



CASE STUDY
Nylon Filter E&L Study

STUDY

The objective of this work was to investigate the extractable and leachables profile of the provided device.

ANALYTICAL STRATEGY

Multiple analytical techniques were employed including QTOF-LCMS, QTOF-GCMS, Headspace GCMS, HPLC, and ICP-MS. ISO 10993 guidelines were followed for this analysis.

CONCLUSIONS

A full list of the leachables (37°C, 72Hrs) and extractables (Soxhlet, 12 Hrs) recovered from the device is shown in **Table 2**.

Read the following report to see the full analysis.



Final Report

Company Name

Date:

Released by:
Dr. Mark Jordi
President
Jordi Labs LLC

Report Number: J#####

Company Name Confidential



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Date

| | |
|--------------|-------|
| Client Name | Email |
| Company Name | |
| Address | |

Dear Valued Client,

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

1 - Nylon syringe filter

The following tests were performed:

1. Headspace Gas Chromatography Mass Spectrometry (HGCMS)
2. Gas Chromatography Mass Spectrometry (GCMS)
3. Liquid Chromatography Mass Spectrometry (LCMS)
4. High Performance Liquid Chromatography (HPLC)
5. Inductively Coupled Plasma-Mass Spectrometry (ICP-MS)

Objective

The objective of this work was to investigate the extractable and leachables profile of the provided device. ISO 10993 guidelines were followed for this analysis.

Summary of Results

Leachables (37°C, 72Hrs) and extractables (Soxhlet, 12 Hrs) were recovered from the device using the indicated conditions. **Table 1** includes the gravimetric results for the exhaustive extraction.

| Table 1 Summary of Exhaustive Extraction Results | | |
|---|----------|-------------|
| Extraction | Solvent | Extractable |
| Exhaustive | Hexane | 0.66% |
| | Methanol | 268 ppm |

Both leachable and exhaustive extracts showed compounds consistent with various oligomers of Nylon 6. In addition to these compounds, the exhaustive extracts showed a number of additional compounds consistent with methyl esters of fatty acids, glycerol fatty acid esters and a variety of alkanes. The common polymer antioxidant Irgafos 168 was detected in the extracts as well. The majority of this compound was found in its oxidized form in the collected extracts.

| Table 2 Summary of Results | | | |
|--|--------------------|------------|----------------|
| Compound | Class/Purpose | CAS | Detected by |
| <i>Leachables</i> | | | |
| Caprolactam dimer | Oligomer | 56403-09-9 | LCMS |
| Adipic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| Caprolactam tetramer | Oligomer | 5834-63-9 | LCMS |
| Heptanedioic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| Caprolactam hexamer | Oligomer | -- | LCMS |
| Octanedioic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| Na | Ion | -- | ICP-MS |
| Ca | Ion | -- | ICP-MS |
| Mg | Ion | -- | ICP-MS |
| <i>Exhaustive</i> | | | |
| Linear and Branched Alkanes | Additive/Oligomer | Var. | HGCMS, GC-QTOF |
| 1,4-Benzenedicarboxylic acid, dimethyl ester | Degradant | 120-61-6 | GC-QTOF |
| Methyl palmitate | Additive | 112-39-0 | GC-QTOF, LCMS |
| Methyl stearate | Additive | 112-61-8 | GC-QTOF, LCMS |
| Octadecanitrile | Additive Degradant | 638-65-3 | GC-QTOF |
| Oxidized Irgafos 168 | Additive | -- | GC-QTOF, LCMS |
| Phenol, 2,4-bis(1,1-dimethylethyl)- | Additive degradant | 96-76-4 | GC-QTOF |
| Glycerol 1-palmitate | Additive | 542-44-9 | GC-QTOF, LCMS |
| Glycerol Stearate | Additive | 123-94-4 | GC-QTOF, LCMS |
| Irgafos 168 | Antioxidant | 31570-04-4 | GC-QTOF, LCMS |
| Caprolactam dimer | Oligomer | 56403-09-9 | LCMS |
| Adipic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| Caprolactam tetramer | Oligomer | 5834-63-9 | LCMS |
| Heptanedioic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| Caprolactam hexamer | Oligomer | -- | LCMS |
| Octanedioic acid – Nylon 6 dimer | Polymer degradant | -- | LCMS |
| $C_{21}H_{38}N_2O_8$ | -- | -- | LCMS |
| $C_{20}H_{36}N_2O_7$ | -- | -- | LCMS |
| caprolactam octamer | Oligomer | -- | LCMS |
| caprolactam decamer | Oligomer | -- | LCMS |
| Stearic acid | Additive | 57-11-4 | LCMS |
| $C_{35}H_{71}NO_3$ | -- | -- | LCMS |
| $C_{36}H_{72}N_2O_2$ | -- | -- | LCMS |
| $C_{38}H_{76}N_2O_2$ | -- | -- | LCMS |
| $C_{42}H_{85}NO$ | -- | -- | LCMS |

Table 2
Summary of Results

| Compound | Class/Purpose | CAS | Detected by |
|-----------------------------|---------------|------------|-------------|
| Distearylamine | | 112-99-2 | LCMS |
| Glycerol distearate | Additive | 1323-83-7 | LCMS |
| Glycerol stearate palmitate | Additive | 29593-61-1 | LCMS |

Next Steps

This report details the identification of the extractables and leachables profiles from the device. Following identification, quantification of the amounts of each component would now be performed.

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.

Equipment and Materials

| <i>Solvents</i> | |
|----------------------------|--|
| Methanol | Pharmco HPLC Grade; Lot C1404116; Batch 14104-1 |
| Hexane | Pharmco Reagent ACS Grade; Lot PB005810HX95; Batch 13247-30 |
| Water | Distilled, deionized water; generated by Symbron Barnstead P/N 16508 Reverse Osmosis DI water system |
| Saline | 0.9% in distilled water (NaCl, Sigma Aldrich; Lot# MKBF1522V) |
| <i>Consumables</i> | |
| Extraction Thimbles | Whatman #2800-432, Lot 1300926 |
| <i>Instrumentation</i> | |
| GC-QTOF | Agilent 7200 QTOF Mass Spectrometer, Agilent 7890B GC |
| ICP-MS | Perkin Elmer Elan DRC II equipped with a Cetac ASX-520 autosampler |
| LCMS | Agilent 6520 QTOF LCMS with Agilent 1200 HPLC system |
| HGCMS | Agilent 7694 Headspace sampler Agilent 5890 GC, Agilent 5972 MSD |
| Solvent Evaporation System | Genevac Rocket 4D |

Sample Preparation

Leachables

The provided devices were subject to leachables testing in water and saline solutions. The extractions were performed at 37°C ($\pm 1^\circ\text{C}$) for a total of 72 hours. The extracts were agitated through the use of a shaker oven. Extractions were performed in borosilicate glass vials (40 ml)

with PTFE lined caps. Because borosilicate glasses will inevitably introduce contamination of silicon and boron, extractions intended for analysis by ICP-MS were extracted in polypropylene (50 ml) vials. Samples were cut such that they would fit into the vials and ensure complete submersion of the entire device. Because the samples represent irregular molded parts, the solvent volume was chosen based on mass. **Table 3** includes the specific extraction parameters.

| Table 3 Summary of Extraction Parameters Leachables | | | | |
|--|----------|-----------------|---------------------|----------------------|
| Sample | Mass (g) | Solvent | Solvent Volume (ml) | Solvent Ratio (g/ml) |
| Nylon syringe filter | 6.4964 | Water | 32 | 0.203 |
| | 6.6282 | Saline | 32 | 0.207 |
| | 6.4615 | Water (ICP-MS) | 32 | 0.202 |
| | 6.3151 | Saline (ICP-MS) | 32 | 0.197 |

Exhaustive

Exhaustive extractions of the devices were performed using Soxhlet extraction. Extractions were performed in polar (methanol) and non-polar (n-hexane) solvents. The extractions were allowed to continue for 12 hours. A volume of 300 ml was used for each solvent. Specific extraction parameters are summarized in **Table 4**. The extract was concentrated via vacuum assisted evaporation, followed by complete drying at room temperature under a stream of nitrogen.

| Table 4 Summary of Extraction Parameters Exhaustive | | | |
|--|----------|----------|---------------------|
| Sample | Mass (g) | Solvent | Solvent Volume (ml) |
| Nylon syringe filter | 6.3200 | Hexane | 300 |
| | 6.4111 | Methanol | 300 |

Following the initial extraction, the extract solvent was replaced and the extraction was continued using fresh solvent. By definition (ISO 10993-12:2012(E)), an extraction is exhaustive if repeat extraction produces less than 10% of the original extracted amount measured gravimetrically. The repeat extraction was allowed to continue for 12 hours, after which the extract was concentrated in the same manner as the original extraction. **Table 5** includes a comparison of the gravimetric data collected from the initial and subsequent extractions.

| Table 5 Summary of Extraction Parameters Exhaustive | | | | | | | | |
|--|----------------------------|------------------------|----------------------------|---------------------------------|----------------------------|---------------------------------|----------------------------|---------------------------------|
| Sample | 1 st Extraction | | 2 nd Extraction | | 3 rd Extraction | | 4 th Extraction | |
| | Solvent | Extractables Mass (mg) | Extract Mass (mg) | % of 1 st Extraction | Extract Mass (mg) | % of 1 st Extraction | Extract Mass m(g) | % of 1 st Extraction |
| Nylon syringe filter | Hexane | 27.988 | 8.432 | 30.1 | 4.286 | 15.3 | 1.038 | 3.7 |
| | Methanol | 1.228 | 0.492 | 40.0* | -- | -- | -- | -- |

* - The mass of the 2nd methanol extract is within the variability of the balance, and is therefore considered complete following the 1st extraction.

HGCMS

The sample was analyzed directly by HGCMS in order to investigate the volatile components which were evolved. **Figure 1** includes the chromatograms collected. The mass spectra observed were searched against the NIST mass spectral database. The resulting best matching compounds are summarized in **Table 6**.

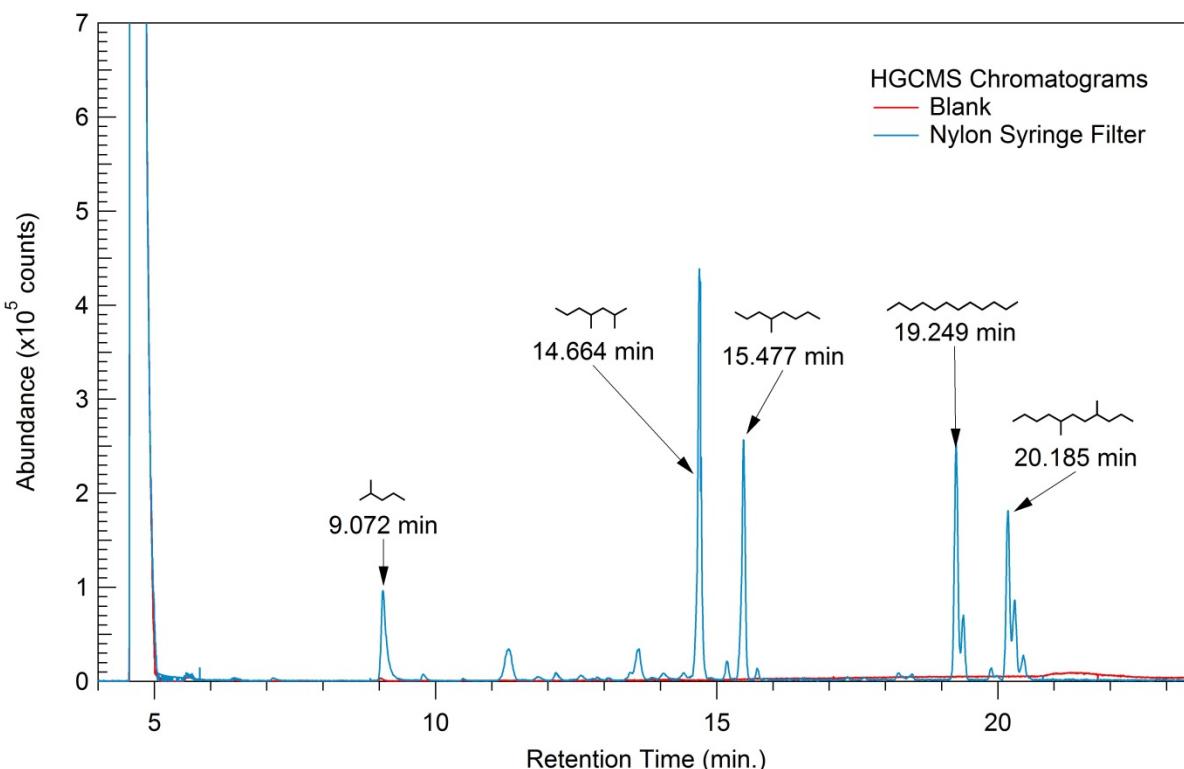


Figure 1 - Overlay of HGCMS chromatograms collected.

Table 6
Summary of HGCMS Results

| RT | Best Match | Score | CAS |
|--------|------------------------------|-------|-------------|
| 9.077 | 2-methylpentane | 880 | 107-83-5 |
| 9.789 | hexane | 928 | 110-54-3 |
| 11.298 | 4,6-dimethyldodecane | 899 | 61141-72-8 |
| 13.591 | 2,3,5,8-tetramethyldecanoate | 892 | 192823-15-7 |
| 14.664 | 2,4-dimethylheptane | 925 | 2213-23-2 |
| 15.187 | 2,4-dimethyl-1-heptene | 860 | 19549-87-2 |
| 15.477 | 4-methyloctane | 943 | 2216-34-4 |
| 15.726 | 2,4-dimethylhexane | 872 | 589-43-5 |
| 19.249 | dodecane | 880 | 112-40-3 |
| 19.397 | 3,5-dimethyloctane | 883 | 15869-93-9 |
| 19.880 | 2-methyl-2-undecanethiol | 781 | 10059-13-9 |
| 20.185 | 4,7,dimethylundecane | 884 | 17301-32-5 |
| 20.292 | undecane | 893 | 1120-21-4 |
| 20.449 | 2,3,6,7-tetramethyloctane | 878 | 52670-34-5 |

GC-QTOF

Leachables

The water and saline leachable extracts were subjected to liquid-liquid extraction in dichloromethane (DCM). A 5 mL aliquot of the prepared extract was added to 5 mL of DCM. The solution was agitated for approximately 2 minutes followed by removal of the DCM layer. This procedure was repeated three (3) times and each of the collected DCM extracts were combined. The resulting DCM extract solution was dried with gentle heating under a stream of nitrogen, followed by reconstitution in 5 mL of freshly distilled DCM.

The collected extracts were analyzed by GC-QTOF. There we no unique compounds detected in the leachables extracts by GC-QTOF.

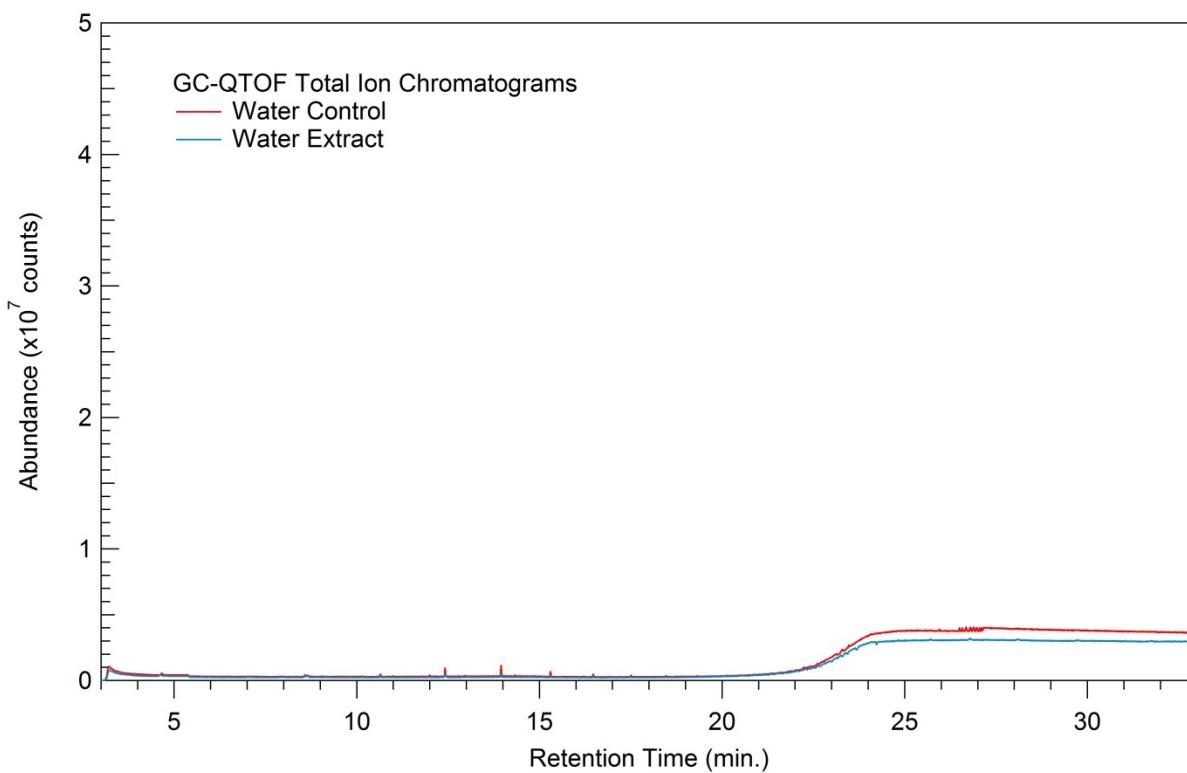


Figure 2 – GC-QTOF chromatograms collected from the leachables extraction performed with water.

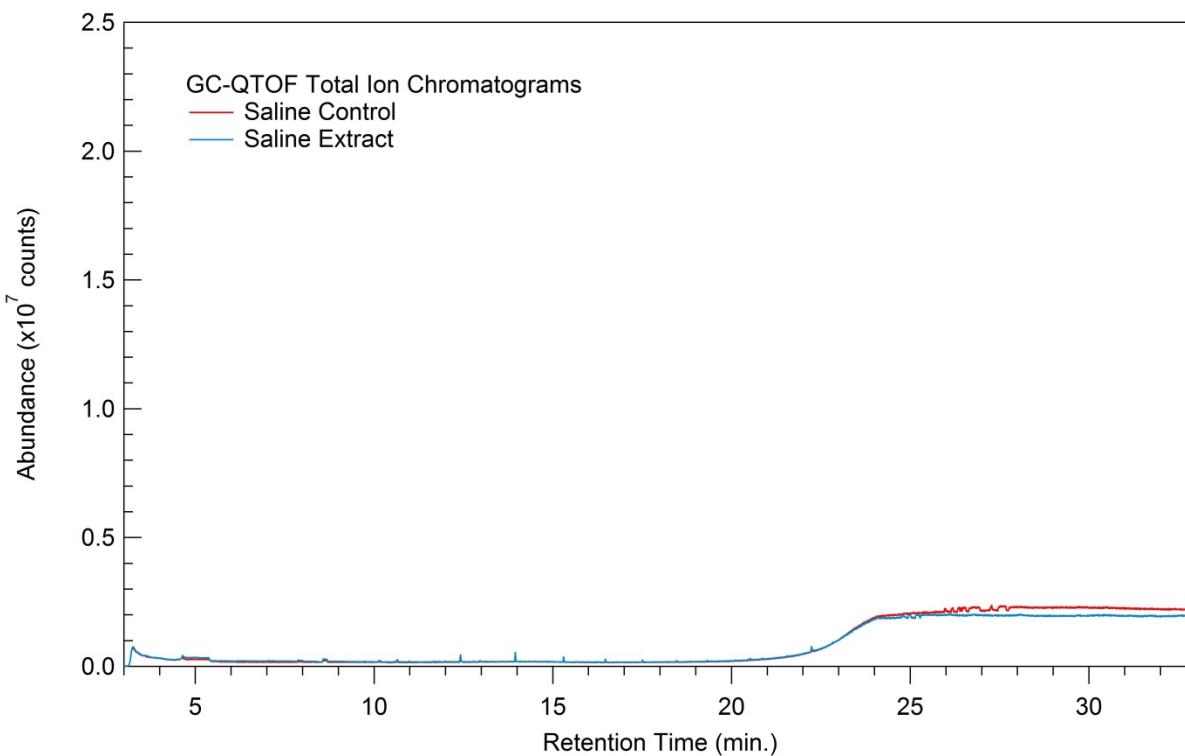


Figure 3 – GC-QTOF chromatograms collected from the leachables extraction performed with saline.

Exhaustive

The dried methanol extract was reconstituted in 2 mL of fresh solvent prior to analysis by GCMS. The hexane extract was reconstituted in 50 mL of fresh solvent prior to analysis. In each case, the control extract was reconstituted in the same solvent volume.

Several compounds observed in the extracts are not well matched by the NIST mass spectral database. In many cases, the accurate mass data collected from the GC-QTOF allows determination of molecular formulas using the molecular formula generation (MFG) algorithm. Determination of the molecular formulas of the fragments observed in the electron impact (EI) mass spectra collected allows determination of likely structures.

A variety of alkanes are detected in the hexane extract. Electron impact (EI) mass spectra of higher molecular weight alkanes show minimal differences, making definitive identification of these components difficult even with accurate mass data. However, the mass spectra observed are easily identified as saturated alkanes. Determination of their chain length could be performed via a soft ionization technique such as chemical ionization.

Table 7
Summary of GCMS Results – Methanol Extract

| RT | Best Match | Score | CAS | ID type |
|--------|--|-------|----------|----------|
| 14.046 | 1,4-Benzenedicarboxylic acid, dimethyl ester | 871 | 120-61-6 | NIST |
| 14.096 | Phenol, 2,4-bis(1,1-dimethylethyl)- | 861 | 96-76-4 | NIST |
| 17.181 | Methyl palmitate | 699 | 112-39-0 | NIST/MFG |

Table 7
Summary of GCMS Results – Methanol Extract

| RT | Best Match | Score | CAS | ID type |
|--------|-------------------------------------|-------|-----------|---------|
| 17.775 | 9-Octadecen-1-ol, (Z)- | 807 | 143-28-2 | NIST |
| 18.249 | Methyl stearate | 783 | 112-61-8 | NIST |
| 18.386 | Octadecanitrile | 853 | 638-65-3 | NIST |
| 18.762 | Eicosane, 2-methyl- | 798 | 1560-84-5 | NIST |
| 19.316 | 1,8-Diazacyclotetradecane-2,9-dione | 573 | 5776-79-4 | NIST |
| 26.815 | Oxidized Irgafos 168 | -- | -- | MFG |

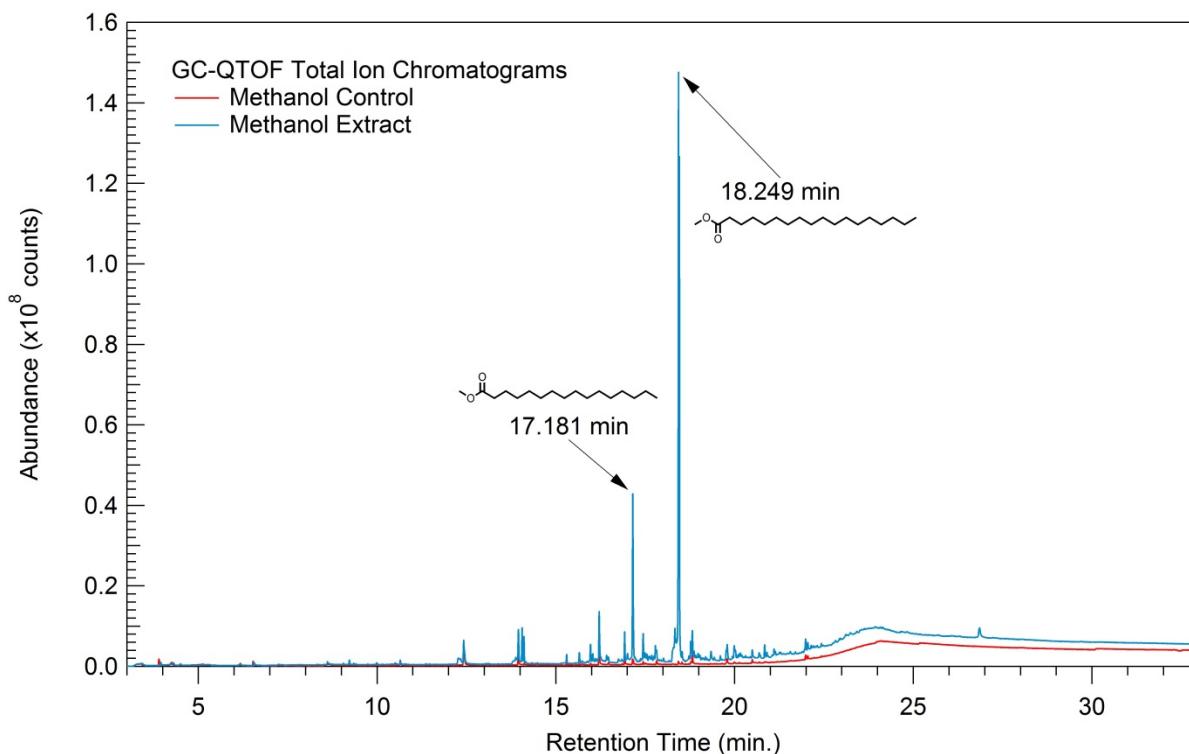


Figure 4 – GC-QTOF chromatograms collected from the methanol extract and associated control.

Table 8
Summary of GCMS Results – Hexane Extract

| RT | Best Match | Score | CAS | ID type |
|--------|---|-------|------------|---------|
| 11.982 | Hexadecane | 849 | 544-76-3 | NIST |
| 14.083 | Phenol, 2,4-bis(1,1-dimethylethyl)- | 812 | 96-76-4 | NIST |
| 14.302 | Heptacosane | 843 | 593-49-7 | NIST |
| 14.392 | Dodecane, 2,6,11-trimethyl- | 847 | 31295-56-4 | NIST |
| 15.638 | Eicosane, 2-methyl- | 851 | 1560-84-5 | NIST |
| 15.950 | Octadecane, 3-ethyl-5-(2-ethylbutyl)- | 622 | 55282-12-7 | NIST |
| 16.400 | Pentadecanal | 839 | 2765-11-9 | NIST |
| 17.135 | Heptacosane | 817 | 593-49-7 | NIST |
| 17.524 | Heptadecane, 2,6,10,15-tetramethyl- | 823 | 54833-46-6 | NIST |
| 17.772 | 1-Octadecyne | 840 | 629-89-0 | NIST |
| 18.555 | Heptacosane | 842 | 593-49-7 | NIST |
| 19.750 | Ethanol, 2-(octadecyloxy)- | 679 | 2136-72-3 | NIST |
| 19.948 | 1,7-Dimethyl-4-(1-methylethyl)cyclododecane | 718 | 645-10-3 | NIST |

Table 8
Summary of GCMS Results – Hexane Extract

| RT | Best Match | Score | CAS | ID type |
|--------|-------------------------------------|-------|------------|---------|
| 20.605 | Glycerol 1-palmitate | 774 | 542-44-9 | NIST |
| 20.887 | Octadecane, 2-methyl- | 849 | 1560-88-9 | NIST |
| 21.089 | Octacosane | 777 | 630-02-4 | NIST |
| 21.656 | Glycerol Stearate | 736 | 123-94-4 | NIST |
| 21.941 | Heptadecane, 2,6,10,15-tetramethyl- | 760 | 54833-48-6 | NIST |
| 22.915 | Heptacosane | 832 | 593-49-7 | NIST |
| 23.110 | Octadecane, 2-methyl- | 793 | 1560-88-9 | NIST |
| 24.110 | Octacosane | 747 | 630-02-4 | NIST |
| 25.291 | Irgafos 168 | -- | 31570-04-4 | MFG |
| 26.913 | Oxidized Irgafos 168 | -- | -- | MFG |

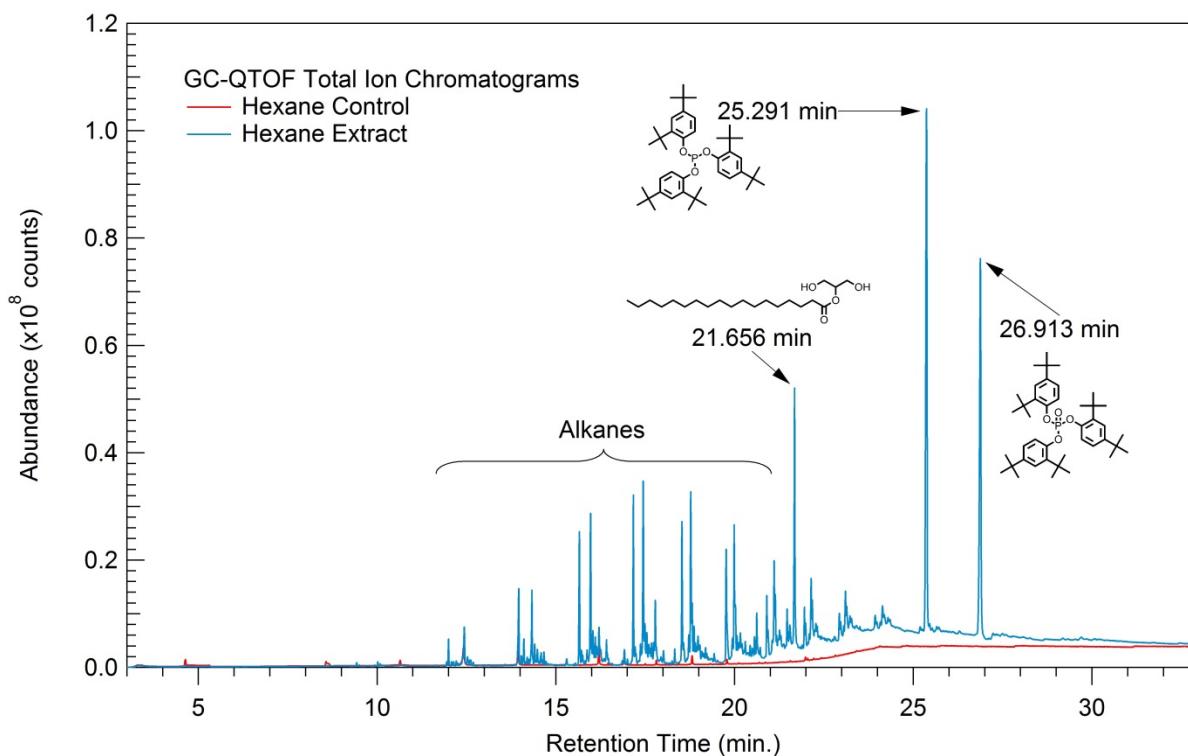


Figure 5 – GC-QTOF chromatograms collected from the hexane extract and associated control.

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⁺, NH₄⁺ 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

Leachables

The extracts prepared were analyzed directly by LCMS with no further sample preparation. **Tables 9** and **10** include a summary of the compounds detected in the water and saline leachables extracts.

Table 9
Summary of LCMS Results
Leachables - Water

| RT | Positive m/z | Negative m/z | Mass | Best Match | Score | Diff. | Possible ID | ID type |
|-----|--------------|--------------|----------|---|-------|-------|-----------------------------------|---------|
| 4.4 | 227.1757 | | 226.1684 | C ₁₂ H ₂₂ N ₂ O ₂ | 98.94 | -1.3 | caprolactam dimer | DB |
| 6.2 | 373.2335 | | 372.2262 | C ₁₈ H ₃₂ N ₂ O ₆ | 99.2 | 0.44 | adipic acid – Nylon 6 dimer | MFG |
| 6.5 | 453.3452 | | 452.3377 | C ₂₄ H ₄₄ N ₄ O ₄ | 93.14 | -3.2 | caprolactam tetramer | DB |
| 6.9 | 387.2499 | | 386.2425 | C ₁₉ H ₃₄ N ₂ O ₆ | 96.79 | -2.06 | heptanedioic acid – Nylon 6 dimer | MFG |
| 7.3 | 679.5131 | | 678.5056 | C ₃₆ H ₆₆ N ₆ O ₆ | 95.7 | -1.85 | caprolactam hexamer | DB |
| 7.6 | 401.2651 | | 400.2573 | C ₂₀ H ₃₆ N ₂ O ₆ | 98.49 | -0.96 | octanedioic acid – Nylon 6 dimer | MFG |

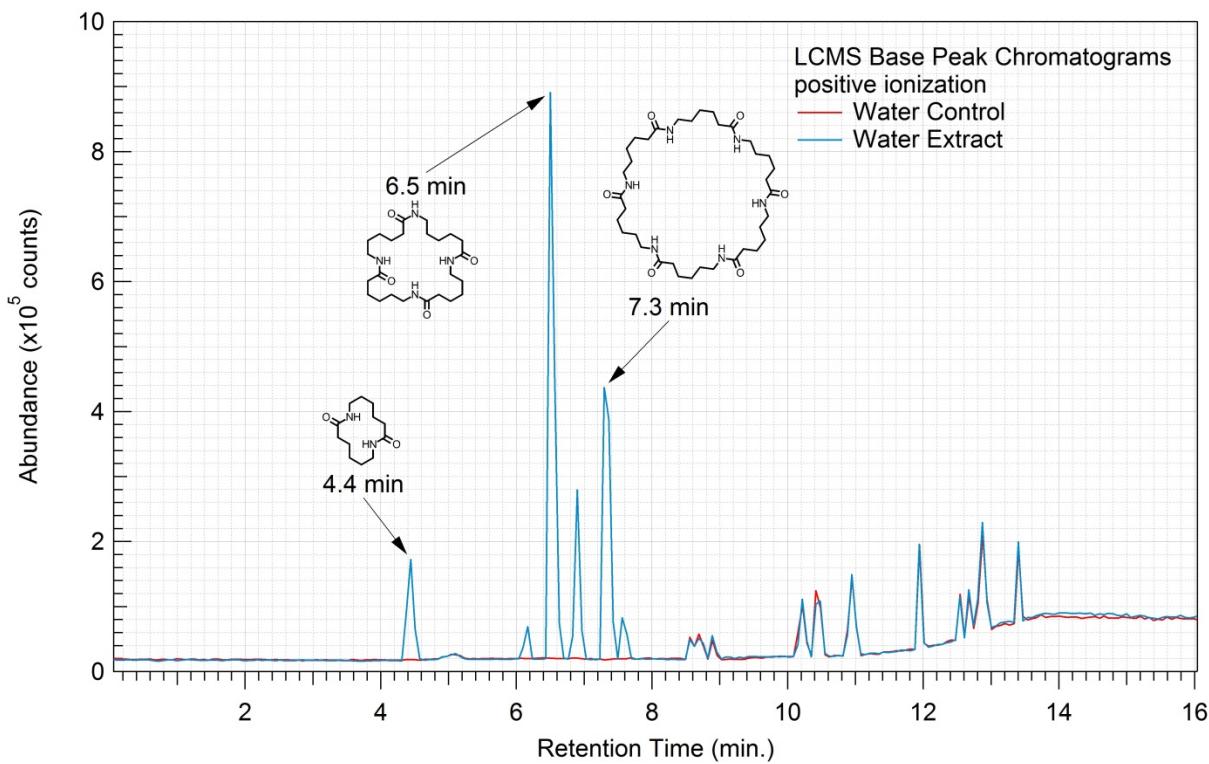


Figure 6 – LCMS base peak chromatograms, positive ionization.

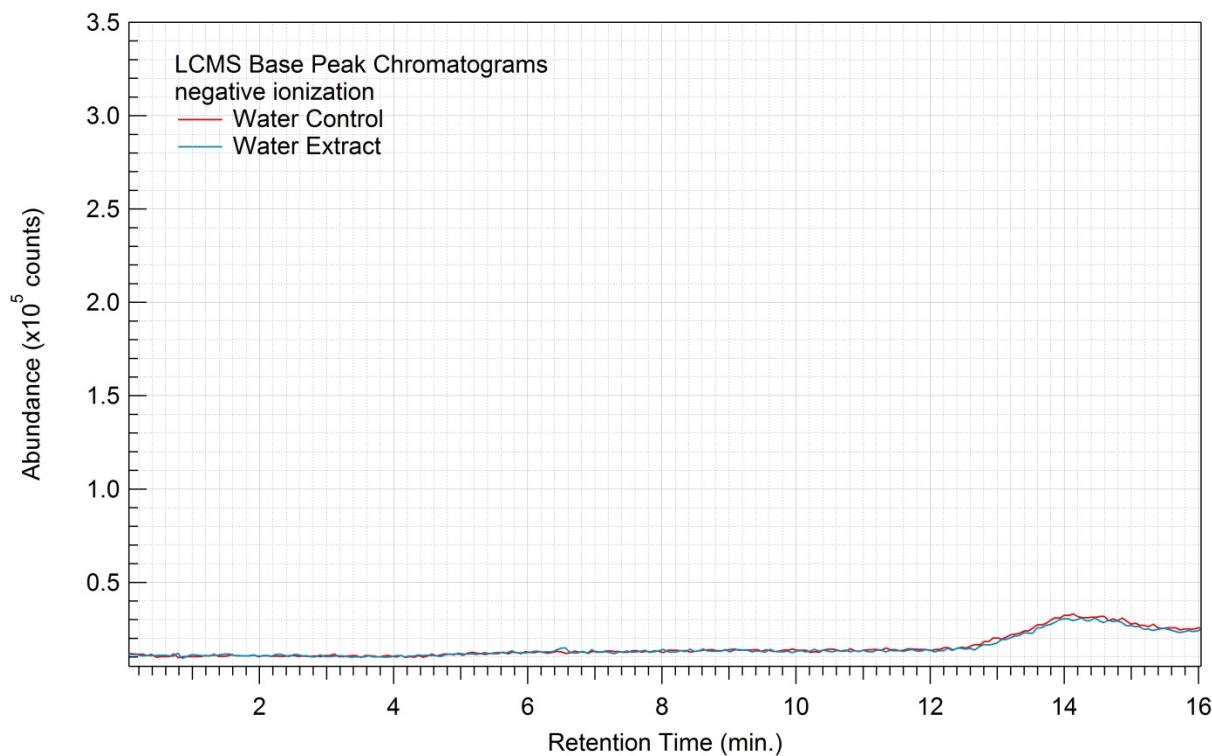


Figure 7 – LCMS base peak chromatograms, negative ionization.

Table 10
Summary of LCMS Results
Leachables – Saline

| RT | Positive m/z | Negative m/z | Mass | Best Match | Score | Diff. | Possible ID | ID type |
|-----|--------------|--------------|----------|---|-------|-------|-----------------------------------|---------|
| 4.5 | 227.1753 | | 226.1679 | C ₁₂ H ₂₂ N ₂ O ₂ | 97.97 | 1.06 | caprolactam dimer | DB |
| 6.2 | 373.2335 | | 372.2262 | C ₁₈ H ₃₂ N ₂ O ₆ | 99.34 | -0.35 | adipic acid – Nylon 6 dimer | MFG |
| 6.5 | 453.3438 | | 452.3365 | C ₂₄ H ₄₄ N ₄ O ₄ | 97.36 | -0.49 | caprolactam tetramer | DB |
| 6.9 | 387.2489 | | 286.2416 | C ₁₉ H ₃₄ N ₂ O ₆ | 99.36 | 0.35 | heptanedioic acid – Nylon 6 dimer | MFG |
| 7.3 | 679.5134 | | 678.5058 | C ₃₆ H ₆₆ N ₆ O ₆ | 94.61 | -2.07 | caprolactam hexamer | DB |
| 7.6 | 401.2649 | | 400.2576 | C ₂₀ H ₃₆ N ₂ O ₆ | 99.3 | -0.56 | octanedioic acid – Nylon 6 dimer | MFG |

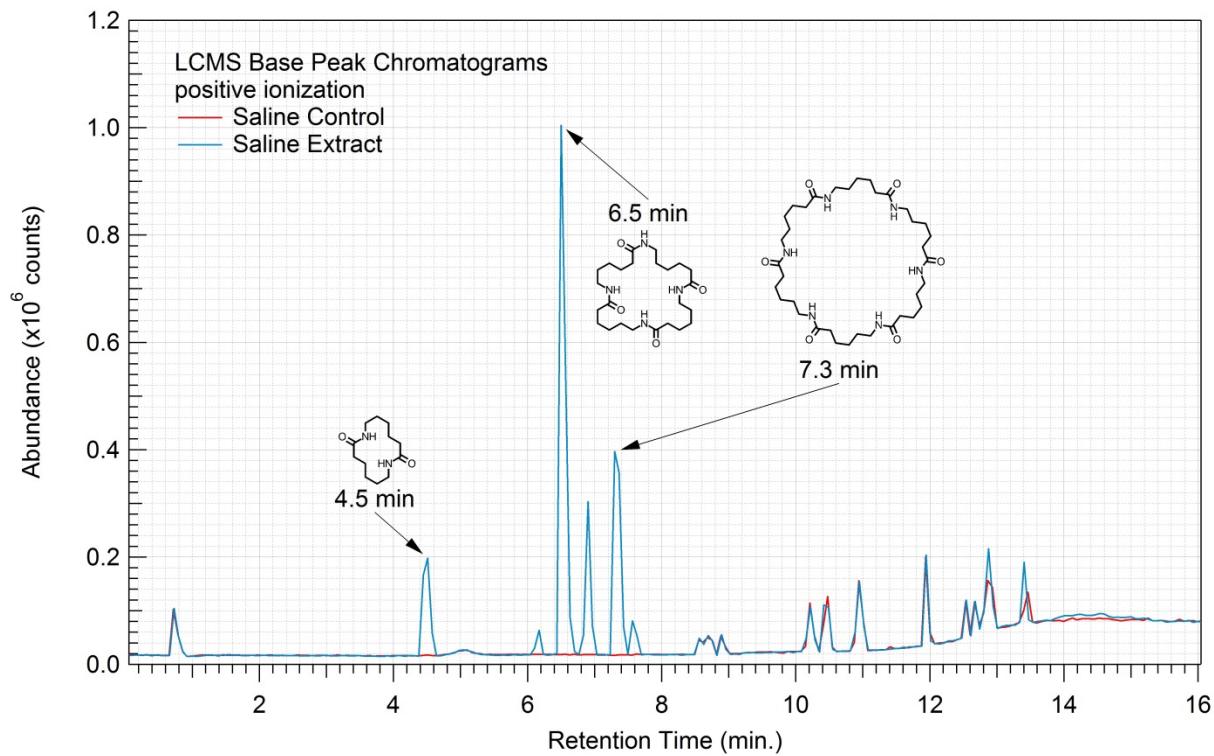


Figure 8 – LCMS base peak chromatograms, positive ionization.

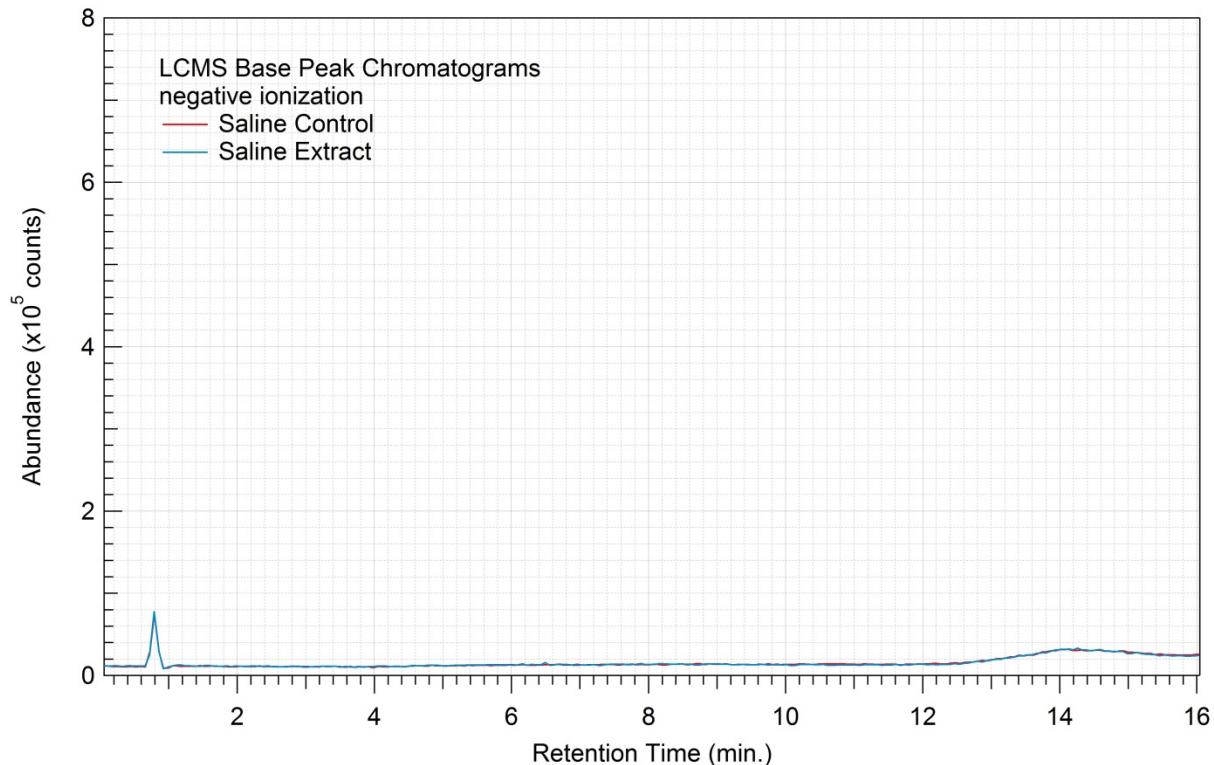


Figure 9 – LCMS base peak chromatograms, negative ionization.

Exhaustive

The methanol extract was analyzed following reconstitution in a 2 ml aliquot of freshly distilled methanol. The hexane extract was first reconstituted in 50 mL of freshly distilled hexane. A 1 mL portion of the extract solution was collected and taken to complete dryness under a stream of nitrogen. The residue was reconstituted in 1 mL of freshly distilled methanol for analysis by LCMS.

Table 11
Summary of LCMS Results
Exhaustive - Methanol

| RT | Positive <i>m/z</i> | Negative <i>m/z</i> | Mass | Best Match | Score | Diff. | Possible ID | ID type |
|------|------------------------|------------------------|----------|--|-------|-------|----------------------------------|---------|
| 4.4 | 227.1760 | | 226.1687 | C ₁₂ H ₂₂ N ₂ O ₂ | 98.01 | -2.69 | caprolactam dimer | DB |
| 6.0 | 447.2708 | | 446.2634 | C ₂₁ H ₃₈ N ₂ O ₈ | 97.87 | -1.39 | | MFG |
| 6.2 | 373.2342 | 371.2190 | 372.2268 | C ₁₈ H ₃₂ N ₂ O ₆ | 96.22 | -2.15 | adipic acid-Nylon 6 dimer | MFG |
| 6.2 | 439.2412 | | 416.2523 | C ₂₀ H ₃₆ N ₂ O ₇ | 97.46 | -0.14 | | MFG |
| 6.5 | 453.3449 | 487.3046 | 452.3376 | C ₂₄ H ₄₄ N ₄ O ₄ | 95.61 | -1.37 | caprolactam tetramer | DB |
| 6.9 | 387.2497 | 385.2351 | 386.2427 | C ₁₉ H ₃₄ N ₂ O ₆ | 95.84 | -2.5 | heptandioic acid – Nylon 6 dimer | MFG |
| 7.4 | 679.5133 | 723.5024 | 678.5059 | C ₃₆ H ₆₆ N ₆ O ₆ | 95.95 | -1.61 | caprolactam hexamer | DB |
| 7.6 | 401.2659 | 445.2551 | 400.2587 | C ₂₀ H ₃₆ N ₂ O ₆ | 95.09 | -3.41 | octanedioic acid – Nylon 6 dimer | MFG |
| 7.8 | 905.6794 | 949.6702 | 904.672 | C ₄₈ H ₈₈ N ₈ O ₈ | 99.24 | 0.6 | caprolactam octamer | MFG |
| 8.1 | 1131.8464 | | 1130.839 | C ₆₀ H ₁₁₀ N ₁₀ O ₁₀ | 93.07 | 1.45 | caprolactam decamer | MFG |
| 10.1 | 288.2909 | | 270.2569 | C ₁₇ H ₃₄ O ₂ | 92.03 | -1.41 | methyl palmitate | DB |
| 10.7 | 316.3217 | | 298.2878 | C ₁₉ H ₃₈ O ₂ | 97.06 | -0.74 | methyl stearate | DB |
| 12.7 | | 283.2645 | 284.2716 | C ₁₈ H ₃₆ O ₂ | 95.33 | -0.12 | stearic acid | DB |
| 13.3 | 554.5539 | | 553.5462 | C ₃₅ H ₇₁ N O ₃ | 84.24 | -5.05 | | MFG |
| 13.4 | | 609.5582 | 564.5596 | C ₃₆ H ₇₂ N ₂ O ₂ | 95.36 | -0.34 | acidic | MFG |
| 13.5 | | 637.5890 | 592.5904 | C ₃₈ H ₇₆ N ₂ O ₂ | 94.96 | 0.43 | acidic | MFG |
| 13.5 | 663.4574 | | 662.4501 | C ₄₂ H ₆₃ O ₄ P | 83.25 | -3.75 | oxidized Irgafos 168 | DB |
| 13.7 | 536.5786 | | 536.5786 | C ₃₆ H ₇₃ N O | 91.8 | -3.31 | N-stearylstearamide | MFG |
| 13.9 | 647.4606 | | 646.453 | C ₄₂ H ₆₃ O ₃ P | 95.43 | -1.88 | Irgafos 168 | DB |

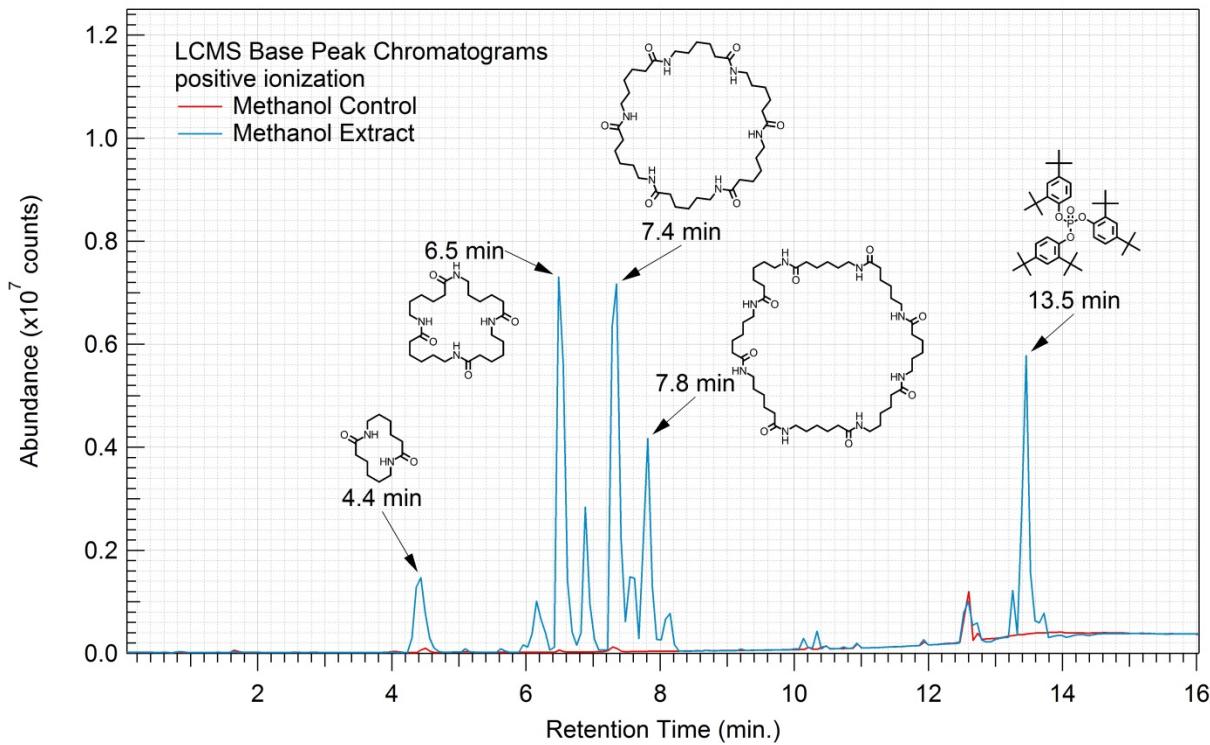


Figure 10 – LCMS base peak chromatograms, positive ionization.

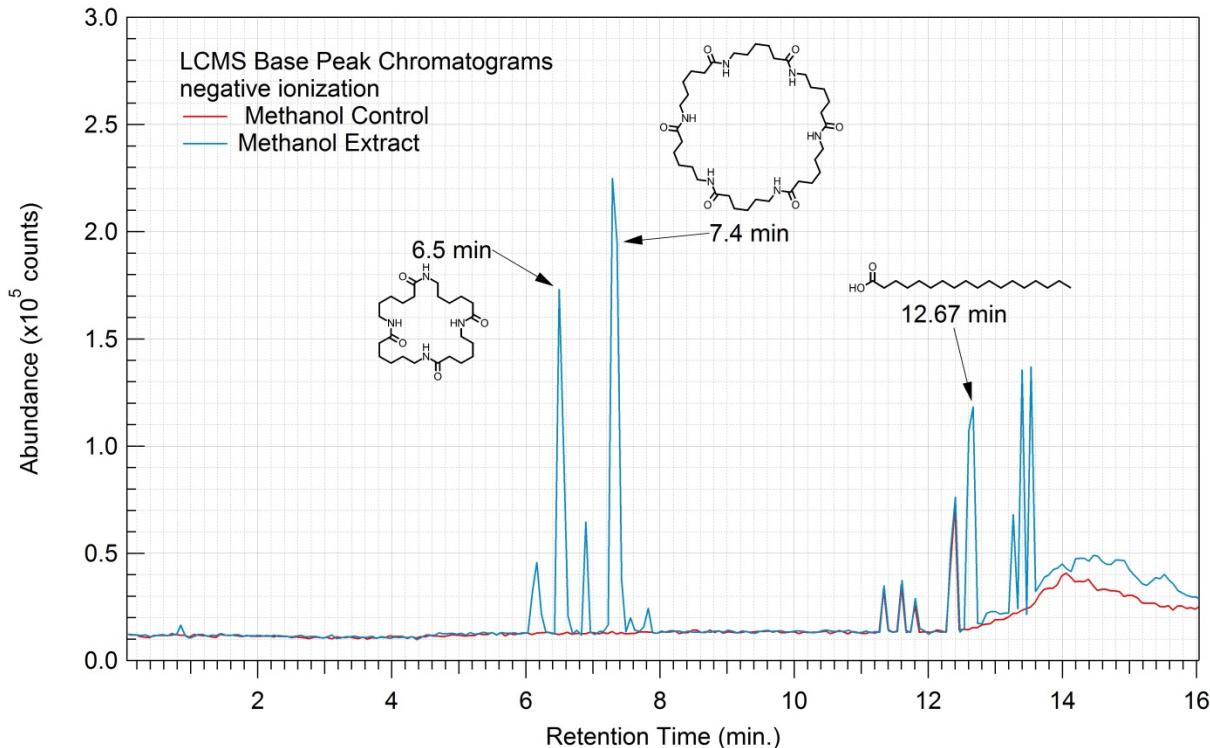


Figure 11 – LCMS base peak chromatograms, negative ionization.

