



CASE STUDY
Headspace Gas Spectroscopy
vs.
Desorption Mass Spectroscopy

OBJECTIVE

The purpose of this work was to compare Headspace Gas Spectroscopy (HS-GCMS) and Desorption Mass Spectroscopy (DMS) while characterizing and identifying the organic volatiles from an unknown sample reported to be a buildup on an extruder used for polyolefin processing.

CONCLUSIONS

DMS is a very sensitive technique which provides valuable information about trace volatile and semi-volatile components. When analyzed by HS-GCMS the low boiling compounds are preferentially evolved into the headspace gas. In general, the signal strength for the most volatile components is increased in HS-GCMS as compared to DMS due to the ability to increase sample size and its selectivity for component with higher vapor pressures.

Read the following report to see the full analysis.



Final Report

Jordi Labs LLC
Case Study
Headspace Gas Spectroscopy
vs.
Desorption Mass Spectroscopy

Date: 11/10/10

Prepared by:
Dr. Mark Jordi
President
Jordi Labs LLC

Report Number: J5169

Jordi Labs LLC Confidential





Date

Client Name
Company Name
Address

Dear Valued Client:

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

1. Unknown Extruder Build-up

The following tests were performed:

1. Desorption Mass Spectroscopy (DMS)
2. Headspace Gas Chromatography Mass Spectroscopy (HS-GCMS)

Objectives

The purpose of this work was to characterize and identify the organic volatiles from an unknown sample reported to be a buildup on an extruder used for polyolefin processing.

Summary of Results

A large variety of components are detected in the sample by DMS including olefinic oligomers, fatty amides, and acid esters. The most abundant species included a series of lubricants including stearamide. **Table 1** shows a list of the components identified.

Background

DMS is a very sensitive technique which provides valuable information about trace volatile and semi-volatile components. When analyzed by HS-GCMS the low boiling compounds are preferentially evolved into the headspace gas. Because only these components are evolved, they can be identified easily and are not subject to interference by additional sample components.

In general, the signal strength for the most volatile components is increased in HS-GCMS as compared to DMS due to the ability to increase sample size and its selectivity for component with higher vapor pressures. The advantage of DMS is that a broader range of analytes can be detected with this method.

Individual Test Results

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

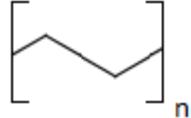
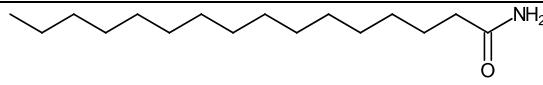
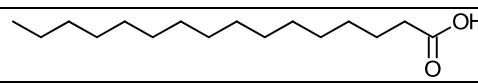
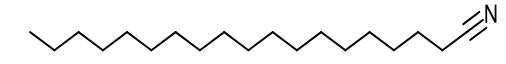
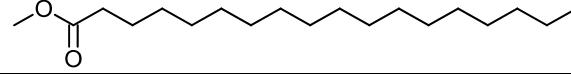
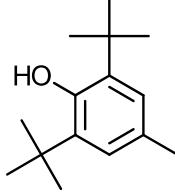
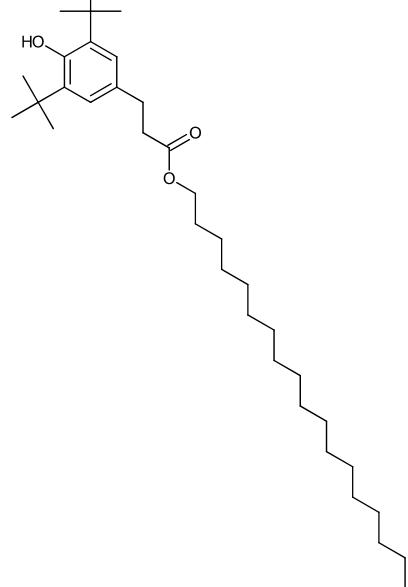
DMS: – Samples were analyzed by desorption mass spectrometry using an injection port temperature of 310°C. This technique is very sensitive for the determination of residual solvents and additives. The mass spectrum of each peak was collected and identified using the best matching database spectrum. Identifications are based on comparison with the NIST spectral library of over 197,000 compounds.

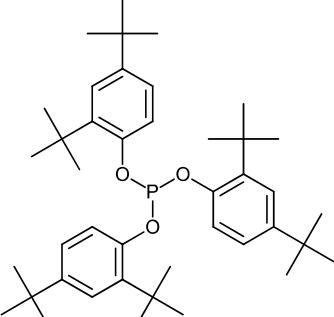
Over 50 different compounds were observed using DMS (due to the technique's heightened sensitivity). This method is excellent for trace component analysis. A large number of the observed compounds were olefinic oligomers, fatty amides, and acid esters of various hydrocarbon tail lengths. Olefinic oligomers varied from length C₁₀ to C₄₄, and included both linear and branched structures.

The antioxidant BHT and the two other related antioxidants were also observed in DMS. The solvents trichlorobenzene (2 isomer peaks), tetrahydrofuran, and isopropanol were also detected by DMS.

A list of observed components can be found in **Table 1**. Compounds of a similar nature are listed as a single category (example: all fatty amides). The best two matches for all 50 of the observed components can be seen in the data section of this report.

Table 1: Components Observed by DMS

<u>Component</u>	<u>Number of Peaks</u>	<u>Purpose</u>	<u>Structure</u>
Olefinic Oligomers	15	Residual Polymer	
Fatty Amides (Saturated & Unsaturated)	16	Slip Agent	
Fatty Acids	7	Slip Agent	
Fatty Nitriles	6	Impurities	
Hydrocarbon Acid Esters	6	Unknown	
BHT	1	Antioxidant	
Irganox 1076	1	Antioxidant	

Irgafos 168	1	Antioxidant	
Solvents	4	Solvents	NA

HS-GCMS – Approximately 10mg of the sample was hermetically sealed into a headspace sampling vial. The sample is then gently heated (70°C), increasing the concentration of volatile components in the gasses trapped above the sample. A precise aliquot of the headspace gasses are then transferred to the GCMS and analyzed.

The major components detected by HS-GCMS were the solvents isopropanol, tetrahydrofuran (THF), and trichlorobenzene. These components were also observed in DMS analysis, however because these compounds are preferentially evolved at the lower temperature used they are easier to identify. Headspace showed a dramatic increase in signal strength for these components and thus a lower detection limit. Also detected by HS-GCMS were a few of the shorter chain aliphatic compounds, as well as dichlorobenzene. We did not observe any of the antioxidants or higher molecular weight components. A list of observed components can be found in **Table 2**.

Table 2: Components Observed by HS-GCMS

<u>Best Matching Component</u>	<u>Retention Time</u>	<u>Match Score</u>	<u>Structure</u>
Isopropanol	1.455	857	
Tetrahydrofuran	2.026	933	
Methyl-nonane	6.673, 6.810	895	
Decane	7.187	952	
Dichlorobenzene	7.598	897	
Trichlorobenzene	9.025	954	

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 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,

Mark Jordi

Mark Jordi, Ph. D.
President
Jordi Labs LLC

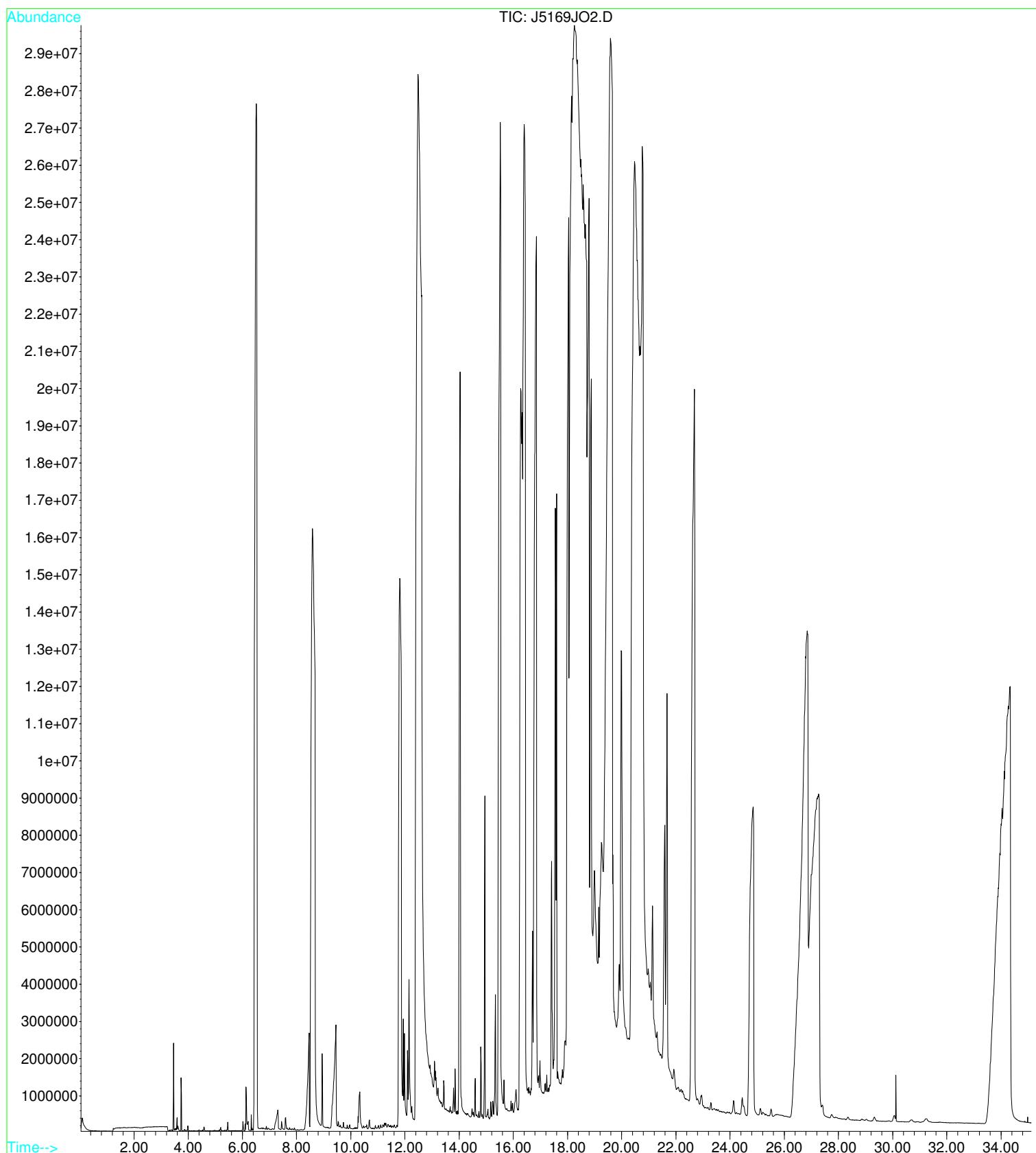
Appendix

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- Pages 9-67 – DMS Data
- Pages 68-80 – Headspace GCMS Data

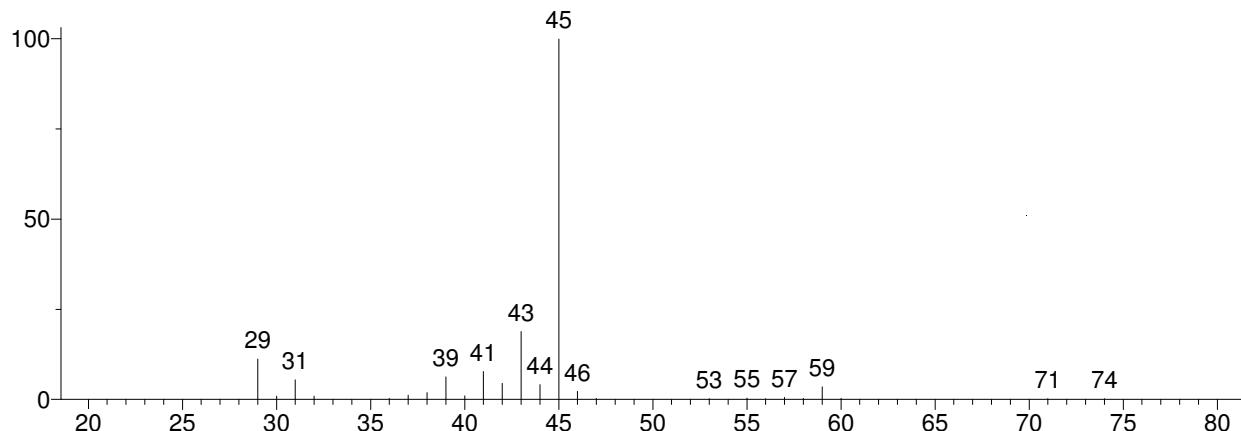
DMS RESULTS

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Operator : Kevin Rowland
Acquired : 1 Oct 2010 13:38 using AcqMethod DESORP2
Instrument : DMS Instr
Sample Name: J5169 Jordi In House Sample Deform - Run 2
Misc Info : Desorp2: 50C to 320C at 15C/Min
Vial Number: 1

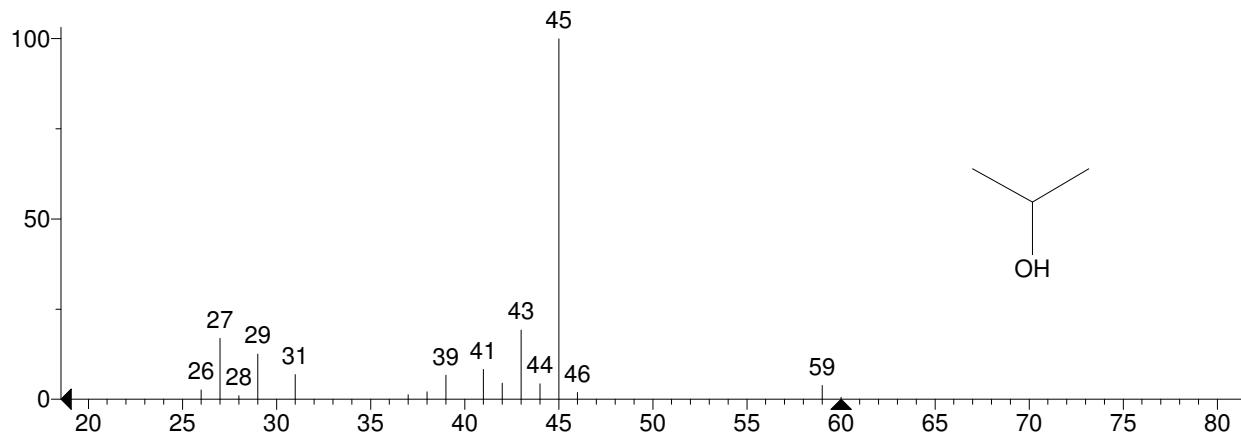


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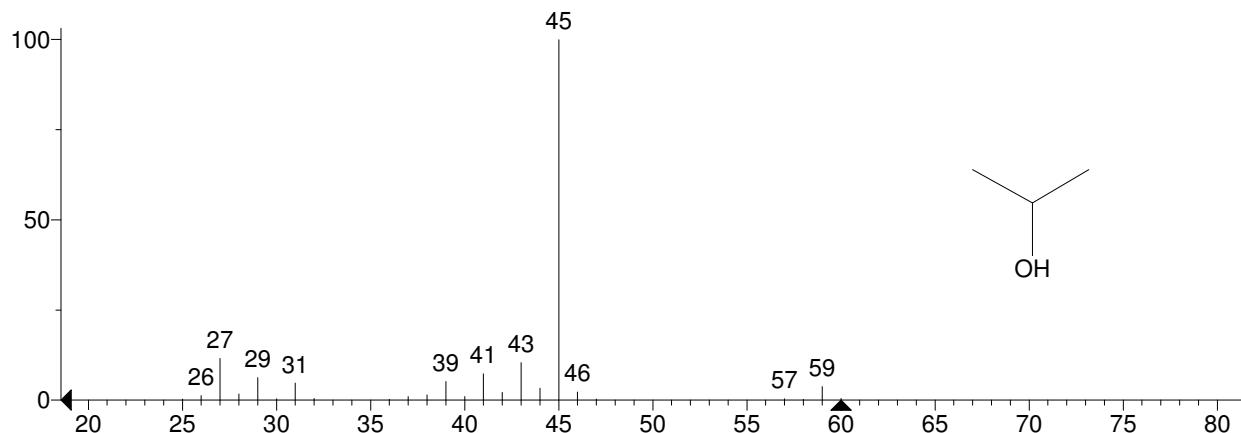
Unknown: Scan 301 (3.463 min): J5169JO2.D
Compound in Library Factor = 405



Hit 1 : Isopropyl Alcohol
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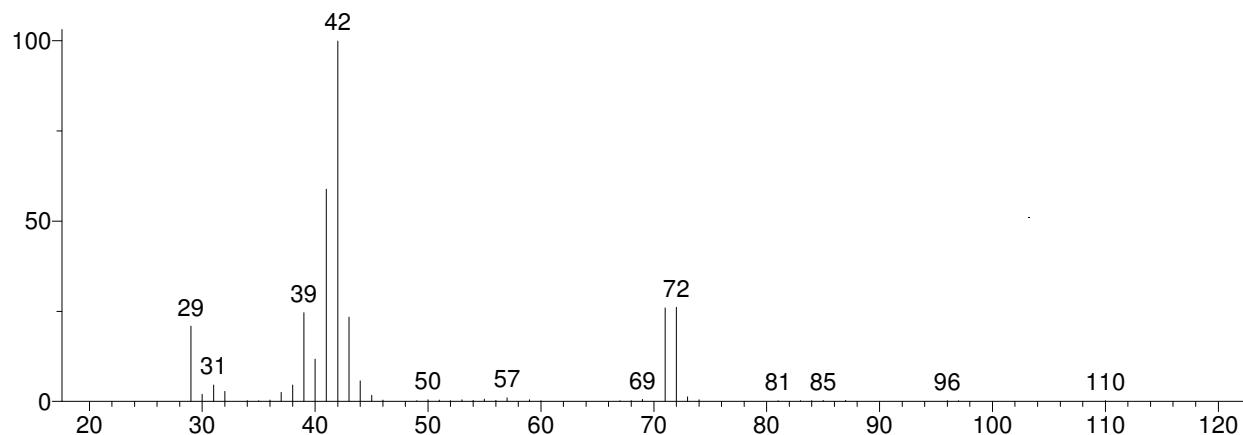


Hit 2 : Isopropyl Alcohol
C₃H₈O; MF: 926; RMF: 927; Prob 77.4%; CAS: 67-63-0; Lib: mainlib; ID: 14532.

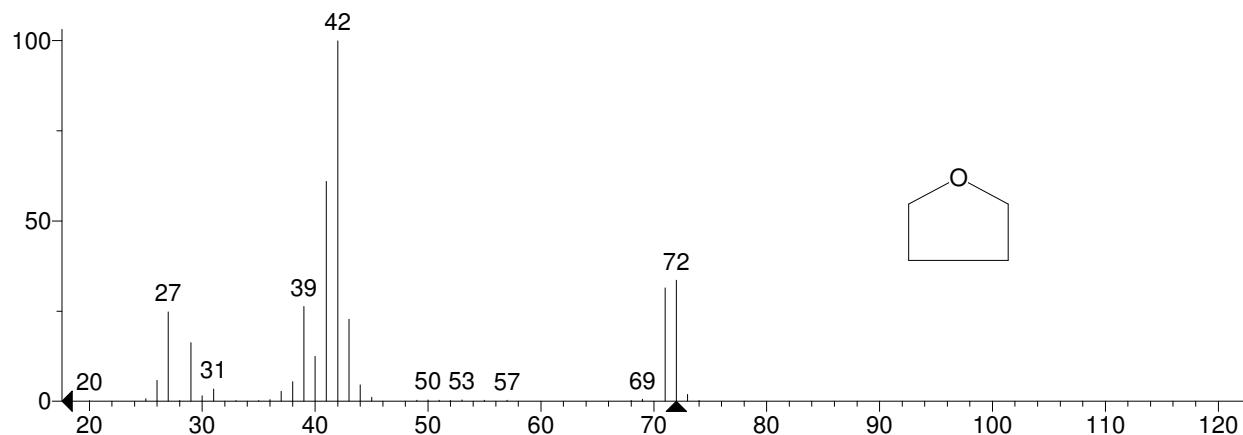


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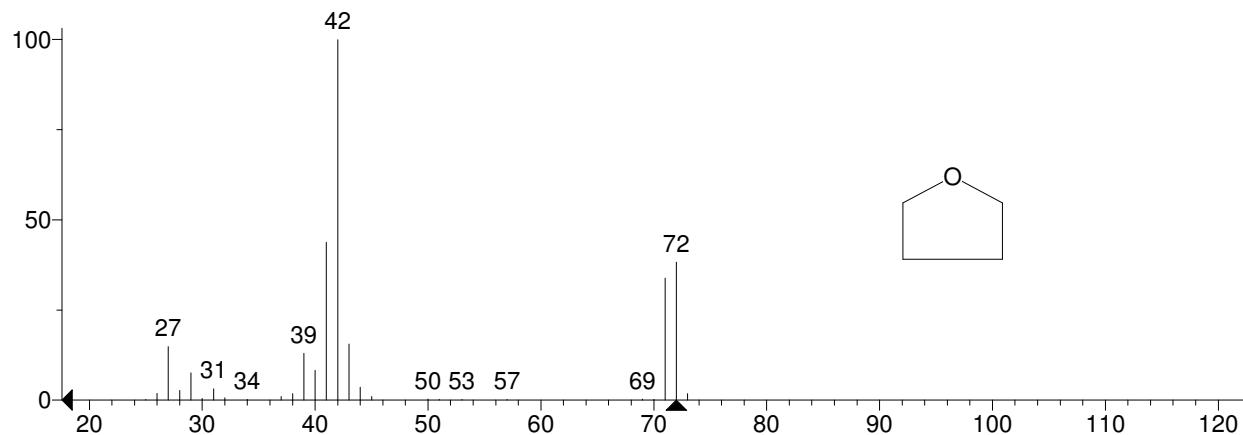
Unknown: Scan 325 (3.737 min): J5169JO2.D
Compound in Library Factor = 237



Hit 1 : Furan, tetrahydro-
C4H8O; MF: 939; RMF: 946; Prob 86.9%; CAS: 109-99-9; Lib: replib; ID: 1325.

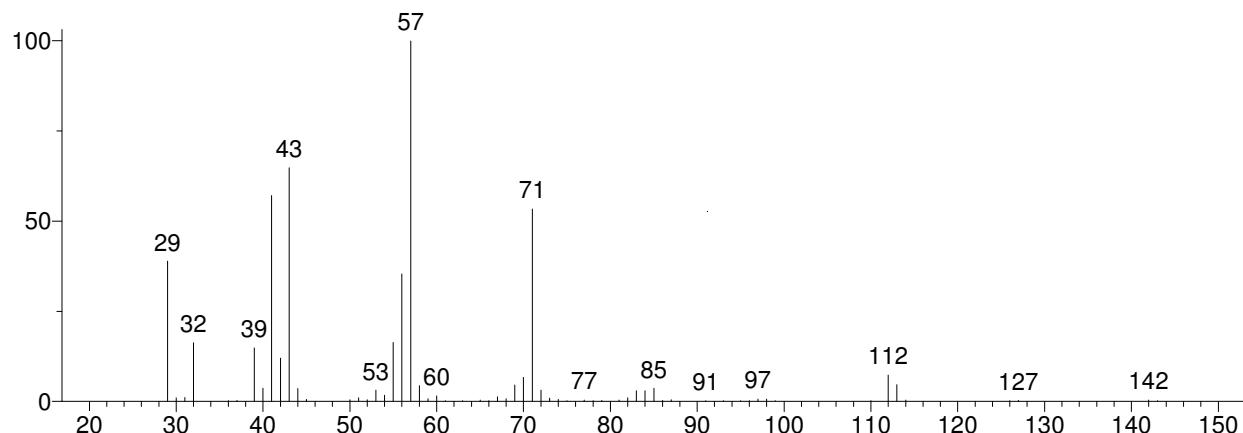


Hit 2 : Furan, tetrahydro-
C4H8O; MF: 904; RMF: 910; Prob 86.9%; CAS: 109-99-9; Lib: mainlib; ID: 4018.

