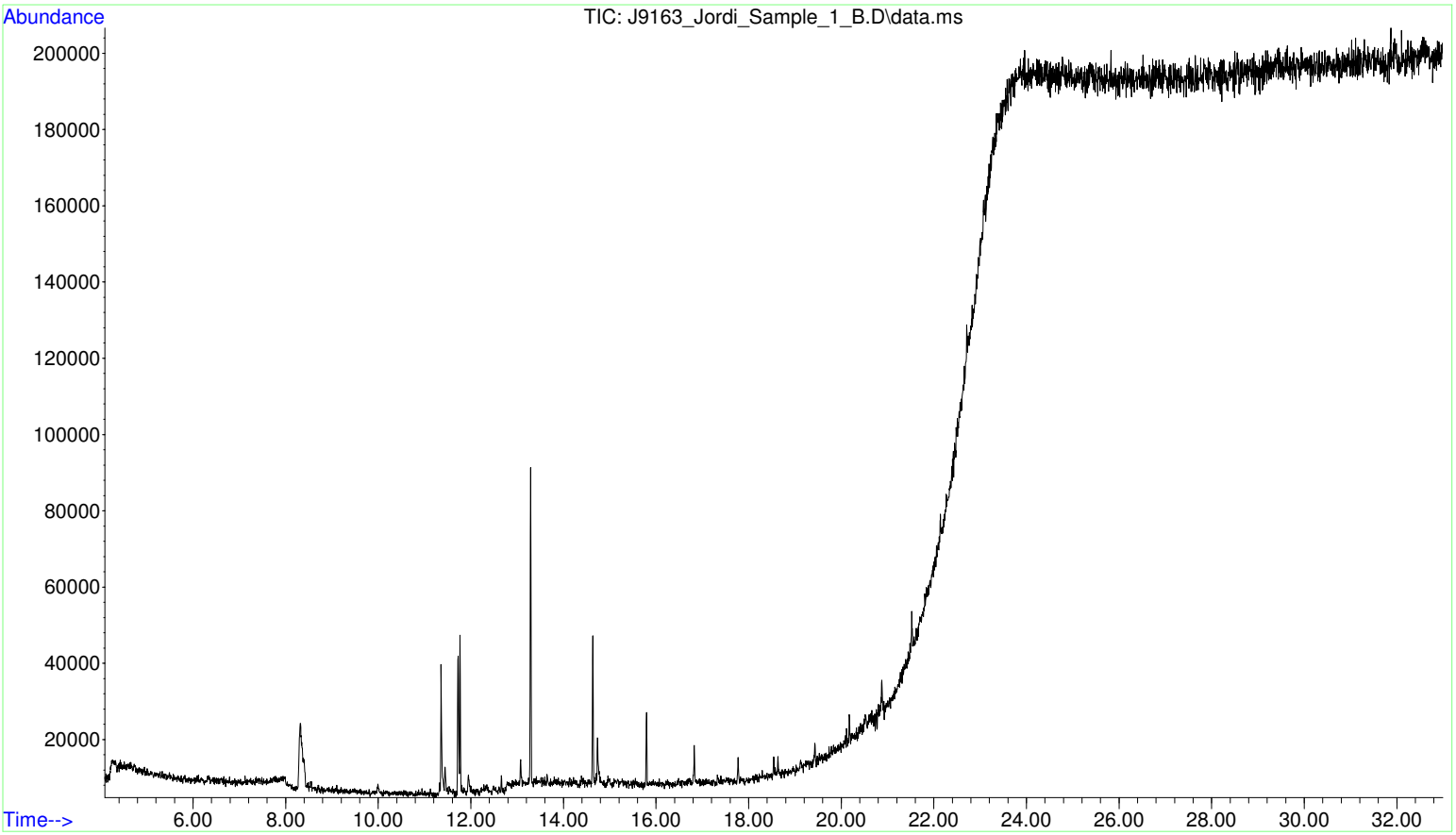
Hit 2 : Hexadecane
C16H34; MF: 607; RMF: 896; Prob 6.20%; CAS: 544-76-3; Lib: replib; ID: 5556.



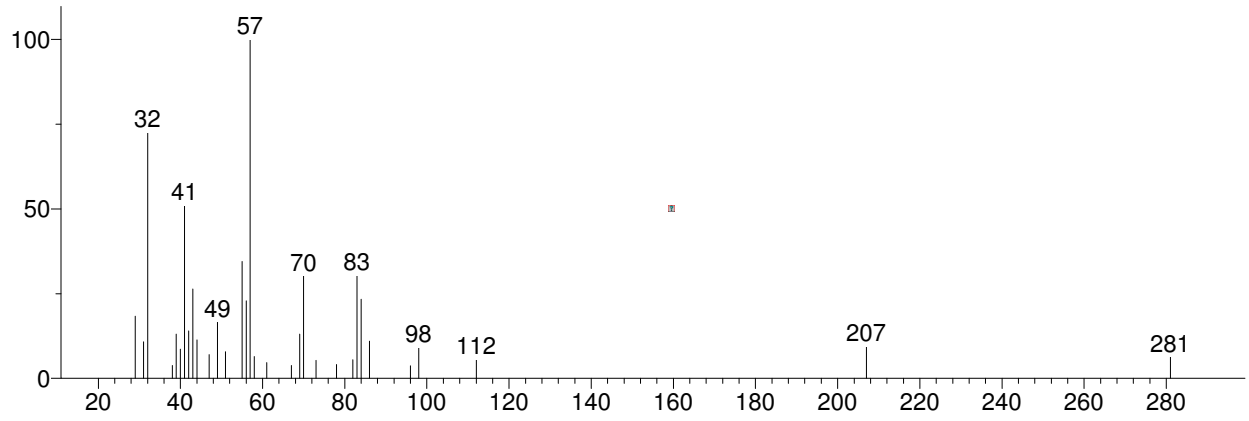
GCMS Data

File :D:\msdchem\1\data\2014\J9163 Jordi\102714\J9163_Jordi_Sample
... _1_B.D
Operator : Courtney McGowan
Instrument : 7890
Acquired : 28 Oct 2014 16:30 using AcqMethod GCMS.M
Sample Name: J9163 Jordi Sample 1
Misc Info :

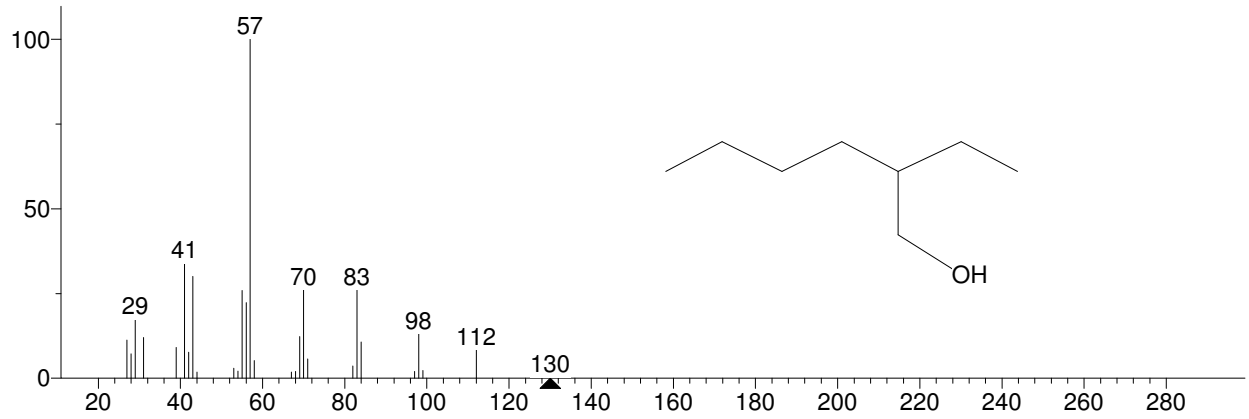
PVC bag in water



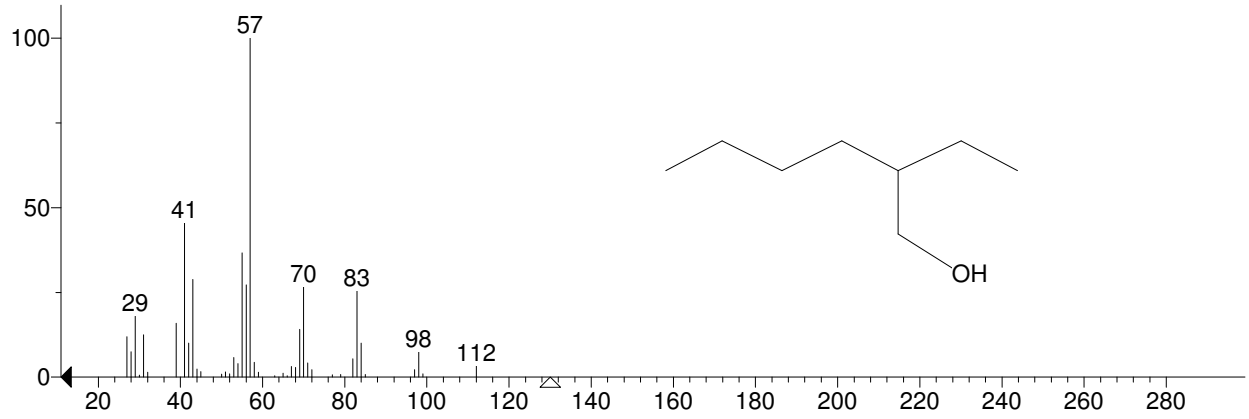
Unknown: Scan 712 (8.320 min): J9163_Jordi_Sample_1_B.D\data.ms
Compound in Library Factor = -695



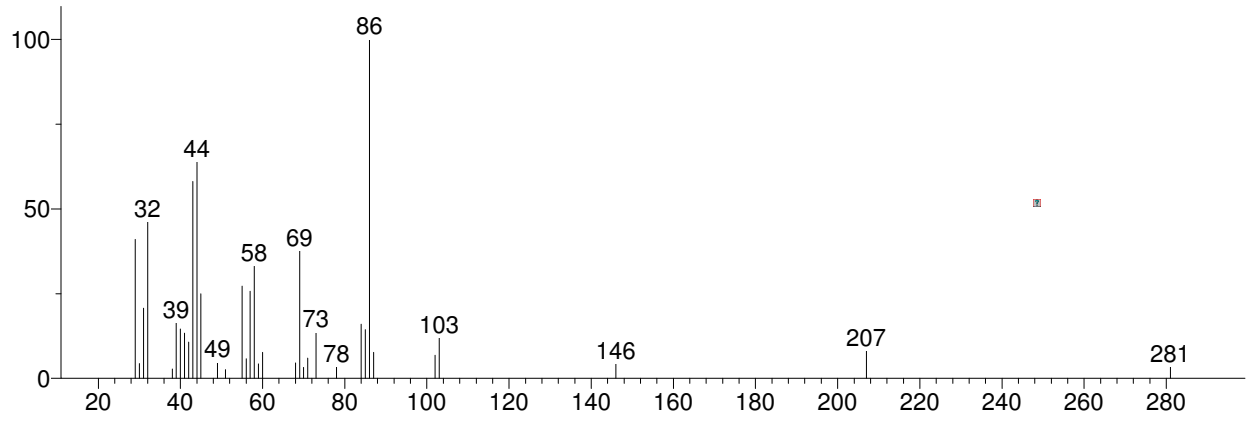
Hit 1 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 712; RMF: 890; Prob 35.4%; CAS: 104-76-7; Lib: replib; ID: 5259.



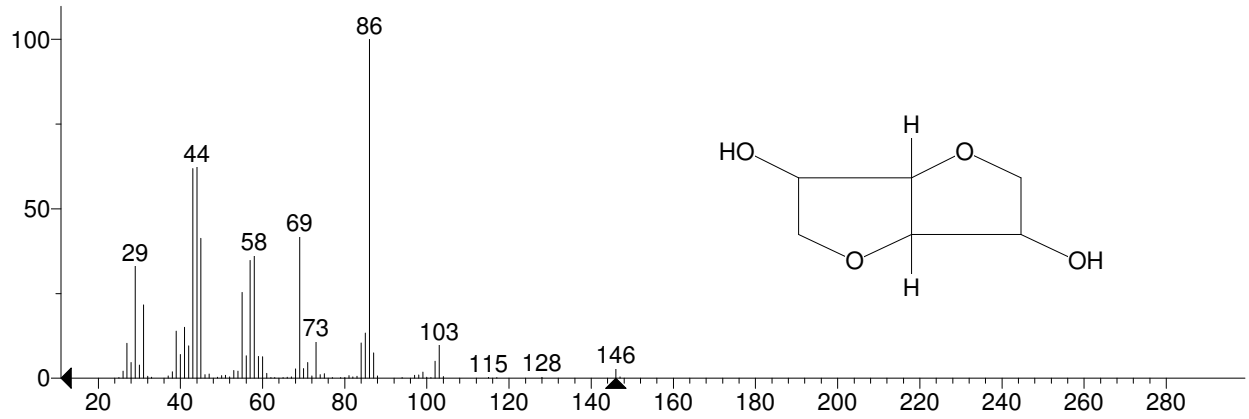
Hit 2 : 1-Hexanol, 2-ethyl-
C8H18O; MF: 701; RMF: 825; Prob 35.4%; CAS: 104-76-7; Lib: replib; ID: 5289.



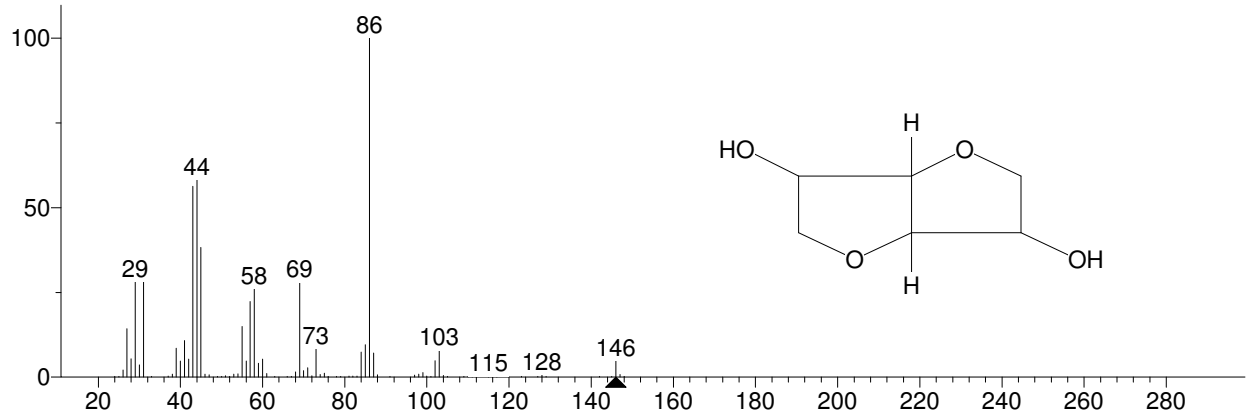
Unknown: Scan 1223 (11.359 min): J9163_Jordi_Sample_1_B.D\data.ms
Compound in Library Factor = 181



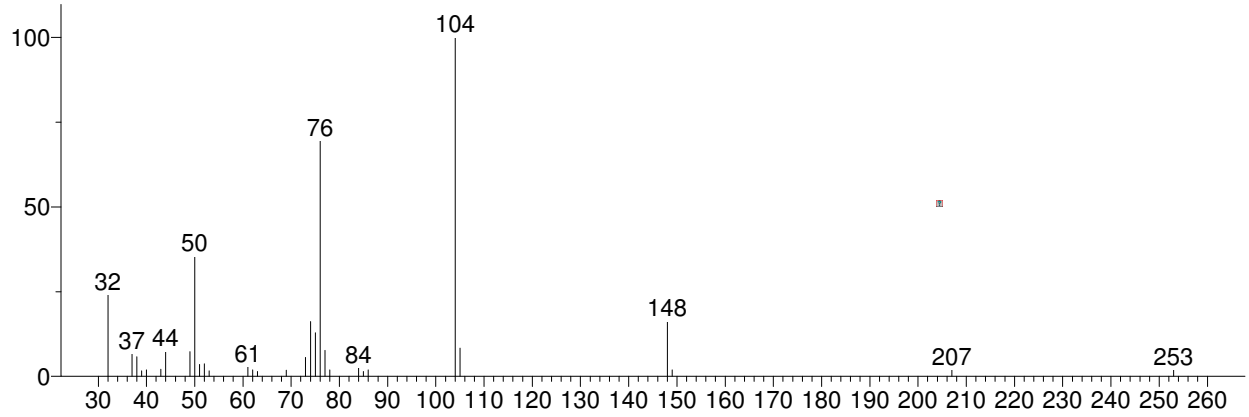
Hit 1 : Isosorbide
C6H10O4; MF: 854; RMF: 892; Prob 73.5%; CAS: 652-67-5; Lib: mainlib; ID: 47618.



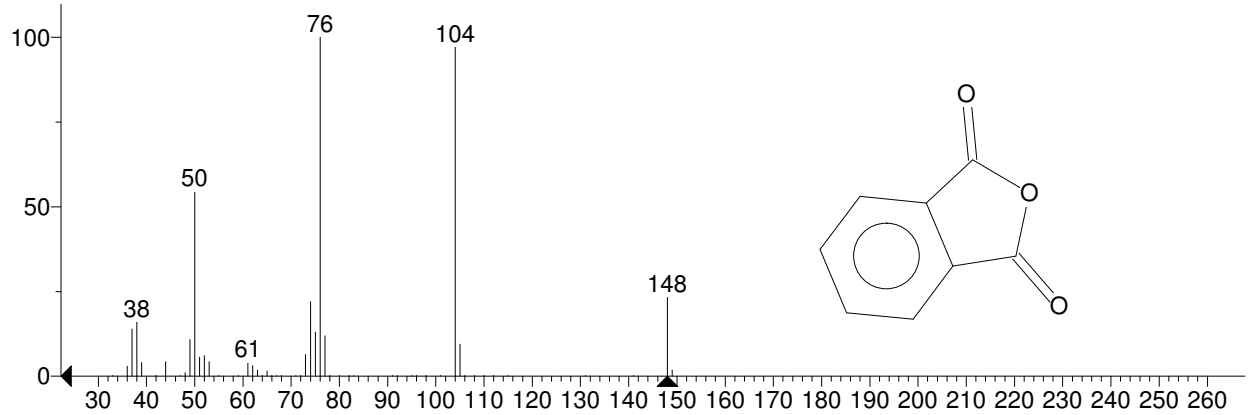
Hit 2 : Isosorbide
C6H10O4; MF: 837; RMF: 896; Prob 73.5%; CAS: 652-67-5; Lib: replib; ID: 10769.



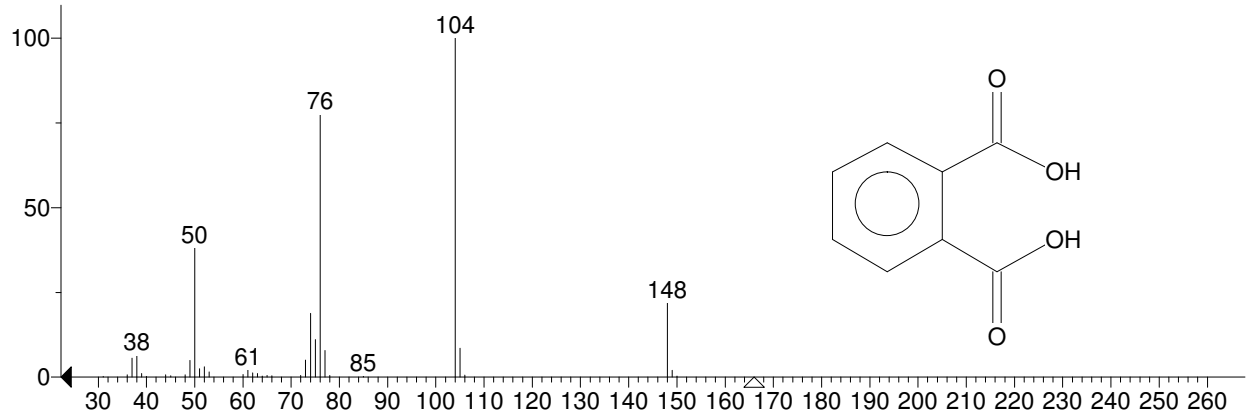
Unknown: Scan 1284 (11.721 min): J9163_Jordi_Sample_1_B.D\data.ms
Compound in Library Factor = -101



Hit 1 : Phthalic anhydride
C8H4O3; MF: 889; RMF: 937; Prob 51.5%; CAS: 85-44-9; Lib: replib; ID: 9355.

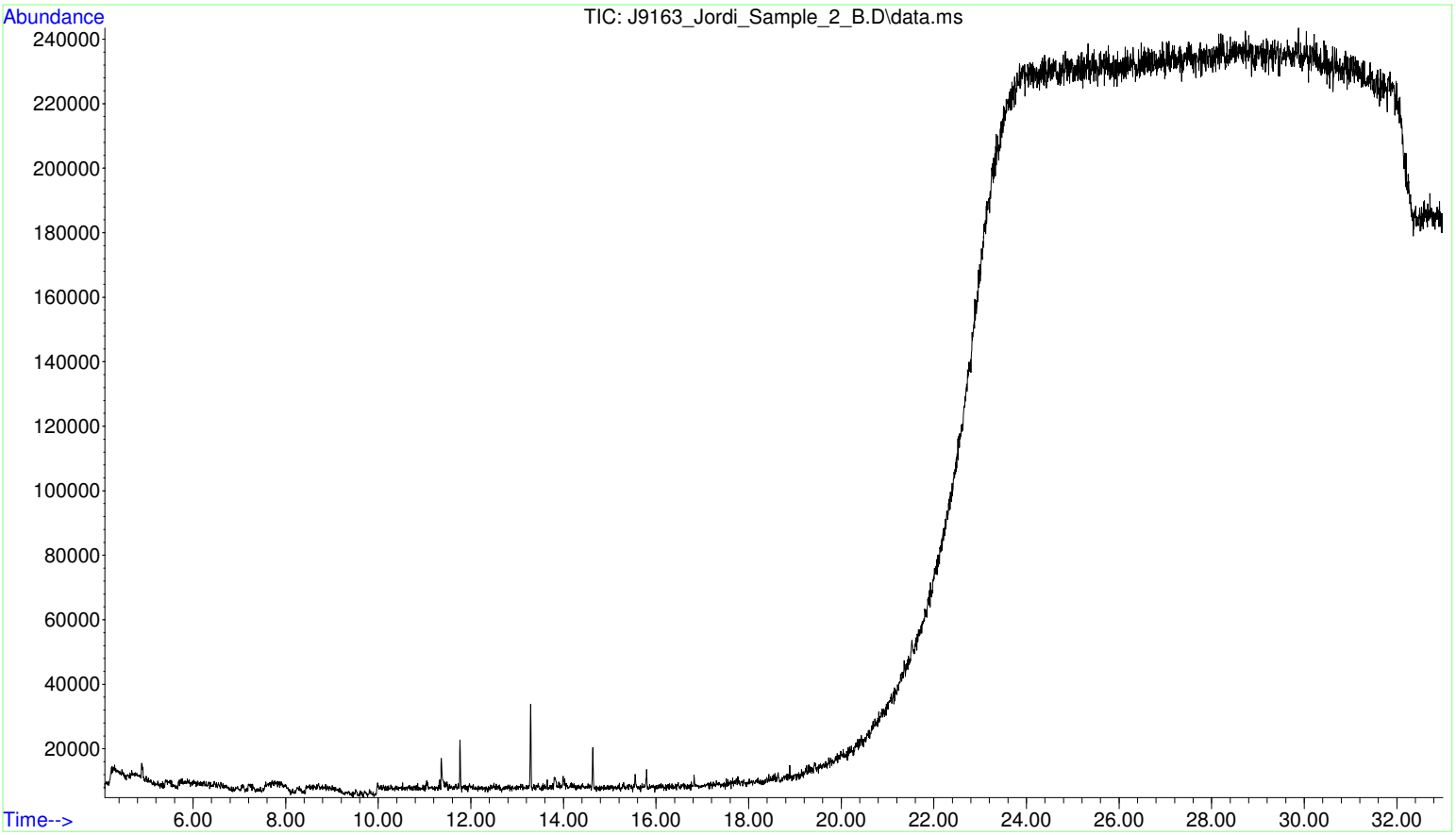


Hit 2 : 1,2-Benzenedicarboxylic acid
C8H6O4; MF: 878; RMF: 922; Prob 35.3%; CAS: 88-99-3; Lib: replib; ID: 13464.