Table 12
Summary of LCMS Results
Extractables - Hexane

| Extractables - Hexane | | | | | | | | |
|-----------------------|--------------|--------------|----------|--|-------|--------|-----------------------------|---------|
| RT | Positive m/z | Negative m/z | Mass | Best Match | Score | Diff. | Possible ID | ID type |
| 12.1 | 331.2862 | 375.2752 | 330.2788 | C ₁₉ H ₃₈ O ₄ | 89.69 | -1.94 | glycerol palmitate | DB |
| 12.5 | 376.3429 | 403.3079 | 358.3092 | C ₂₁ H ₄₂ O ₄ | 97.57 | -2.38 | glycerol stearate | DB |
| 12.7 | | 283.2645 | 284.2714 | C ₁₈ H ₃₆ O ₂ | 96.3 | -0.59 | stearic acid | DB |
| 12.7 | 554.5532 | | 553.5460 | C ₃₅ H ₇₁ NO ₃ | 88.79 | -4.67 | | MFG |
| 12.8 | 522.5982 | | | C ₃₆ H ₇₆ N | 97.5 | -1.73 | distearylamine | MFG |
| 13.5 | | 641.5369 | 596.5383 | C ₃₇ H ₇₂ O ₅ | 94.75 | -0.72 | glycerol stearate palmitate | DB |
| 13.5 | 663.4569 | | 662.4493 | C ₄₂ H ₆₃ O ₄ P | 86.54 | -3.22 | oxidized Irgafos 168 | DB |
| 13.7 | | 669.5692 | 624.5706 | C ₃₉ H ₇₆ O ₅ | 94.39 | --1.75 | glycerol distearate | DB |
| 13.7 | 637.7007 | | 619.6663 | C ₄₂ H ₈₅ NO | 84.00 | -5.11 | | MFG |
| 13.9 | 647.4620 | | 646.4547 | C ₄₂ H ₆₃ O ₃ P | 85.83 | -3.27 | Irgafos 168 | DB |

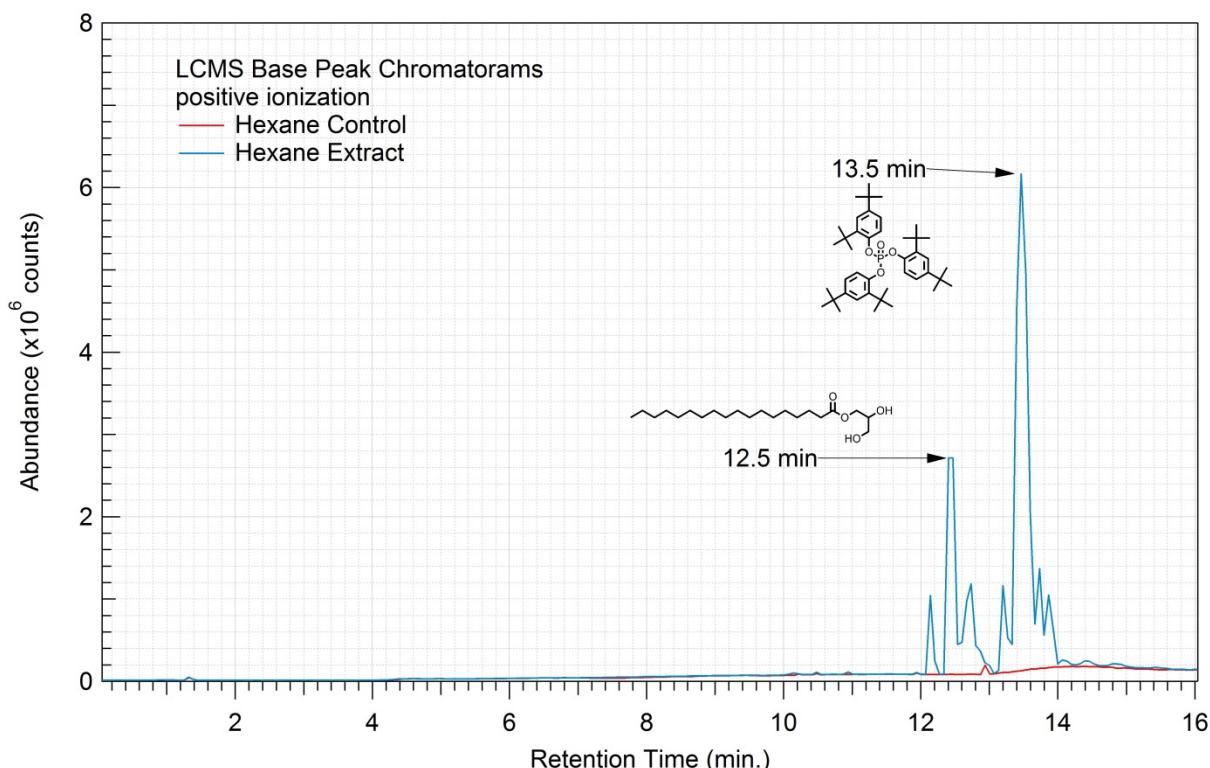


Figure 12 – LCMS base peak chromatograms, positive ionization.

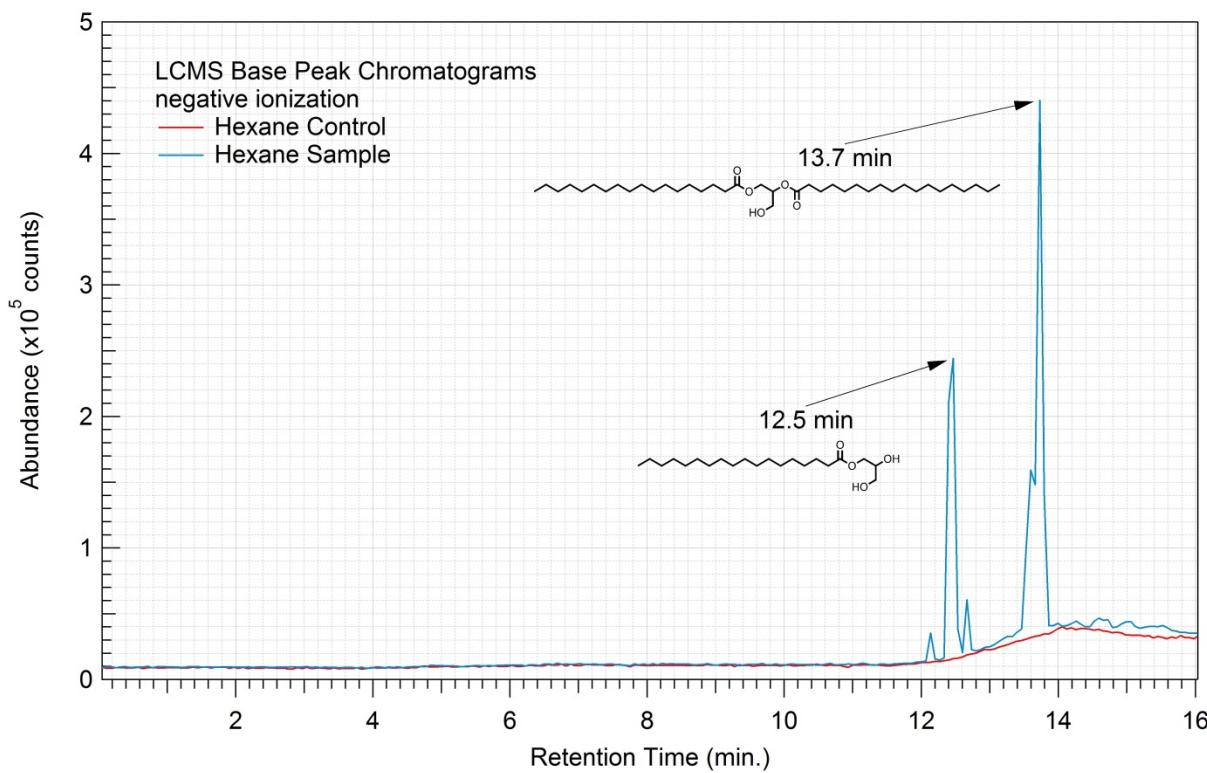


Figure 13 – LCMS base peak chromatograms, negative ionization.

ICP-MS

The leachables extracts prepared were analyzed by ICP-MS in order to investigate their inorganic content. The analysis performed is capable of simultaneous identification and quantification of the elements listed. In general, the instrument used is capable of a 10 µg/L detection limit for most elements. Specific detection limits, as well as the analytical results are listed in **Table 13**.

Table 13
ICP-MS Results

| Sample: | Control Water | Water Extract | | Control Saline | Saline Extract | |
|---------------------|---------------|---------------|------------------|----------------|----------------|--------|
| mass extracted (g): | -- | 6.4615 g | | -- | 6.3151 g | |
| Element | µg/L | µg/L | ppm ¹ | µg/L | µg/L | ppm |
| Li | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Be | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| B | 30 | 30 | 0.149 | 20 | 30 | 0.152 |
| Na | 150 | 230 | 1.14 | Matrix | Matrix | -- |
| Mg | 20 | 120 | 0.594 | 20 | 70 | 0.355 |

Table 13
ICP-MS Results

| Sample: | Control Water | Water Extract | | Control Saline | Saline Extract | |
|---------------------|---------------|---------------|------------------|----------------|----------------|--------|
| mass extracted (g): | -- | 6.4615 g | | -- | 6.3151 g | |
| Element | µg/L | µg/L | ppm ¹ | µg/L | µg/L | ppm |
| Al | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Si | < 100 | < 100 | < 0.5 | < 100 | < 100 | < 0.05 |
| P | < 100 | < 100 | < 0.5 | < 100 | < 100 | < 0.5 |
| K | < 100 | < 100 | < 0.5 | < 100 | < 100 | < 0.5 |
| Ca | < 100 | 960 | 4.75 | 120 | 530 | 2.69 |
| Sc | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ti | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| V | < 10 | < 10 | < 0.05 | 60 | 60 | 0.304 |
| Cr | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Mn | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Fe | < 100 | < 100 | < 0.5 | < 100 | < 100 | < 0.5 |
| Co | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ni | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Cu | < 10 | < 10 | < 0.05 | 20 | 20 | 0.101 |
| Zn | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ga | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ge | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| As | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Se | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Rb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Sr | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Y | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Zr | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Nb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Mo | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ru | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Rh | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Pd | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ag | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Cd | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| In | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Sn | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Sb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |

Table 13
ICP-MS Results

| Sample: | Control Water | Water Extract | | Control Saline | Saline Extract | |
|---------------------|---------------|---------------|------------------|----------------|----------------|--------|
| mass extracted (g): | -- | 6.4615 g | | -- | 6.3151 g | |
| Element | µg/L | µg/L | ppm ¹ | µg/L | µg/L | ppm |
| Te | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Cs | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ba | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| La | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ce | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Pr | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Nd | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Sm | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Eu | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Gd | < 10 | < 10 | < 0.05 | 40 | 30 | 0.152 |
| Tb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Dy | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ho | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Er | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Tm | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Yb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Lu | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Hf | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ta | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| W | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Re | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Os | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Ir | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Pt | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Au | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Hg | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Tl | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Pb | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Bi | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| Th | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |
| U | < 10 | < 10 | < 0.05 | < 10 | < 10 | < 0.05 |

¹ “ppm” refers to the calculated mass ratio in the original sample [(volume***µg/mL”)/ sample mass] where volume = 32 mL)

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

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

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,

Kevin Rowland

Kevin Rowland, M.S
Senior Chemist
Jordi Labs LLC

Mark Jordi

Mark Jordi, Ph. D.
President
Jordi Labs LLC

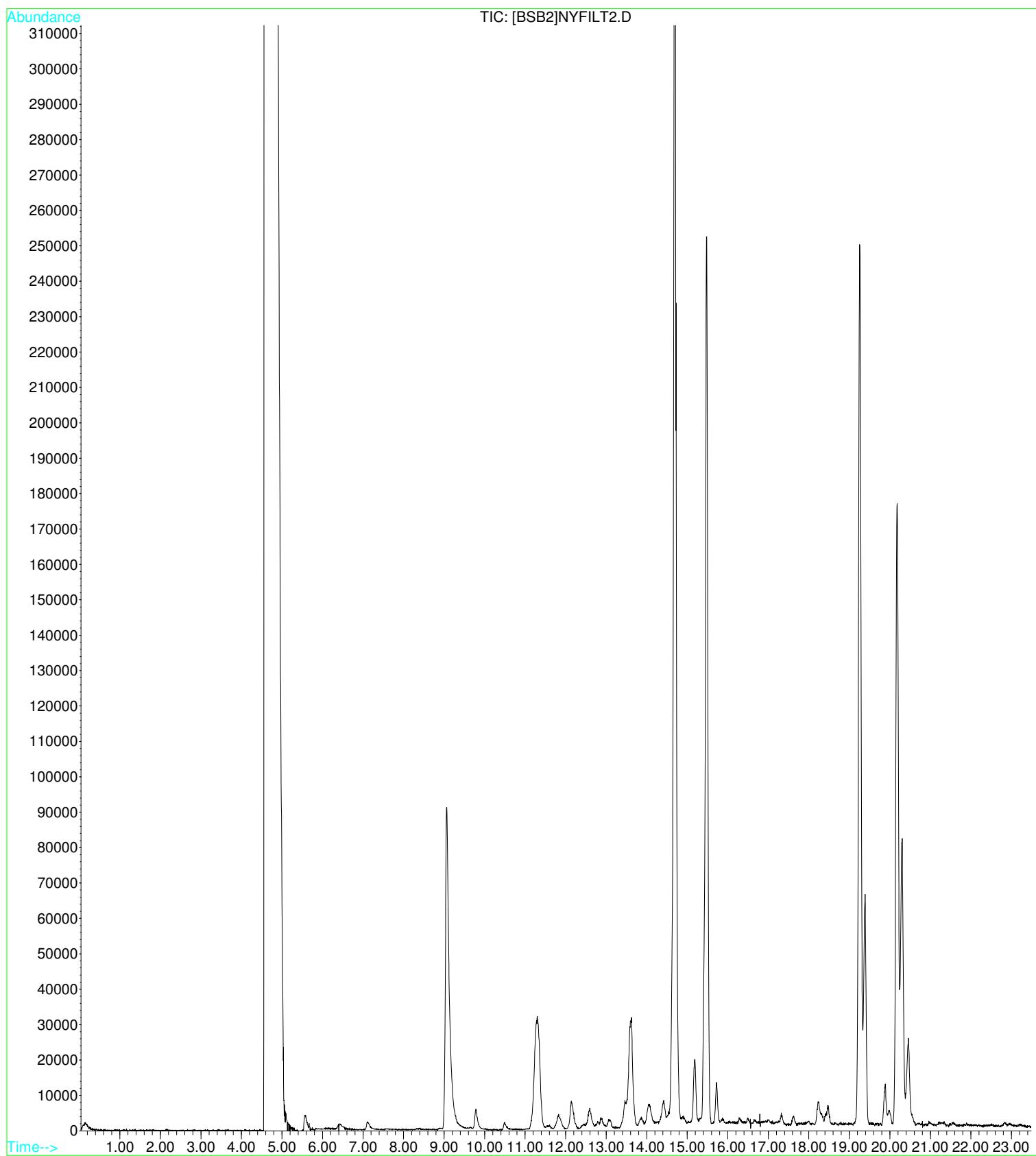
Appendix

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- Pages 44 - 81 QTOF-GCMS Exhaustive
- Pages 82 - 94 QTOF-LCMS Leachables
- Pages 95 - 117 QTOF-LCMS Exhaustive

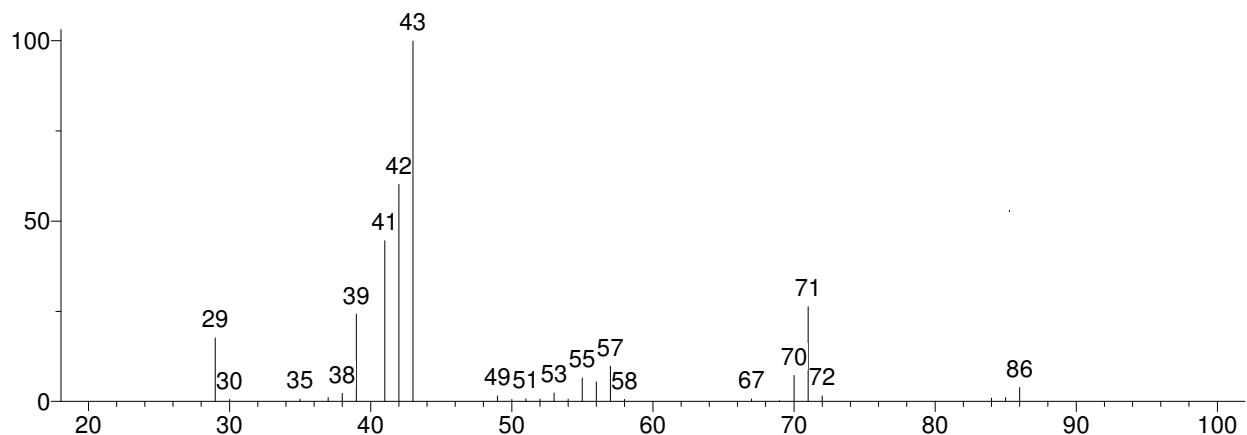
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Instrument : Purity An
Sample Name: Nylon Syringe
Misc Info :
Vial Number: 100

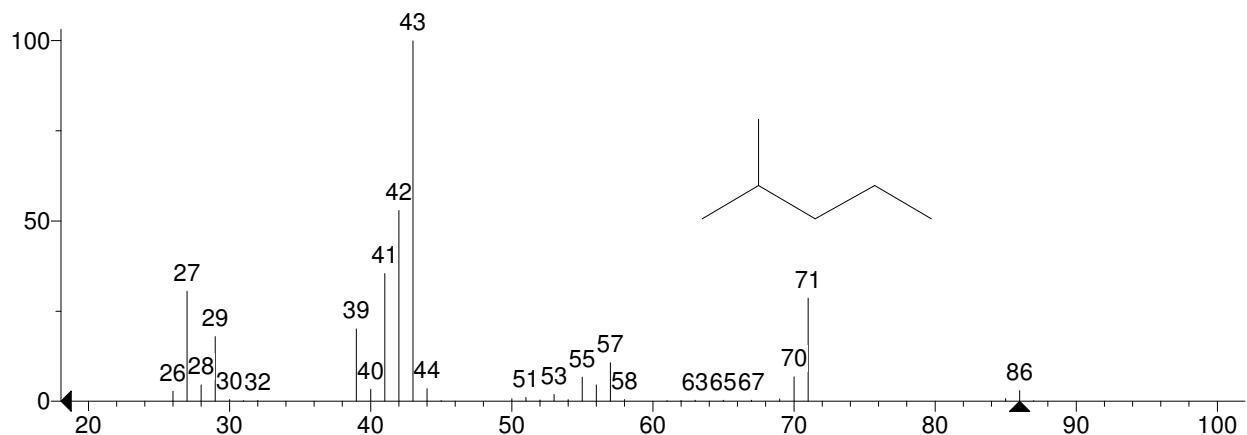


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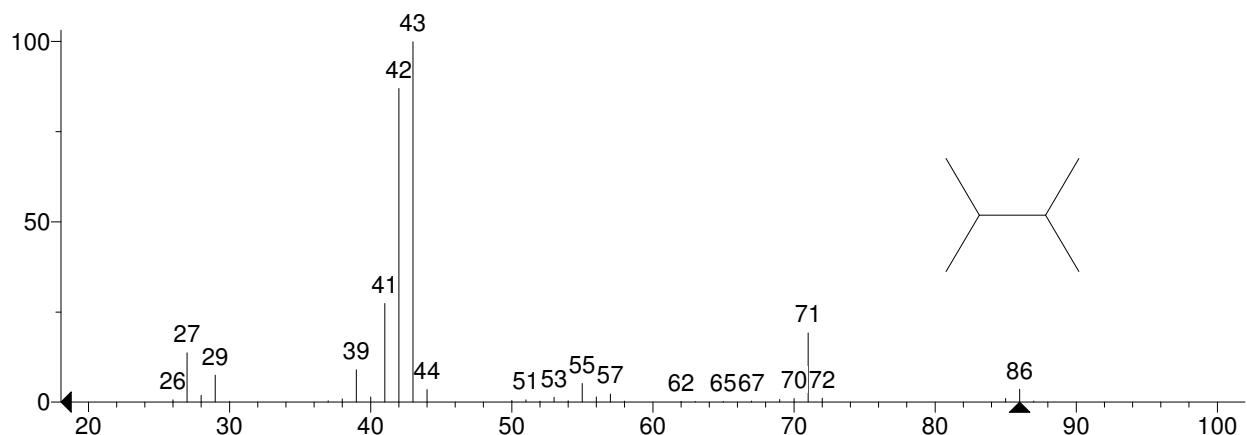
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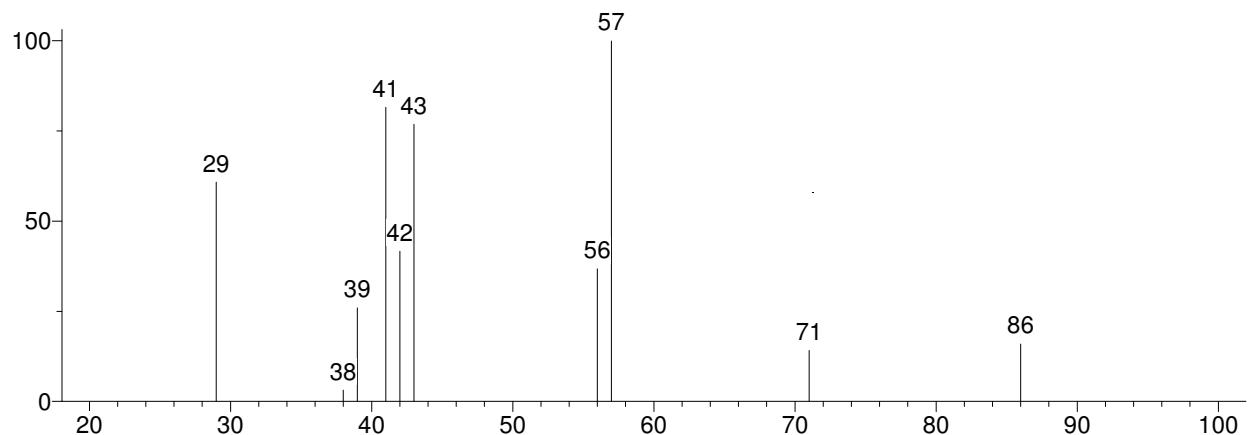


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 C6H14; MF: 829; RMF: 835; Prob 13.8%; CAS: 79-29-8; Lib: mainlib; ID: 5866.

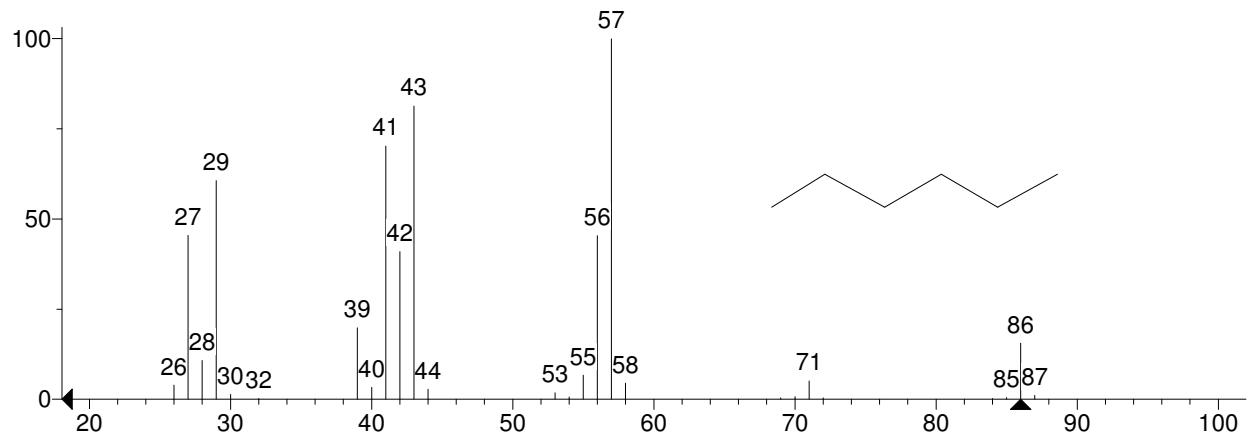


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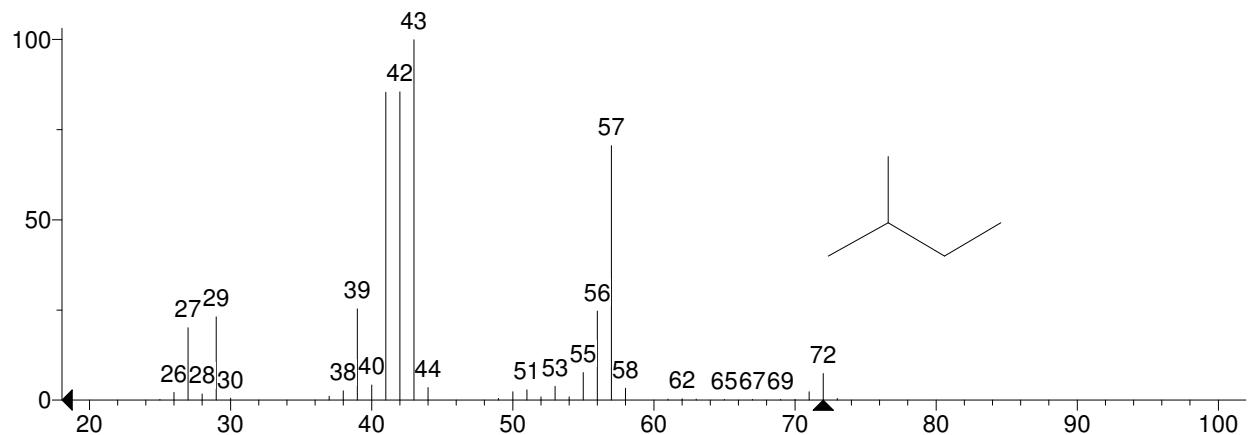
Unknown: Scan 1919 (9.789 min): NYFILT2.D
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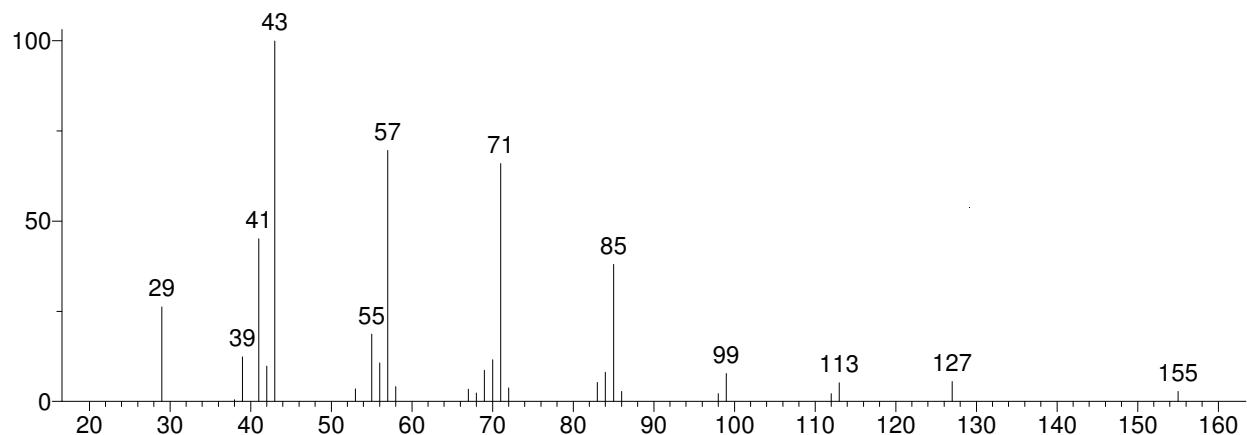


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 C5H12; MF: 810; RMF: 847; Prob 4.92%; CAS: 78-78-4; Lib: replib; ID: 1799.

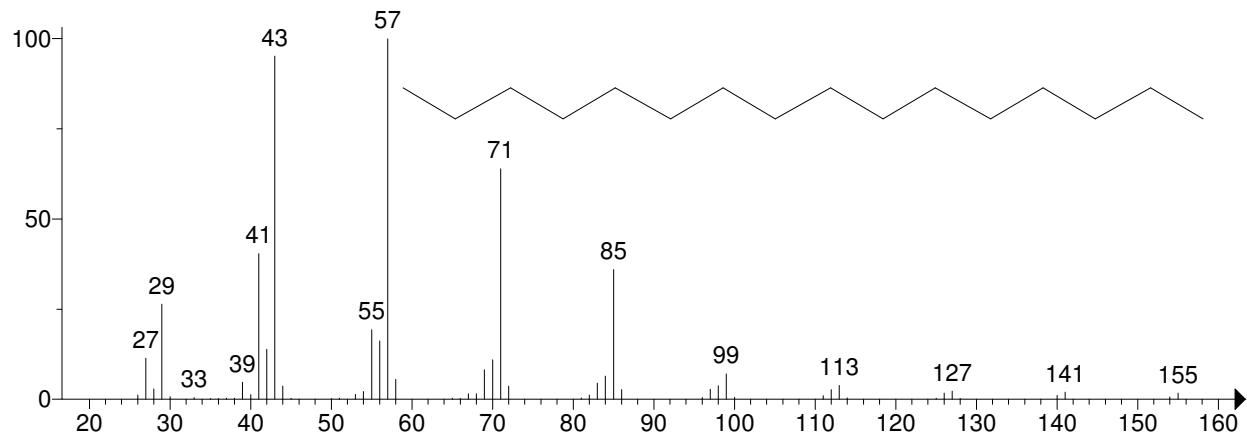


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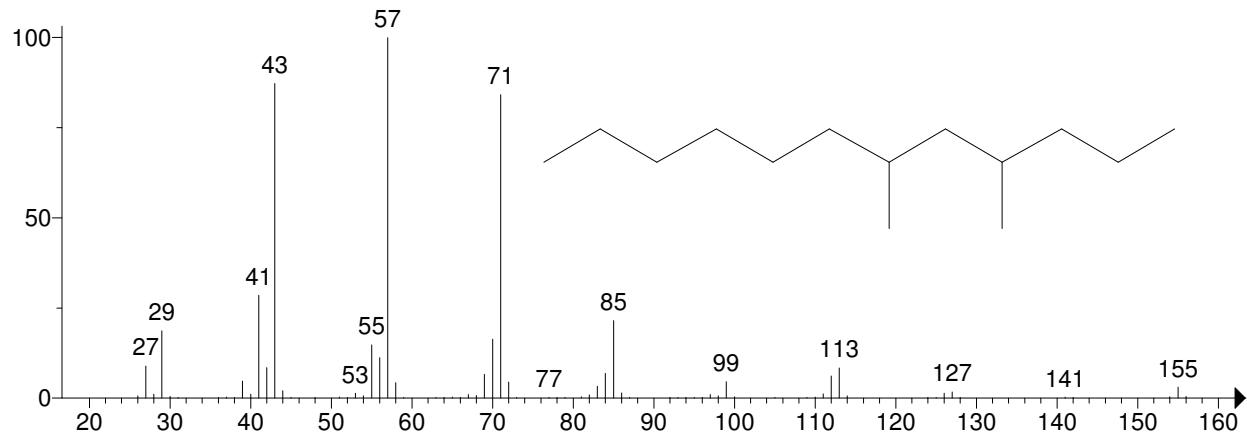
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Compound in Library Factor = -151



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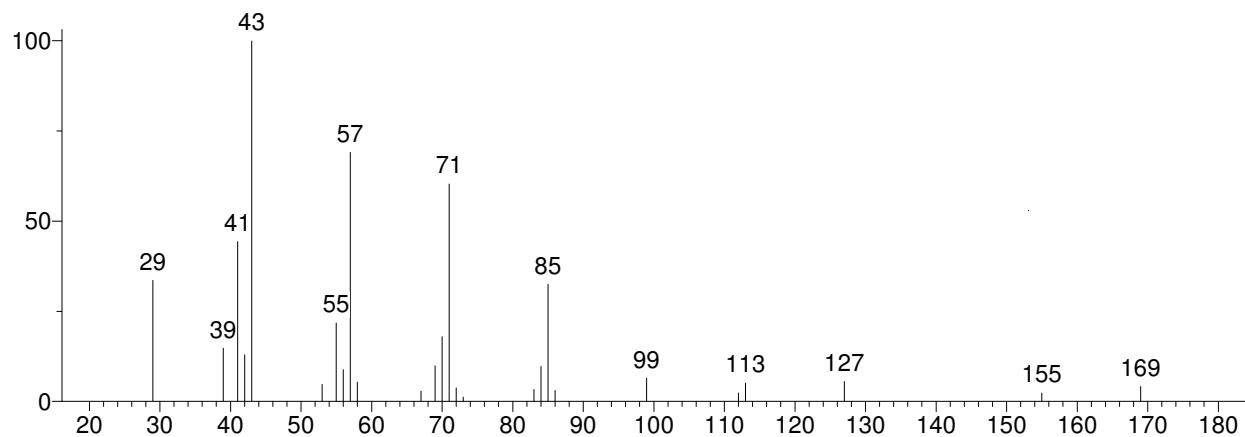


Hit 2 : Dodecane, 4,6-dimethyl-
C₁₄H₃₀; MF: 889; RMF: 889; Prob 6.37%; CAS: 61141-72-8; Lib: mainlib; ID: 20934.

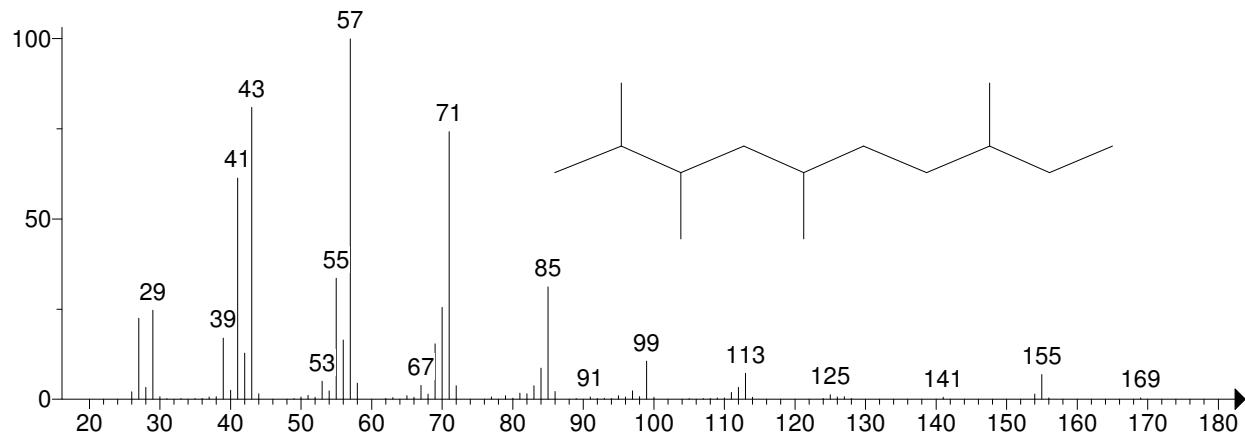


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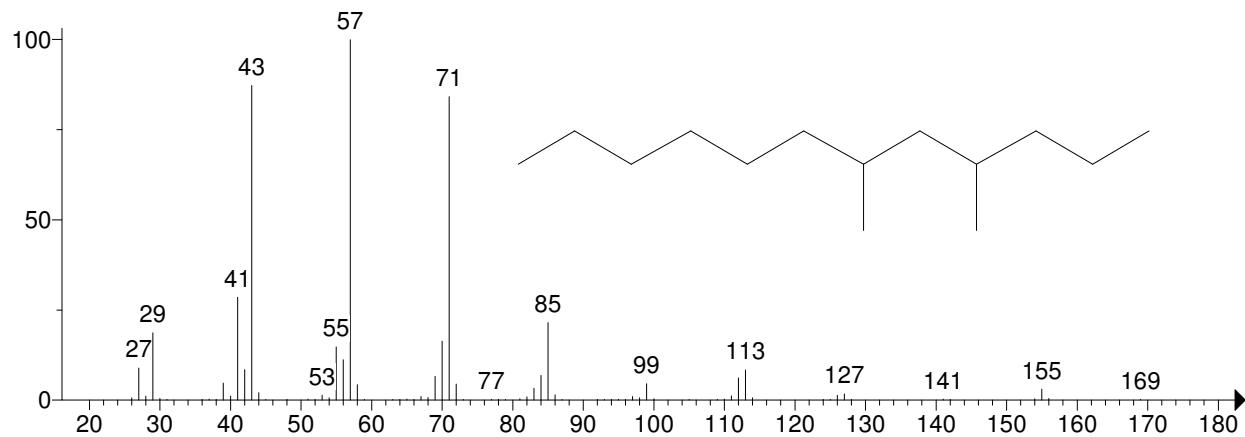
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Compound in Library Factor = -138



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C14H30; MF: 892; RMF: 894; Prob 18.1%; CAS: 192823-15-7; Lib: mainlib; ID: 20874.

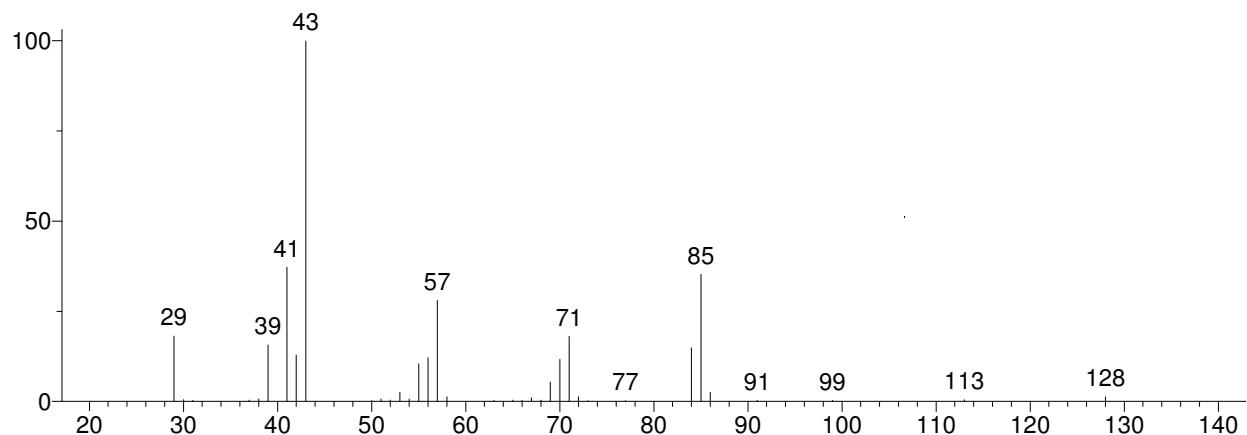


Hit 2 : Dodecane, 4,6-dimethyl-
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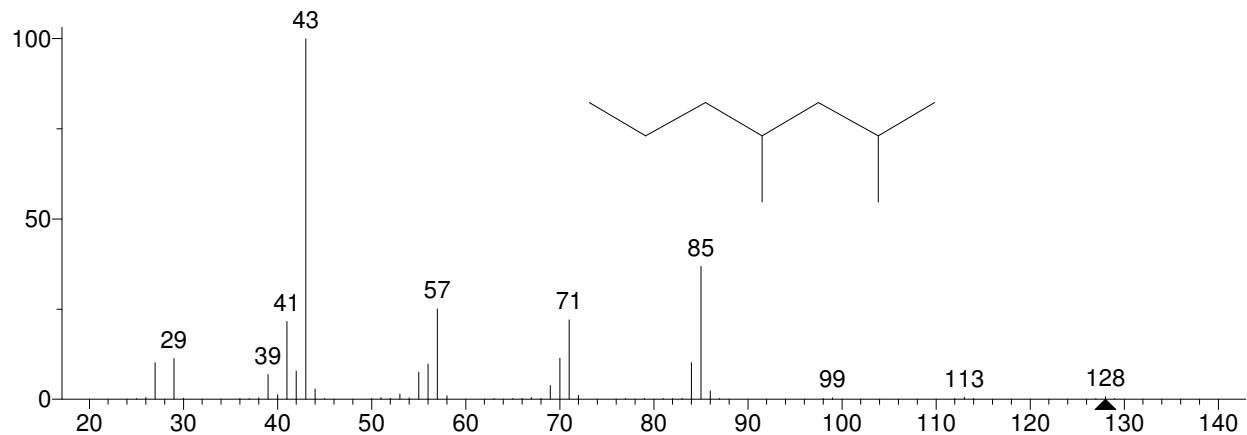


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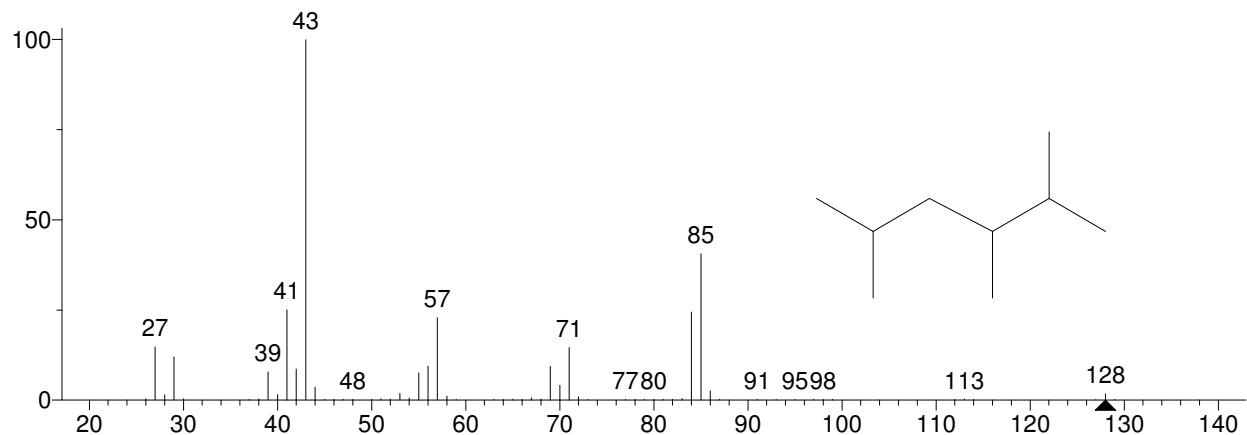
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 Compound in Library Factor = -117



Hit 1 : Heptane, 2,4-dimethyl-
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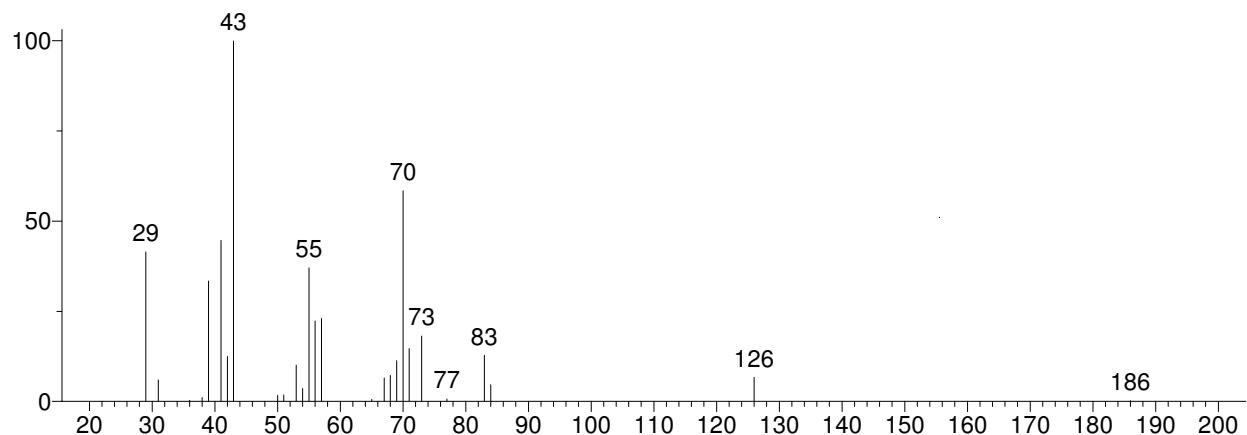


Hit 2 : Hexane, 2,3,5-trimethyl-
 C9H20; MF: 907; RMF: 908; Prob 11.1%; CAS: 1069-53-0; Lib: mainlib; ID: 8733.

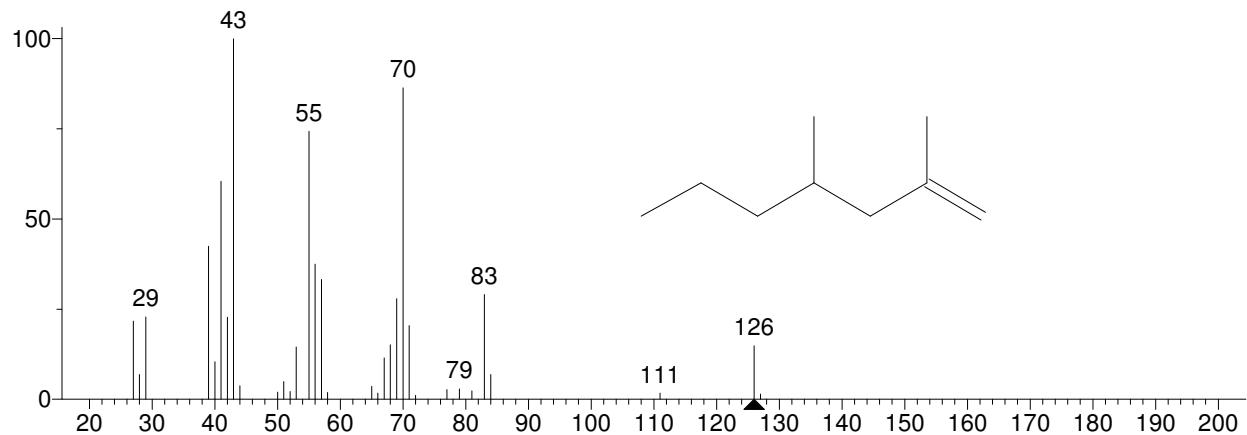


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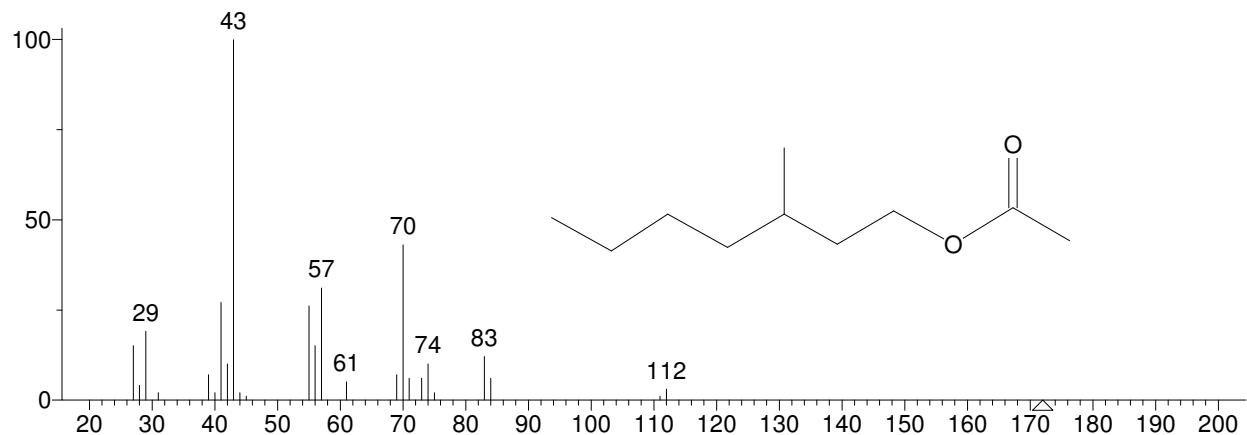
Unknown: Scan 2981 (15.187 min): NYFILT2.D
 Compound in Library Factor = -155



Hit 1 : 2,4-Dimethyl-1-heptene
 C9H18; MF: 860; RMF: 903; Prob 48.0%; CAS: 19549-87-2; Lib: replib; ID: 2334.

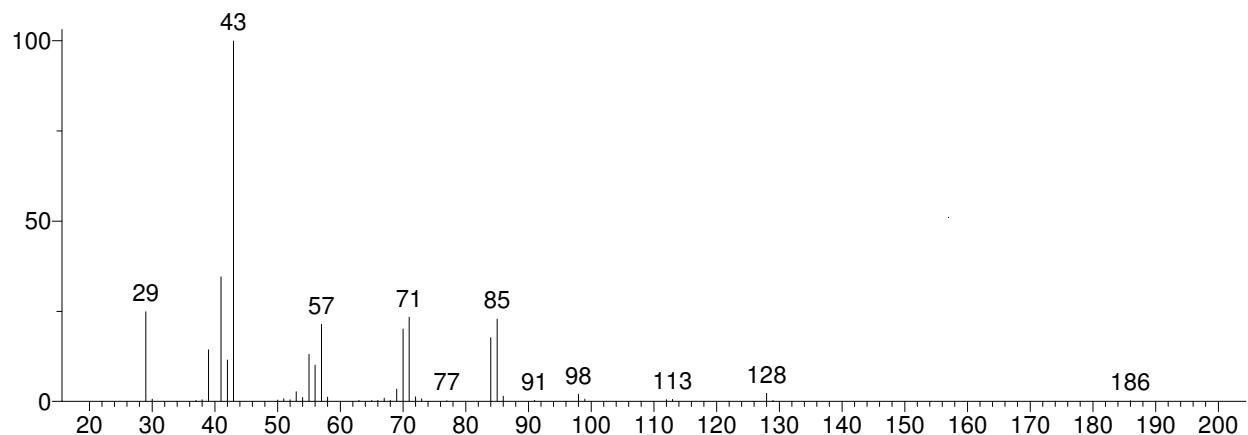


Hit 2 : 3-Methylheptyl acetate
 C10H20O2; MF: 860; RMF: 860; Prob 8.67%; CAS: 72218-58-7; Lib: mainlib; ID: 7754.

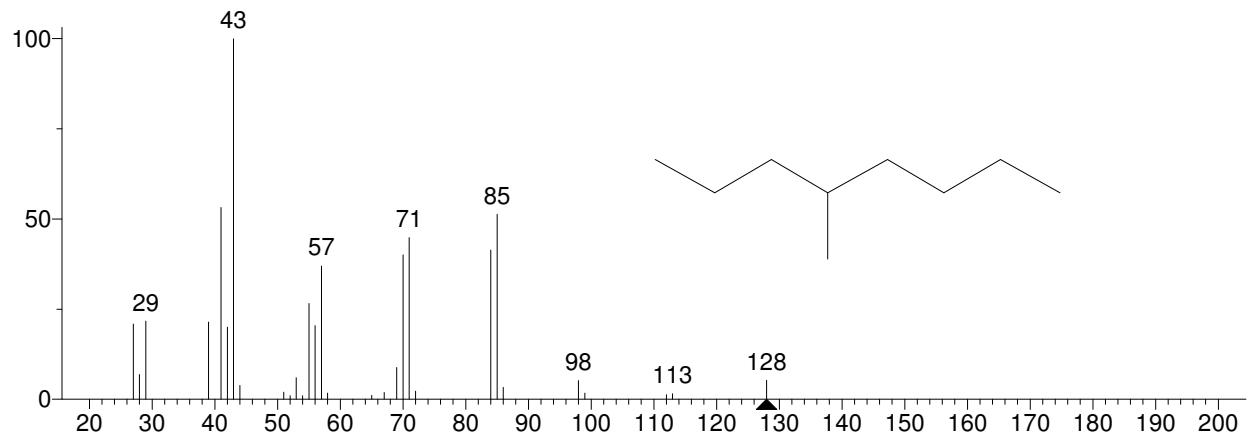


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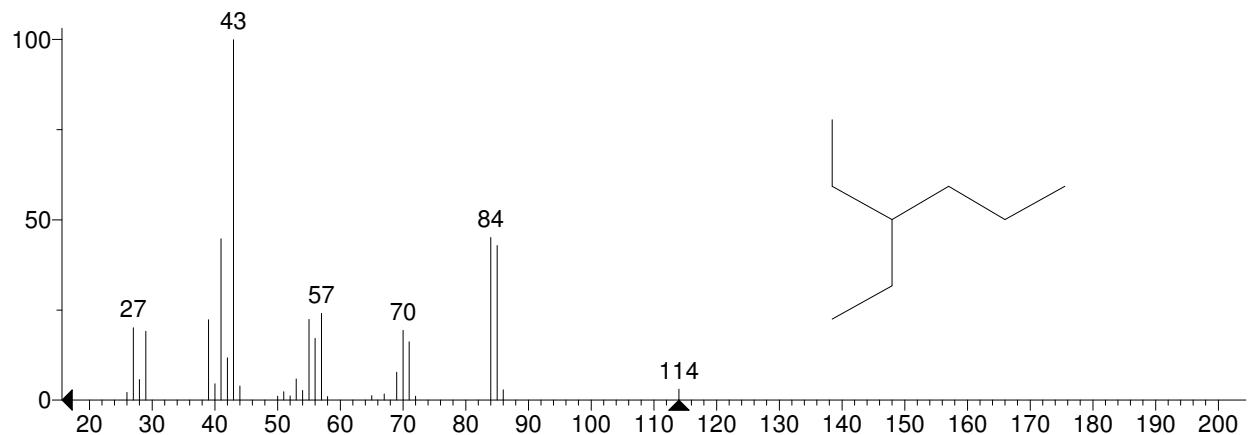
Unknown: Scan 3038 (15.477 min): NYFILT2.D
Compound in Library Factor = 165



Hit 1 : Octane, 4-methyl-
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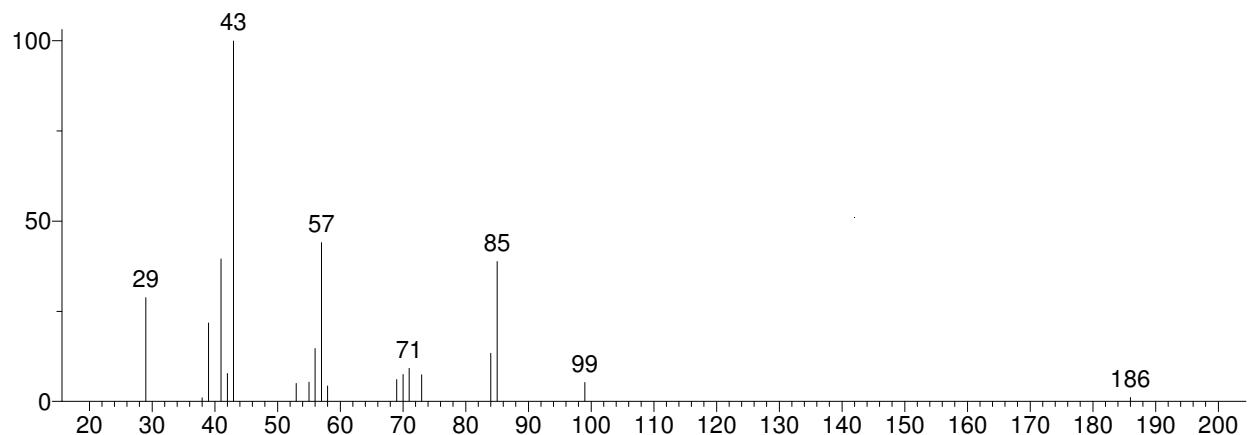


Hit 2 : Hexane, 3-ethyl-
C8H18; MF: 887; RMF: 912; Prob 9.33%; CAS: 619-99-8; Lib: replib; ID: 2594.