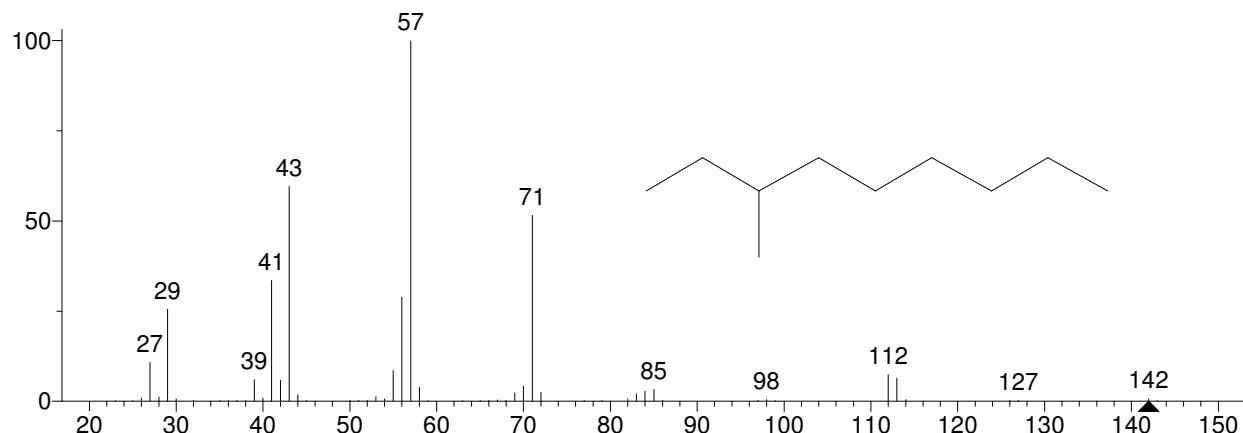


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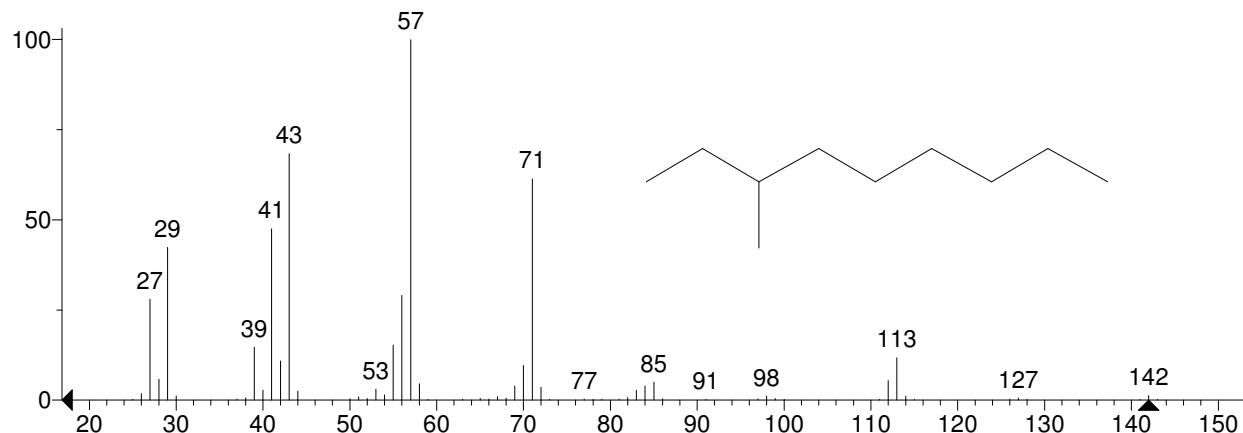
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Hit 1 : Nonane, 3-methyl-
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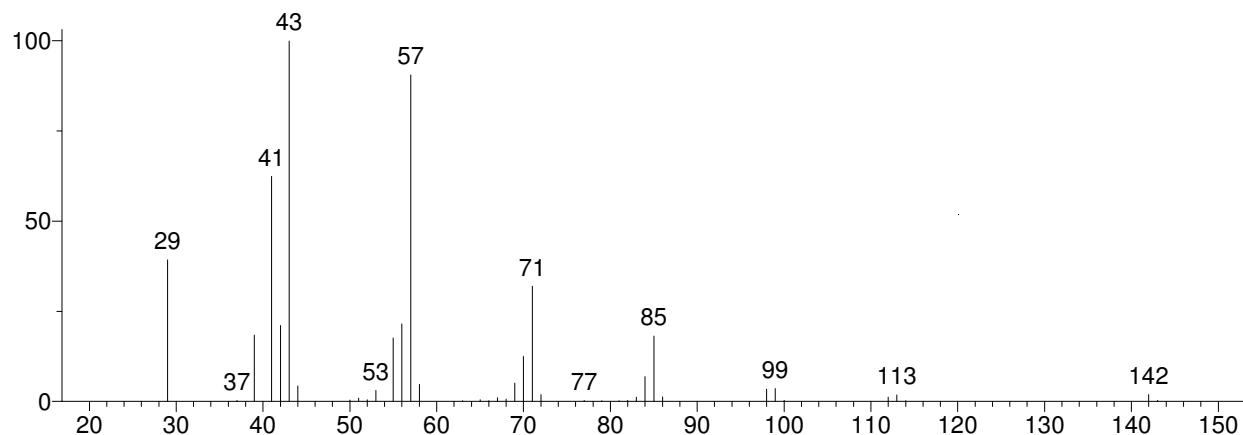


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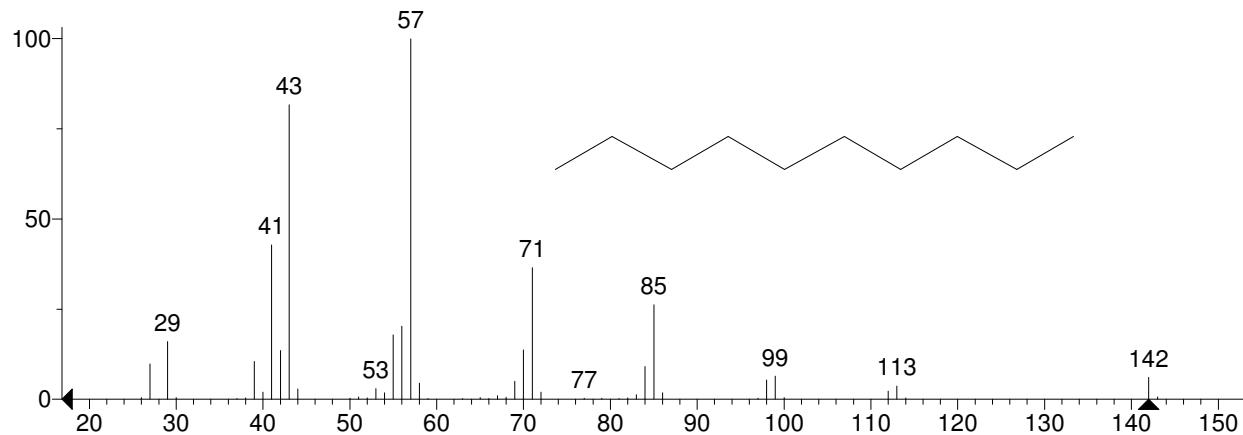


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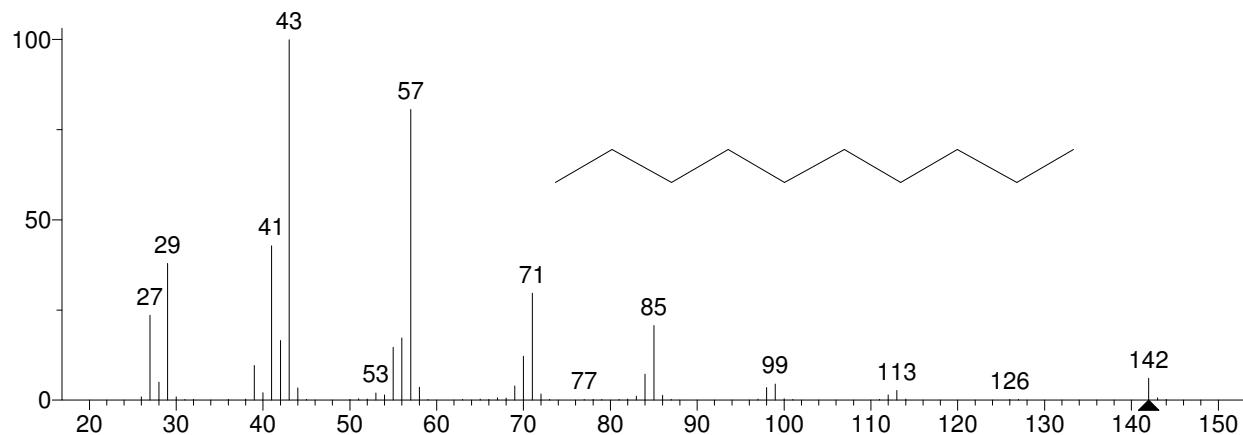
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Hit 1 : Decane
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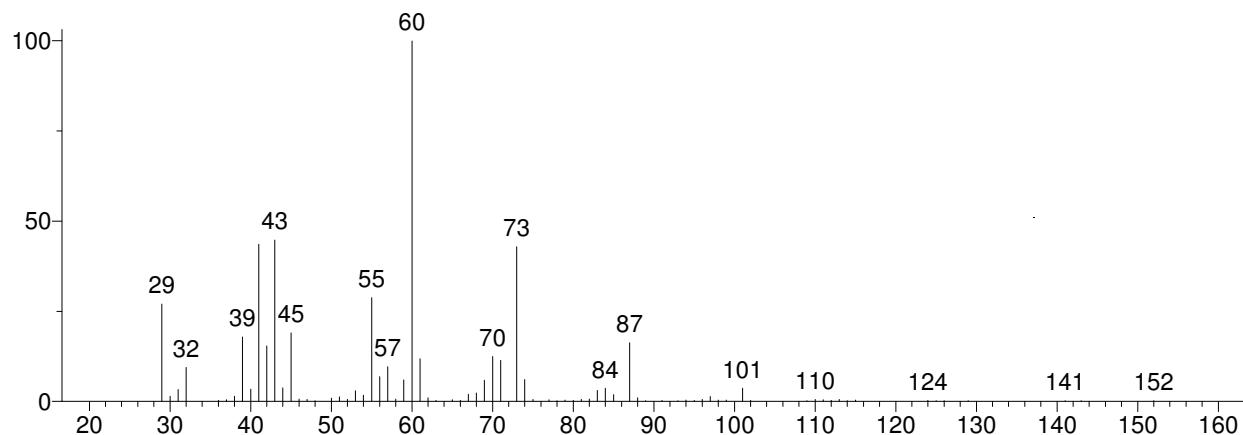


Hit 2 : Decane
C10H22; MF: 937; RMF: 937; Prob 34.6%; CAS: 124-18-5; Lib: mainlib; ID: 6868.

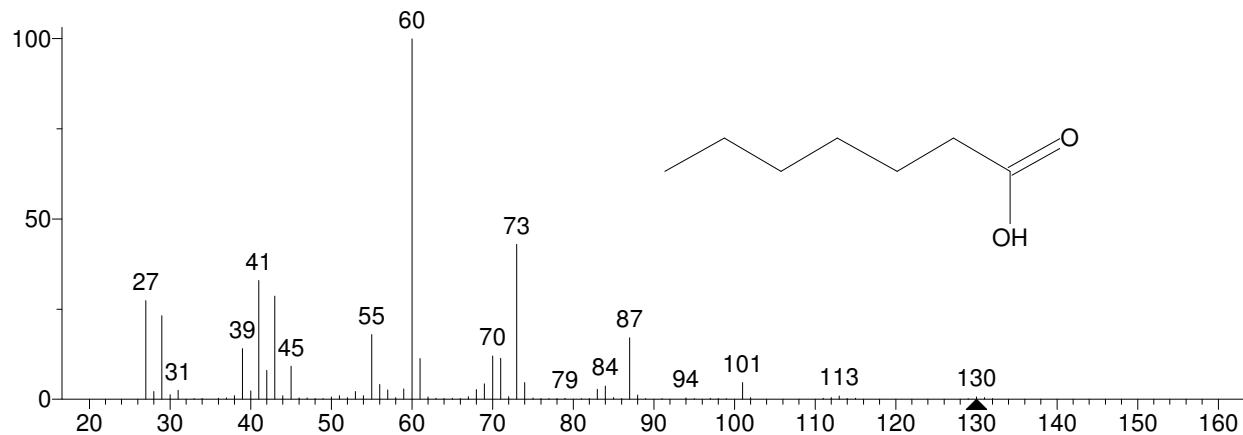


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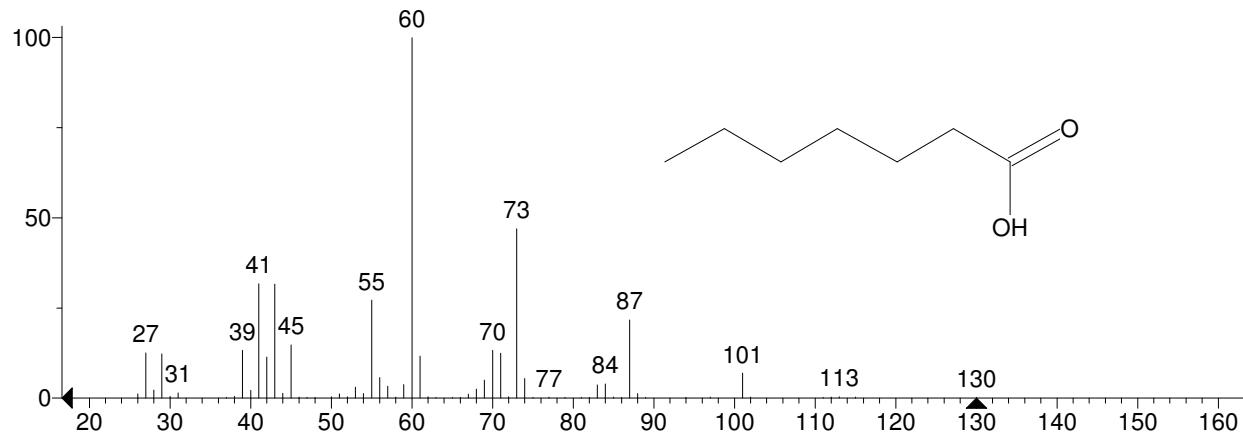
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 Compound in Library Factor = -168



Hit 1 : Heptanoic acid
 C7H14O2; MF: 878; RMF: 889; Prob 71.4%; CAS: 111-14-8; Lib: replib; ID: 6687.

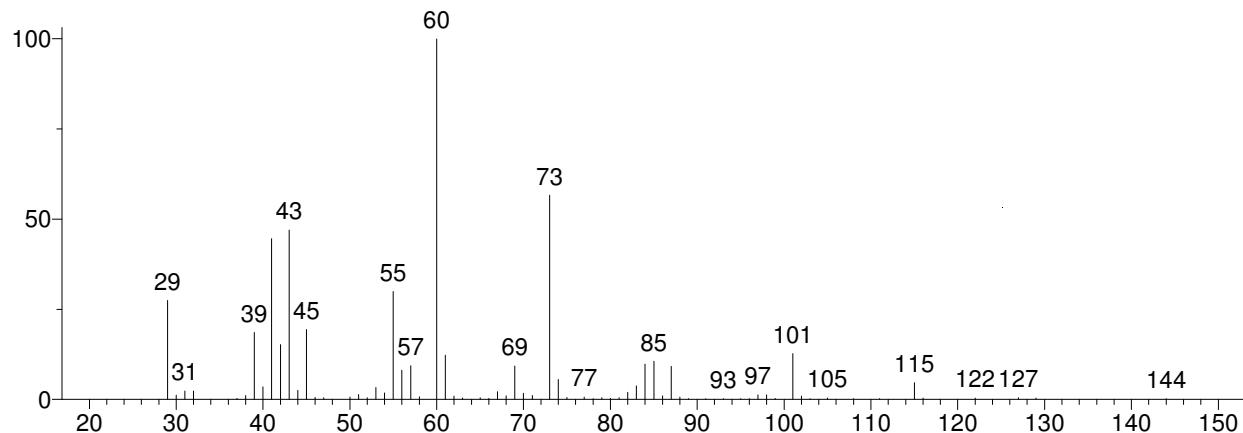


Hit 2 : Heptanoic acid
 C7H14O2; MF: 865; RMF: 875; Prob 71.4%; CAS: 111-14-8; Lib: replib; ID: 6688.

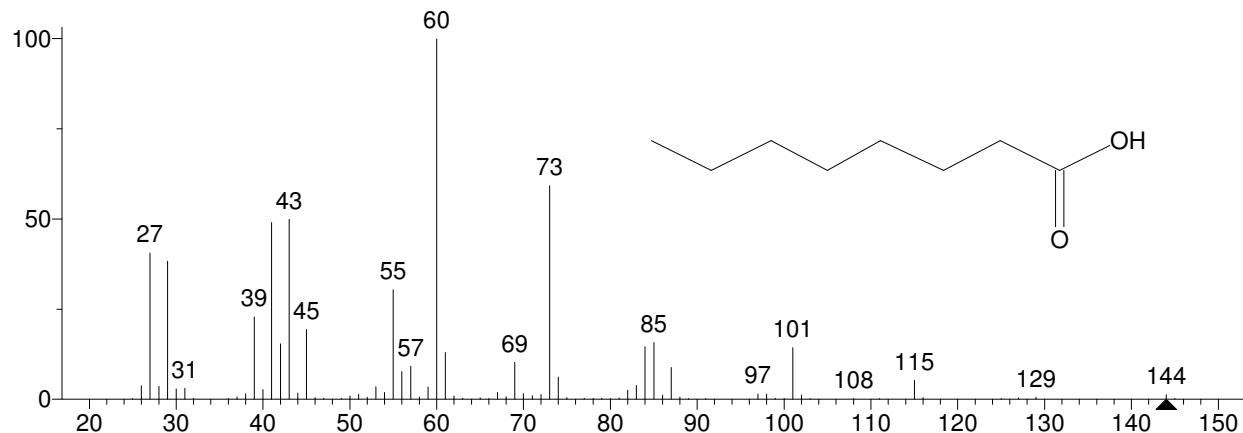


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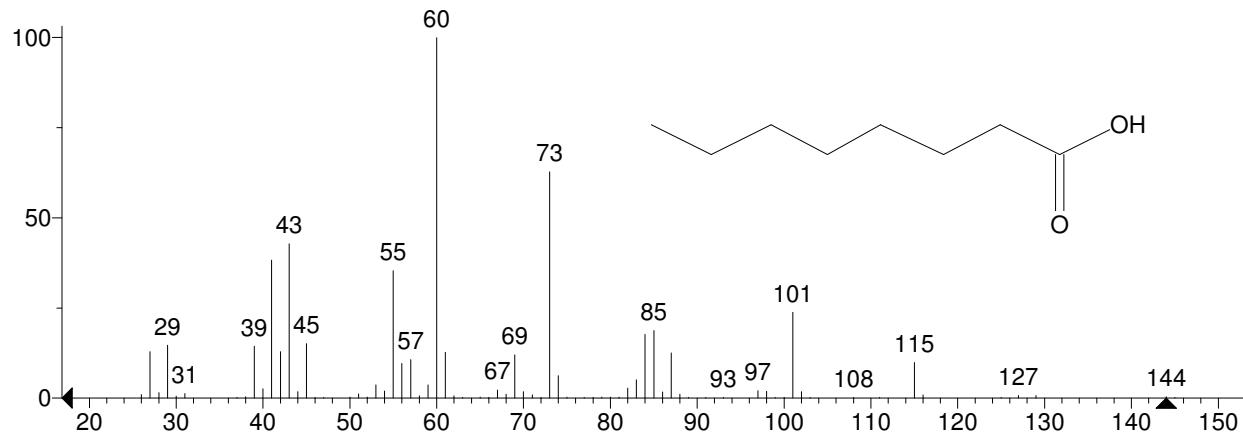
Unknown: Scan 739 (8.464 min): J5169JO2.D
 Compound in Library Factor = 284



Hit 1 : Octanoic Acid
 C8H16O2; MF: 916; RMF: 917; Prob 82.8%; CAS: 124-07-2; Lib: replib; ID: 6701.

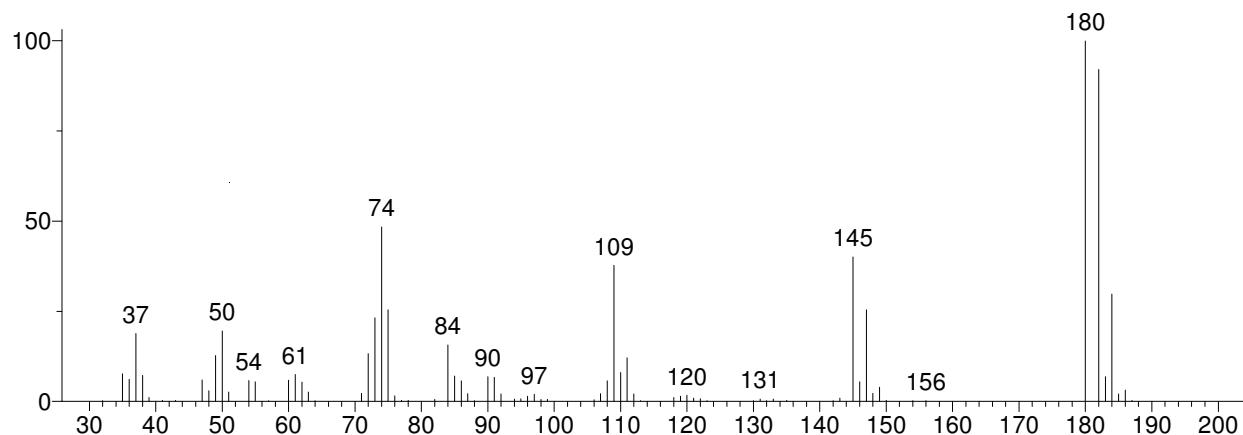


Hit 2 : Octanoic Acid
 C8H16O2; MF: 905; RMF: 907; Prob 82.8%; CAS: 124-07-2; Lib: replib; ID: 6702.

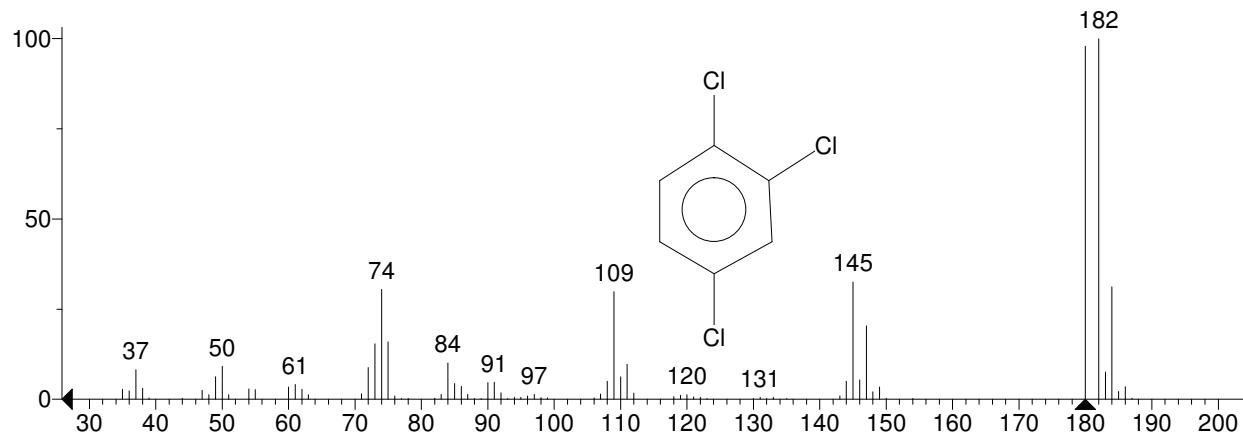


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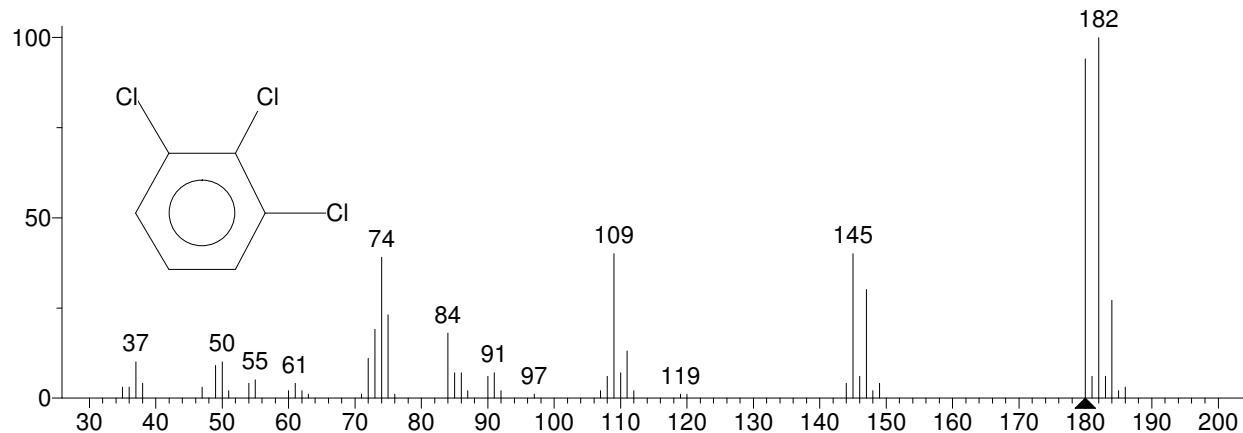
Unknown: Scan 750 (8.589 min): J5169JO2.D
 Compound in Library Factor = 1047



Hit 1 : Benzene, 1,2,4-trichloro-
 C6H3Cl3; MF: 961; RMF: 961; Prob 56.5%; CAS: 120-82-1; Lib: replib; ID: 22722.

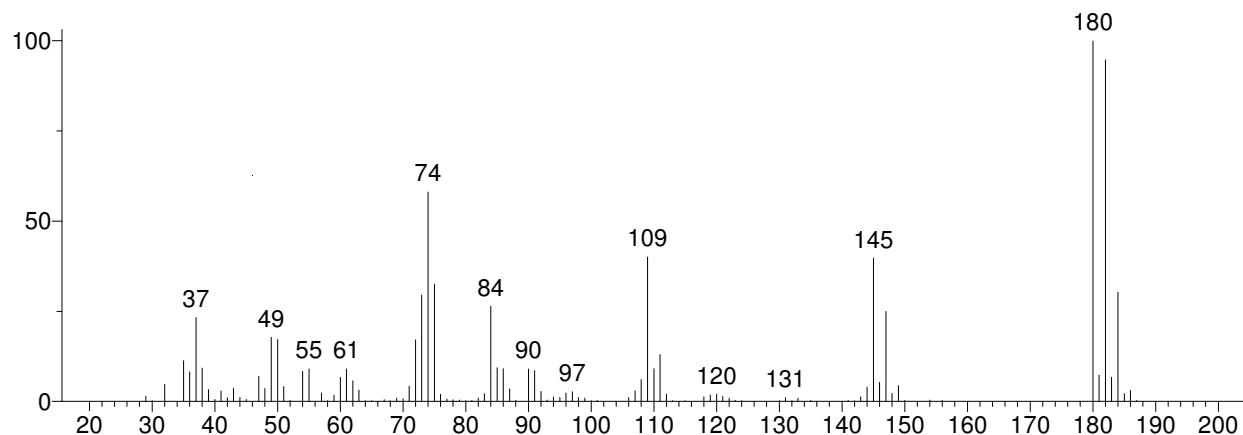


Hit 2 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 940; RMF: 949; Prob 24.1%; CAS: 87-61-6; Lib: replib; ID: 22721.