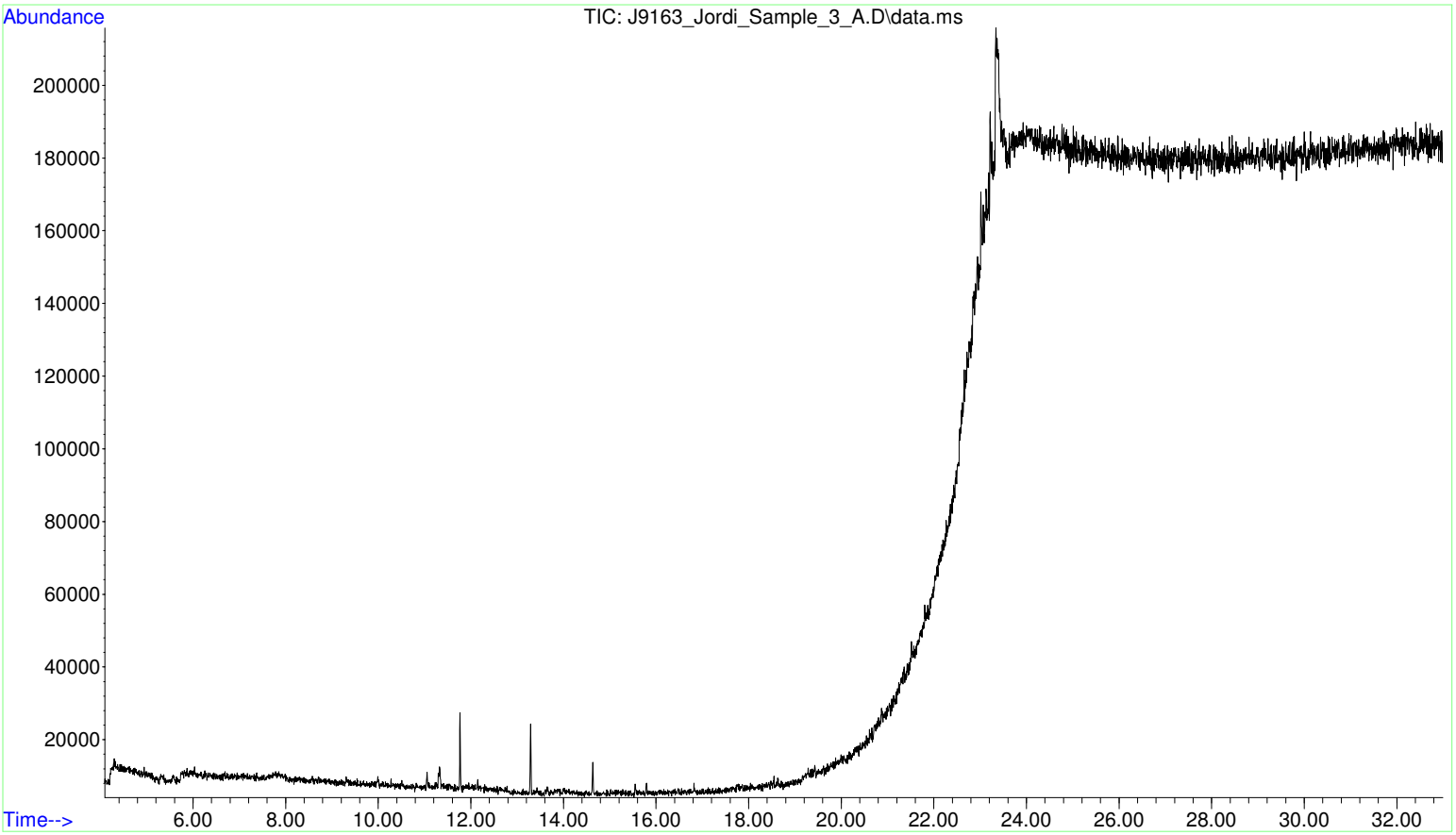
File :D:\msdchem\1\data\2014\J9163 Jordi\102714\J9163_Jordi_Sample
... _2_B.D
Operator : Courtney McGowan
Instrument : 7890
Acquired : 28 Oct 2014 18:23 using AcqMethod GCMS.M
Sample Name: J9163 Jordi Sample 2
Misc Info :

EVA bag in saline

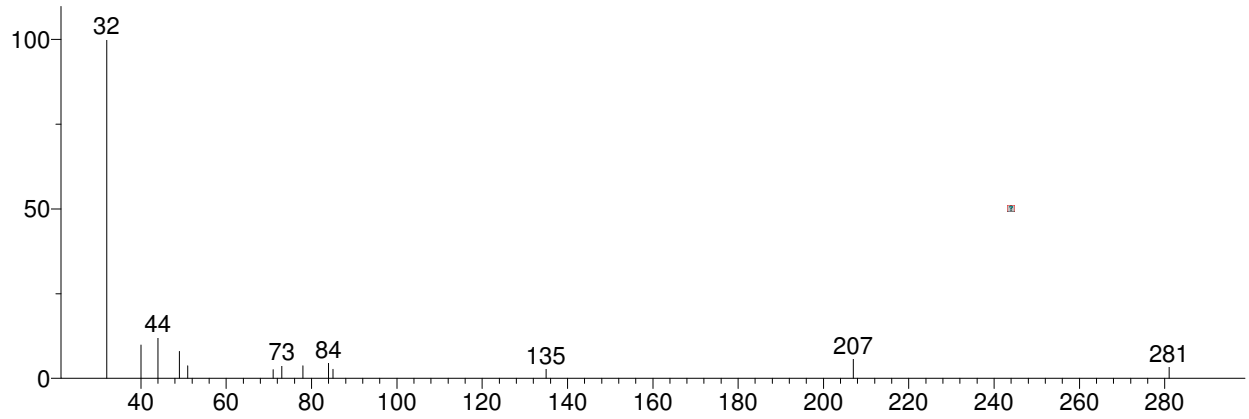


File :D:\msdchem\1\data\2014\J9163 Jordi\102714\J9163_Jordi_Sample
... _3_A.D
Operator : Courtney McGowan
Instrument : 7890
Acquired : 28 Oct 2014 19:38 using AcqMethod GCMS.M
Sample Name: J9163 Jordi Sample 3
Misc Info :

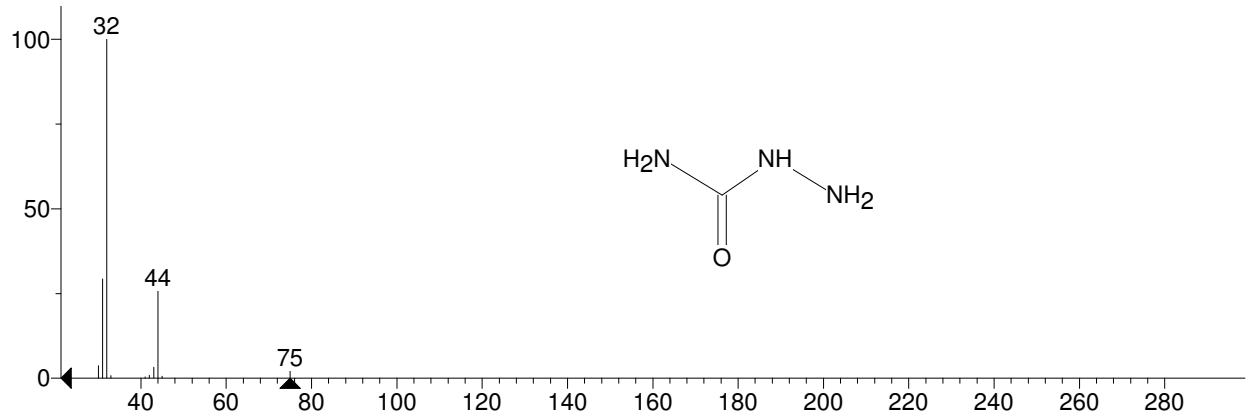
EVA bag in water



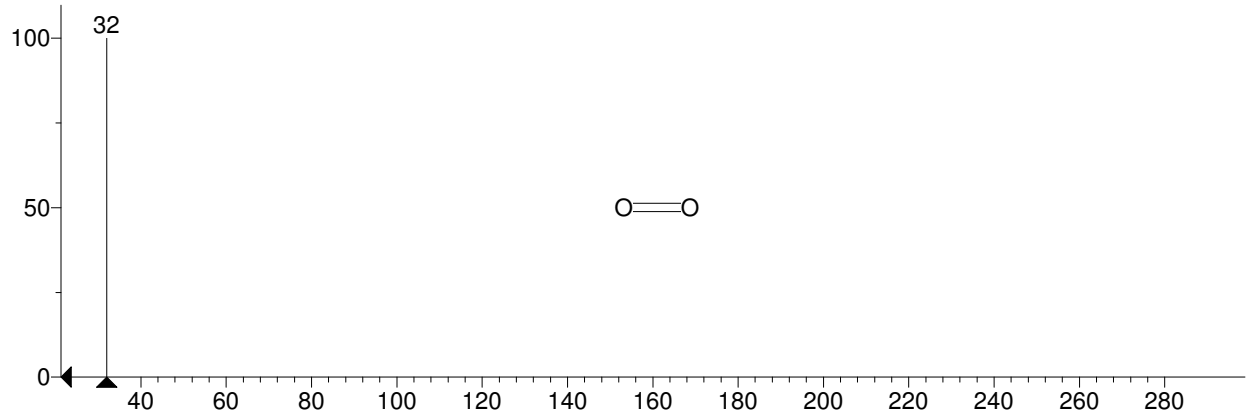
Unknown: Scan 1215 (11.311 min): J9163_Jordi_Sample_3_A.D\data.ms
Compound in Library Factor = -1428



Hit 1 : Hydrazinecarboxamide
CH5N3O; MF: 394; RMF: 898; Prob 31.3%; CAS: 57-56-7; Lib: mainlib; ID: 1457.



Hit 2 : Oxygen
O2; MF: 377; RMF: 999; Prob 17.1%; CAS: 7782-44-7; Lib: mainlib; ID: 1449.



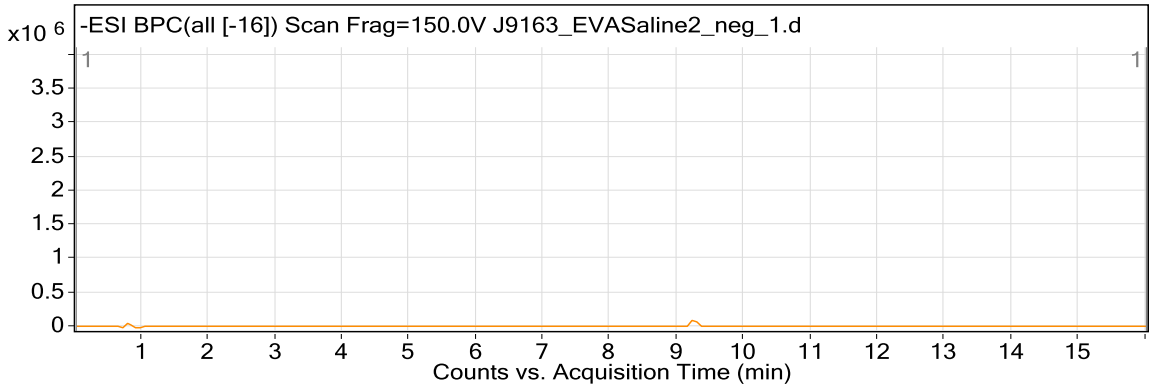
LCMS Data

Qualitative Analysis Report

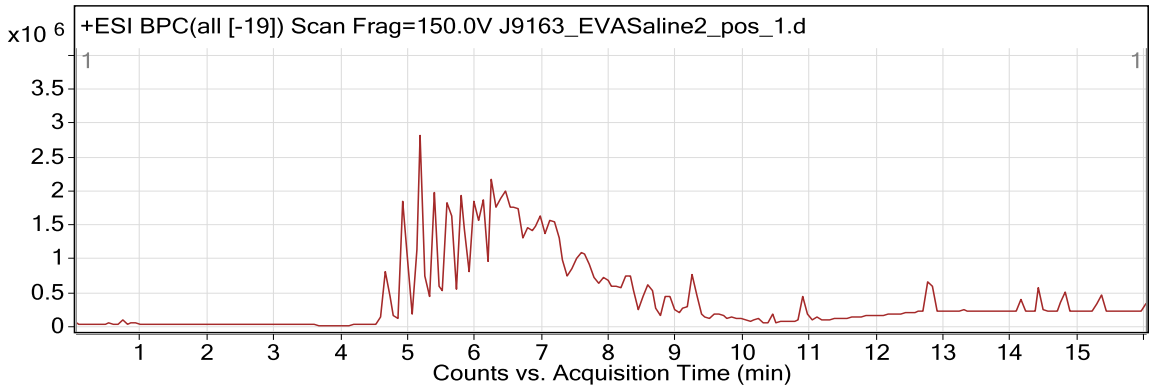
Data Filename	J9163_EVASaline2_neg_1.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 96
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-neg.m	**Acquired Time**	11/11/2014 3:04:03 PM
IRM Calibration Status	Some Ions Missed	**DA Method**	Default.m
Comment			
Data Filename	J9163_EVASaline2_pos_1.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 96
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-pos.m	**Acquired Time**	11/11/2014 1:48:51 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Data Filename	J9163_EVAWater3_neg_1.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 94
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-neg.m	**Acquired Time**	11/11/2014 9:58:36 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Data Filename	J9163_EVAWater3_pos_1.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 94
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-pos.m	**Acquired Time**	11/11/2014 8:39:22 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Data Filename	J9163_PVCWater1_neg_1.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 93
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-neg.m	**Acquired Time**	11/11/2014 7:48:59 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			
Data Filename	J9163_PVCWater1_pos_2.d	**Sample Name**	Control
Sample Type	Blank	**Position**	Vial 93
Instrument Name	Instrument 1	**User Name**	
Acq Method	Default-DualESI-pos.m	**Acquired Time**	11/11/2014 6:54:07 AM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

User Chromatograms

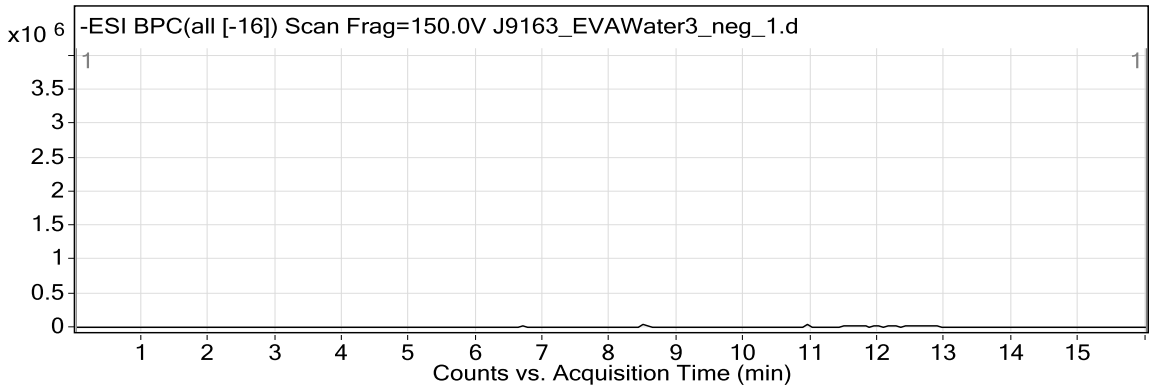
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



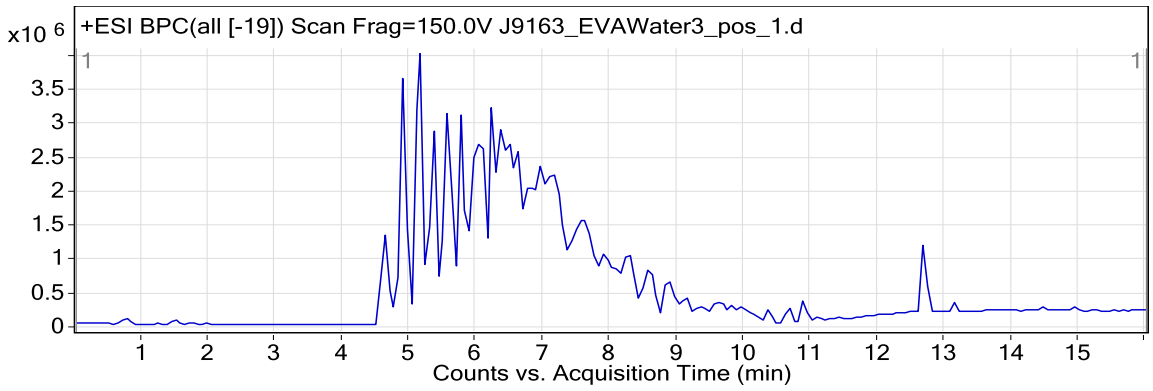
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



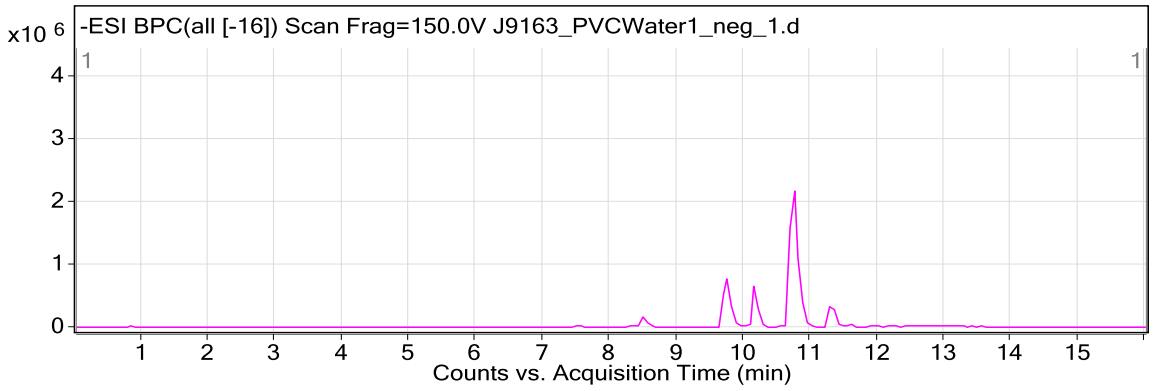
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



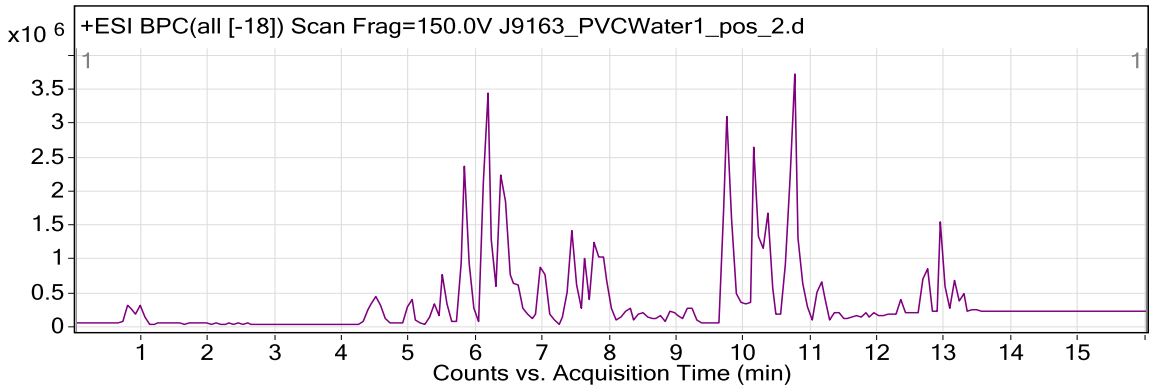
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

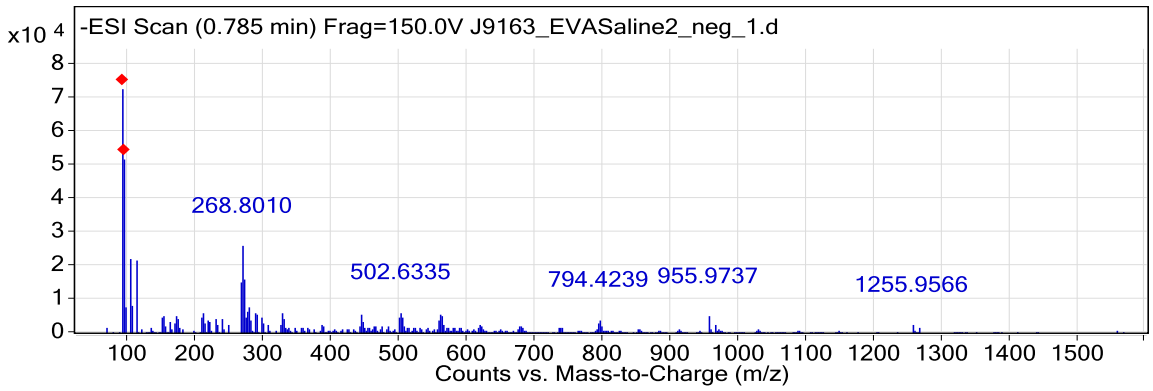


Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

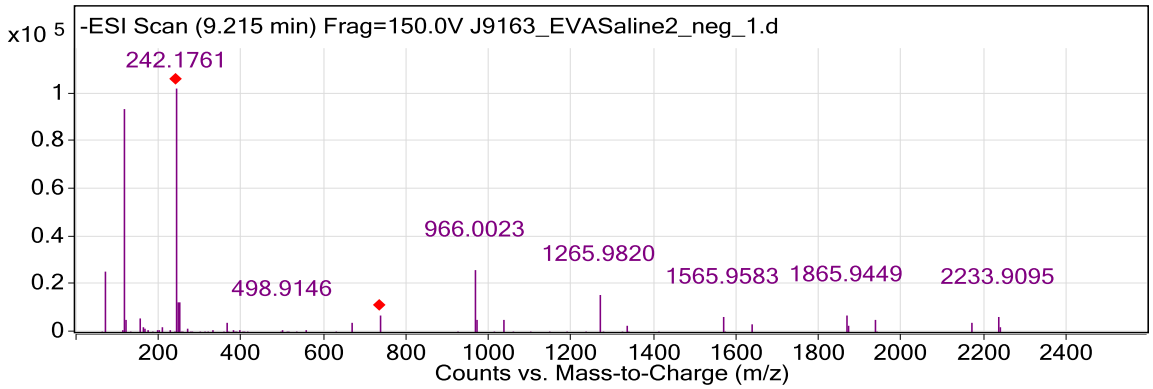


User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



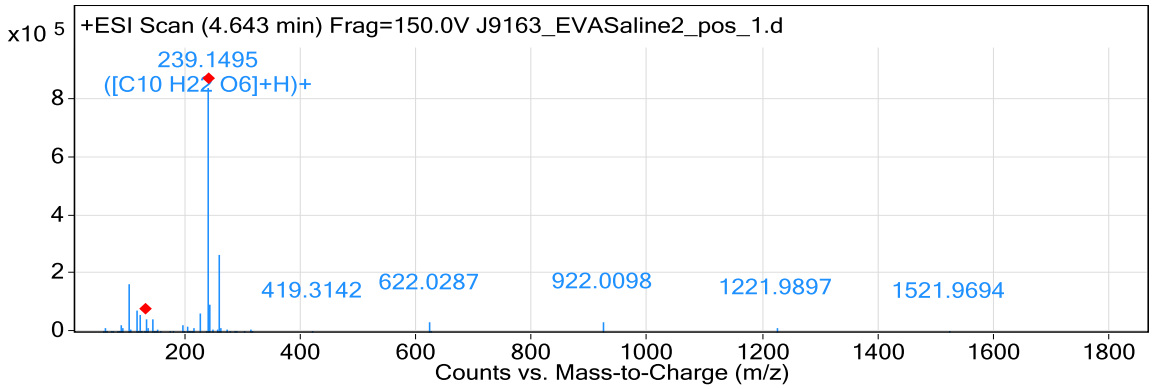
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
253.1449	254.1522	C14 H22 O4	47.15	-1.34	C14 H21 O4
255.1236	256.1309	C13 H20 O5	47.45	0.8	C13 H19 O5