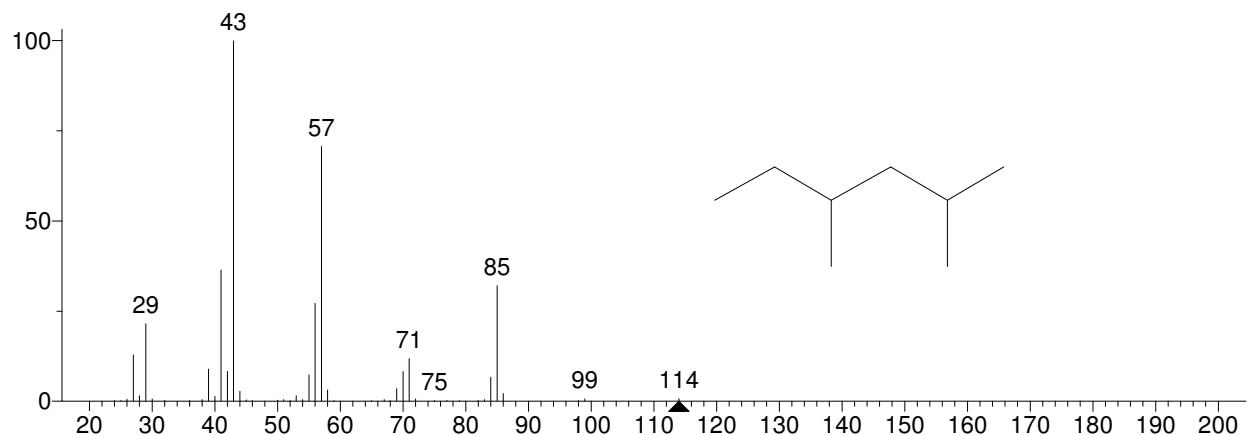


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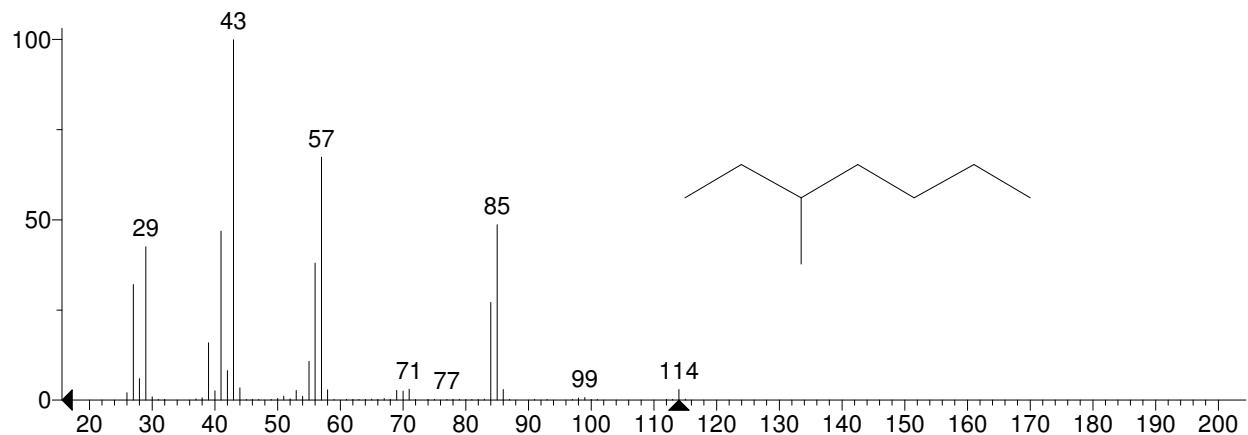
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 Compound in Library Factor = -197



Hit 1 : Hexane, 2,4-dimethyl-
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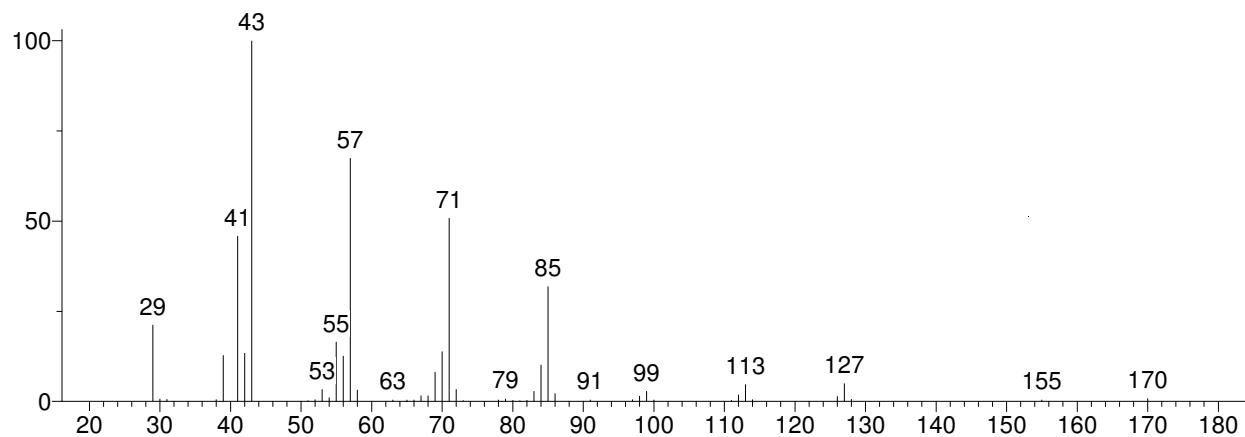


Hit 2 : Heptane, 3-methyl-
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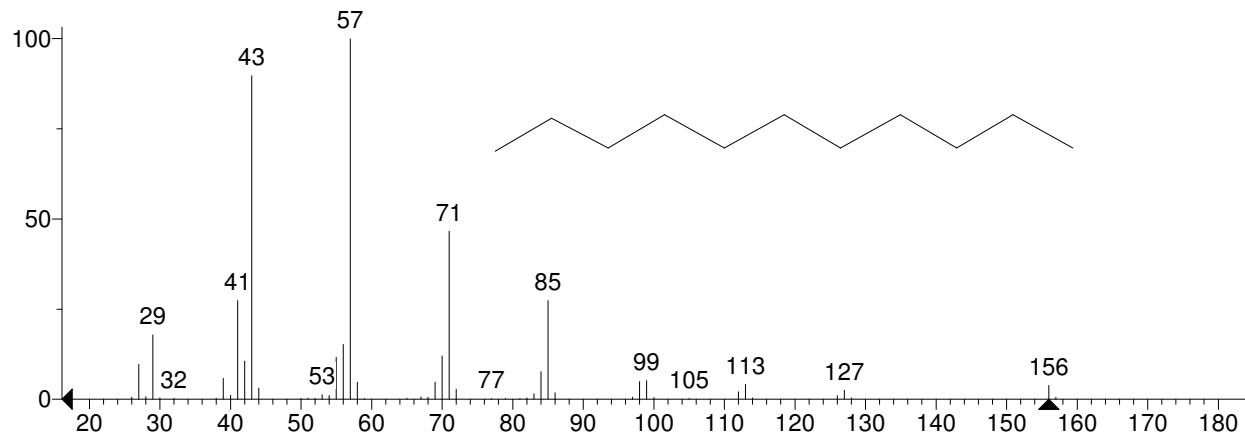


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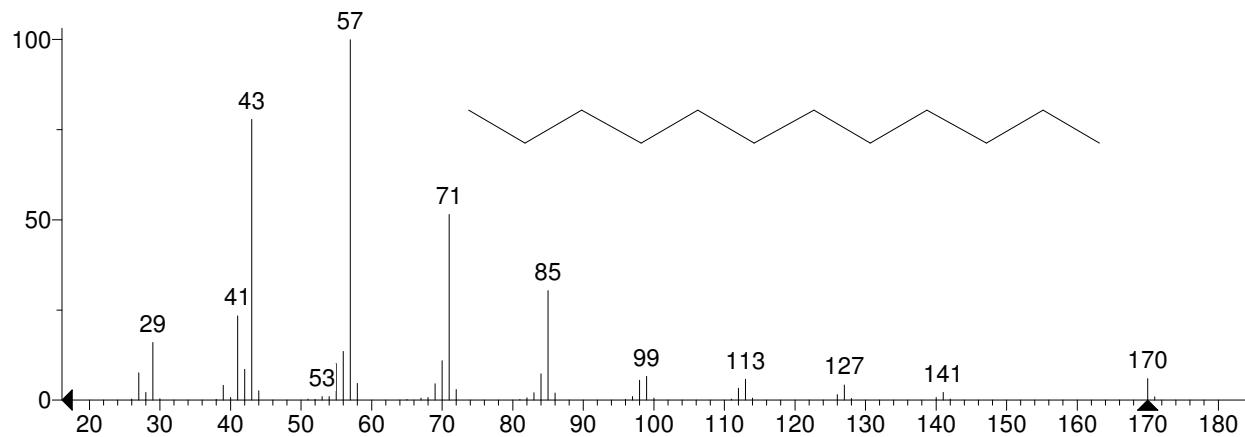
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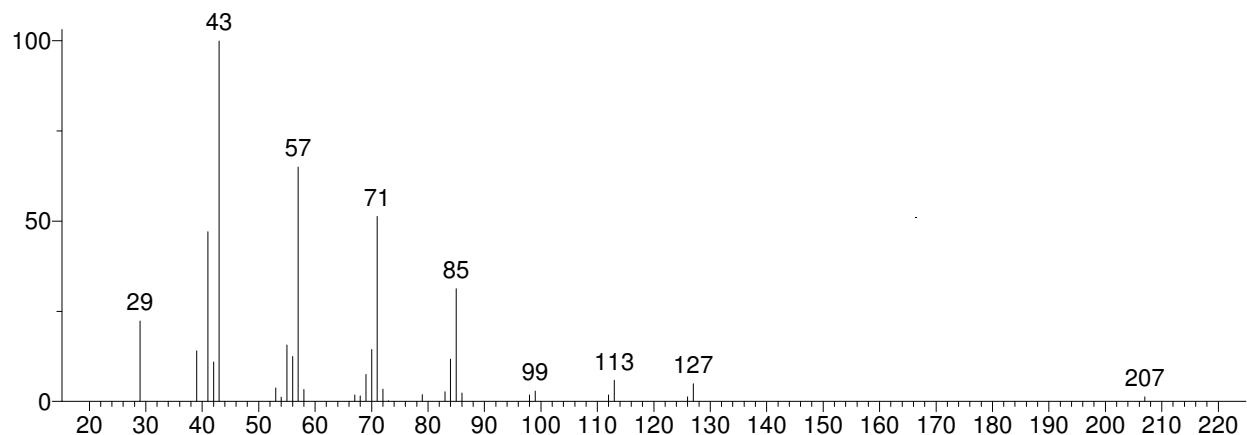


Hit 2 : Dodecane
C12H26; MF: 880; RMF: 884; Prob 6.37%; CAS: 112-40-3; Lib: mainlib; ID: 20794.

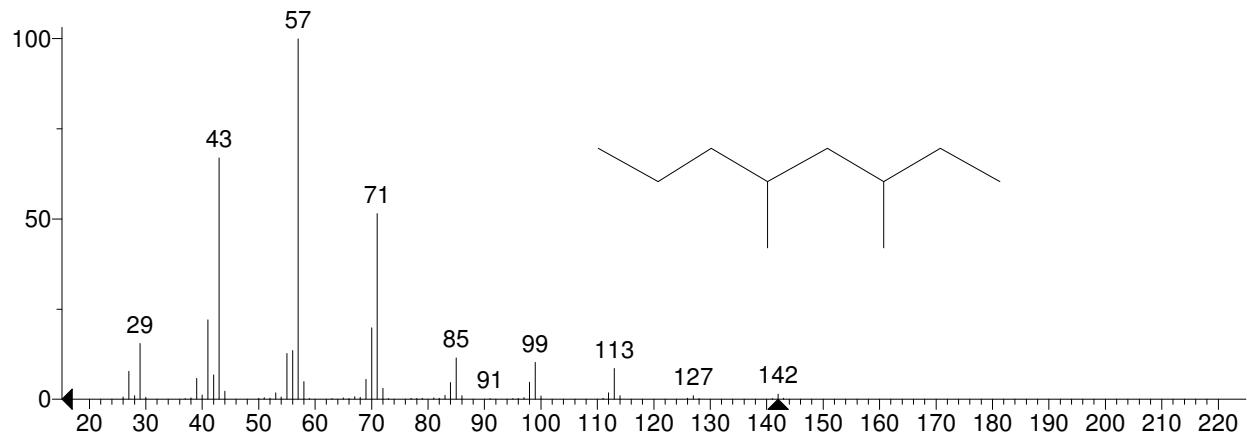


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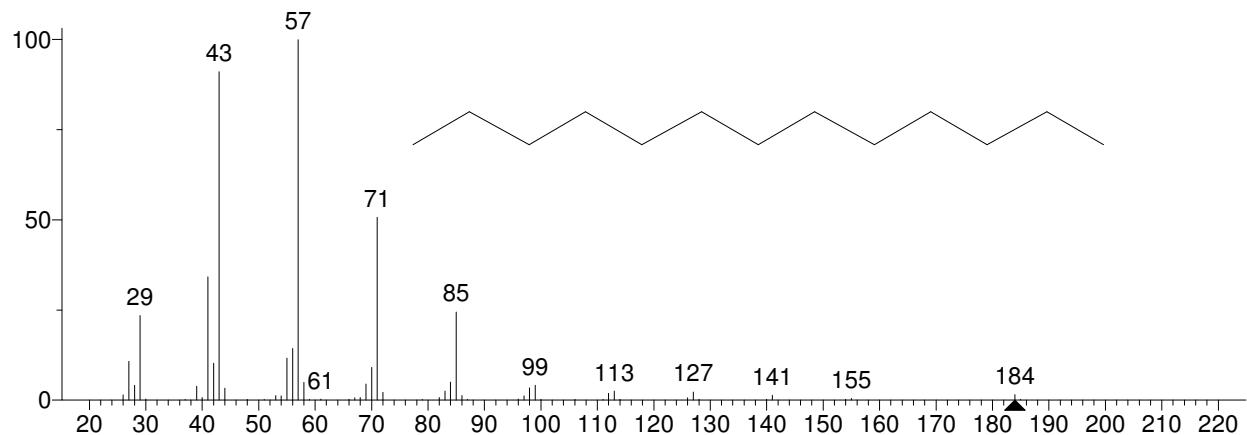
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 Compound in Library Factor = -185



Hit 1 : Octane, 3,5-dimethyl-
 C10H22; MF: 883; RMF: 889; Prob 9.61%; CAS: 15869-93-9; Lib: mainlib; ID: 20946.

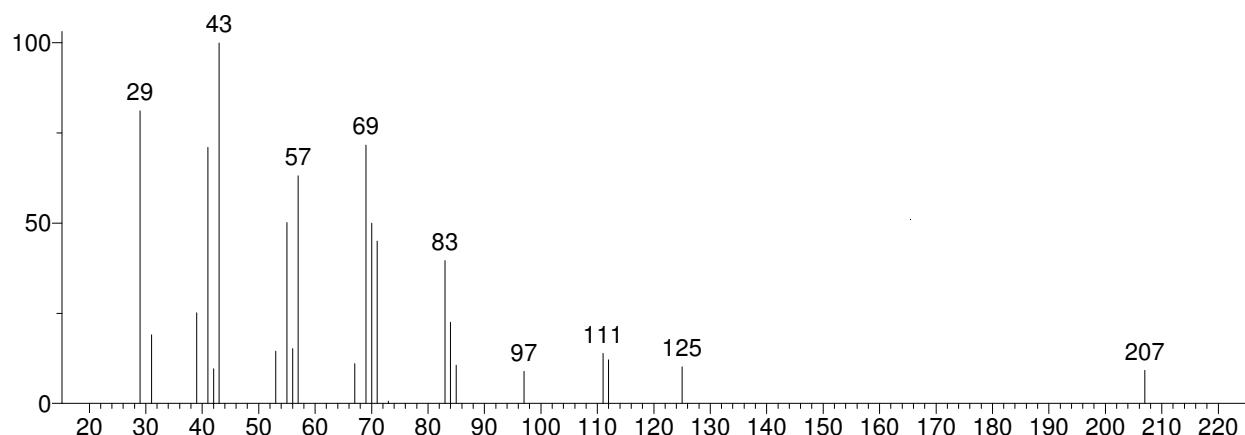


Hit 2 : Tridecane
 C13H28; MF: 879; RMF: 887; Prob 8.12%; CAS: 629-50-5; Lib: mainlib; ID: 20782.

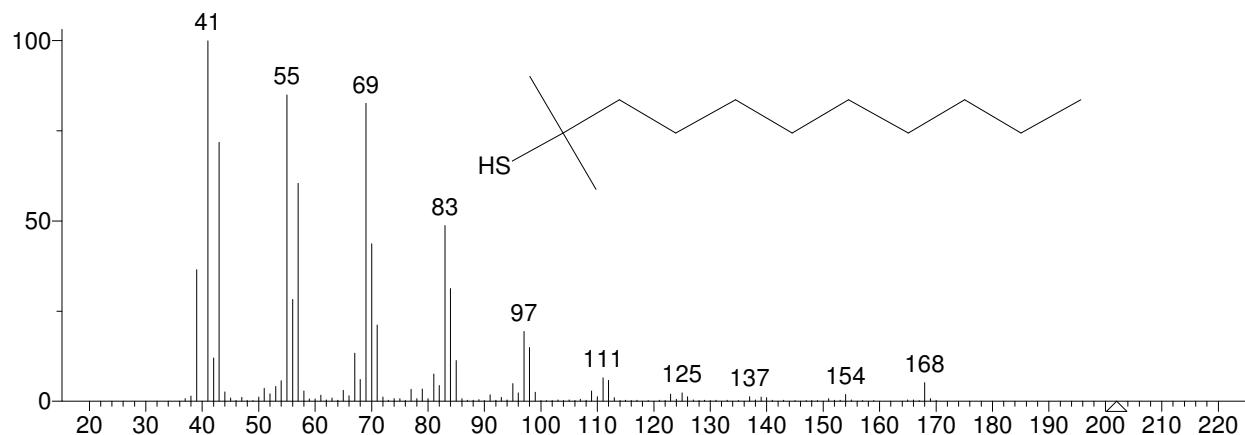


** Search Report Page 1 of 1 **

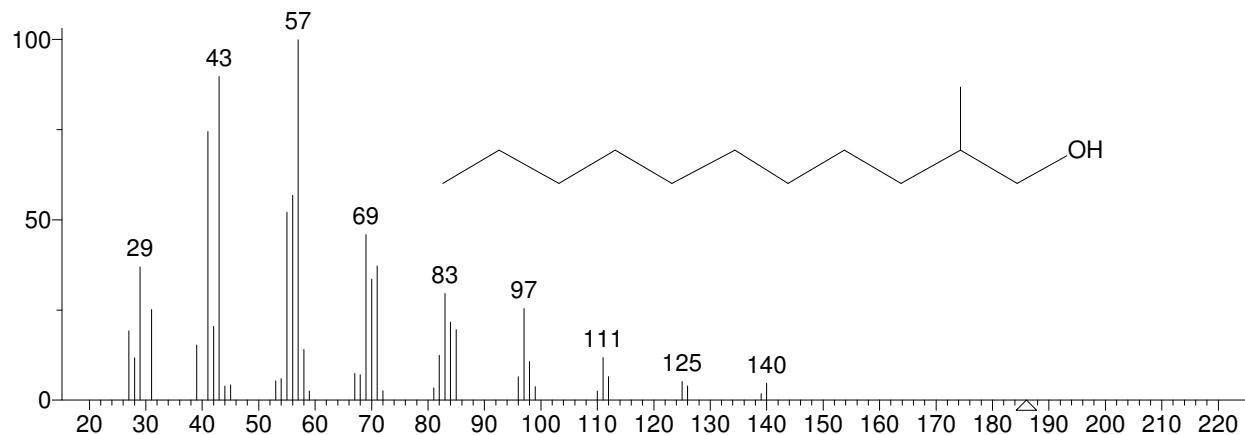
Unknown: Scan 3904 (19.880 min): NYFILT2.D
 Compound in Library Factor = -713



Hit 1 : 2-Undecanethiol, 2-methyl-
 C12H26S; MF: 781; RMF: 803; Prob 4.62%; CAS: 10059-13-9; Lib: mainlib; ID: 2530.

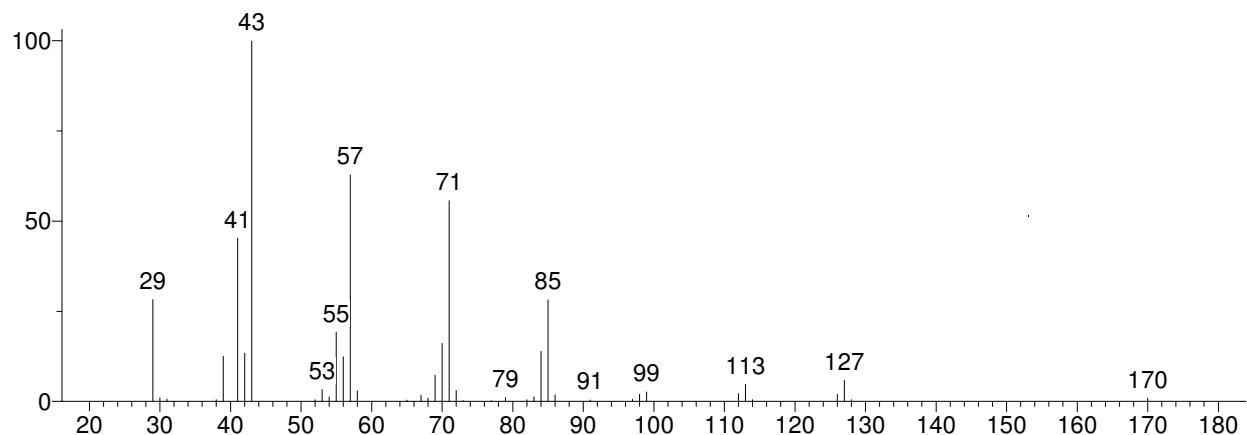


Hit 2 : 2-Methyl-1-undecanol
 C12H26O; MF: 774; RMF: 796; Prob 3.54%; CAS: 10522-26-6; Lib: mainlib; ID: 20662.

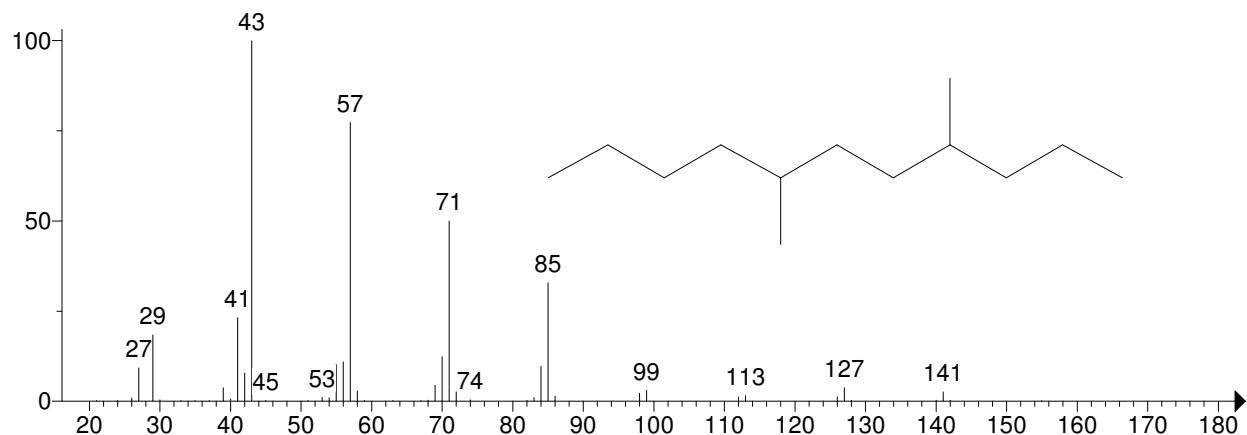


** Search Report Page 1 of 1 **

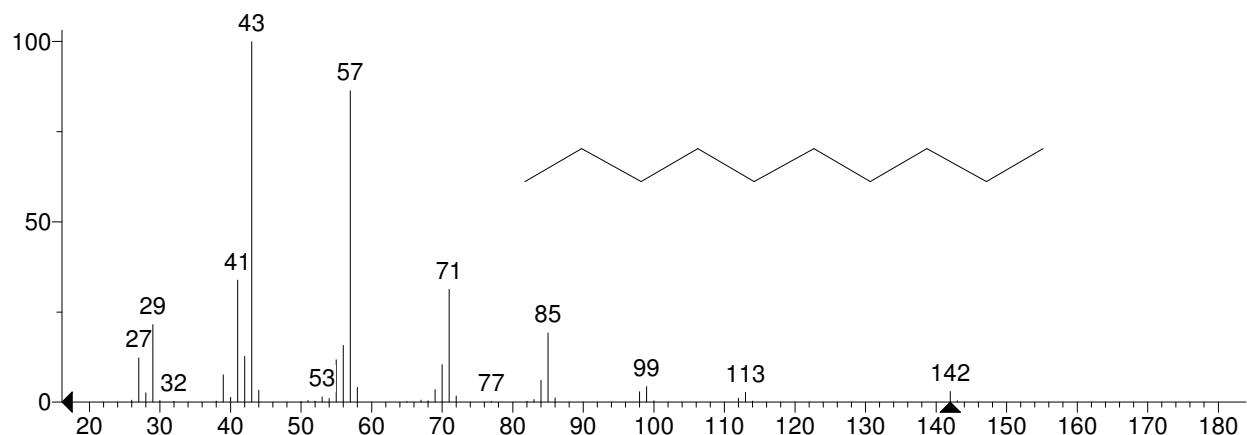
Unknown: Scan 3964 (20.185 min): NYFILT2.D
 Compound in Library Factor = -185



Hit 1 : Undecane, 4,7-dimethyl-
 C13H28; MF: 884; RMF: 893; Prob 8.40%; CAS: 17301-32-5; Lib: mainlib; ID: 7064.

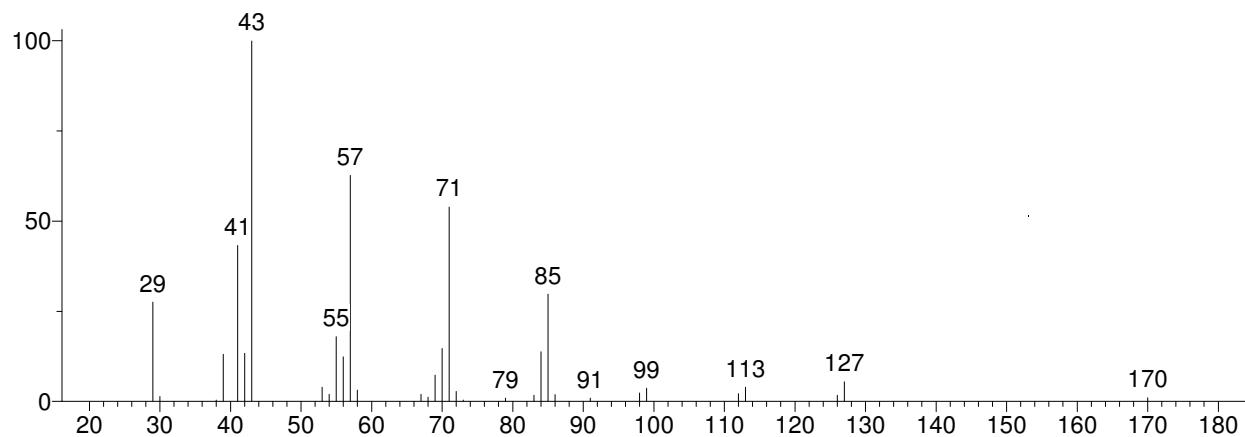


Hit 2 : Decane
 C10H22; MF: 882; RMF: 908; Prob 7.74%; CAS: 124-18-5; Lib: replib; ID: 2036.

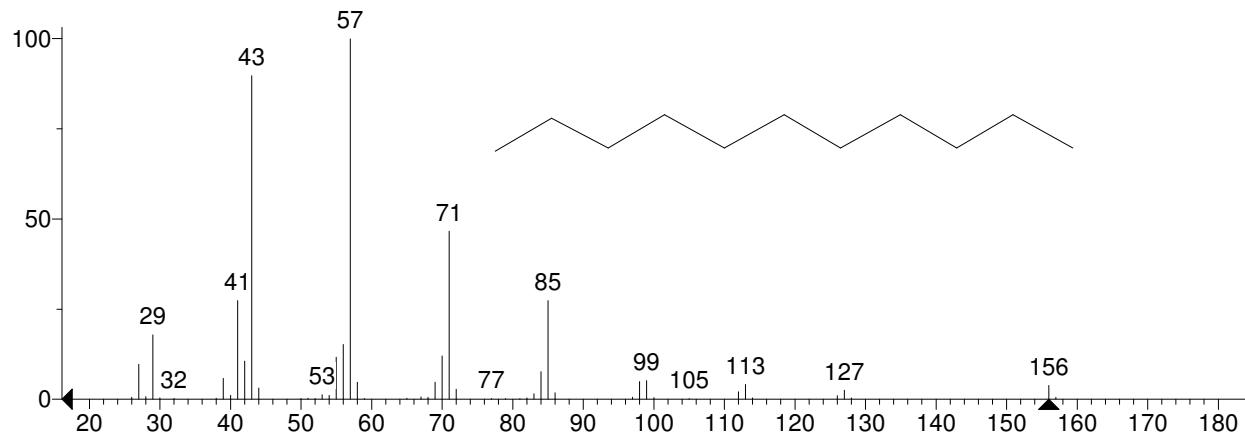


** Search Report Page 1 of 1 **

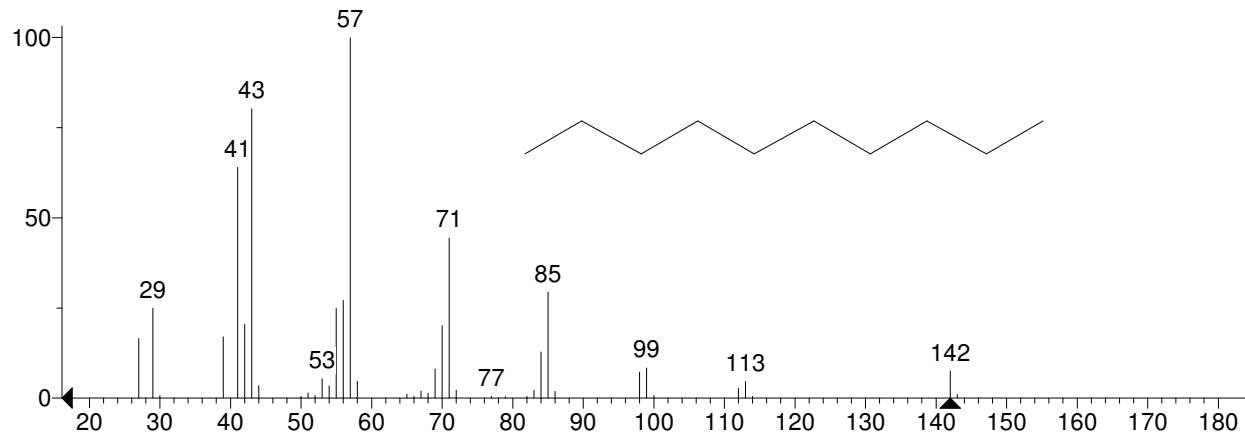
Unknown: Scan 3985 (20.292 min): NYFILT2.D
Compound in Library Factor = -151



Hit 1 : Undecane
C11H24; MF: 893; RMF: 898; Prob 10.1%; CAS: 1120-21-4; Lib: mainlib; ID: 20927.

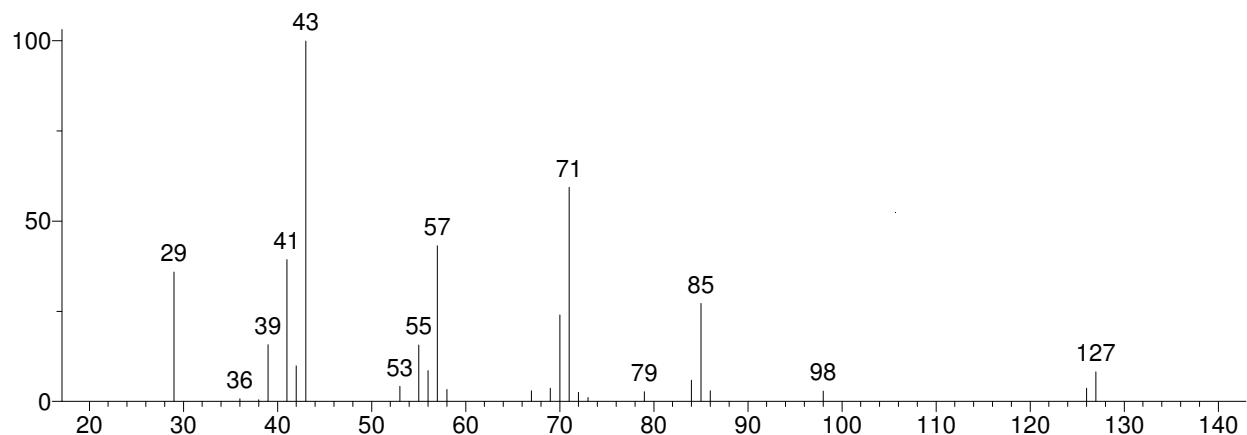


Hit 2 : Decane
C10H22; MF: 888; RMF: 912; Prob 8.10%; CAS: 124-18-5; Lib: replib; ID: 5328.

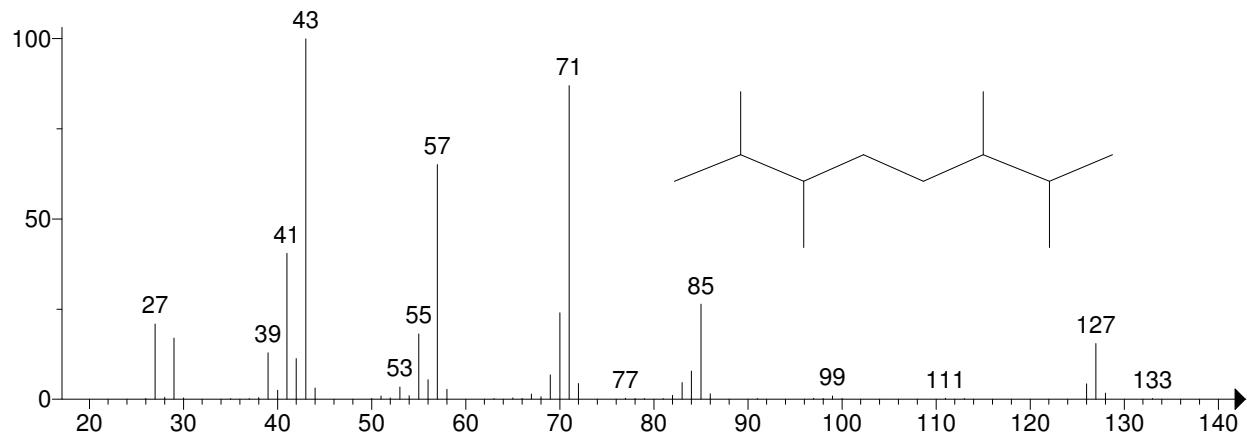


** Search Report Page 1 of 1 **

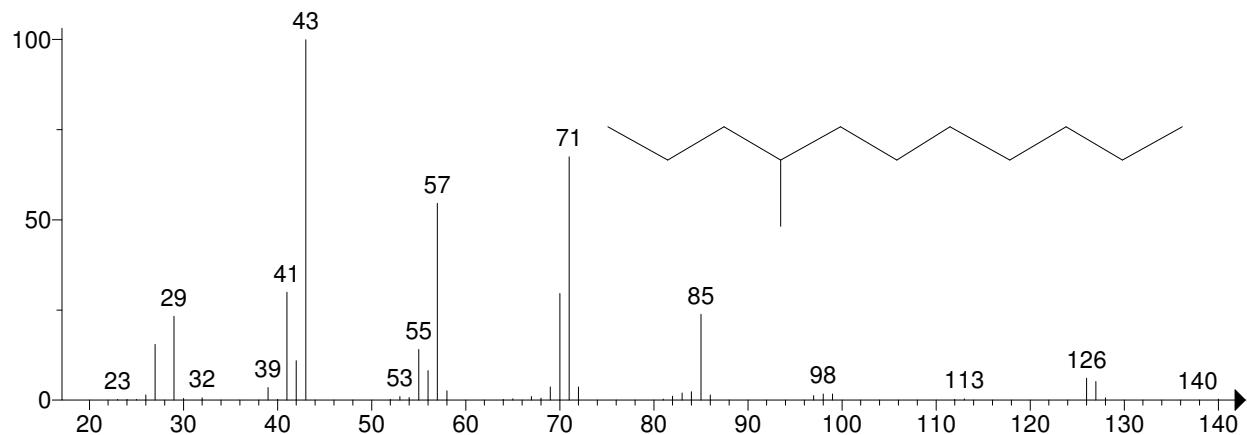
Unknown: Scan 4016 (20.449 min): NYFILT2.D
 Compound in Library Factor = -197



Hit 1 : Octane, 2,3,6,7-tetramethyl-
 C12H26; MF: 878; RMF: 881; Prob 20.9%; CAS: 52670-34-5; Lib: mainlib; ID: 7935.



Hit 2 : Undecane, 4-methyl-
 C12H26; MF: 864; RMF: 871; Prob 13.1%; CAS: 2980-69-0; Lib: mainlib; ID: 7931.



QTOF-GCMS

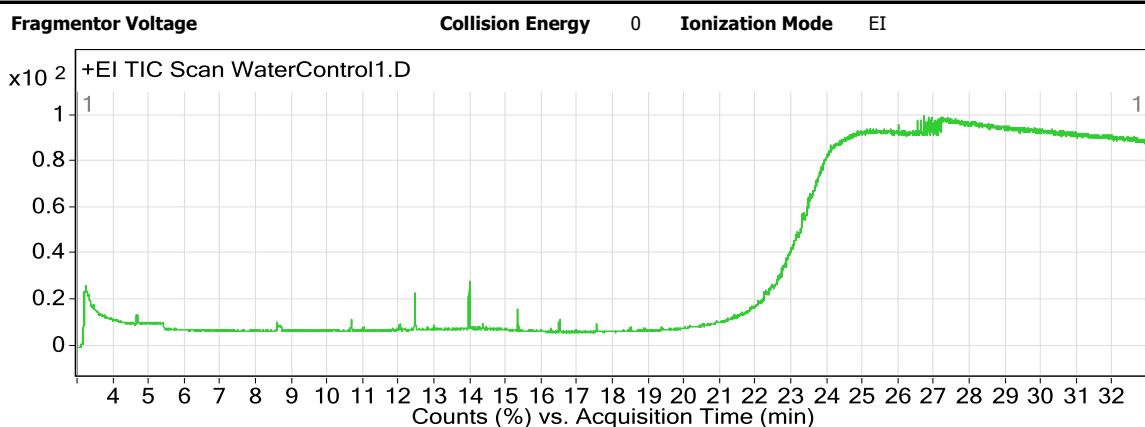
Leachables

Data

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | WaterControl1.D | Sample Name | Water Control |
| Sample Type | | Position | 11 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/19/2014 5:54:56 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms

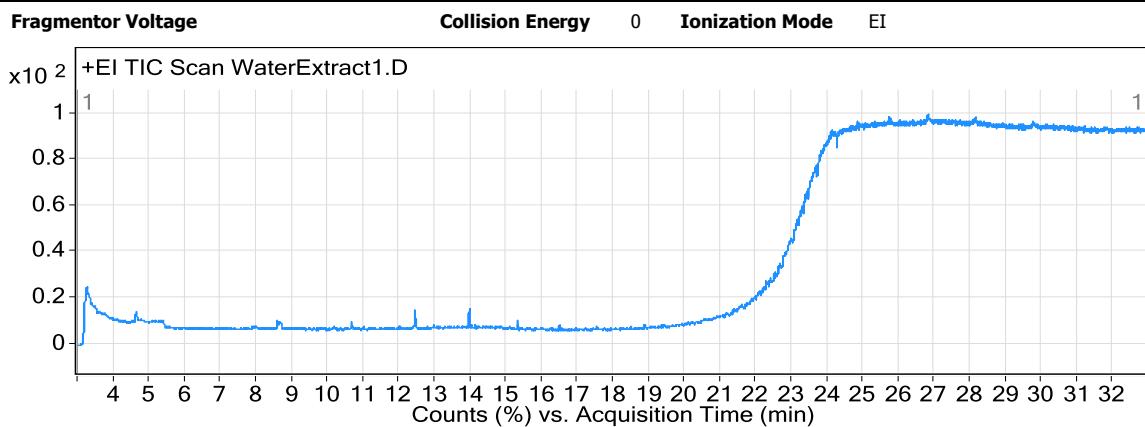


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | WaterExtract1.D | Sample Name | Water Extract |
| Sample Type | | Position | 12 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/19/2014 7:58:11 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atuses.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms

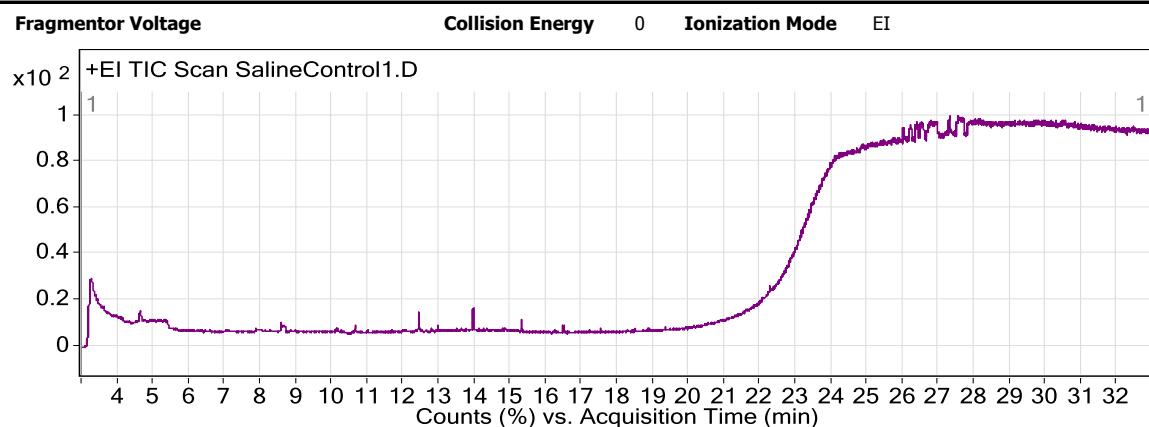


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | SalineControl1.D | Sample Name | Saline Control |
| Sample Type | | Position | 14 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 12:04:28 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms

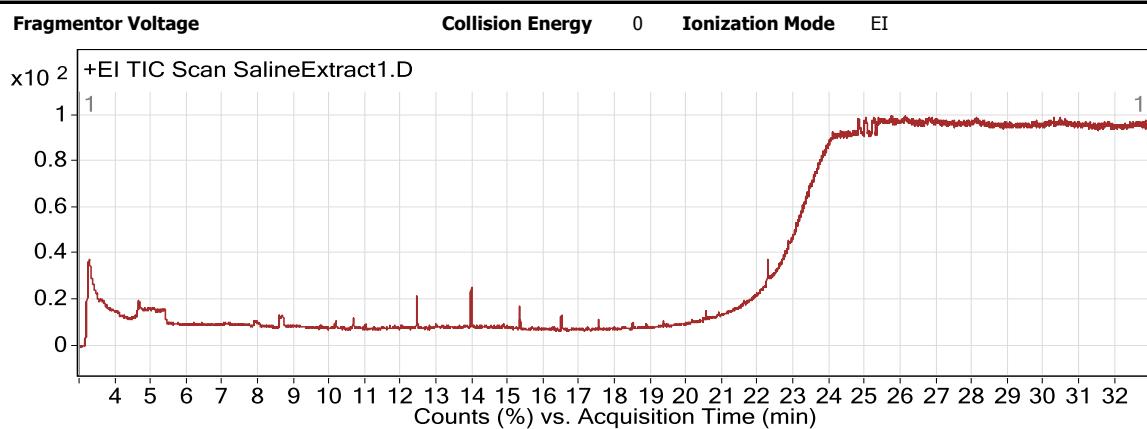


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | SalineExtract1.D | Sample Name | Saline Extract |
| Sample Type | | Position | 15 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 2:07:21 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms



--- End Of Report ---

QTOF-GCMS

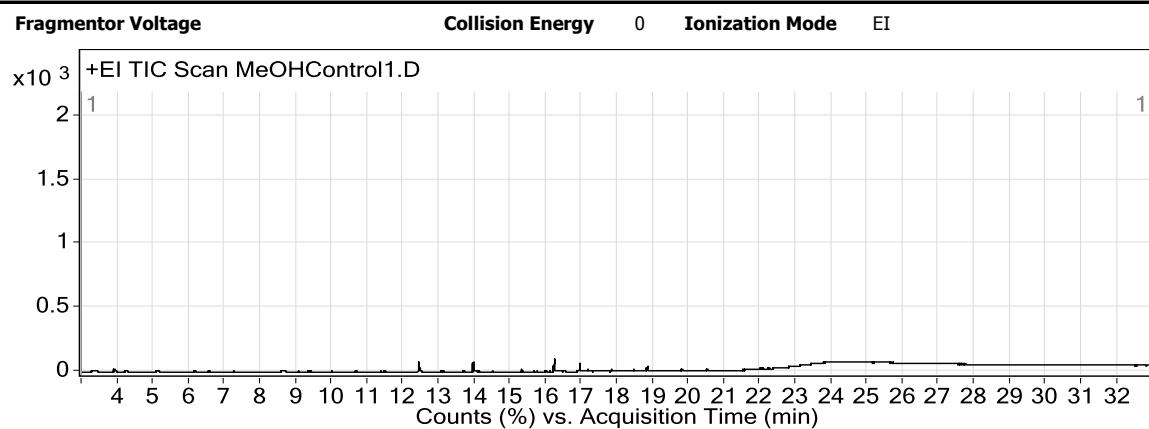
Exhaustive

Data

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | MeOHControl1.D | Sample Name | MeOH Control |
| Sample Type | | Position | 61 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 6:12:40 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms

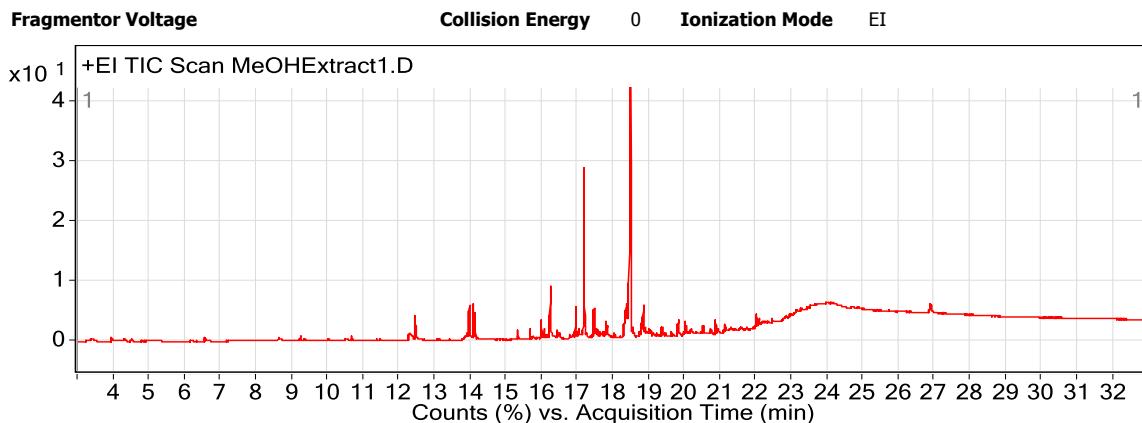


--- End Of Report ---

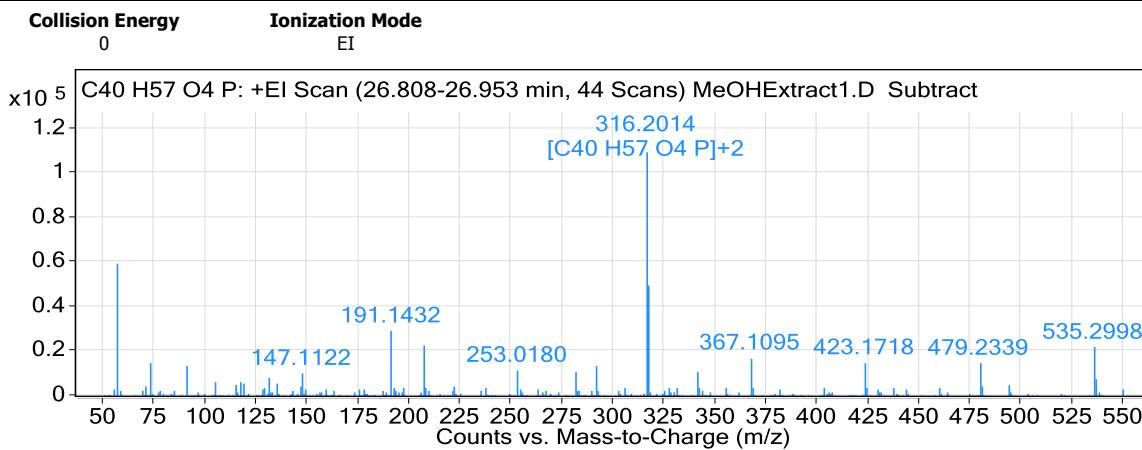
Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | MeOHExtract1.D | Sample Name | MeOH Extract |
| Sample Type | | Position | 62 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 8:15:38 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms



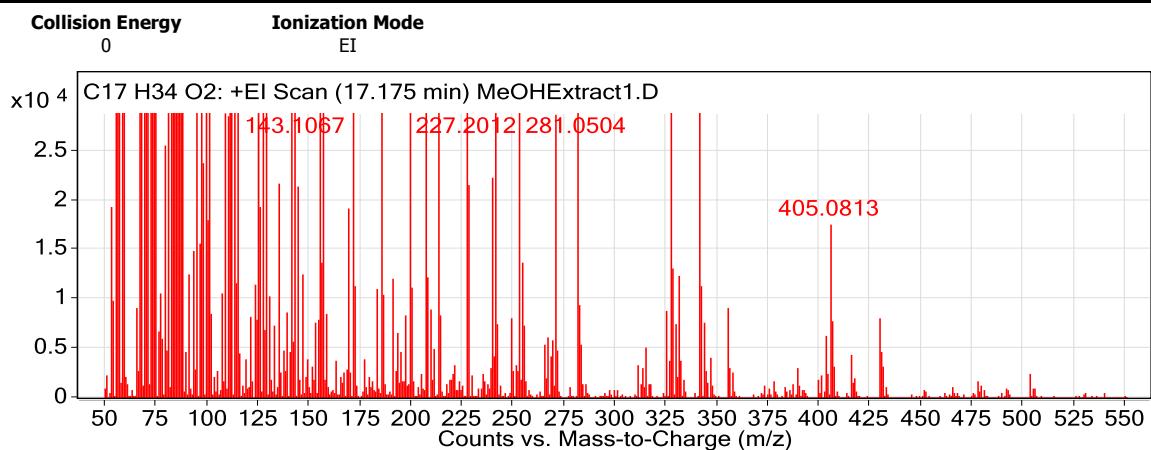
User Spectra



MFG Results

Qualitative Analysis Report

| <i>m/z</i> | Mass | Best Match | Score | Diff. | Ion Form. |
|-------------------|-------------|-------------------|--------------|--------------|------------------|
| 316.2014 | 632.404 | C40 H57 O4 P | 85.33 | -7.15 | C40 H57 O4 P |

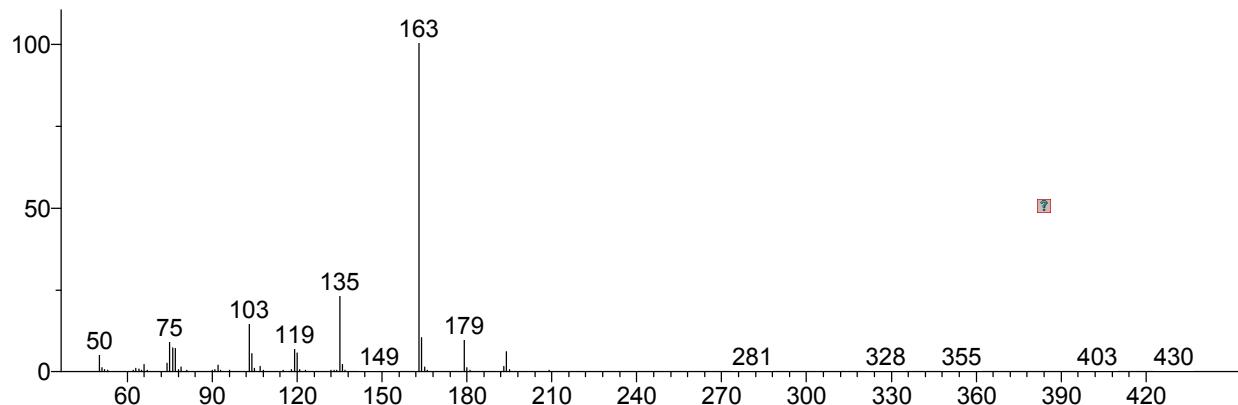
**MFG Results**

| <i>m/z</i> | Mass | Best Match | Score | Diff. | Ion Form. |
|-------------------|-------------|-------------------|--------------|--------------|------------------|
| 270.2556 | 270.256 | C17 H34 O2 | 97.6 | -0.58 | C17 H34 O2 |

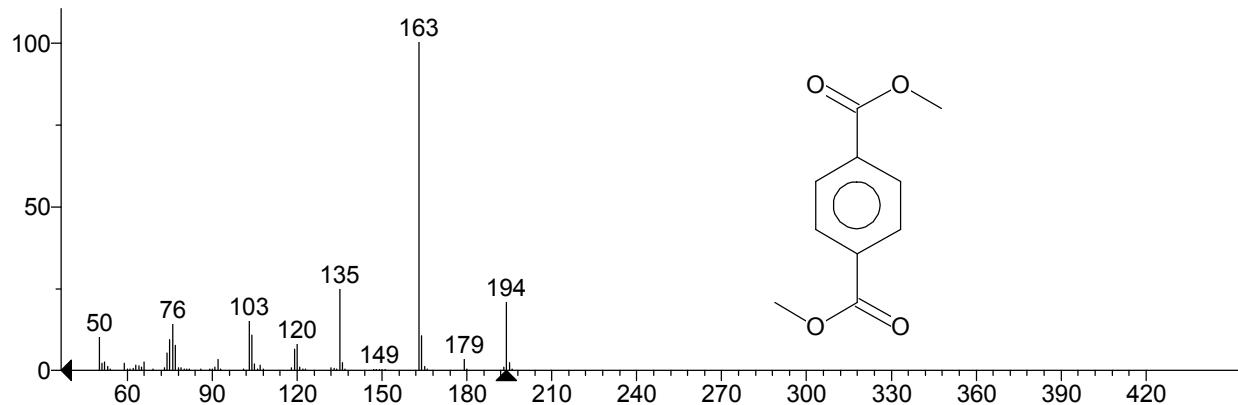
--- End Of Report ---

** Search Report Page 1 of 1 **

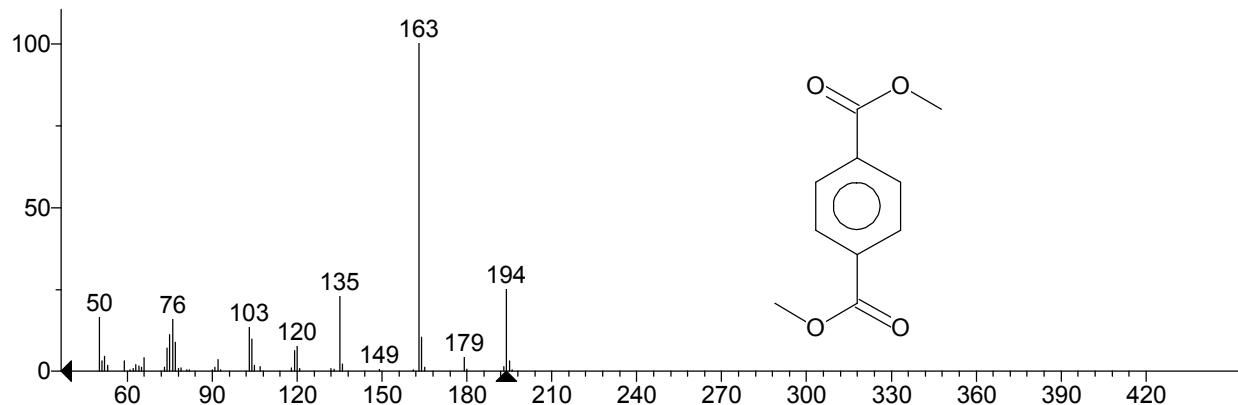
Unknown: +EI Scan (14.046, 14.076 min, 2 Scans) MeOHExtract1.D Subtract
 Compound in Library Factor = -119



Hit 1 : 1,4-Benzenedicarboxylic acid, dimethyl ester
 C10H10O4; MF: 871; RMF: 873; Prob 67.0%; CAS: 120-61-6; Lib: replib; ID: 23341.

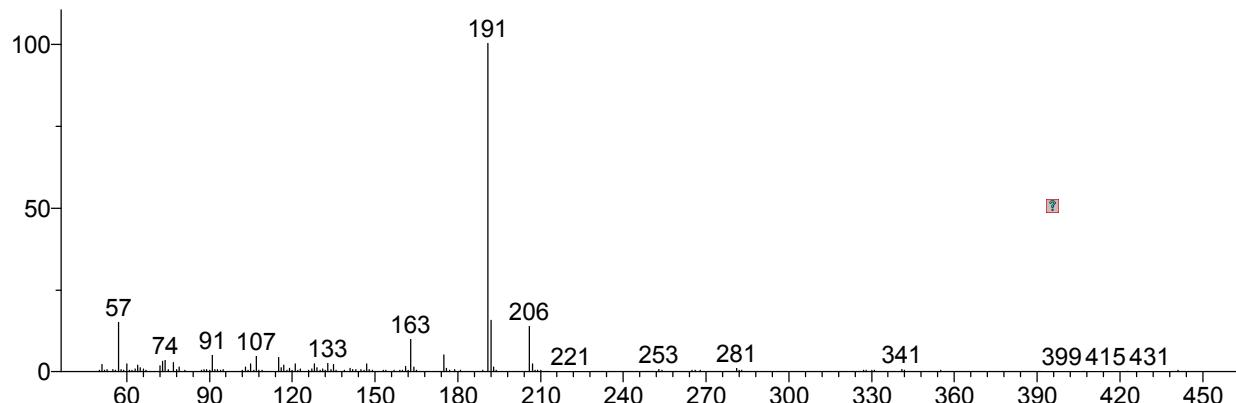


Hit 2 : 1,4-Benzenedicarboxylic acid, dimethyl ester
 C10H10O4; MF: 861; RMF: 864; Prob 67.0%; CAS: 120-61-6; Lib: replib; ID: 23383.