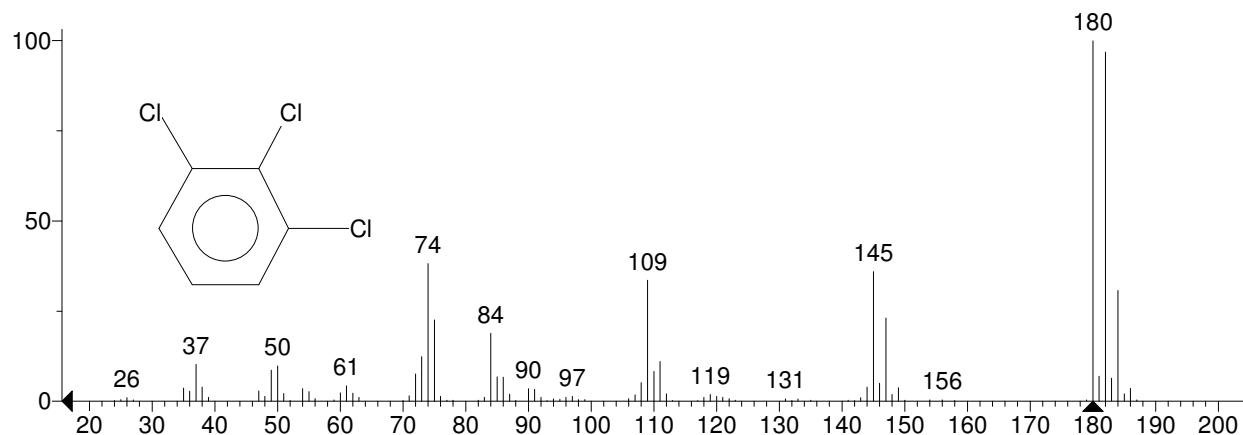


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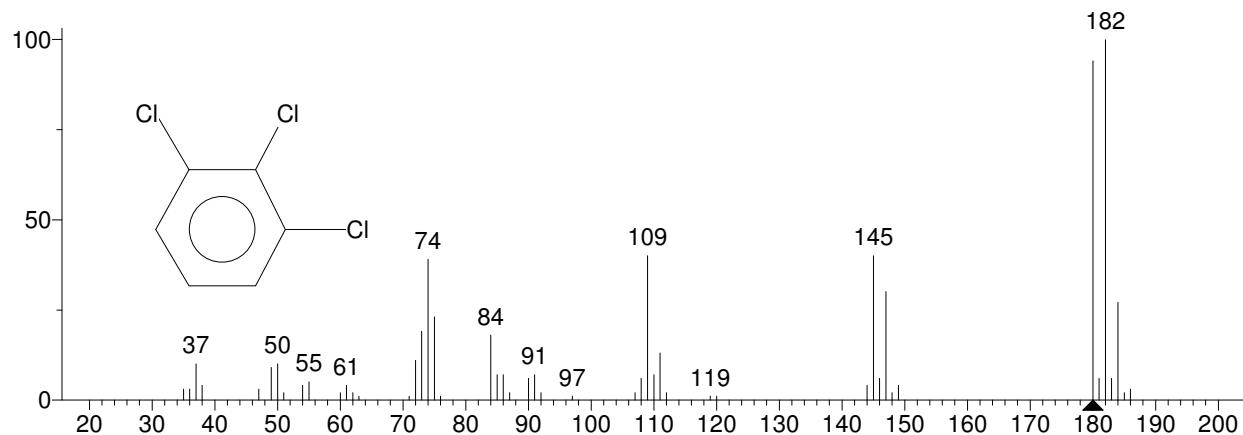
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 Compound in Library Factor = 1045



Hit 1 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 943; RMF: 948; Prob 57.4%; CAS: 87-61-6; Lib: replib; ID: 22558.

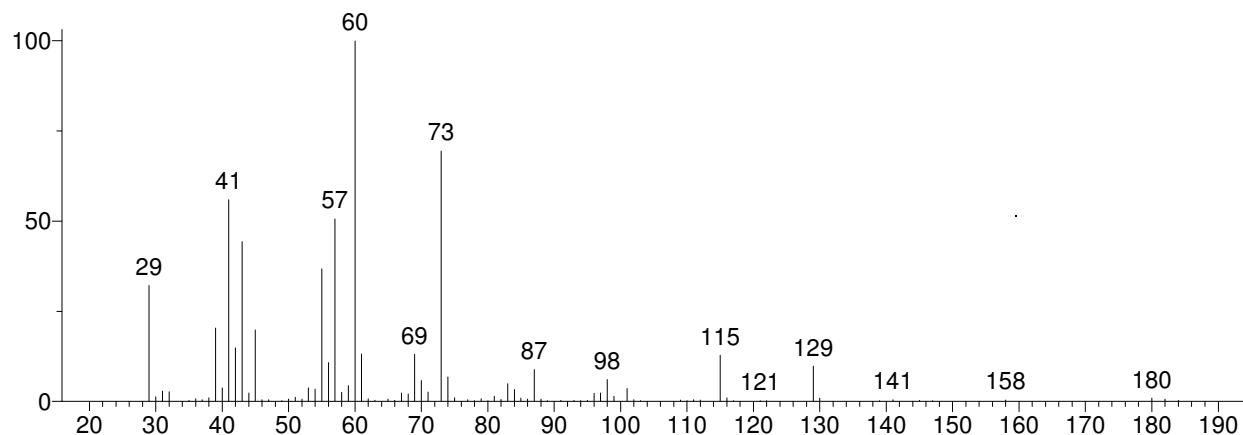


Hit 2 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 942; RMF: 962; Prob 57.4%; CAS: 87-61-6; Lib: replib; ID: 22721.

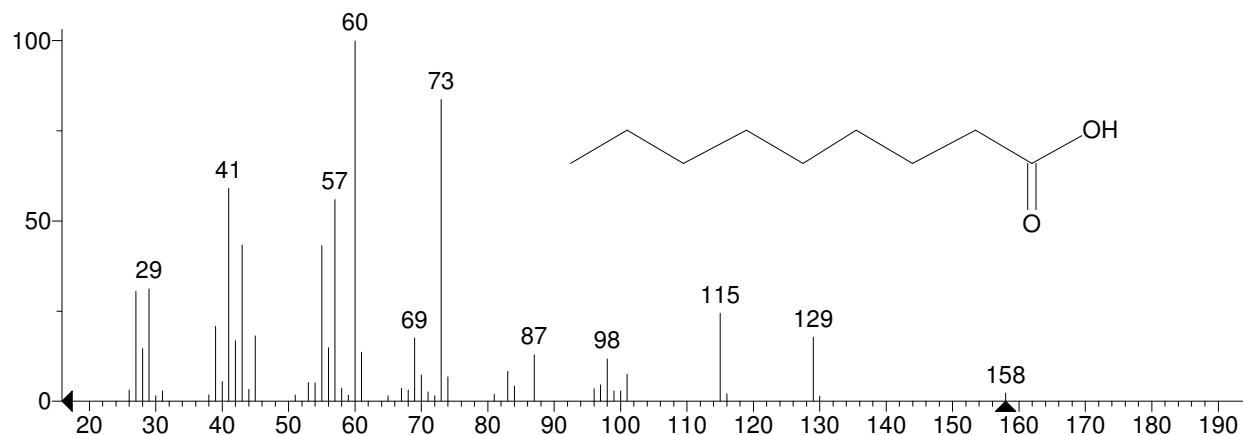


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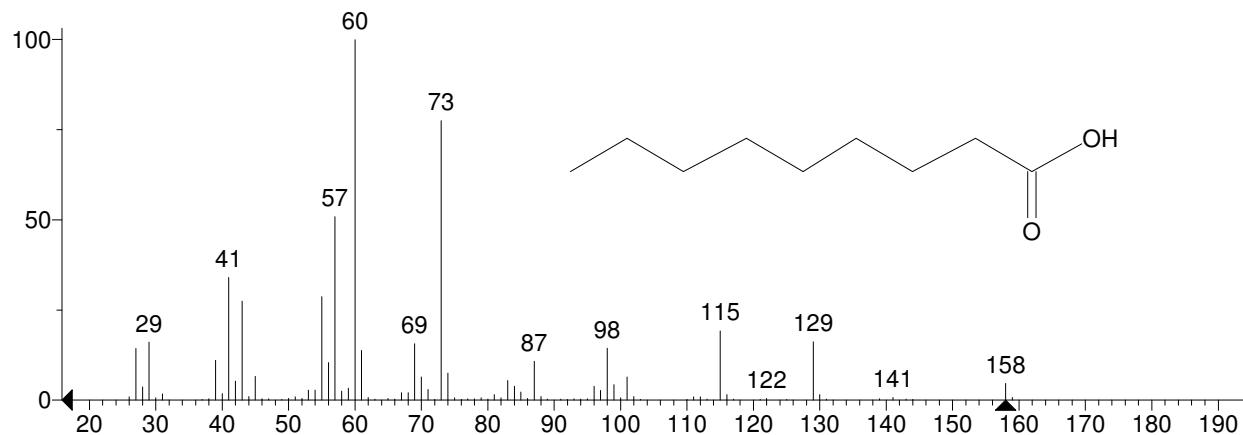
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Compound in Library Factor = 256



Hit 1 : Nonanoic acid
C9H18O2; MF: 921; RMF: 942; Prob 85.6%; CAS: 112-05-0; Lib: replib; ID: 6695.

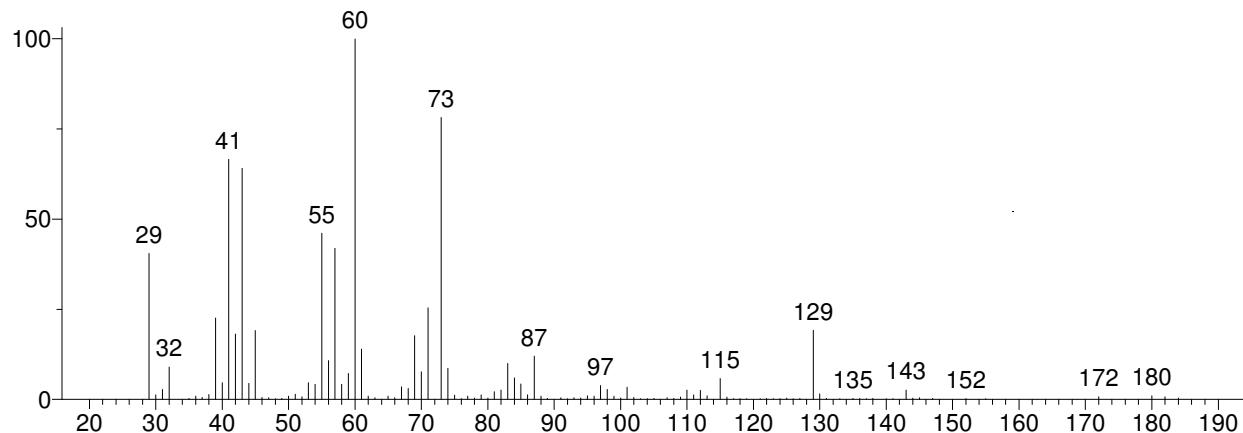


Hit 2 : Nonanoic acid
C9H18O2; MF: 892; RMF: 898; Prob 85.6%; CAS: 112-05-0; Lib: mainlib; ID: 25519.

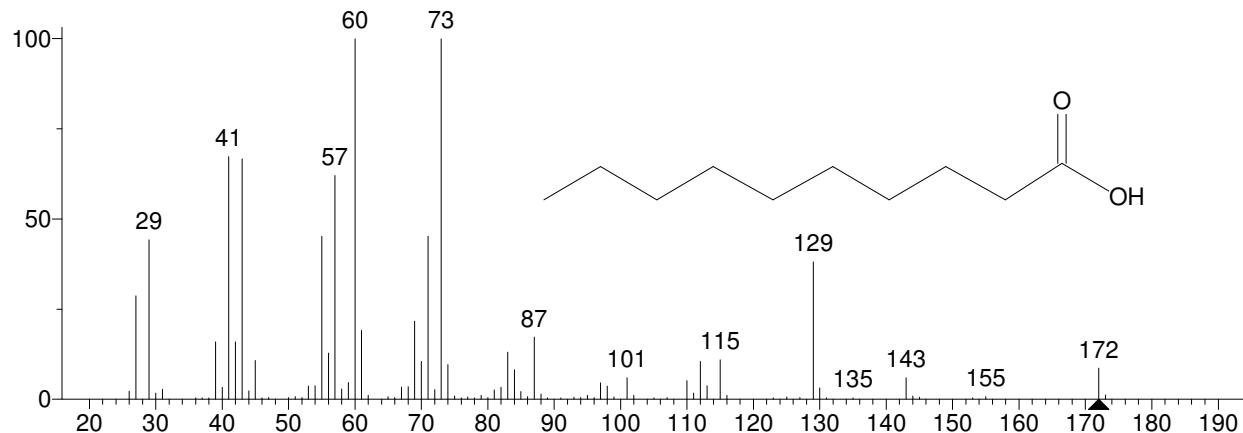


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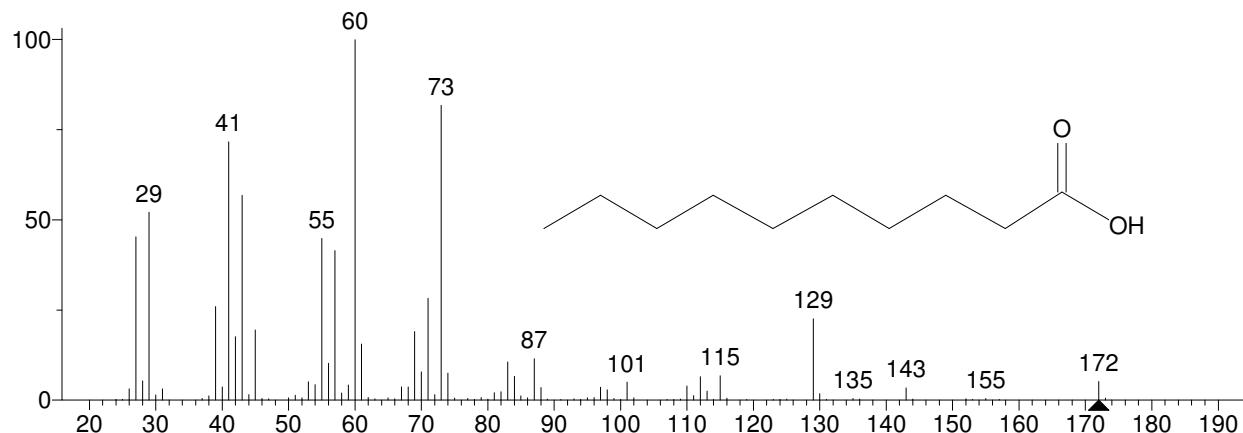
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Hit 1 : n-Decanoic acid
 C10H20O2; MF: 894; RMF: 904; Prob 70.3%; CAS: 334-48-5; Lib: replib; ID: 6692.

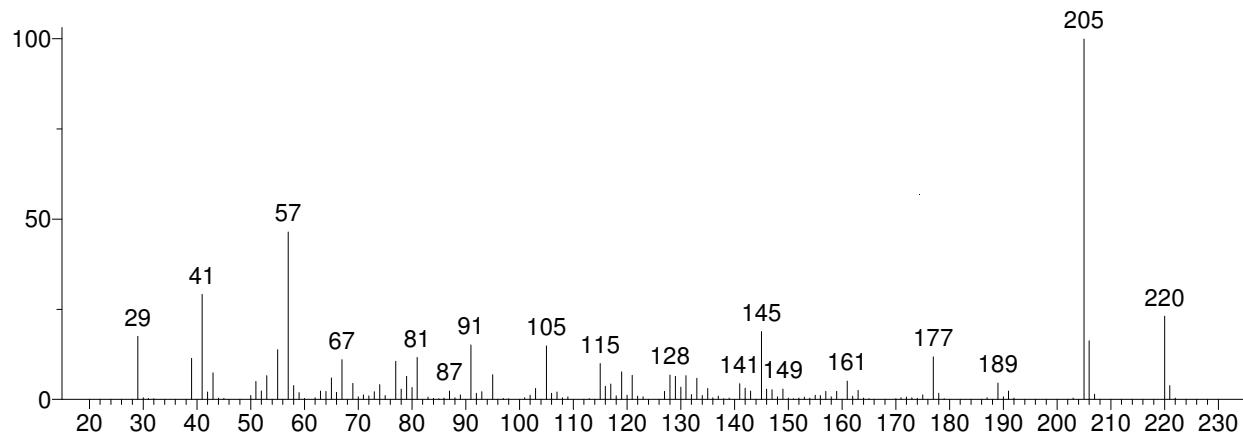


Hit 2 : n-Decanoic acid
 C10H20O2; MF: 892; RMF: 904; Prob 70.3%; CAS: 334-48-5; Lib: replib; ID: 6691.

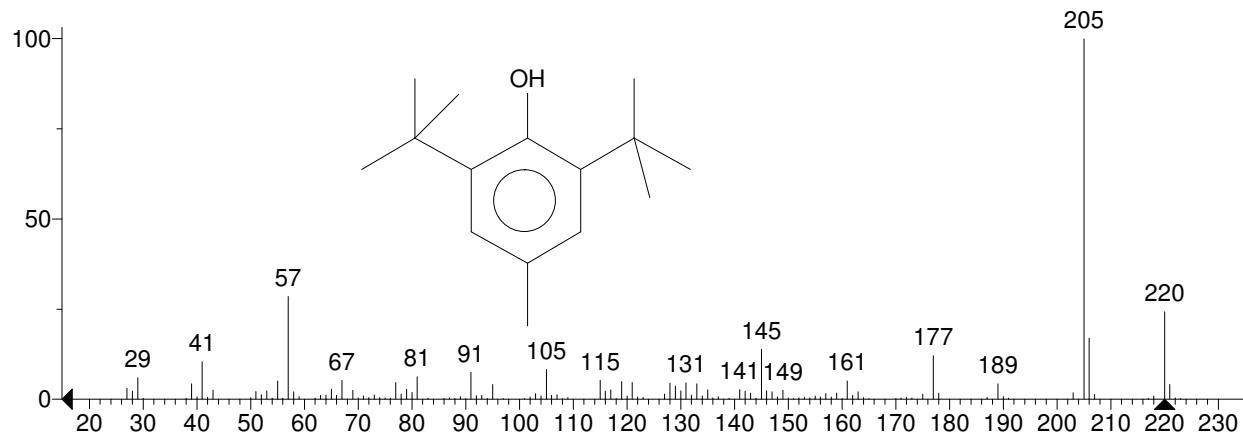


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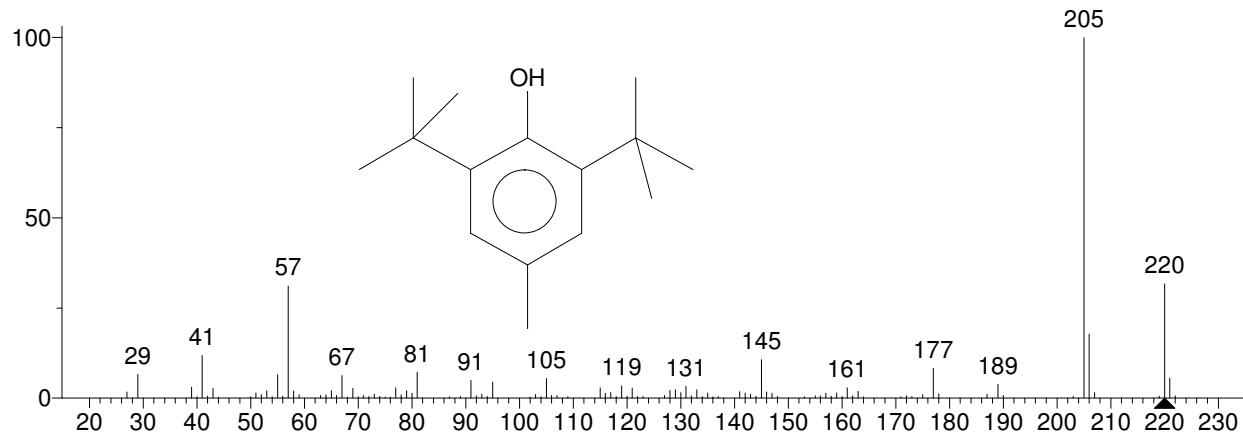
Unknown: Scan 1032 (11.809 min): J5169JO2.D
Compound in Library Factor = 167



Hit 1 : Butylated Hydroxytoluene
C15H24O; MF: 920; RMF: 921; Prob 75.9%; CAS: 128-37-0; Lib: mainlib; ID: 125747.

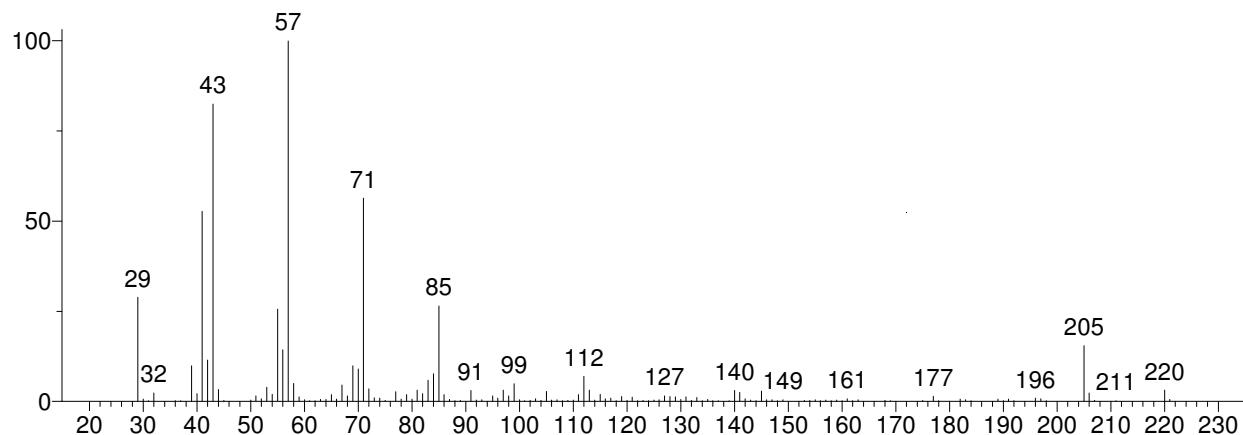


Hit 2 : Butylated Hydroxytoluene
C15H24O; MF: 908; RMF: 919; Prob 75.9%; CAS: 128-37-0; Lib: replib; ID: 24147.

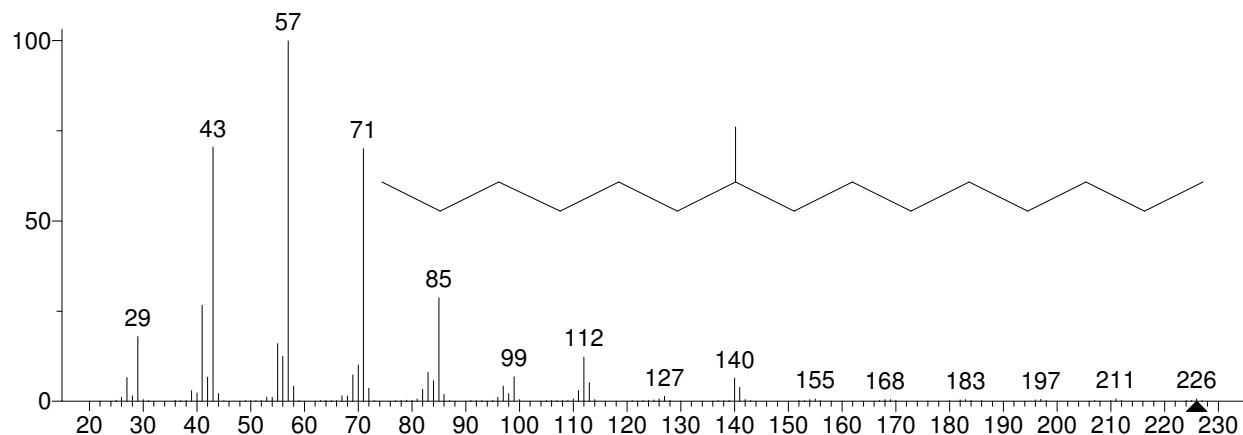


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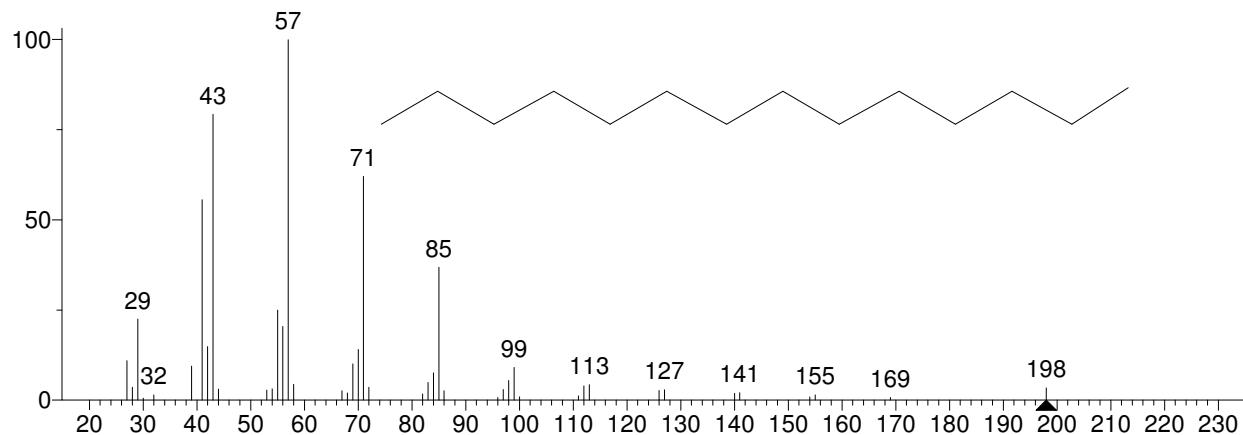
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Compound in Library Factor = -1067



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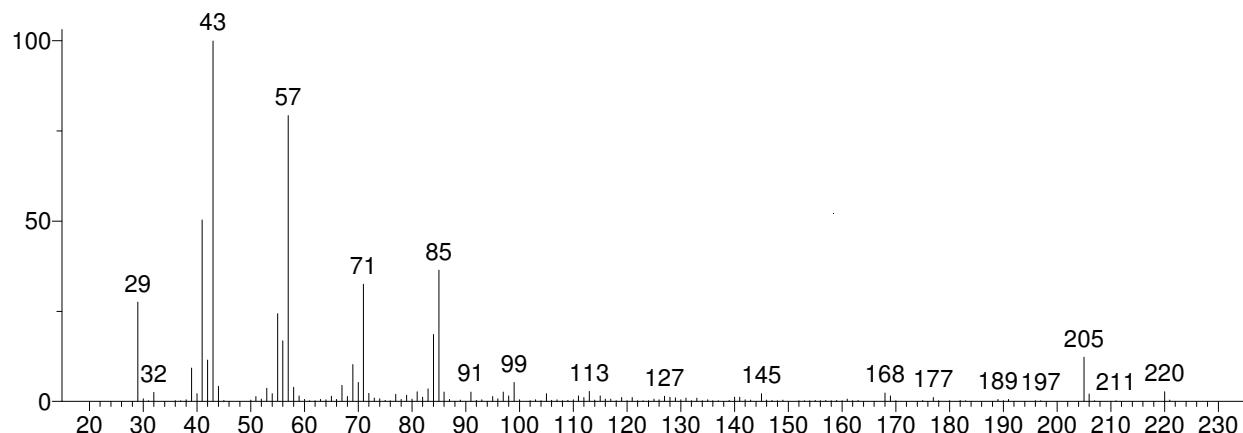


Hit 2 : Tetradecane
C14H30; MF: 759; RMF: 908; Prob 5.57%; CAS: 629-59-4; Lib: replib; ID: 5464.