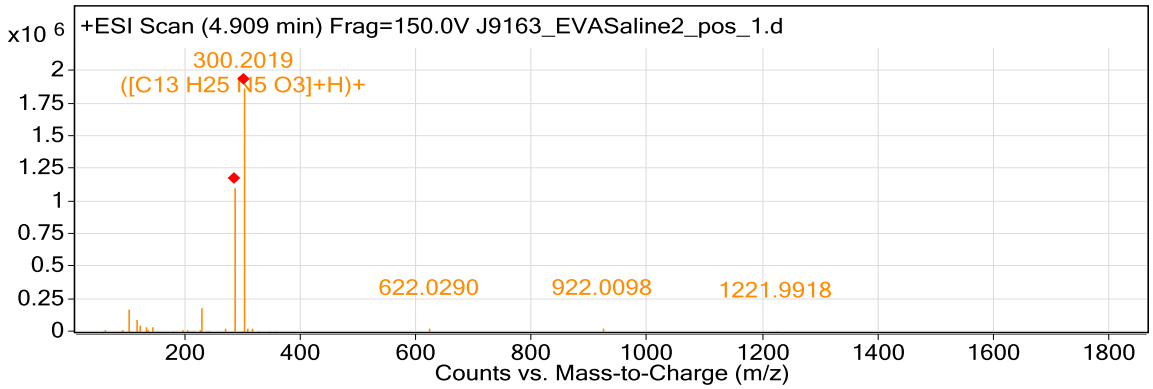
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
236.1011	235.0938	C6 H14 Cl N7 O	43.49	4.25	C6 H15 Cl N7 O
237.2093	236.2018	C13 H24 N4	73.61	-7.29	C13 H25 N4
239.1495	238.1421	C10 H22 O6	96.64	-1.73	C10 H23 O6
245.1004	244.0931	C6 H17 Cl N4 O4	45.57	2.9	C6 H18 Cl N4 O4
247.1333	246.1281	C12 H22 O3 S	56.71	3.33	C12 H23 O3 S
253.1274	252.1218	C11 H24 O2 S2	65.46	-0.06	C11 H25 O2 S2
256.1755	255.1683	C11 H21 N5 O2	90.99	4.7	C11 H22 N5 O2
261.1307	260.1239	C8 H16 N6 O4	87.99	-2.33	C8 H17 N6 O4

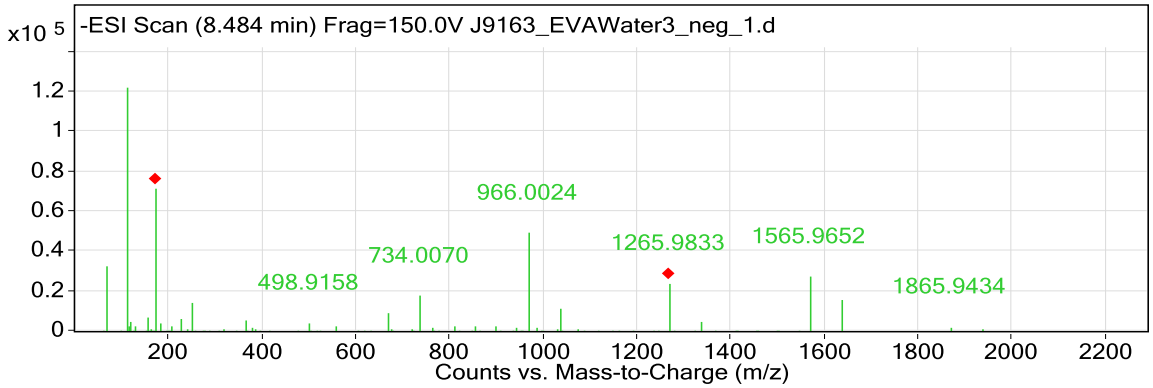
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
283.1758	282.1684	C13 H22 N4 O3	96.47	2.81	C13 H23 N4 O3
284.1779	283.1706	C14 H25 N3 O S	87.46	4.22	C14 H26 N3 O S
297.1554	296.1481	C13 H28 O3 S2	47.57	-0.38	C13 H29 O3 S2
298.1552	297.1487	C17 H19 N3 O2	73.49	-3.39	C17 H20 N3 O2
300.9018	299.8946	C5 H2 Cl2 N4 O3 S2	47.62	-0.07	C5 H3 Cl2 N4 O3 S2
300.5662	599.1165	C22 H33 N O12 S3	79.91	0.05	C22 H35 N O12 S3
300.2019	299.1947	C13 H25 N5 O3	93.99	3.49	C13 H26 N5 O3
301.2054	300.1979	C14 H28 N4 O S	90.89	1.61	C14 H29 N4 O S
305.1571	304.1505	C11 H16 N10 O	87.01	1.07	C11 H17 N10 O
314.1817	313.1746	C13 H23 N5 O4	82.7	1.15	C13 H24 N5 O4

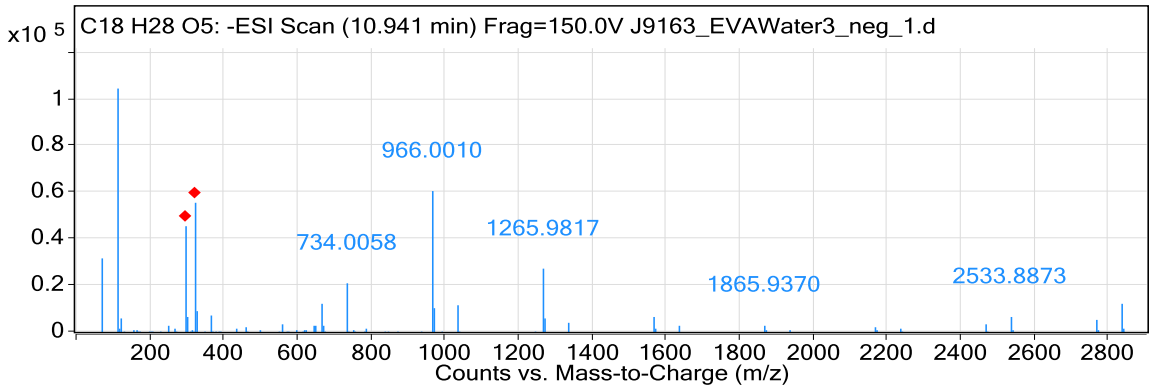
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
171.1022	172.1094	C9 H16 O3	98.14	2.93	C9 H15 O3

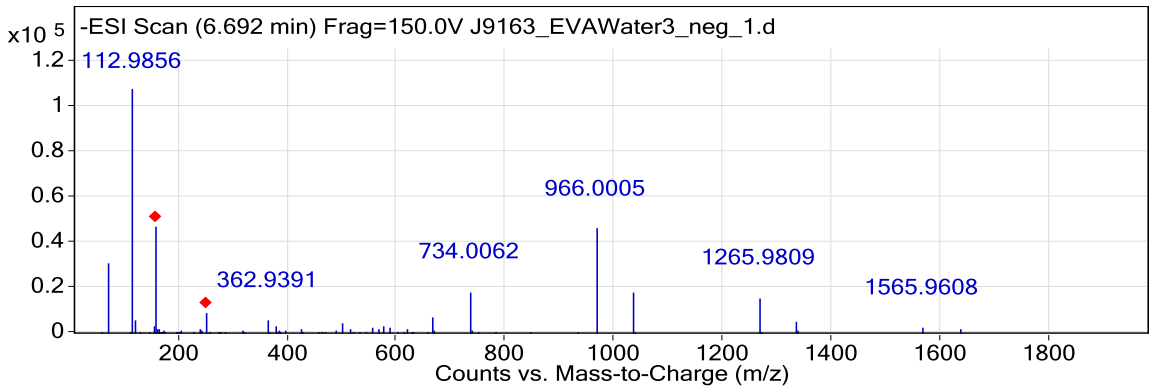
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
323.1891	324.1959	C18 H28 O5	72.12	-6.76	C18 H27 O5

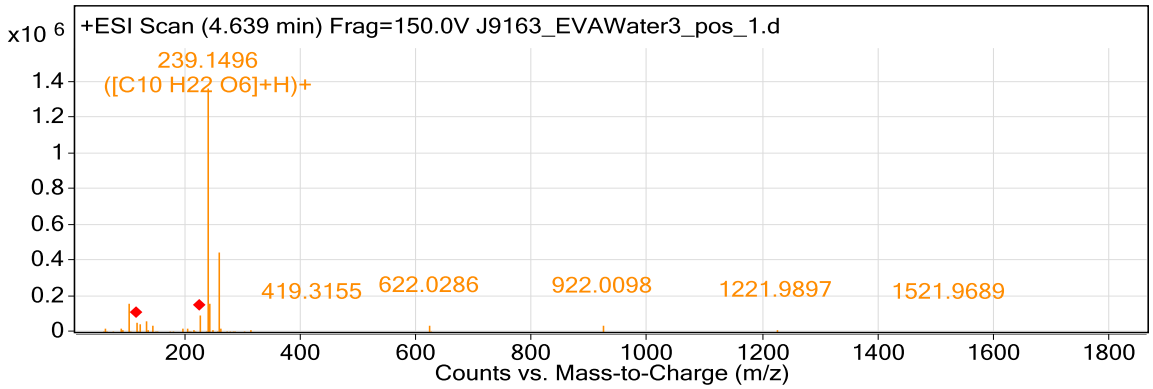
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
157.0864	158.0938	C8 H14 O3	97.74	3.35	C8 H13 O3

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

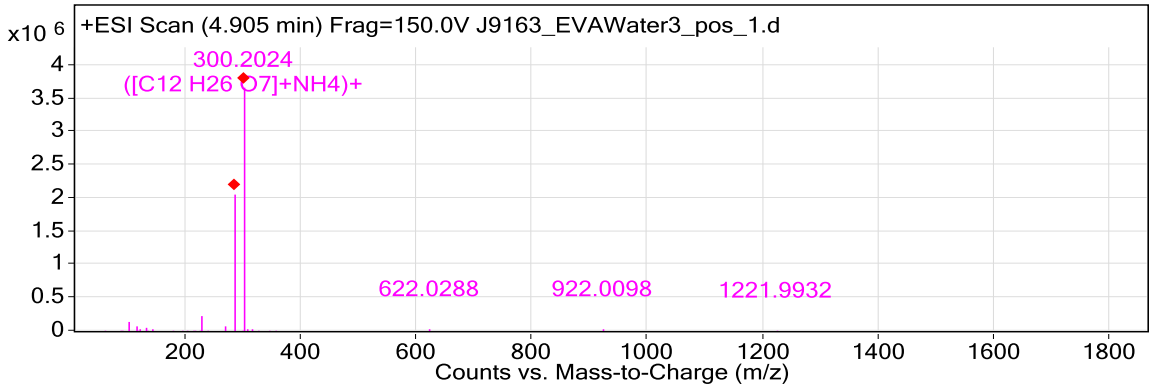


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
239.1496	238.1422	C10 H22 O6	97.43	-2.51	C10 H23 O6

261.1309	238.1421	C10 H22 O6	89.19	-1.99	C10 H22 Na O6
256.176	238.142	C10 H22 O6	98.22	-1.66	C10 H26 N O6

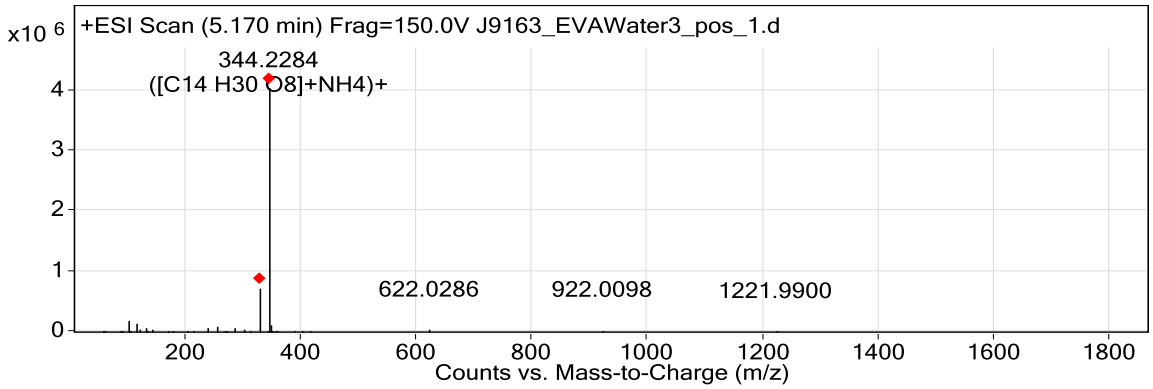
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
283.1757	282.1682	C12 H26 O7	95.27	-1.29	C12 H27 O7
305.1576	282.1685	C12 H26 O7	96.92	-2.29	C12 H26 Na O7
300.2024	282.1686	C12 H26 O7	97.29	-2.71	C12 H30 N O7

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

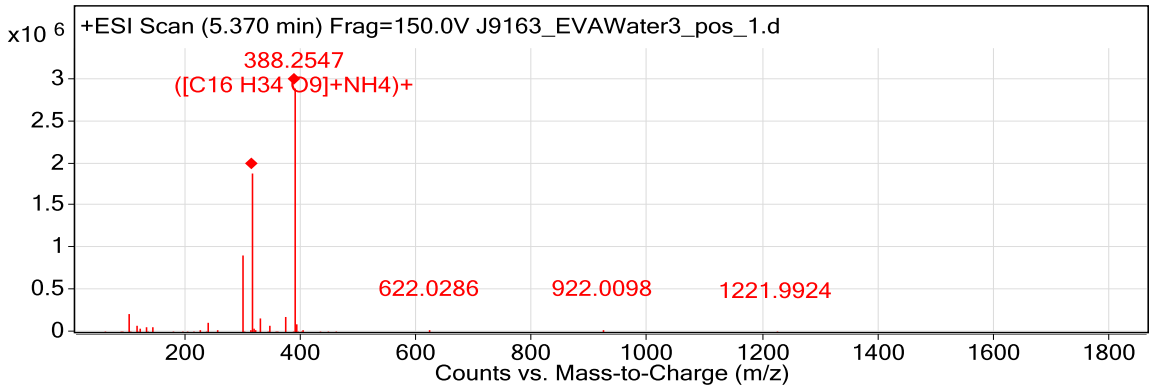


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
327.2025	326.1942	C14 H30 O8	70.23	-0.32	C14 H31 O8
349.1834	326.194	C14 H30 O8	96.91	0.26	C14 H30 Na O8
344.2284	326.1947	C14 H30 O8	97.79	-1.96	C14 H34 N O8

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

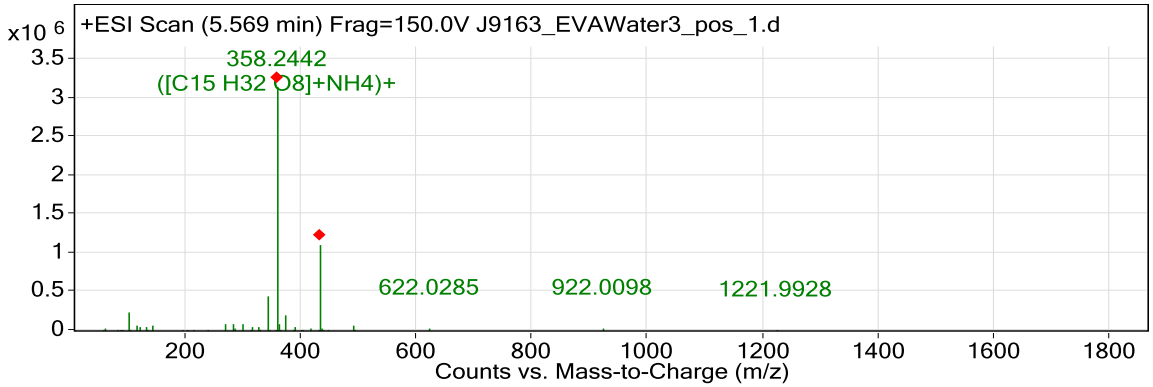
Qualitative Analysis Report



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
371.2283	370.2202	C16 H34 O9	78.15	0.14	C16 H35 O9
393.2101	370.221	C16 H34 O9	96.83	-1.82	C16 H34 Na O9
388.2547	370.221	C16 H34 O9	97.94	-1.9	C16 H38 N O9

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

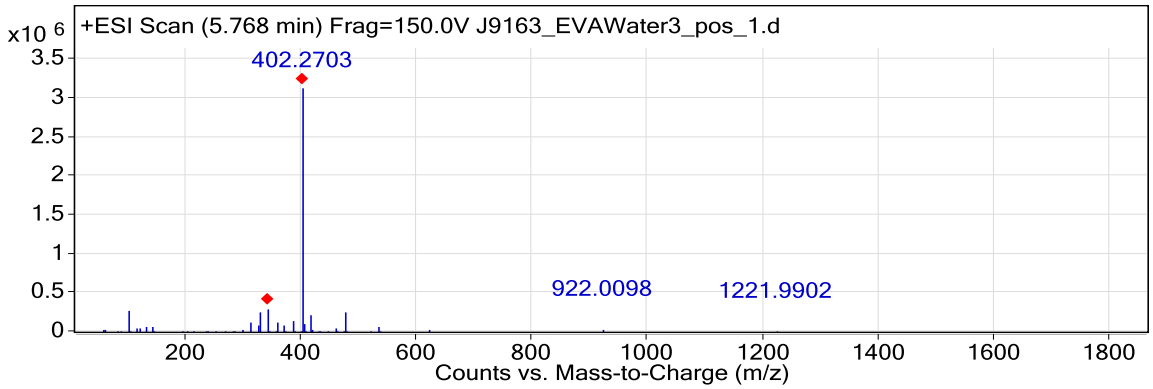


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
341.2182	340.2107	C15 H32 O8	94.79	-2.78	C15 H33 O8
363.1993	362.1919	C17 H30 O8	82.18	5.87	C17 H31 O8
415.2539	414.2466	C18 H38 O10	47.56	-0.35	C18 H39 O10
437.2355	436.2284	C20 H36 O10	83.45	5.71	C20 H37 O10
363.1993	340.21	C15 H32 O8	91.15	-0.84	C15 H32 Na O8
437.2355	414.2464	C18 H38 O10	93.41	0.2	C18 H38 Na O10
344.2281	326.194	C14 H30 O8	91.01	0.35	C14 H34 N O8
358.2442	340.2105	C15 H32 O8	97.53	-2.19	C15 H36 N O8
360.2495	342.2153	C22 H30 O3	43.43	12.15	C22 H34 N O3
372.2237	354.1898	C15 H30 O9	97.56	-2.37	C15 H34 N O9
386.2346	368.2005	C23 H28 O4	72.53	-4.72	C23 H32 N O4
388.2543	370.2204	C16 H34 O9	99.7	-0.33	C16 H38 N O9
402.2473	384.2135	C20 H32 O7	83.96	3.47	C20 H36 N O7
416.2521	398.219	C17 H34 O10	36.67	-9.62	C17 H38 N O10
430.2291	412.1956	C17 H32 O11	75.5	-2.67	C17 H36 N O11
432.2817	414.2477	C18 H38 O10	96.03	-2.96	C18 H42 N O10
444.2779	426.2439	C19 H38 O10	68.49	6.1	C19 H42 N O10
446.2593	428.2261	C18 H36 O11	83	-0.71	C18 H40 N O11

341.2182	312.1794	C13 H28 O8	94.79	-3.03	C15 H33 O8
363.1993	334.1606	C15 H26 O8	82.18	6.36	C17 H31 O8
415.2539	386.2153	C16 H34 O10	47.56	-0.38	C18 H39 O10
437.2355	408.1971	C18 H32 O10	83.45	6.1	C20 H37 O10
341.2182	300.1794	C12 H28 O8	94.79	-3.15	C15 H33 O8
363.1993	322.1606	C14 H26 O8	82.18	6.6	C17 H31 O8
437.2355	396.1971	C17 H32 O10	83.45	6.29	C20 H37 O10
341.2182	284.1481	C11 H24 O8	94.79	-3.33	C15 H33 O8
363.1993	306.1293	C13 H22 O8	82.18	6.94	C17 H31 O8
415.2539	358.184	C14 H30 O10	47.56	-0.41	C18 H39 O10
437.2355	380.1658	C16 H28 O10	83.45	6.55	C20 H37 O10

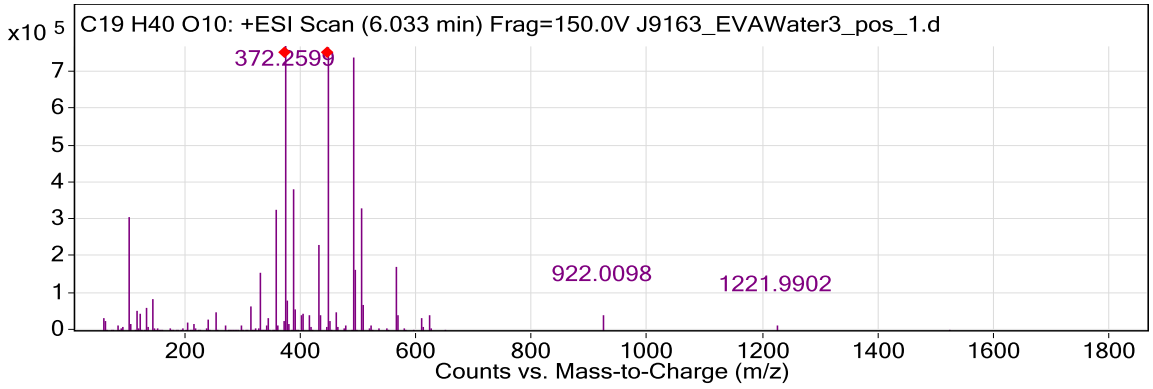
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
416.2496	398.2157	C17 H34 O10	98.76	-1.2	C17 H38 N O10

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



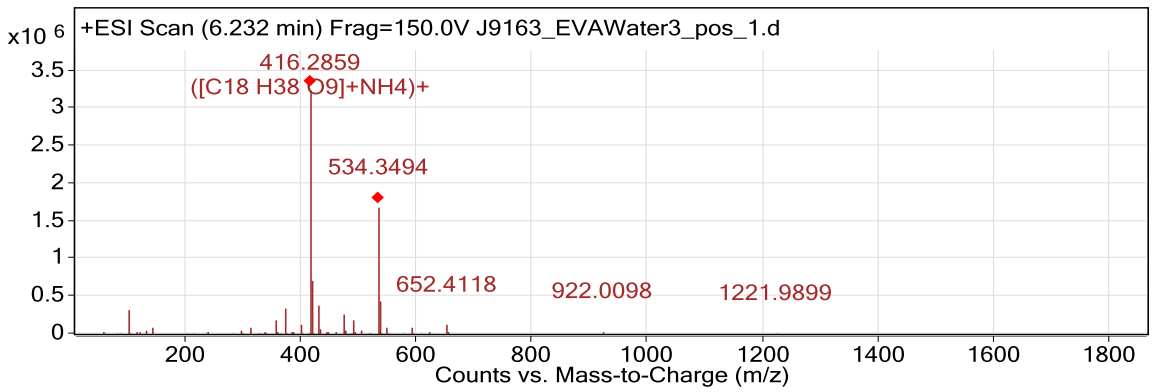
MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
429.2701	428.2628	C19 H40 O10	46.49	-1.59	C19 H41 O10
446.2976	428.2636	C19 H40 O10	94.59	-3.36	C19 H44 N O10