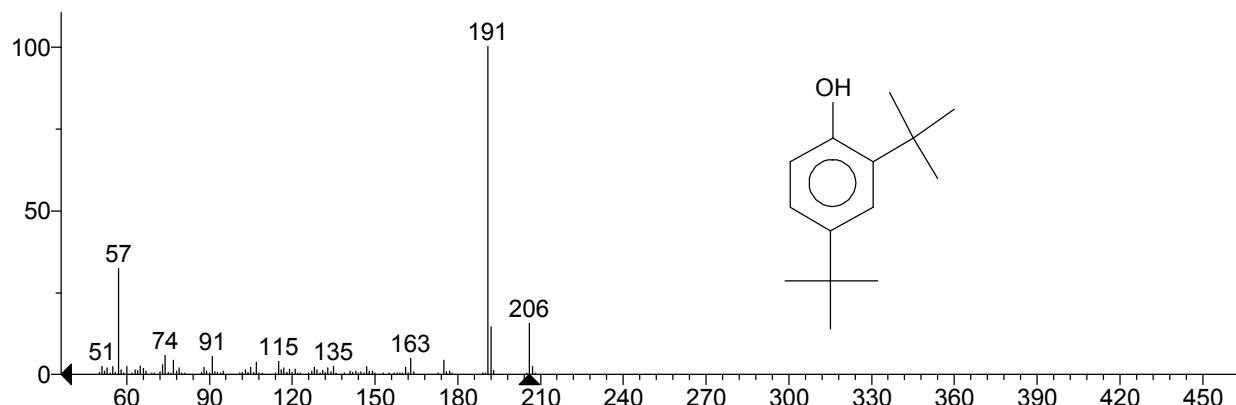


** Search Report Page 1 of 1 **

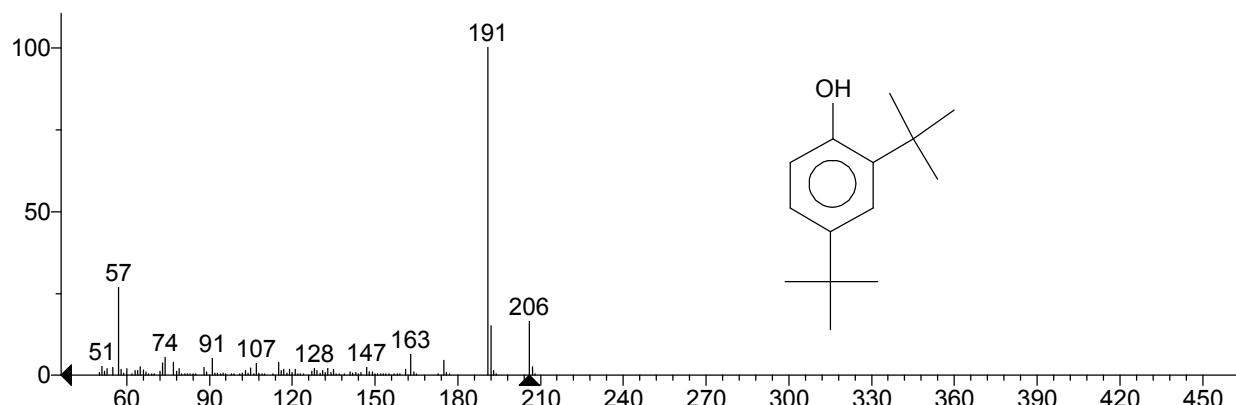
Unknown: +EI Scan (14.096-14.100, 14.123-14.127 min, 4 Scans) MeOHExtract1.D Subtract
Compound in Library Factor = -157



Hit 1 : Phenol, 2,4-bis(1,1-dimethylethyl)-
C14H22O; MF: 861; RMF: 878; Prob 46.3%; CAS: 96-76-4; Lib: mainlib; ID: 156338.

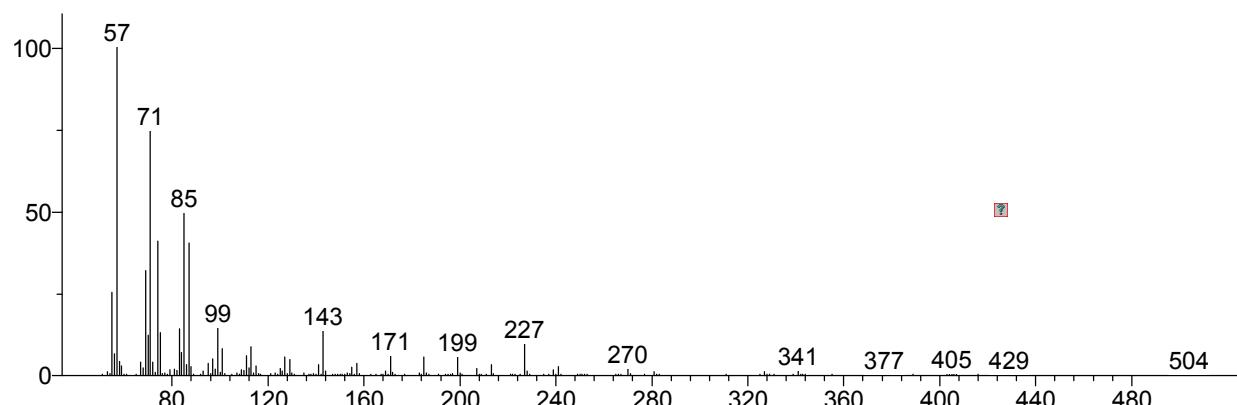


Hit 2 : Phenol, 2,4-bis(1,1-dimethylethyl)-
C14H22O; MF: 859; RMF: 878; Prob 46.3%; CAS: 96-76-4; Lib: replib; ID: 25771.



** Search Report Page 1 of 1 **

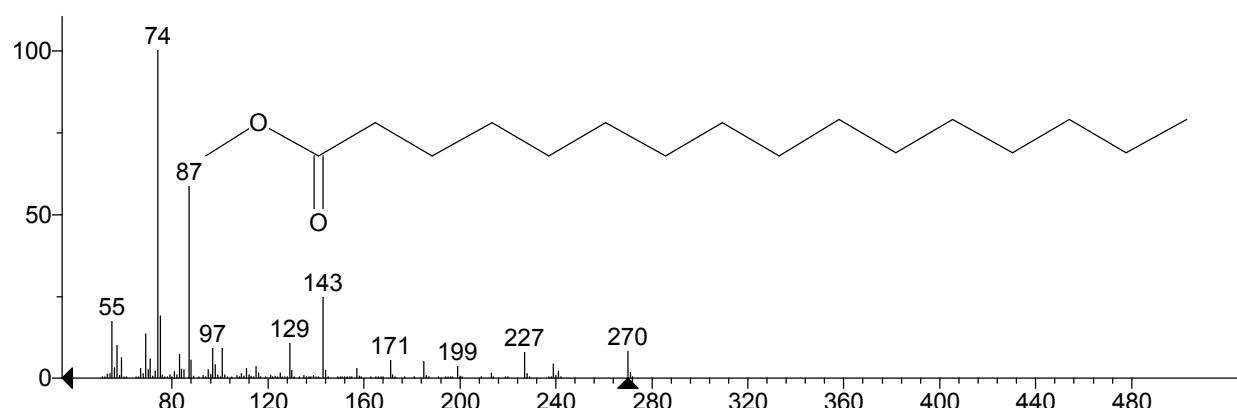
Unknown: +EI Scan (17.181 min) MeOHExtract1.D Subtract
 Compound in Library Factor = -632



Hit 1 : Tridecanoic acid, 4,8,12-trimethyl-, methyl ester
 C17H34O2; MF: 732; RMF: 802; Prob 42.3%; CAS: 10339-74-9; Lib: replib; ID: 11872.

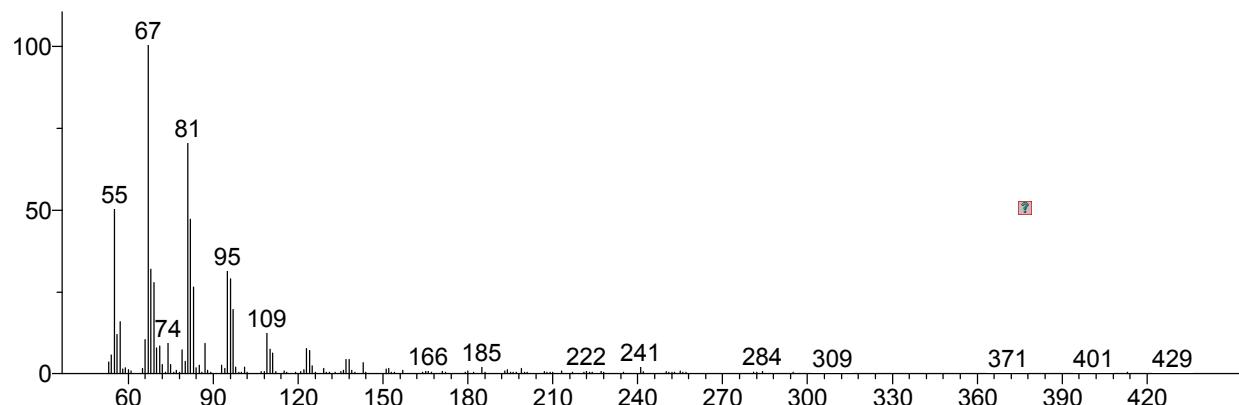


Hit 2 : Hexadecanoic acid, methyl ester
 C17H34O2; MF: 699; RMF: 728; Prob 11.1%; CAS: 112-39-0; Lib: replib; ID: 9769.

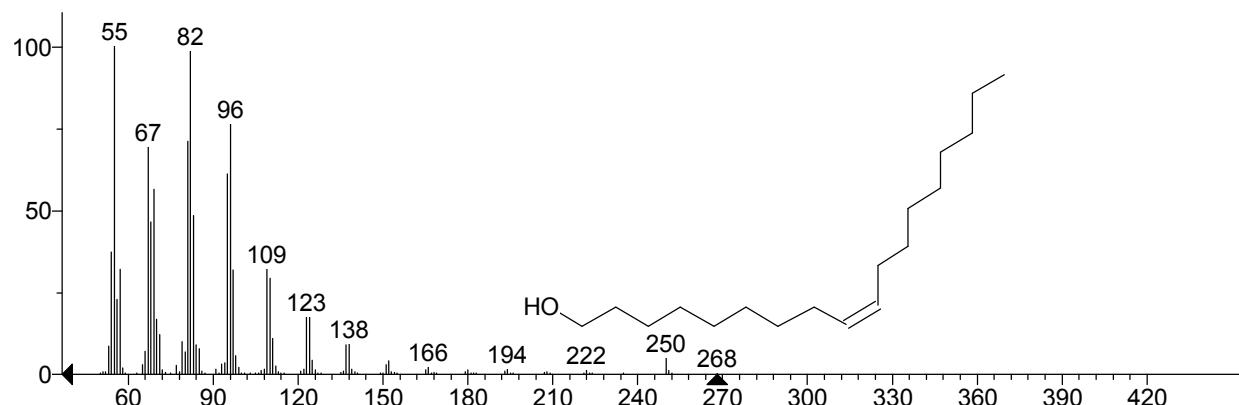


** Search Report Page 1 of 1 **

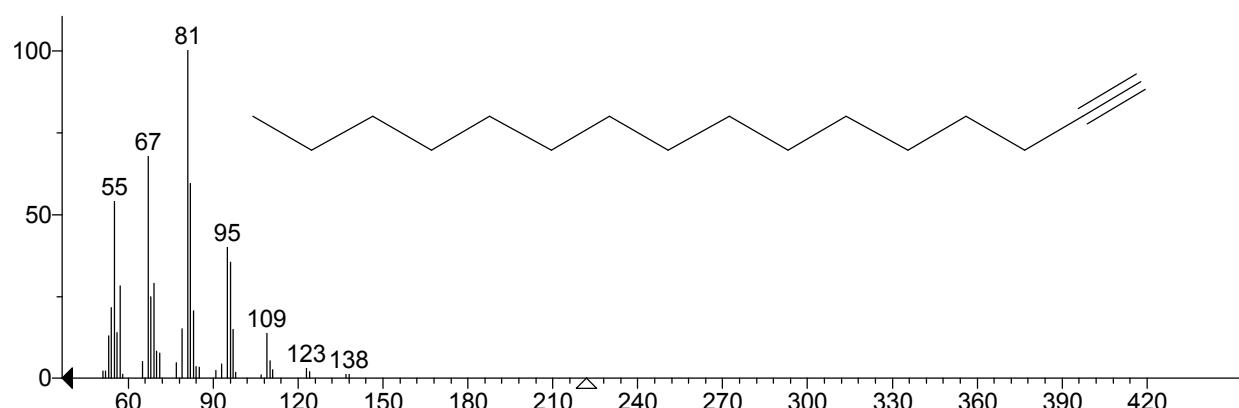
Unknown: +EI Scan (17.775-17.809 min, 11 Scans) MeOHExtract1.D Subtract
 Compound in Library Factor = -688



Hit 1 : 9-Octadecen-1-ol, (Z)-
 C18H36O; MF: 807; RMF: 848; Prob 4.41%; CAS: 143-28-2; Lib: mainlib; ID: 19267.

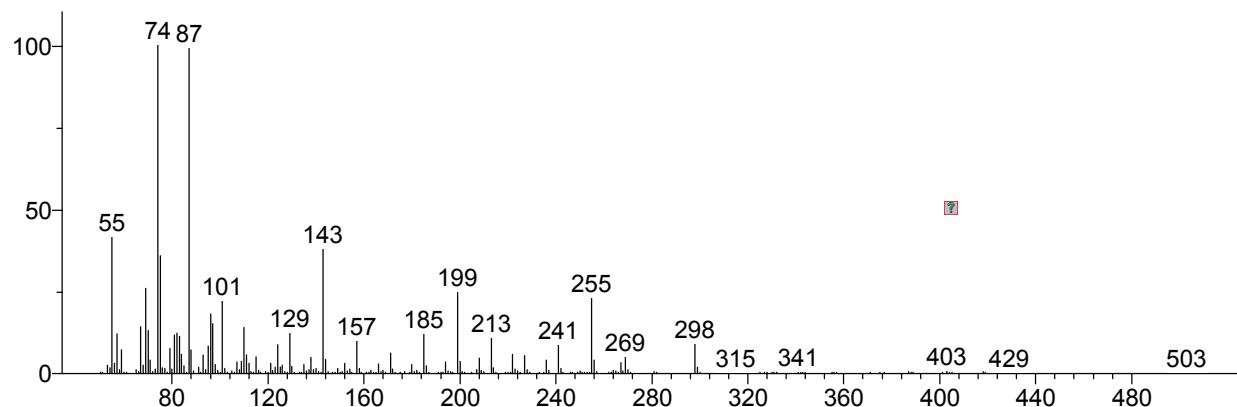


Hit 2 : 1-Hexadecyne
 C16H30; MF: 801; RMF: 907; Prob 3.47%; CAS: 629-74-3; Lib: replib; ID: 10761.

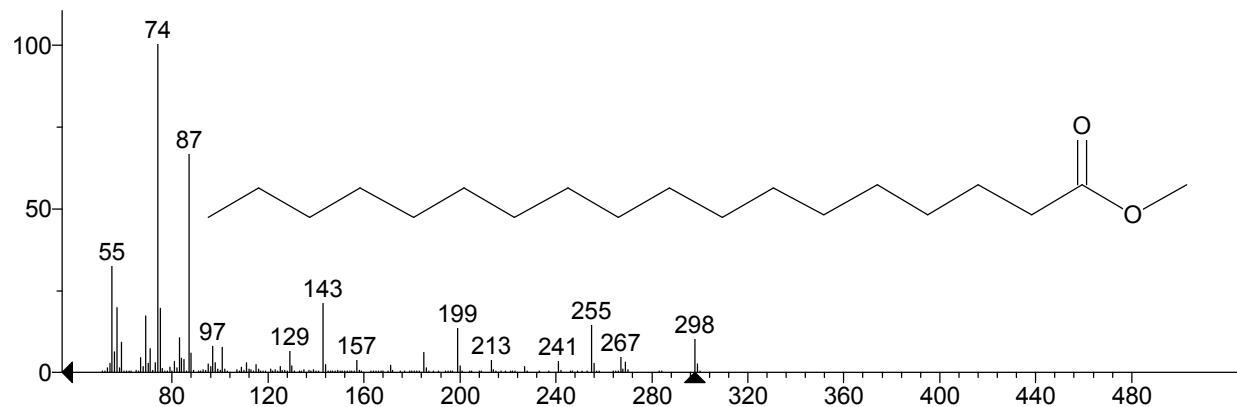


** Search Report Page 1 of 1 **

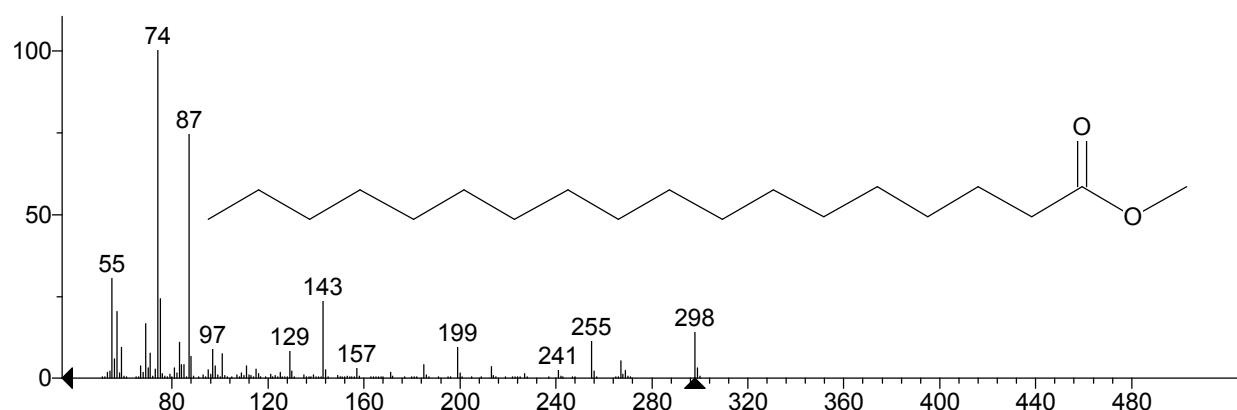
Unknown: +EI Scan (18.249-18.376 min, 39 Scans) MeOHExtract1.D Subtract
 Compound in Library Factor = -285



Hit 1 : Methyl stearate
 C₁₉H₃₈O₂; MF: 783; RMF: 814; Prob 58.6%; CAS: 112-61-8; Lib: replib; ID: 9808.

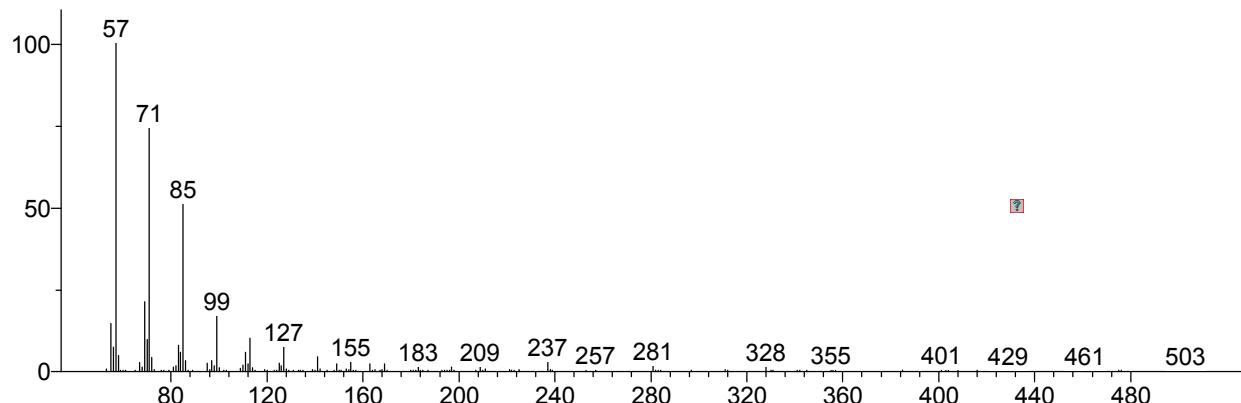


Hit 2 : Methyl stearate
 C₁₉H₃₈O₂; MF: 766; RMF: 792; Prob 58.6%; CAS: 112-61-8; Lib: mainlib; ID: 40712.

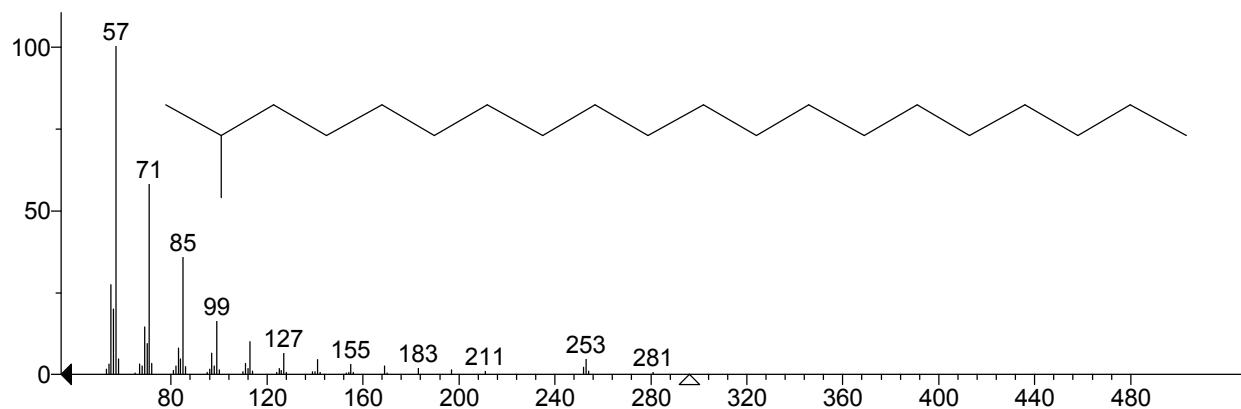


** Search Report Page 1 of 1 **

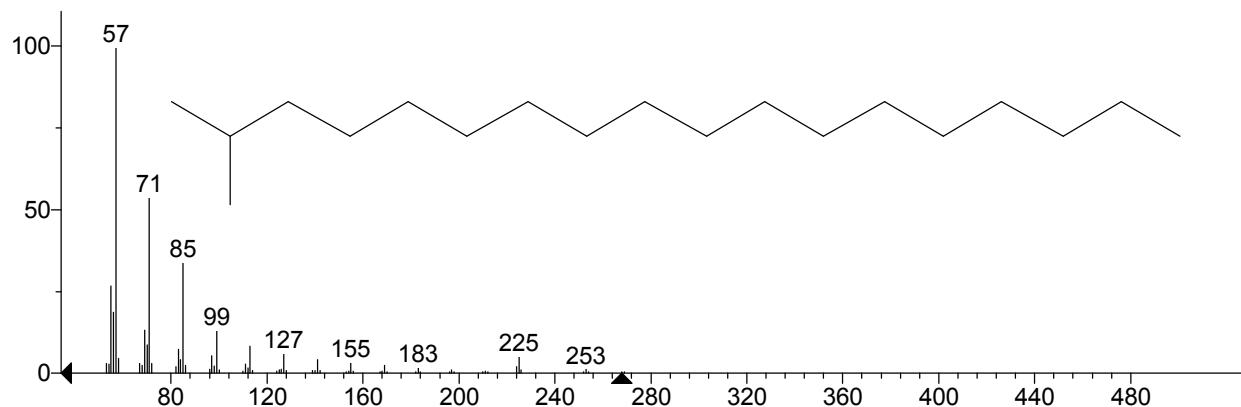
Unknown: +EI Scan (18.762-18.769, 18.789-18.799 min, 7 Scans) MeOHExtract1.D Subtract
Compound in Library Factor = -509



Hit 1 : Eicosane, 2-methyl-
C₂₁H₄₄; MF: 798; RMF: 869; Prob 6.78%; CAS: 1560-84-5; Lib: mainlib; ID: 22547.

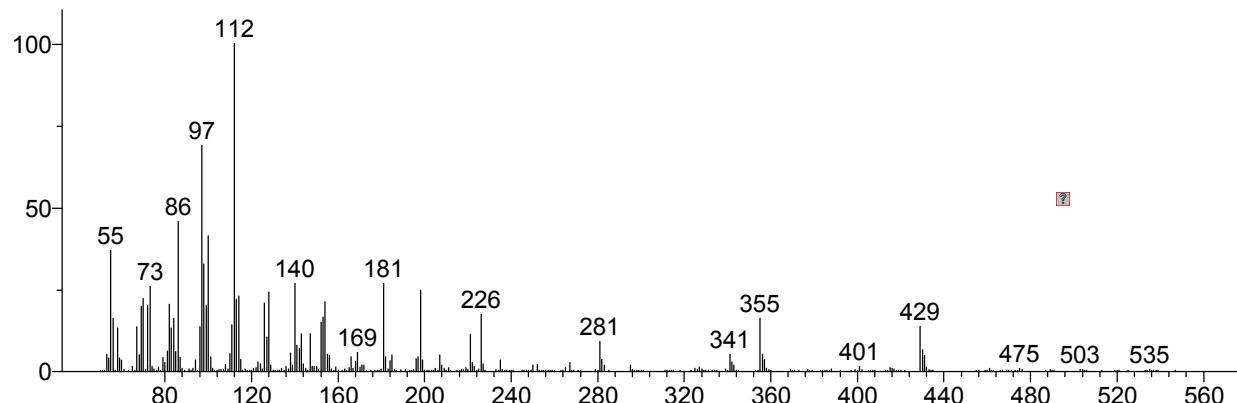


Hit 2 : Octadecane, 2-methyl-
C₁₉H₄₀; MF: 797; RMF: 875; Prob 6.52%; CAS: 1560-88-9; Lib: replib; ID: 2198.

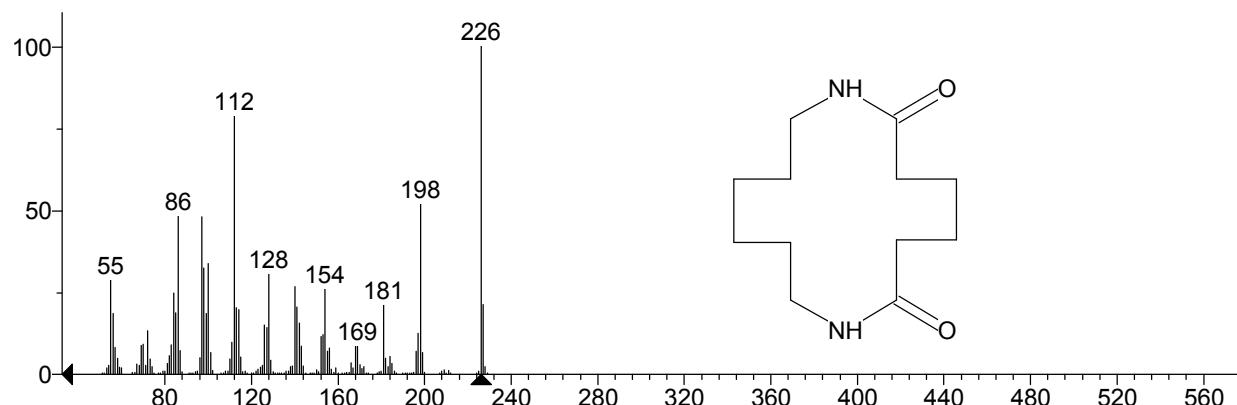


** Search Report Page 1 of 1 **

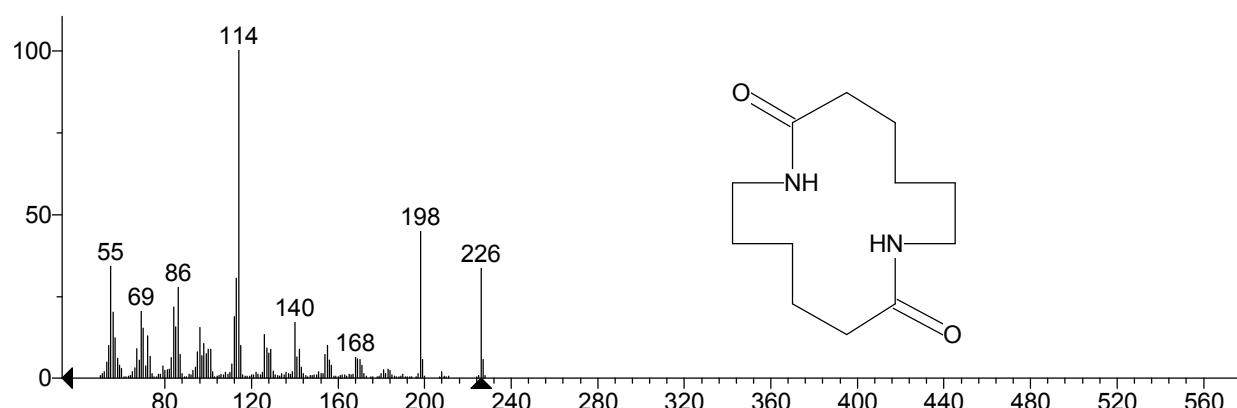
Unknown: +EI Scan (19.316-19.393 min, 24 Scans) MeOHExtract1.D Subtract
 Compound in Library Factor = -550



Hit 1 : 1,8-Diazacyclotetradecane-2,7-dione
 C12H22N2O2; MF: 650; RMF: 776; Prob 69.7%; CAS: 4266-66-4; Lib: mainlib; ID: 175001.

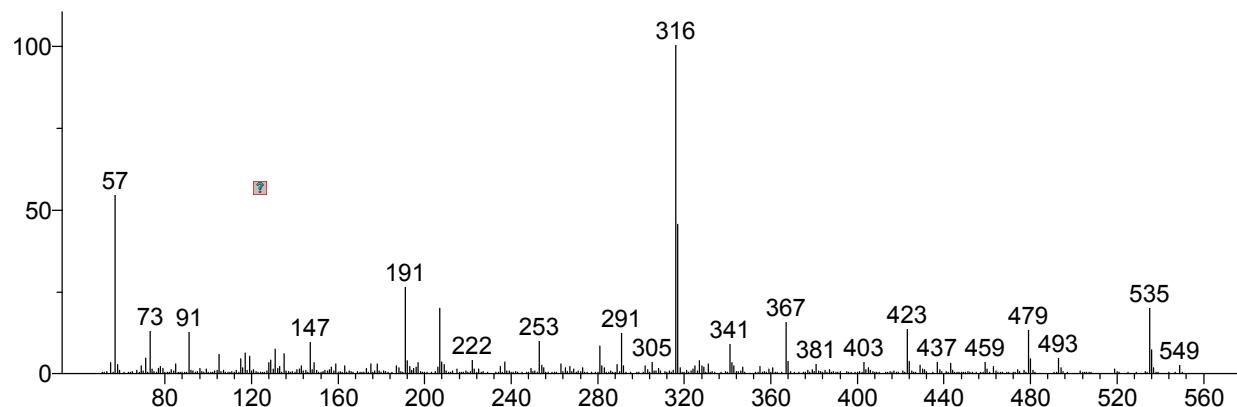


Hit 2 : 1,8-Diazacyclotetradecane-2,9-dione
 C12H22N2O2; MF: 573; RMF: 682; Prob 8.49%; CAS: 5776-79-4; Lib: mainlib; ID: 82198.



** Search Report Page 1 of 1 **

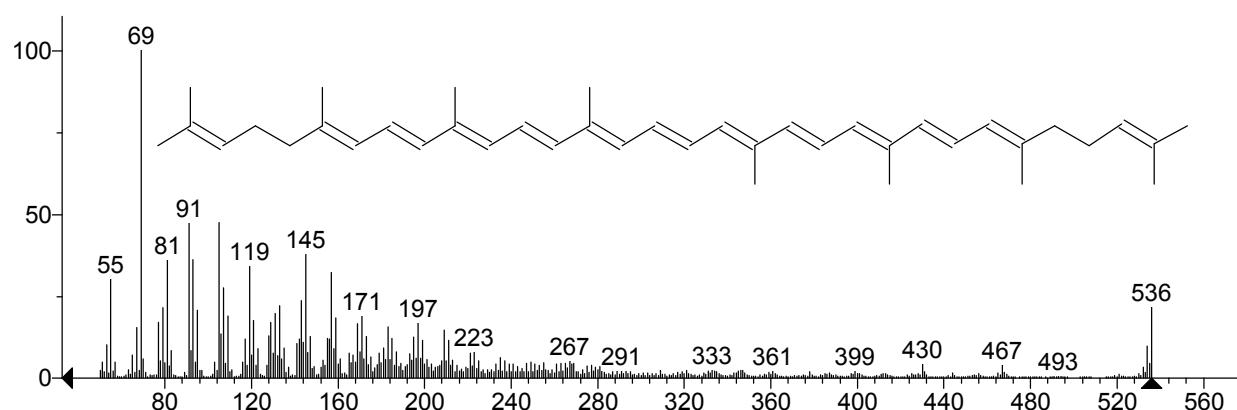
Unknown: +EI Scan (26.815-26.946 min, 40 Scans) MeOHExtract1.D Subtract
 Compound in Library Factor = -1774



Hit 1 : Lycoxanthin
 C₄₀H₅₆O; MF: 459; RMF: 459; Prob 7.54%; CAS: 19891-74-8; Lib: mainlib; ID: 53605.



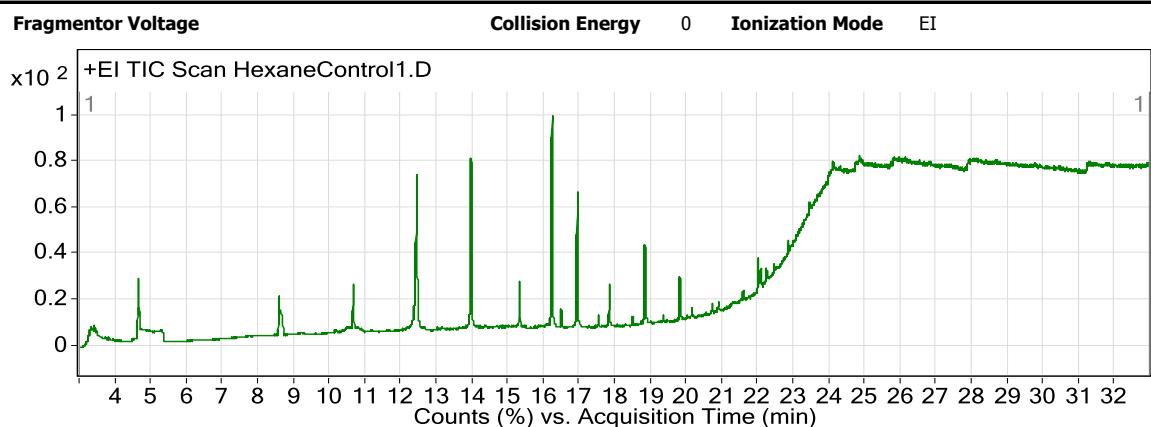
Hit 2 : Lycopene
 C₄₀H₅₆; MF: 456; RMF: 459; Prob 6.66%; CAS: 502-65-8; Lib: replib; ID: 8053.



Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | HexaneControl1.D | Sample Name | Hexane Control |
| Sample Type | | Position | 63 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 10:18:27 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Chromatograms

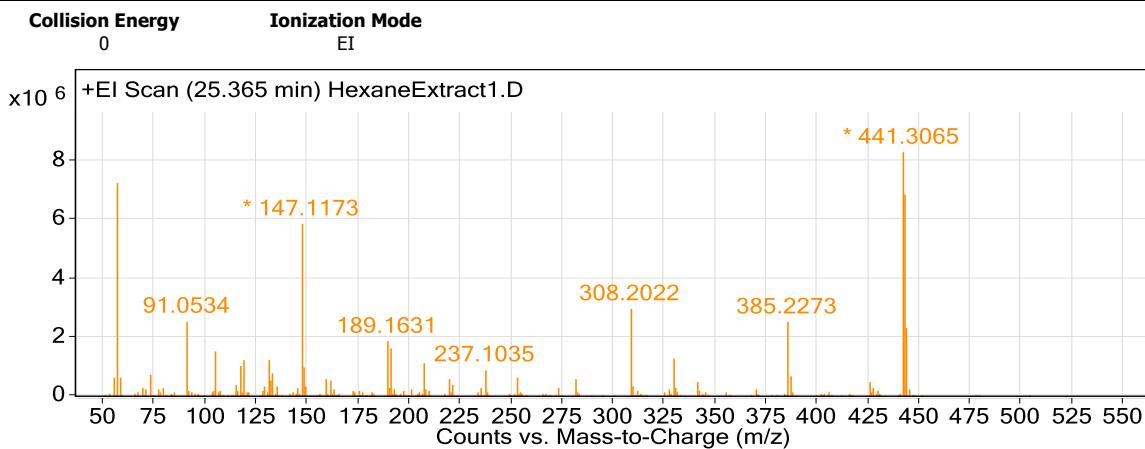


--- End Of Report ---

Qualitative Analysis Report

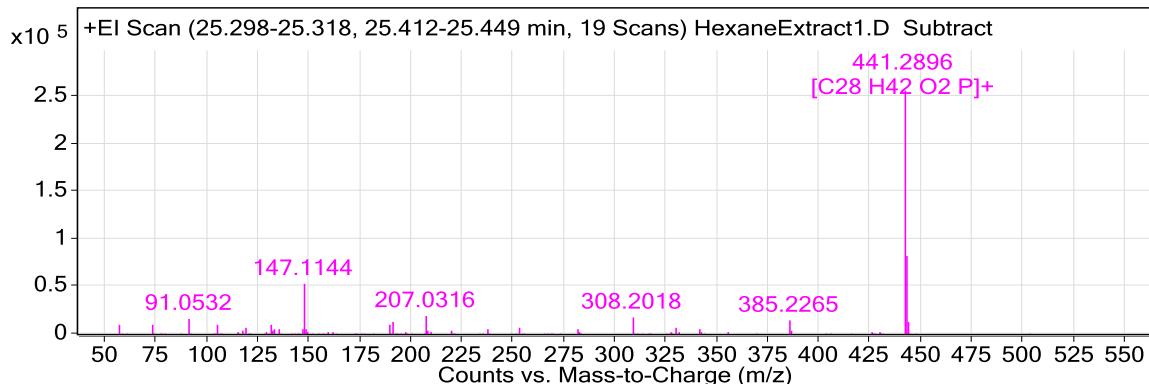
| | | | |
|-------------------------------|----------------------------|-------------------------------|--|
| Data Filename | HexaneExtract1.D | Sample Name | Hexane Extract |
| Sample Type | | Position | 64 |
| Instrument Name | GC-QTOF | User Name | |
| Acq Method | GCMS.M | Acquired Time | 5/20/2014 12:21:02 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |
| Expected Barcode | | Sample Amount | |
| Dual Inj Vol | 1 | TuneName | atunes.ei.tune.xml |
| TunePath | D:\MassHunter\GCMS\1\7200\ | TuneTimeStamp | 41778.82672 |
| | \ | | |
| MSFirmwareVersion | G.7200.01.14 | OperatorName | |
| RunCompletedFlag | TRUE | Acquisition SW Version | MassHunter GC/MS Acquisition B.07.00 SP2.1654 29-Aug-2013 Copyright © 1989-2013 Agilent Technologies, Inc. |

User Spectra

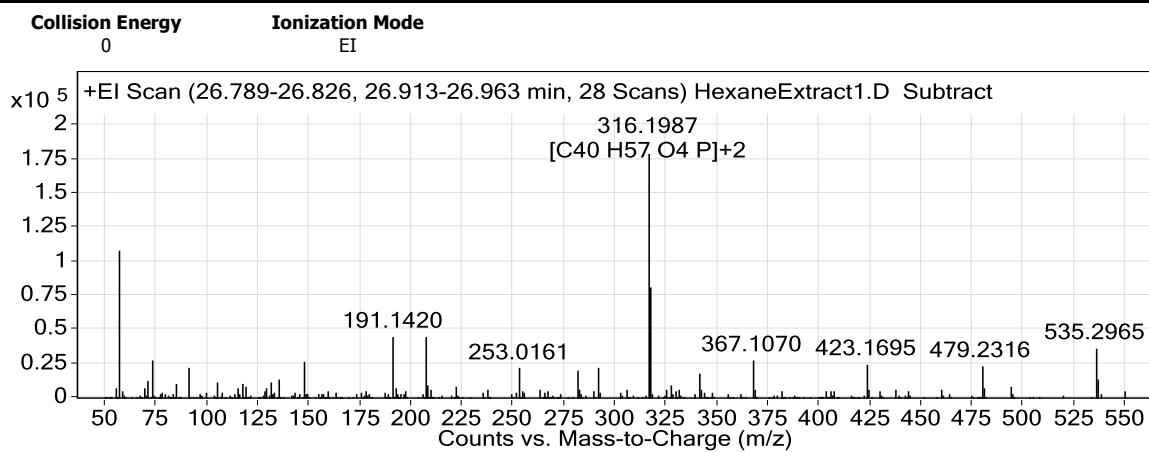


| | |
|-------------------------|------------------------|
| Collision Energy | Ionization Mode |
| 0 | EI |

Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|--|-------|-------|--|
| 441.2896 | 441.2902 | C ₂₈ H ₄₂ O ₂ P | 90.93 | 4.57 | C ₂₈ H ₄₂ O ₂ P |

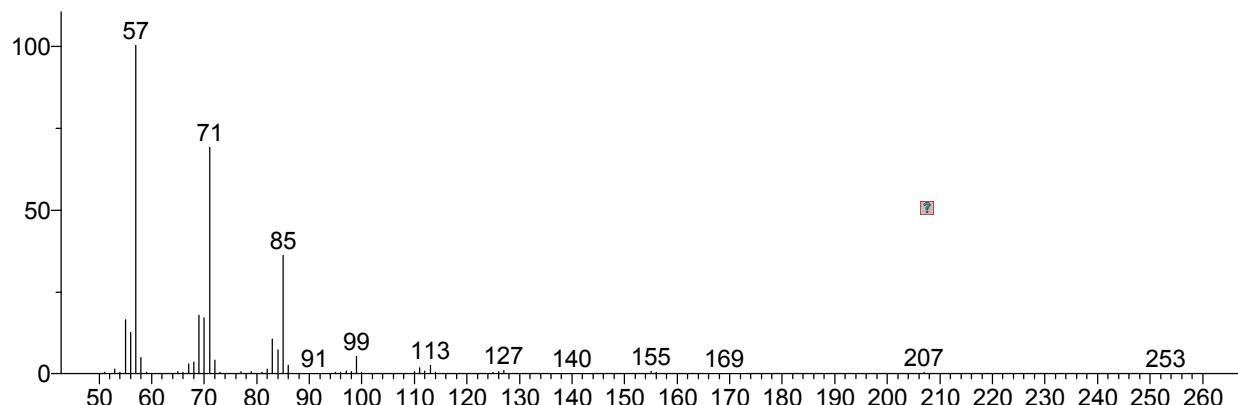
**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|--|-------|-------|--|
| 316.1987 | 632.3988 | C ₄₀ H ₅₇ O ₄ P | 99.18 | 0.99 | C ₄₀ H ₅₇ O ₄ P |

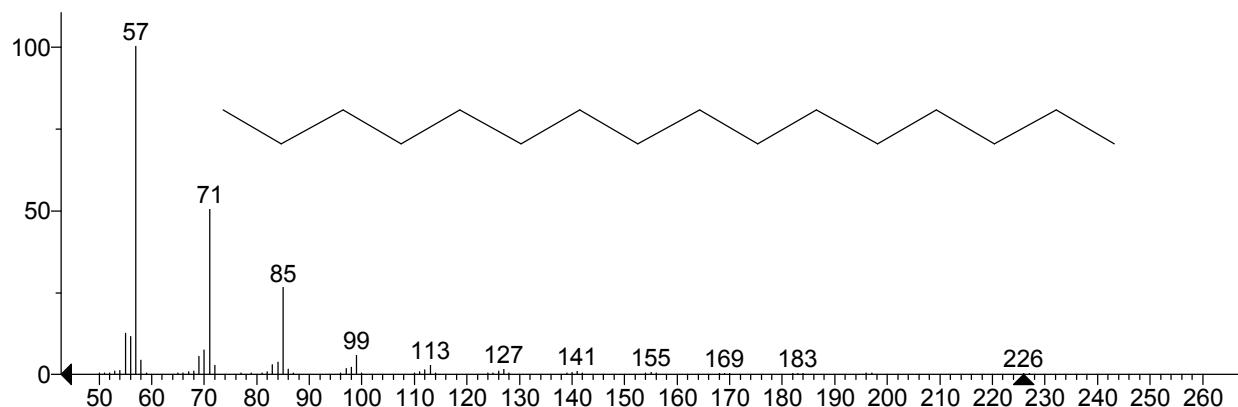
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** Search Report Page 1 of 1 **

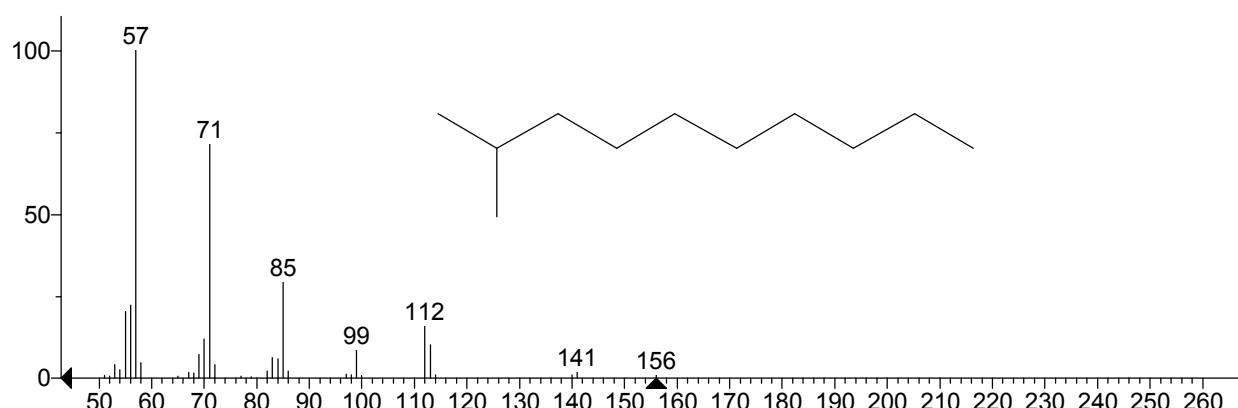
Unknown: +EI Scan (11.982-11.989, 12.009-12.016 min, 6 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -331



Hit 1 : Hexadecane
C16H34; MF: 849; RMF: 856; Prob 6.40%; CAS: 544-76-3; Lib: replib; ID: 5859.

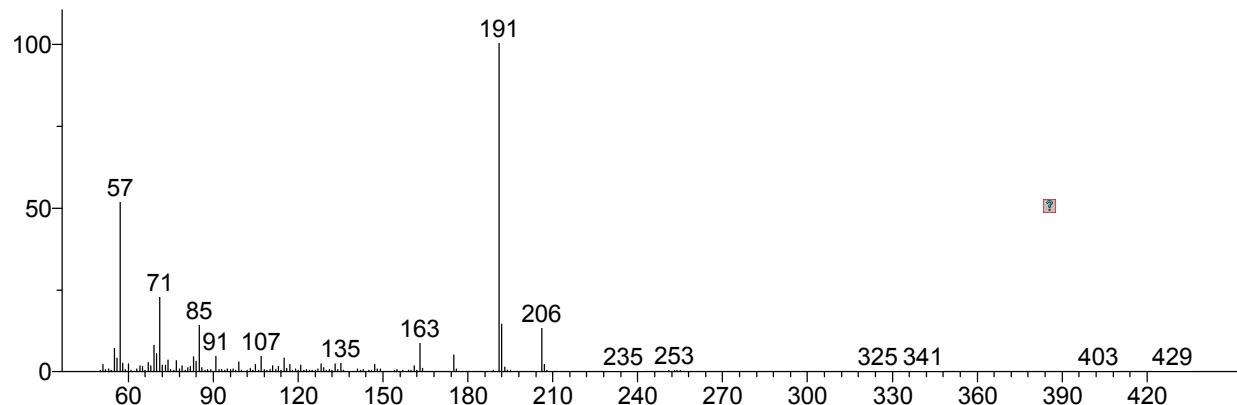


Hit 2 : Decane, 2-methyl-
C11H24; MF: 848; RMF: 865; Prob 6.15%; CAS: 6975-98-0; Lib: mainlib; ID: 22701.

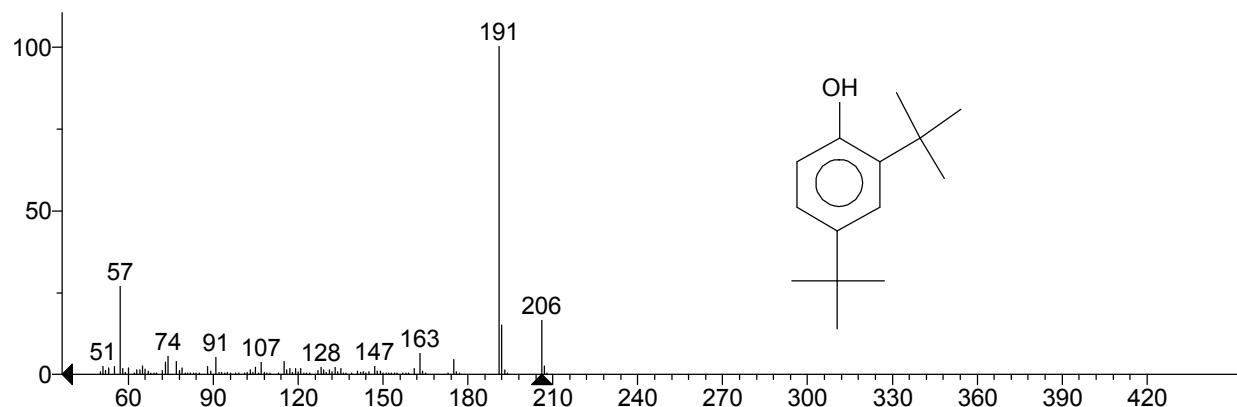


** Search Report Page 1 of 1 **

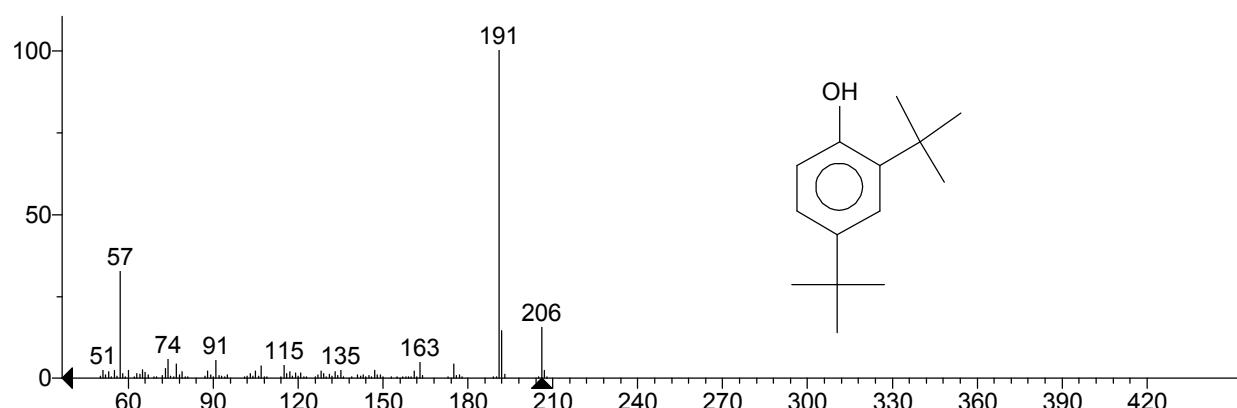
Unknown: +EI Scan (14.083-14.097, 14.120-14.124 min, 7 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -259



Hit 1 : Phenol, 2,4-bis(1,1-dimethylethyl)-
C14H22O; MF: 812; RMF: 876; Prob 40.7%; CAS: 96-76-4; Lib: replib; ID: 25771.

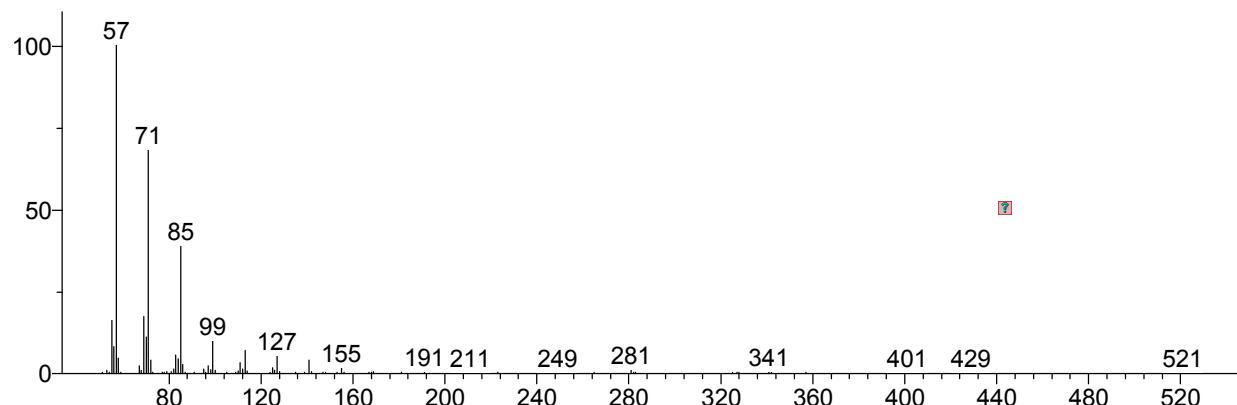


Hit 2 : Phenol, 2,4-bis(1,1-dimethylethyl)-
C14H22O; MF: 803; RMF: 862; Prob 40.7%; CAS: 96-76-4; Lib: mainlib; ID: 156338.

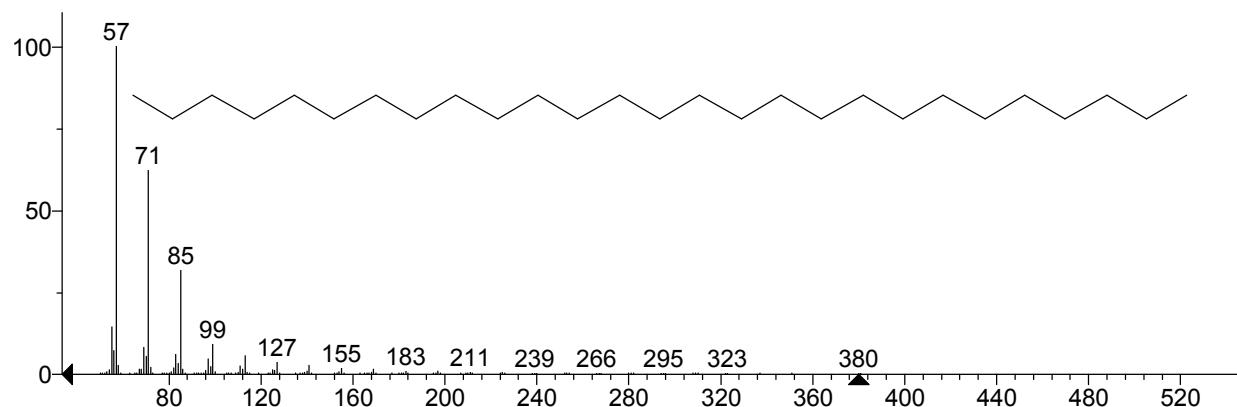


** Search Report Page 1 of 1 **

Unknown: +EI Scan (14.302-14.308, 14.349-14.362 min, 8 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -454



Hit 1 : Heptacosane
C₂₇H₅₆; MF: 843; RMF: 853; Prob 5.46%; CAS: 593-49-7; Lib: replib; ID: 5812.