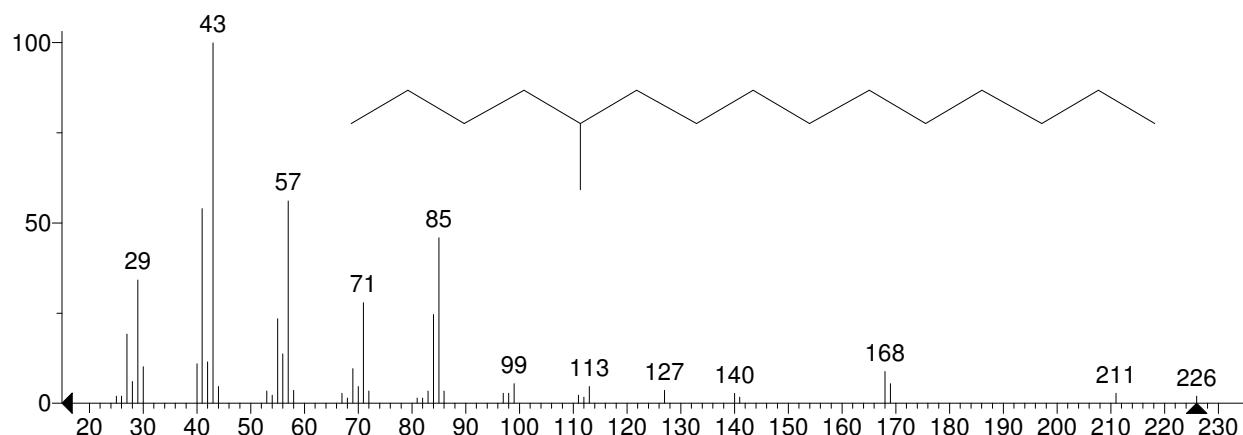


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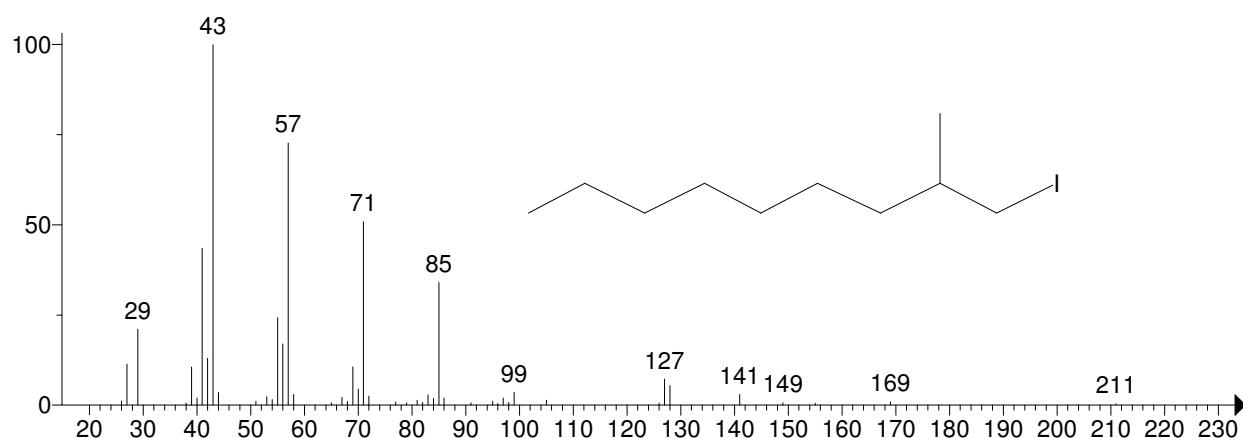
Unknown: Scan 1047 (11.980 min): J5169JO2.D
 Compound in Library Factor = -591



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 C16H34; MF: 778; RMF: 907; Prob 8.23%; CAS: 25117-33-3; Lib: mainlib; ID: 6899.

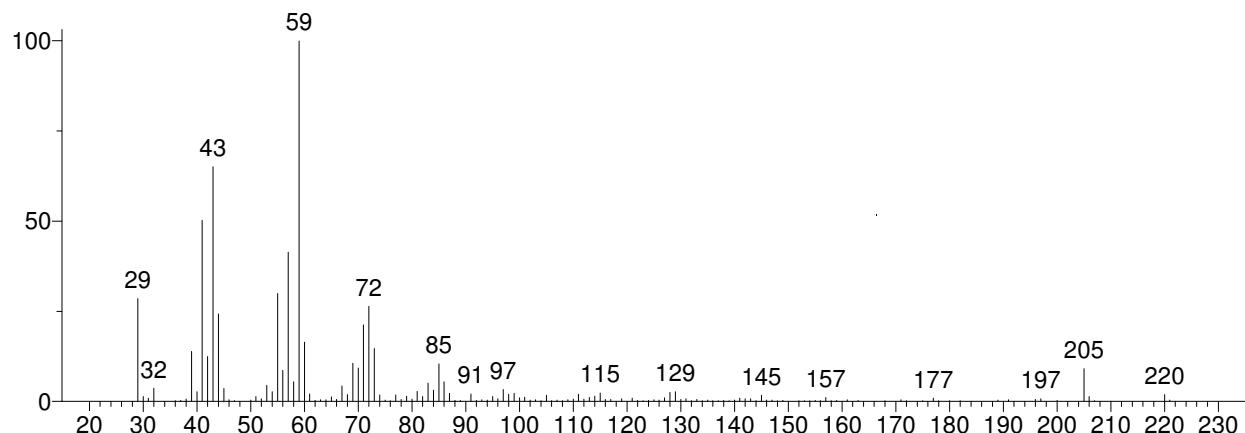


Hit 2 : 1-Iodo-2-methylnonane
 C10H21I; MF: 763; RMF: 890; Prob 4.99%; Lib: mainlib; ID: 7023.

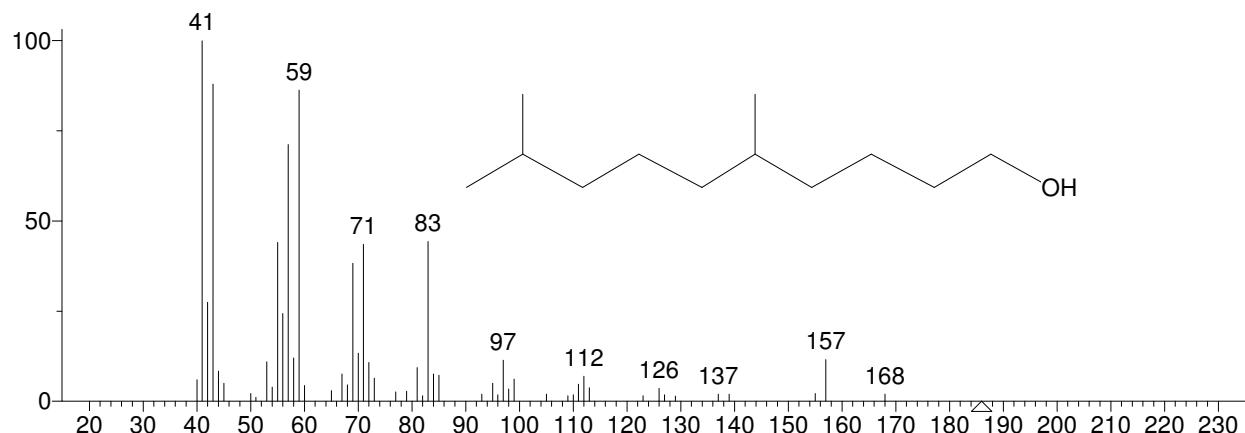


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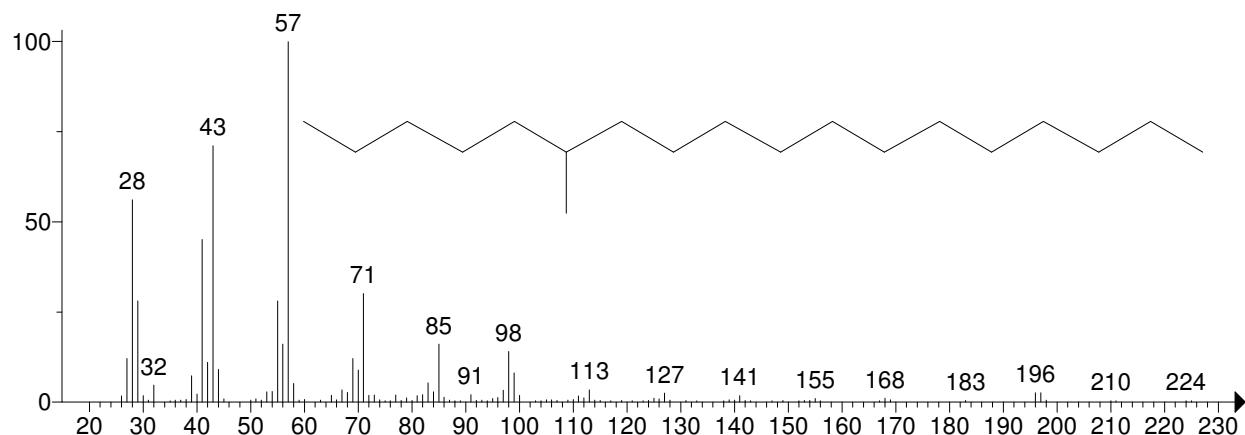
Unknown: Scan 1057 (12.094 min): J5169JO2.D
 Compound in Library Factor = -918



Hit 1 : 1-Decanol, 5,9-dimethyl-
 C12H26O; MF: 693; RMF: 795; Prob 15.4%; CAS: 91482-38-1; Lib: mainlib; ID: 2196.

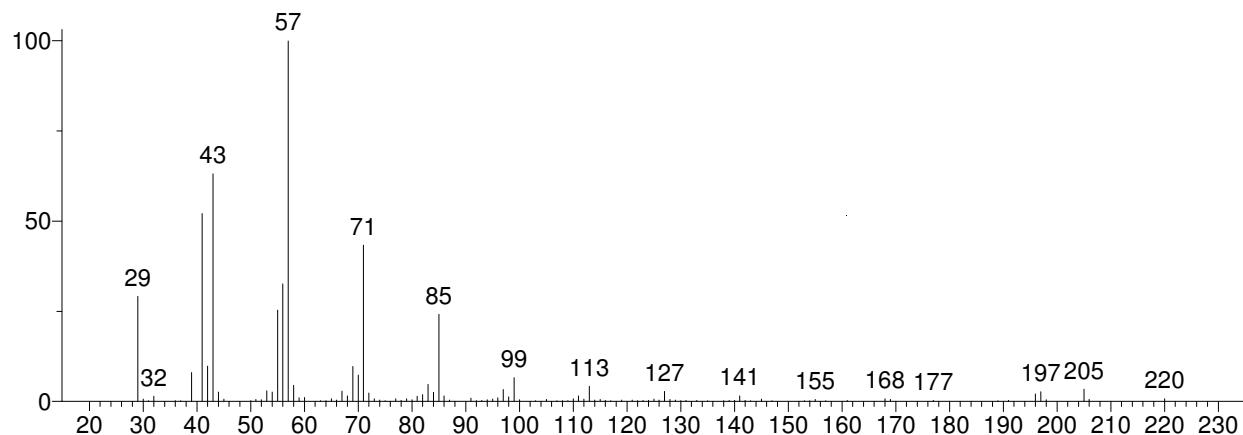


Hit 2 : Octadecane, 6-methyl-
 C19H40; MF: 670; RMF: 712; Prob 5.62%; CAS: 10544-96-4; Lib: mainlib; ID: 20572.

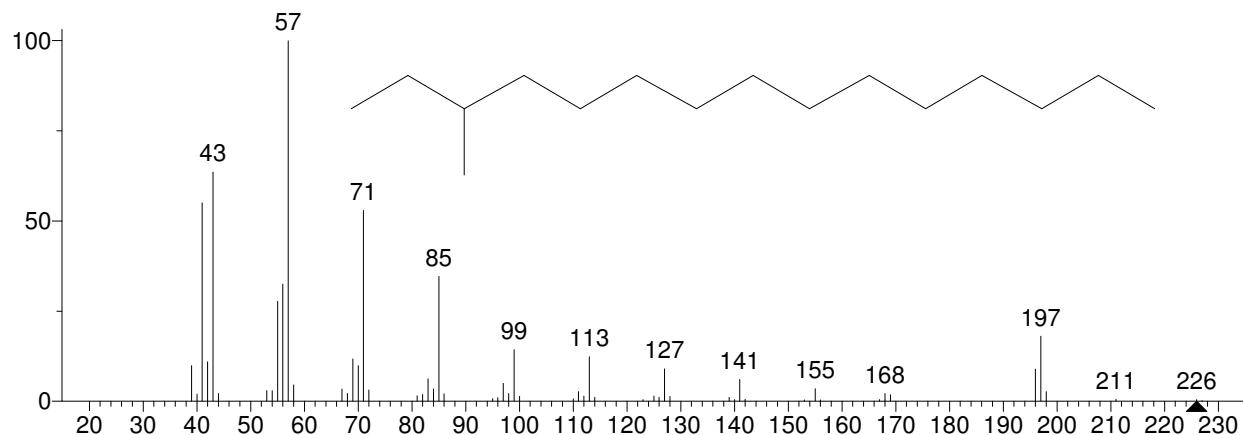


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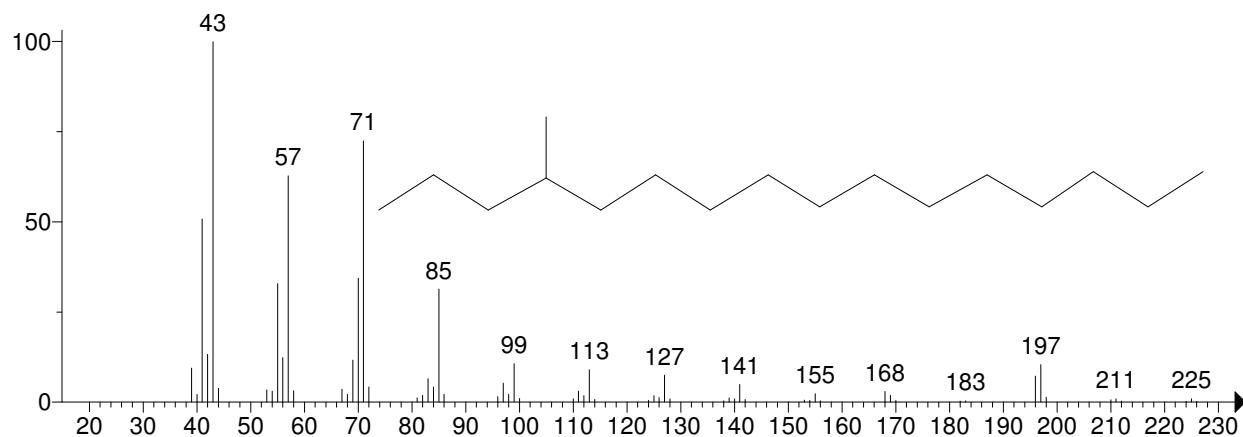
Unknown: Scan 1062 (12.151 min): J5169JO2.D
Compound in Library Factor = -246



Hit 1 : Pentadecane, 3-methyl-
C16H34; MF: 862; RMF: 900; Prob 11.0%; CAS: 2882-96-4; Lib: mainlib; ID: 20661.

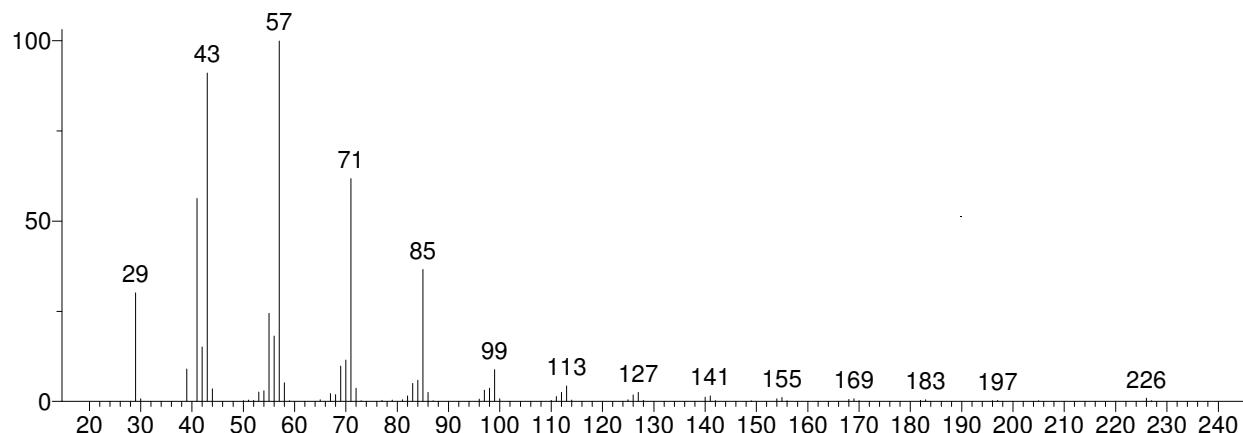


Hit 2 : Hexadecane, 4-methyl-
C17H36; MF: 848; RMF: 885; Prob 6.88%; CAS: 25117-26-4; Lib: mainlib; ID: 7930.

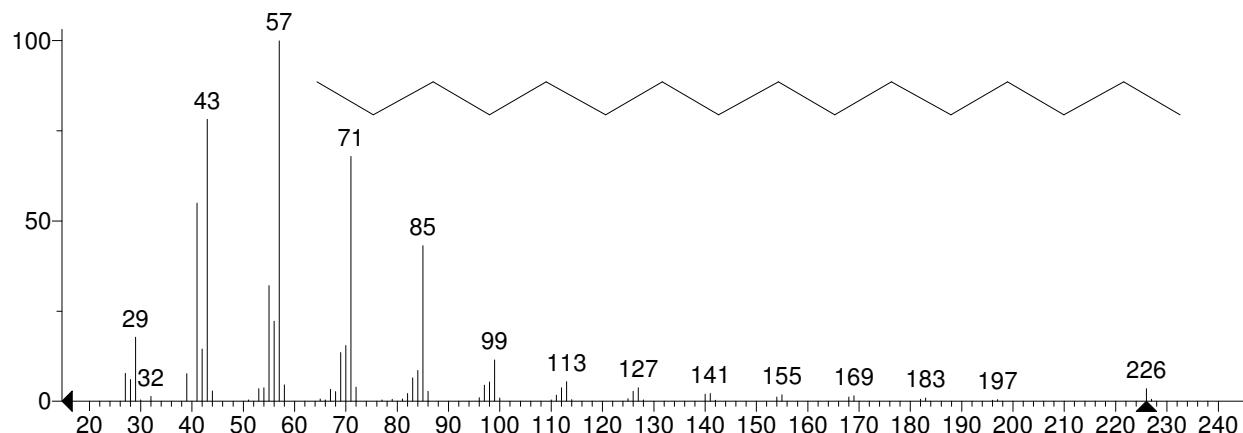


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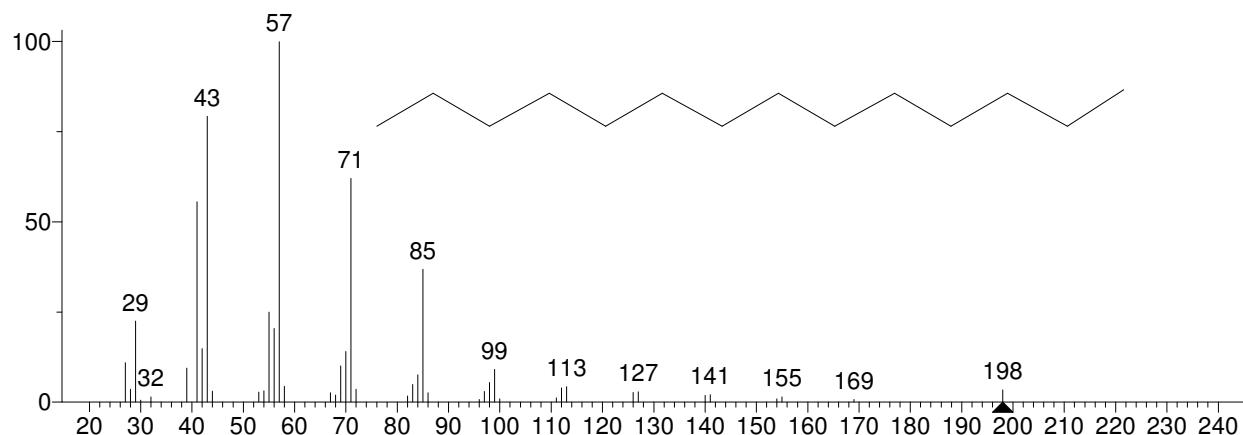
Unknown: Scan 1091 (12.482 min): J5169JO2.D
Compound in Library Factor = 101



Hit 1 : Hexadecane
C₁₆H₃₄; MF: 953; RMF: 953; Prob 24.5%; CAS: 544-76-3; Lib: replib; ID: 5518.

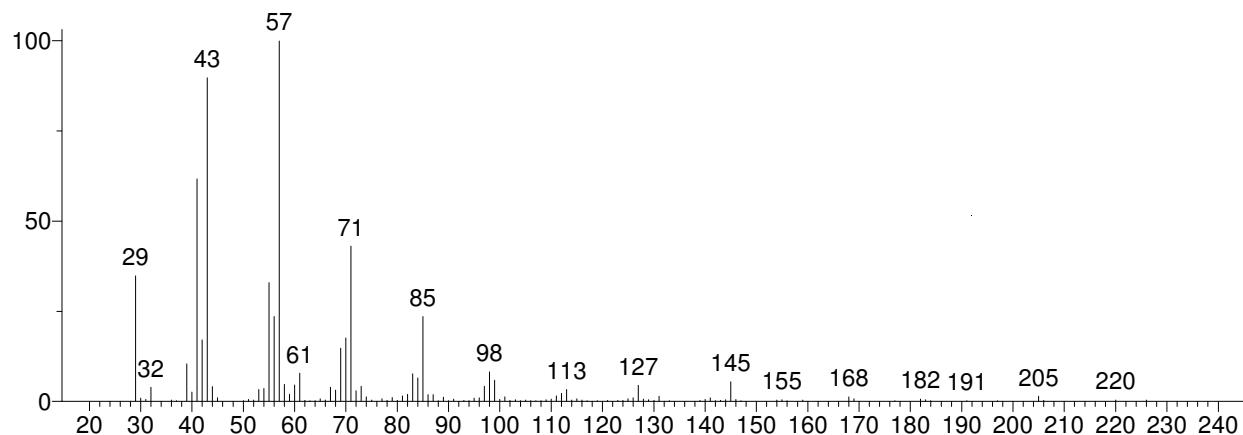


Hit 2 : Tetradecane
C₁₄H₃₀; MF: 933; RMF: 944; Prob 11.2%; CAS: 629-59-4; Lib: replib; ID: 5464.