Fragmentor Voltage **Collision Energy** **Ionization Mode**

Qualitative Analysis Report

150 0 ESI

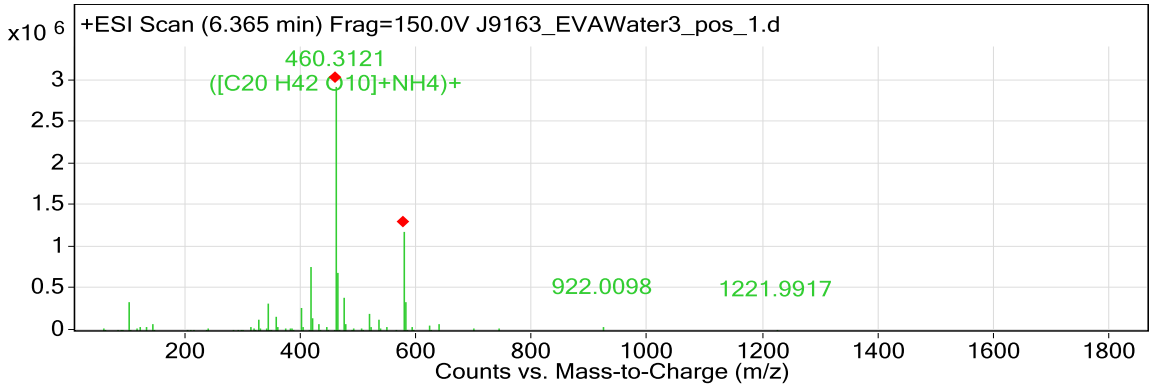


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
399.2593	398.251	C18 H38 O9	70.42	1.53	C18 H39 O9
421.2409	398.2517	C18 H38 O9	47.6	-0.22	C18 H38 Na O9
416.2859	398.2523	C18 H38 O9	97.67	-1.76	C18 H42 N O9

Fragmentor Voltage **Collision Energy** **Ionization Mode**

150 0 ESI



MFG Results

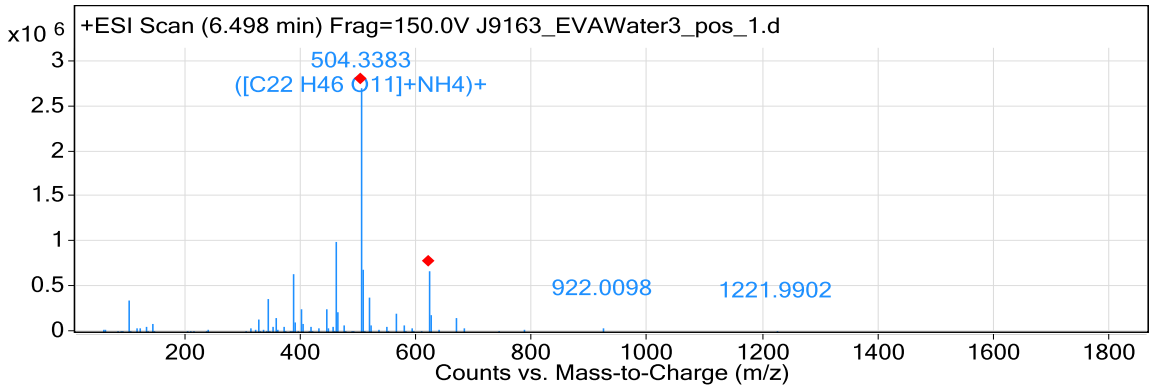
m/z	Mass	Best Match	Score	Diff.	Ion Form.
460.9129	459.9056	C13 O19	37.83	-4.78	C13 H O19
465.2658	464.2581	C29 H36 O5	77.76	-3.9	C29 H37 O5
475.2944	474.287	C24 H42 O9	70.7	-8.63	C24 H43 O9
519.3207	518.3138	C26 H46 O10	69.42	-9.01	C26 H47 O10
579.3791	578.3714	C29 H54 O11	55.27	-8.33	C29 H55 O11
460.9658	437.9767	C27 H2 O7	46.32	7.66	C27 H2 Na O7
465.2658	442.2762	C20 H42 O10	87.32	3.66	C20 H42 Na O10
475.2944	452.305	C33 H40 O	65.52	6.44	C33 H40 Na O
519.3207	496.3318	C35 H44 O2	77.81	4.69	C35 H44 Na O2
460.3121	442.2784	C20 H42 O10	98.13	-1.42	C20 H46 N O10
474.4849	456.4515	C29 H60 O3	50.65	6.09	C29 H64 N O3
474.292	456.258	C20 H40 O11	96.35	-2.05	C20 H44 N O11
488.2902	470.2567	C35 H34 O	38.94	9.03	C35 H38 N O
490.3211	472.2875	C21 H44 O11	95.21	1.88	C21 H48 N O11
502.3187	484.2846	C29 H40 O6	66.26	-4.41	C29 H44 N O6
504.3334	486.2989	C29 H42 O6	80.49	-1.67	C29 H46 N O6
518.3177	500.284	C22 H44 O12	96.97	-1.37	C22 H48 N O12

532.2984	514.2646	C22 H42 O13	72.02	-4.07	C22 H46 N O13
534.3486	516.3146	C23 H48 O12	99.63	-0.02	C23 H52 N O12
548.3328	530.2976	C34 H42 O5	35.9	10.62	C34 H46 N O5
578.3762	560.3422	C25 H52 O13	96.01	-2.56	C25 H56 N O13
592.354	574.3201	C25 H50 O14	98.28	-0.1	C25 H54 N O14
465.2658	436.2268	C27 H32 O5	77.76	-4.15	C29 H37 O5
475.2944	446.2557	C22 H38 O9	70.7	-9.17	C24 H43 O9
519.3207	490.2825	C24 H42 O10	69.42	-9.52	C26 H47 O10
465.2658	424.2268	C26 H32 O5	77.76	-4.27	C29 H37 O5
475.2944	434.2557	C21 H38 O9	70.7	-9.43	C24 H43 O9
519.3207	478.2825	C23 H42 O10	69.42	-9.76	C26 H47 O10
465.2658	408.1955	C25 H28 O5	77.76	-4.43	C29 H37 O5
475.2944	418.2244	C20 H34 O9	70.7	-9.79	C24 H43 O9
519.3207	462.2512	C22 H38 O10	69.42	-10.1	C26 H47 O10

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
ESI



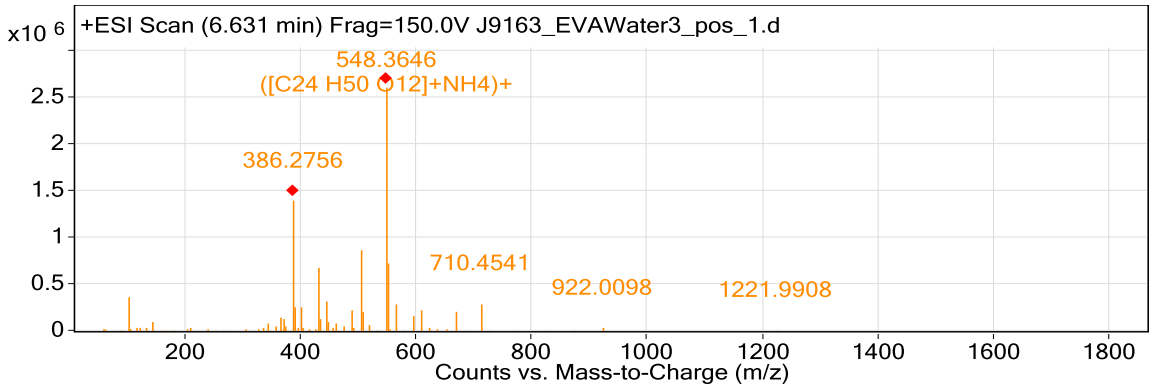
MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
504.9169	503.9096	C18 O18	45.14	-2.21	C18 H O18
509.293	508.2854	C24 H44 O11	78.24	5.75	C24 H45 O11
519.3207	518.3135	C26 H46 O10	64.72	-8.51	C26 H47 O10
623.4049	622.3971	C31 H58 O12	58.09	-6.89	C31 H59 O12
509.293	486.3035	C22 H46 O11	91.14	1.05	C22 H46 Na O11
490.321	472.2867	C21 H44 O11	89.37	3.46	C21 H48 N O11
504.3383	486.3047	C22 H46 O11	98.16	-1.4	C22 H50 N O11
518.3181	500.2841	C22 H44 O12	96.63	-1.74	C22 H48 N O12
534.3473	516.3135	C23 H48 O12	97.16	2.01	C23 H52 N O12
548.3614	530.3274	C24 H50 O12	85.78	5.39	C24 H54 N O12

Qualitative Analysis Report

m/z	Mass	Best Match	Score	Diff.	Ion Form.
562.3438	544.31	C24 H48 O13	97.9	-0.91	C24 H52 N O13
576.3234	558.289	C24 H46 O14	72.76	-0.47	C24 H50 N O14
578.3744	560.3403	C25 H52 O13	99.36	0.79	C25 H56 N O13
590.3739	572.3373	C33 H48 O8	55.58	-4.17	C33 H52 N O8
622.0289	603.9949	C24 H12 O19	81.37	3.92	C24 H16 N O19
622.4023	604.3682	C27 H56 O14	96.51	-2	C27 H60 N O14
509.293	480.2541	C22 H40 O11	78.24	6.08	C24 H45 O11
519.3207	490.2822	C24 H42 O10	64.72	-9	C26 H47 O10
623.4049	594.3658	C29 H54 O12	58.09	-7.21	C31 H59 O12
509.293	468.2541	C21 H40 O11	78.24	6.24	C24 H45 O11
519.3207	478.2822	C23 H42 O10	64.72	-9.22	C26 H47 O10
623.4049	582.3658	C28 H54 O12	58.09	-7.36	C31 H59 O12
509.293	452.2228	C20 H36 O11	78.24	6.46	C24 H45 O11
519.3207	462.2509	C22 H38 O10	64.72	-9.54	C26 H47 O10
623.4049	566.3345	C27 H50 O12	58.09	-7.57	C31 H59 O12

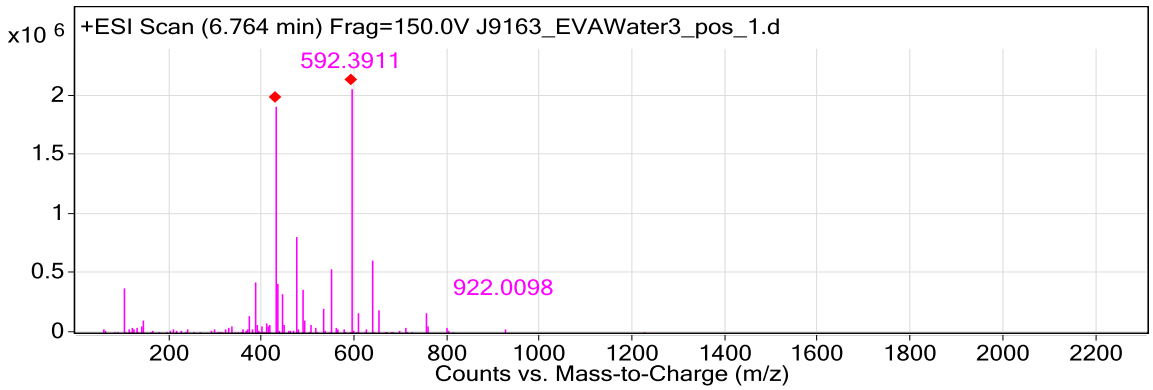
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
553.3187	530.3295	C24 H50 O12	97.63	1.29	C24 H50 Na O12
548.3646	530.331	C24 H50 O12	97.82	-1.46	C24 H54 N O12

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

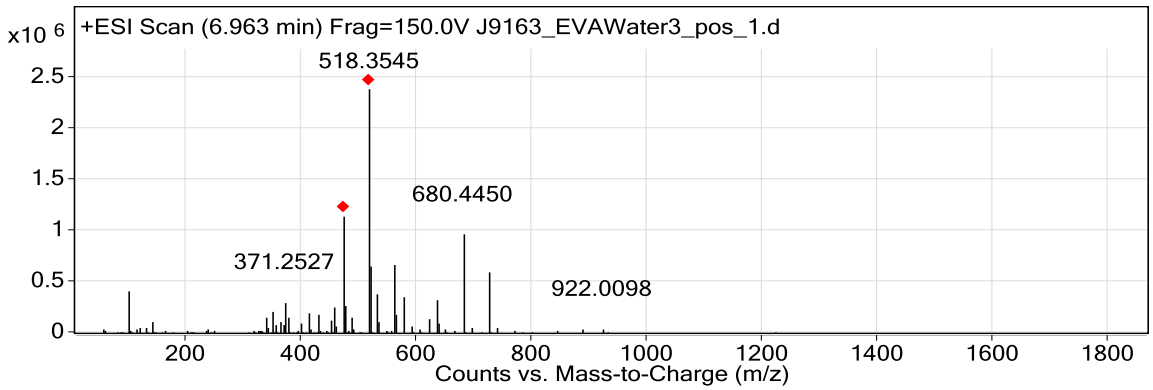


MFG Results

Qualitative Analysis Report

m/z	Mass	Best Match	Score	Diff.	Ion Form.
430.3015	412.2678	C19 H40 O9	98.53	-1.42	C19 H44 N O9

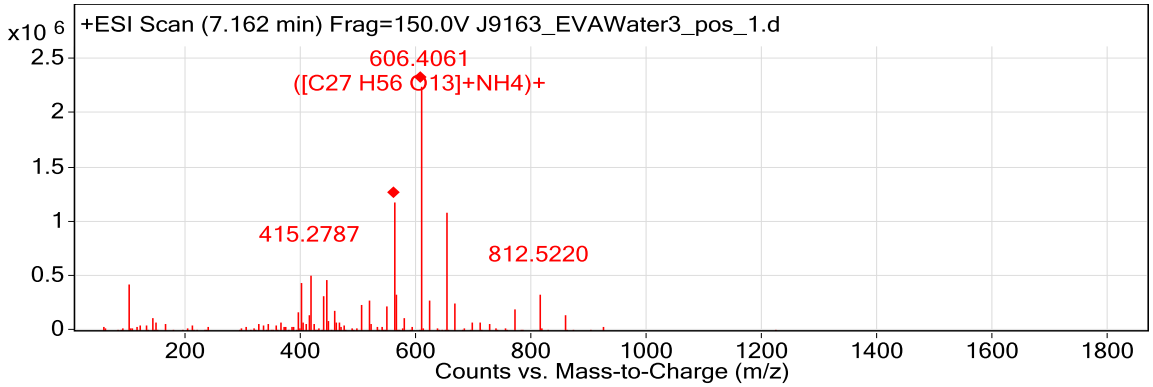
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
474.3284	456.2944	C21 H44 O10	97.61	-2.14	C21 H48 N O10

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

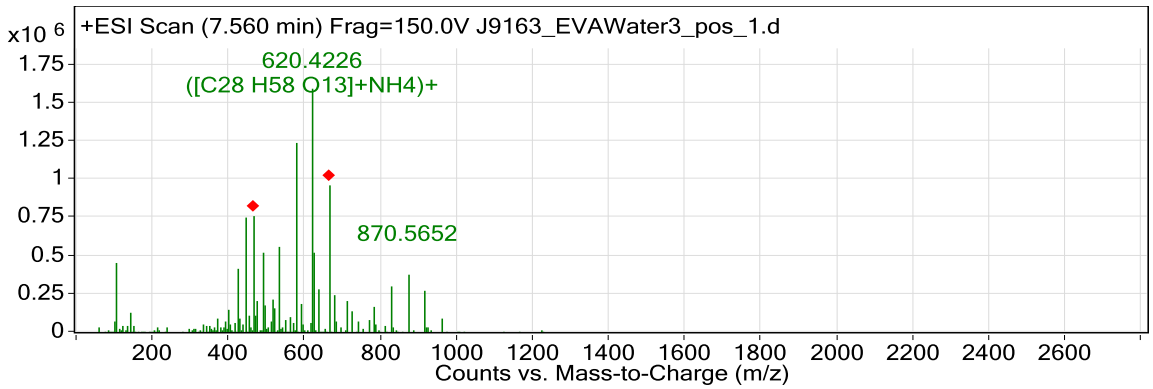


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
563.3835	562.3758	C29 H54 O10	58.44	-7.25	C29 H55 O10
651.436	650.4283	C33 H62 O12	58.94	-6.34	C33 H63 O12
562.3801	544.3462	C25 H52 O12	99.53	-0.68	C25 H56 N O12
576.3589	558.3251	C25 H50 O13	93.26	0.11	C25 H54 N O13
606.4061	588.3725	C27 H56 O13	98.58	-0.71	C27 H60 N O13
606.6187	588.5855	C40 H76 O2	80.01	-1.64	C40 H80 N O2
620.3854	602.3517	C27 H54 O14	98.62	-0.54	C27 H58 N O14
622.0275	603.9934	C24 H12 O19	43.61	6.5	C24 H16 N O19
650.4332	632.3991	C29 H60 O14	98.27	-1.26	C29 H64 N O14
563.3835	534.3445	C27 H50 O10	58.44	-7.63	C29 H55 O10
651.436	622.397	C31 H58 O12	58.94	-6.63	C33 H63 O12
563.3835	522.3445	C26 H50 O10	58.44	-7.8	C29 H55 O10
651.436	610.397	C30 H58 O12	58.94	-6.76	C33 H63 O12
563.3835	506.3132	C25 H46 O10	58.44	-8.05	C29 H55 O10

651.436	594.3657	C29 H54 O12	58.94	-6.94	C33 H63 O12

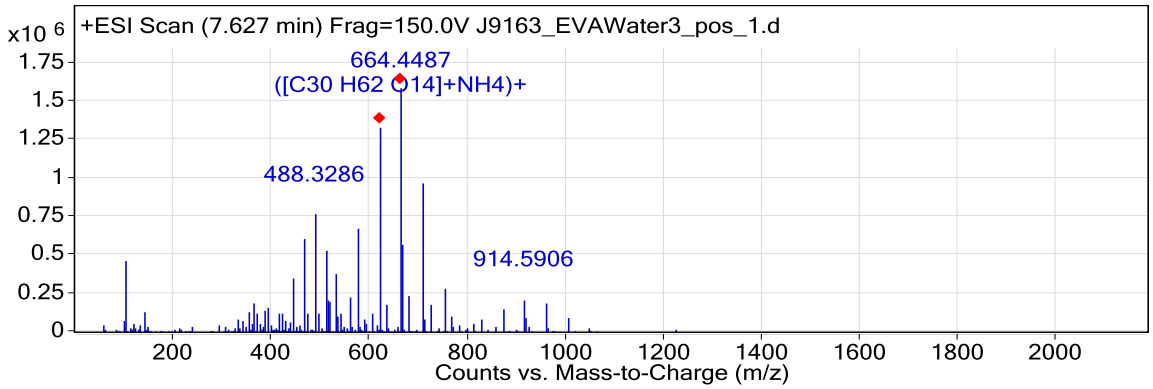
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
620.4226	602.3888	C28 H58 O13	97.62	-1.81	C28 H62 N O13

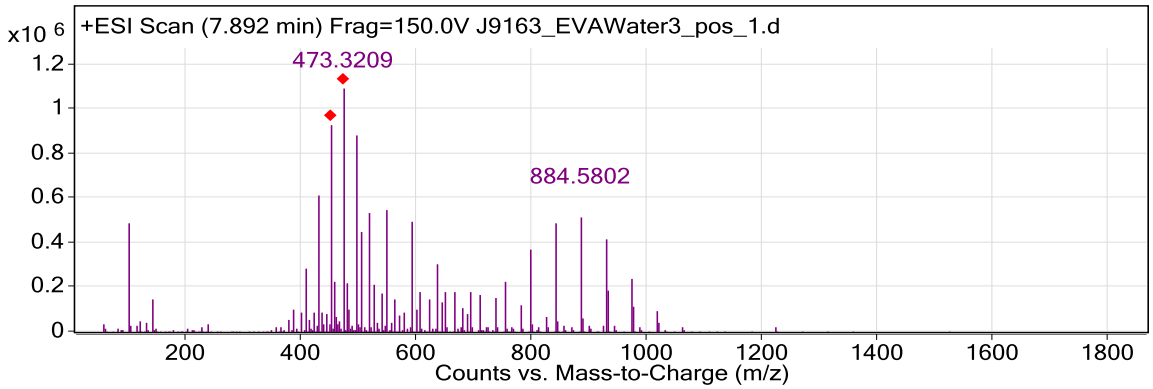
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
664.4487	646.4149	C30 H62 O14	97.87	-1.45	C30 H66 N O14

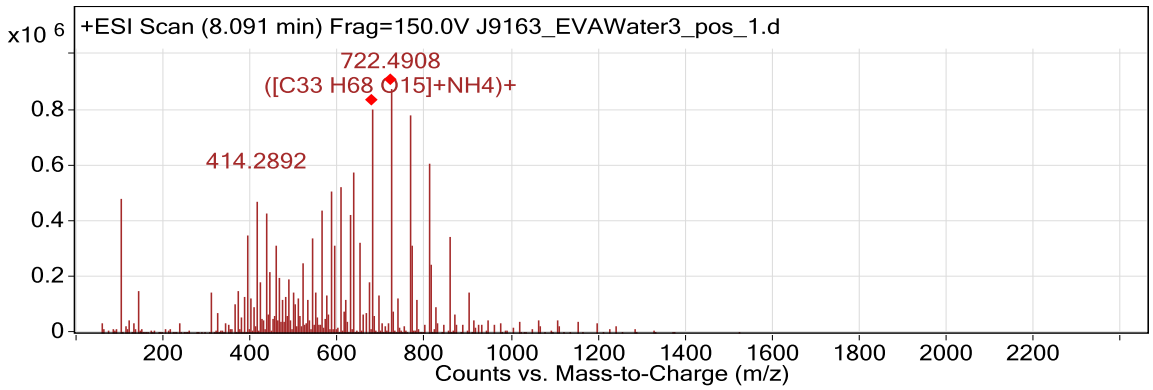
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
451.3085	900.6019	C45 H88 O17	98.55	0.29	C45 H90 O17

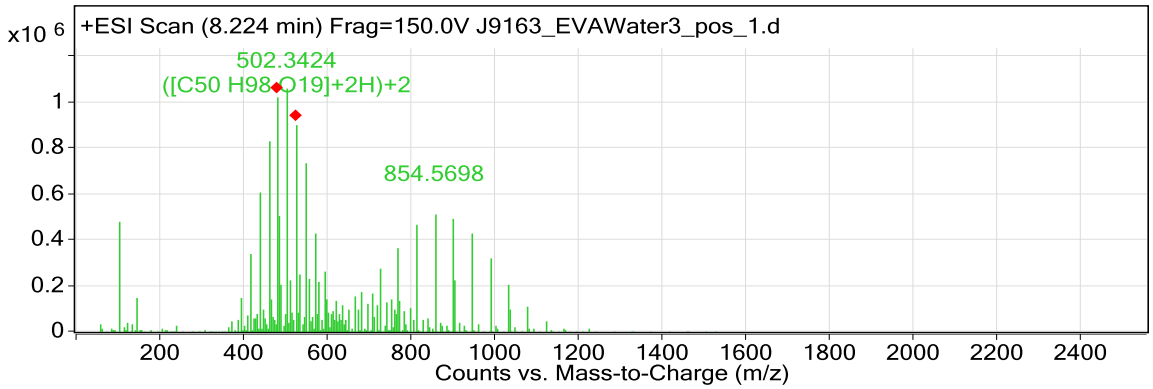
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
671.4384	1340.8613	C65 H128 O27	95.16	2.22	C65 H130 O27
671.4384	1296.8974	C68 H128 O22	79.92	-5.93	C68 H128 Na2 O22
671.4384	1306.8083	C60 H122 O29	98.84	-0.85	C60 H130 N2 O29
678.464	660.4298	C31 H64 O14	98.72	-0.35	C31 H68 N O14
692.4421	674.4083	C31 H62 O15	47.11	0.9	C31 H66 N O15
722.4908	704.4566	C33 H68 O15	98.07	-1.08	C33 H72 N O15
736.4688	718.4354	C33 H66 O16	91.15	-0.49	C33 H70 N O16
671.4384	1284.7987	C61 H120 O27	95.16	2.32	C65 H130 O27
671.4384	1260.7987	C59 H120 O27	95.16	2.36	C65 H130 O27
671.4384	1228.7361	C57 H112 O27	95.16	2.42	C65 H130 O27