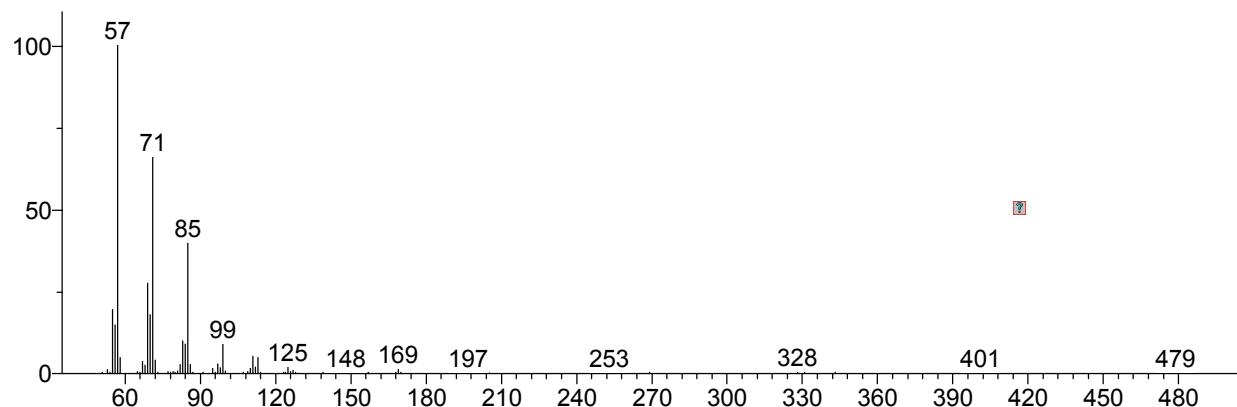


Hit 2 : Heptadecane, 2,6,10,15-tetramethyl-
C₂₁H₄₄; MF: 839; RMF: 848; Prob 4.62%; CAS: 54833-48-6; Lib: mainlib; ID: 23564.



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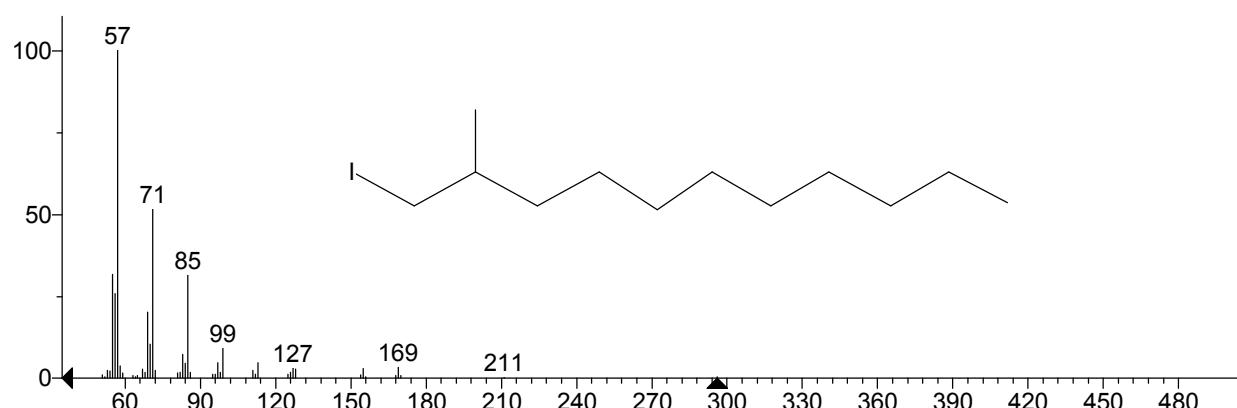
Unknown: +EI Scan (14.392-14.402, 14.419-14.439 min, 11 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -331



Hit 1 : Dodecane, 2,6,11-trimethyl-
C15H32; MF: 847; RMF: 869; Prob 7.73%; CAS: 31295-56-4; Lib: replib; ID: 6070.

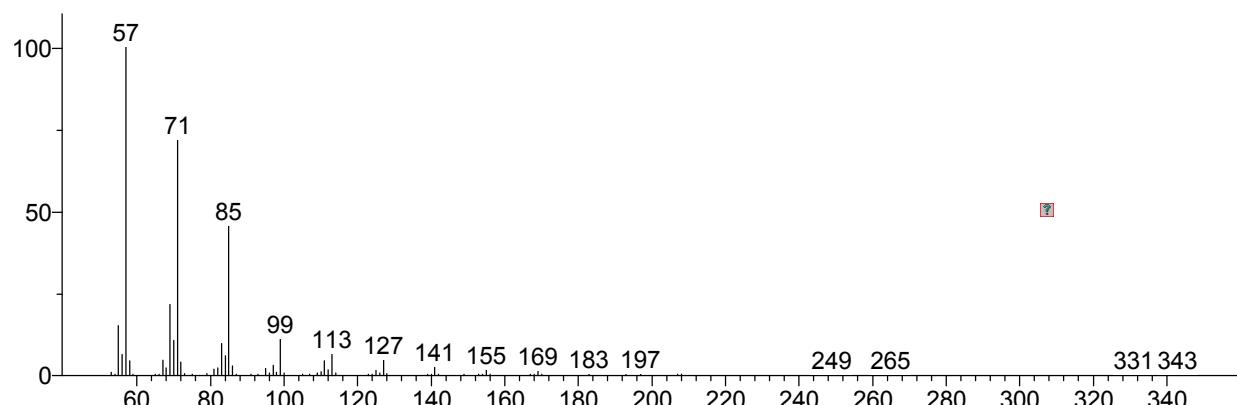


Hit 2 : 1-Iodo-2-methylundecane
C12H25I; MF: 844; RMF: 859; Prob 6.83%; CAS: 73105-67-6; Lib: mainlib; ID: 22546.

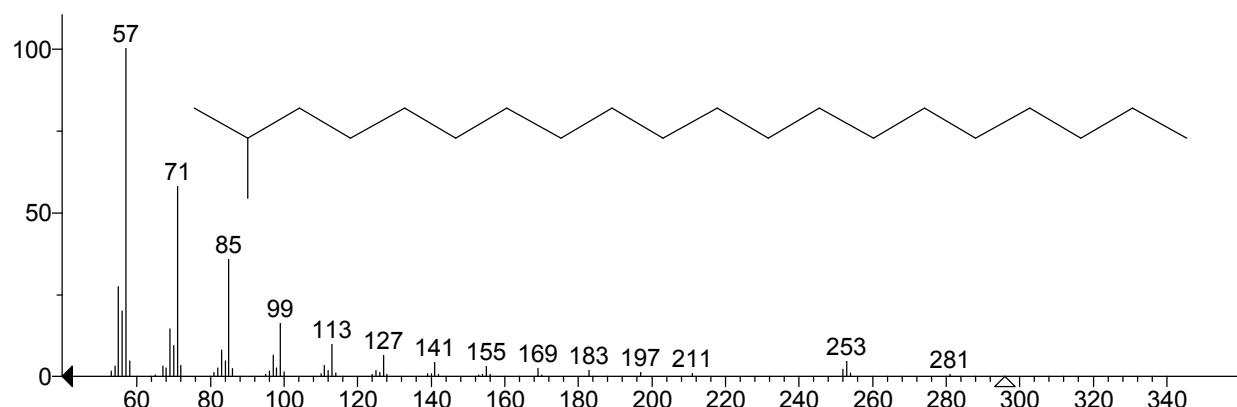


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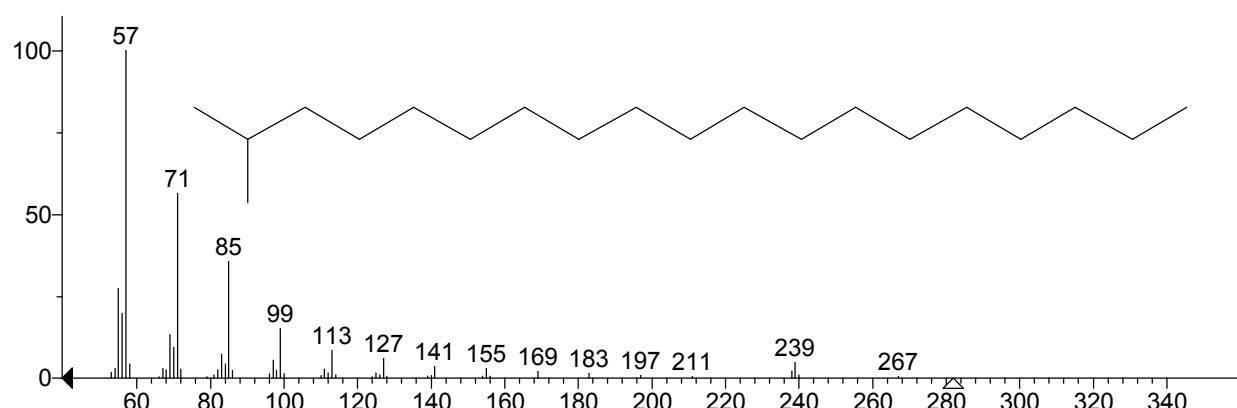
Unknown: +EI Scan (15.638, 15.678 min, 2 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -389



Hit 1 : Eicosane, 2-methyl-
C₂₁H₄₄; MF: 851; RMF: 857; Prob 5.83%; CAS: 1560-84-5; Lib: mainlib; ID: 22547.

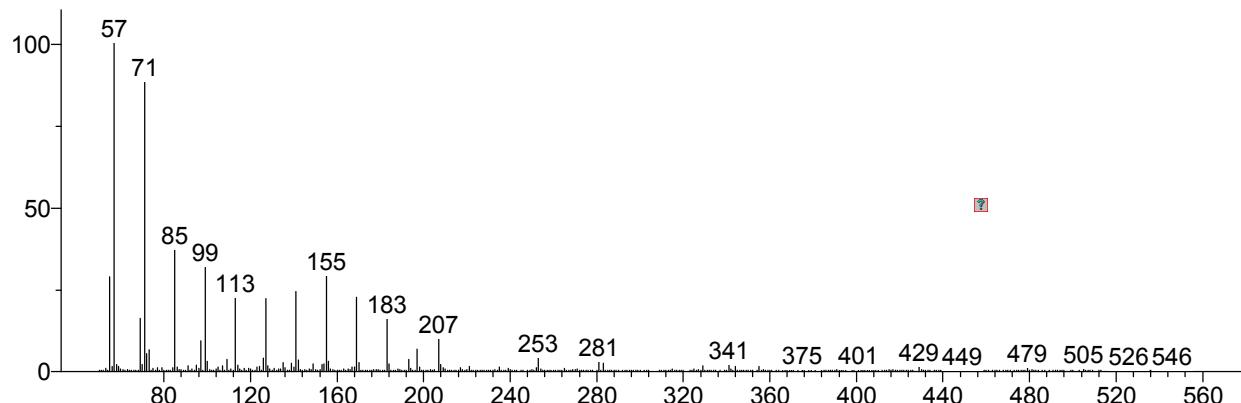


Hit 2 : Nonadecane, 2-methyl-
C₂₀H₄₂; MF: 848; RMF: 858; Prob 5.15%; CAS: 1560-86-7; Lib: mainlib; ID: 22565.

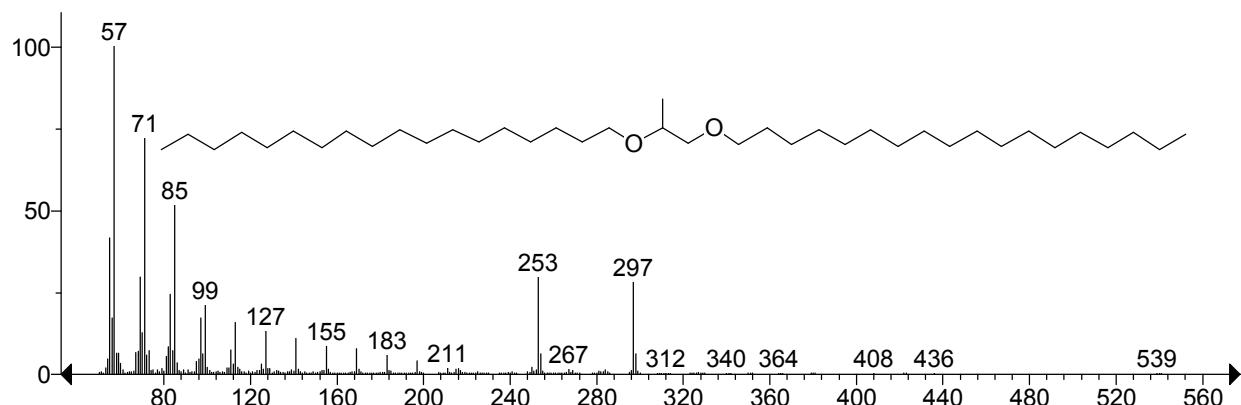


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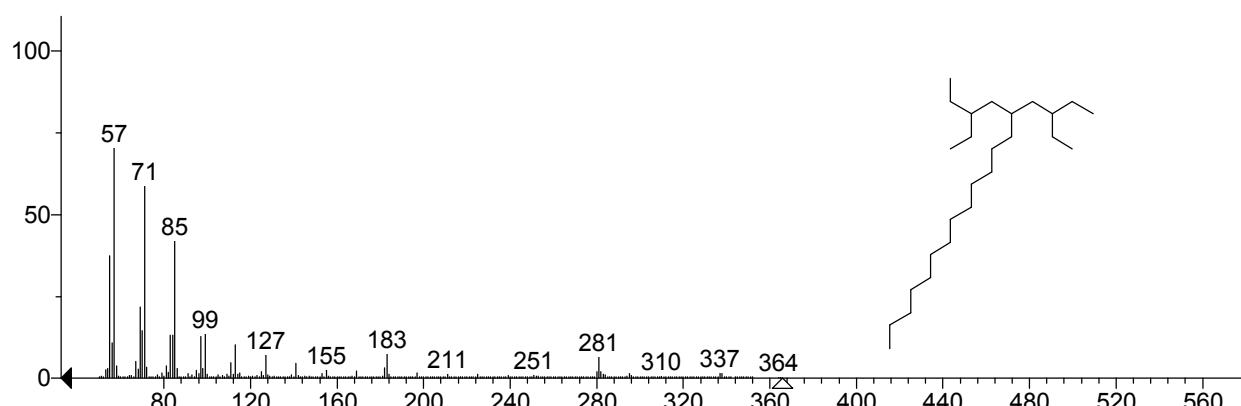
Unknown: +EI Scan (15.950, 15.997-16.013 min, 7 Scans) HexaneExtract1.D Subtract
 Compound in Library Factor = -1302



Hit 1 : Octadecane, 1,1'-(1-methyl-1,2-ethanediyl)bis(oxy)]bis-
 C39H80O2; MF: 630; RMF: 666; Prob 8.30%; CAS: 35545-51-8; Lib: mainlib; ID: 22665.

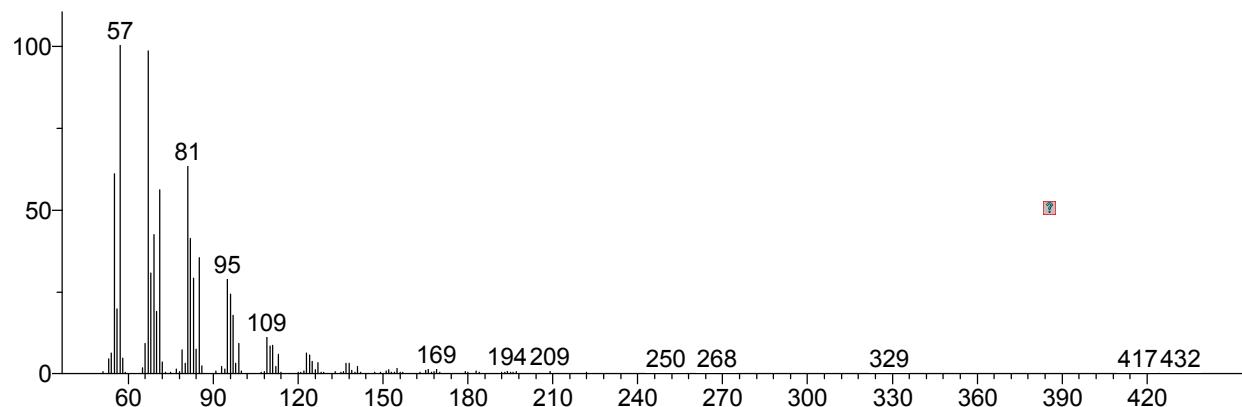


Hit 2 : Octadecane, 3-ethyl-5-(2-ethylbutyl)-
 C26H54; MF: 622; RMF: 652; Prob 6.19%; CAS: 55282-12-7; Lib: mainlib; ID: 7471.

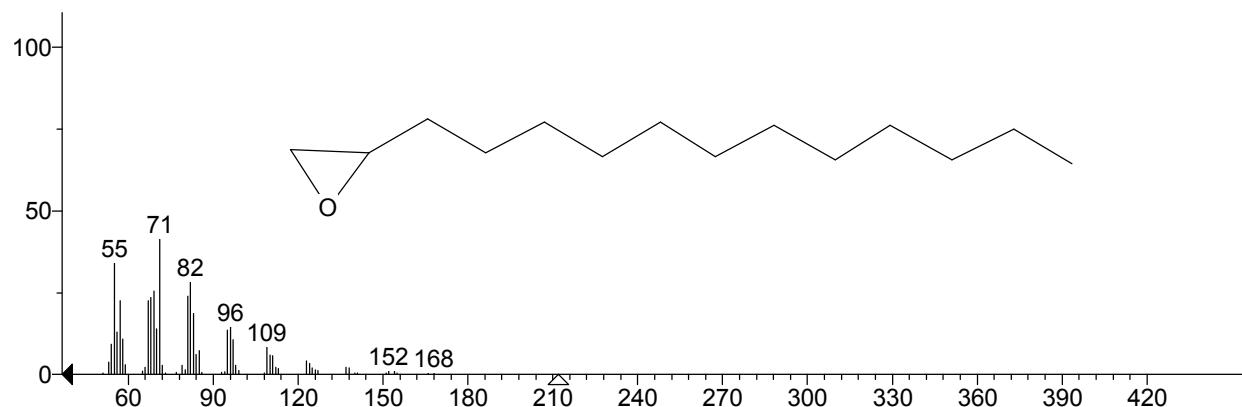


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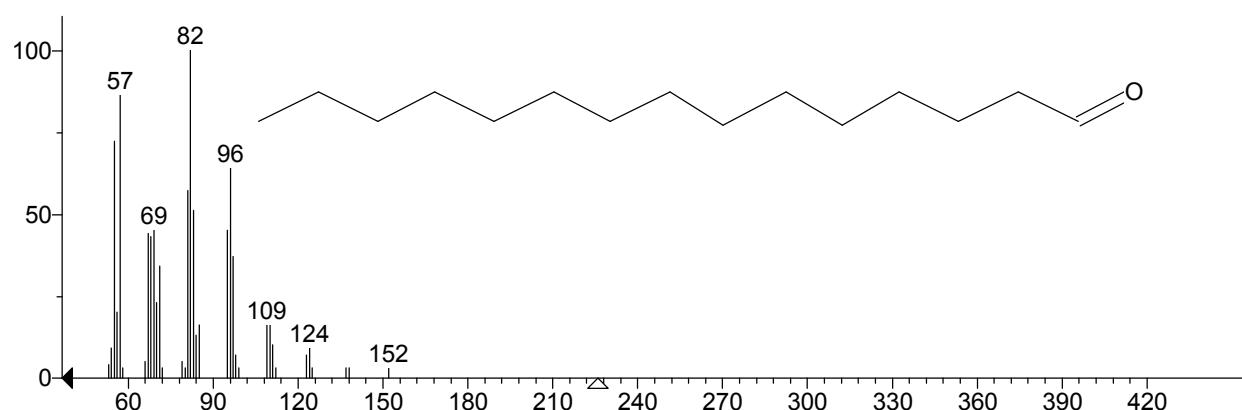
Unknown: +EI Scan (16.400-16.457 min, 18 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -331



Hit 1 : Oxirane, dodecyl-
C14H28O; MF: 844; RMF: 865; Prob 12.7%; CAS: 3234-28-4; Lib: replib; ID: 835.

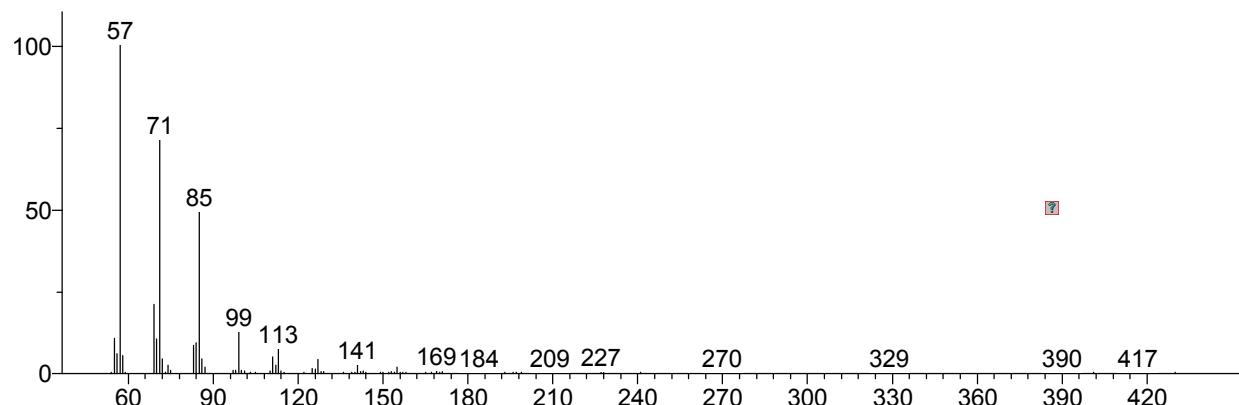


Hit 2 : Pentadecanal-
C15H30O; MF: 839; RMF: 880; Prob 10.3%; CAS: 2765-11-9; Lib: replib; ID: 10961.

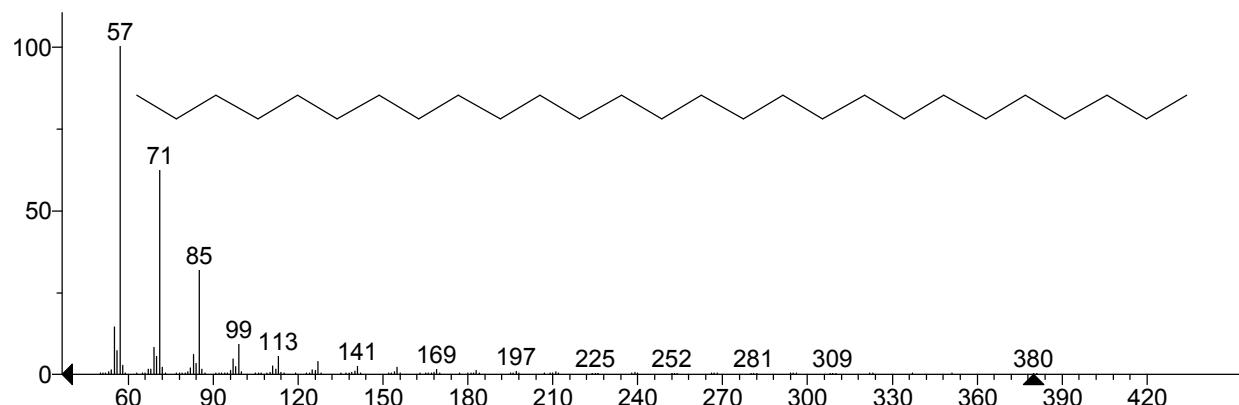


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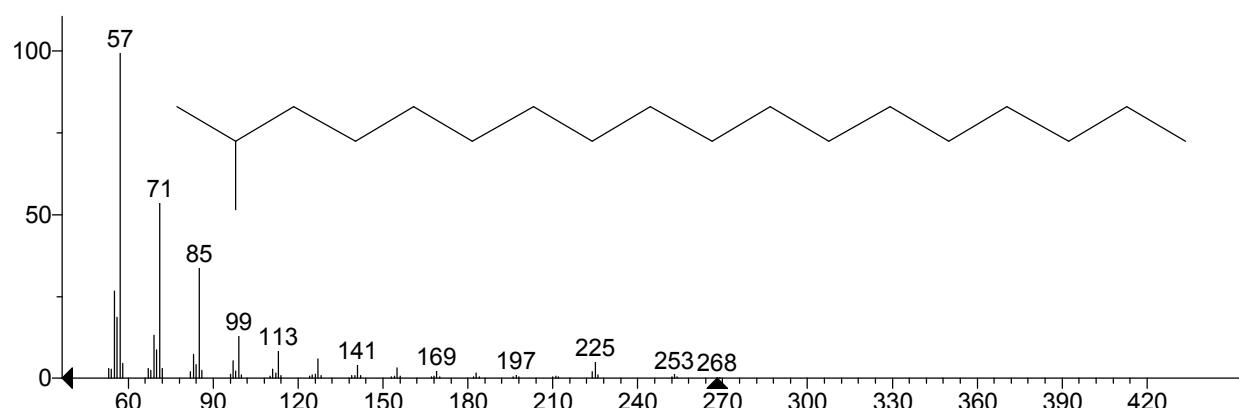
Unknown: +EI Scan (17.135-17.148, 17.188 min, 6 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -407



Hit 1 : Heptacosane
C₂₇H₅₆; MF: 817; RMF: 838; Prob 5.43%; CAS: 593-49-7; Lib: replib; ID: 5812.

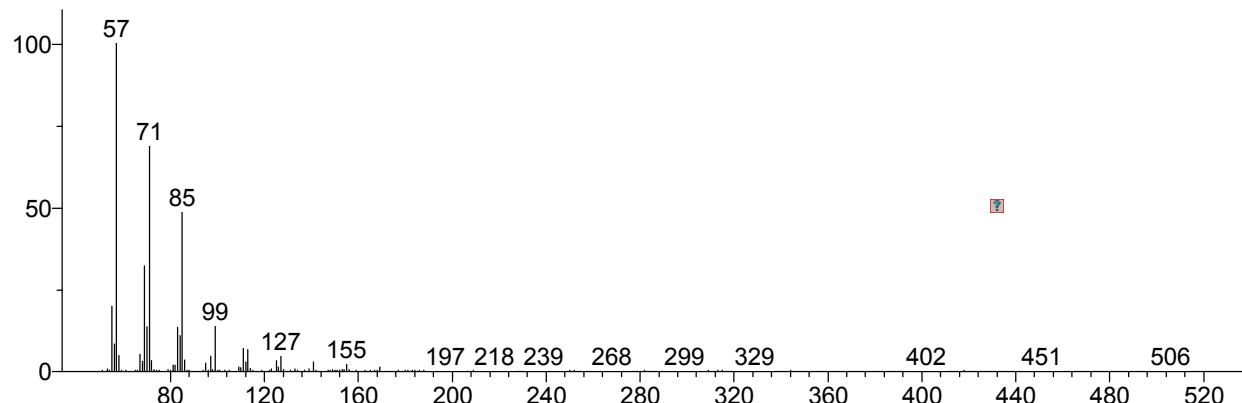


Hit 2 : Octadecane, 2-methyl-
C₁₉H₄₀; MF: 806; RMF: 826; Prob 3.73%; CAS: 1560-88-9; Lib: replib; ID: 2198.

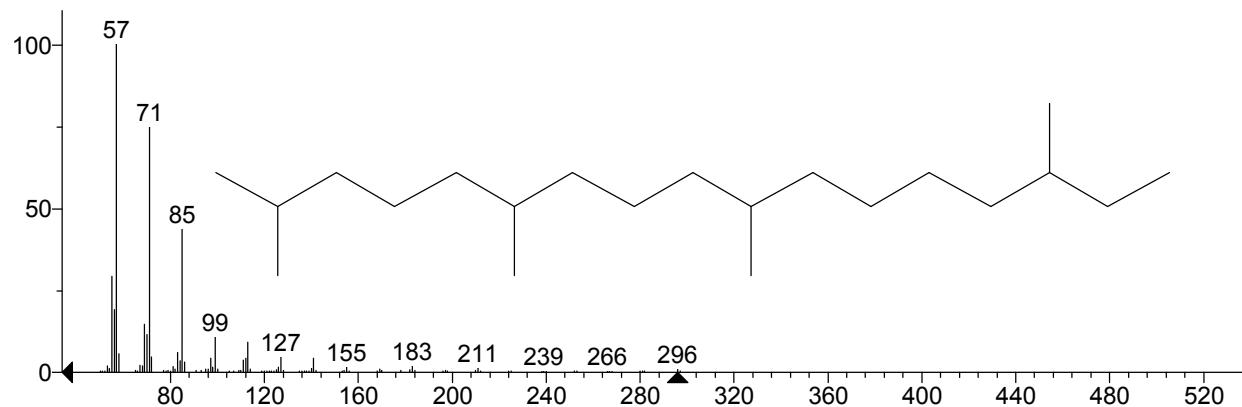


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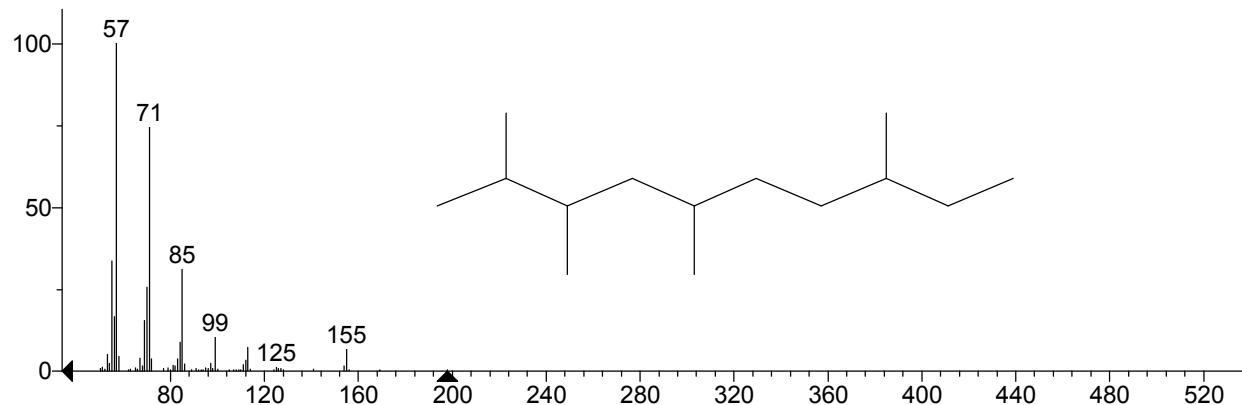
Unknown: +EI Scan (17.524-17.537, 17.564-17.571 min, 8 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -367



Hit 1 : Heptadecane, 2,6,10,15-tetramethyl-
C21H44; MF: 823; RMF: 830; Prob 7.75%; CAS: 54833-48-6; Lib: mainlib; ID: 23564.

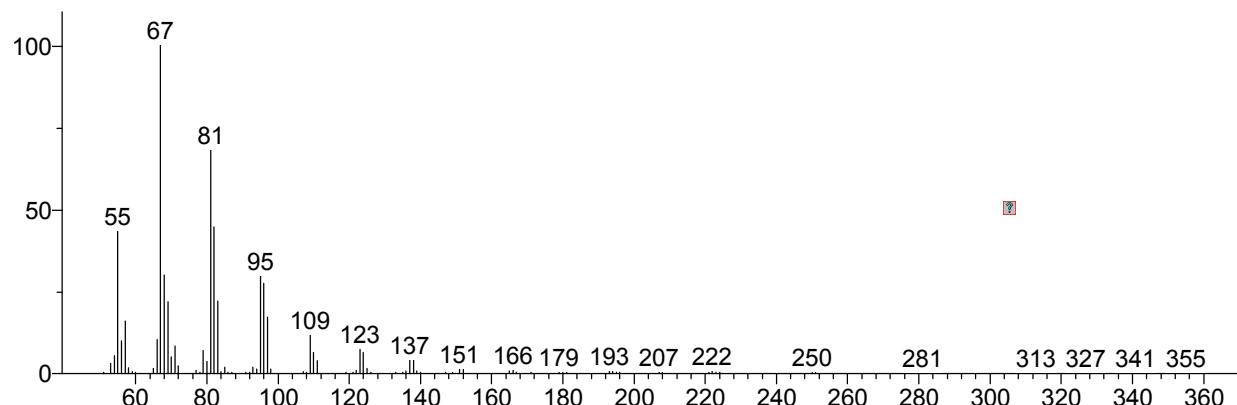


Hit 2 : Decane, 2,3,5,8-tetramethyl-
C14H30; MF: 812; RMF: 828; Prob 5.31%; CAS: 192823-15-7; Lib: mainlib; ID: 22632.

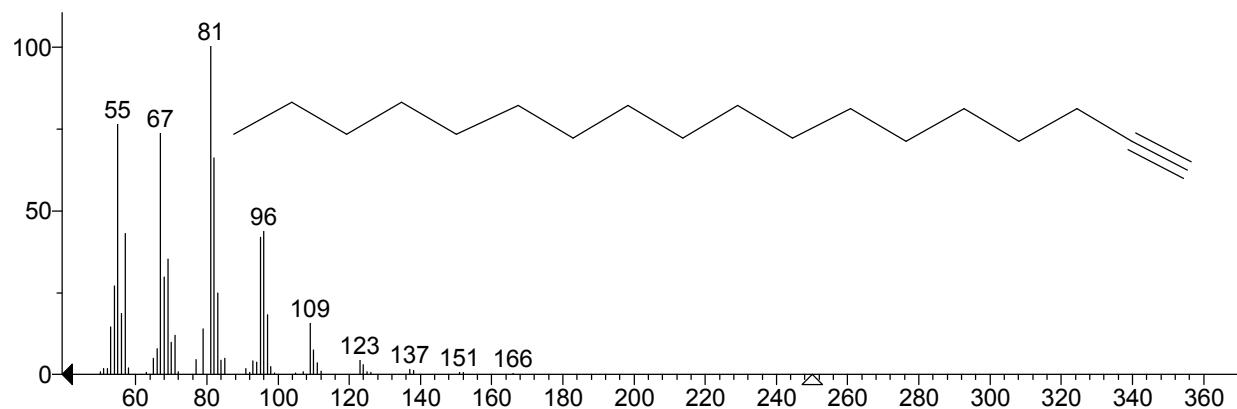


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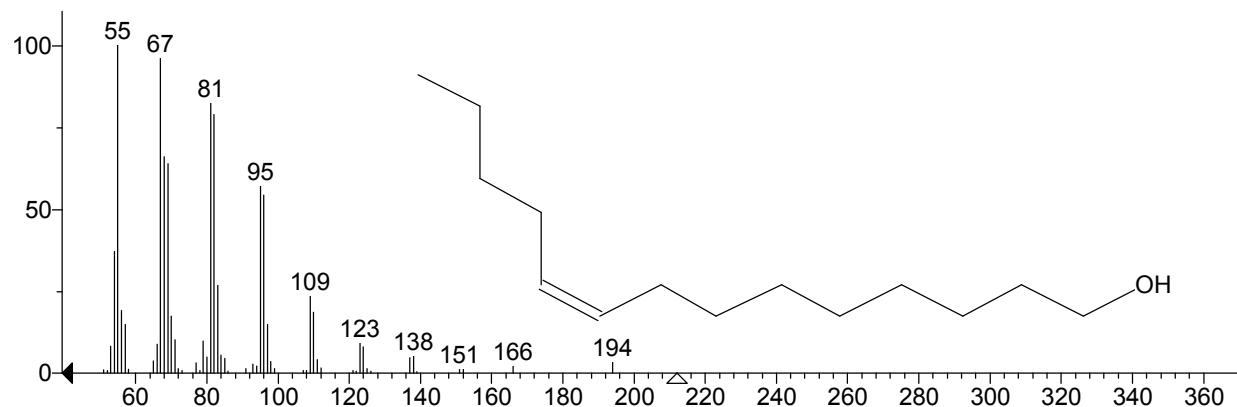
Unknown: +EI Scan (17.772-17.776, 17.796-17.806 min, 6 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -493



Hit 1 : 1-Octadecyne
C₁₈H₃₄; MF: 840; RMF: 864; Prob 3.79%; CAS: 629-89-0; Lib: mainlib; ID: 45296.

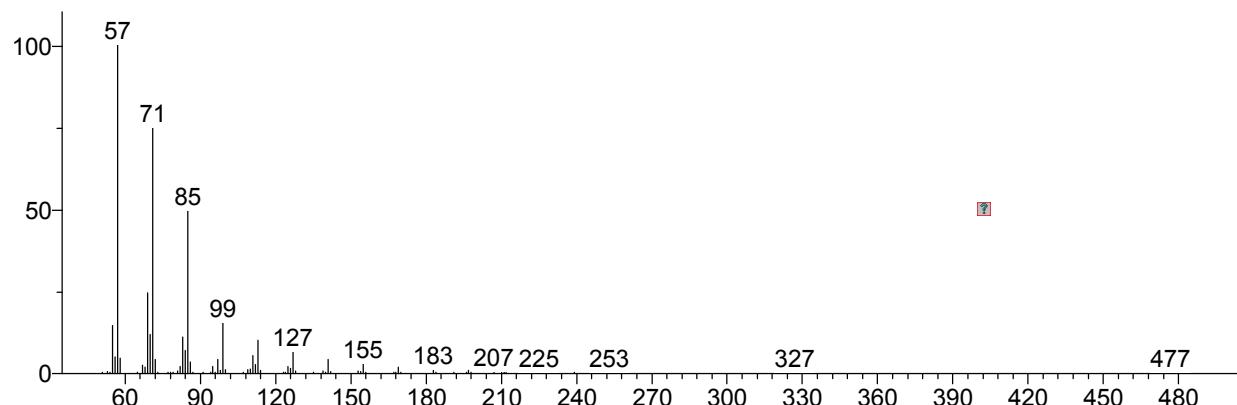


Hit 2 : cis-9-Tetradecen-1-ol
C₁₄H₂₈O; MF: 840; RMF: 854; Prob 3.79%; CAS: 35153-15-2; Lib: replib; ID: 4690.

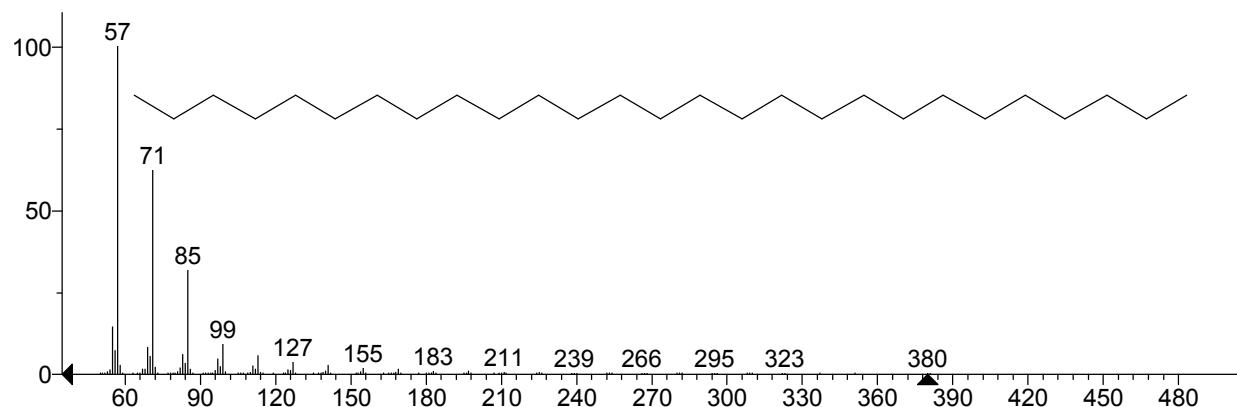


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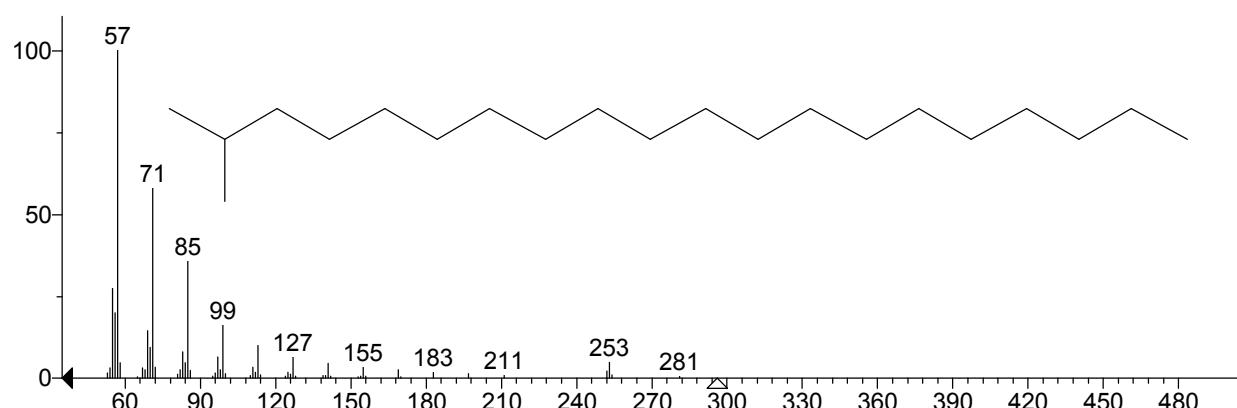
Unknown: +EI Scan (18.555-18.568, 18.578-18.581 min, 7 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -331



Hit 1 : Heptacosane
C₂₇H₅₆; MF: 842; RMF: 845; Prob 6.05%; CAS: 593-49-7; Lib: replib; ID: 5812.

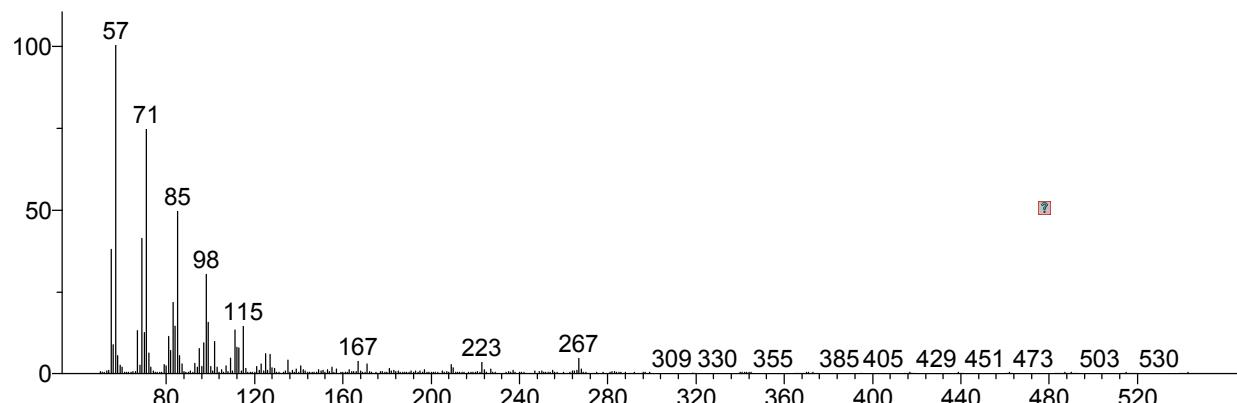


Hit 2 : Eicosane, 2-methyl-
C₂₁H₄₄; MF: 840; RMF: 848; Prob 5.58%; CAS: 1560-84-5; Lib: mainlib; ID: 22547.

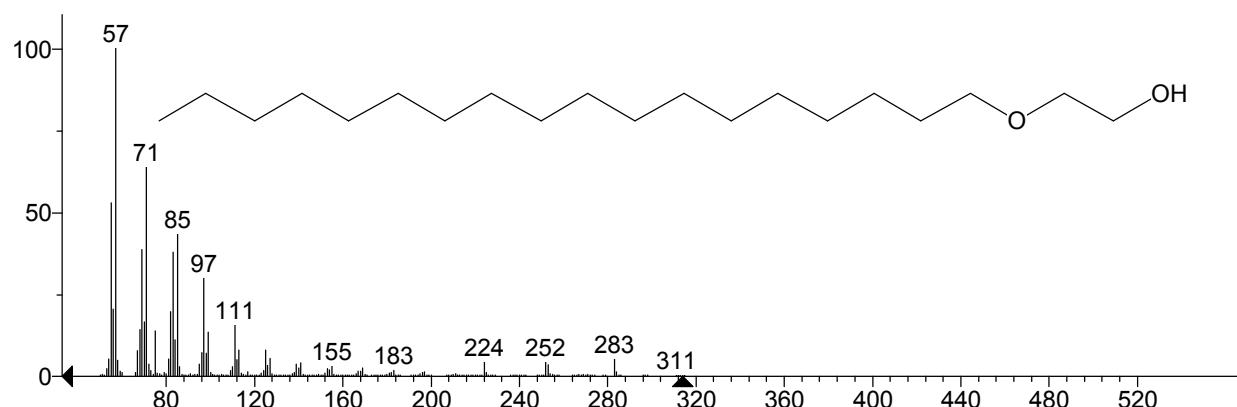


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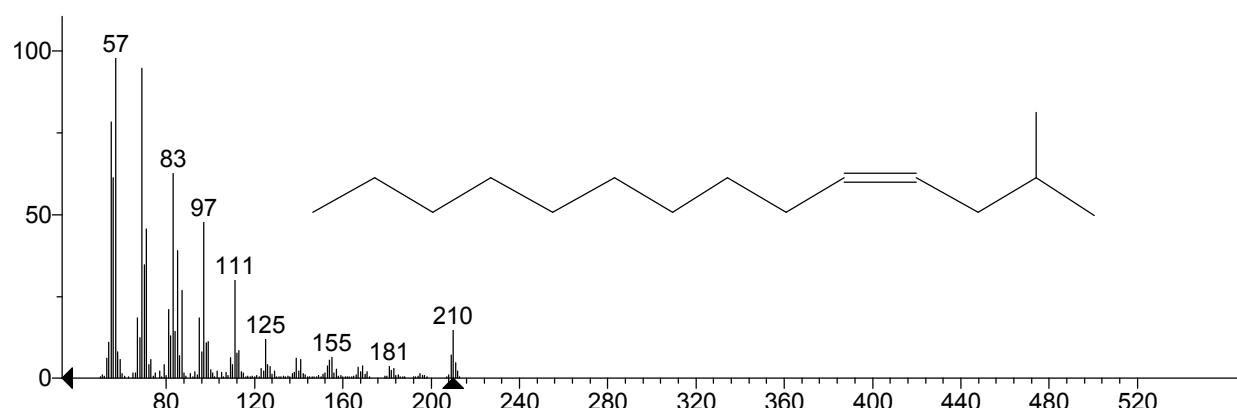
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 Compound in Library Factor = -1149



Hit 1 : Ethanol, 2-(octadecyloxy)-
 C₂₀H₄₂O₂; MF: 679; RMF: 691; Prob 5.72%; CAS: 2136-72-3; Lib: mainlib; ID: 22653.

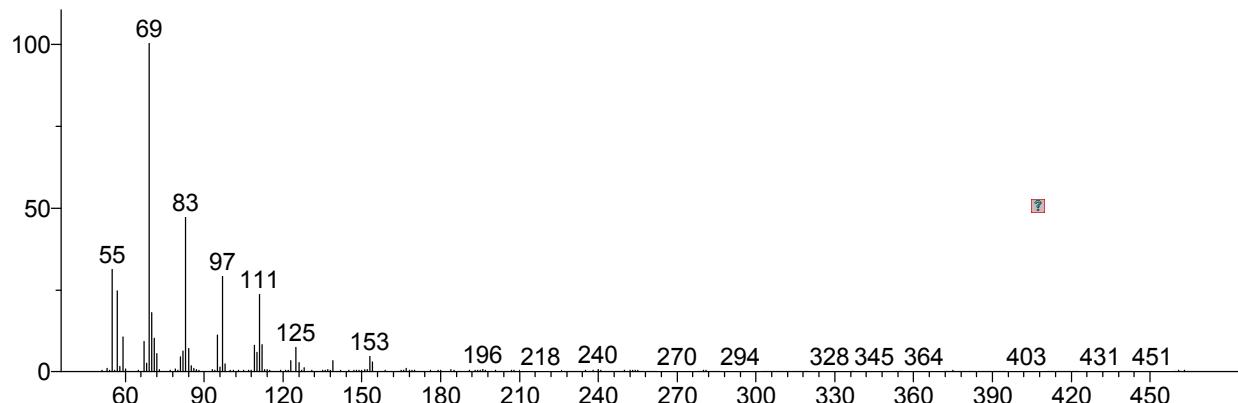


Hit 2 : 2-Methyl-Z-4-tetradecene
 C₁₅H₃₀; MF: 678; RMF: 731; Prob 5.50%; Lib: mainlib; ID: 7391.

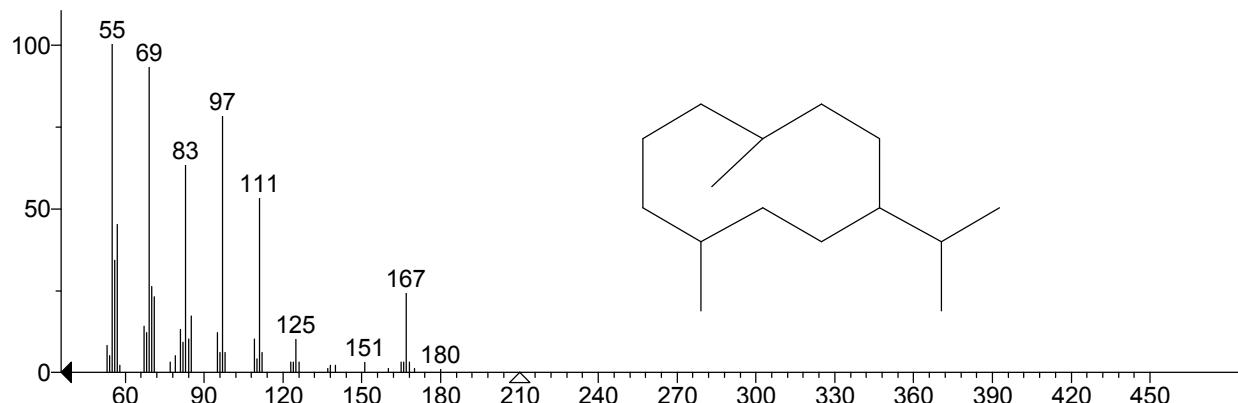


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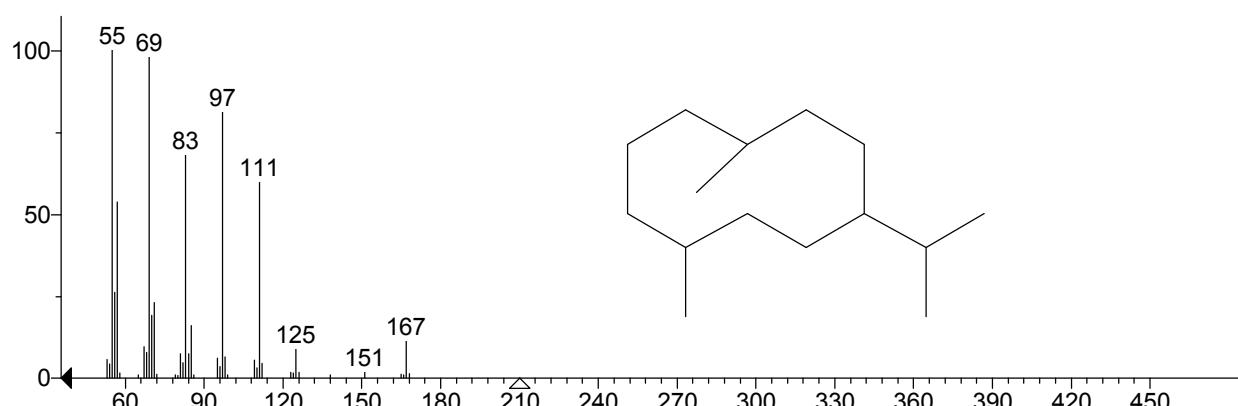
Unknown: +EI Scan (19.948-19.971 min, 8 Scans) HexaneExtract1.D Subtract
 Compound in Library Factor = -1231



Hit 1 : 1,7-Dimethyl-4-(1-methylethyl)cyclodecane
 C15H30; MF: 718; RMF: 783; Prob 6.97%; CAS: 645-10-3; Lib: replib; ID: 4735.

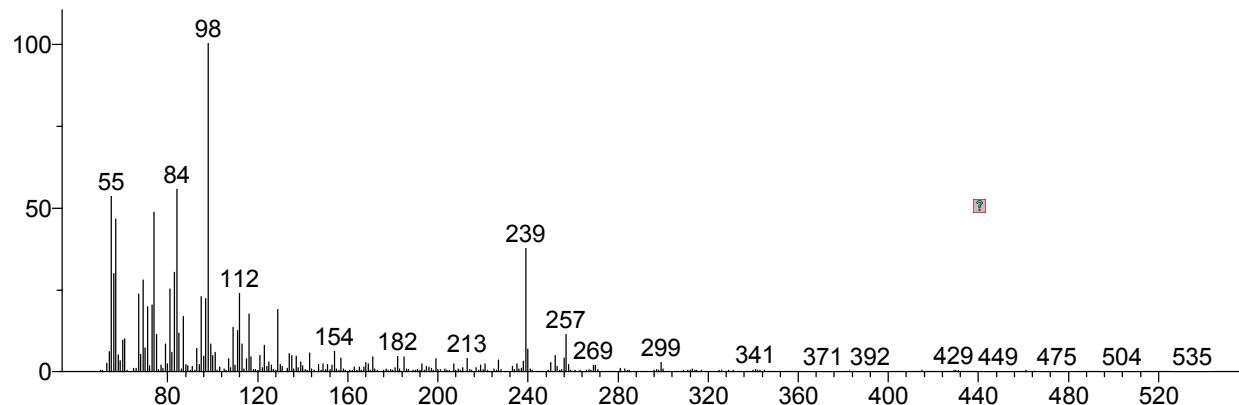


Hit 2 : 1,7-Dimethyl-4-(1-methylethyl)cyclodecane
 C15H30; MF: 716; RMF: 774; Prob 6.97%; CAS: 645-10-3; Lib: mainlib; ID: 18985.

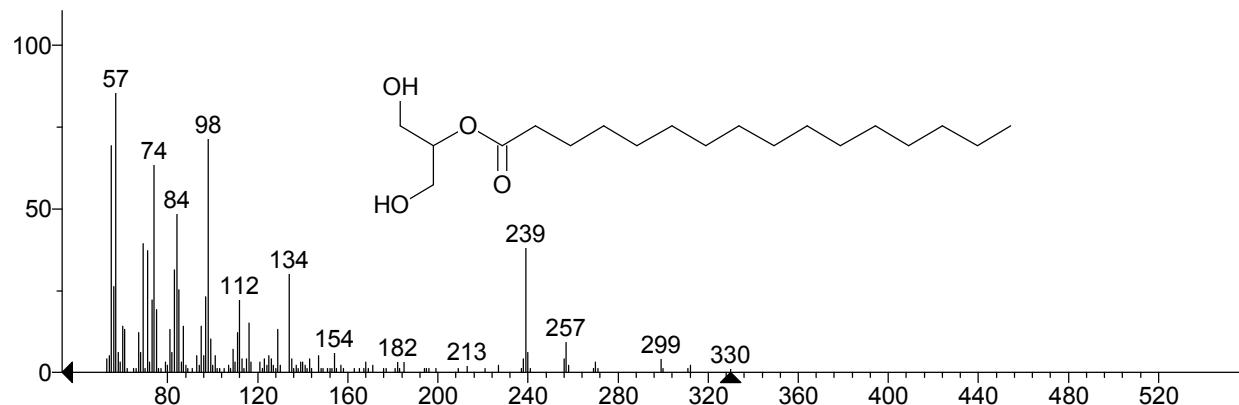


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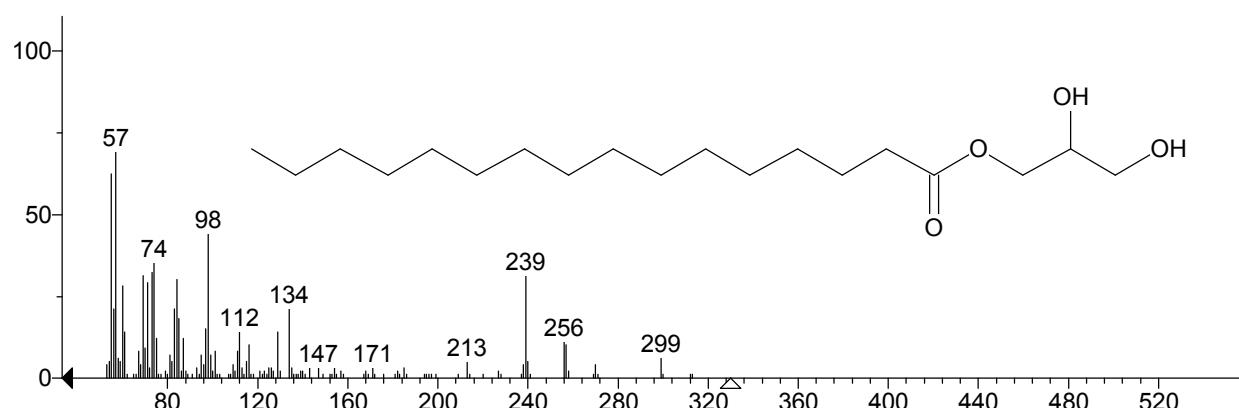
Unknown: +EI Scan (20.605-20.659 min, 17 Scans) HexaneExtract1.D Subtract
 Compound in Library Factor = -243



Hit 1 : Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester
 C19H38O4; MF: 793; RMF: 840; Prob 55.3%; CAS: 23470-00-0; Lib: mainlib; ID: 7272.