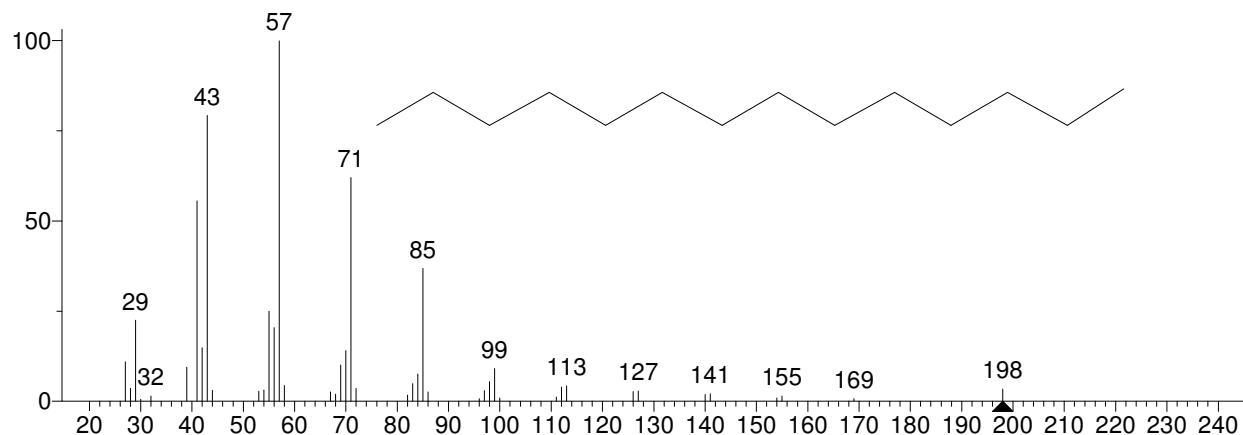


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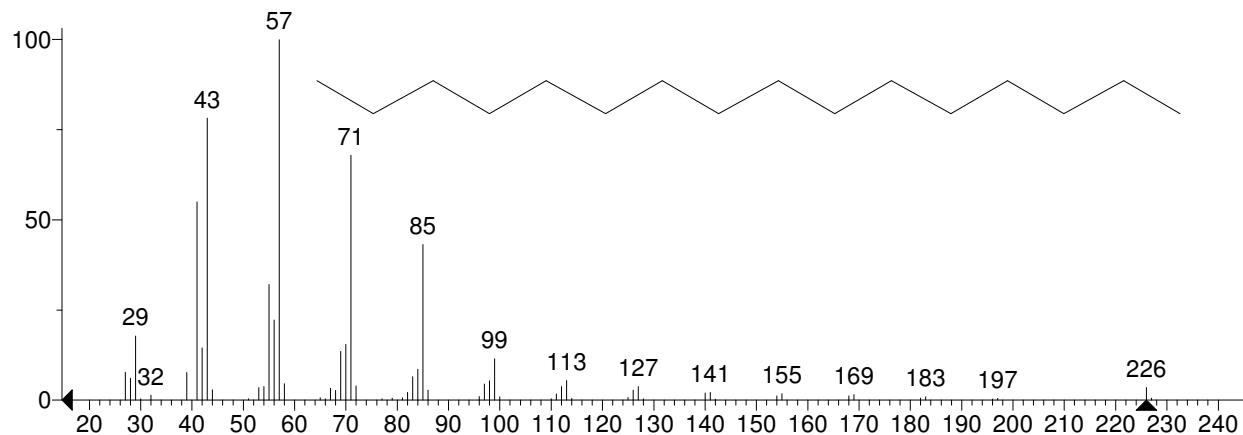
Unknown: Scan 1144 (13.087 min): J5169JO2.D
Compound in Library Factor = -493



Hit 1 : Tetradecane
C14H30; MF: 834; RMF: 913; Prob 7.89%; CAS: 629-59-4; Lib: replib; ID: 5464.

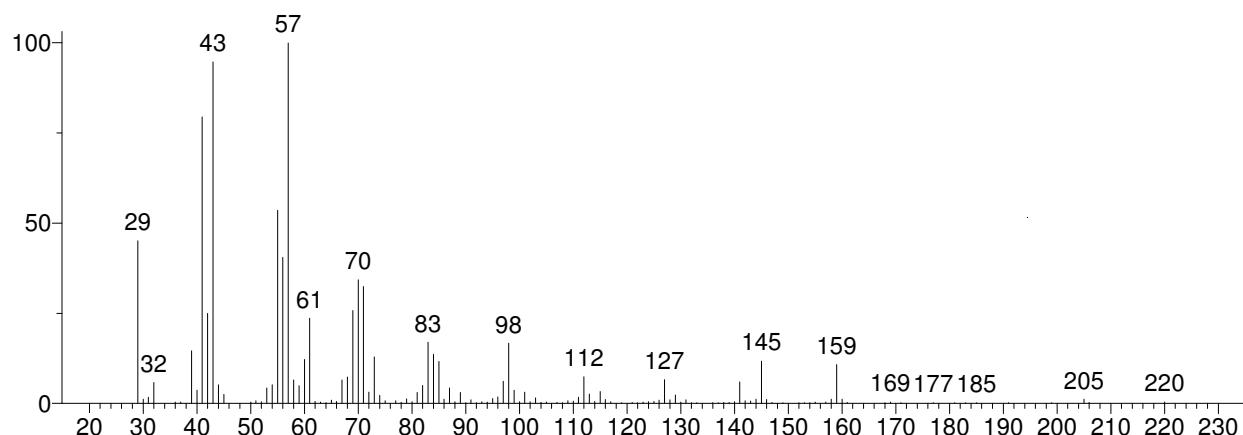


Hit 2 : Hexadecane
C16H34; MF: 833; RMF: 895; Prob 7.58%; CAS: 544-76-3; Lib: replib; ID: 5518.

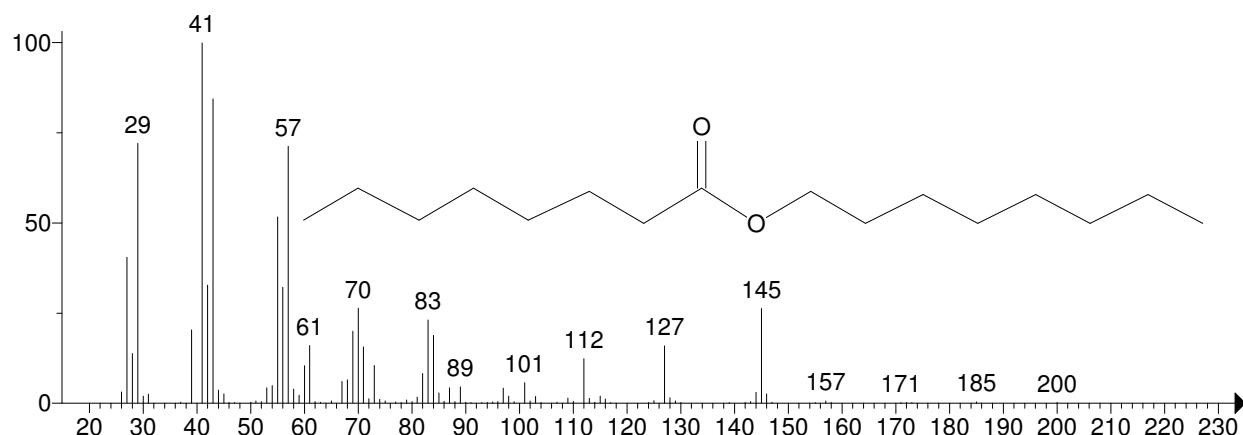


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Unknown: Scan 1211 (13.852 min): J5169JO2.D
 Compound in Library Factor = -457



Hit 1 : Octanoic acid, octyl ester
 C16H32O2; MF: 801; RMF: 840; Prob 29.1%; CAS: 2306-88-9; Lib: replib; ID: 776.

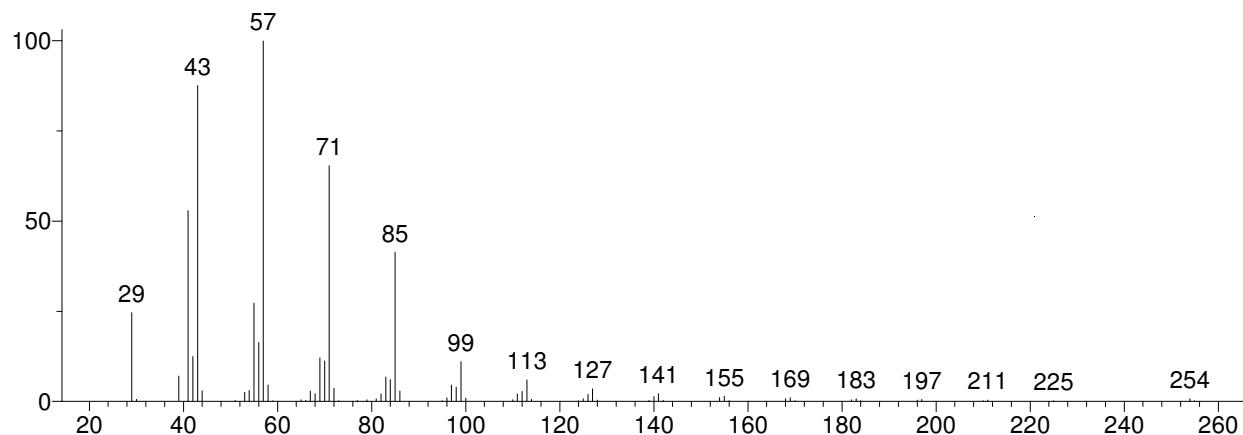


Hit 2 : Octanoic acid, 2-ethylhexyl ester
 C16H32O2; MF: 772; RMF: 798; Prob 8.25%; CAS: 63321-70-0; Lib: replib; ID: 5152.

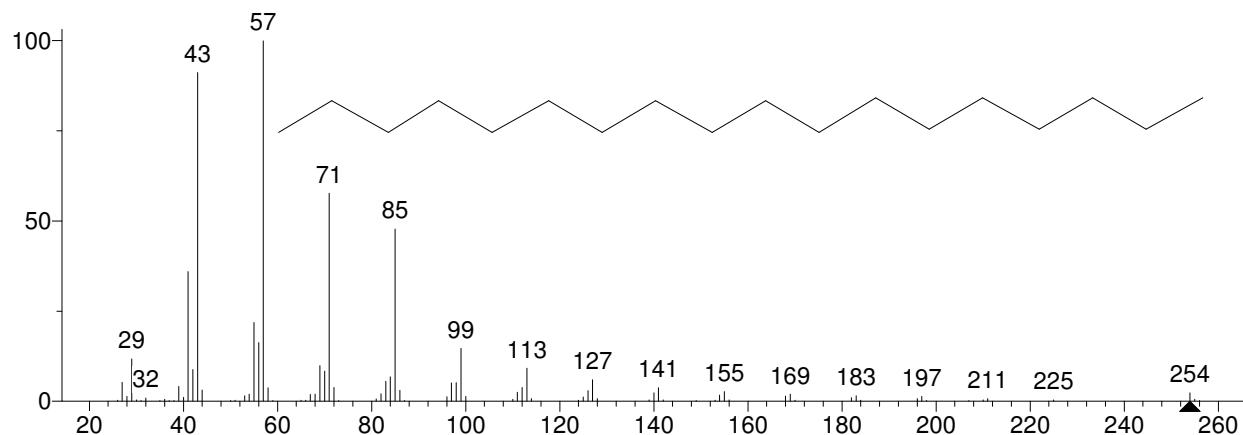


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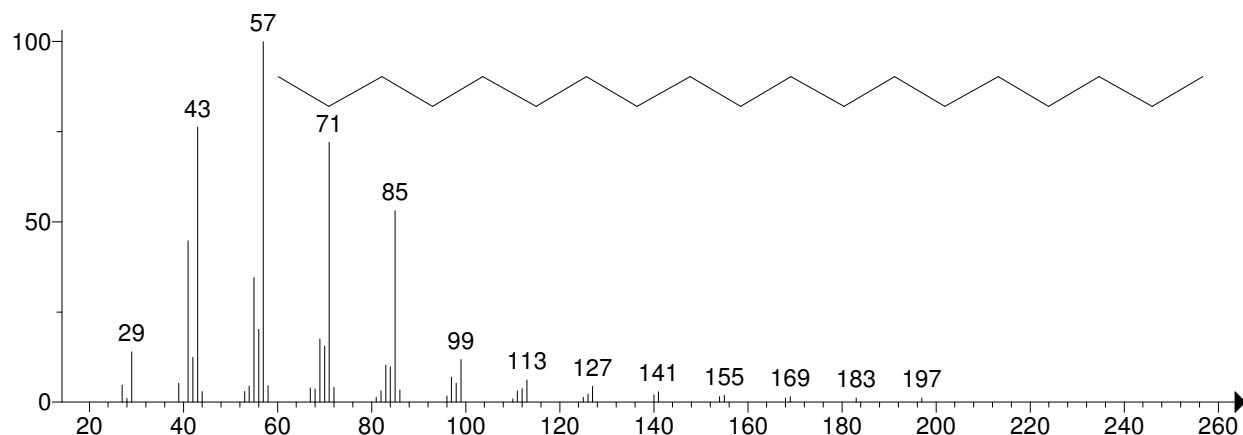
Unknown: Scan 1227 (14.035 min): J5169JO2.D
Compound in Library Factor = -110



Hit 1 : Octadecane
C18H38; MF: 942; RMF: 943; Prob 15.6%; CAS: 593-45-3; Lib: replib; ID: 5445.

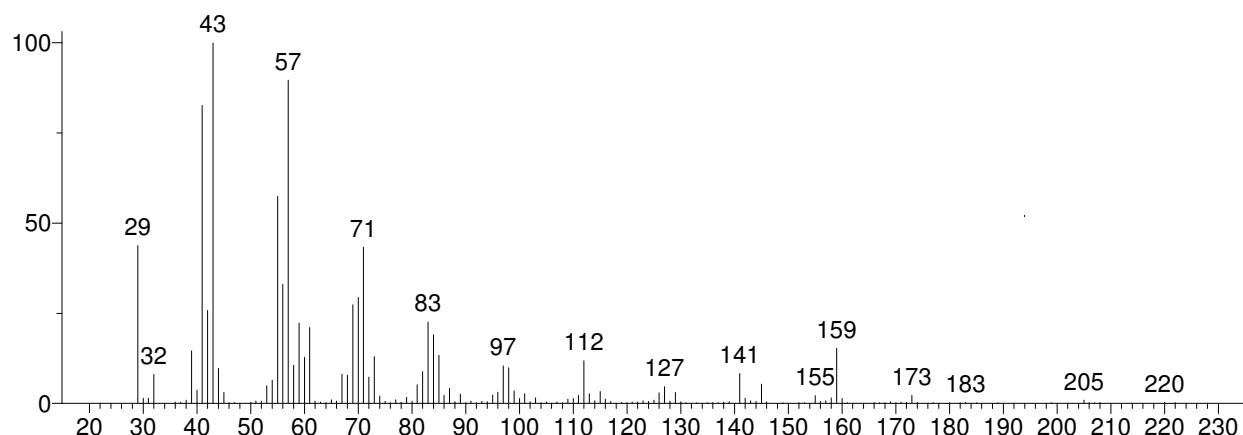


Hit 2 : Nonadecane
C19H40; MF: 939; RMF: 951; Prob 13.8%; CAS: 629-92-5; Lib: replib; ID: 5489.

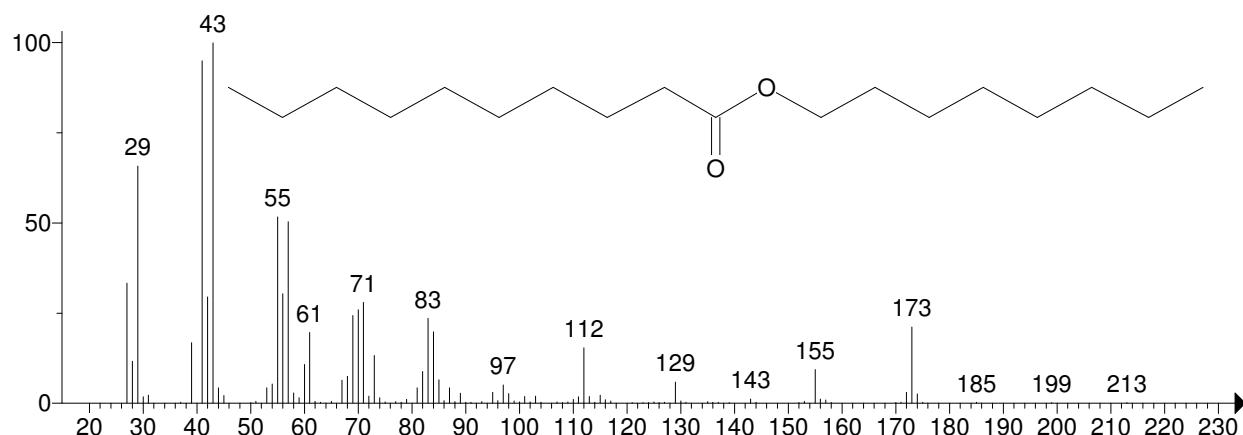


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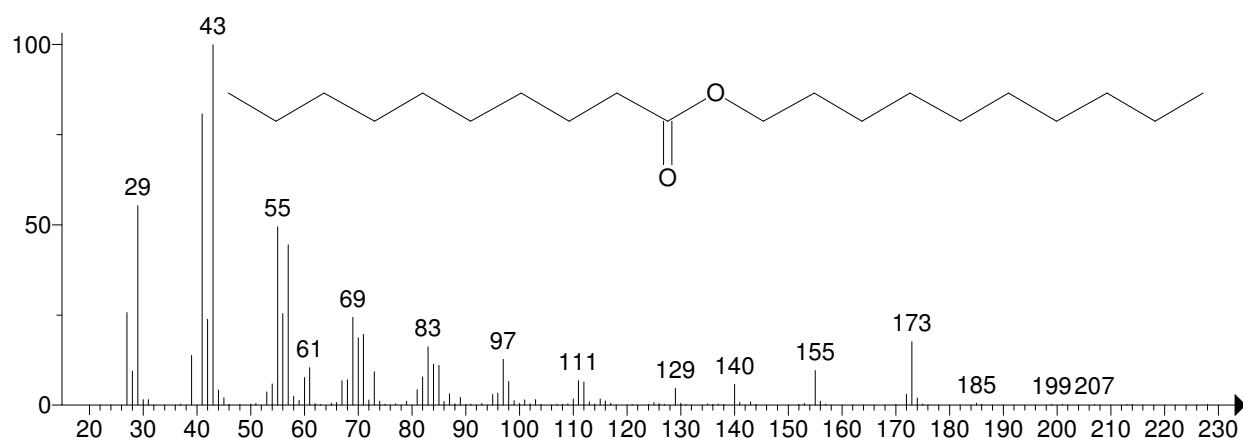
Unknown: Scan 1276 (14.594 min): J5169JO2.D
 Compound in Library Factor = -591



Hit 1 : Decanoic acid, octyl ester
 $C_{18}H_{36}O_2$; MF: 774; RMF: 823; Prob 10.7%; CAS: 2306-92-5; Lib: mainlib; ID: 5210.

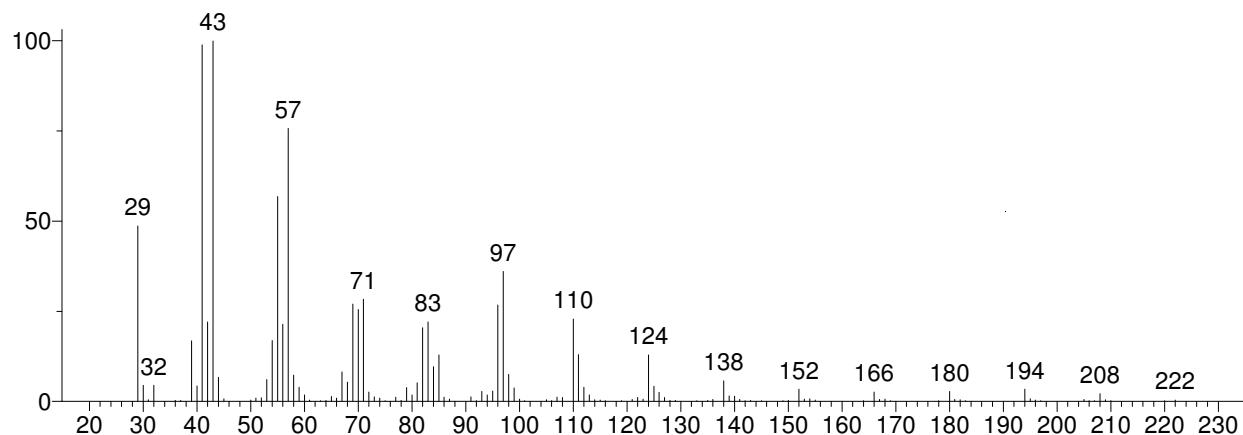


Hit 2 : Decanoic acid, decyl ester
 $C_{20}H_{40}O_2$; MF: 767; RMF: 809; Prob 8.15%; CAS: 1654-86-0; Lib: replib; ID: 1614.

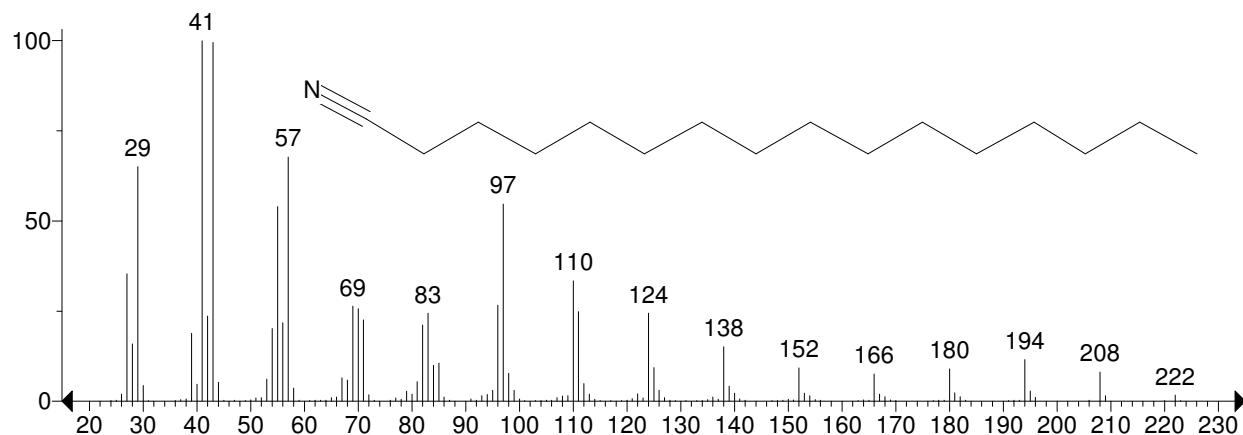


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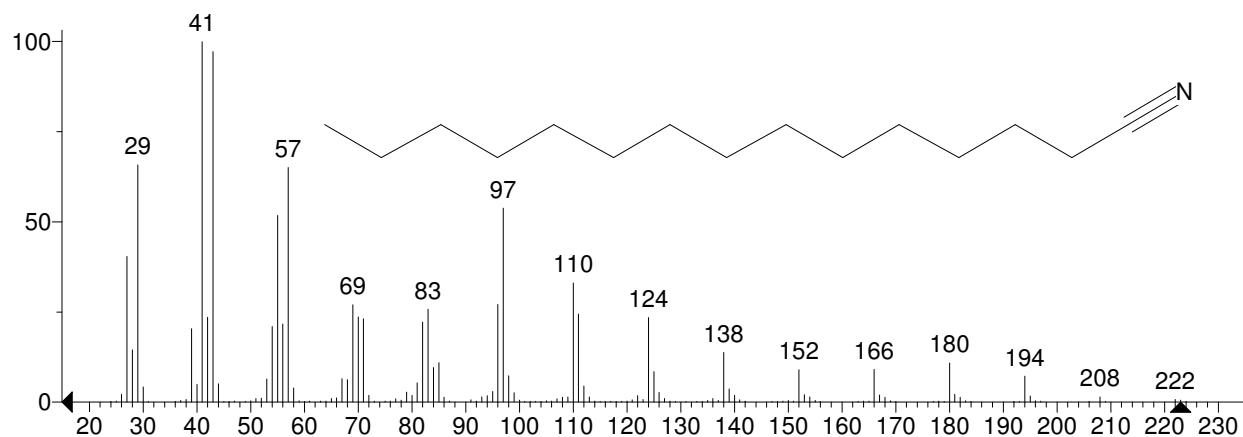
Unknown: Scan 1294 (14.800 min): J5169JO2.D
Compound in Library Factor = -197



Hit 1 : Hexadecanenitrile
C₁₆H₃₁N; MF: 879; RMF: 883; Prob 23.2%; CAS: 629-79-8; Lib: replib; ID: 806.

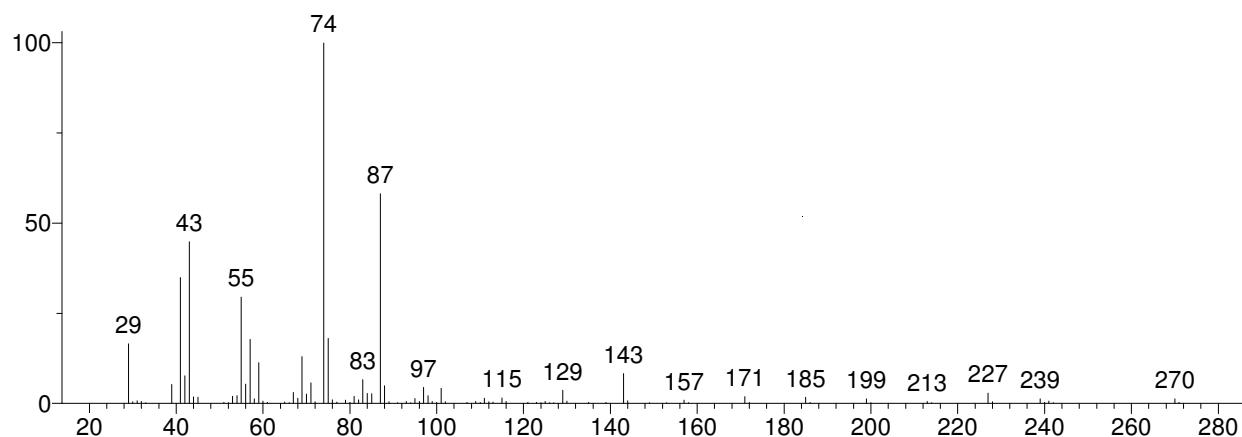


Hit 2 : Pentadecanenitrile
C₁₅H₂₉N; MF: 878; RMF: 880; Prob 22.3%; CAS: 18300-91-9; Lib: mainlib; ID: 2068.