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

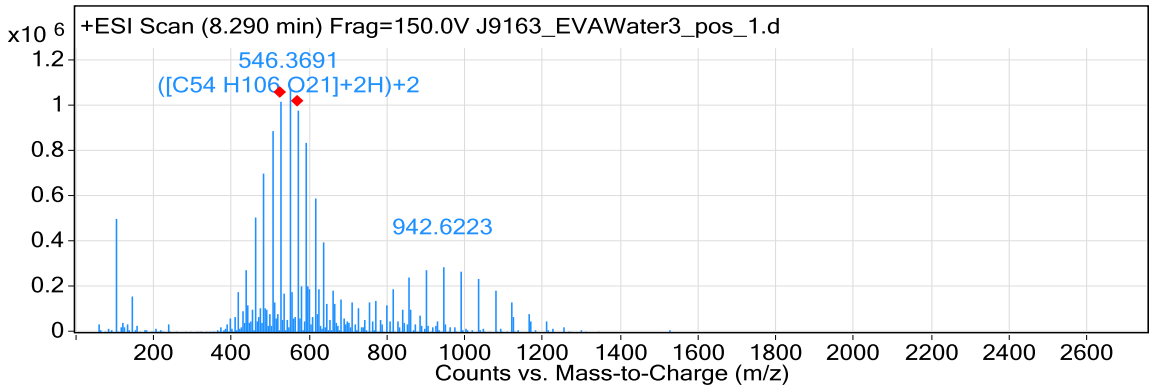


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
480.3295	958.6439	C48 H94 O18	98.46	0.17	C48 H96 O18
482.9888	481.9814	C14 H10 O19	78.57	0.54	C14 H11 O19
487.3191	972.6226	C48 H92 O19	95.66	0.66	C48 H94 O19
502.3424	1002.6698	C50 H98 O19	98.36	0.39	C50 H100 O19
509.3318	1016.6481	C50 H96 O20	95.2	1.37	C50 H98 O20
524.3557	1046.6961	C52 H102 O20	98.84	0.31	C52 H104 O20
527.0146	526.0072	C16 H14 O20	91.05	1.26	C16 H15 O20
531.3454	1060.6753	C52 H100 O21	90.35	0.39	C52 H102 O21
480.3295	914.6799	C55 H94 O10	82.07	5.22	C55 H94 Na2 O10
487.3191	928.6587	C55 H92 O11	77.76	5.66	C55 H92 Na2 O11
502.3424	958.7059	C57 H98 O11	81.69	5.22	C57 H98 Na2 O11
509.3318	972.6842	C57 H96 O12	74.92	6.18	C57 H96 Na2 O12
524.3557	1002.7322	C59 H102 O12	84.65	4.92	C59 H102 Na2 O12
527.0146	504.0252	C14 H16 O20	88.54	-3.46	C14 H16 Na O20
531.3454	1016.7114	C59 H100 O13	74.85	4.95	C59 H100 Na2 O13
480.3295	924.5908	C43 H88 O20	92.05	-4.24	C43 H96 N2 O20
487.3191	938.5696	C43 H86 O21	91.08	-3.66	C43 H94 N2 O21
502.3424	968.6168	C45 H92 O21	93.28	-3.81	C45 H100 N2 O21
509.3318	982.5951	C45 H90 O22	94.55	-2.74	C45 H98 N2 O22
512.3387	494.3054	C24 H46 O10	47.41	7.56	C24 H50 N O10
524.3557	1012.6431	C47 H96 O22	92.64	-3.72	C47 H104 N2 O22
531.3454	1026.6223	C47 H94 O23	85.71	-3.58	C47 H102 N2 O23
480.3295	902.5812	C44 H86 O18	98.46	0.18	C48 H96 O18
487.3191	916.56	C44 H84 O19	95.66	0.7	C48 H94 O19
502.3424	946.6072	C46 H90 O19	98.36	0.41	C50 H100 O19
509.3318	960.5855	C46 H88 O20	95.2	1.45	C50 H98 O20
524.3557	990.6335	C48 H94 O20	98.84	0.32	C52 H104 O20
527.0146	497.9759	C14 H10 O20	91.05	1.33	C16 H15 O20
531.3454	1004.6127	C48 H92 O21	90.35	0.41	C52 H102 O21
480.3295	878.5812	C42 H86 O18	98.46	0.19	C48 H96 O18
487.3191	892.56	C42 H84 O19	95.66	0.72	C48 H94 O19
502.3424	922.6072	C44 H90 O19	98.36	0.43	C50 H100 O19
509.3318	936.5855	C44 H88 O20	95.2	1.49	C50 H98 O20
524.3557	966.6335	C46 H94 O20	98.84	0.33	C52 H104 O20
531.3454	980.6127	C46 H92 O21	90.35	0.42	C52 H102 O21
480.3295	846.5186	C40 H78 O18	98.46	0.2	C48 H96 O18
487.3191	860.4974	C40 H76 O19	95.66	0.75	C48 H94 O19
502.3424	890.5446	C42 H82 O19	98.36	0.44	C50 H100 O19

509.3318	904.5229	C42 H80 O20	95.2	1.54	C50 H98 O20
524.3557	934.5709	C44 H86 O20	98.84	0.34	C52 H104 O20
531.3454	948.5501	C44 H84 O21	90.35	0.44	C52 H102 O21

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

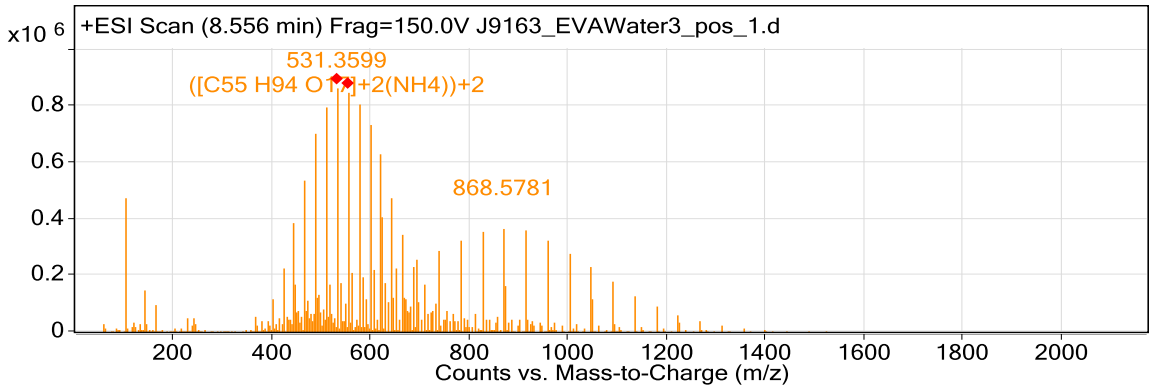


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
524.3558	1046.6964	C52 H102 O20	99.05	0.09	C52 H104 O20
531.3458	1060.6757	C52 H100 O21	90.43	-0.01	C52 H102 O21
546.3691	1090.7232	C54 H106 O21	99.27	-0.45	C54 H108 O21
553.3578	1104.7005	C54 H104 O22	98.22	1.29	C54 H106 O22
568.3824	1134.7493	C56 H110 O22	99.03	-0.41	C56 H112 O22
571.0407	570.0332	C18 H18 O21	75.02	1.57	C18 H19 O21
575.3722	1148.7285	C56 H108 O23	89.4	-0.29	C56 H110 O23
524.3558	1002.7324	C59 H102 O12	85.3	4.69	C59 H102 Na2 O12
531.3458	1016.7118	C59 H100 O13	75.65	4.53	C59 H100 Na2 O13
546.3691	1046.7592	C61 H106 O13	88.59	3.93	C61 H106 Na2 O13
553.3578	1060.7366	C61 H104 O14	81.32	5.69	C61 H104 Na2 O14
568.3824	1090.7854	C63 H110 O14	89.28	3.8	C63 H110 Na2 O14
571.0407	548.0512	C16 H20 O21	73.17	-2.75	C16 H20 Na O21
575.3722	1104.7645	C63 H108 O15	77.55	3.88	C63 H108 Na2 O15
524.3558	1012.6433	C47 H96 O22	92.34	-3.94	C47 H104 N2 O22
531.3458	1026.6227	C47 H94 O23	85.02	-4	C47 H102 N2 O23
546.5732	1057.0814	C71 H140 O4	70.21	-5.86	C71 H148 N2 O4
546.3691	1056.6701	C49 H100 O23	90.81	-4.33	C49 H108 N2 O23
553.3578	1070.6475	C49 H98 O24	96.3	-2.49	C49 H106 N2 O24
568.3824	1100.6962	C69 H96 O11	91.27	-0.87	C69 H104 N2 O11
575.3722	1114.6754	C51 H102 O25	83.02	-3.97	C51 H110 N2 O25
524.3558	990.6338	C48 H94 O20	99.05	0.09	C52 H104 O20
531.3458	1004.6131	C48 H92 O21	90.43	-0.01	C52 H102 O21
546.3691	1034.6606	C50 H98 O21	99.27	-0.48	C54 H108 O21
553.3578	1048.6379	C50 H96 O22	98.22	1.36	C54 H106 O22
568.3824	1078.6867	C52 H102 O22	99.03	-0.43	C56 H112 O22
571.0407	542.0019	C16 H14 O21	75.02	1.65	C18 H19 O21
575.3722	1092.6659	C52 H100 O23	89.4	-0.3	C56 H110 O23
524.3558	966.6338	C46 H94 O20	99.05	0.09	C52 H104 O20
531.3458	980.6131	C46 H92 O21	90.43	-0.01	C52 H102 O21
546.3691	1010.6606	C48 H98 O21	99.27	-0.49	C54 H108 O21
553.3578	1024.6379	C48 H96 O22	98.22	1.39	C54 H106 O22

568.3824	1054.6867	C50 H102 O22	99.03	-0.44	C56 H112 O22
571.0407	530.0019	C15 H14 O21	75.02	1.69	C18 H19 O21
575.3722	1068.6659	C50 H100 O23	89.4	-0.31	C56 H110 O23
524.3558	934.5712	C44 H86 O20	99.05	0.1	C52 H104 O20
531.3458	948.5505	C44 H84 O21	90.43	-0.01	C52 H102 O21
546.3691	978.598	C46 H90 O21	99.27	-0.5	C54 H108 O21
553.3578	992.5753	C46 H88 O22	98.22	1.43	C54 H106 O22
568.3824	1022.6241	C48 H94 O22	99.03	-0.45	C56 H112 O22
575.3722	1036.6033	C48 H92 O23	89.4	-0.32	C56 H110 O23

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

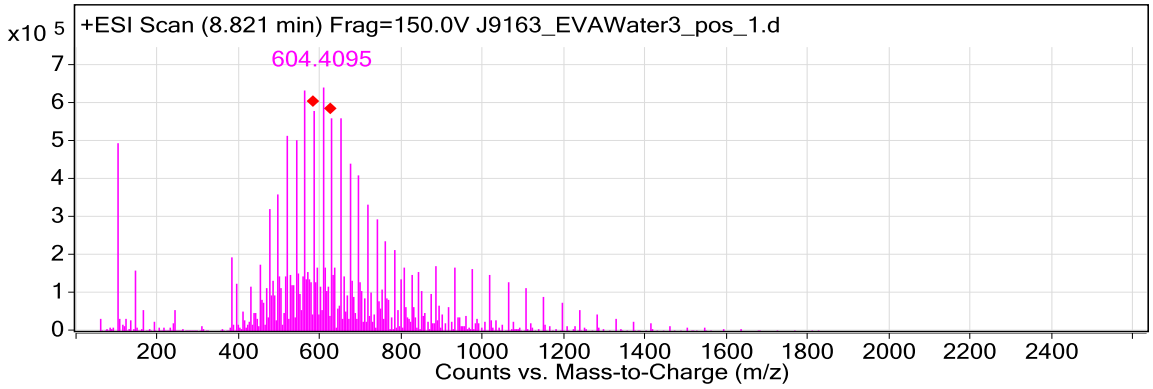


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
531.3599	1060.7043	C60 H100 O15	92.82	1.81	C60 H102 O15
538.3487	1074.6823	C60 H98 O16	92.32	2.99	C60 H100 O16
553.3731	1104.7307	C62 H104 O16	95.16	1.55	C62 H106 O16
560.3676	1118.7161	C55 H106 O22	62.18	1.29	C55 H108 O22
531.3599	1016.7404	C56 H104 O15	92.72	-2.84	C56 H104 Na2 O15
538.3487	1030.7184	C56 H102 O16	96.85	-1.55	C56 H102 Na2 O16
553.3731	1060.7668	C58 H108 O16	94.24	-2.93	C58 H108 Na2 O16
531.3599	1026.6513	C55 H94 O17	94.87	-2.1	C55 H102 N2 O17
538.3487	1040.6292	C55 H92 O18	98.09	-0.83	C55 H100 N2 O18
546.3597	528.3258	C28 H48 O9	55.73	7.55	C28 H52 N O9
553.3731	1070.6777	C57 H98 O18	96.11	-2.22	C57 H106 N2 O18
531.3599	1004.6417	C56 H92 O15	92.82	1.92	C60 H102 O15
538.3487	1018.6197	C56 H90 O16	92.32	3.16	C60 H100 O16
553.3731	1048.6681	C58 H96 O16	95.16	1.63	C62 H106 O16
560.3676	1062.6535	C51 H98 O22	62.18	1.36	C55 H108 O22
531.3599	980.6417	C54 H92 O15	92.82	1.96	C60 H102 O15
538.3487	994.6197	C54 H90 O16	92.32	3.23	C60 H100 O16
553.3731	1024.6681	C56 H96 O16	95.16	1.67	C62 H106 O16
560.3676	1038.6535	C49 H98 O22	62.18	1.39	C55 H108 O22
531.3599	948.5791	C52 H84 O15	92.82	2.03	C60 H102 O15
538.3487	962.5571	C52 H82 O16	92.32	3.34	C60 H100 O16
553.3731	992.6055	C54 H88 O16	95.16	1.72	C62 H106 O16
560.3676	1006.5909	C47 H90 O22	62.18	1.44	C55 H108 O22

Fragmentor Voltage **Collision Energy** **Ionization Mode**

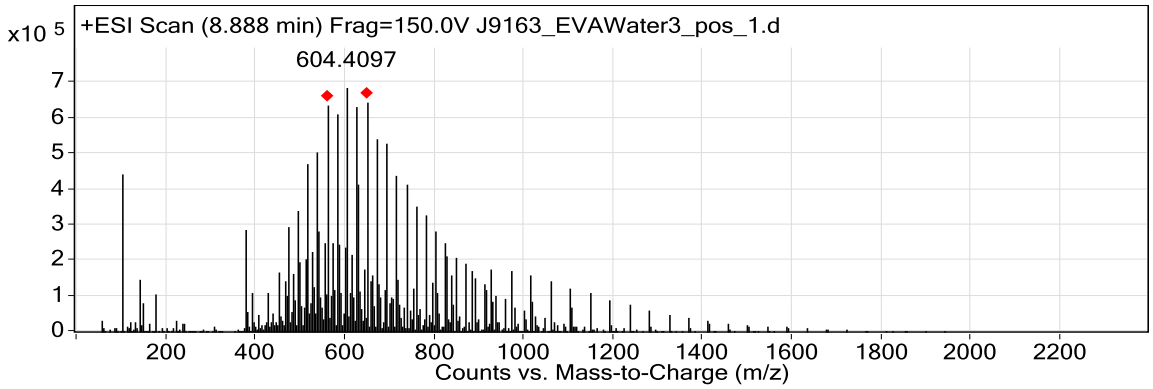
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
626.4237	1250.8319	C62 H122 O24	98.73	0.54	C62 H124 O24

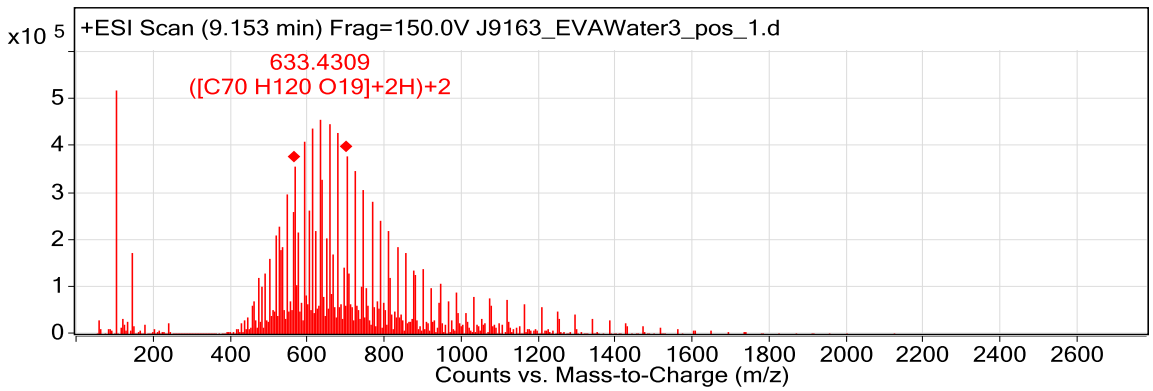
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
582.3974	1162.7795	C58 H114 O22	98.63	0.56	C58 H116 O22

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



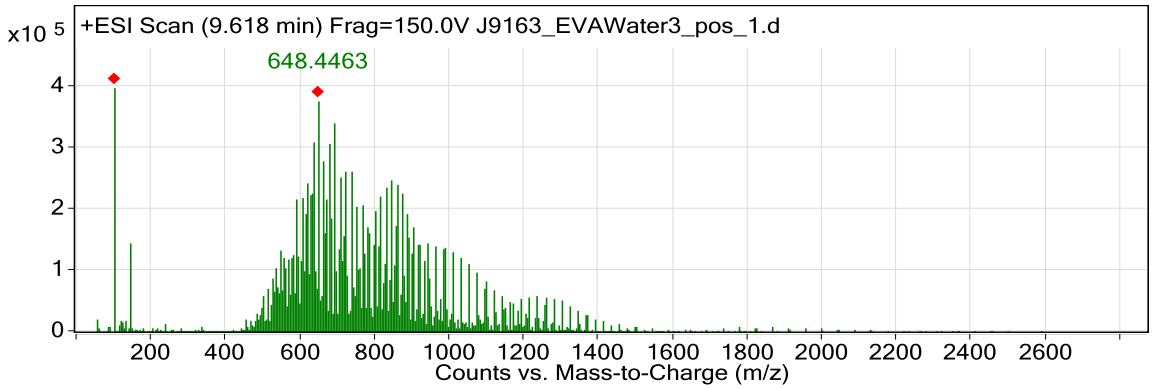
MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.

567.3915	1132.7653	C64 H108 O16	89.98	-1.39	C64 H110 O16
575.0548	574.0473	C21 H18 O19	76.71	-5.29	C21 H19 O19
589.4041	1176.7889	C66 H112 O17	65.24	0.92	C66 H114 O17
611.4179	1220.8185	C68 H116 O18	91.71	-1.88	C68 H118 O18
619.0803	618.0727	C23 H22 O20	83.14	-3.59	C23 H23 O20
633.4309	1264.843	C70 H120 O19	72.28	-0.48	C70 H122 O19
655.4441	1308.8717	C65 H128 O25	95.13	2.1	C65 H130 O25
663.1049	662.0974	C25 H26 O21	90.41	-1.05	C25 H27 O21
677.4569	1352.8957	C74 H128 O21	79.27	-0.69	C74 H130 O21
699.4699	1396.924	C69 H136 O27	95.72	2.09	C69 H138 O27
707.1304	706.1227	C27 H30 O22	88.03	0.19	C27 H31 O22
567.3915	1088.8014	C71 H108 O8	85.32	2.78	C71 H108 Na2 O8
575.0548	552.0653	C30 H16 O11	58.11	7.14	C30 H16 Na O11
589.4041	1132.8249	C73 H112 O9	53.89	5.04	C73 H112 Na2 O9
611.4179	1176.8545	C75 H116 O10	88.26	1.97	C75 H116 Na2 O10
619.0803	596.0907	C21 H24 O20	66.2	-7.75	C21 H24 Na O20
633.4309	1220.8791	C77 H120 O11	66.59	3.29	C77 H120 Na2 O11
655.4441	1264.9078	C72 H128 O17	79.41	5.81	C72 H128 Na2 O17
663.1049	640.1154	C23 H28 O21	79.42	-4.84	C23 H28 Na O21
677.4569	1308.9319	C70 H132 O21	67.97	-4.4	C70 H132 Na2 O21
699.4699	1352.9601	C72 H136 O22	81.24	-5.72	C72 H136 Na2 O22
707.1304	684.1408	C25 H32 O22	80.57	-3.32	C25 H32 Na O22
560.3774	542.3432	C29 H50 O9	66.45	4.23	C29 H54 N O9
567.3915	1098.7123	C52 H106 O23	87.17	0.17	C52 H114 N2 O23
589.4041	1142.7358	C61 H106 O19	61.61	-2.64	C61 H114 N2 O19
604.4038	586.3696	C31 H54 O10	70.98	3.5	C31 H58 N O10
611.4179	1186.7653	C56 H114 O25	94.06	-0.28	C56 H122 N2 O25
618.4076	600.3738	C28 H56 O13	43.24	-2.83	C28 H60 N O13
633.4309	1230.79	C58 H118 O26	70.15	0.91	C58 H126 N2 O26
648.4303	630.396	C33 H58 O11	76	3.09	C33 H62 N O11
655.4441	1274.8187	C60 H122 O27	97.06	-1.05	C60 H130 N2 O27
677.4569	1318.8428	C62 H126 O28	77.59	0.61	C62 H134 N2 O28
699.4699	1362.8707	C64 H130 O29	98.81	-0.67	C64 H138 N2 O29
567.3915	1076.7027	C60 H100 O16	89.98	-1.46	C64 H110 O16
575.0548	546.016	C19 H14 O19	76.71	-5.56	C21 H19 O19
589.4041	1120.7263	C62 H104 O17	65.24	0.96	C66 H114 O17
611.4179	1164.7559	C64 H108 O18	91.71	-1.97	C68 H118 O18
619.0803	590.0414	C21 H18 O20	83.14	-3.76	C23 H23 O20
633.4309	1208.7804	C66 H112 O19	72.28	-0.5	C70 H122 O19
655.4441	1252.8091	C61 H120 O25	95.13	2.19	C65 H130 O25
663.1049	634.0661	C23 H22 O21	90.41	-1.1	C25 H27 O21
677.4569	1296.8331	C70 H120 O21	79.27	-0.72	C74 H130 O21
699.4699	1340.8614	C65 H128 O27	95.72	2.18	C69 H138 O27
707.1304	678.0914	C25 H26 O22	88.03	0.2	C27 H31 O22
567.3915	1052.7027	C58 H100 O16	89.98	-1.49	C64 H110 O16
575.0548	534.016	C18 H14 O19	76.71	-5.69	C21 H19 O19
589.4041	1096.7263	C60 H104 O17	65.24	0.99	C66 H114 O17
611.4179	1140.7559	C62 H108 O18	91.71	-2.01	C68 H118 O18
619.0803	578.0414	C20 H18 O20	83.14	-3.84	C23 H23 O20
633.4309	1184.7804	C64 H112 O19	72.28	-0.51	C70 H122 O19
655.4441	1228.8091	C59 H120 O25	95.13	2.23	C65 H130 O25
663.1049	622.0661	C22 H22 O21	90.41	-1.12	C25 H27 O21