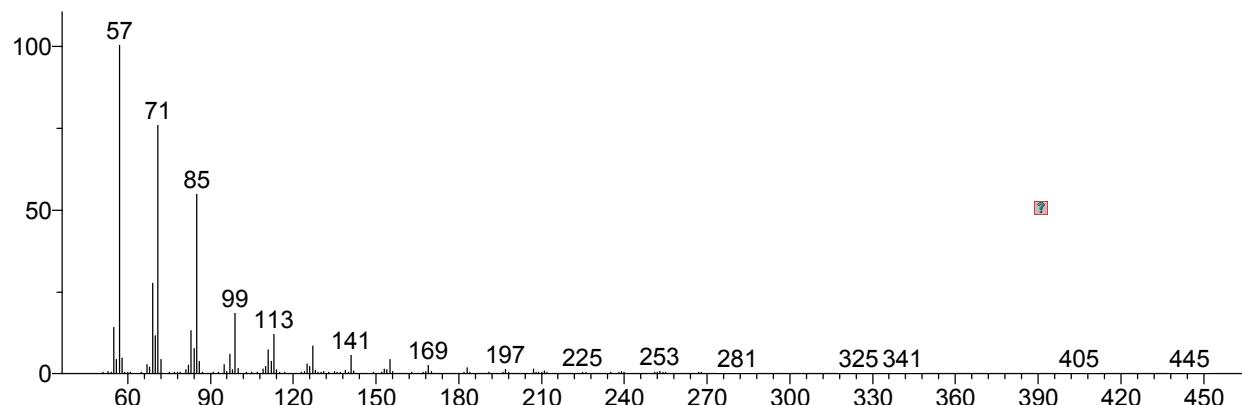


Hit 2 : Glycerol 1-palmitate
 C19H38O4; MF: 774; RMF: 823; Prob 26.9%; CAS: 542-44-9; Lib: mainlib; ID: 7291.

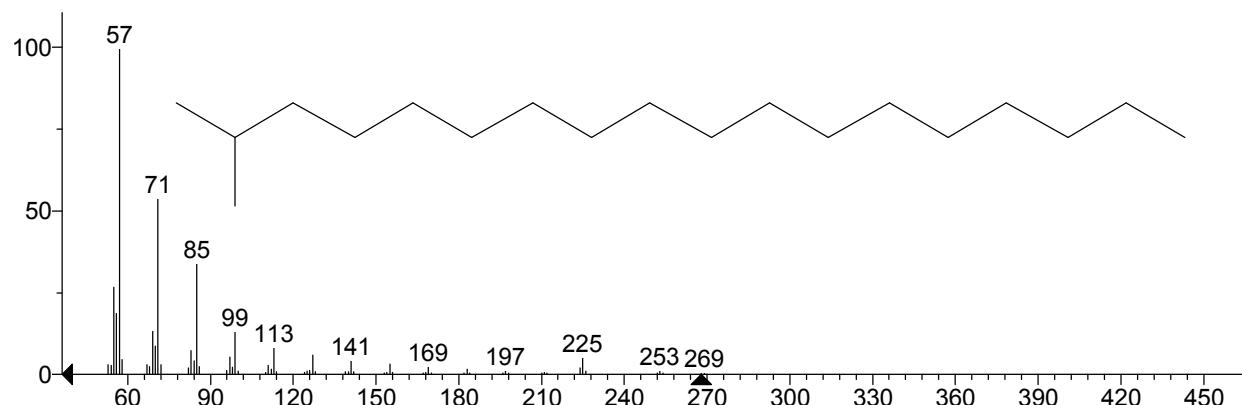


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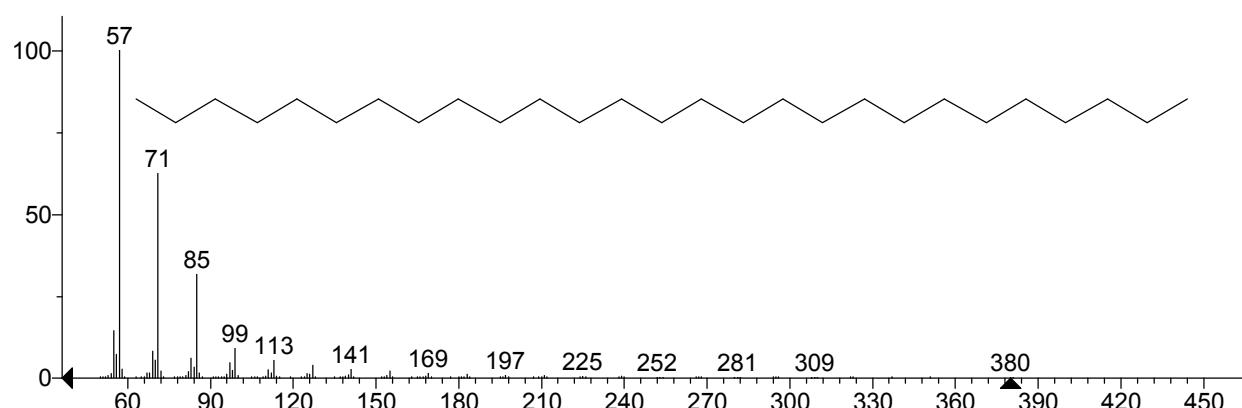
Unknown: +EI Scan (20.887-20.891, 20.924 ... min, 8 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -331



Hit 1 : Octadecane, 2-methyl-
C19H40; MF: 849; RMF: 870; Prob 9.53%; CAS: 1560-88-9; Lib: replib; ID: 2198.

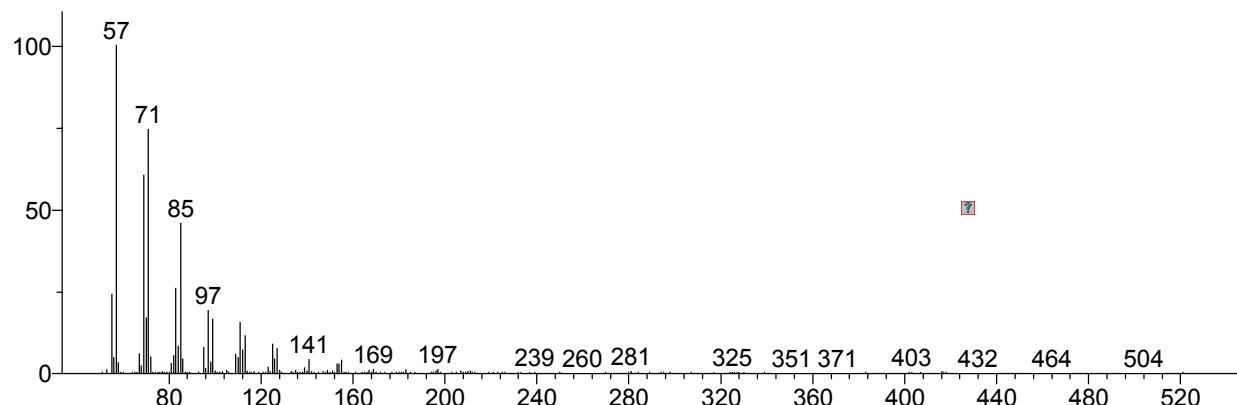


Hit 2 : Heptacosane
C27H56; MF: 845; RMF: 859; Prob 8.05%; CAS: 593-49-7; Lib: replib; ID: 5812.

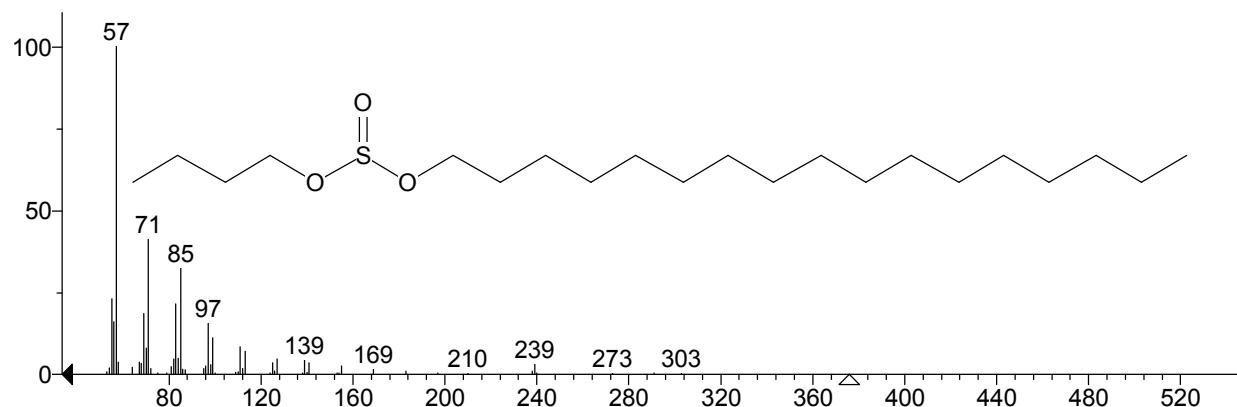


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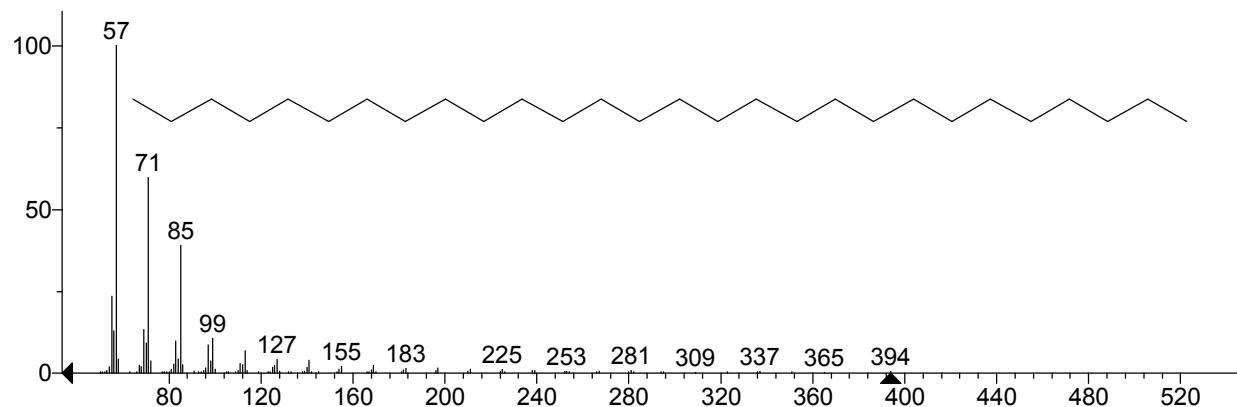
Unknown: +EI Scan (21.089 min) HexaneExtract1.D Subtract
Compound in Library Factor = -811



Hit 1 : Sulfurous acid, butyl heptadecyl ester
C₂₁H₄₄O₃S; MF: 778; RMF: 822; Prob 5.12%; Lib: mainlib; ID: 23670.

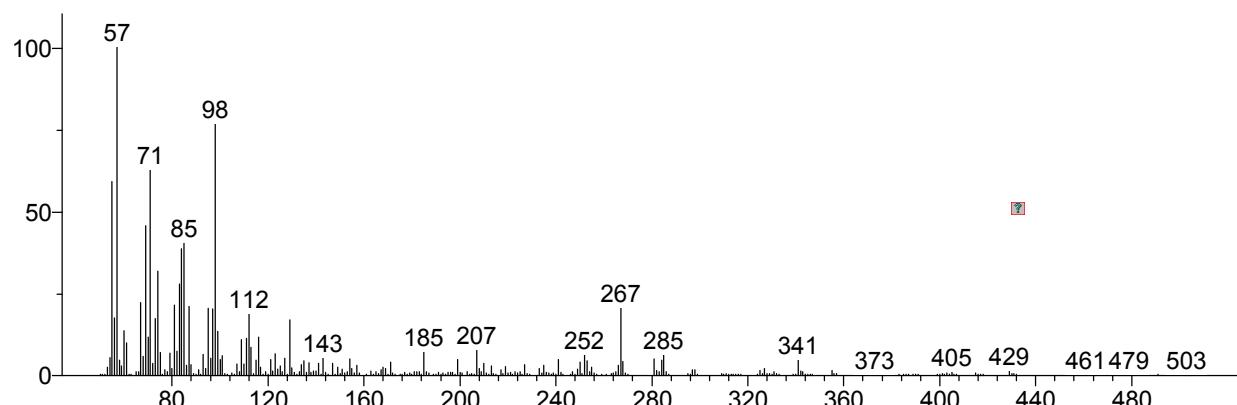


Hit 2 : Octacosane
C₂₈H₅₈; MF: 777; RMF: 804; Prob 4.92%; CAS: 630-02-4; Lib: replib; ID: 5775.

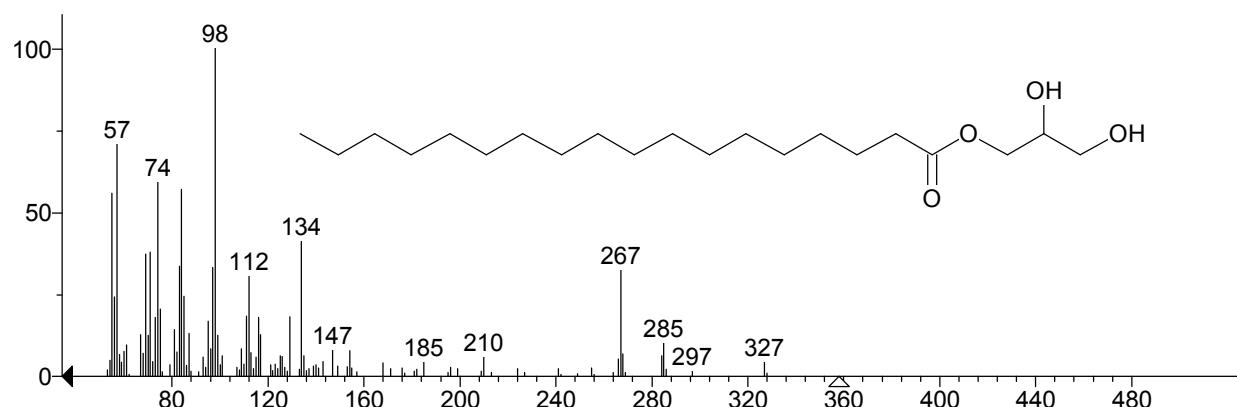


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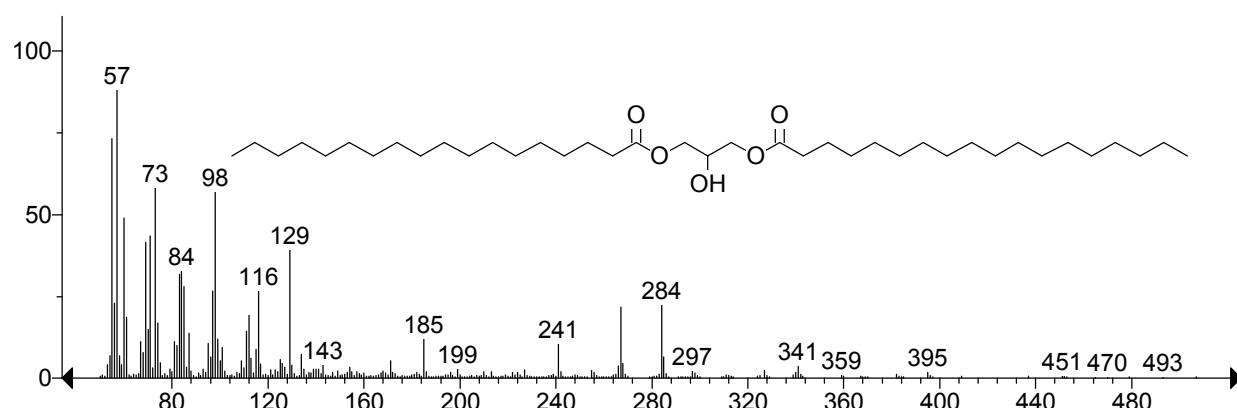
Unknown: +EI Scan (21.656-21.659, 21.700-21.706 min, 5 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -744



Hit 1 : Octadecanoic acid, 2,3-dihydroxypropyl ester
C₂₁H₄₂O₄; MF: 736; RMF: 859; Prob 33.4%; CAS: 123-94-4; Lib: replib; ID: 13886.

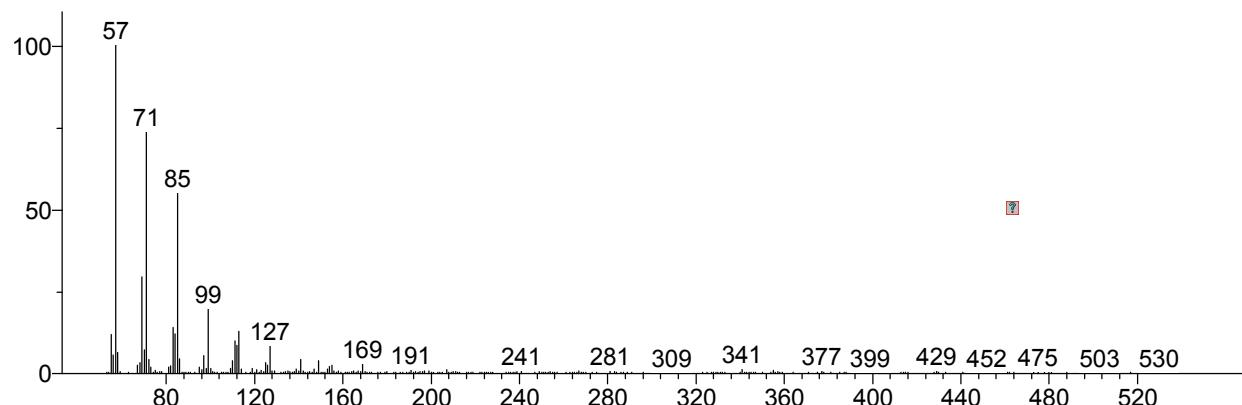


Hit 2 : Octadecanoic acid, 2-hydroxy-1,3-propanediyl ester
C₃₉H₇₆O₅; MF: 725; RMF: 742; Prob 22.9%; CAS: 504-40-5; Lib: replib; ID: 2171.

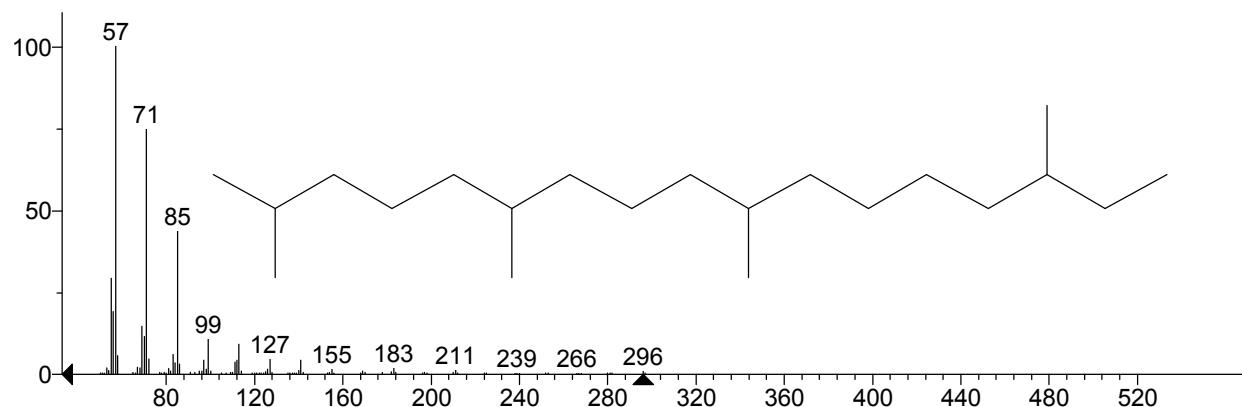


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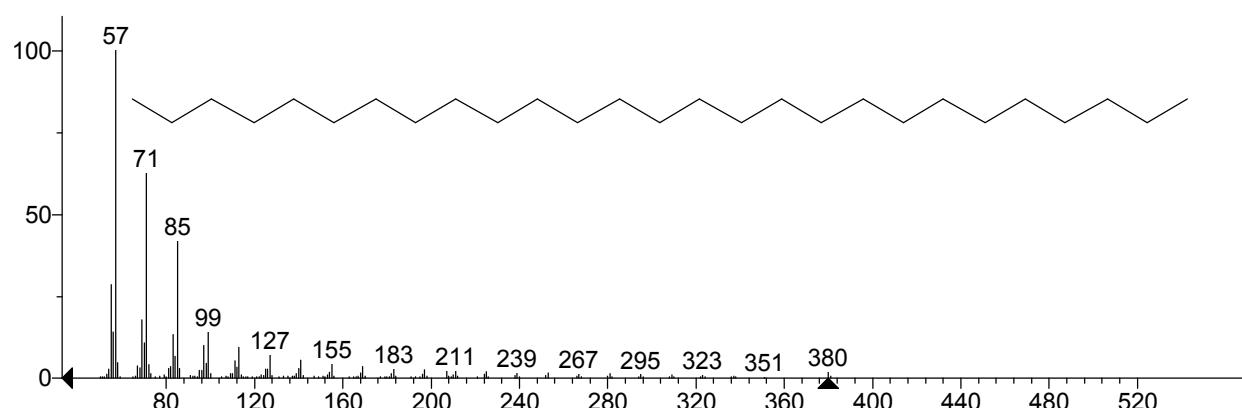
Unknown: +EI Scan (21.941-21.945, 21.972-21.978 min, 5 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -1067



Hit 1 : Heptadecane, 2,6,10,15-tetramethyl-
C21H44; MF: 760; RMF: 846; Prob 7.86%; CAS: 54833-48-6; Lib: mainlib; ID: 23564.

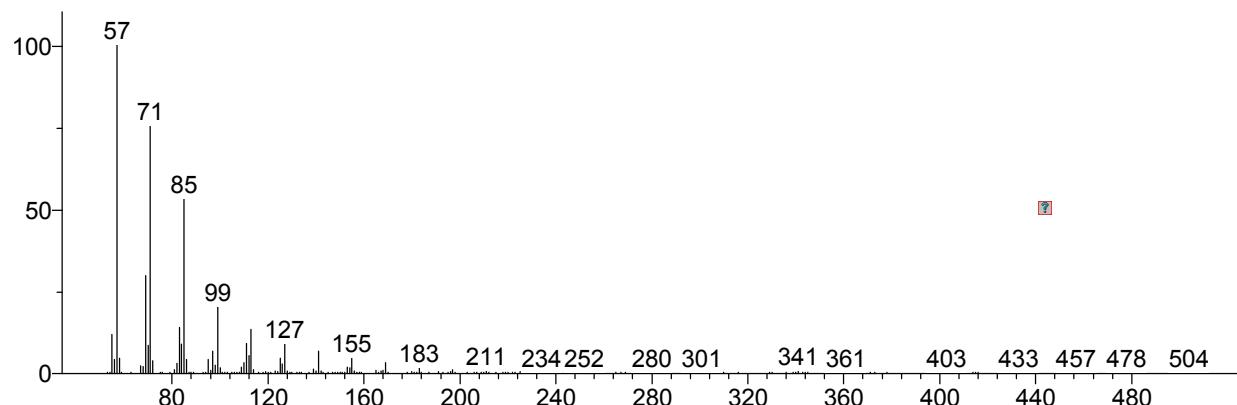


Hit 2 : Heptacosane
C27H56; MF: 751; RMF: 808; Prob 5.71%; CAS: 593-49-7; Lib: replib; ID: 5811.

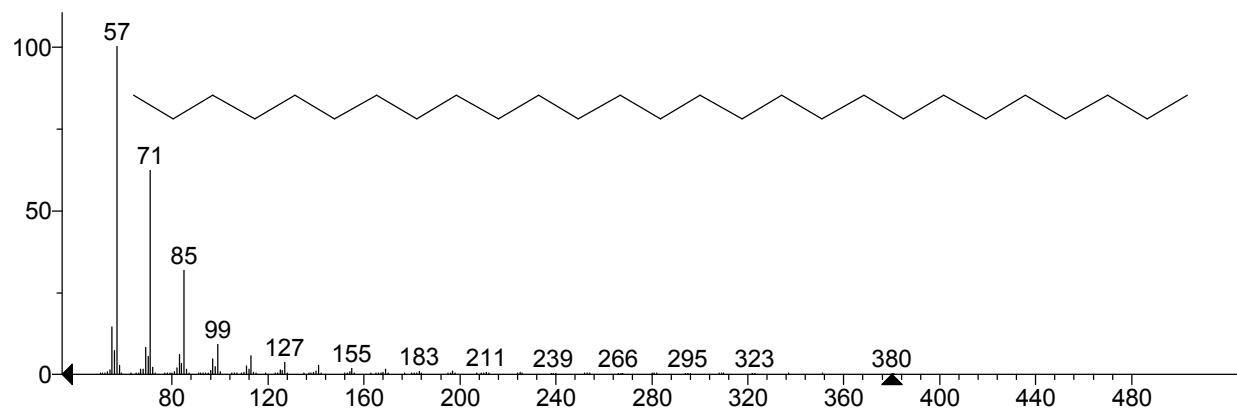


** Search Report Page 1 of 1 **

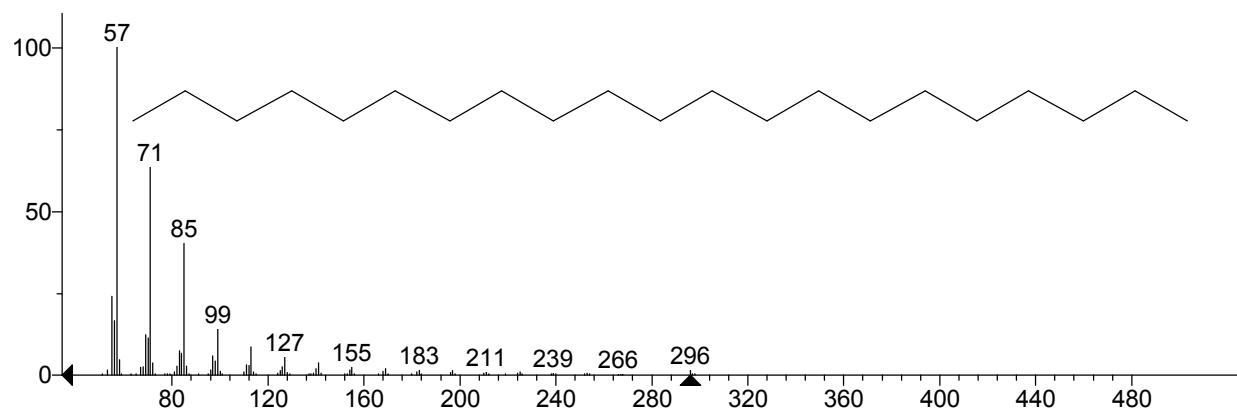
Unknown: +EI Scan (22.915-22.925, 22.942-22.948 min, 7 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -359



Hit 1 : Heptacosane
C₂₇H₅₆; MF: 832; RMF: 856; Prob 7.37%; CAS: 593-49-7; Lib: replib; ID: 5812.

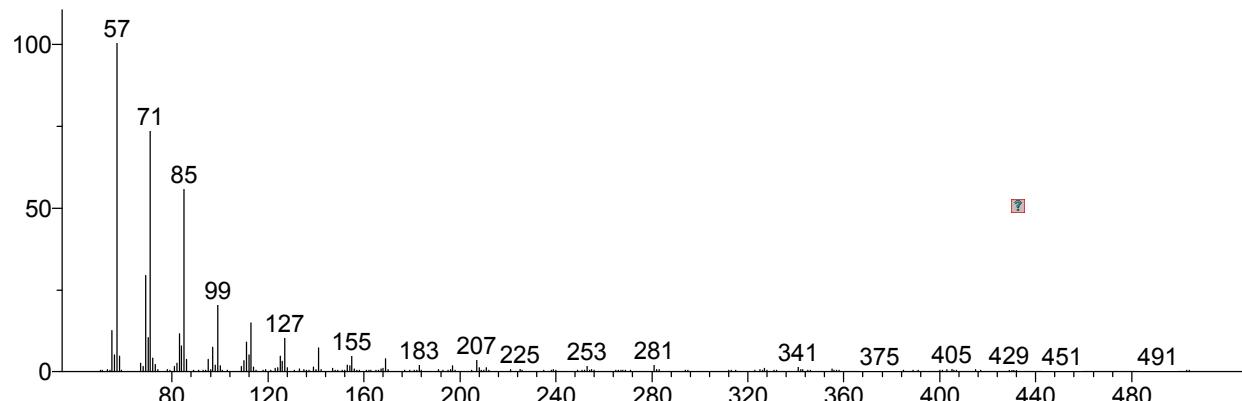


Hit 2 : Heneicosane
C₂₁H₄₄; MF: 825; RMF: 852; Prob 5.65%; CAS: 629-94-7; Lib: replib; ID: 5845.

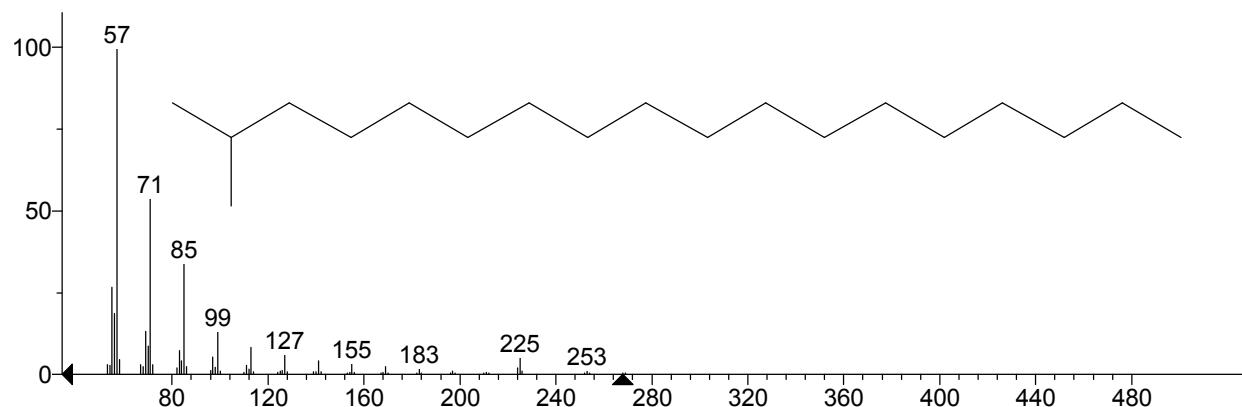


** Search Report Page 1 of 1 **

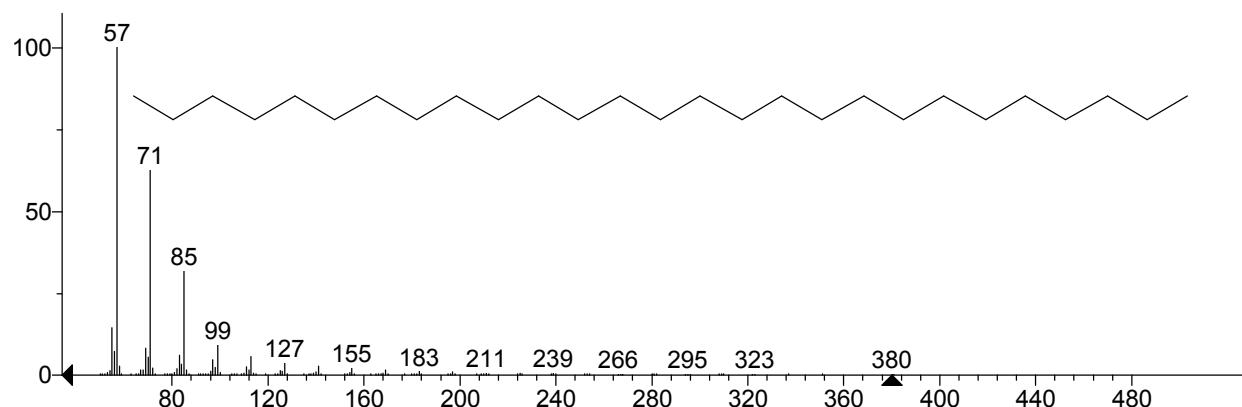
Unknown: +EI Scan (23.110 min) HexaneExtract1.D Subtract
Compound in Library Factor = -509



Hit 1 : Octadecane, 2-methyl-
C19H40; MF: 793; RMF: 875; Prob 9.13%; CAS: 1560-88-9; Lib: replib; ID: 2198.

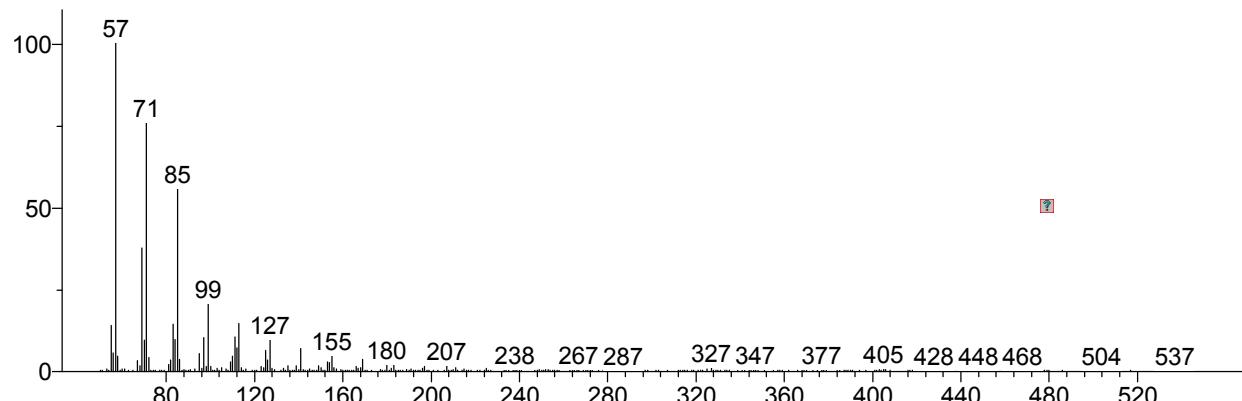


Hit 2 : Heptacosane
C27H56; MF: 781; RMF: 849; Prob 6.08%; CAS: 593-49-7; Lib: replib; ID: 5812.

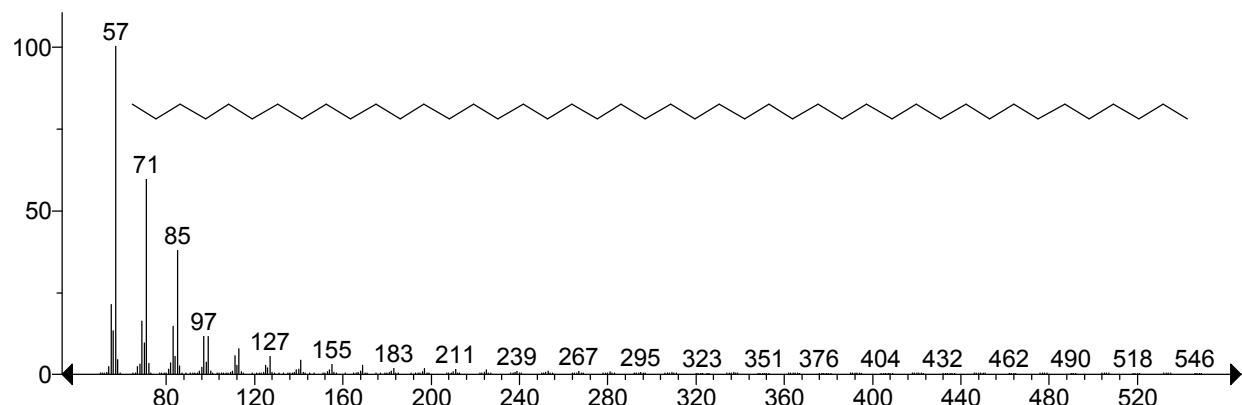


** Search Report Page 1 of 1 **

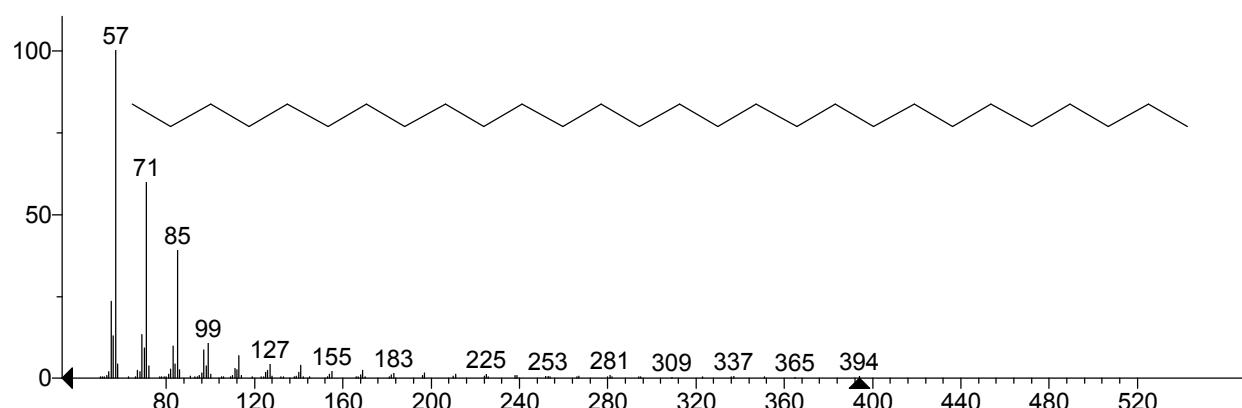
Unknown: +EI Scan (24.110-24.137, 24.150-24.174 min, 17 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -778



Hit 1 : Tetratetracontane
C44H90; MF: 751; RMF: 789; Prob 6.40%; CAS: 7098-22-8; Lib: replib; ID: 5823.

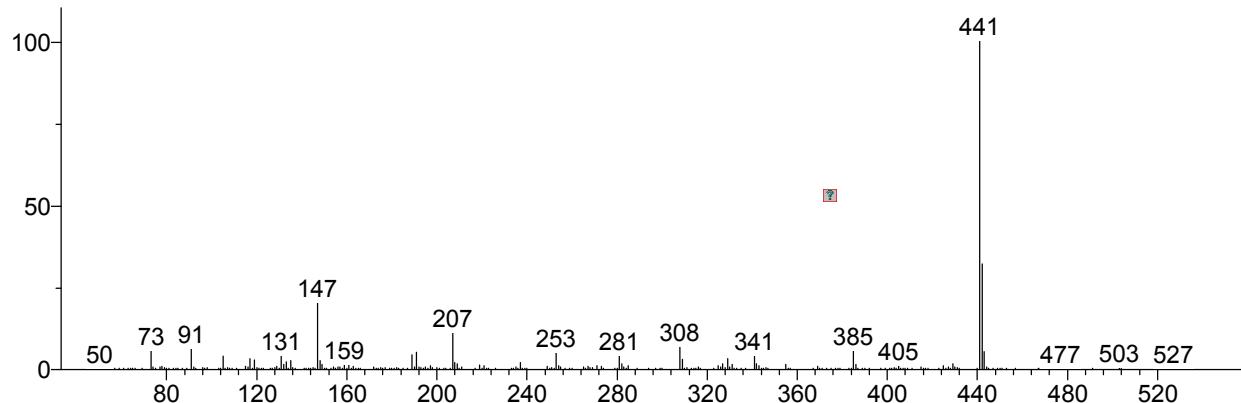


Hit 2 : Octacosane
C28H58; MF: 747; RMF: 837; Prob 5.40%; CAS: 630-02-4; Lib: replib; ID: 5775.

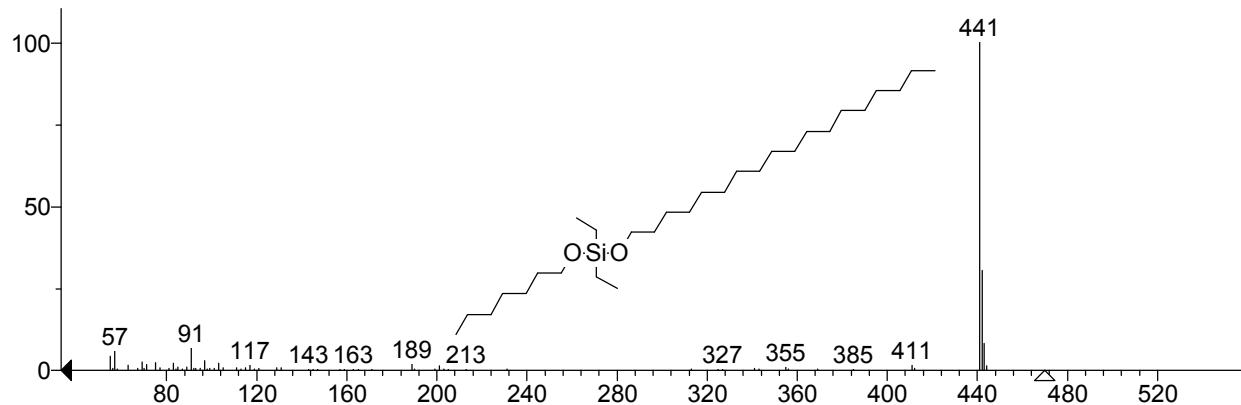


** Search Report Page 1 of 1 **

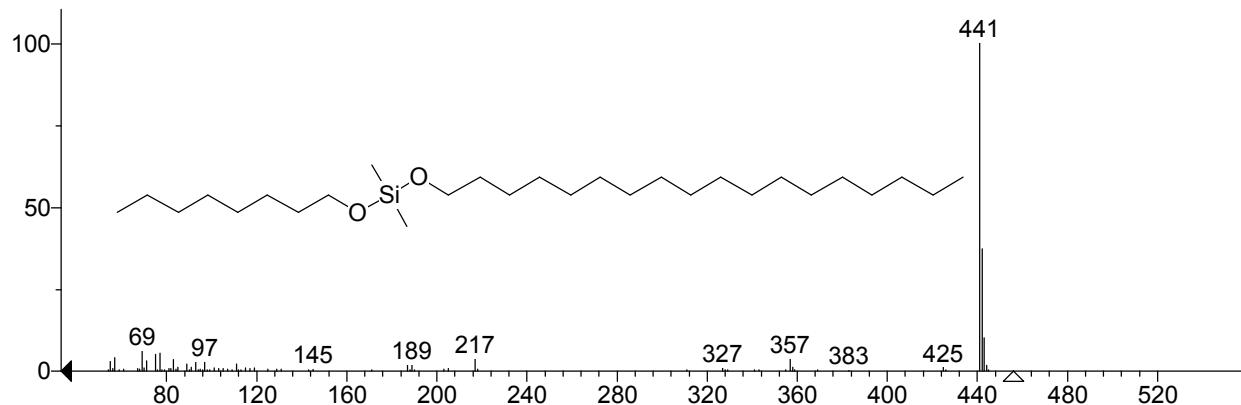
Unknown: +EI Scan (25.291-25.318, 25.412-25.443 min, 19 Scans) HexaneExtract1.D Subtract
Compound in Library Factor = -1066



Hit 1 : Silane, diethylheptyloxyoctadecyloxy-
C₂₉H₆₂O₂Si; MF: 663; RMF: 841; Prob 22.8%; Lib: mainlib; ID: 210918.

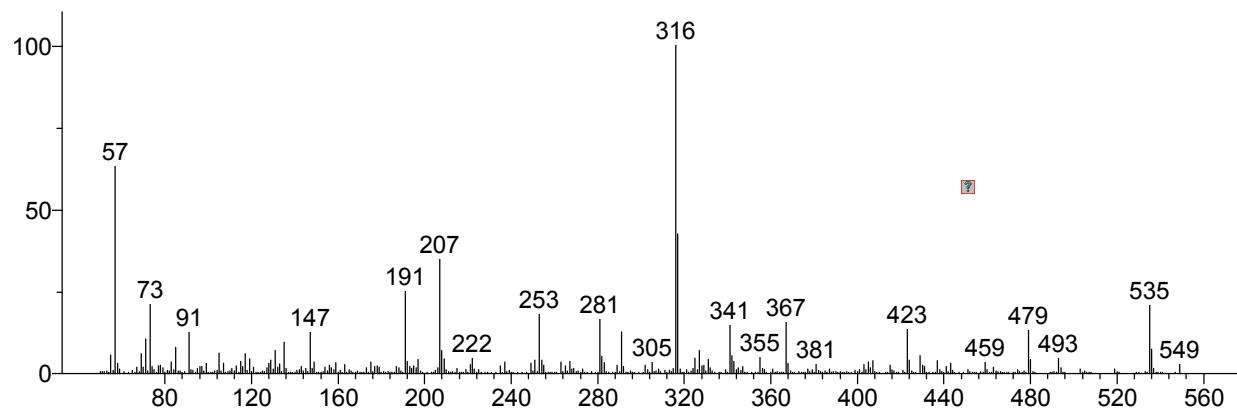


Hit 2 : Silane, dimethyloctyloxyoctadecyloxy-
C₂₈H₆₀O₂Si; MF: 645; RMF: 847; Prob 11.7%; Lib: mainlib; ID: 210914.

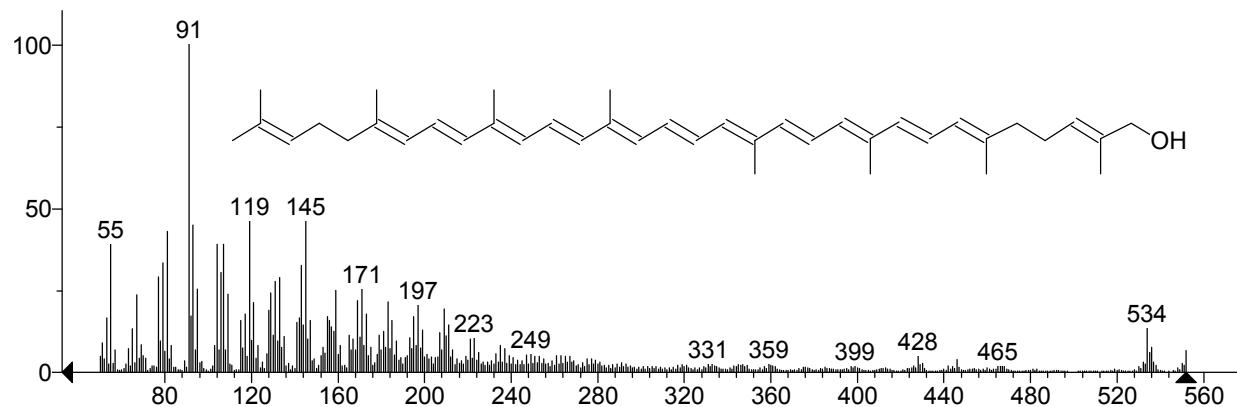


** Search Report Page 1 of 1 **

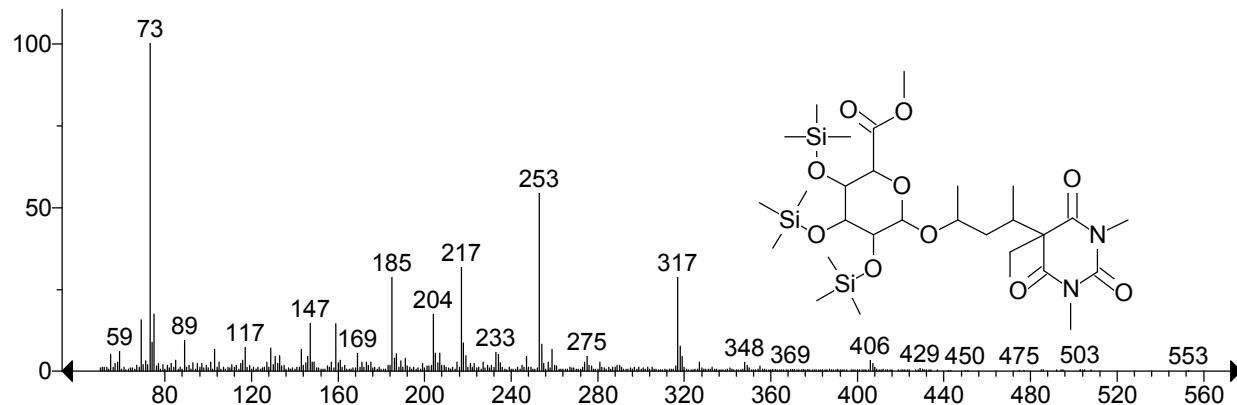
Unknown: +EI Scan (26.913 min) HexaneExtract1.D Subtract
 Compound in Library Factor = -1709



Hit 1 : Lycoxanthin
 C40H56O; MF: 482; RMF: 482; Prob 7.55%; CAS: 19891-74-8; Lib: mainlib; ID: 53605.



Hit 2 : D-Glucopyranosiduronic acid, 3-(5-ethylhexahydro-1,3-dimethyl-2,4,6-trioxo-5-pyrimidinyl)-1-methylbutyl 2,3-C29H56N2O10Si3; MF: 479; RMF: 520; Prob 6.67%; CAS: 55556-79-1; Lib: mainlib; ID: 39728.