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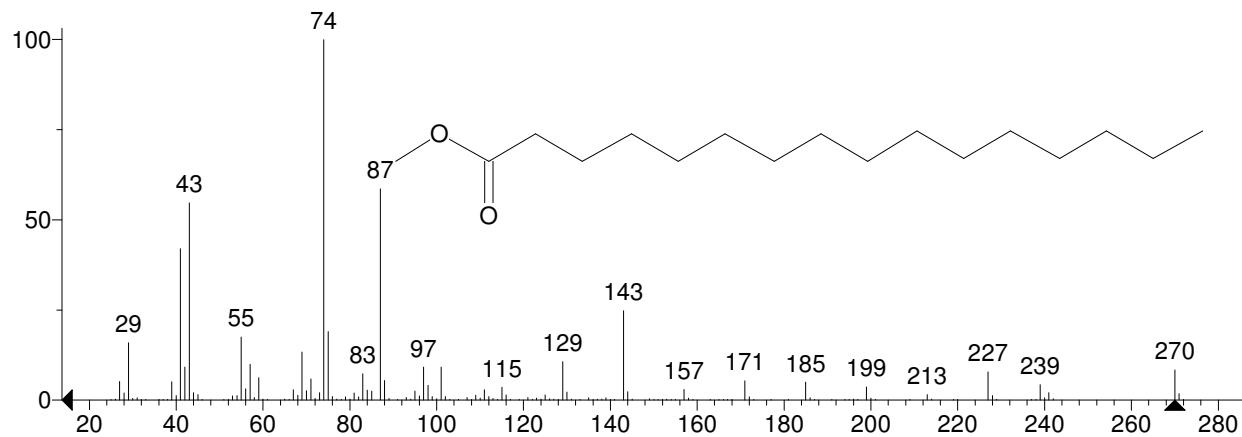
Unknown: Scan 1307 (14.948 min): J5169JO2.D
Compound in Library Factor = -113



Hit 1 : Hexadecanoic acid, methyl ester
C17H34O2; MF: 915; RMF: 916; Prob 42.0%; CAS: 112-39-0; Lib: replib; ID: 9000.

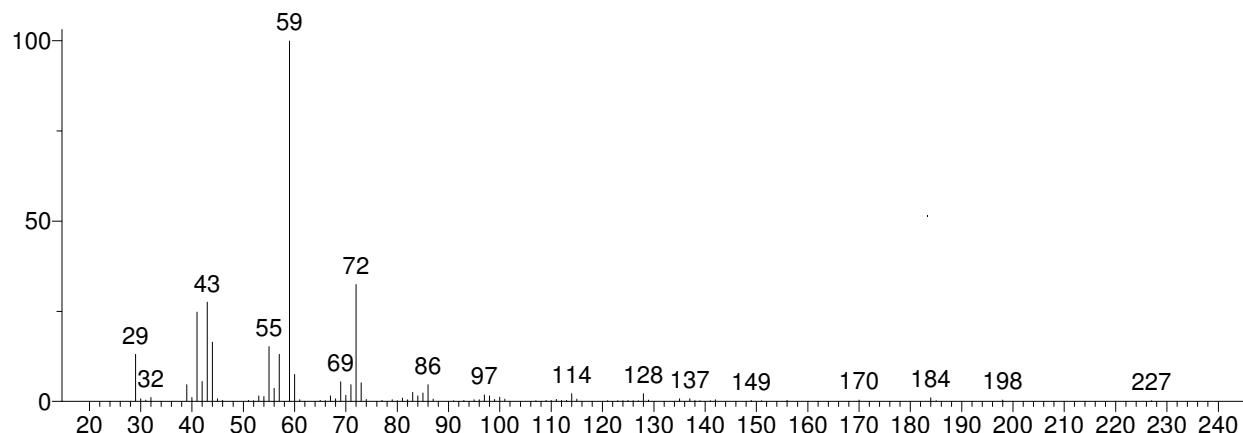


Hit 2 : Hexadecanoic acid, methyl ester
C17H34O2; MF: 901; RMF: 902; Prob 42.0%; CAS: 112-39-0; Lib: replib; ID: 9001.

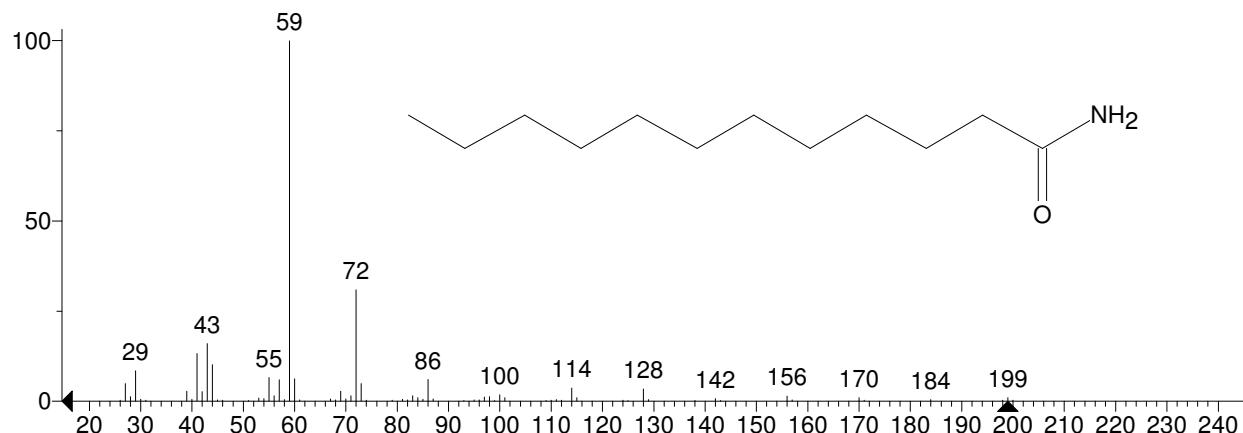


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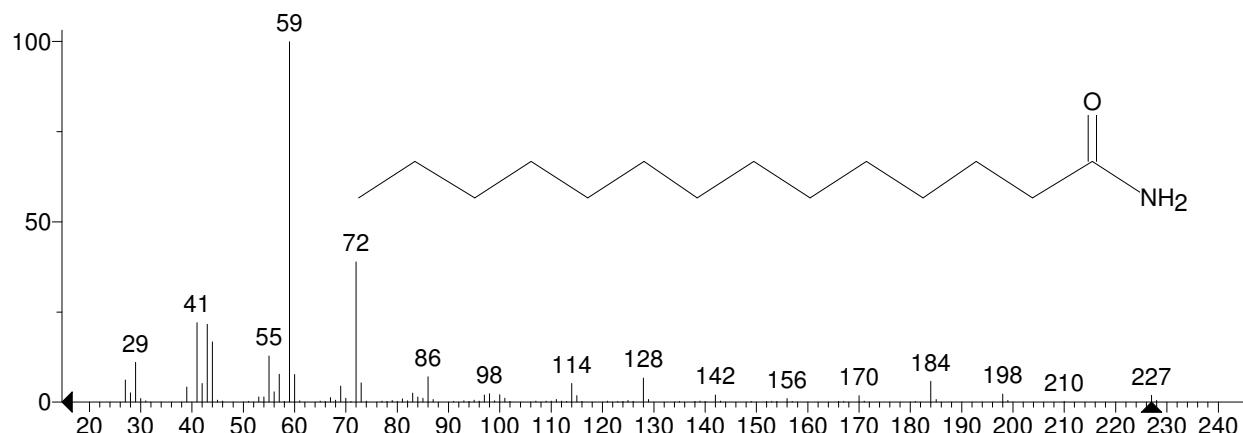
Unknown: Scan 1341 (15.336 min): J5169JO2.D
 Compound in Library Factor = -168



Hit 1 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 872; RMF: 880; Prob 64.8%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

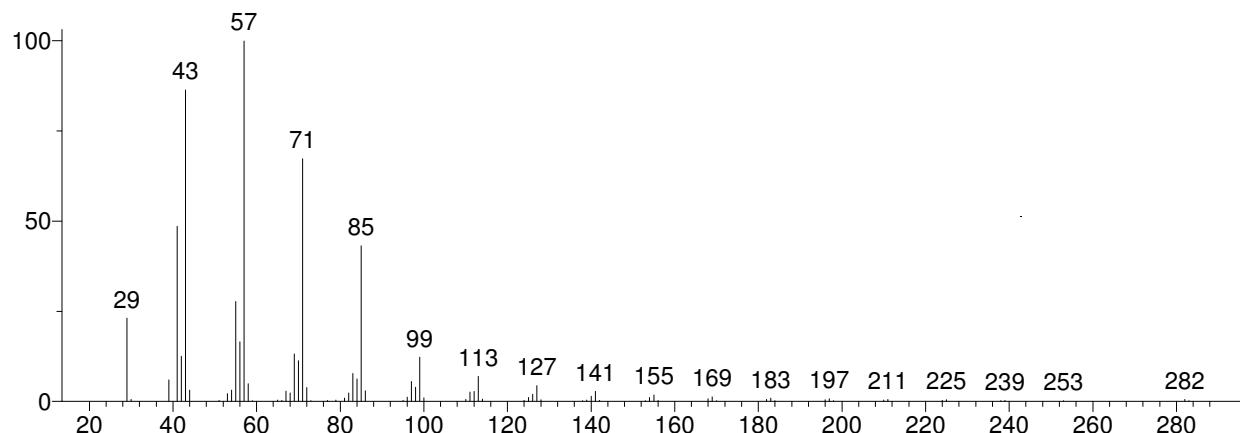


Hit 2 : Tetradecanamide
 $C_{14}H_{29}NO$; MF: 845; RMF: 849; Prob 19.1%; CAS: 638-58-4; Lib: mainlib; ID: 24922.

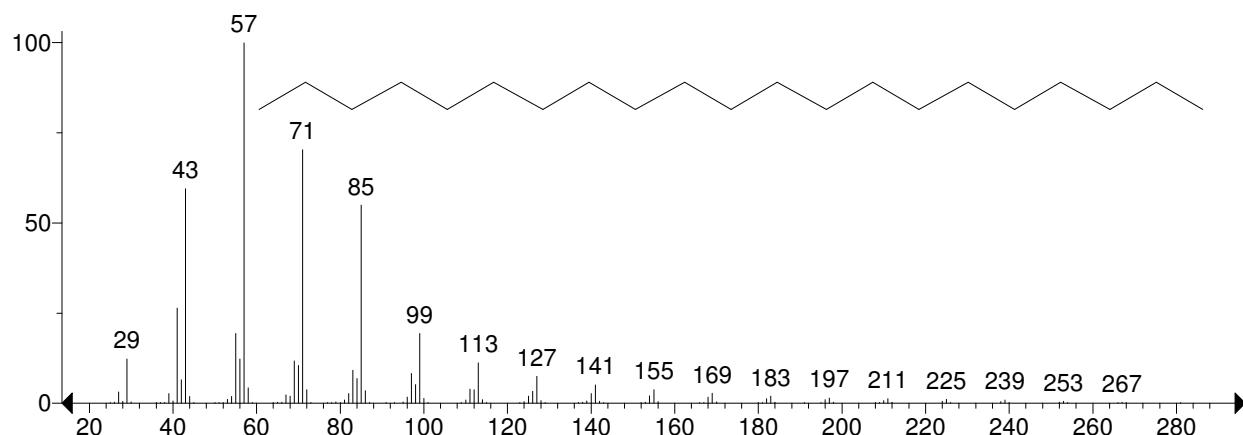


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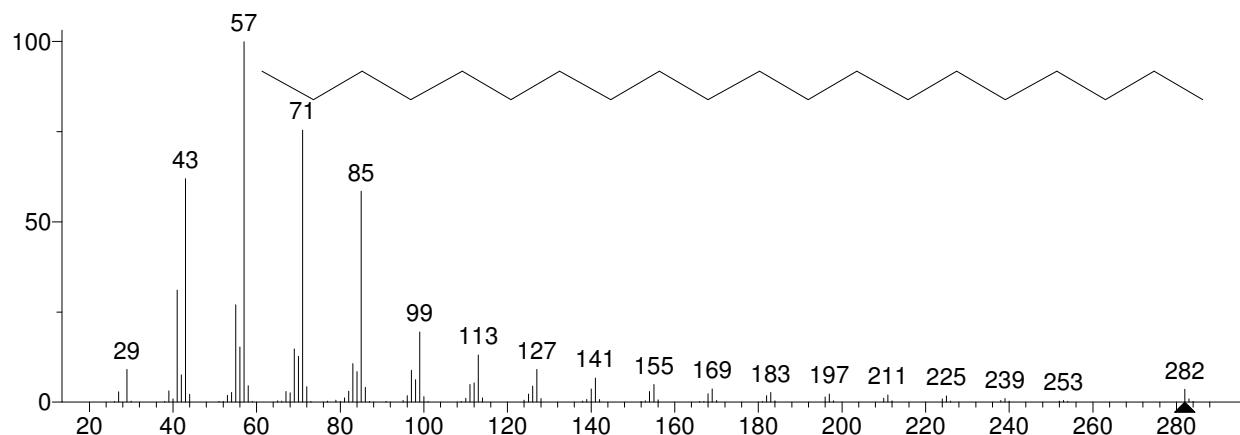
Unknown: Scan 1357 (15.519 min): J5169JO2.D
Compound in Library Factor = -113



Hit 1 : Heneicosane
C₂₁H₄₄; MF: 940; RMF: 942; Prob 13.2%; CAS: 629-94-7; Lib: replib; ID: 5723.

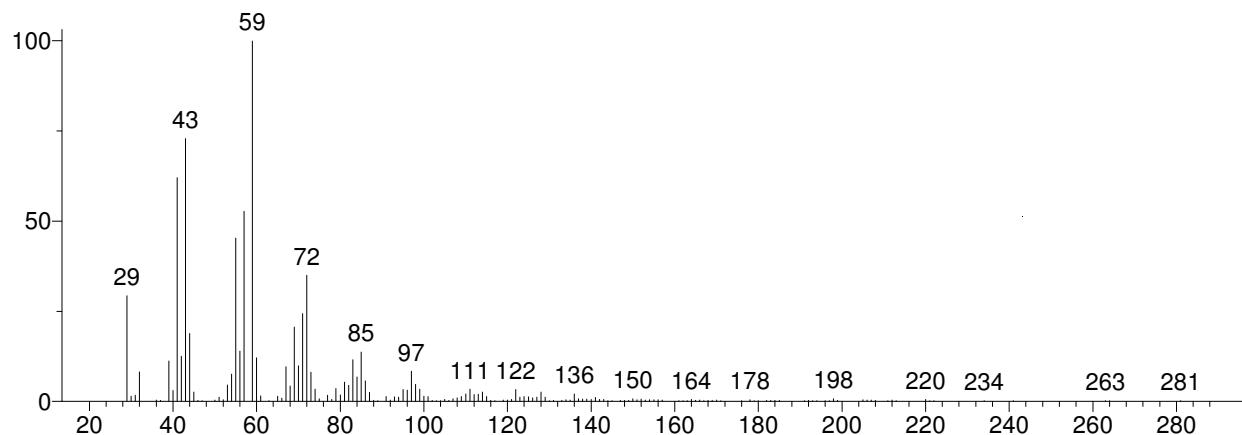


Hit 2 : Eicosane
C₂₀H₄₂; MF: 940; RMF: 940; Prob 13.2%; CAS: 112-95-8; Lib: replib; ID: 5706.

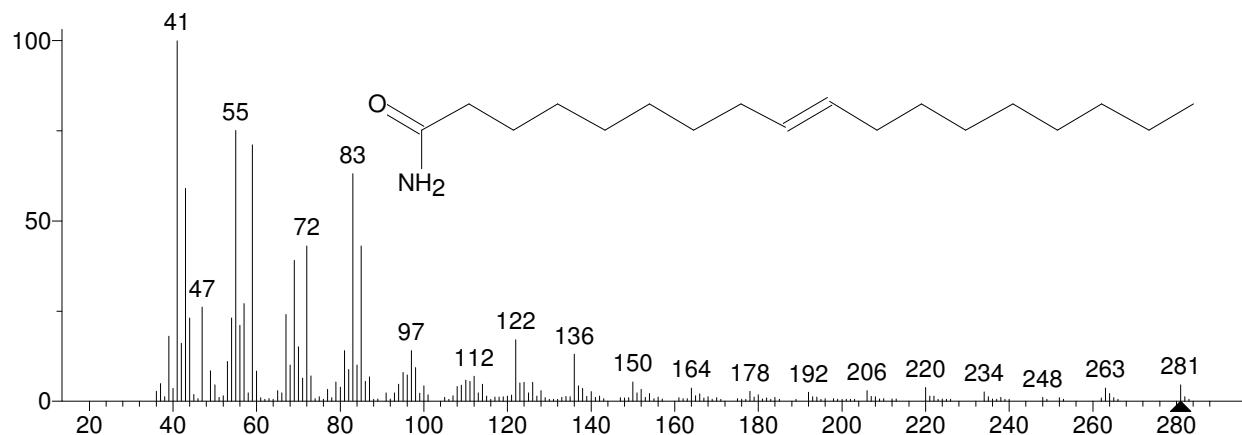


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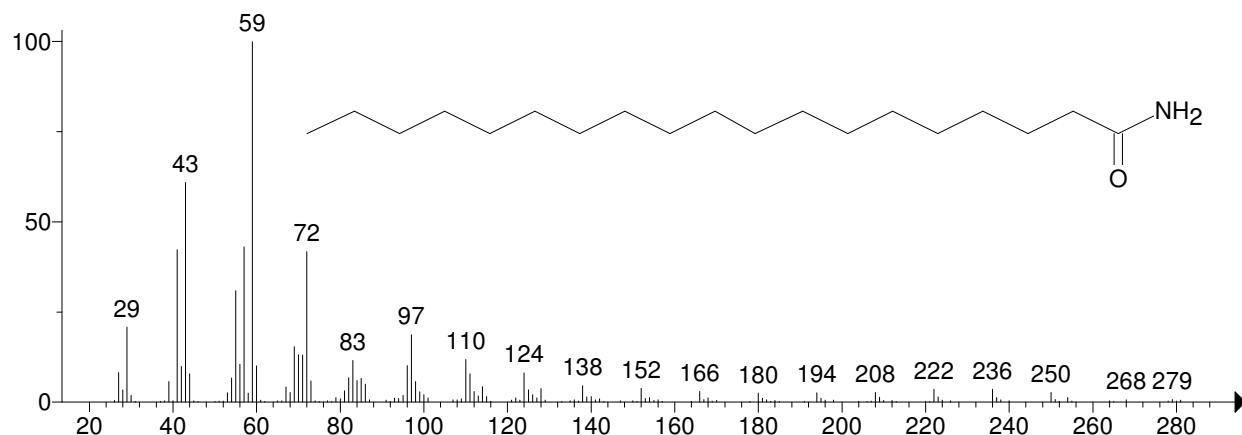
Unknown: Scan 1408 (16.101 min): J5169JO2.D
 Compound in Library Factor = -377



Hit 1 : 9-Octadecenamide
 $C_{18}H_{35}NO$; MF: 772; RMF: 773; Prob 33.4%; CAS: 3322-62-1; Lib: mainlib; ID: 2451.

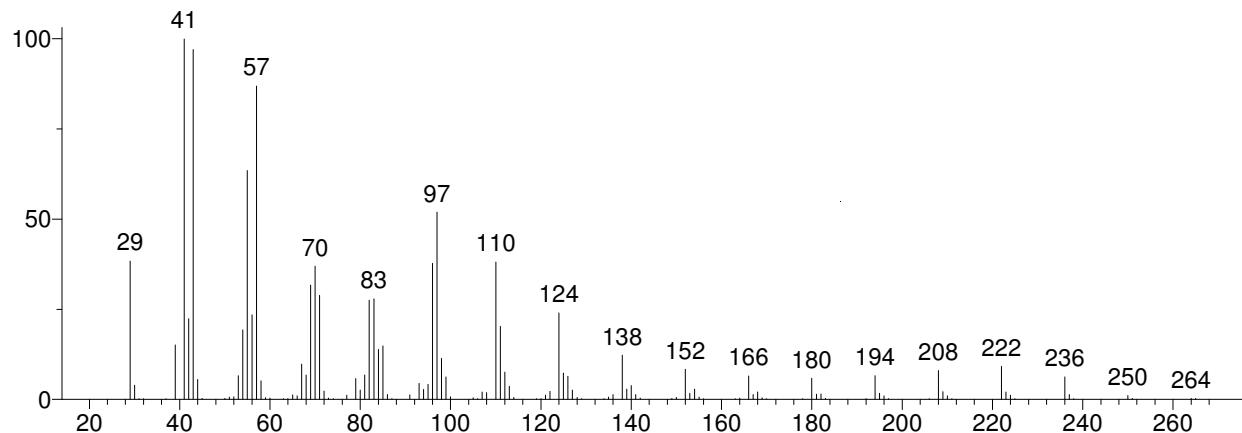


Hit 2 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 732; RMF: 745; Prob 7.74%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

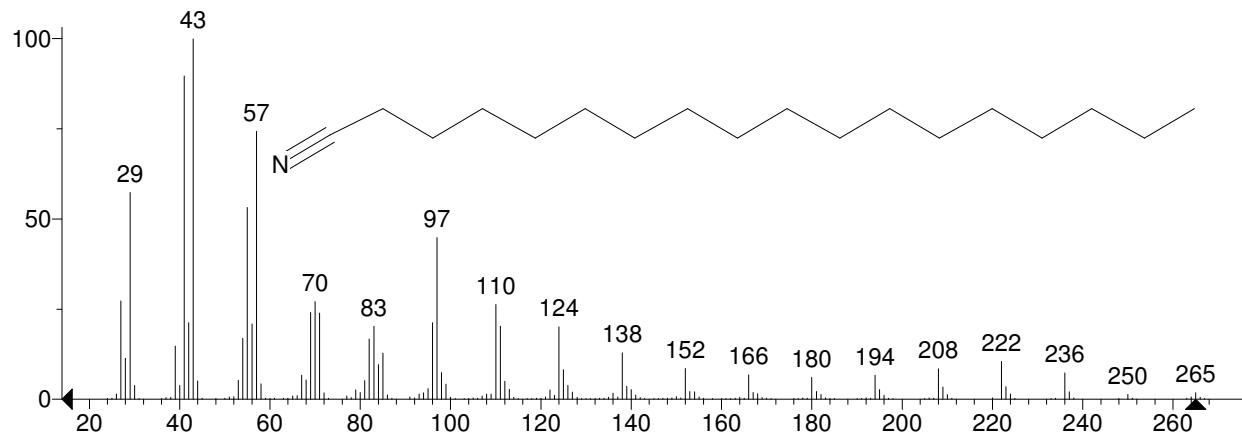


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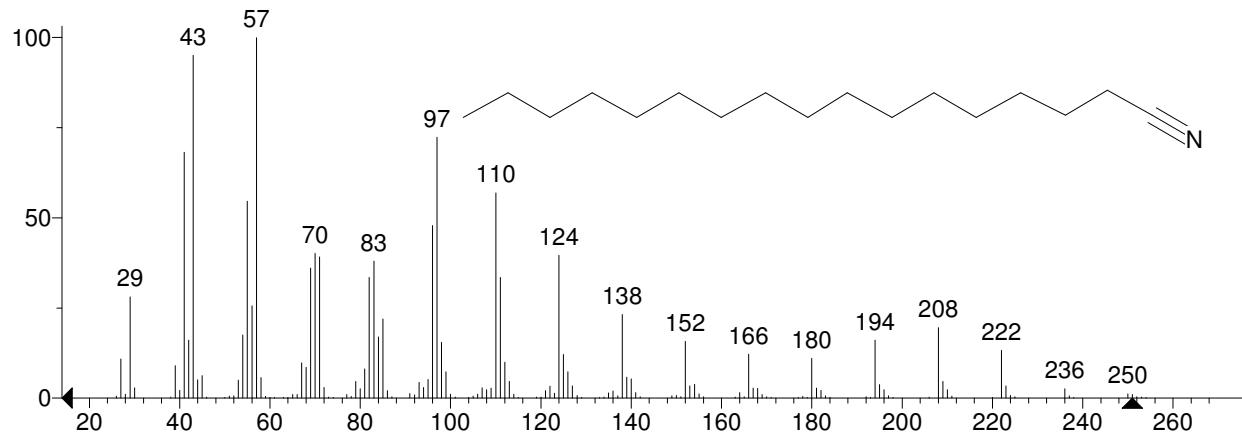
Unknown: Scan 1423 (16.272 min): J5169JO2.D
 Compound in Library Factor = -117



Hit 1 : Octadecanenitrile
 C18H35N; MF: 899; RMF: 899; Prob 27.0%; CAS: 638-65-3; Lib: replib; ID: 1691.

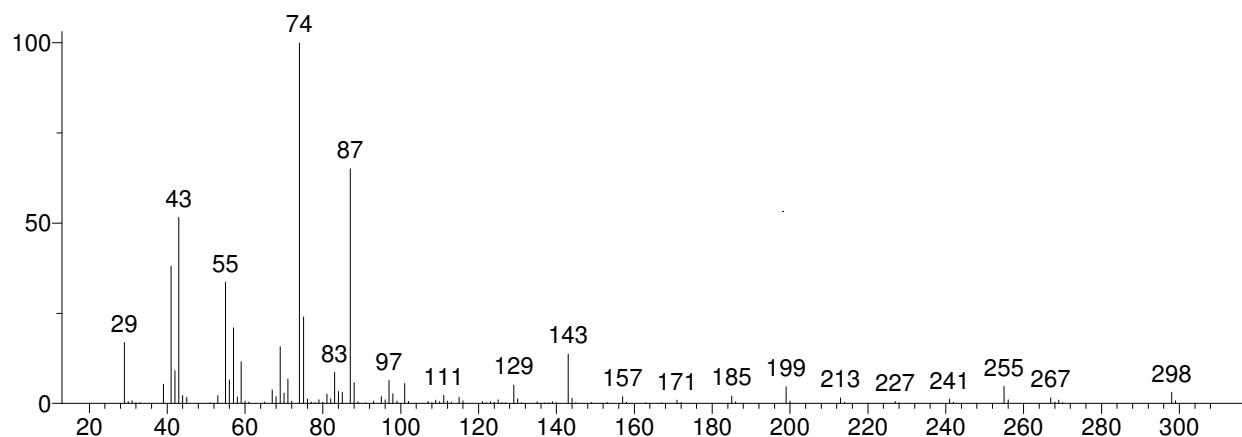


Hit 2 : Heptadecanenitrile
 C17H33N; MF: 892; RMF: 893; Prob 20.7%; CAS: 5399-02-0; Lib: replib; ID: 5535.