677.4569	1272.8331	C68 H120 O21	79.27	-0.74	C74 H130 O21
699.4699	1316.8614	C63 H128 O27	95.72	2.22	C69 H138 O27
707.1304	666.0914	C24 H26 O22	88.03	0.2	C27 H31 O22
567.3915	1020.6401	C56 H92 O16	89.98	-1.54	C64 H110 O16
575.0548	517.9847	C17 H10 O19	76.71	-5.86	C21 H19 O19
589.4041	1064.6637	C58 H96 O17	65.24	1.02	C66 H114 O17
611.4179	1108.6933	C60 H100 O18	91.71	-2.07	C68 H118 O18
619.0803	562.0101	C19 H14 O20	83.14	-3.94	C23 H23 O20
633.4309	1152.7178	C62 H104 O19	72.28	-0.53	C70 H122 O19
655.4441	1196.7465	C57 H112 O25	95.13	2.29	C65 H130 O25
663.1049	606.0348	C21 H18 O21	90.41	-1.15	C25 H27 O21
677.4569	1240.7705	C66 H112 O21	79.27	-0.76	C74 H130 O21
699.4699	1284.7988	C61 H120 O27	95.72	2.27	C69 H138 O27
707.1304	650.0601	C23 H22 O22	88.03	0.21	C27 H31 O22

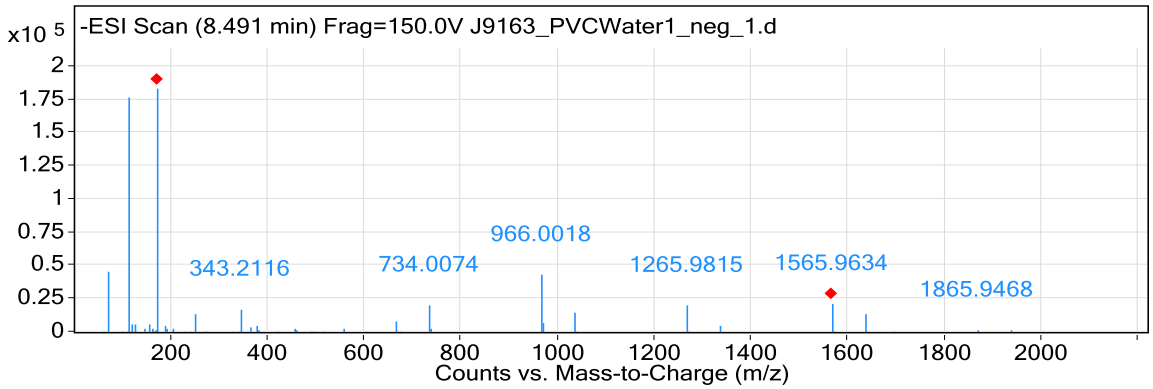
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
648.1616	630.1278	C22 H30 O21	47.58	0.27	C22 H34 N O21

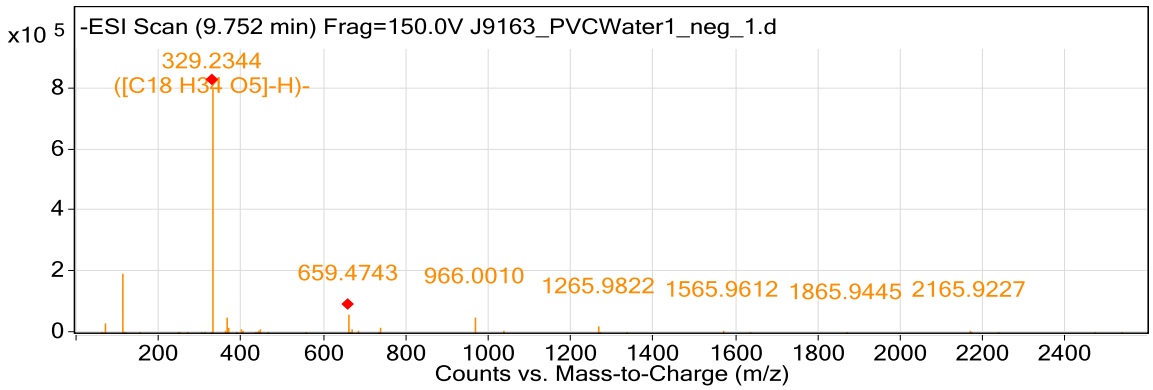
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
171.1023	172.1095	C9 H16 O3	97.81	2.51	C9 H15 O3

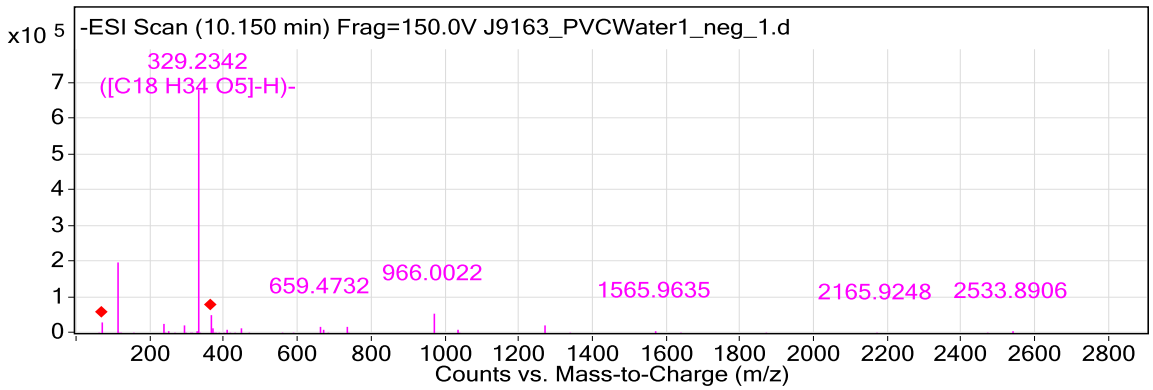
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
329.2344	330.2416	C18 H34 O5	95.56	-2.86	C18 H33 O5

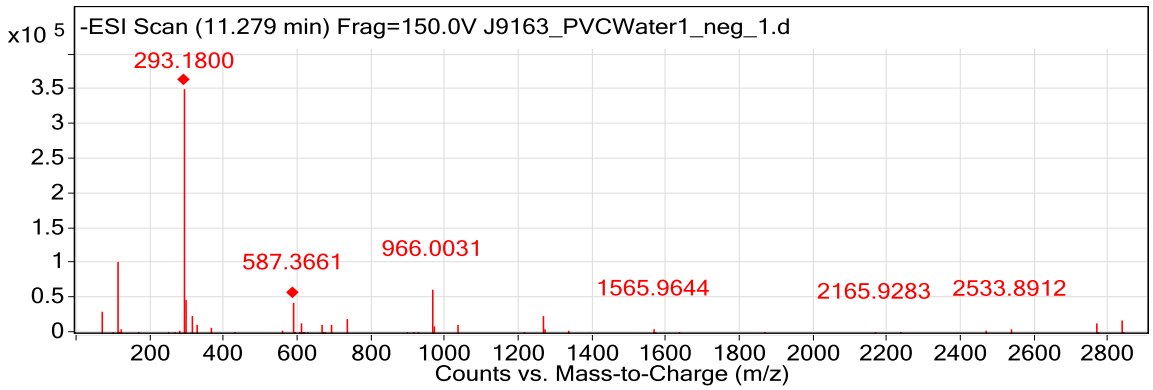
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
329.2342	330.2414	C18 H34 O5	96.42	-2.41	C18 H33 O5

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

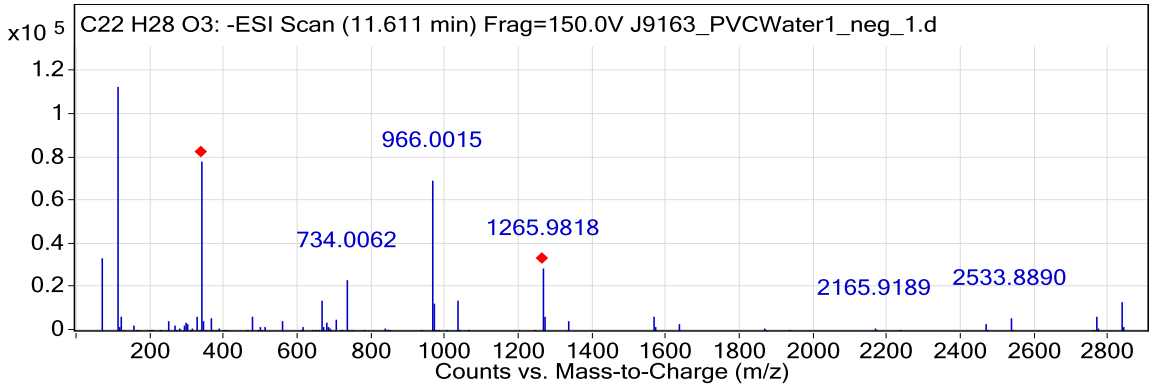


Qualitative Analysis Report

MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
277.1438	278.1513	C16 H22 O4	82.61	1.73	C16 H21 O4

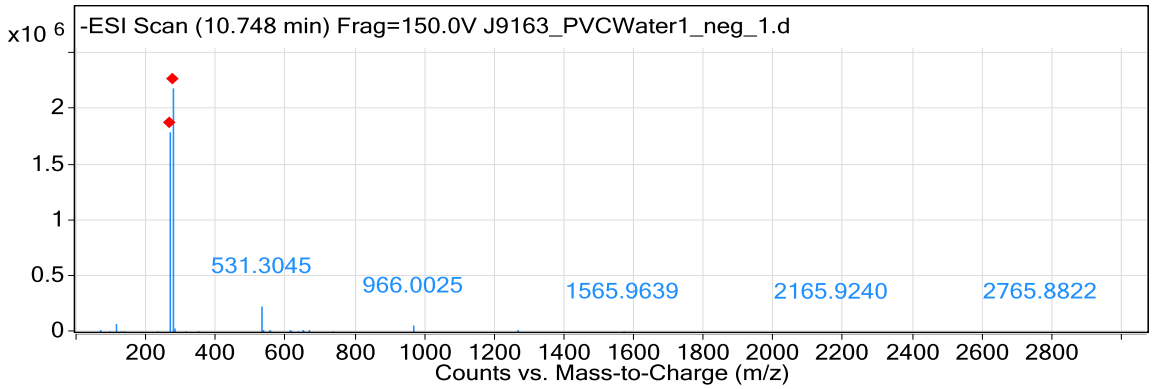
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
339.1996	340.2065	C22 H28 O3	68.45	-7.68	C22 H27 O3
341.1994	342.2063	C18 H30 O6	67.83	-6.02	C18 H29 O6

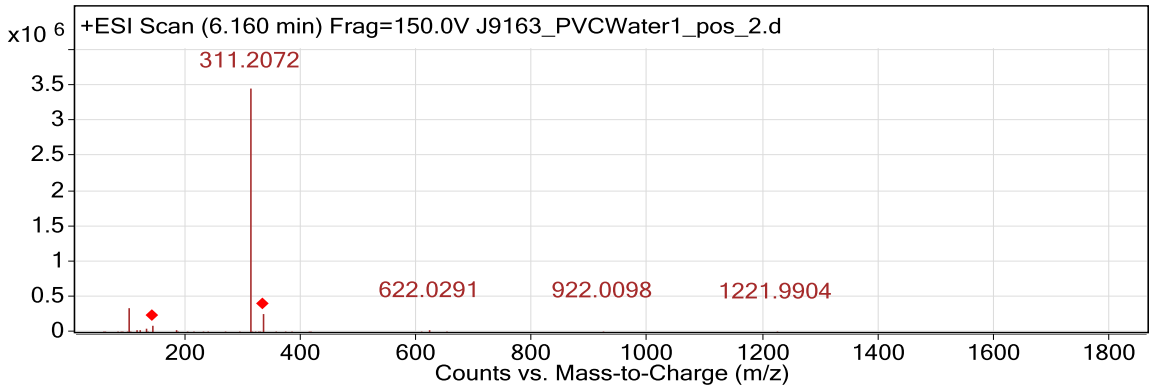
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
257.1749	258.1824	C14 H26 O4	81.47	2.64	C14 H25 O4
265.293	266.3	C19 H38	53.02	-10.01	C19 H37
267.1468	268.1538	C11 H24 O7	84.52	-6.11	C11 H23 O7
277.1451	278.1524	C16 H22 O4	98.75	-1.97	C16 H21 O4

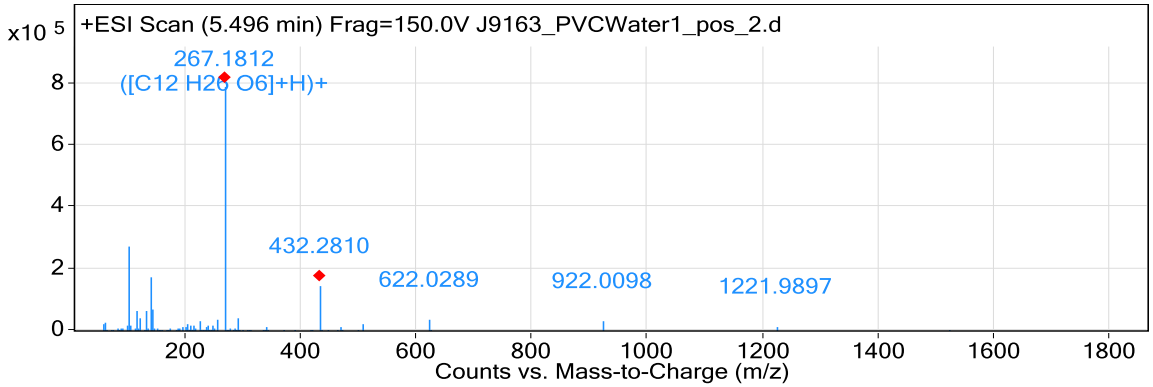
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
333.1894	332.1821	C16 H28 O7	78.74	4.13	C16 H29 O7
333.1894	310.2002	C14 H30 O7	82.47	-3.32	C14 H30 Na O7
328.2333	310.1991	C14 H30 O7	76.55	0.02	C14 H34 N O7

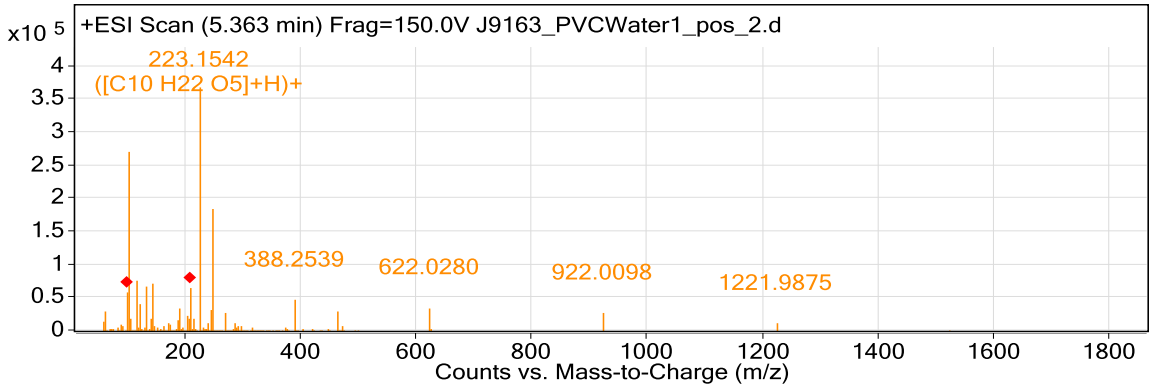
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
267.1812	266.1738	C12 H26 O6	95.99	-3.07	C12 H27 O6

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

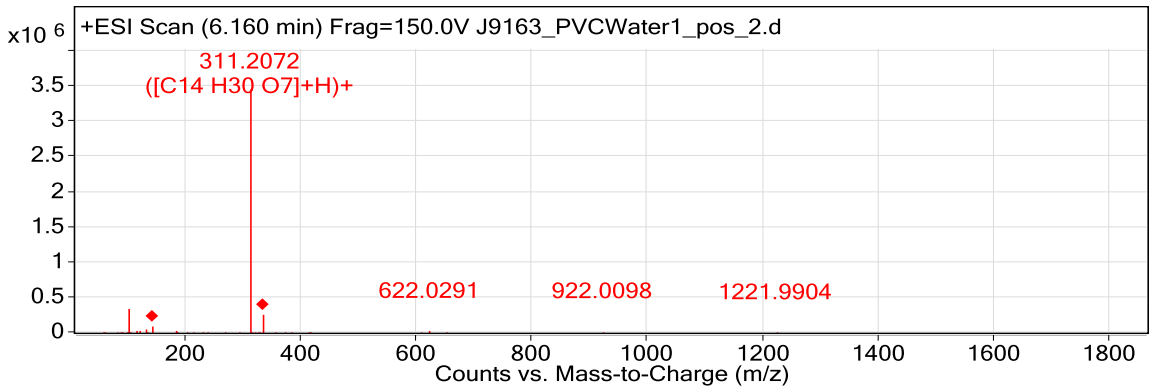


MFG Results

Qualitative Analysis Report

m/z	Mass	Best Match	Score	Diff.	Ion Form.
223.1542	222.1461	C10 H22 O5	70.39	2.79	C10 H23 O5

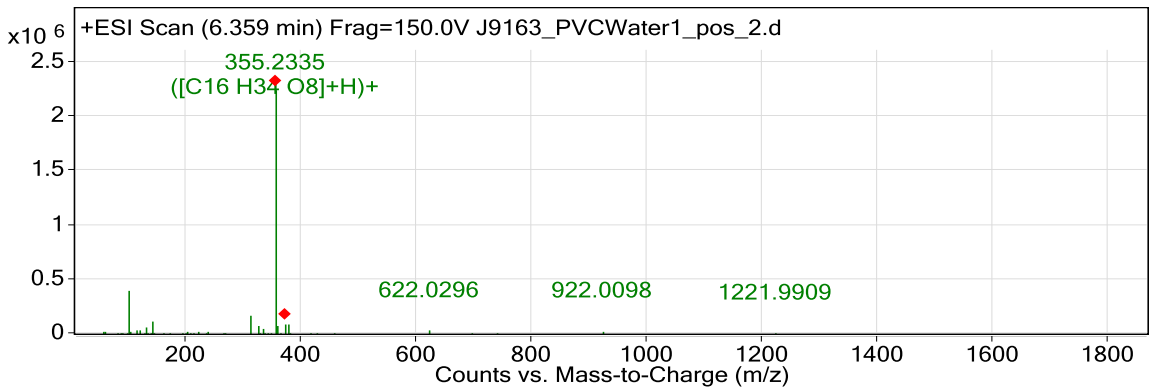
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
289.1639	288.1566	C14 H24 O6	45.84	2.45	C14 H25 O6
293.1971	292.1882	C14 H28 O6	67.14	1.2	C14 H29 O6
311.2072	310.2	C14 H30 O7	97.09	-2.71	C14 H31 O7
333.1894	332.1821	C16 H28 O7	78.74	4.13	C16 H29 O7
289.1639	266.1746	C12 H26 O6	38.19	-6.39	C12 H26 Na O6
313.2122	290.2229	C19 H30 O2	77.3	5.89	C19 H30 Na O2
333.1894	310.2002	C14 H30 O7	82.47	-3.32	C14 H30 Na O7
328.2333	310.1991	C14 H30 O7	76.55	0.02	C14 H34 N O7
289.1639	260.1253	C12 H20 O6	45.84	2.71	C14 H25 O6
293.1971	264.1569	C12 H24 O6	67.14	1.32	C14 H29 O6
311.2072	282.1687	C12 H26 O7	97.09	-2.98	C14 H31 O7
333.1894	304.1508	C14 H24 O7	78.74	4.51	C16 H29 O7
289.1639	248.1253	C11 H20 O6	45.84	2.84	C14 H25 O6
293.1971	252.1569	C11 H24 O6	67.14	1.39	C14 H29 O6
333.1894	292.1508	C13 H24 O7	78.74	4.7	C16 H29 O7

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

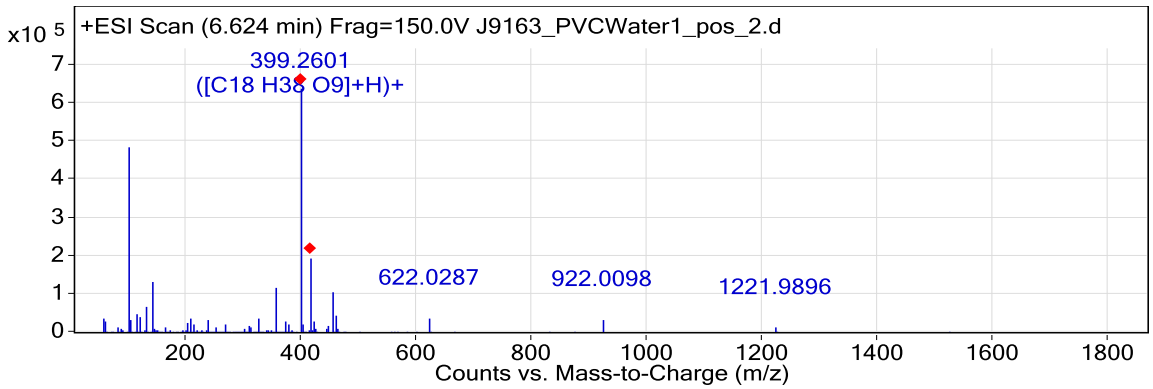


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.