QTOF-LCMS

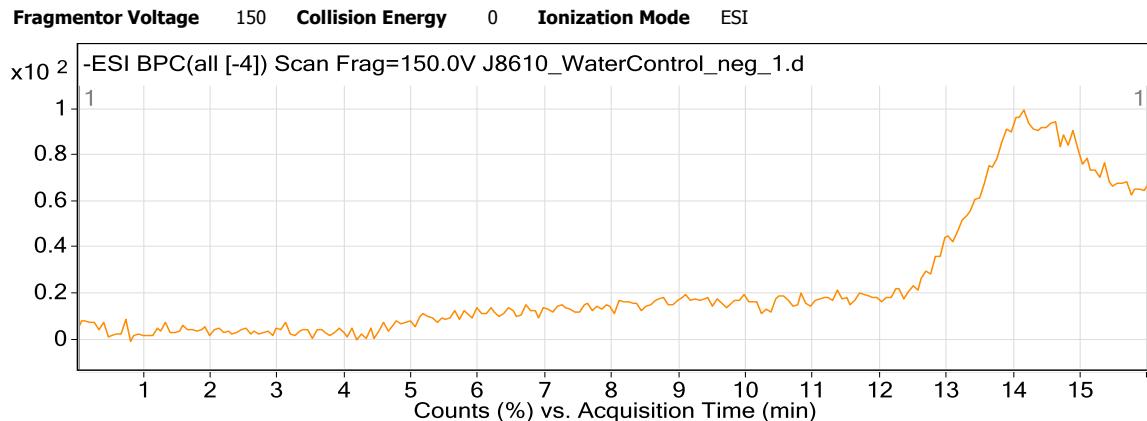
Leachables

Data

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|----------------------|---------------------|
| Data Filename | J8610_WaterControl_neg_1.d | Sample Name | Water Control |
| Sample Type | Blank | Position | Vial 11 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 8:58:23 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

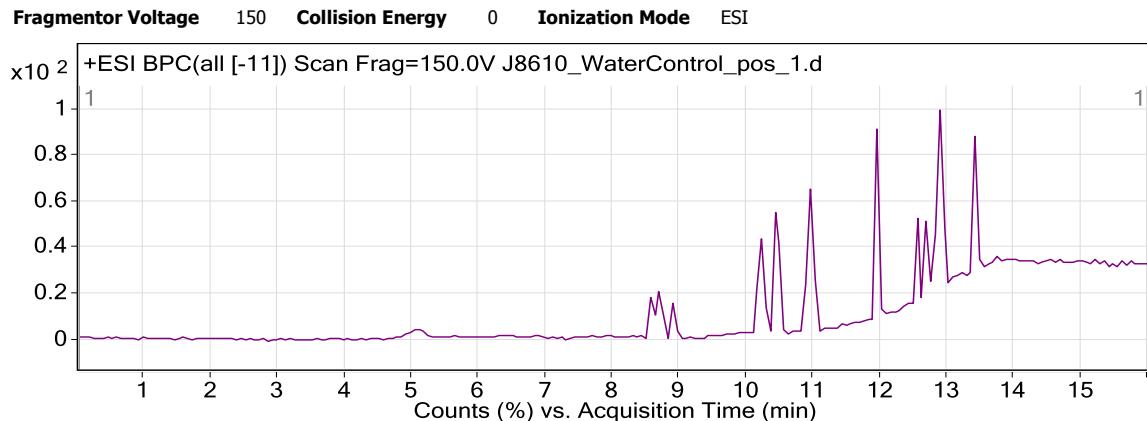


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|----------------------|---------------------|
| Data Filename | J8610_WaterControl_pos_1.d | Sample Name | Water Control |
| Sample Type | Blank | Position | Vial 11 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 8:09:52 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

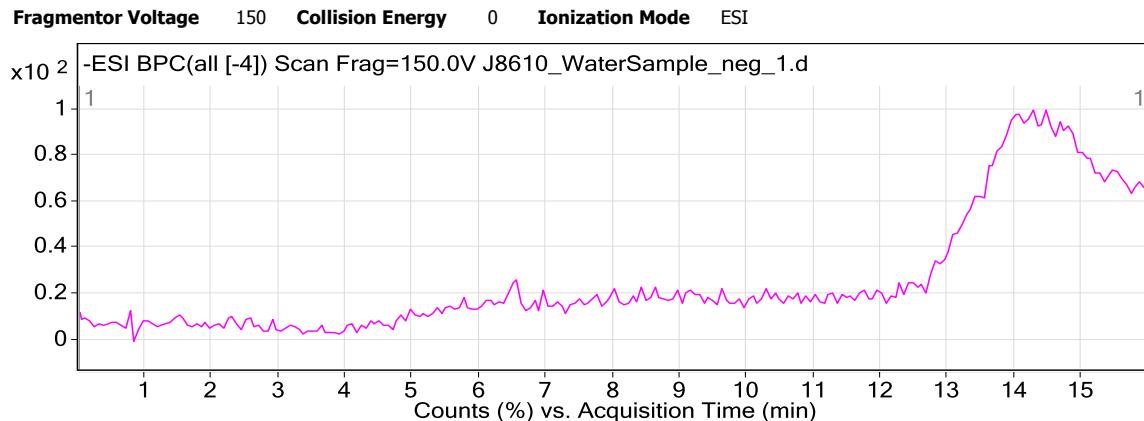


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|---------------------------|----------------------|----------------------|
| Data Filename | J8610_WaterSample_neg_1.d | Sample Name | Water |
| Sample Type | Blank | Position | Vial 12 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 11:24:07 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

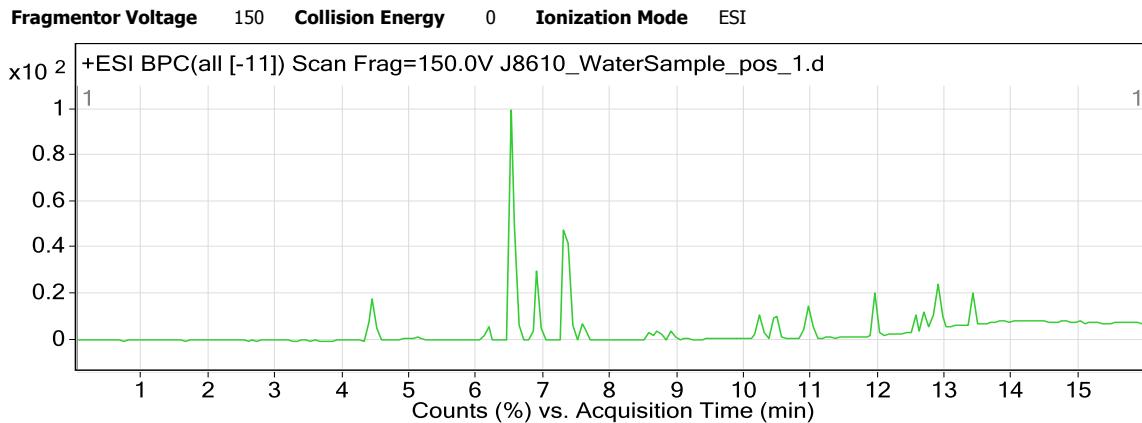


--- End Of Report ---

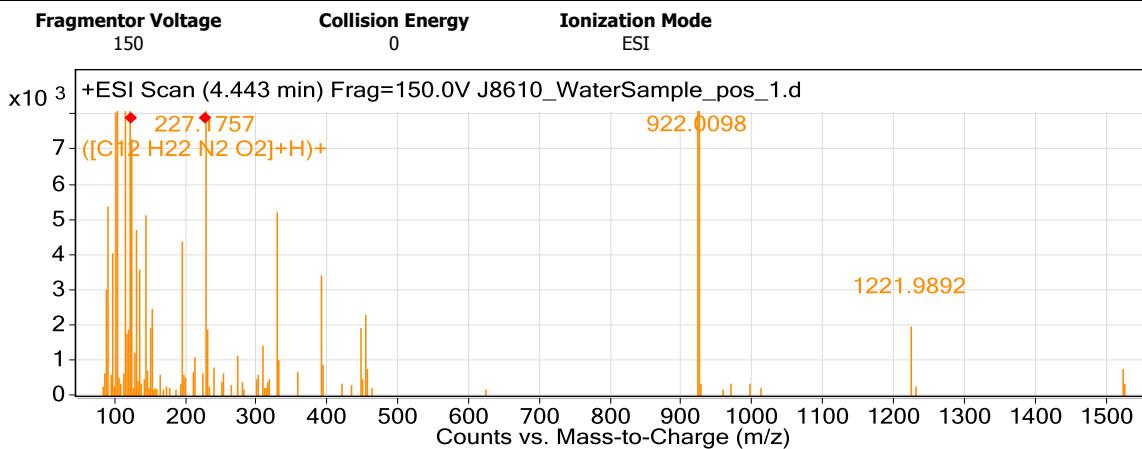
Qualitative Analysis Report

| | | | |
|-------------------------------|---------------------------|----------------------|----------------------|
| Data Filename | J8610_WaterSample_pos_1.d | Sample Name | Water |
| Sample Type | Blank | Position | Vial 12 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 10:35:42 AM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms



User Spectra



MFG Results

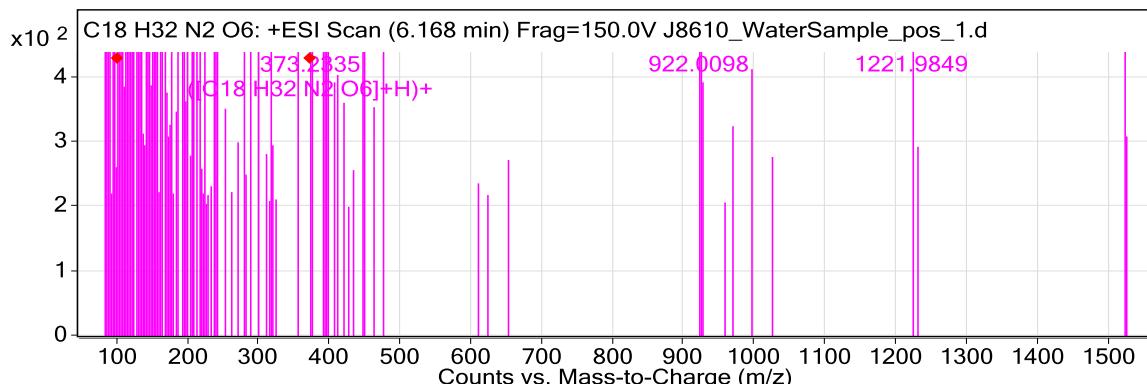
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 227.1757 | 226.1684 | C12 H22 N2 O2 | 98.94 | -1.3 | C12 H23 N2 O2 |

Database Results

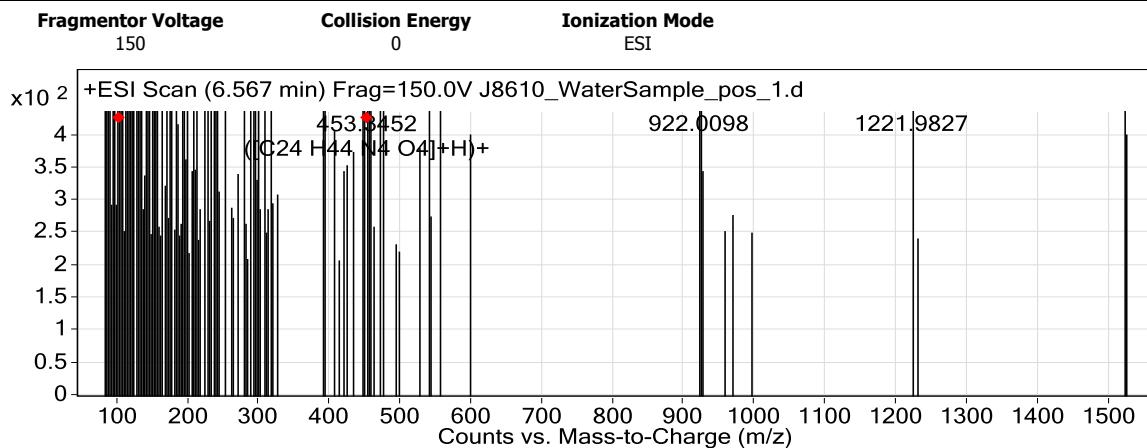
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-------------------|---------------|------------|-----------|------------|----------|
| 227.1757 | caprolactam dimer | C12 H22 N2 O2 | 98.87 | 1 | -0.34 | 226.1684 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report

**MFG Results**

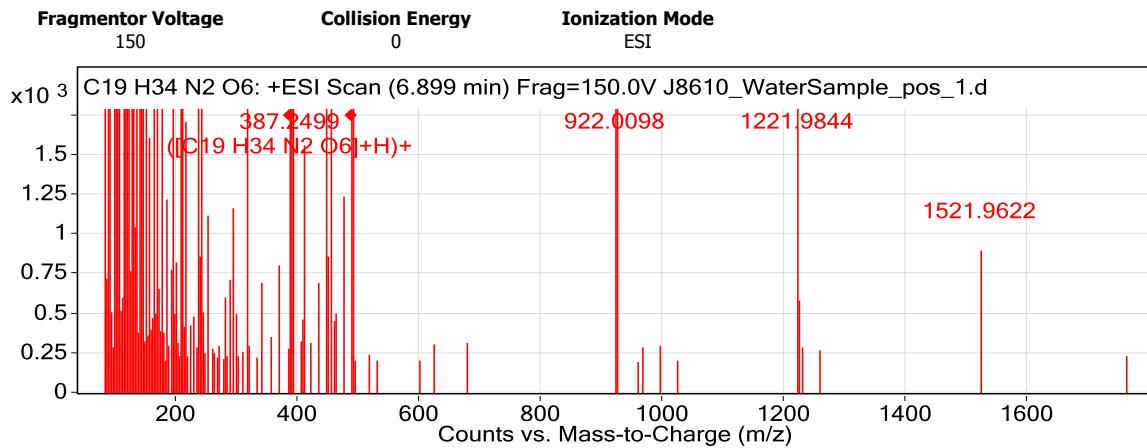
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 373.2335 | 372.2262 | C18 H32 N2 O6 | 99.2 | -0.44 | C18 H33 N2 O6 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 453.3452 | 452.3377 | C24 H44 N4 O4 | 93.01 | -3.2 | C24 H45 N4 O4 |

Database Results

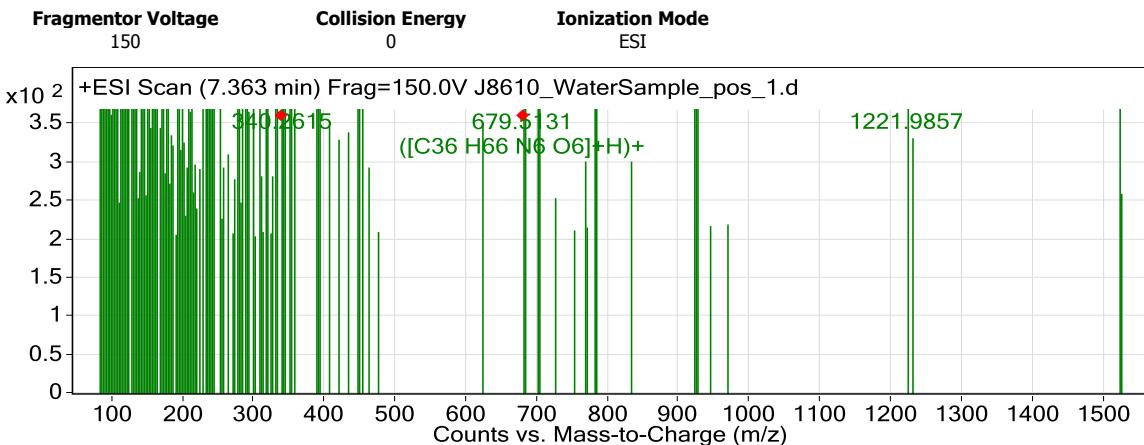
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|----------------------|---------------|------------|-----------|------------|----------|
| 453.3452 | caprolactam tetramer | C24 H44 N4 O4 | 93.27 | 1 | -1.69 | 452.3377 |



Qualitative Analysis Report

MFG Results

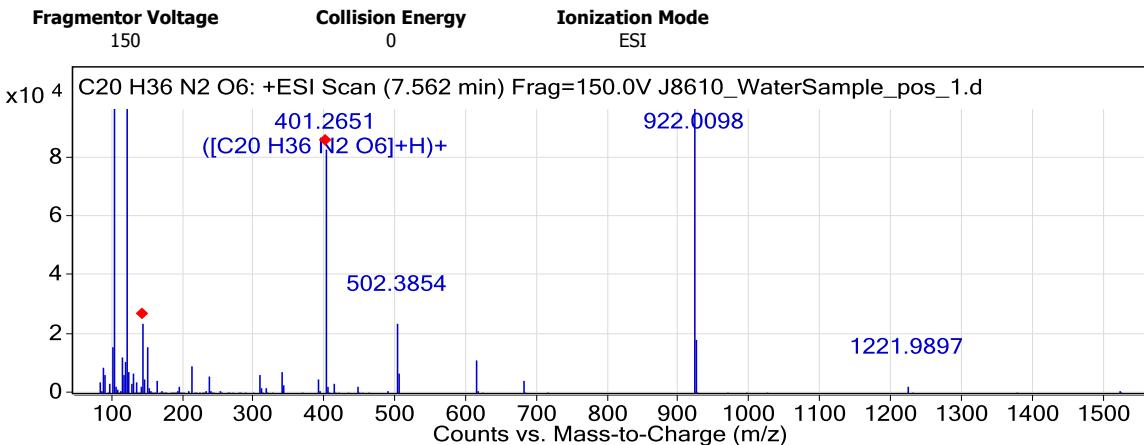
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 387.2499 | 386.2425 | C19 H34 N2 O6 | 96.79 | -2.06 | C19 H35 N2 O6 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 679.5131 | 678.5056 | C36 H66 N6 O6 | 95.7 | -1.85 | C36 H67 N6 O6 |

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|------------|---------------------|----------------|-------------------|------------------|-------------------|-------------|
| 679.5131 | caprolactam hexamer | C36 H66 N6 O6 | 95.83 | 1 | -1.48 | 678.5056 |

**MFG Results**

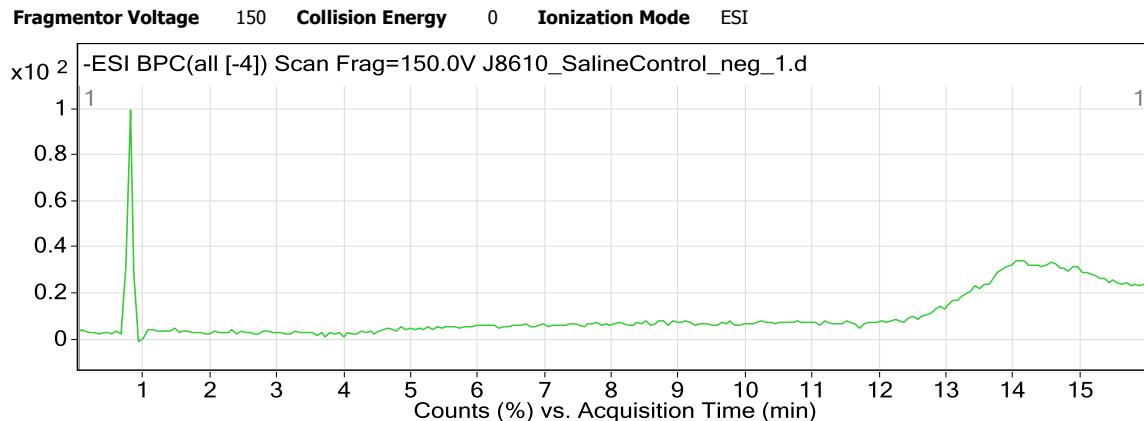
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 401.2651 | 400.2577 | C20 H36 N2 O6 | 98.49 | -0.96 | C20 H37 N2 O6 |

--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|---------------------|
| Data Filename | J8610_SalineControl_neg_1.d | Sample Name | Saline Control |
| Sample Type | Blank | Position | Vial 13 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 1:50:07 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

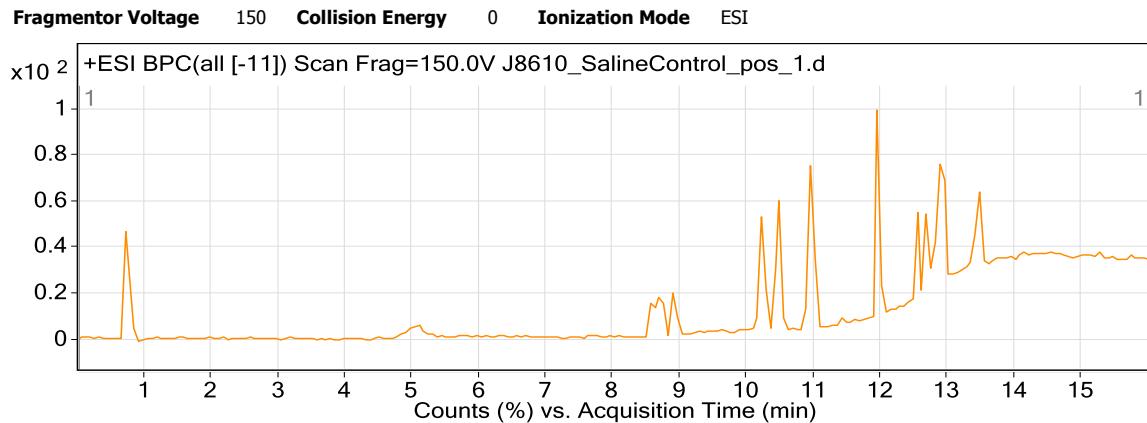


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|---------------------|
| Data Filename | J8610_SalineControl_pos_1.d | Sample Name | Saline Control |
| Sample Type | Blank | Position | Vial 13 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 1:01:28 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

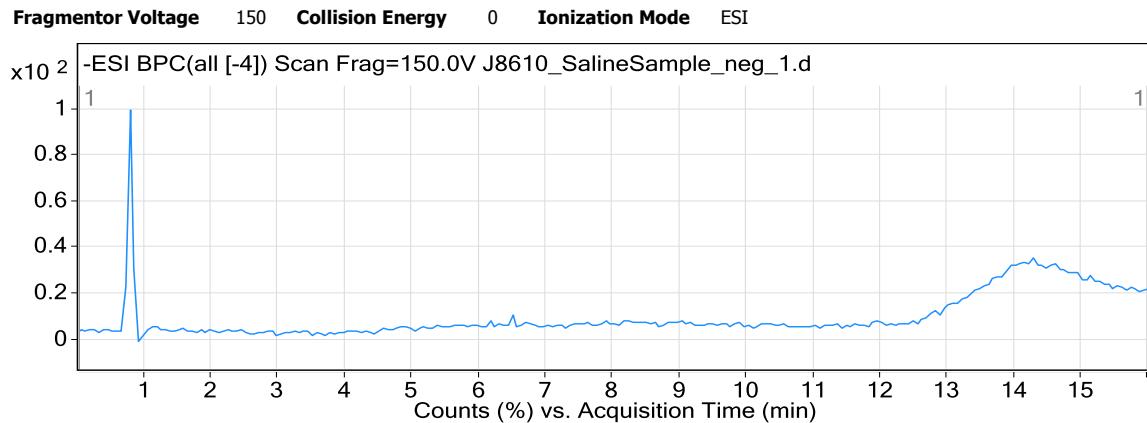


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|----------------------------|----------------------|---------------------|
| Data Filename | J8610_SalineSample_neg_1.d | Sample Name | Saline |
| Sample Type | Blank | Position | Vial 14 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 4:16:01 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

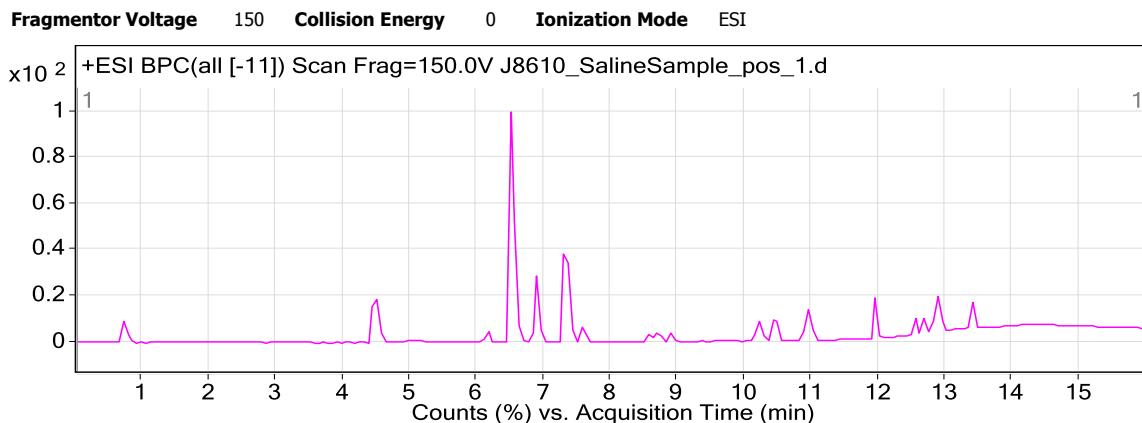
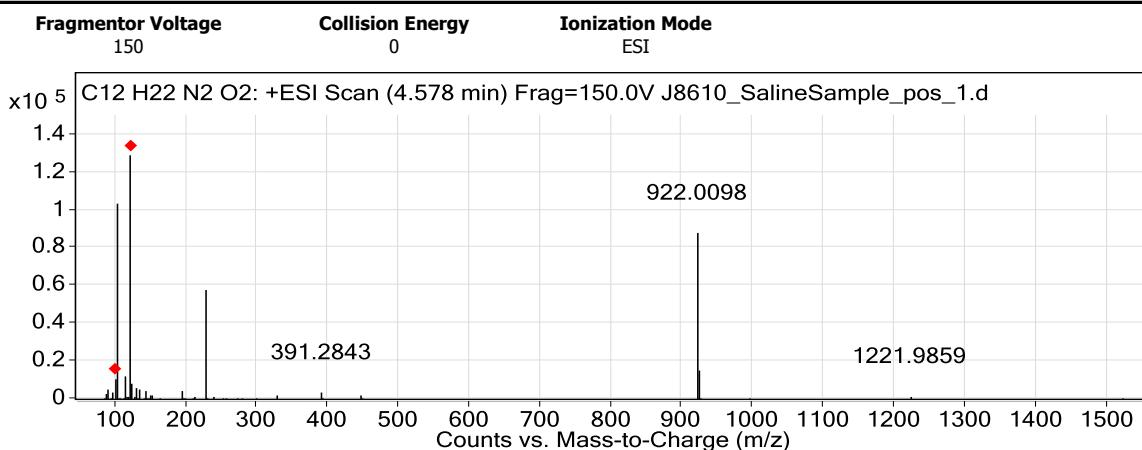
User Chromatograms



--- End Of Report ---

Qualitative Analysis Report

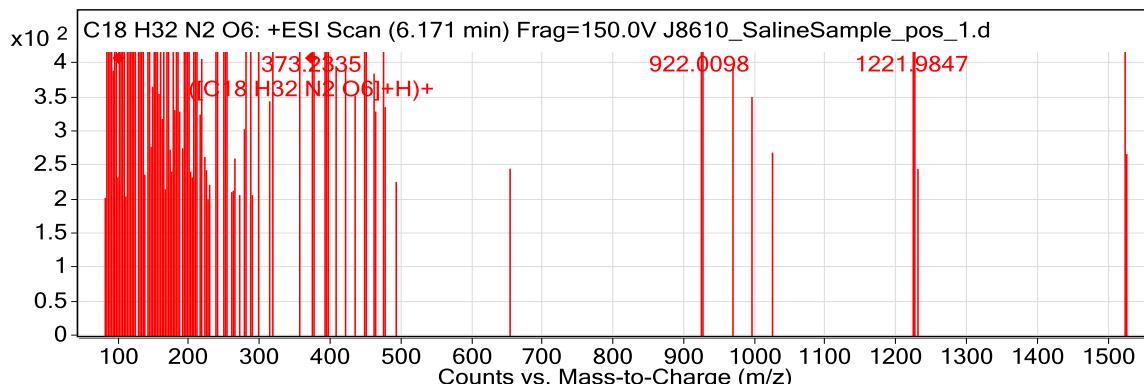
| | | | |
|-------------------------------|----------------------------|----------------------|---------------------|
| Data Filename | J8610_SalineSample_pos_1.d | Sample Name | Saline |
| Sample Type | Blank | Position | Vial 14 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 3:27:34 PM |
| IRM Calibration Status | Success | DA Method | neg.m |

Comment**User Chromatograms****User Spectra****MFG Results**

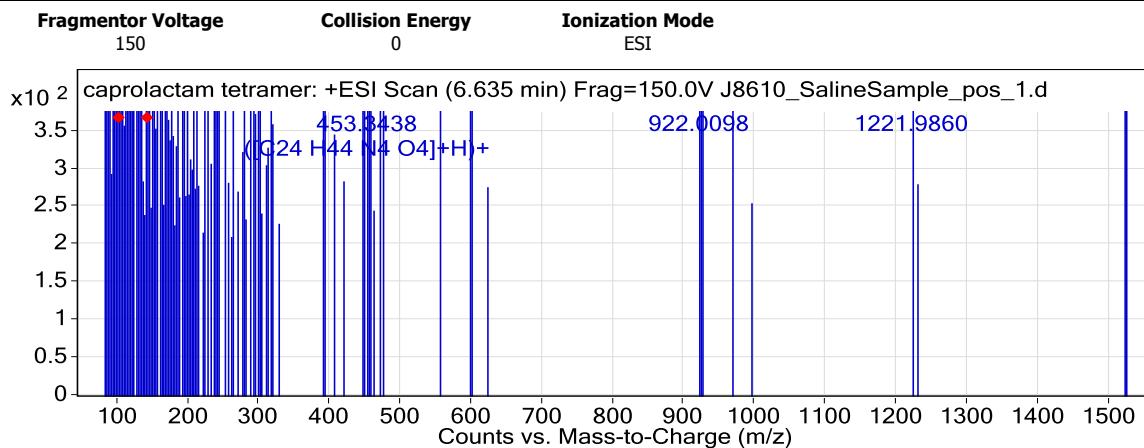
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 227.1753 | 226.1679 | C12 H22 N2 O2 | 97.97 | 1.06 | C12 H23 N2 O2 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report

**MFG Results**

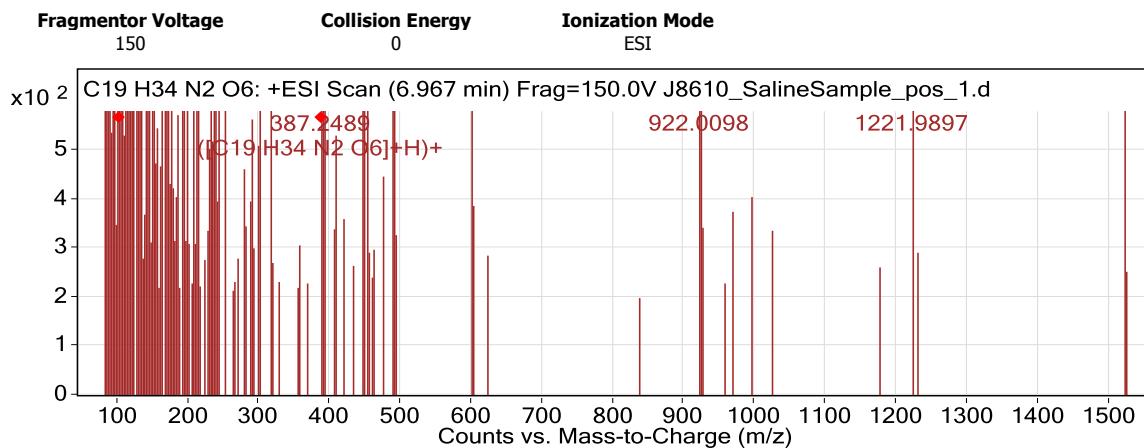
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 373.2335 | 372.2262 | C18 H32 N2 O6 | 99.34 | -0.35 | C18 H33 N2 O6 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 453.3438 | 452.3365 | C24 H44 N4 O4 | 97.36 | -0.49 | C24 H45 N4 O4 |

Database Results

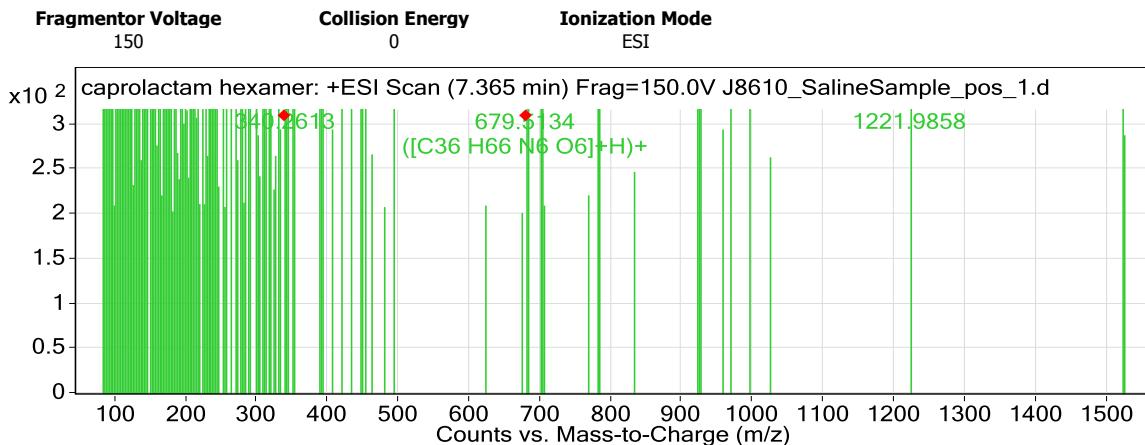
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|----------------------|---------------|------------|-----------|------------|----------|
| 453.3438 | caprolactam tetramer | C24 H44 N4 O4 | 97.45 | 2 | -0.3 | 452.3365 |



Qualitative Analysis Report

MFG Results

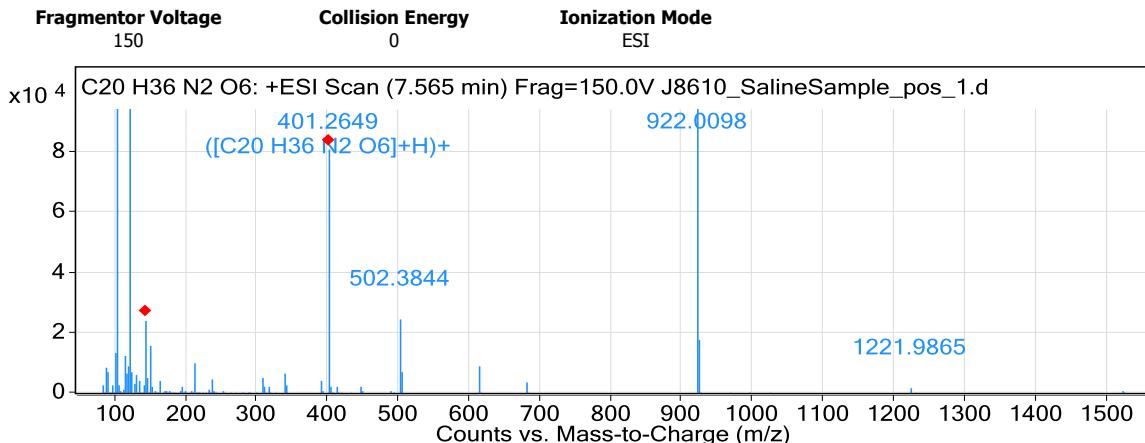
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 387.2489 | 386.2416 | C19 H34 N2 O6 | 99.36 | 0.35 | C19 H35 N2 O6 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 679.5134 | 678.5058 | C36 H66 N6 O6 | 94.53 | -2.07 | C36 H67 N6 O6 |

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|------------|---------------------|----------------|-------------------|------------------|-------------------|-------------|
| 679.5134 | caprolactam hexamer | C36 H66 N6 O6 | 94.7 | 1 | -1.79 | 678.5058 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|------------|-------------|-------------------|--------------|--------------|------------------|
| 401.2649 | 400.2576 | C20 H36 N2 O6 | 99.3 | -0.56 | C20 H37 N2 O6 |

--- End Of Report ---

QTOF-LCMS

Exhaustive

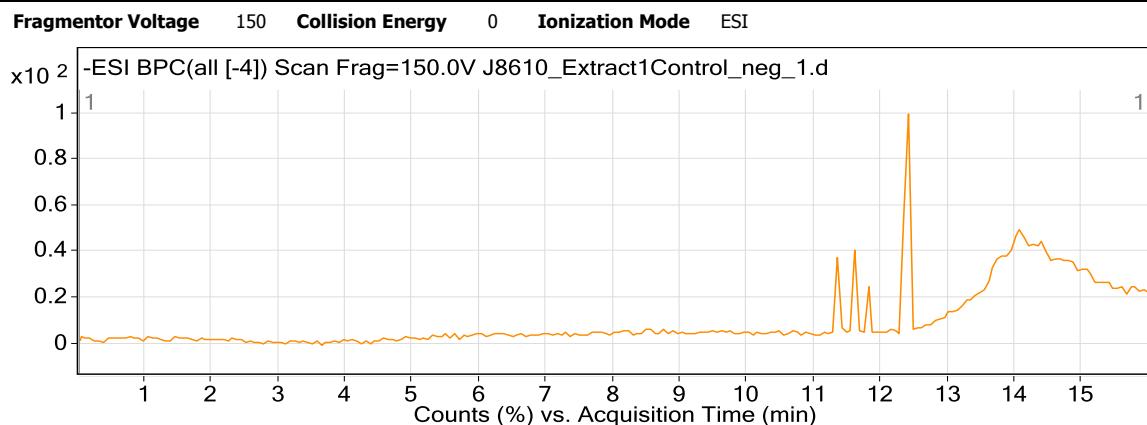
Data

Qualitative Analysis Report

| | | | |
|-------------------------------|-------------------------------|----------------------|---------------------|
| Data Filename | J8610_MethanolControl_neg_1.d | Sample Name | Extract 1 Blank |
| Sample Type | Blank | Position | Vial 15 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 6:41:52 PM |
| IRM Calibration Status | Success | DA Method | neg.m |

Comment

User Chromatograms

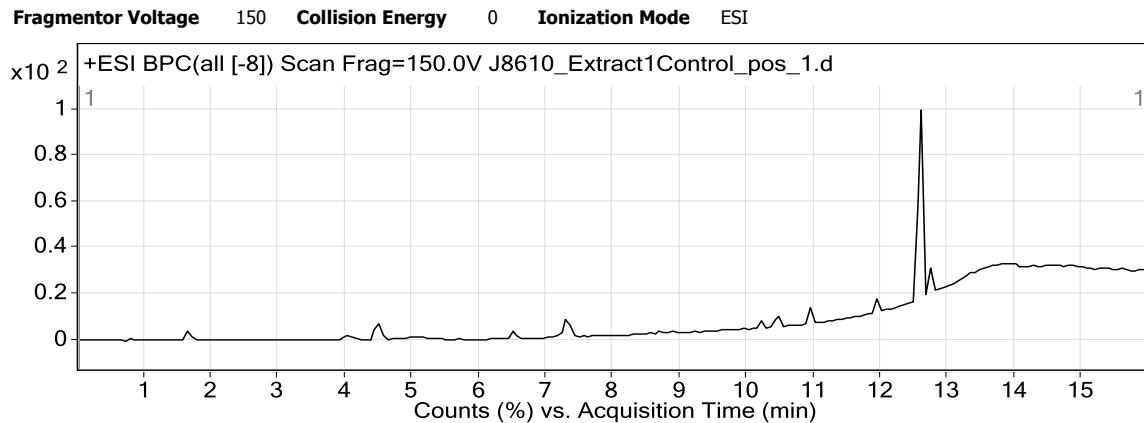


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-------------------------------|----------------------|---------------------|
| Data Filename | J8610_MethanolControl_pos_1.d | Sample Name | Extract 1 Blank |
| Sample Type | Blank | Position | Vial 15 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 5:53:21 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms



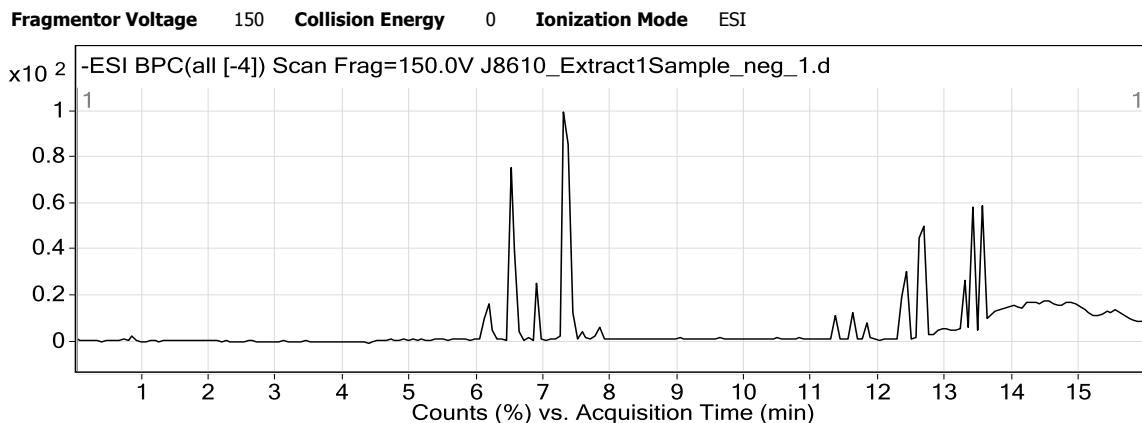
--- End Of Report ---

Qualitative Analysis Report

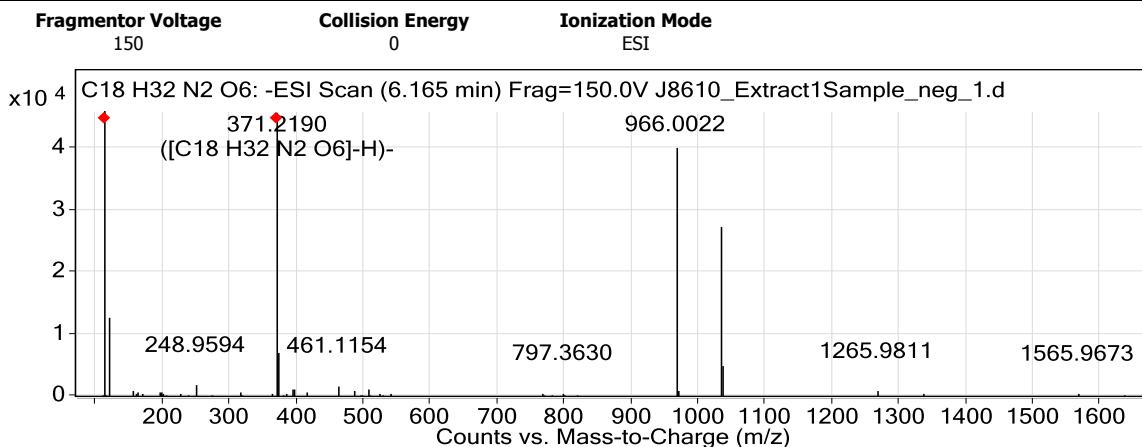
| | | | |
|-------------------------------|-------------------------------|----------------------|---------------------|
| Data Filename | J8610_MethanolExtract_neg_1.d | Sample Name | Extract 1 Sample |
| Sample Type | Blank | Position | Vial 16 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/7/2014 9:07:45 PM |
| IRM Calibration Status | Success | DA Method | neg.m |

Comment

User Chromatograms



User Spectra

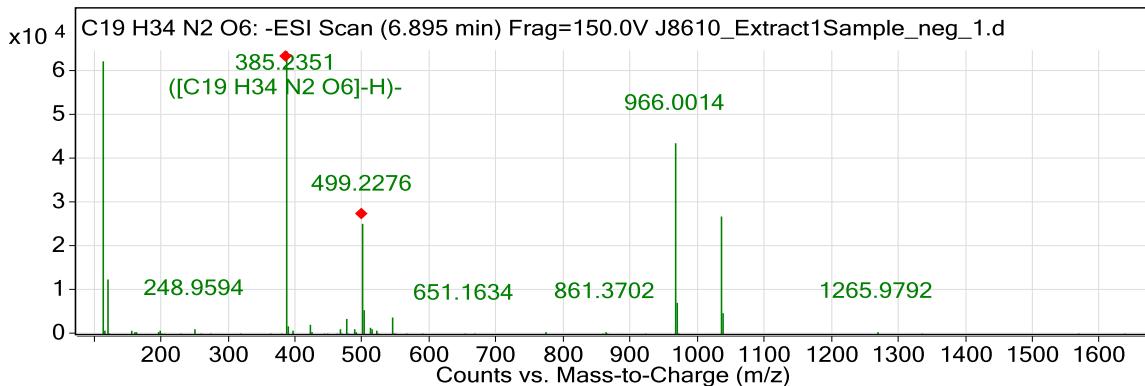


MFG Results

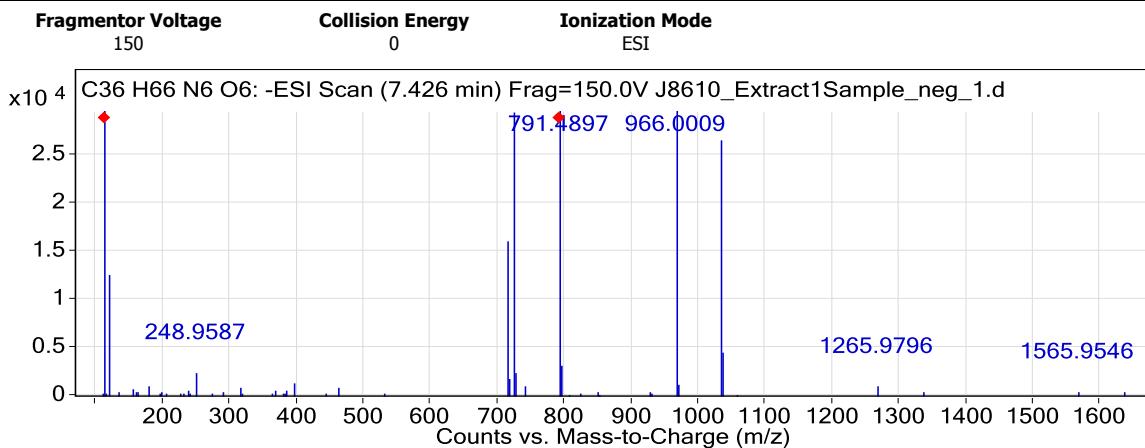
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|---------|----------|---------------|-------|-------|---------------|
| 371.219 | 372.2263 | C18 H32 N2 O6 | 93.64 | -0.76 | C18 H31 N2 O6 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

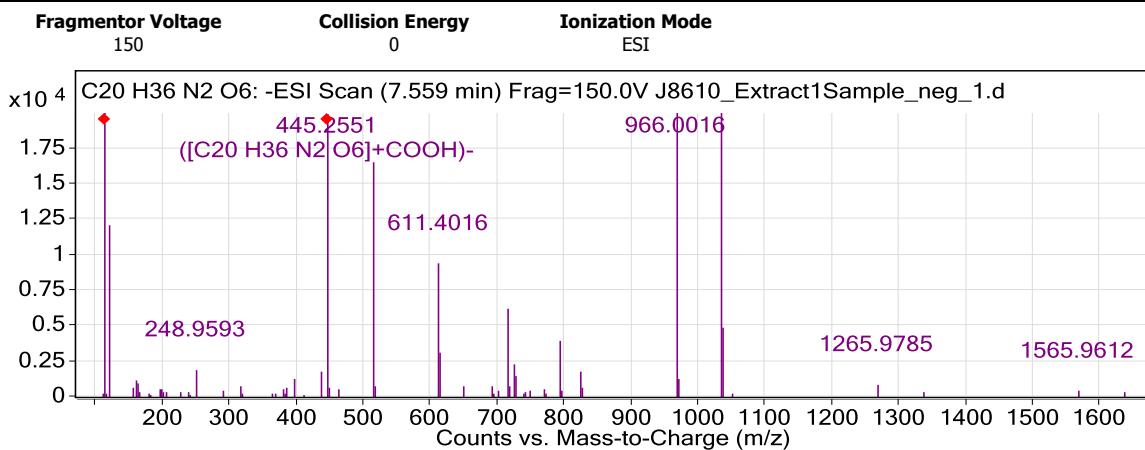
Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 385.2351 | 386.2422 | C19 H34 N2 O6 | 95.61 | -1.27 | C19 H33 N2 O6 |

**MFG Results**

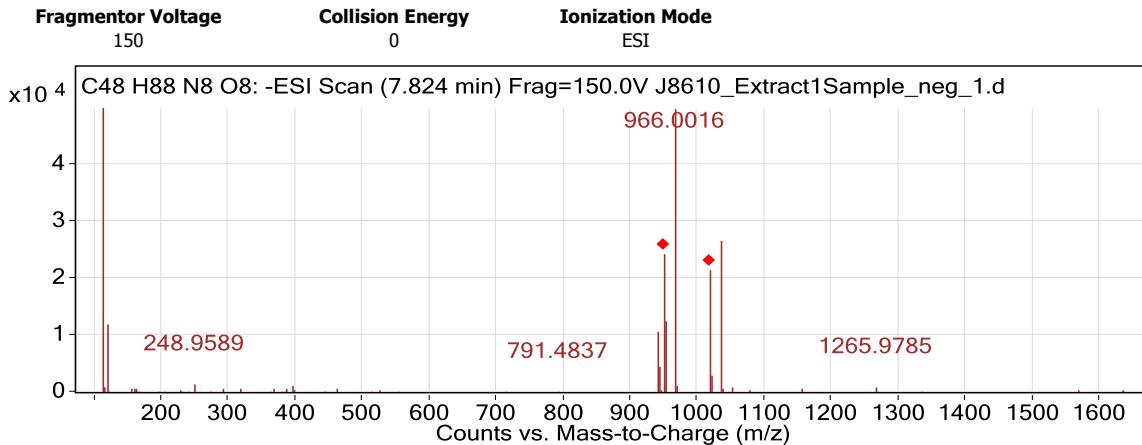
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|------------------|
| 713.4727 | 678.5036 | C36 H66 N6 O6 | 96.62 | 1.19 | C36 H66 Cl N6 O6 |
| 723.5024 | 678.5038 | C36 H66 N6 O6 | 95.5 | 0.85 | C37 H67 N6 O8 |

**MFG Results**

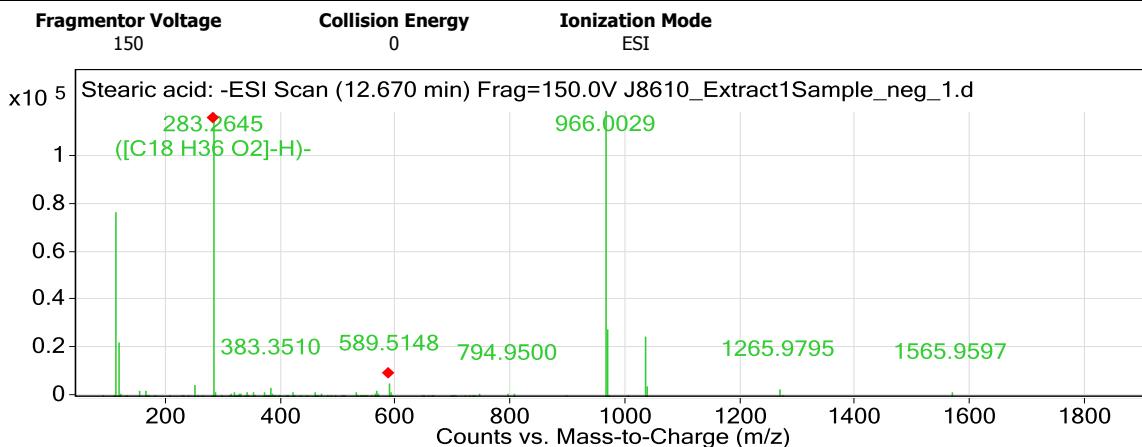
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|-----|------|------------|-------|-------|-----------|
| | | | | | |

Qualitative Analysis Report

| | | | | | |
|----------|----------|---------------|-------|-------|------------------|
| 435.2272 | 400.2579 | C20 H36 N2 O6 | 83.44 | -1.33 | C20 H36 Cl N2 O6 |
| 445.2551 | 400.2568 | C20 H36 N2 O6 | 95.87 | 1.26 | C21 H37 N2 O8 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|------------------|
| 939.6407 | 904.6707 | C48 H88 N8 O8 | 94.12 | 1.97 | C48 H88 Cl N8 O8 |
| 949.6702 | 904.672 | C48 H88 N8 O8 | 95.5 | 0.6 | C49 H89 N8 O10 |

**MFG Results**

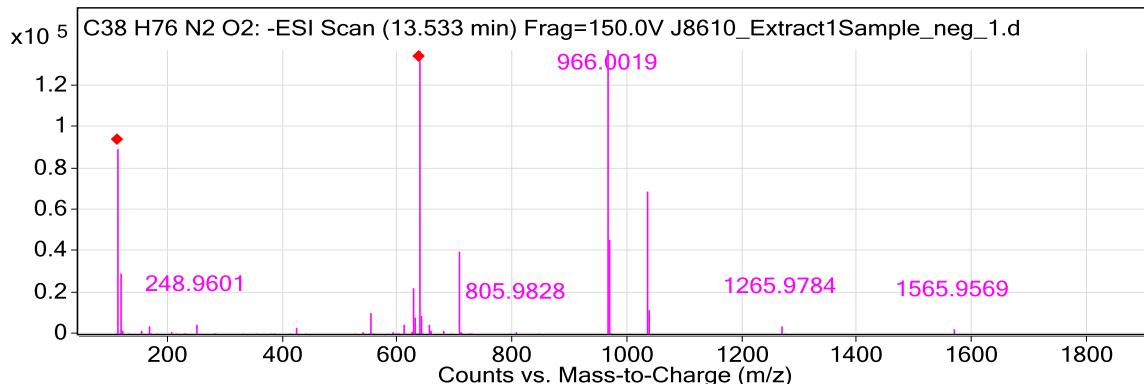
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|------------|
| 283.2645 | 284.2716 | C18 H36 O2 | 95.33 | -0.12 | C18 H35 O2 |

Database Results

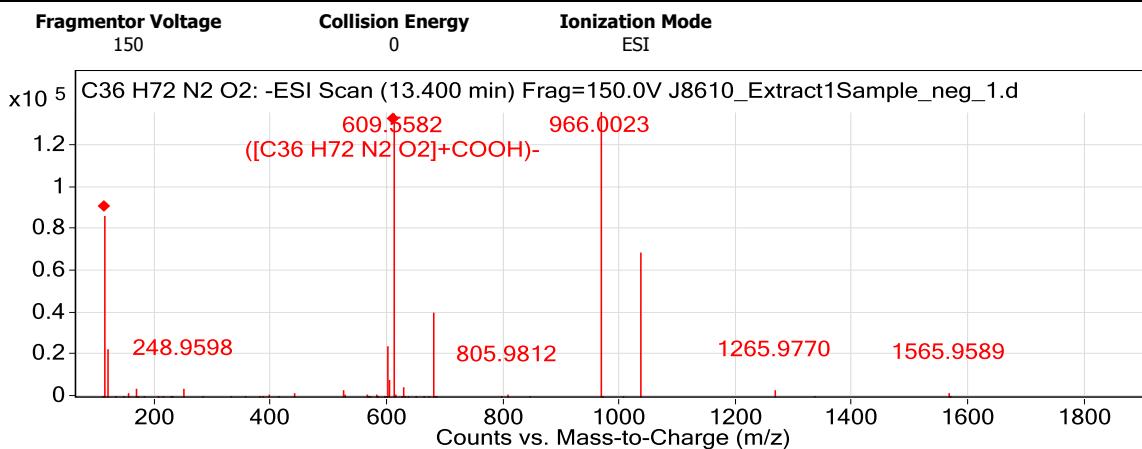
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|--------------|------------|------------|-----------|------------|----------|
| 283.2645 | Stearic acid | C18 H36 O2 | 95.26 | 1 | -0.2 | 284.2716 |

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

Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|------------------|
| 627.5591 | 592.5892 | C38 H76 N2 O2 | 76.06 | 2.48 | C38 H76 Cl N2 O2 |
| 637.589 | 592.5904 | C38 H76 N2 O2 | 94.96 | 0.43 | C39 H77 N2 O4 |

**MFG Results**

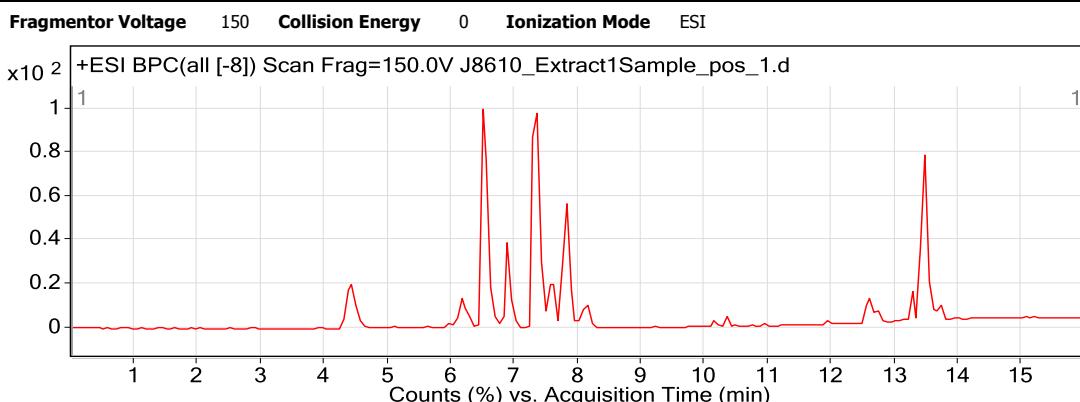
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|------------------|
| 599.5277 | 564.5581 | C36 H72 N2 O2 | 94.73 | 2.35 | C36 H72 Cl N2 O2 |
| 609.5582 | 564.5596 | C36 H72 N2 O2 | 95.36 | -0.34 | C37 H73 N2 O4 |

--- End Of Report ---

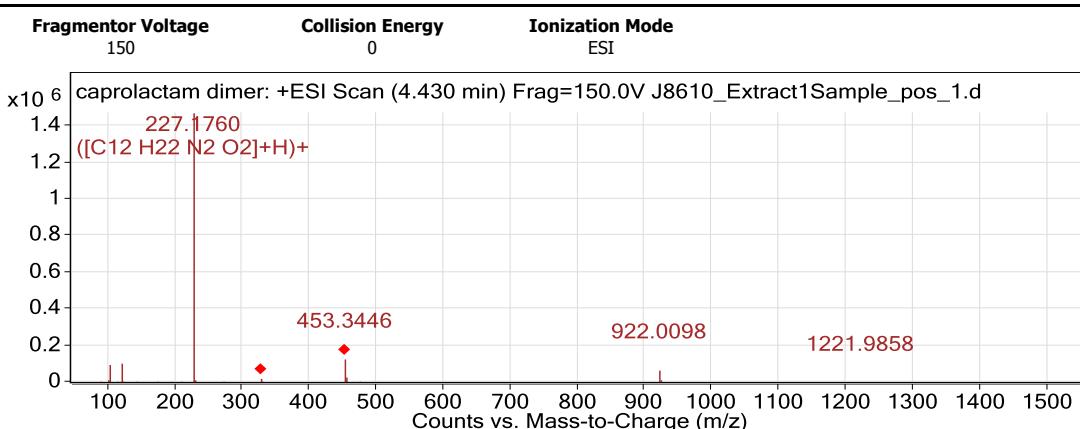
Qualitative Analysis Report

| | | | |
|-------------------------------|-------------------------------|----------------------|---------------------|
| Data Filename | J8610_MethanolExtract_pos_1.d | Sample Name | Extract 1 Sample |
| Sample Type | Blank | Position | Vial 16 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/7/2014 8:19:19 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms



User Spectra



MFG Results

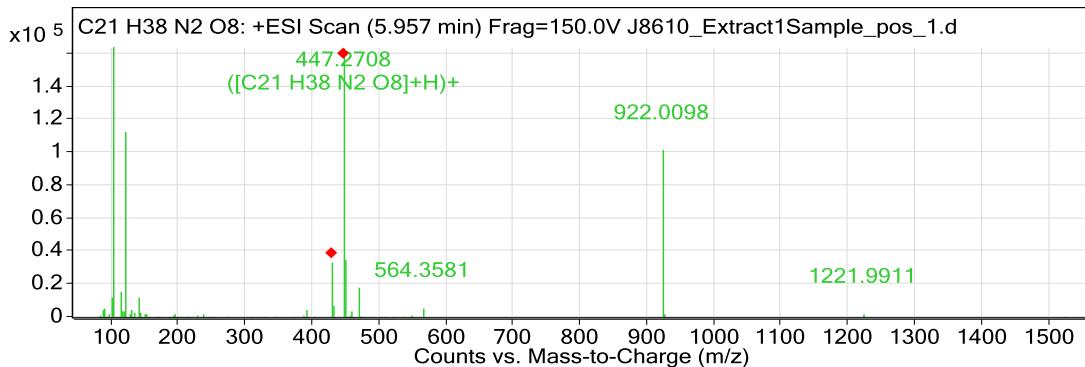
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|---------|----------|---------------|-------|-------|---------------|
| 227.176 | 226.1687 | C12 H22 N2 O2 | 98.01 | -2.69 | C12 H23 N2 O2 |

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|---------|--------------------------------|---------------|------------|-----------|------------|----------|
| 227.176 | N-N-Di(2-hydroxypropyl)aniline | C12 H22 N2 O2 | 97.88 | 2 | -0.61 | 209.1422 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report

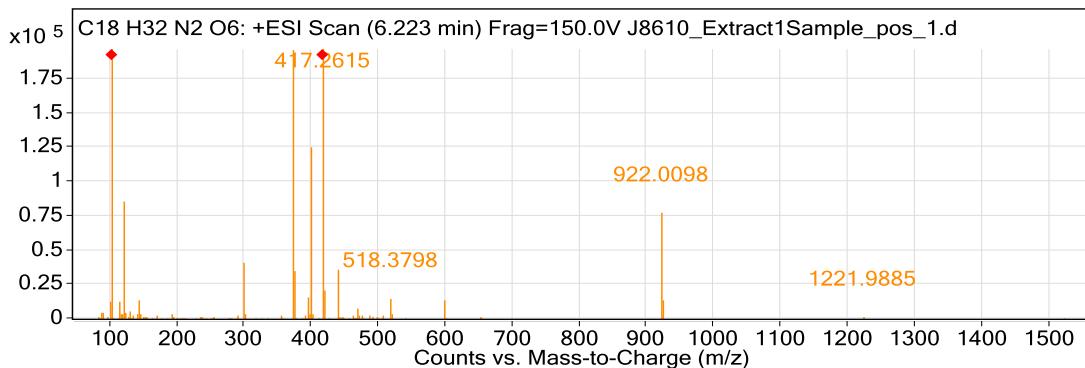
**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|------------------|
| 447.2708 | 446.2634 | C21 H38 N2 O8 | 97.87 | -1.39 | C21 H39 N2 O8 |
| 469.2522 | 446.2628 | C21 H38 N2 O8 | 81.57 | -0.01 | C21 H38 N2 Na O8 |