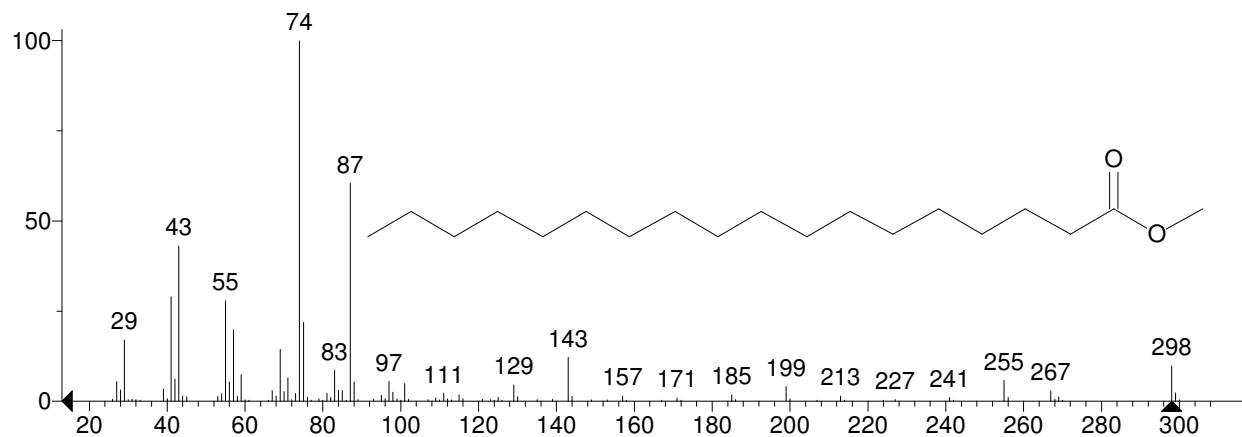


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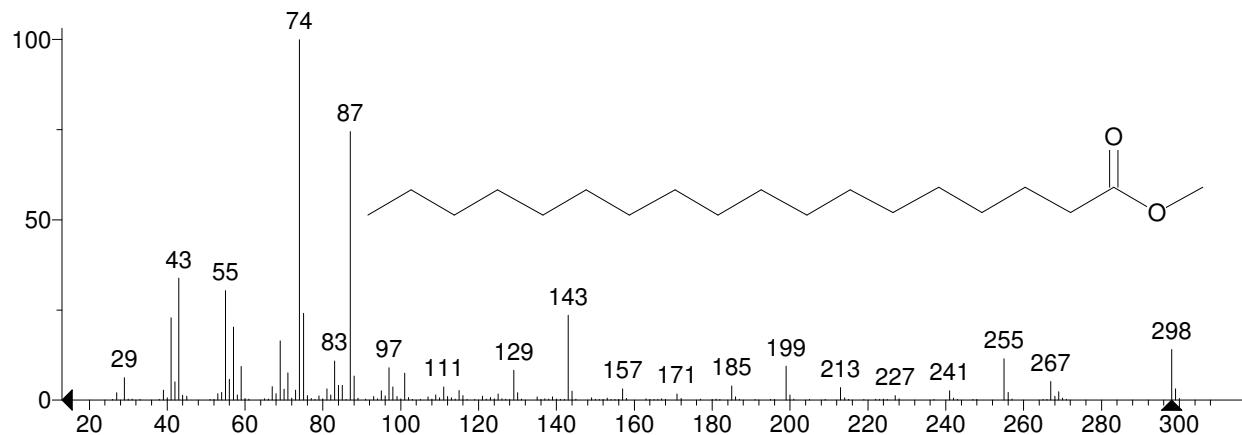
Unknown: Scan 1434 (16.398 min): J5169JO2.D
 Compound in Library Factor = 196



Hit 1 : Octadecanoic acid, methyl ester
 C19H38O2; MF: 938; RMF: 938; Prob 54.9%; CAS: 112-61-8; Lib: mainlib; ID: 35262.

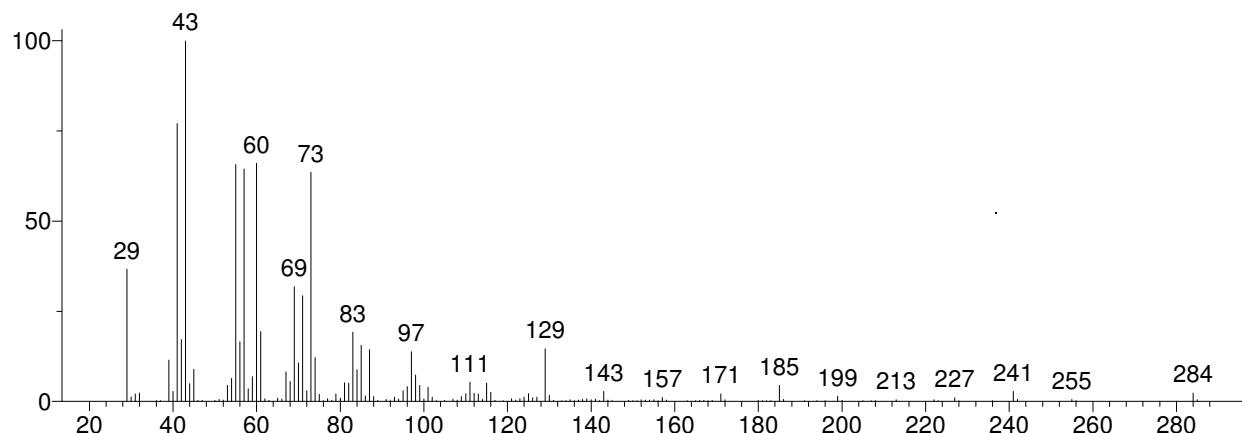


Hit 2 : Octadecanoic acid, methyl ester
 C19H38O2; MF: 927; RMF: 927; Prob 54.9%; CAS: 112-61-8; Lib: replib; ID: 9041.

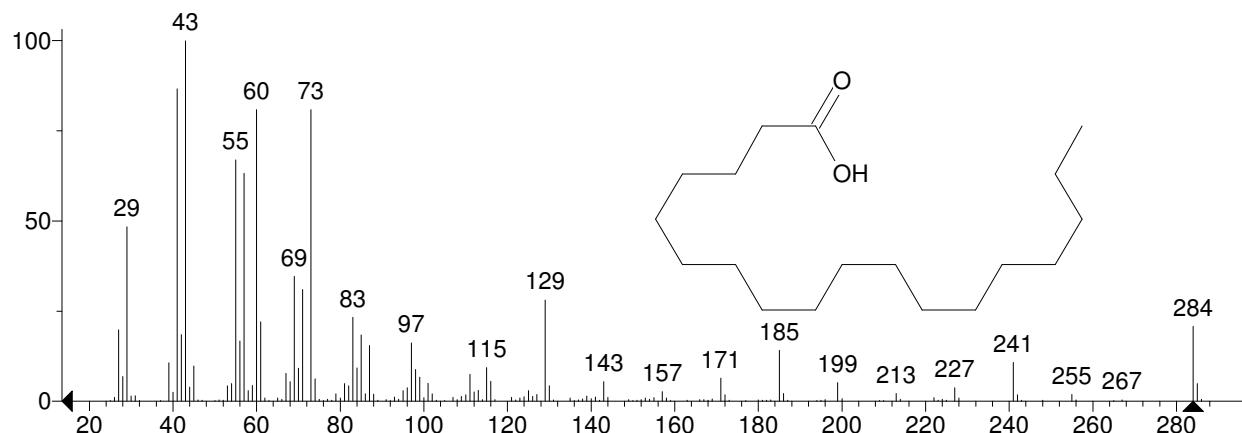


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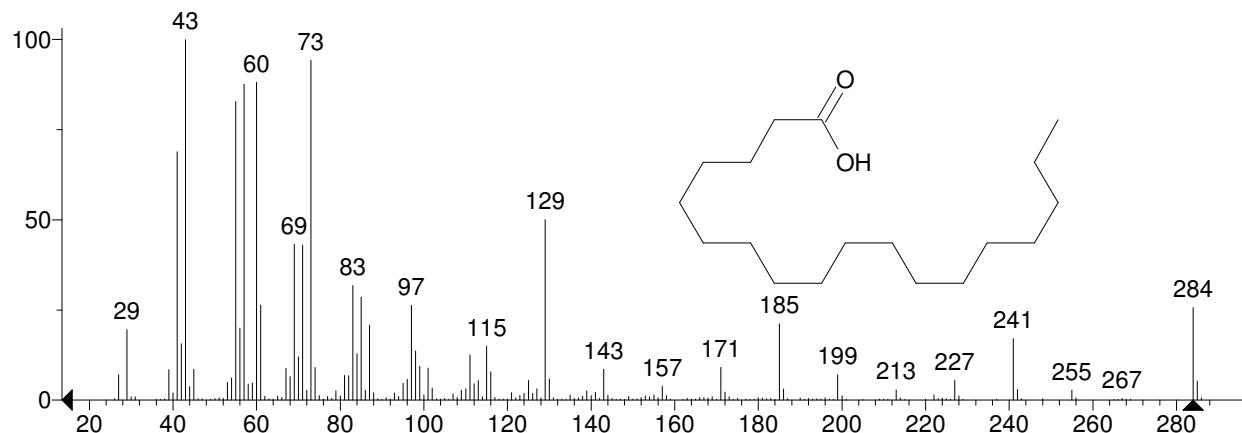
Unknown: Scan 1461 (16.706 min): J5169JO2.D
 Compound in Library Factor = 103



Hit 1 : Octadecanoic acid
 C₁₈H₃₆O₂; MF: 894; RMF: 895; Prob 55.2%; CAS: 57-11-4; Lib: replib; ID: 1699.

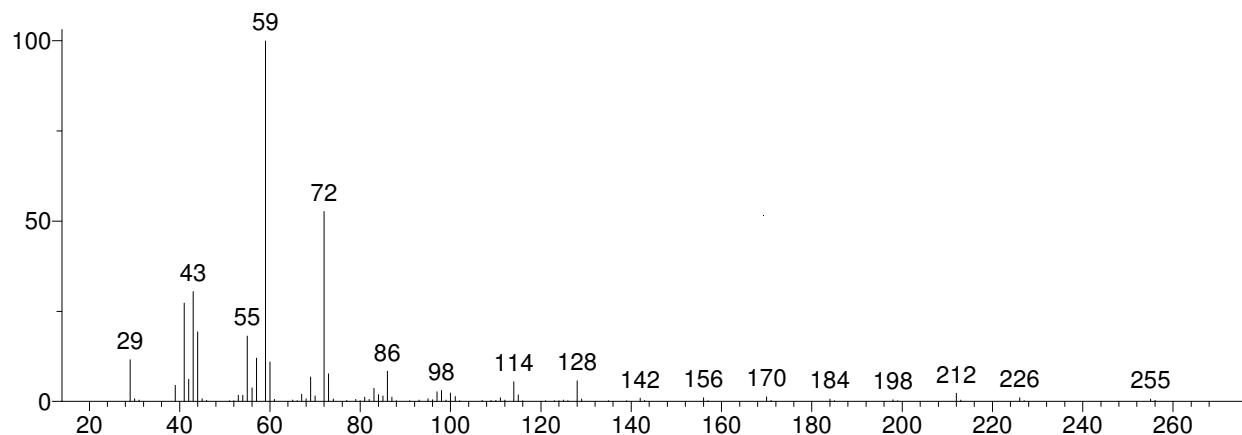


Hit 2 : Octadecanoic acid
 C₁₈H₃₆O₂; MF: 883; RMF: 883; Prob 55.2%; CAS: 57-11-4; Lib: replib; ID: 2523.

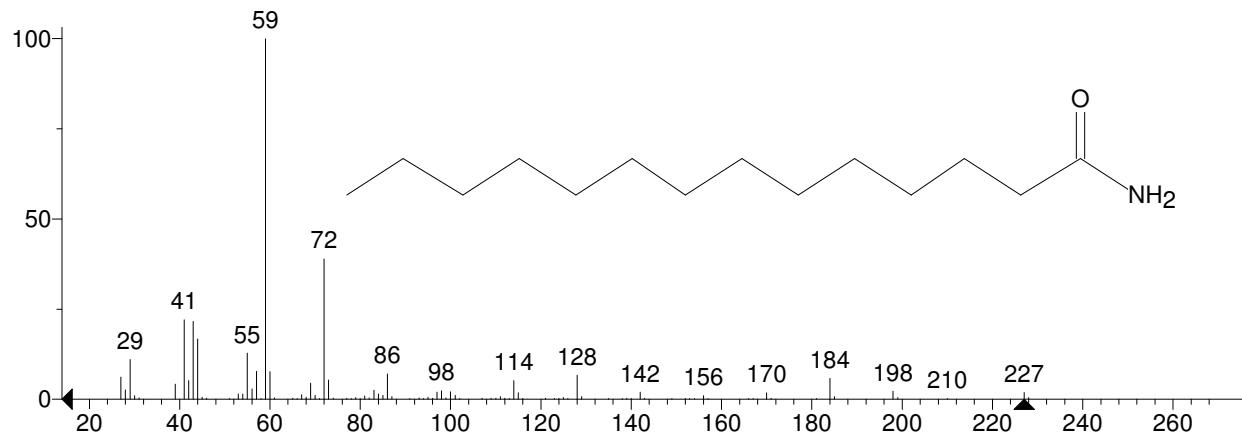


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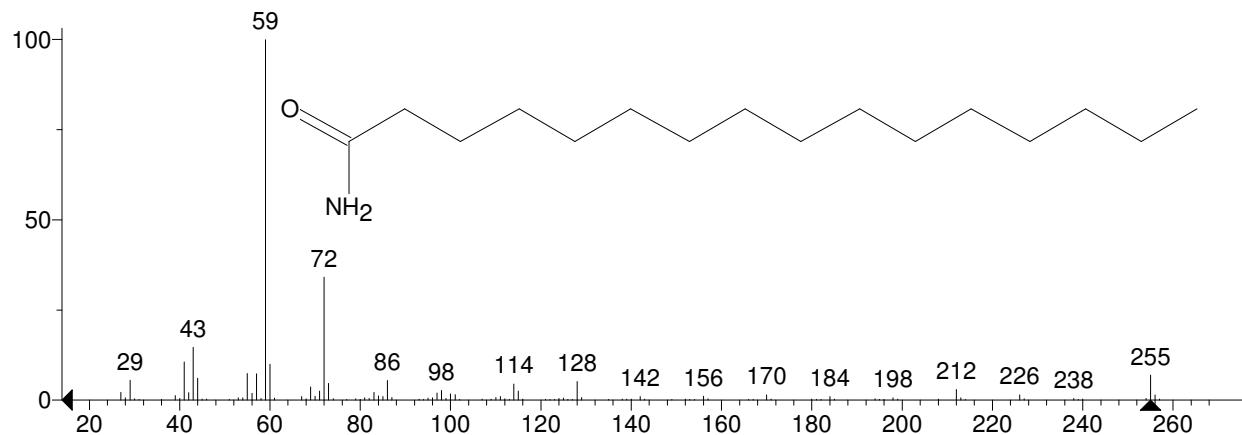
Unknown: Scan 1474 (16.854 min): J5169JO2.D
 Compound in Library Factor = -101



Hit 1 : Tetradecanamide
 $C_{14}H_{29}NO$; MF: 886; RMF: 905; Prob 59.9%; CAS: 638-58-4; Lib: mainlib; ID: 24922.

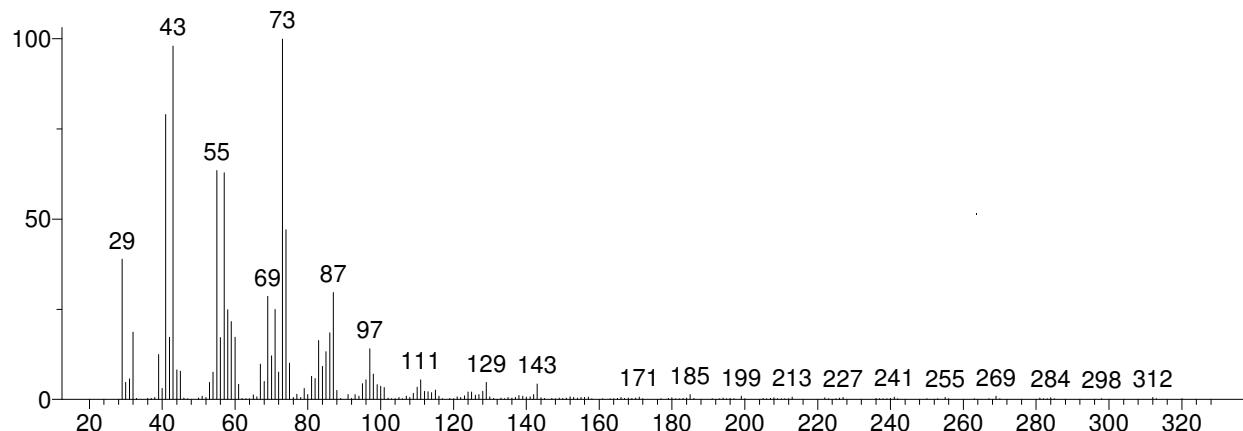


Hit 2 : Hexadecanamide
 $C_{16}H_{33}NO$; MF: 856; RMF: 857; Prob 16.6%; CAS: 629-54-9; Lib: mainlib; ID: 24924.

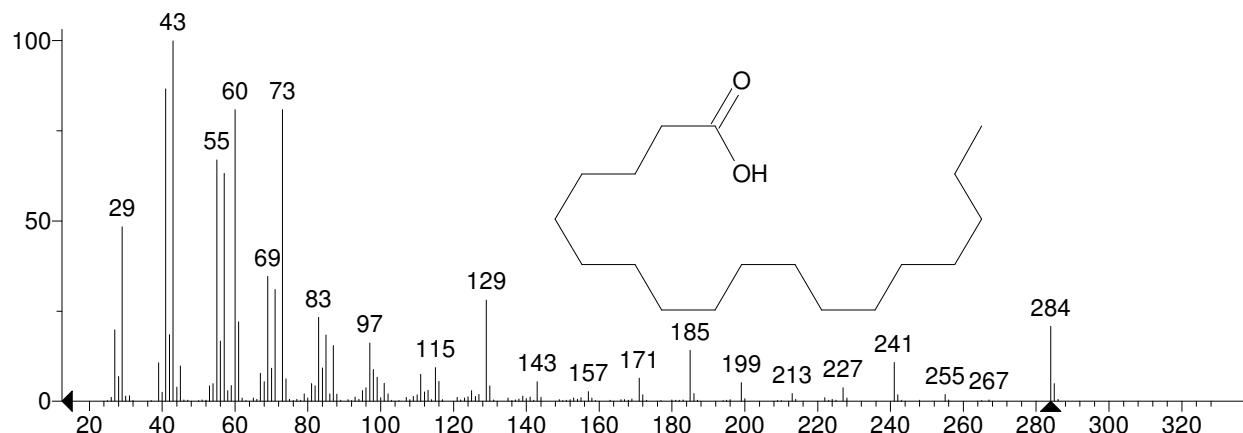


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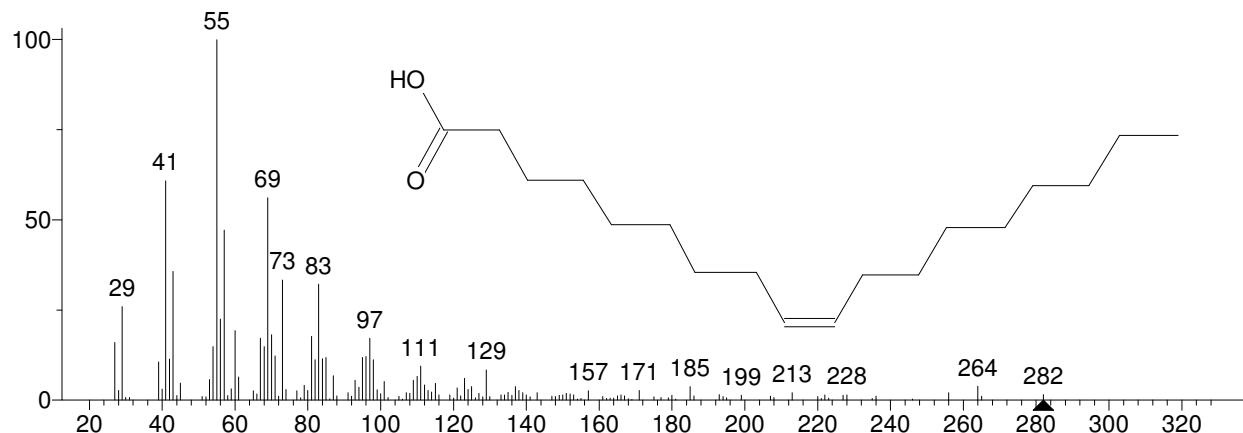
Unknown: Scan 1485 (16.980 min): J5169JO2.D
 Compound in Library Factor = -1120



Hit 1 : Octadecanoic acid
 $C_{18}H_{36}O_2$; MF: 739; RMF: 752; Prob 8.30%; CAS: 57-11-4; Lib: replib; ID: 1699.

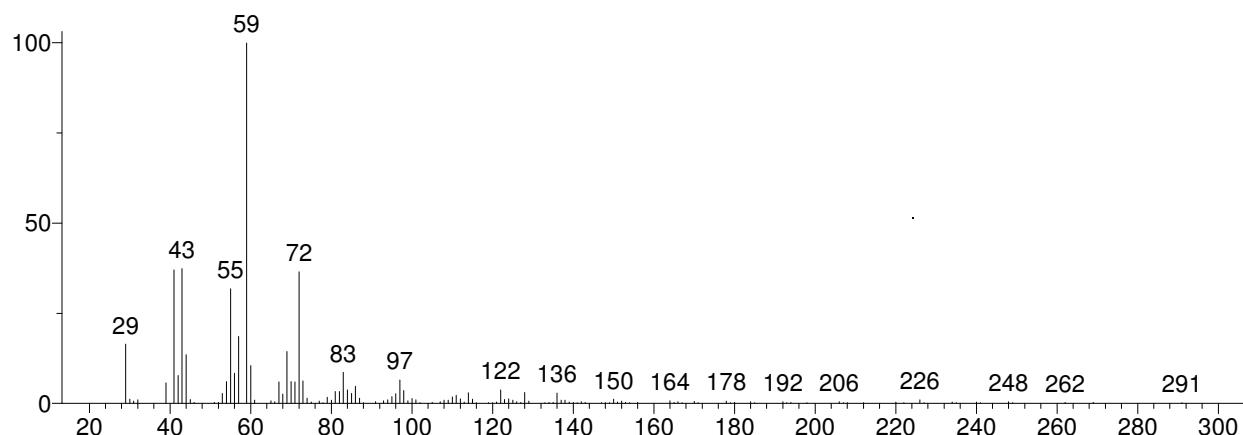


Hit 2 : Oleic Acid
 $C_{18}H_{34}O_2$; MF: 734; RMF: 753; Prob 6.69%; CAS: 112-80-1; Lib: replib; ID: 4240.

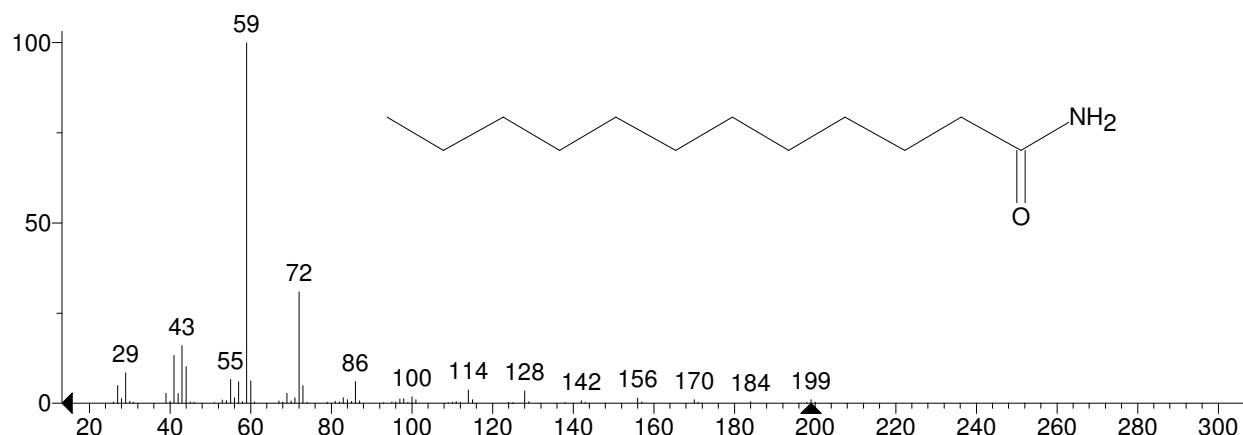


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Unknown: Scan 1523 (17.414 min): J5169JO2.D
 Compound in Library Factor = -602



Hit 1 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 760; RMF: 816; Prob 20.1%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

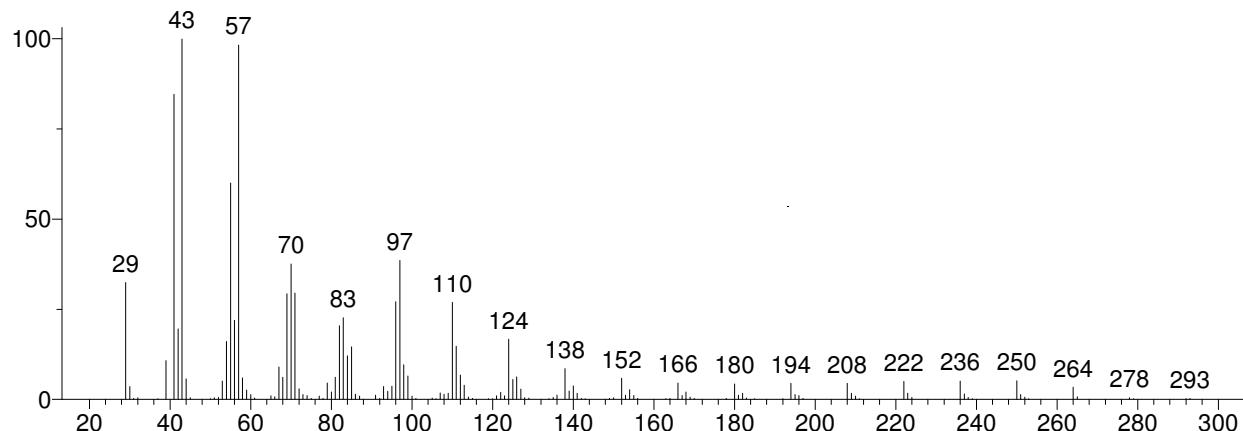


Hit 2 : 9-Octadecenamide
 $C_{18}H_{35}NO$; MF: 758; RMF: 759; Prob 18.6%; CAS: 3322-62-1; Lib: mainlib; ID: 2451.