355.2335	354.2262	C16 H34 O8	97.33	-2.49	C16 H35 O8

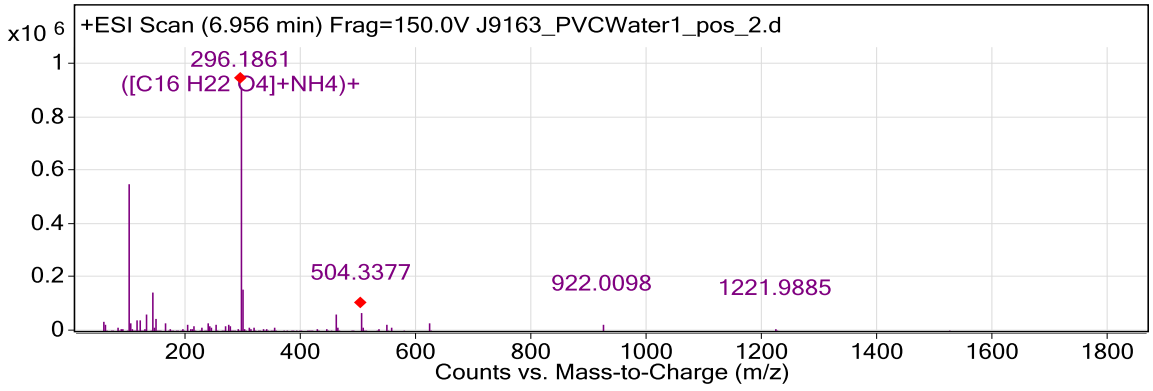
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
377.215	376.2082	C18 H32 O8	70.71	4.1	C18 H33 O8
399.2601	398.2526	C18 H38 O9	96.05	-2.59	C18 H39 O9
417.2883	416.2807	C22 H40 O7	58.22	-7.89	C22 H41 O7
421.2406	420.2336	C20 H36 O9	68.64	5.65	C20 H37 O9
377.215	354.2262	C16 H34 O8	72.56	-2.44	C16 H34 Na O8
401.264	378.2746	C23 H38 O4	66.31	6.5	C23 H38 Na O4
419.3127	396.3199	C24 H44 O4	43.4	10.37	C24 H44 Na O4
421.2406	398.2516	C18 H38 O9	80.7	-0.08	C18 H38 Na O9
400.2626	382.2284	C28 H30 O	74.34	3.3	C28 H34 N O
416.286	398.252	C18 H38 O9	98.09	-0.96	C18 H42 N O9
377.215	348.1769	C16 H28 O8	70.71	4.42	C18 H33 O8
399.2601	370.2213	C16 H34 O9	96.05	-2.79	C18 H39 O9
417.2883	388.2494	C20 H36 O7	58.22	-8.46	C22 H41 O7
421.2406	392.2023	C18 H32 O9	68.64	6.05	C20 H37 O9
377.215	336.1769	C15 H28 O8	70.71	4.58	C18 H33 O8
417.2883	376.2494	C19 H36 O7	58.22	-8.73	C22 H41 O7
421.2406	380.2023	C17 H32 O9	68.64	6.24	C20 H37 O9

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

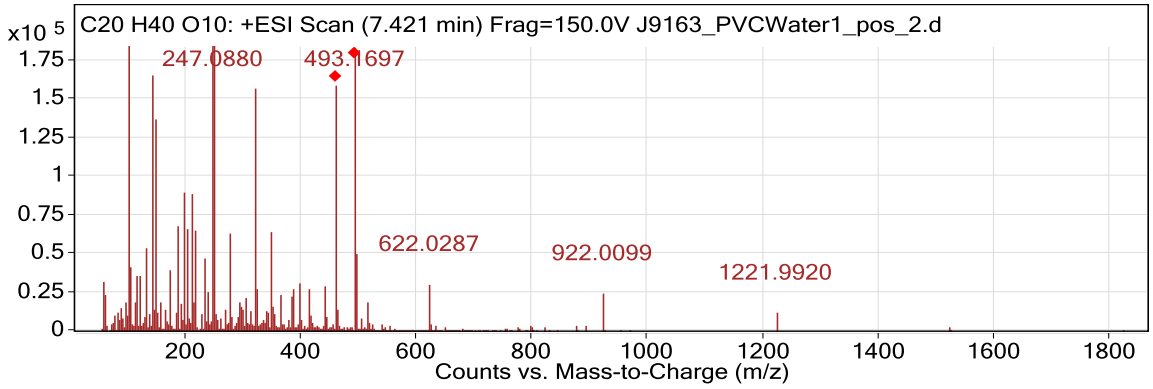


MFG Results

Qualitative Analysis Report

m/z	Mass	Best Match	Score	Diff.	Ion Form.
297.1892	296.1813	C13 H28 O7	74.14	7.47	C13 H29 O7
290.1609	272.1275	C13 H20 O6	61.22	-5.38	C13 H24 N O6
296.1861	278.1521	C16 H22 O4	99.3	-1.15	C16 H26 N O4
302.1946	284.1608	C15 H24 O5	39.77	5.51	C15 H28 N O5
297.1892	268.15	C11 H24 O7	74.14	8.25	C13 H29 O7

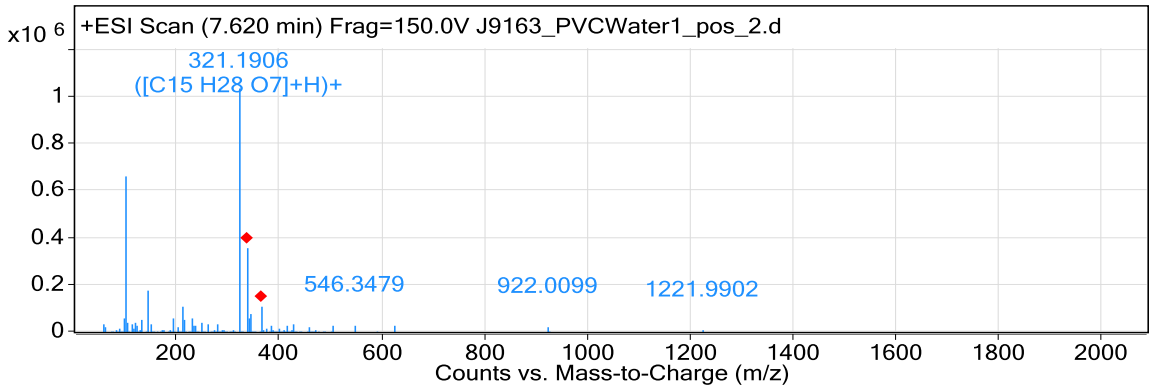
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
441.2695	440.2619	C20 H40 O10	82.71	0.58	C20 H41 O10
463.2521	440.2641	C20 H40 O10	71.23	-4.33	C20 H40 Na O10
458.2962	440.262	C20 H40 O10	96.64	0.27	C20 H44 N O10

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

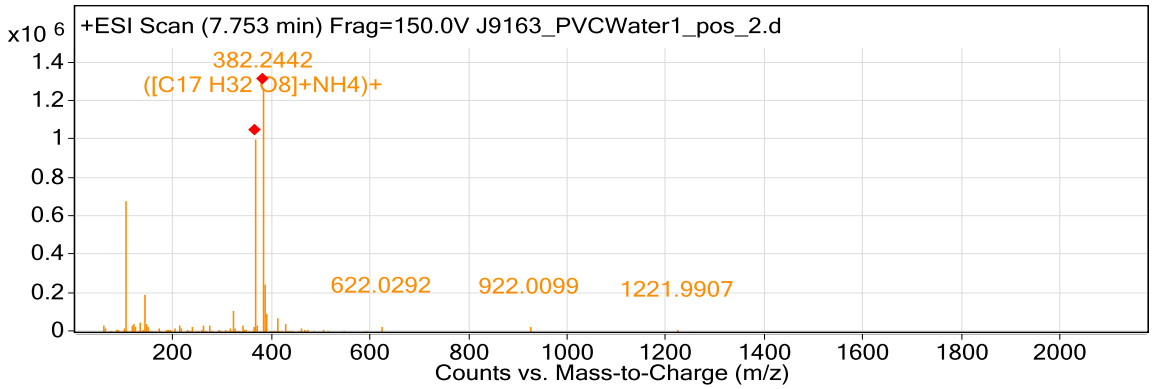


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
321.3499	320.3426	C23 H44	56.59	5.29	C23 H45
321.1906	320.1833	C15 H28 O7	99.19	0.73	C15 H29 O7
339.2189	338.2106	C19 H30 O5	79.04	-3.88	C19 H31 O5
343.1724	342.1653	C17 H26 O7	67.51	7.49	C17 H27 O7
365.2163	364.2096	C17 H32 O8	75.52	0.46	C17 H33 O8
343.1724	320.1833	C15 H28 O7	84.14	0.5	C15 H28 Na O7
338.3794	320.3456	C23 H44	64.72	-4.06	C23 H48 N
338.2168	320.1827	C15 H28 O7	95.15	2.63	C15 H32 N O7

374.1582	356.1244	C20 H20 O6	40.81	4.52	C20 H24 N O6
321.3499	292.3113	C21 H40	56.59	5.8	C23 H45
321.1906	292.152	C13 H24 O7	99.19	0.8	C15 H29 O7
339.2189	310.1793	C17 H26 O5	79.04	-4.23	C19 H31 O5
343.1724	314.134	C15 H22 O7	67.51	8.16	C17 H27 O7
365.2163	336.1783	C15 H28 O8	75.52	0.5	C17 H33 O8
321.3499	280.3113	C20 H40	56.59	6.05	C23 H45
321.1906	280.152	C12 H24 O7	99.19	0.83	C15 H29 O7
339.2189	298.1793	C16 H26 O5	79.04	-4.4	C19 H31 O5
343.1724	302.134	C14 H22 O7	67.51	8.48	C17 H27 O7
365.2163	324.1783	C14 H28 O8	75.52	0.51	C17 H33 O8

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

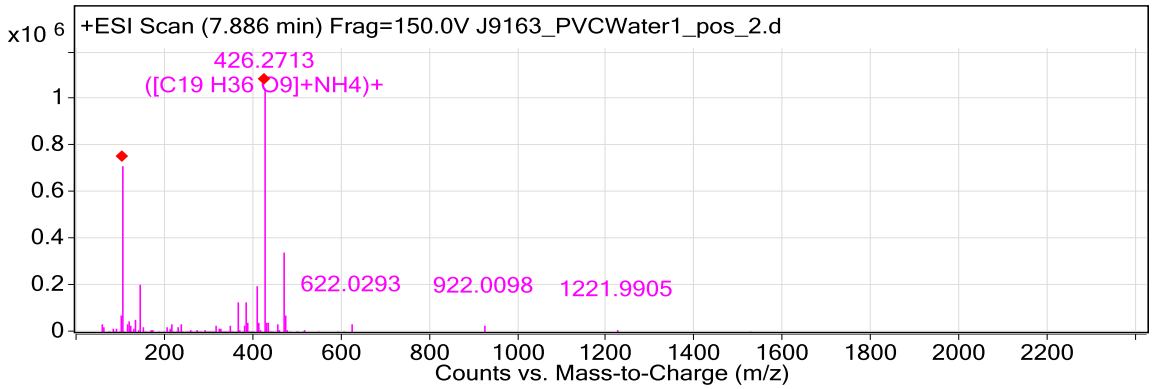


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
363.2382	362.2312	C18 H34 O7	79.38	-2.15	C18 H35 O7
365.2179	364.2105	C17 H32 O8	97.77	-2.15	C17 H33 O8
387.199	386.1923	C19 H30 O8	81.65	4.57	C19 H31 O8
387.199	364.2104	C17 H32 O8	90.17	-1.76	C17 H32 Na O8
366.2208	348.1866	C27 H24	74.42	3.38	C27 H28 N
382.2442	364.2103	C17 H32 O8	98.83	-1.71	C17 H36 N O8
363.2382	334.1999	C16 H30 O7	79.38	-2.33	C18 H35 O7
365.2179	336.1792	C15 H28 O8	97.77	-2.32	C17 H33 O8
387.199	358.161	C17 H26 O8	81.65	4.93	C19 H31 O8
363.2382	322.1999	C15 H30 O7	79.38	-2.42	C18 H35 O7
365.2179	324.1792	C14 H28 O8	97.77	-2.41	C17 H33 O8
387.199	346.161	C16 H26 O8	81.65	5.1	C19 H31 O8

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

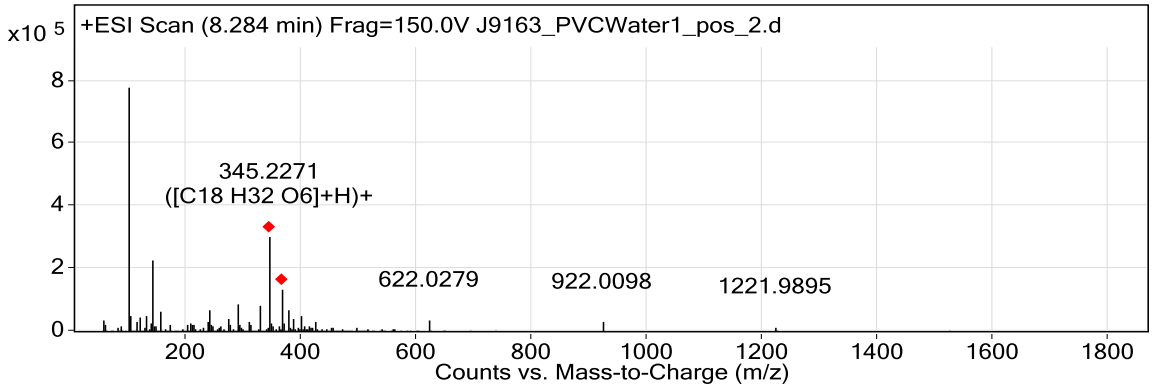
Qualitative Analysis Report



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
409.2438	408.2367	C19 H36 O9	96.37	-1.89	C19 H37 O9
431.2256	430.2195	C21 H34 O9	71.76	1.73	C21 H35 O9
431.2256	408.2376	C19 H36 O9	67	-4.07	C19 H36 Na O9
410.2473	392.2139	C29 H28 O	89.84	0.41	C29 H32 N O
426.2713	408.2373	C19 H36 O9	94.98	-3.33	C19 H40 N O9
428.2764	410.2424	C26 H34 O4	62.97	8.02	C26 H38 N O4
409.2438	380.2054	C17 H32 O9	96.37	-2.03	C19 H37 O9
431.2256	402.1882	C19 H30 O9	71.76	1.85	C21 H35 O9
409.2438	368.2054	C16 H32 O9	96.37	-2.1	C19 H37 O9
431.2256	390.1882	C18 H30 O9	71.76	1.91	C21 H35 O9

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

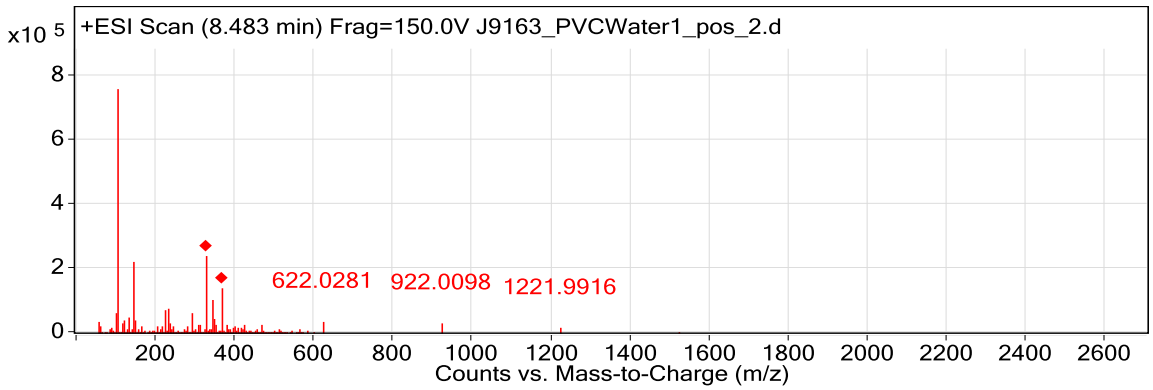


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
343.2066	342.2016	C25 H26 O	42.83	-9.34	C25 H27 O
345.2271	344.2199	C18 H32 O6	85.84	-0.08	C18 H33 O6
347.2368	346.229	C25 H30 O	79.17	2.05	C25 H31 O
351.2163	350.2098	C20 H30 O5	67.07	-1.28	C20 H31 O5
367.2095	366.203	C20 H30 O6	72.84	3.27	C20 H31 O6
369.2229	368.2165	C27 H28 O	50.48	-6.68	C27 H29 O
345.2271	322.238	C16 H34 O6	68.38	-7.58	C16 H34 Na O6
347.2368	324.247	C23 H32 O	69.7	-5.23	C23 H32 Na O
351.2163	328.2278	C18 H32 O5	44.89	-8.69	C18 H32 Na O5
365.2059	342.2171	C22 H30 O3	55.72	6.92	C22 H30 Na O3
367.2095	344.2211	C18 H32 O6	73.2	-3.54	C18 H32 Na O6

369.2229	346.2346	C18 H34 O6	63.7	2.63	C18 H34 Na O6
379.2373	356.2481	C27 H32	35.14	6.38	C27 H32 Na
360.2397	342.2059	C18 H30 O6	40.09	-4.87	C18 H34 N O6
362.2519	344.2181	C18 H32 O6	39.21	5.16	C18 H36 N O6
343.2066	314.1703	C23 H22 O	42.83	-10.17	C25 H27 O
345.2271	316.1886	C16 H28 O6	85.84	-0.09	C18 H33 O6
347.2368	318.1977	C23 H26 O	79.17	2.23	C25 H31 O
351.2163	322.1785	C18 H26 O5	67.07	-1.39	C20 H31 O5
367.2095	338.1717	C18 H26 O6	72.84	3.54	C20 H31 O6
369.2229	340.1852	C25 H24 O	50.48	-7.23	C27 H29 O
343.2066	302.1703	C22 H22 O	42.83	-10.58	C25 H27 O
345.2271	304.1886	C15 H28 O6	85.84	-0.09	C18 H33 O6
347.2368	306.1977	C22 H26 O	79.17	2.31	C25 H31 O
351.2163	310.1785	C17 H26 O5	67.07	-1.45	C20 H31 O5
367.2095	326.1717	C17 H26 O6	72.84	3.67	C20 H31 O6
369.2229	328.1852	C24 H24 O	50.48	-7.49	C27 H29 O

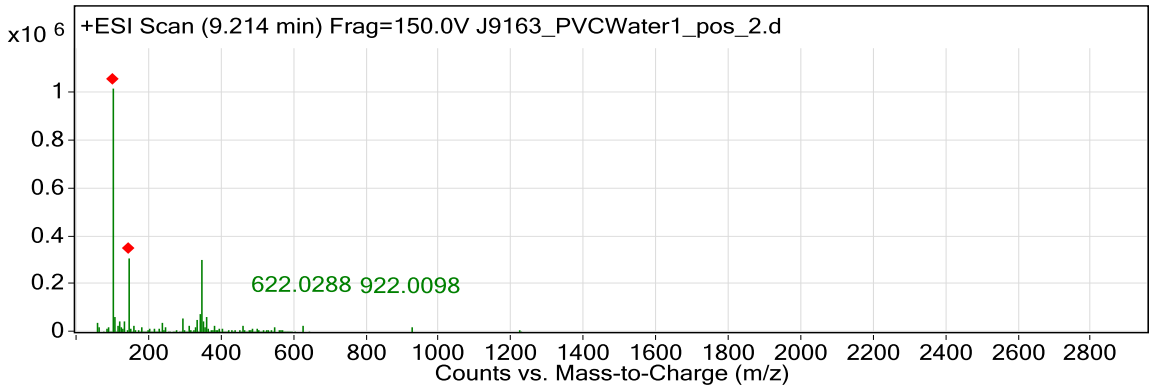
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
327.2161	326.2088	C18 H30 O5	84.31	1.7	C18 H31 O5

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

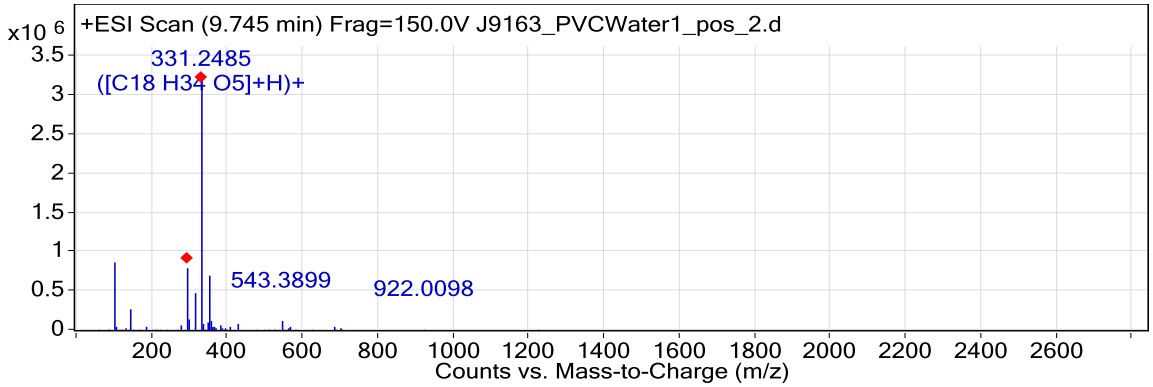


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.

329.2321	328.2251	C18 H32 O5	82.58	-0.39	C18 H33 O5
331.2475	330.2393	C18 H34 O5	63.51	3.89	C18 H35 O5
341.2326	340.2253	C19 H32 O5	93.33	-0.99	C19 H33 O5
345.2458	344.2394	C22 H32 O3	44.71	-12.25	C22 H33 O3
351.2158	350.2091	C20 H30 O5	74.61	0.68	C20 H31 O5
359.2432	358.2365	C19 H34 O6	74.73	-2.6	C19 H35 O6
361.2571	360.2498	C19 H36 O6	67.65	3.81	C19 H37 O6
329.2321	306.2432	C16 H34 O5	64.04	-8.26	C16 H34 Na O5
341.2326	318.2434	C17 H34 O5	73.43	-8.64	C17 H34 Na O5
351.2158	328.2271	C18 H32 O5	59.41	-6.6	C18 H32 Na O5
359.2432	336.2545	C17 H36 O6	51.32	-9.92	C17 H36 Na O6
344.2441	326.2102	C18 H30 O5	89.97	-2.6	C18 H34 N O5
329.2321	300.1938	C16 H28 O5	82.58	-0.42	C18 H33 O5
331.2475	302.208	C16 H30 O5	63.51	4.25	C18 H35 O5
341.2326	312.194	C17 H28 O5	93.33	-1.08	C19 H33 O5
345.2458	316.2081	C20 H28 O3	44.71	-13.34	C22 H33 O3
351.2158	322.1778	C18 H26 O5	74.61	0.74	C20 H31 O5
359.2432	330.2052	C17 H30 O6	74.73	-2.82	C19 H35 O6
361.2571	332.2185	C17 H32 O6	67.65	4.13	C19 H37 O6
329.2321	288.1938	C15 H28 O5	82.58	-0.44	C18 H33 O5
331.2475	290.208	C15 H30 O5	63.51	4.42	C18 H35 O5
341.2326	300.194	C16 H28 O5	93.33	-1.13	C19 H33 O5
345.2458	304.2081	C19 H28 O3	44.71	-13.86	C22 H33 O3
351.2158	310.1778	C17 H26 O5	74.61	0.76	C20 H31 O5
359.2432	318.2052	C16 H30 O6	74.73	-2.93	C19 H35 O6
361.2571	320.2185	C16 H32 O6	67.65	4.28	C19 H37 O6

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

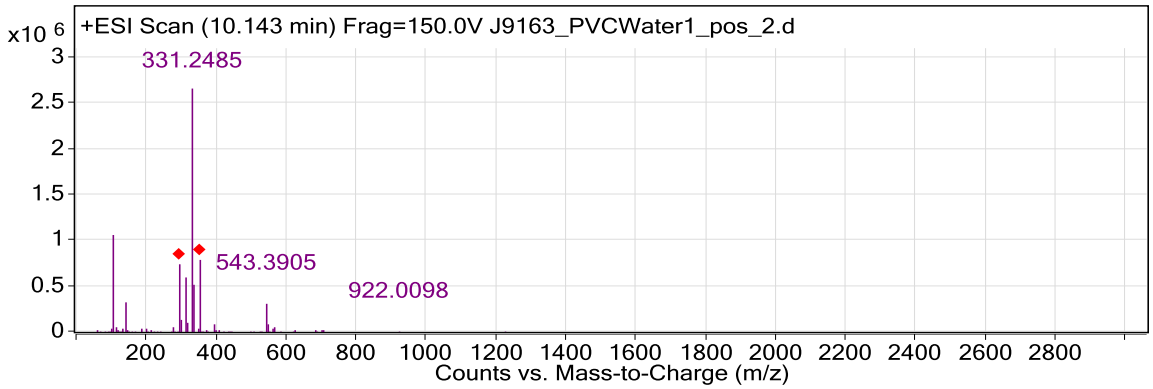


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
277.2139	276.2063	C18 H28 O2	76.77	9.47	C18 H29 O2
291.1952	290.1885	C18 H26 O3	76.46	-1.15	C18 H27 O3
293.2101	292.2028	C18 H28 O3	43.85	3.58	C18 H29 O3
295.2282	294.2208	C18 H30 O3	92.93	-4.31	C18 H31 O3
311.2202	310.2124	C18 H30 O4	59.16	6.34	C18 H31 O4
313.2384	312.2309	C18 H32 O4	96.14	-2.84	C18 H33 O4
329.2344	328.2273	C18 H32 O5	62.82	-6.94	C18 H33 O5
331.2485	330.2414	C18 H34 O5	97.6	-2.2	C18 H35 O5
345.1902	344.183	C17 H28 O7	46.7	1.59	C17 H29 O7