Database Results

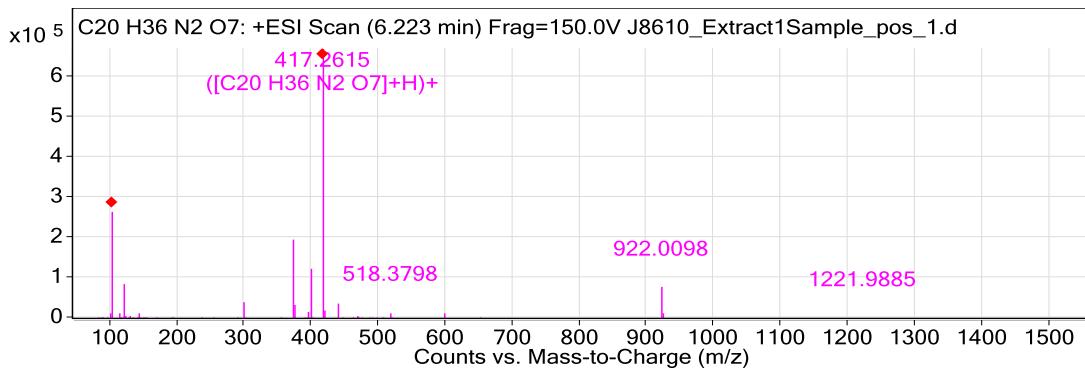
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|------------------------------|---------------|------------|-----------|------------|----------|
| 447.2708 | Irganox 1520 CAS 110553-27-0 | C21 H38 N2 O8 | 74.98 | 1 | -0.7 | 424.2817 |

Fragmentor Voltage Collision Energy Ionization Mode
150 0 ESI

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 373.2342 | 372.2268 | C18 H32 N2 O6 | 96.22 | -2.15 | C18 H33 N2 O6 |

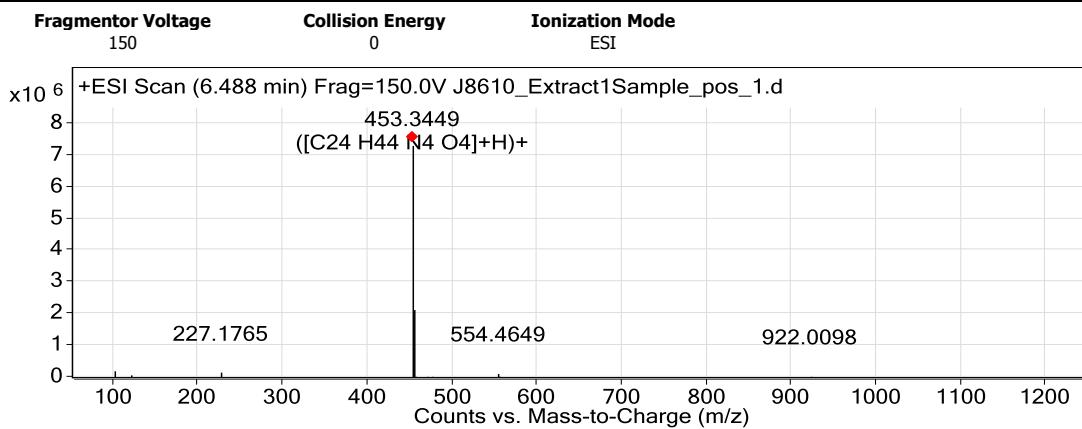
Fragmentor Voltage Collision Energy Ionization Mode
150 0 ESI

**MFG Results**

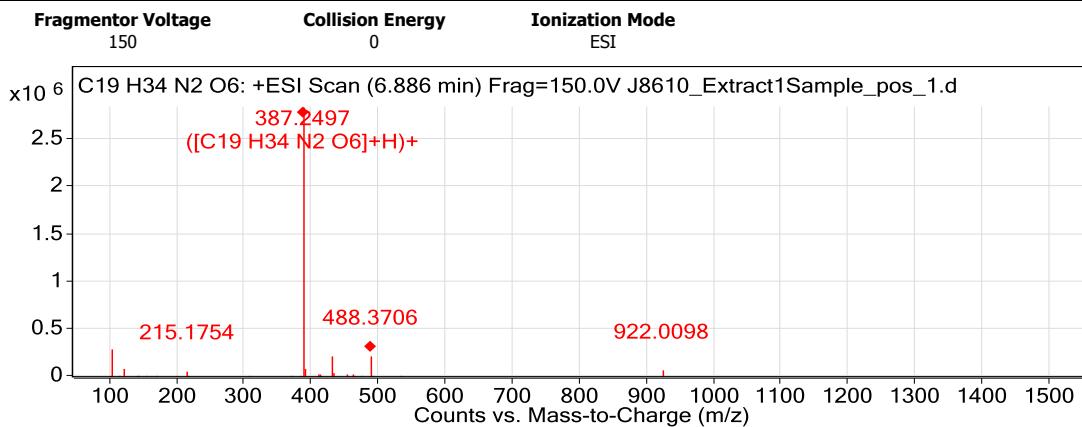
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|-----|------|------------|-------|-------|-----------|
| | | | | | |

Qualitative Analysis Report

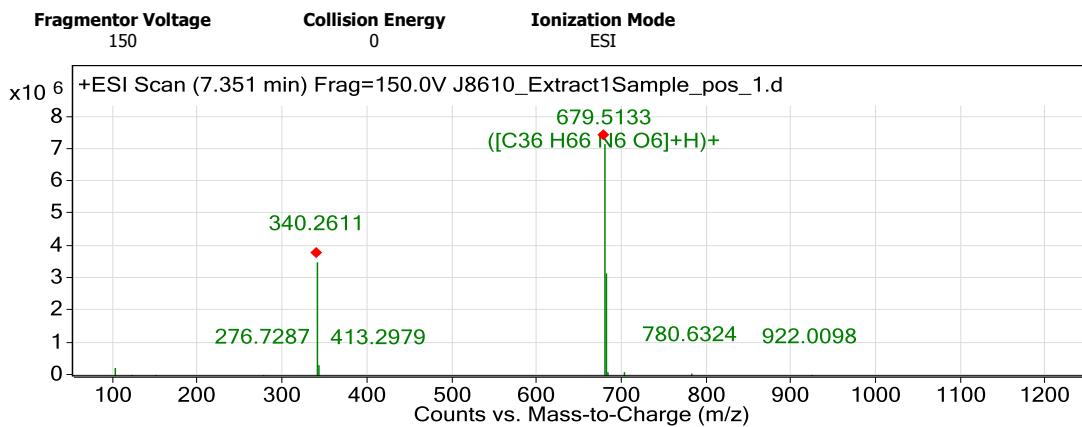
| | | | | | |
|----------|----------|---------------|-------|-------|------------------|
| 417.2615 | 416.254 | C20 H36 N2 O7 | 91.17 | -4.23 | C20 H37 N2 O7 |
| 439.2412 | 416.2523 | C20 H36 N2 O7 | 97.46 | -0.14 | C20 H36 N2 Na O7 |

**Database Results**

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|----------------------|---|------------|-----------|------------|----------|
| 453.3449 | caprolactam tetramer | C ₂₄ H ₄₄ N ₄ O ₄ | 95.61 | 2 | -1.37 | 452.3376 |

**MFG Results**

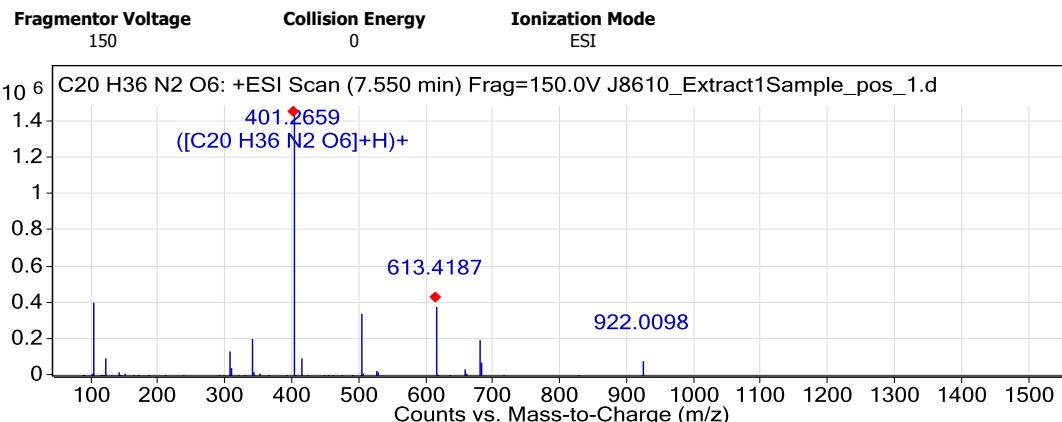
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---|-------|-------|---|
| 387.2497 | 386.2427 | C19 H ₃₄ N ₂ O ₆ | 95.84 | -2.5 | C19 H ₃₅ N ₂ O ₆ |



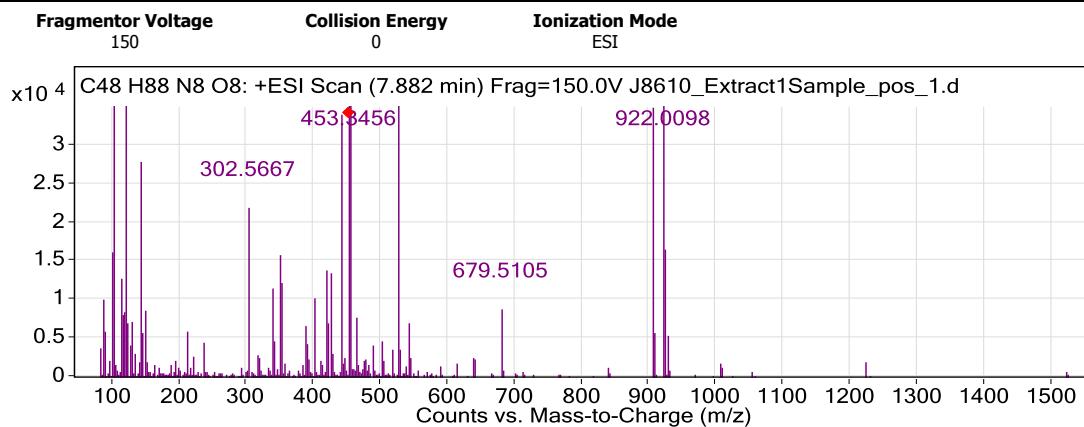
Qualitative Analysis Report

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|---------------------|---------------|------------|-----------|------------|----------|
| 679.5133 | caprolactam hexamer | C36 H66 N6 O6 | 95.95 | 1 | -1.61 | 678.5059 |


MFG Results

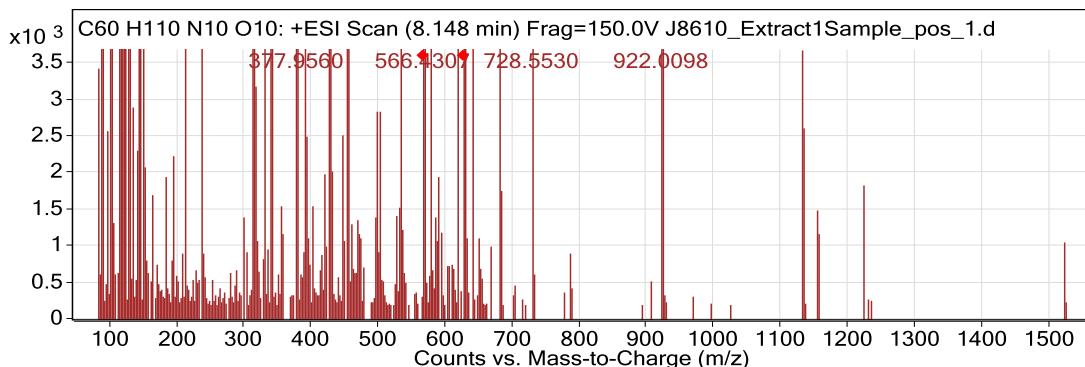
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|---------------|-------|-------|---------------|
| 401.2659 | 400.2587 | C20 H36 N2 O6 | 95.09 | -3.41 | C20 H37 N2 O6 |


MFG Results

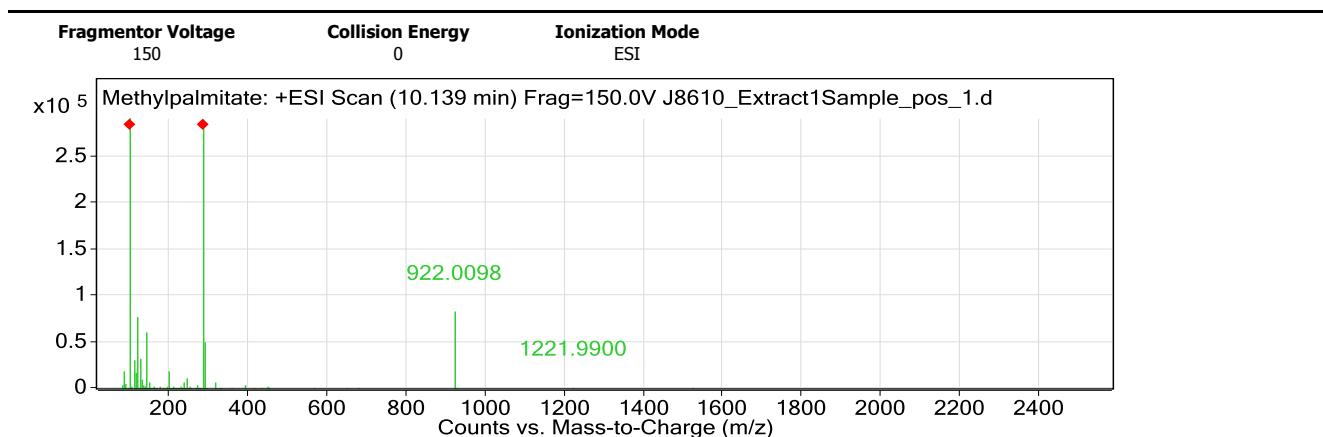
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|---------|---------------|-------|-------|---------------|
| 905.6794 | 904.672 | C48 H88 N8 O8 | 99.24 | 0.6 | C48 H89 N8 O8 |

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

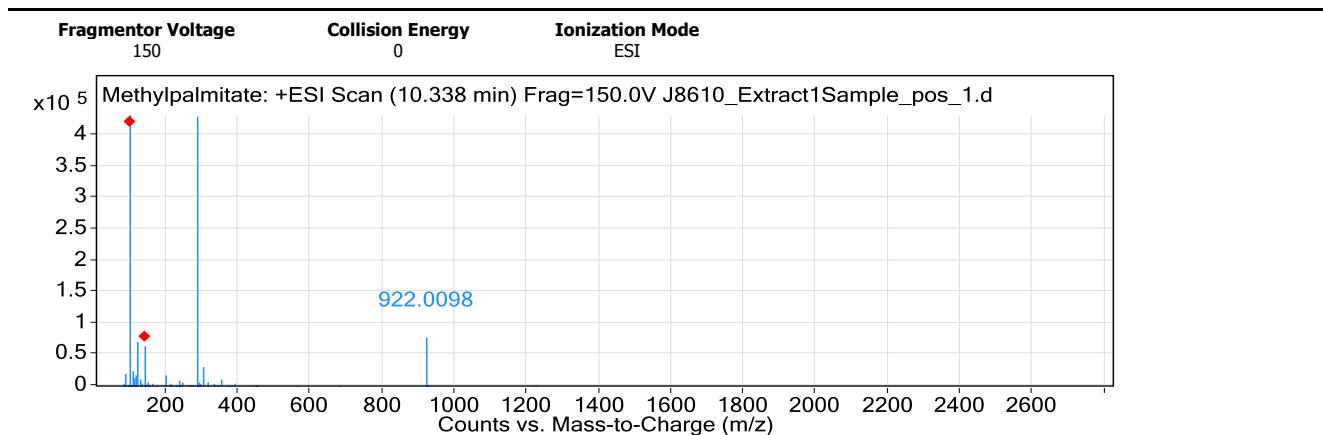
Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|-----------|----------|------------------|-------|-------|------------------|
| 1131.8464 | 1130.839 | C60 H110 N10 O10 | 93.07 | 1.45 | C60 H111 N10 O10 |

**Database Results**

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-----------------|------------|------------|-----------|------------|----------|
| 288.2909 | Methylpalmitate | C17 H34 O2 | 94.27 | 1 | -1.15 | 270.2569 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|--------------|
| 288.2911 | 270.2572 | C17 H34 O2 | 92.21 | -4.76 | C17 H38 N O2 |

Database Results

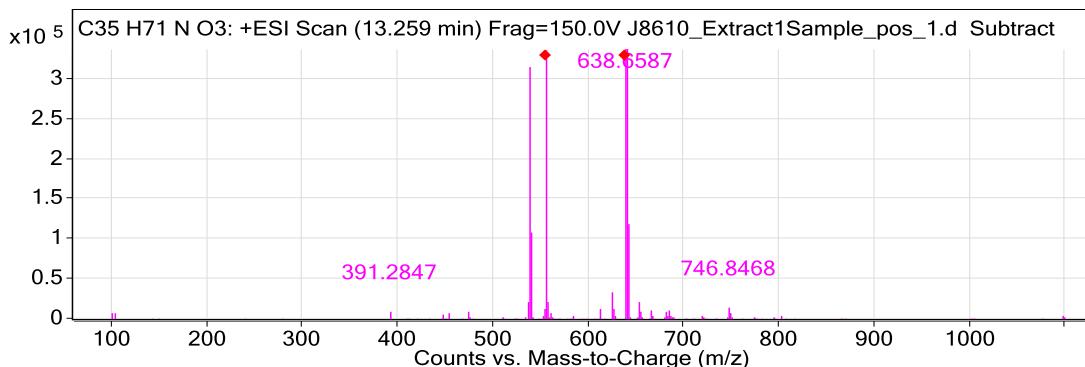
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-----------------|------------|------------|-----------|------------|----------|
| 288.2911 | Methylpalmitate | C17 H34 O2 | 92.03 | 1 | -1.41 | 270.2572 |

Qualitative Analysis Report

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
ESI

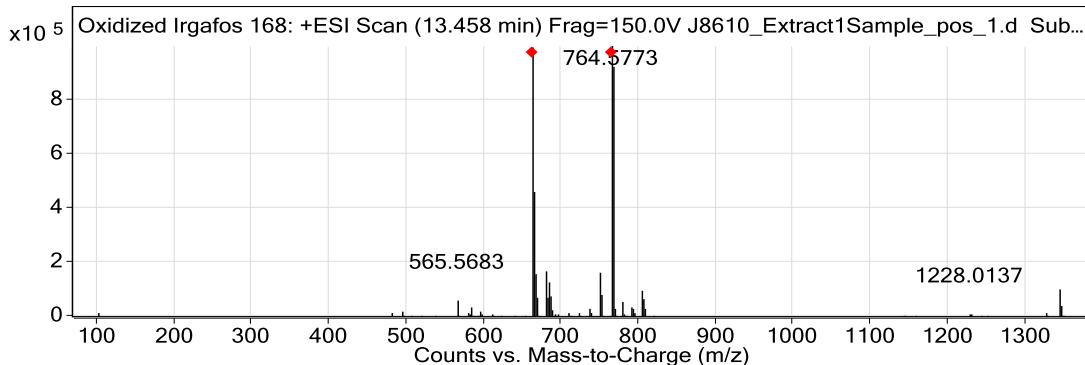

MFG Results

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|--------------|-------|-------|--------------|
| 554.5539 | 553.5462 | C35 H71 N O3 | 84.24 | -5.05 | C35 H72 N O3 |

Fragmentor Voltage
150

Collision Energy
0

Ionization Mode
ESI

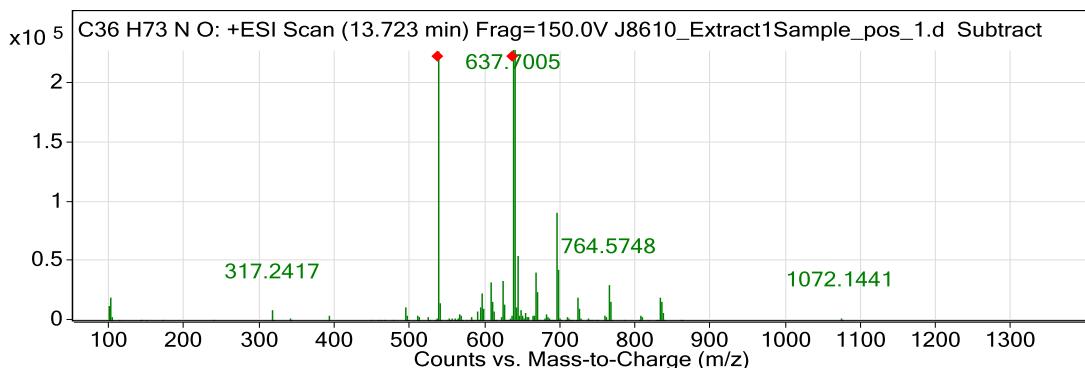

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|----------------------|--------------|------------|-----------|------------|----------|
| 663.4574 | Oxidized Irgafos 168 | C42 H63 O4 P | 83.25 | 2 | -3.75 | 662.4501 |

Fragmentor Voltage
150

Collision Energy
0

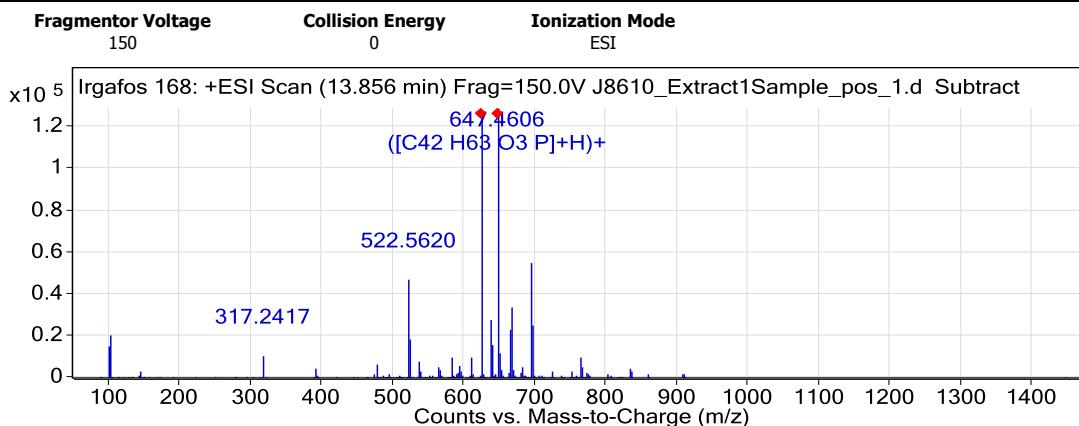
Ionization Mode
ESI


MFG Results

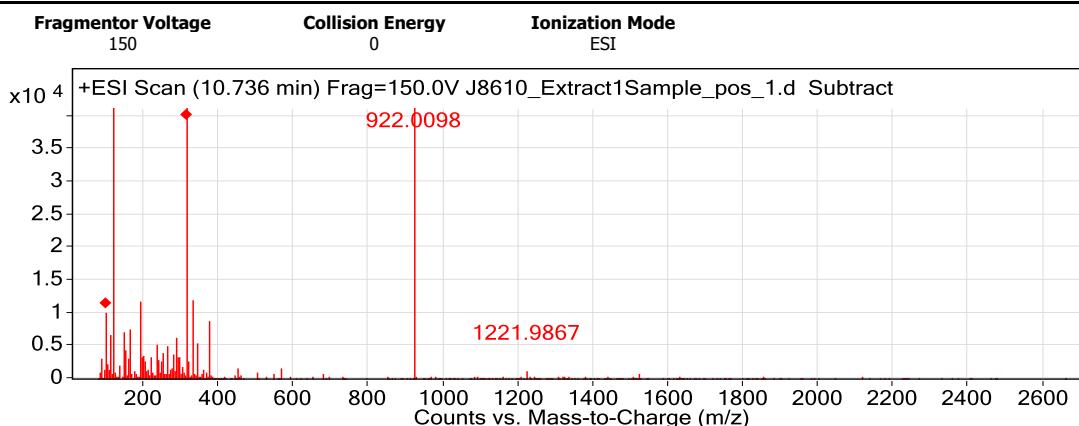
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|---------|-------------|-------|-------|-------------|
| 536.5786 | 535.571 | C36 H73 N O | 91.78 | -3.31 | C36 H74 N O |



Qualitative Analysis Report

**Database Results**

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-------------|--|------------|-----------|------------|---------|
| 647.4606 | Irgafos 168 | C ₄₂ H ₆₃ O ₃ P | 95.43 | 1 | -1.88 | 646.453 |

**Database Results**

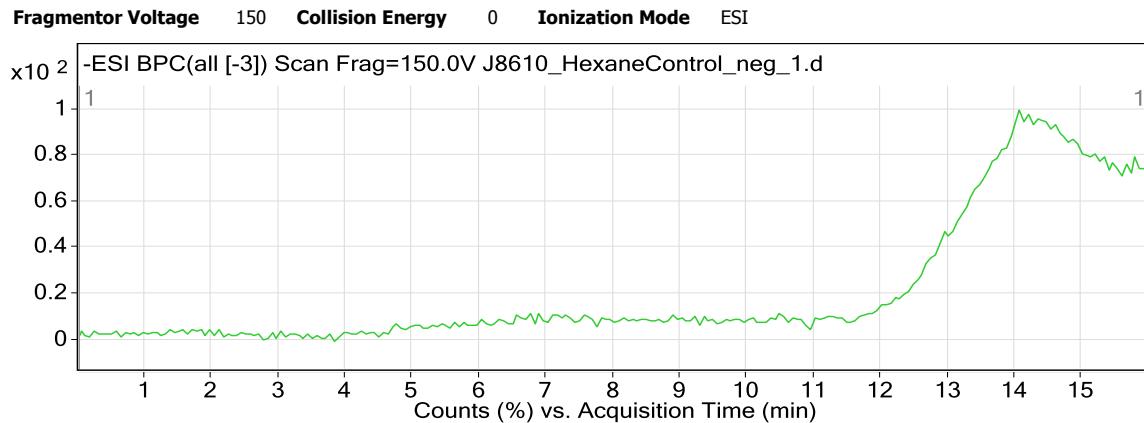
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-----------------|--|------------|-----------|------------|----------|
| 316.3217 | Methyl stearate | C ₁₉ H ₃₈ O ₂ | 97.06 | 1 | -0.74 | 298.2878 |

--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|----------------------|
| Data Filename | J8610_HexaneControl_neg_1.d | Sample Name | Control |
| Sample Type | Blank | Position | Vial 91 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/14/2014 7:10:52 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

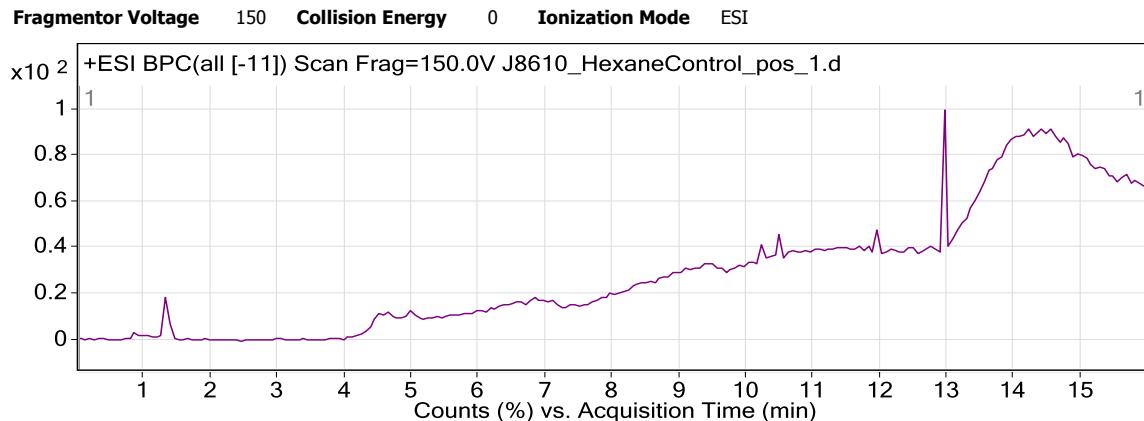


--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|----------------------|
| Data Filename | J8610_HexaneControl_pos_1.d | Sample Name | Control |
| Sample Type | Blank | Position | Vial 91 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/14/2014 6:22:15 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms

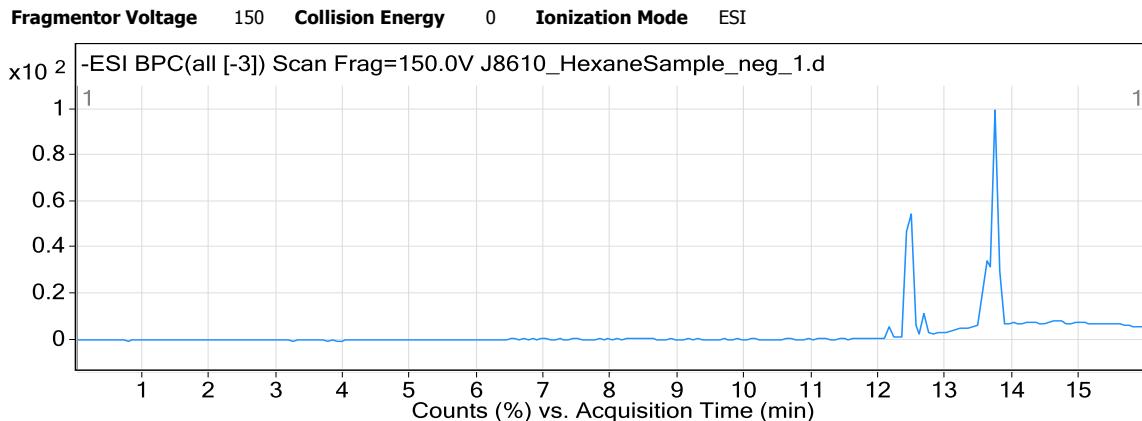


--- End Of Report ---

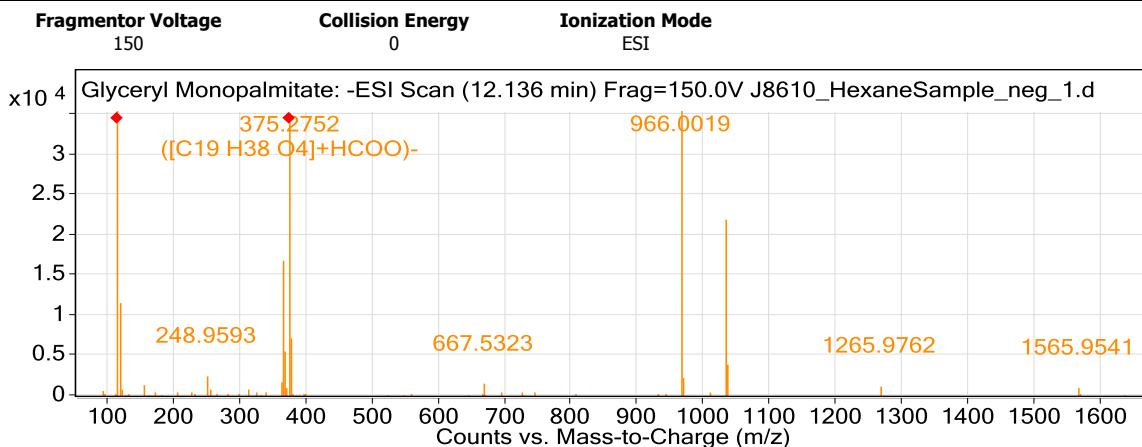
Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|----------------------|
| Data Filename | J8610_HexaneExtract_neg_1.d | Sample Name | Hexane Sample |
| Sample Type | Blank | Position | Vial 92 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-neg.m | Acquired Time | 5/14/2014 9:36:56 PM |
| IRM Calibration Status | Success | DA Method | neg.m |
| Comment | | | |

User Chromatograms



User Spectra



MFG Results

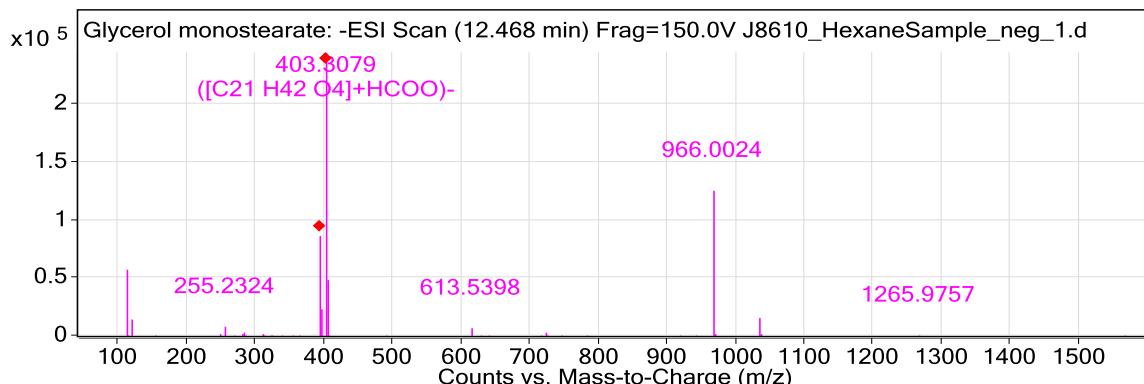
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|---------------|
| 365.2465 | 330.2768 | C19 H38 O4 | 97.62 | 0.77 | C19 H38 Cl O4 |
| 375.2752 | 330.2769 | C19 H38 O4 | 99.21 | 0.39 | C20 H39 O6 |

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|------------------|------------|------------|-----------|------------|----------|
| 375.2752 | PEG4 monolaurate | C19 H38 O4 | 99.25 | 5 | 0.06 | 376.2824 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

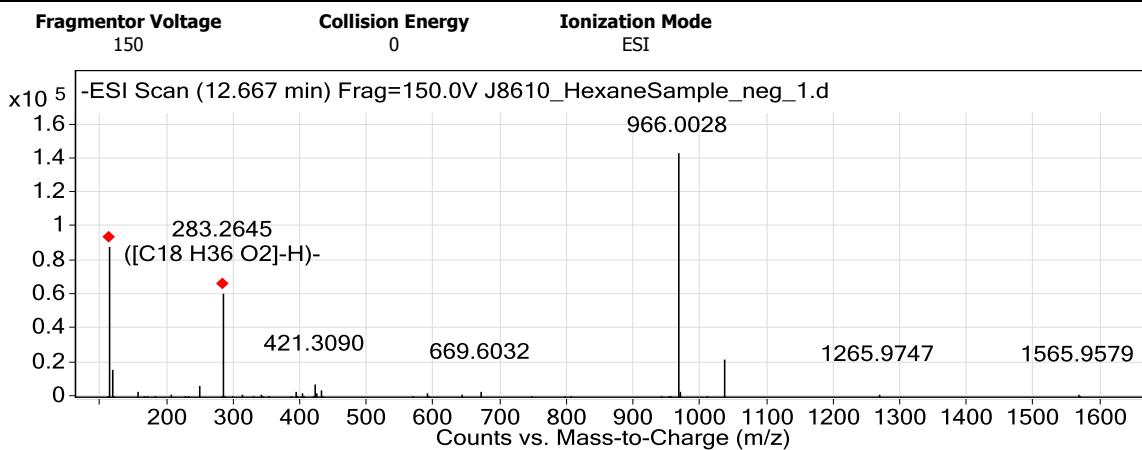
Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|---------------|
| 393.2785 | 358.3087 | C21 H42 O4 | 93.44 | -1.14 | C21 H42 Cl O4 |
| 403.3079 | 358.3095 | C21 H42 O4 | 91.04 | -3.25 | C22 H43 O6 |

Database Results

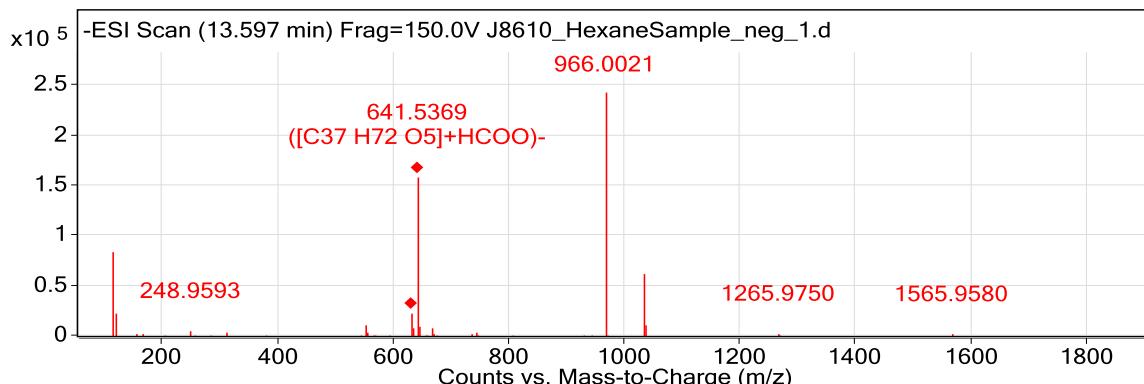
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-----------------------|------------|------------|-----------|------------|----------|
| 403.3079 | Glycerol monostearate | C21 H42 O4 | 90.5 | 2 | -1.4 | 358.3095 |

**Database Results**

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|--------------|------------|------------|-----------|------------|----------|
| 283.2645 | Stearic acid | C18 H36 O2 | 96.3 | 1 | -0.22 | 284.2717 |

Fragmentor Voltage Collision Energy Ionization Mode
150 0 ESI

Qualitative Analysis Report

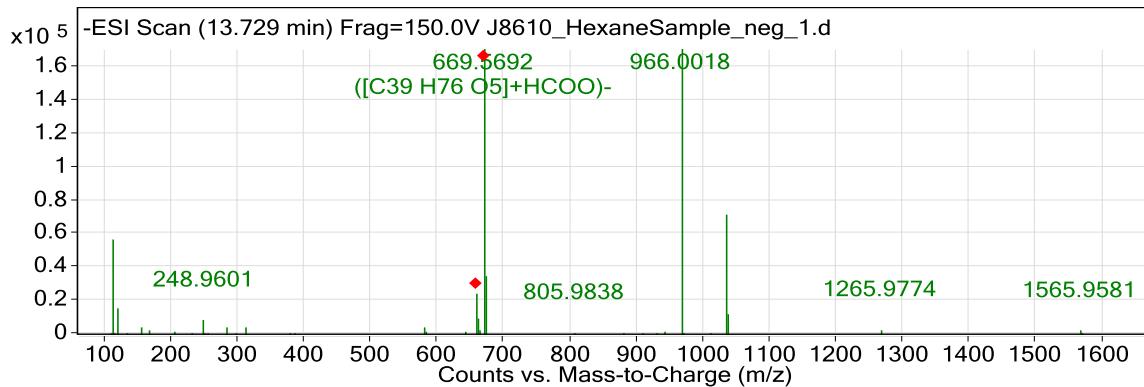
**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|---------------|
| 631.5065 | 596.5365 | C37 H72 O5 | 92.72 | 2.44 | C37 H72 Cl O5 |
| 641.5369 | 596.5384 | C37 H72 O5 | 94.75 | -0.72 | C38 H73 O7 |

Database Results

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|-----------------------|------------|------------|-----------|------------|----------|
| 641.5369 | Diglyceride 18:0-16:0 | C37 H72 O5 | 94.71 | 1 | -0.68 | 596.5384 |

Fragmentor Voltage Collision Energy Ionization Mode
150 0 ESI

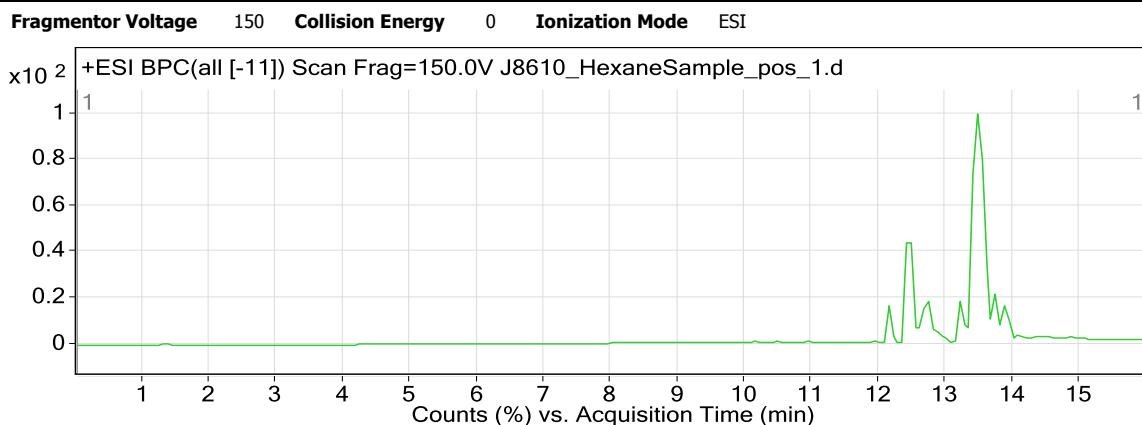
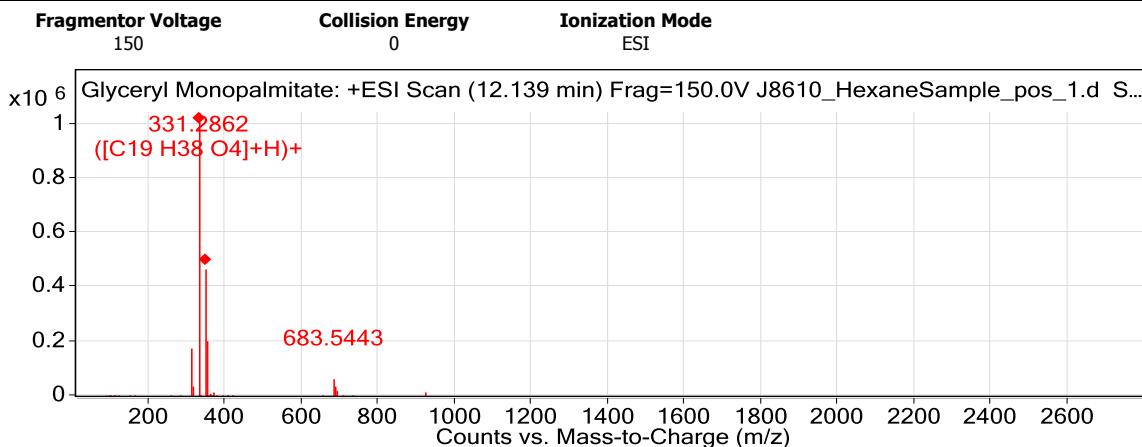
**Database Results**

| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|---------------------|------------|------------|-----------|------------|----------|
| 669.5692 | Glycerol distearate | C39 H76 O5 | 94.39 | 2 | -1.75 | 624.5706 |

--- End Of Report ---

Qualitative Analysis Report

| | | | |
|-------------------------------|-----------------------------|----------------------|----------------------|
| Data Filename | J8610_HexaneExtract_pos_1.d | Sample Name | Hexane Sample |
| Sample Type | Blank | Position | Vial 92 |
| Instrument Name | Instrument 1 | User Name | |
| Acq Method | Default-DualESI-pos.m | Acquired Time | 5/14/2014 8:48:19 PM |
| IRM Calibration Status | Success | DA Method | neg.m |

Comment**User Chromatograms****User Spectra****MFG Results**

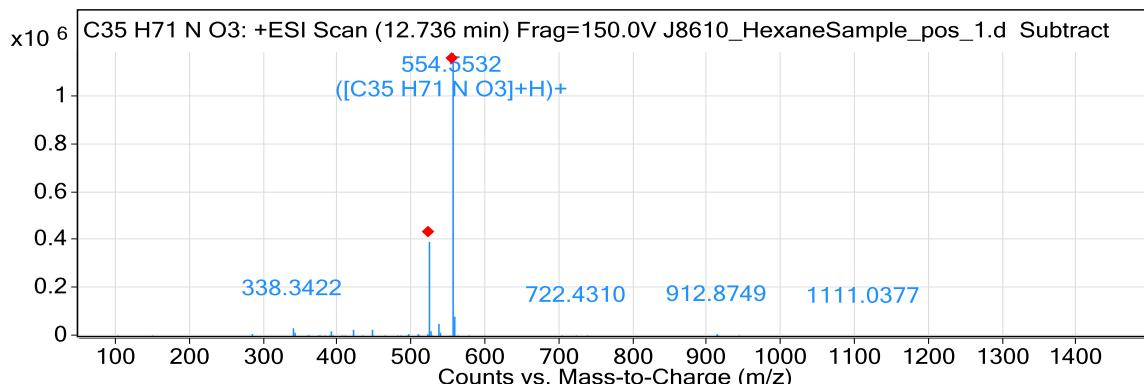
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|---------------|
| 331.2862 | 330.2788 | C19 H38 O4 | 89.75 | -5.33 | C19 H39 O4 |
| 353.2671 | 330.2777 | C19 H38 O4 | 95.49 | -2.19 | C19 H38 Na O4 |
| 348.3124 | 330.2784 | C19 H38 O4 | 92.12 | -4.17 | C19 H42 N O4 |

Database Results

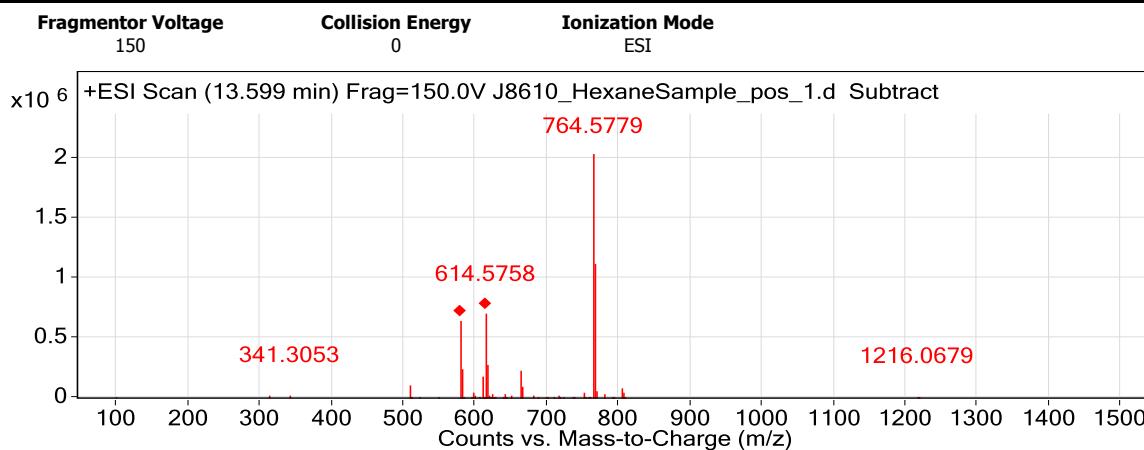
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|------------------------|------------|------------|-----------|------------|----------|
| 331.2862 | Glyceryl Monopalmitate | C19 H38 O4 | 89.69 | 2 | -1.94 | 330.2788 |

Fragmentor Voltage 150 Collision Energy 0 Ionization Mode ESI

Qualitative Analysis Report

**MFG Results**

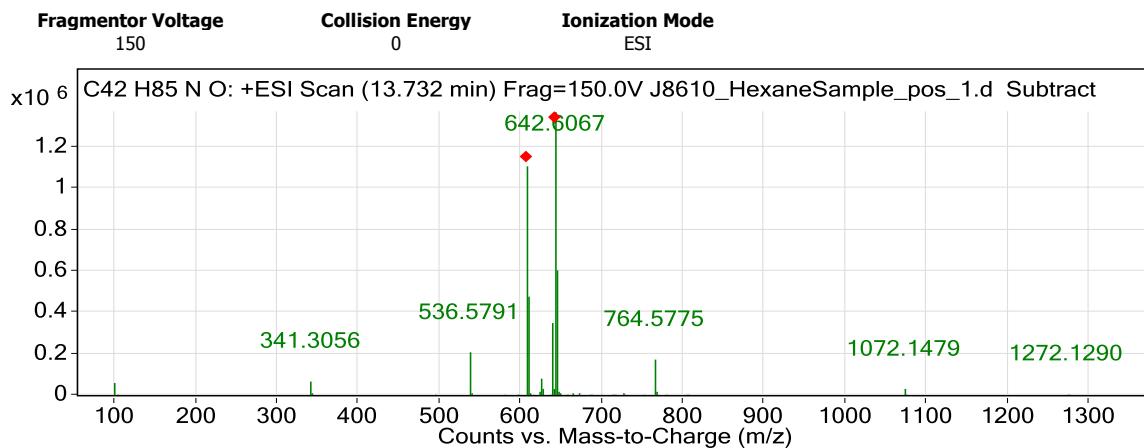
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|---------|--------------|-------|-------|--------------|
| 554.5532 | 553.546 | C35 H71 N O3 | 88.79 | -4.67 | C35 H72 N O3 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|--------------|-------|-------|--------------|
| 663.4569 | 662.4493 | C42 H63 O4 P | 86.62 | -4.4 | C42 H64 O4 P |

Database Results

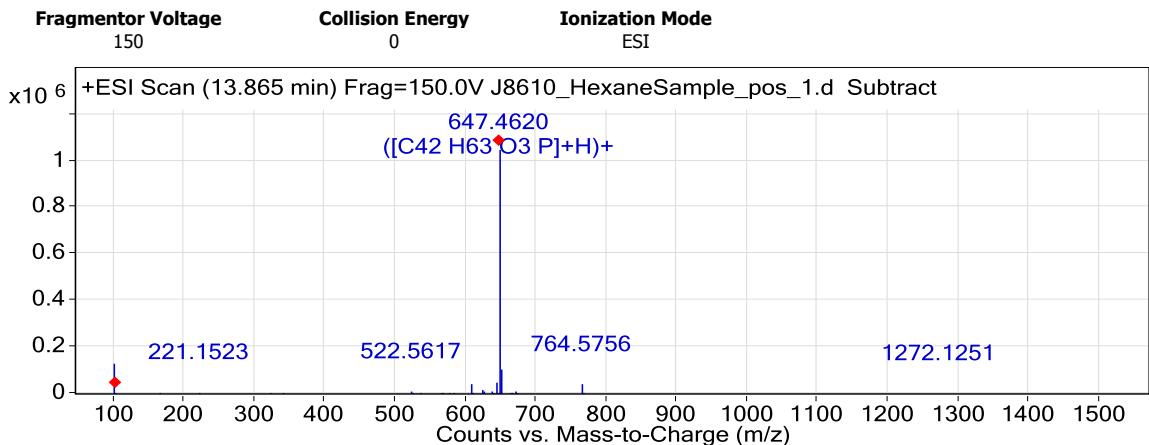
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|----------|----------------------|--------------|------------|-----------|------------|----------|
| 663.4569 | Oxidized Irgafos 168 | C42 H63 O4 P | 86.54 | 1 | -3.22 | 662.4493 |



Qualitative Analysis Report

MFG Results

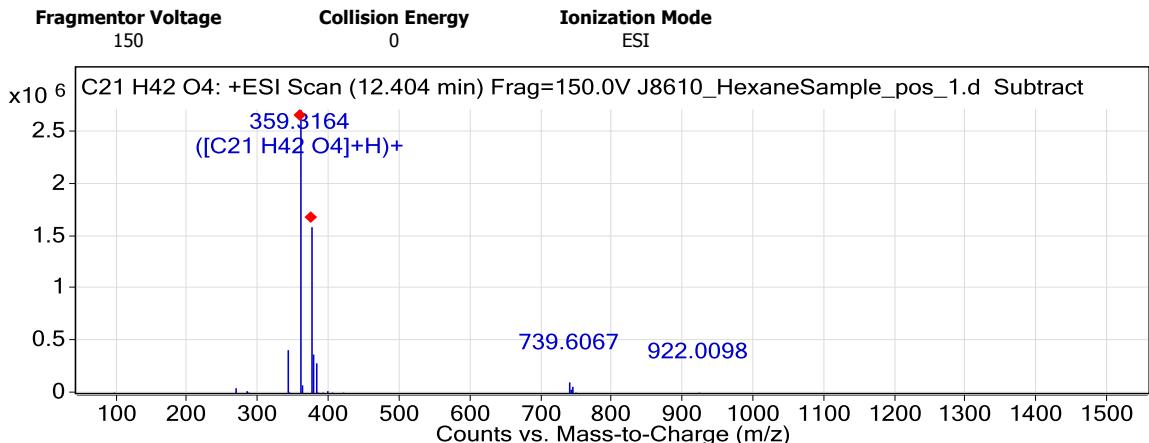
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|-------------|-------|-------|--------------|
| 637.7007 | 619.6663 | C42 H85 N O | 84 | -5.11 | C42 H89 N2 O |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|---------|----------|--------------|-------|-------|--------------|
| 647.462 | 646.4547 | C42 H63 O3 P | 85.77 | -4.99 | C42 H64 O3 P |

Database Results

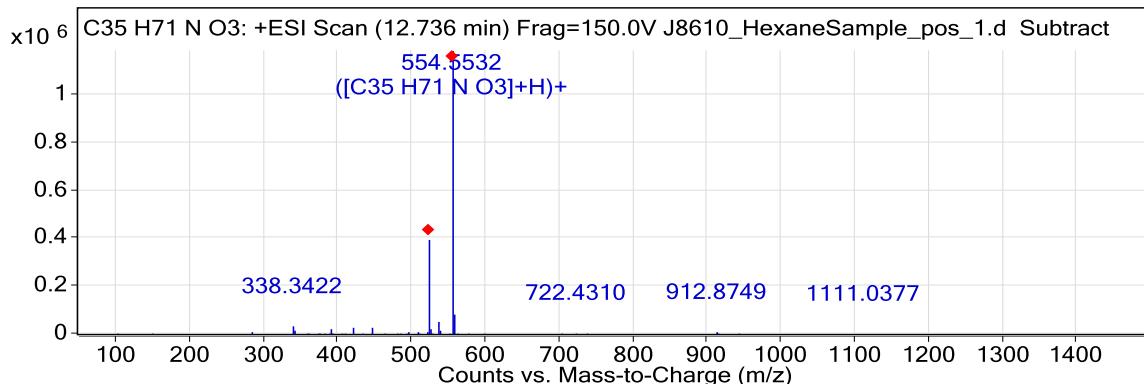
| m/z | Name | Formula | Score (DB) | Hits (DB) | Difference | Mass |
|---------|-------------|--------------|------------|-----------|------------|----------|
| 647.462 | Irgafos 168 | C42 H63 O3 P | 85.83 | 1 | -3.27 | 646.4547 |

**MFG Results**

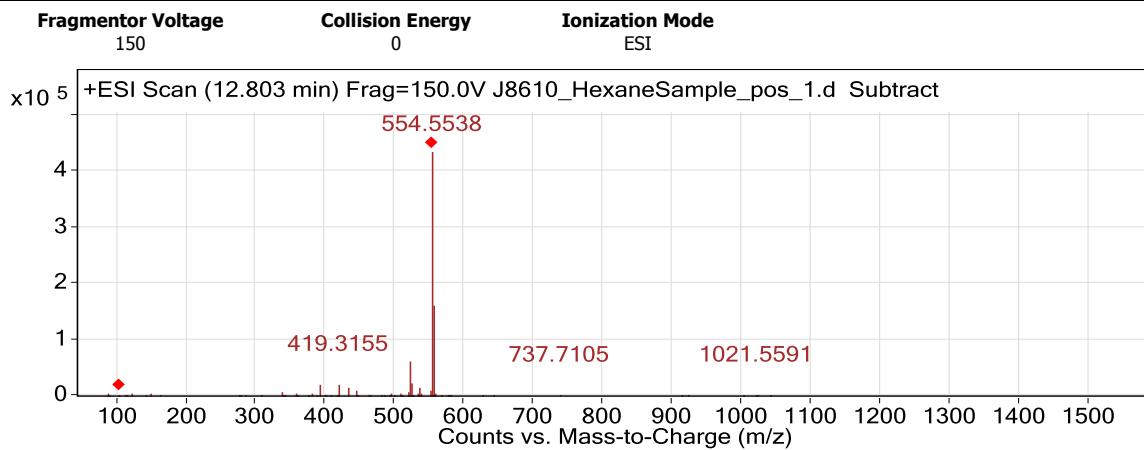
| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|---------------|
| 359.3164 | 358.3093 | C21 H42 O4 | 95.96 | -2.69 | C21 H43 O4 |
| 381.2986 | 358.3089 | C21 H42 O4 | 90.12 | -1.66 | C21 H42 Na O4 |
| 376.3429 | 358.3092 | C21 H42 O4 | 97.57 | -2.38 | C21 H46 N O4 |

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

Qualitative Analysis Report

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|---------|--------------|-------|-------|--------------|
| 554.5532 | 553.546 | C35 H71 N O3 | 88.79 | -4.67 | C35 H72 N O3 |

**MFG Results**

| m/z | Mass | Best Match | Score | Diff. | Ion Form. |
|----------|----------|------------|-------|-------|-----------|
| 522.5982 | 504.5643 | C36 H72 | 97.5 | -1.73 | C36 H76 N |

--- End Of Report ---