353.2312	352.2239	C20 H32 O5	92.73	3.17	C20 H33 O5
365.1936	364.1872	C20 H28 O6	62.16	3.75	C20 H29 O6
369.2075	368.2018	C23 H28 O4	41.12	-8.16	C23 H29 O4
277.2139	254.2244	C16 H30 O2	95.93	0.81	C16 H30 Na O2
291.1952	268.2066	C16 H28 O3	53.59	-10.2	C16 H28 Na O3
293.2101	270.2209	C16 H30 O3	41.42	-5.03	C16 H30 Na O3
311.2202	288.2305	C16 H32 O4	66	-1.52	C16 H32 Na O4
313.2384	290.249	C16 H34 O4	73.14	-11.35	C16 H34 Na O4
345.1902	322.201	C15 H30 O7	38.1	-5.77	C15 H30 Na O7
353.2312	330.2419	C18 H34 O5	94.01	-3.91	C18 H34 Na O5
365.1936	342.2053	C18 H30 O6	60.75	-3.04	C18 H30 Na O6
286.2024	268.1692	C15 H24 O4	56.19	-6.39	C15 H28 N O4
294.2265	276.1927	C14 H28 O5	44.37	3.51	C14 H32 N O5
328.2472	310.2134	C18 H30 O4	44.39	3.28	C18 H34 N O4
348.2749	330.2407	C18 H34 O5	97.54	-0.35	C18 H38 N O5
358.2591	340.2245	C19 H32 O5	68.03	1.35	C19 H36 N O5
277.2139	248.175	C16 H24 O2	76.77	10.54	C18 H29 O2
291.1952	262.1572	C16 H22 O3	76.46	-1.27	C18 H27 O3
293.2101	264.1715	C16 H24 O3	43.85	3.96	C18 H29 O3
295.2282	266.1895	C16 H26 O3	92.93	-4.76	C18 H31 O3
311.2202	282.1811	C16 H26 O4	59.16	6.97	C18 H31 O4
313.2384	284.1996	C16 H28 O4	96.14	-3.12	C18 H33 O4
329.2344	300.196	C16 H28 O5	62.82	-7.58	C18 H33 O5
331.2485	302.2101	C16 H30 O5	97.6	-2.41	C18 H35 O5
345.1902	316.1517	C15 H24 O7	46.7	1.73	C17 H29 O7
353.2312	324.1926	C18 H28 O5	92.73	3.45	C20 H33 O5
365.1936	336.1559	C18 H24 O6	62.16	4.06	C20 H29 O6
369.2075	340.1705	C21 H24 O4	41.12	-8.83	C23 H29 O4
277.2139	236.175	C15 H24 O2	76.77	11.07	C18 H29 O2
291.1952	250.1572	C15 H22 O3	76.46	-1.33	C18 H27 O3
293.2101	252.1715	C15 H24 O3	43.85	4.15	C18 H29 O3
295.2282	254.1895	C15 H26 O3	92.93	-4.99	C18 H31 O3
311.2202	270.1811	C15 H26 O4	59.16	7.28	C18 H31 O4
313.2384	272.1996	C15 H28 O4	96.14	-3.25	C18 H33 O4
329.2344	288.196	C15 H28 O5	62.82	-7.9	C18 H33 O5
331.2485	290.2101	C15 H30 O5	97.6	-2.5	C18 H35 O5
345.1902	304.1517	C14 H24 O7	46.7	1.8	C17 H29 O7
353.2312	312.1926	C17 H28 O5	92.73	3.58	C20 H33 O5
365.1936	324.1559	C17 H24 O6	62.16	4.21	C20 H29 O6
369.2075	328.1705	C20 H24 O4	41.12	-9.15	C23 H29 O4

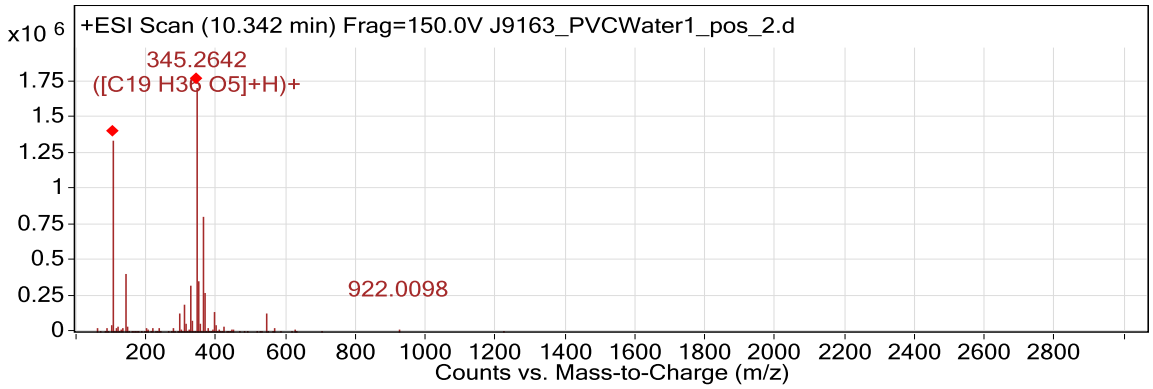
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
353.2314	330.2421	C18 H34 O5	92.92	-4.37	C18 H34 Na O5
348.2743	330.2398	C18 H34 O5	87.83	2.4	C18 H38 N O5

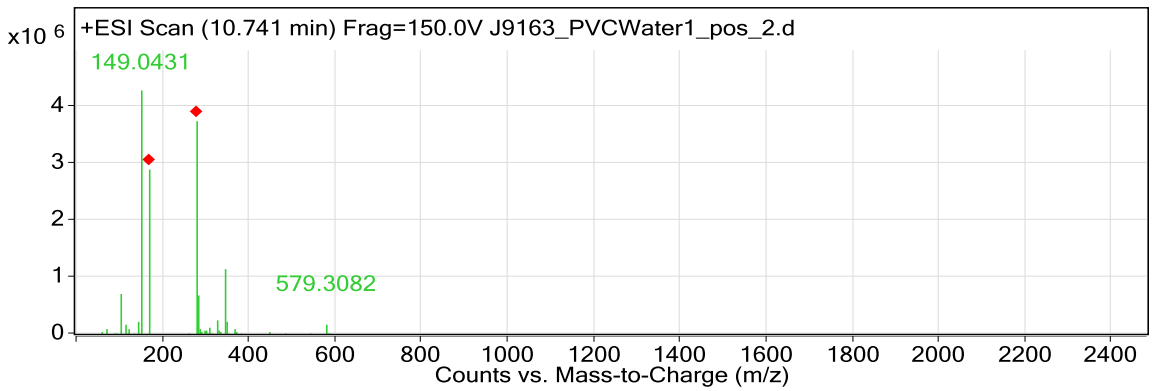
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
345.2642	344.257	C19 H36 O5	98.42	-1.99	C19 H37 O5

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

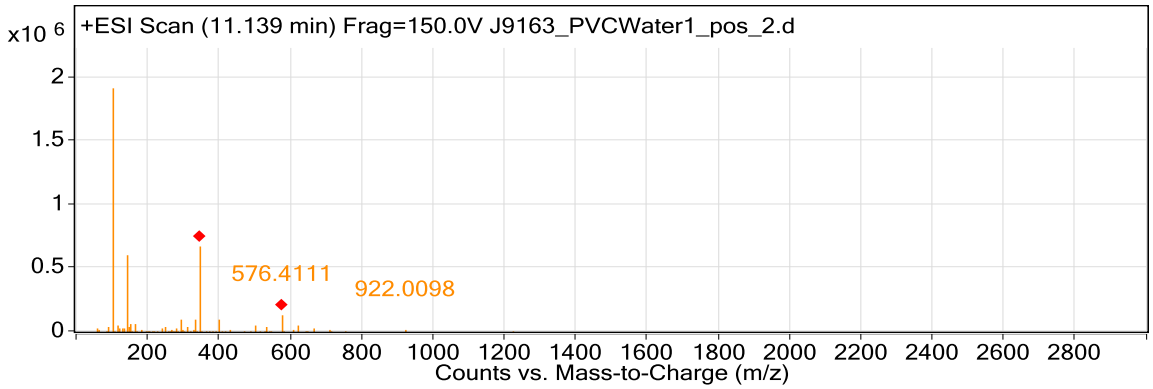


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.

277.2367	276.2297	C15 H32 O4	80.41	1.25	C15 H33 O4
279.1802	278.1731	C13 H26 O6	95.43	-0.47	C13 H27 O6
289.1656	288.1583	C14 H24 O6	80.13	-3.6	C14 H25 O6
289.1656	266.1764	C12 H26 O6	57.78	-12.93	C12 H26 Na O6
284.2102	266.1761	C12 H26 O6	62.29	-12	C12 H30 N O6
277.2367	248.1984	C13 H28 O4	80.41	1.39	C15 H33 O4
279.1802	250.1418	C11 H22 O6	95.43	-0.52	C13 H27 O6
289.1656	260.127	C12 H20 O6	80.13	-3.99	C14 H25 O6
277.2367	236.1984	C12 H28 O4	80.41	1.46	C15 H33 O4
279.1802	238.1418	C10 H22 O6	95.43	-0.55	C13 H27 O6
289.1656	248.127	C11 H20 O6	80.13	-4.18	C14 H25 O6

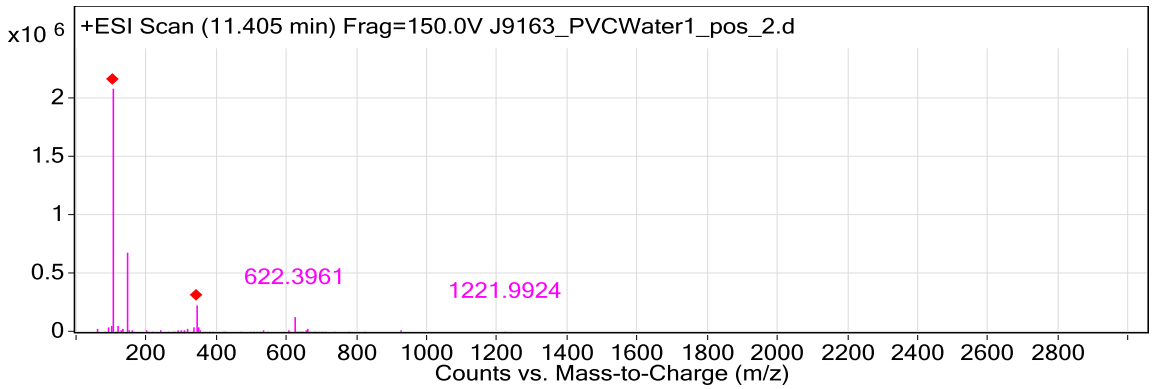
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
327.2527	326.2457	C19 H34 O4	73.4	-0.04	C19 H35 O4
349.2336	326.2434	C19 H34 O4	50.98	6.95	C19 H34 Na O4
344.2807	326.2466	C19 H34 O4	95.25	-2.71	C19 H38 N O4

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

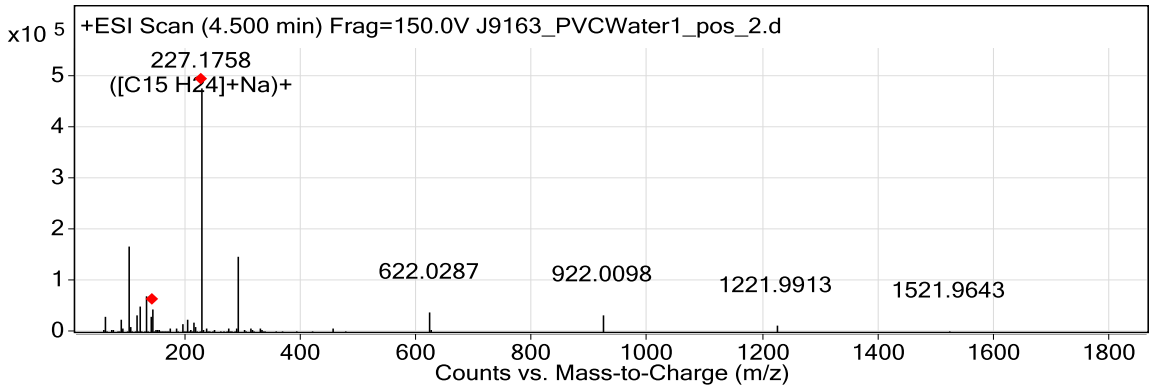


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
331.2843	330.2764	C19 H38 O4	87.68	1.85	C19 H39 O4
345.2307	344.2216	C18 H32 O6	58.57	-4.92	C18 H33 O6
349.1815	348.1746	C23 H24 O3	68.88	-5.8	C23 H25 O3

349.1815	326.1926	C14 H30 O8	65.88	4.47	C14 H30 Na O8
344.391	326.3568	C22 H46 O	69.96	-6	C22 H50 N O
344.2265	326.1926	C14 H30 O8	82.03	4.55	C14 H34 N O8
331.2843	302.2451	C17 H34 O4	87.68	2.03	C19 H39 O4
345.2307	316.1903	C16 H28 O6	58.57	-5.36	C18 H33 O6
349.1815	320.1433	C21 H20 O3	68.88	-6.31	C23 H25 O3
331.2843	290.2451	C16 H34 O4	87.68	2.11	C19 H39 O4
345.2307	304.1903	C15 H28 O6	58.57	-5.57	C18 H33 O6
349.1815	308.1433	C20 H20 O3	68.88	-6.55	C23 H25 O3

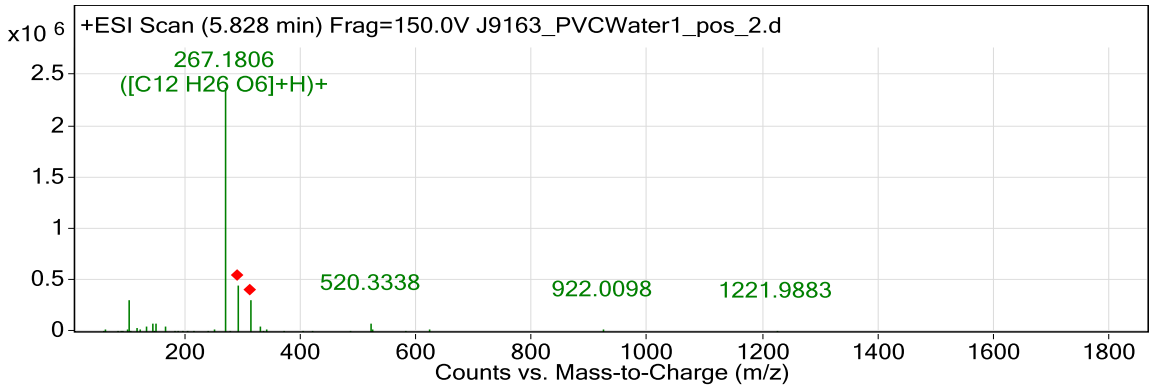
Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
227.1758	204.1865	C15 H24	87.88	6.5	C15 H24 Na

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

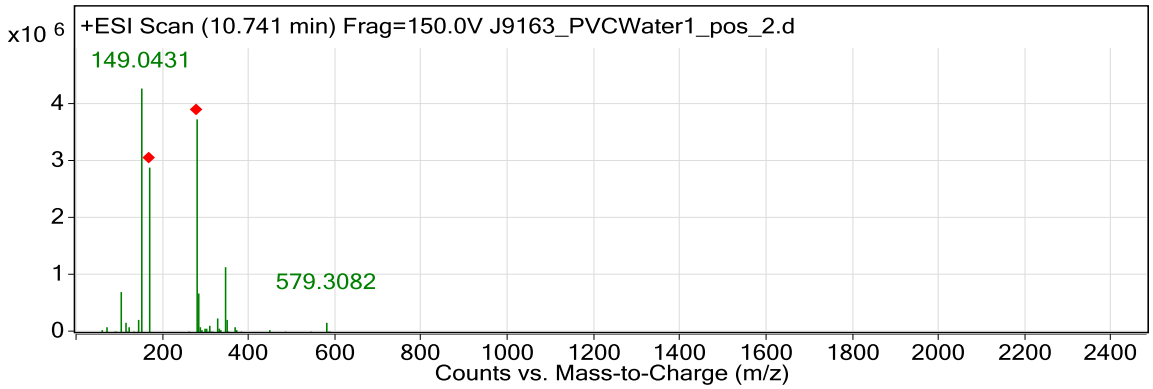


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
267.1806	266.1734	C12 H26 O6	98.82	-1.72	C12 H27 O6
289.1631	266.1738	C12 H26 O6	96.22	-3.25	C12 H26 Na O6

Fragmentor Voltage 150 **Collision Energy** 0 **Ionization Mode** ESI

Qualitative Analysis Report

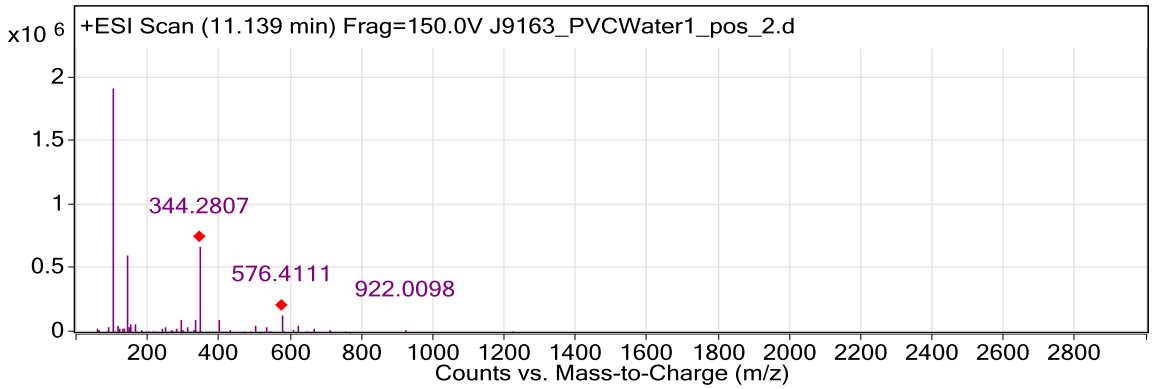


MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
277.2367	276.2297	C15 H32 O4	80.41	1.25	C15 H33 O4
279.4898	556.9681	C15 H11 N9 O7 S4	77.71	-2.94	C15 H13 N9 O7 S4
279.5724	557.1258	C22 H15 N13 O6	66.22	1.9	C22 H17 N13 O6
279.8475	278.8402	C4 Cl3 N O3 S2	37.78	-6.15	C4 H Cl3 N O3 S2
279.1802	278.1731	C13 H26 O6	95.43	-0.47	C13 H27 O6
284.2102	283.2028	C13 H25 N5 O2	74.22	-6.85	C13 H26 N5 O2
289.1656	288.1584	C15 H20 N4 O2	80.3	0.83	C15 H21 N4 O2
295.2477	294.2404	C16 H30 N4 O	39.76	5.27	C16 H31 N4 O
296.2461	295.2388	C15 H29 N5 O	39.27	-5.44	C15 H30 N5 O
297.2622	296.2555	C19 H36 S	79.4	-5.94	C19 H37 S
301.23	300.223	C16 H32 N2 O S	73.63	1.86	C16 H33 N2 O S
301.162	300.1547	C11 H20 N6 O4	82.19	-0.4	C11 H21 N6 O4
309.2633	308.2561	C17 H32 N4 O	77.61	4.88	C17 H33 N4 O
313.257	312.2509	C12 H28 N10	66.64	-3.48	C12 H29 N10
324.238	323.2308	C15 H33 N O6	47.62	0.05	C15 H34 N O6
327.2739	326.2667	C13 H30 N10	93.26	-3.65	C13 H31 N10
331.2291	330.2218	C10 H30 N6 O6	45.28	2.62	C10 H31 N6 O6
332.2961	331.2885	C22 H37 N O	91.17	-3.08	C22 H38 N O
333.2223	332.2149	C24 H28 O	71.96	-2.73	C24 H29 O
345.2846	344.2774	C17 H36 N4 O3	94.45	3.88	C17 H37 N4 O3
349.2341	348.2272	C12 H29 Cl N10	83.42	-1.94	C12 H30 Cl N10
352.2673	351.2594	C21 H37 N O S	88.33	0.47	C21 H38 N O S
366.262	365.2547	C10 H31 N13 S	47.59	-0.28	C10 H32 N13 S
367.2646	366.2573	C19 H40 Cl2 N2	46.92	-1.35	C19 H41 Cl2 N2
368.2606	367.2539	C13 H33 N7 O5	88.31	1.24	C13 H34 N7 O5
380.2986	379.2902	C23 H41 N O S	80.22	1.73	C23 H42 N O S

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

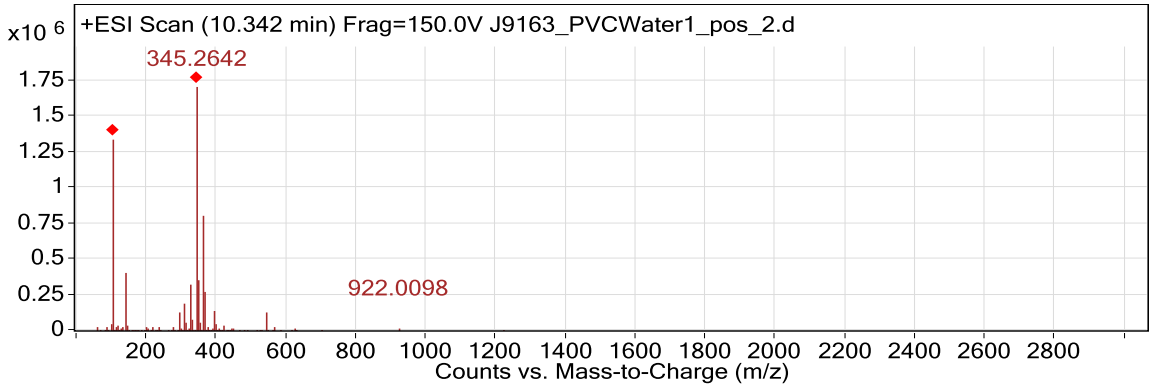
Qualitative Analysis Report



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
399.251	398.2436	C25 H34 O4	64.37	5.22	C25 H35 O4
405.2643	404.2571	C24 H36 O5	46.07	-1.92	C24 H37 O5
399.251	376.2617	C23 H36 O4	78.18	-0.86	C23 H36 Na O4

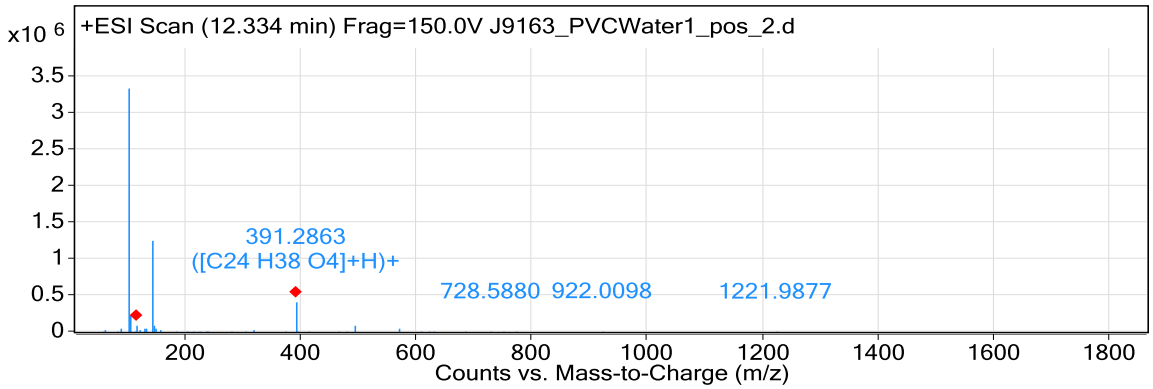
Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
390.319	372.2824	C28 H36	70.02	-1.95	C28 H40 N
396.235	378.2015	C21 H30 O6	76.99	7.36	C21 H34 N O6
406.3164	388.2823	C21 H40 O6	70.42	0.6	C21 H44 N O6

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



MFG Results

m/z	Mass	Best Match	Score	Diff.	Ion Form.
391.2863	390.279	C24 H38 O4	89.37	-4.97	C24 H39 O4

--- End Of Report ---