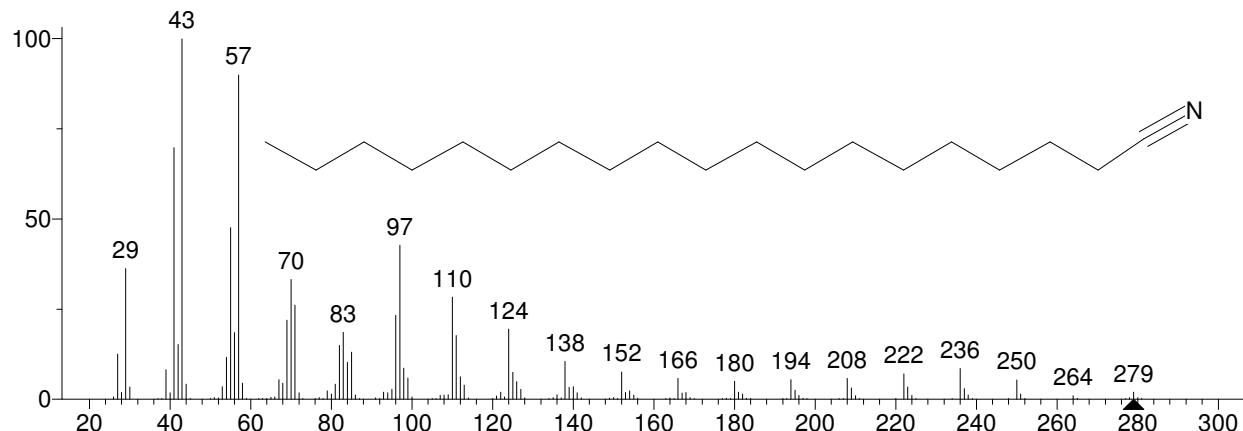


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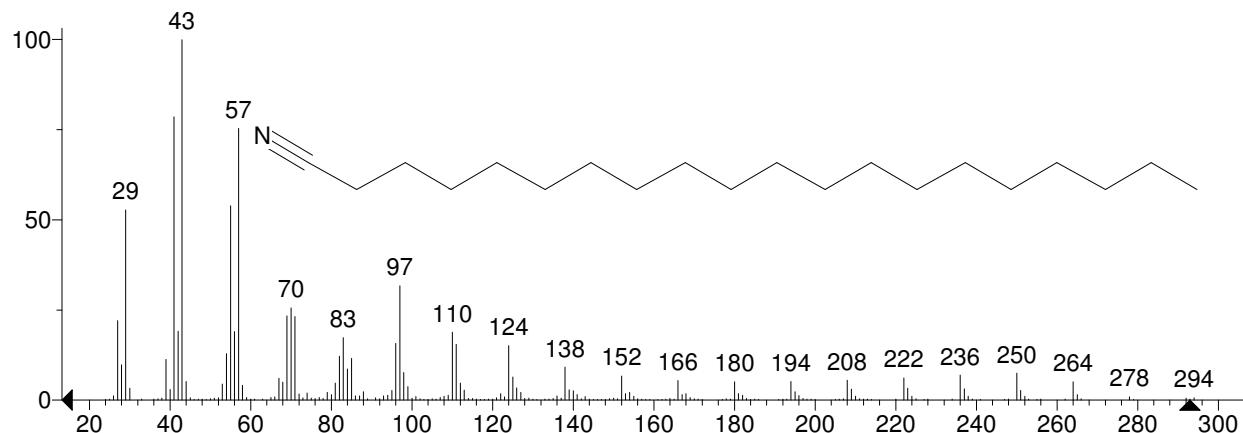
Unknown: Scan 1535 (17.551 min): J5169JO2.D
 Compound in Library Factor = -104



Hit 1 : Nonadecanenitrile
 $C_{19}H_{37}N$; MF: 906; RMF: 911; Prob 36.9%; CAS: 28623-46-3; Lib: mainlib; ID: 6885.

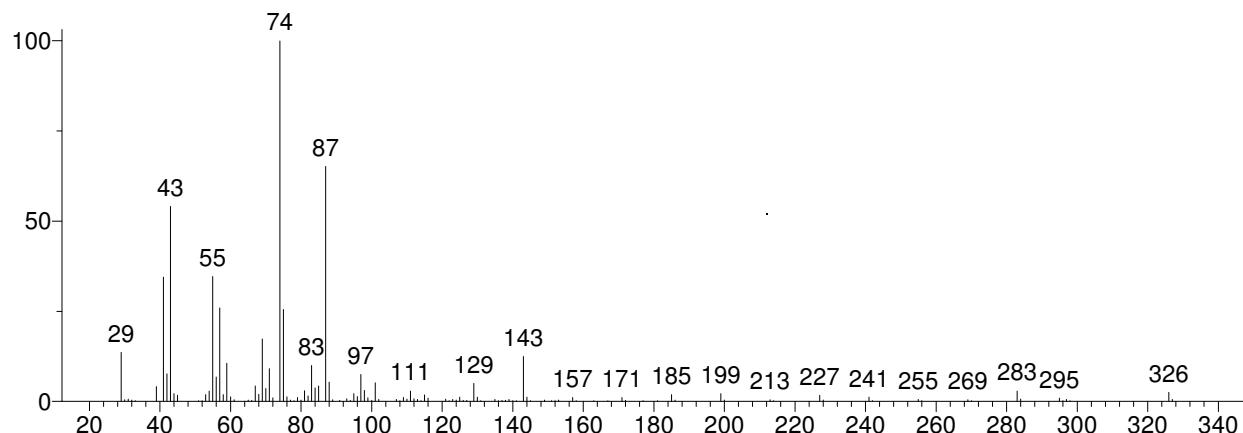


Hit 2 : Eicosanenitrile
 $C_{20}H_{39}N$; MF: 890; RMF: 890; Prob 21.2%; CAS: 4616-73-3; Lib: mainlib; ID: 5477.

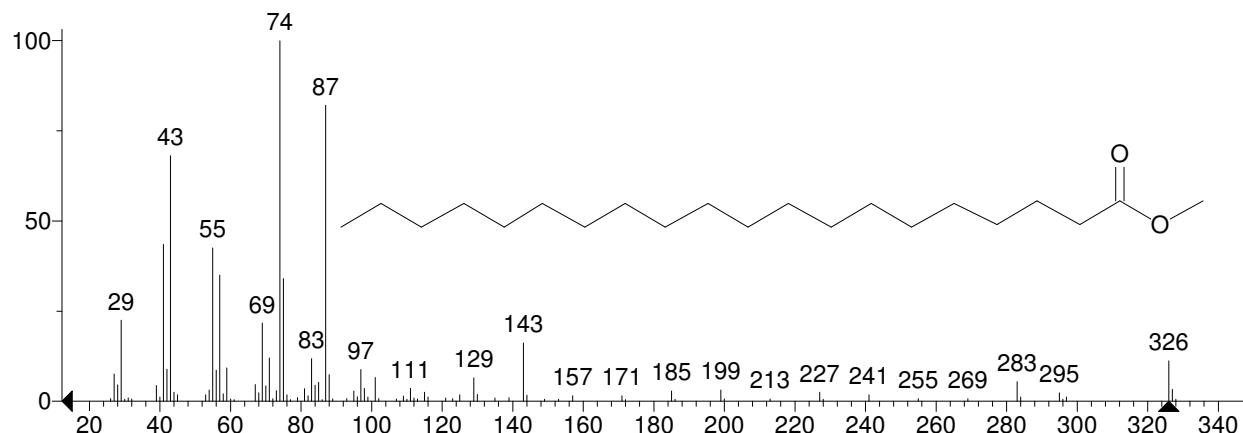


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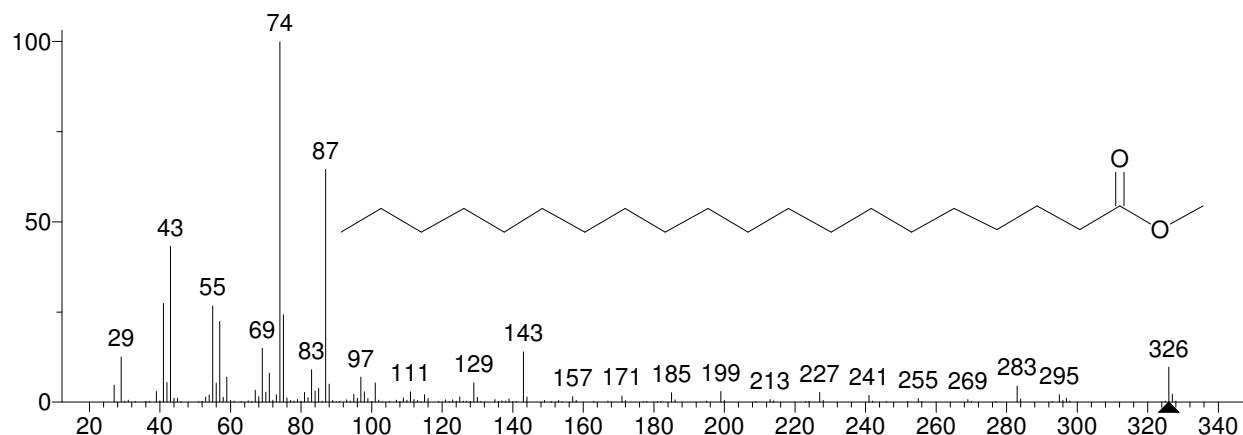
Unknown: Scan 1539 (17.596 min): J5169JO2.D
 Compound in Library Factor = 177



Hit 1 : Eicosanoic acid, methyl ester
 C₂₁H₄₂O₂; MF: 930; RMF: 933; Prob 56.4%; CAS: 1120-28-1; Lib: replib; ID: 9005.

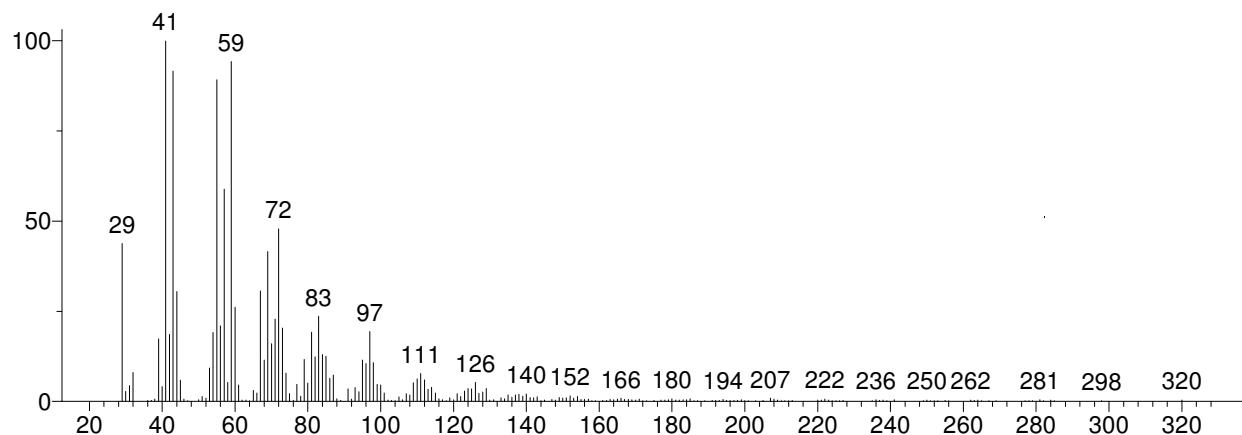


Hit 2 : Eicosanoic acid, methyl ester
 C₂₁H₄₂O₂; MF: 921; RMF: 921; Prob 56.4%; CAS: 1120-28-1; Lib: replib; ID: 9006.

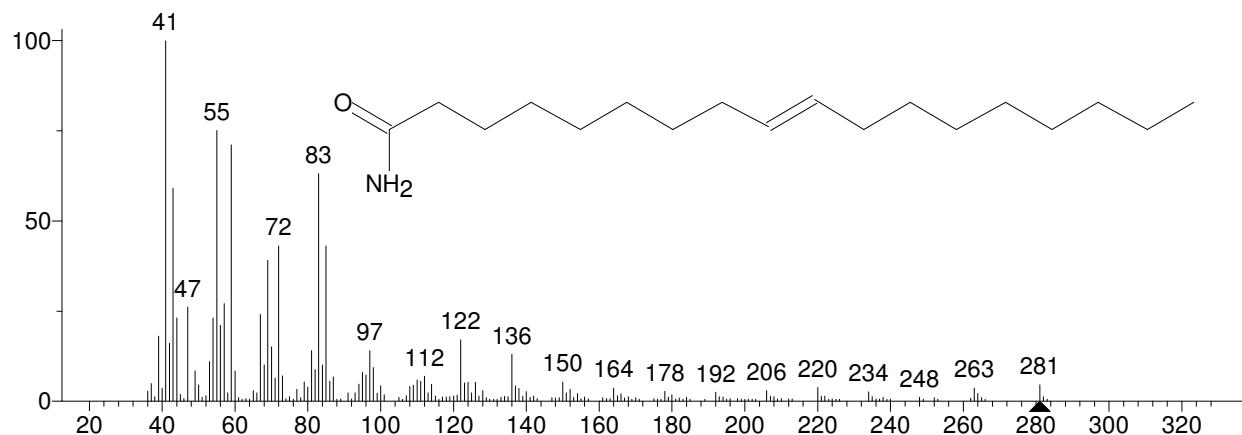


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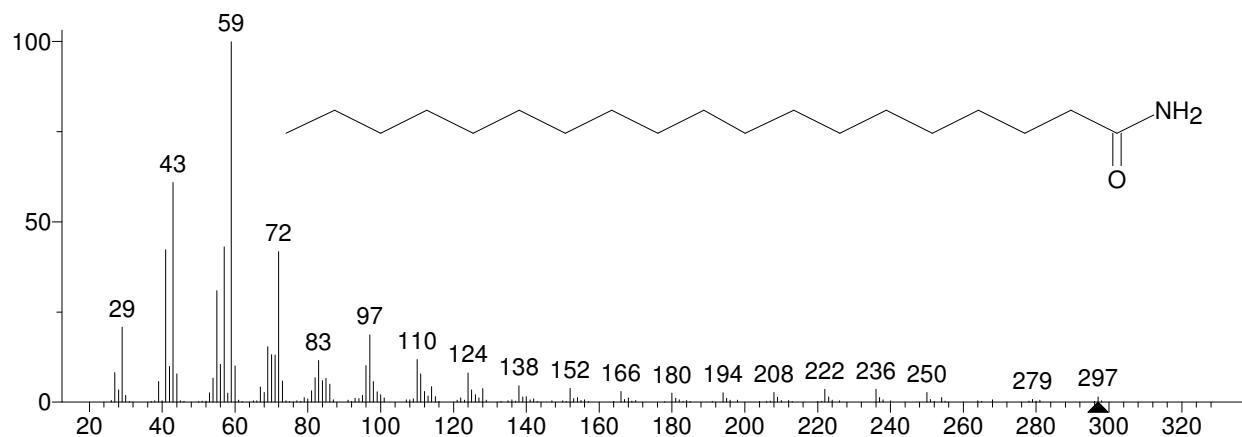
Unknown: Scan 1566 (17.905 min): J5169JO2.D
 Compound in Library Factor = -625



Hit 1 : 9-Octadecenamide
 C18H35NO; MF: 765; RMF: 769; Prob 10.1%; CAS: 3322-62-1; Lib: mainlib; ID: 2451.

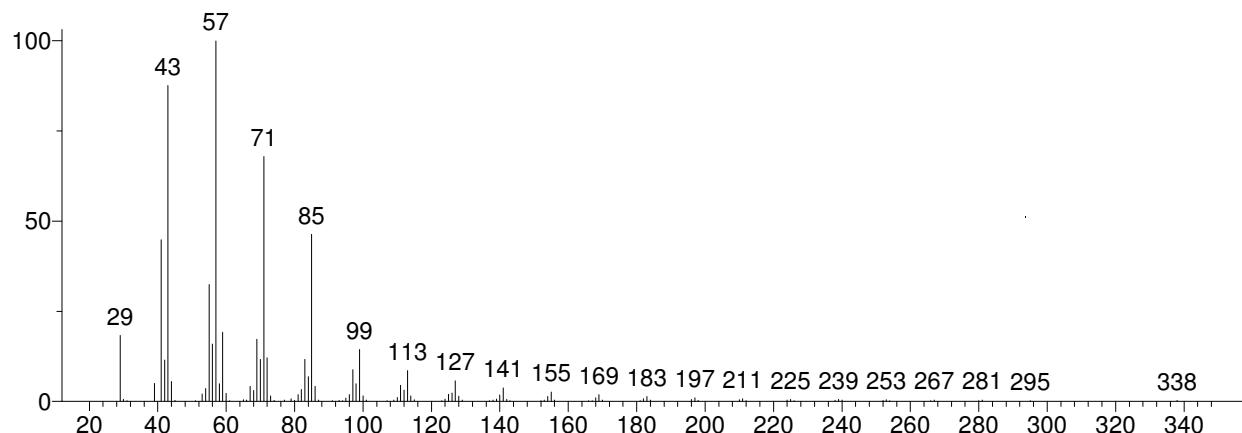


Hit 2 : Nonadecanamide
 C19H39NO; MF: 759; RMF: 778; Prob 7.91%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

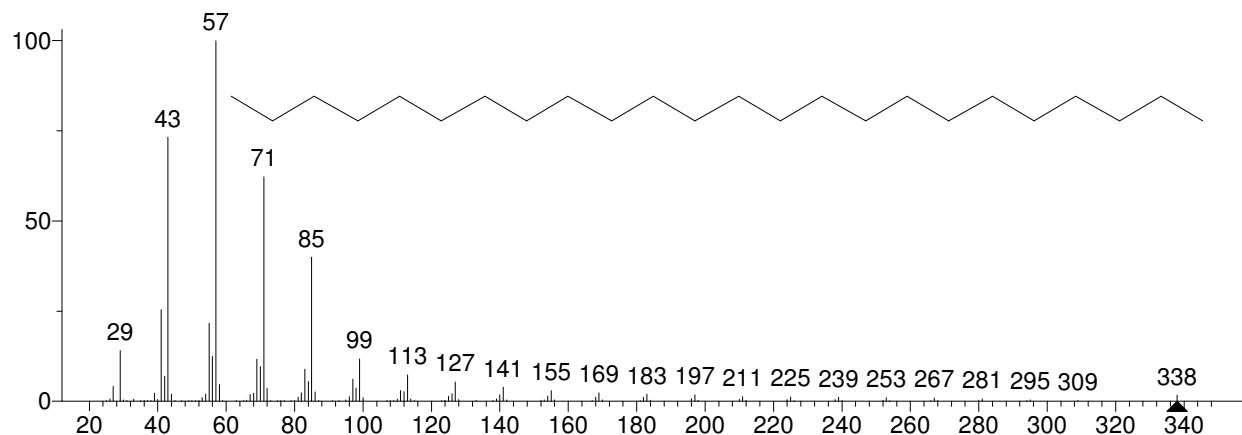


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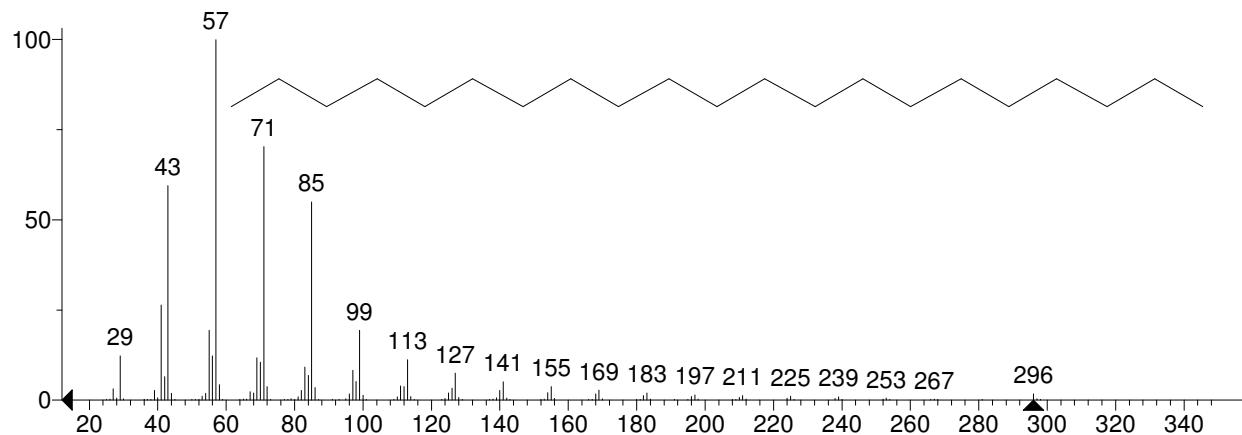
Unknown: Scan 1578 (18.042 min): J5169JO2.D
 Compound in Library Factor = -253



Hit 1 : Tetracosane
 C₂₄H₅₀; MF: 883; RMF: 902; Prob 8.16%; CAS: 646-31-1; Lib: replib; ID: 5493.

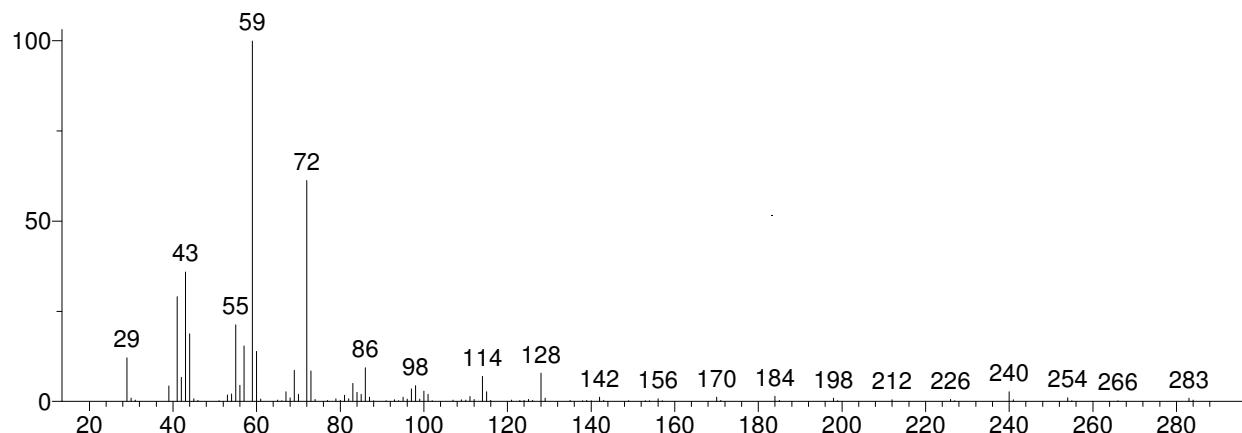


Hit 2 : Heneicosane
 C₂₁H₄₄; MF: 879; RMF: 885; Prob 6.89%; CAS: 629-94-7; Lib: replib; ID: 5723.

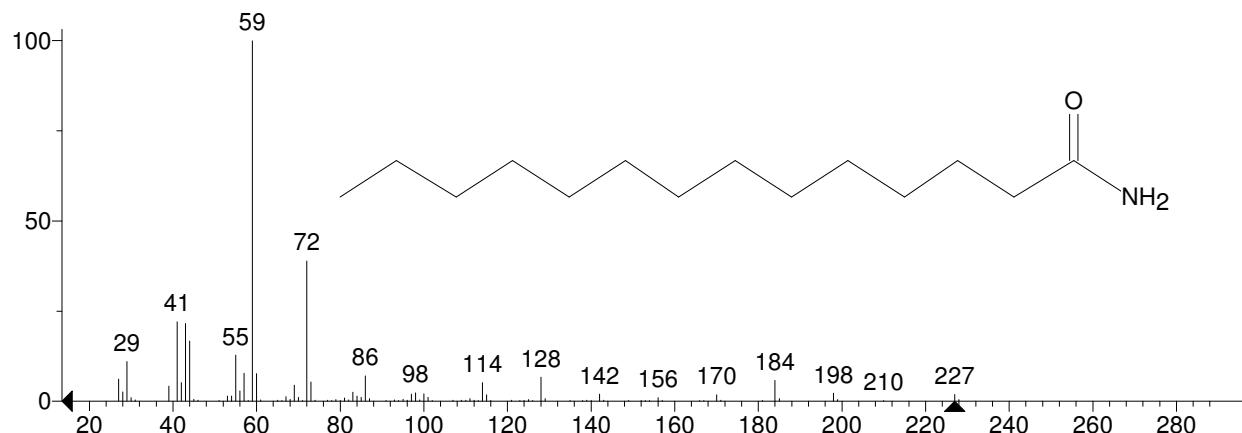


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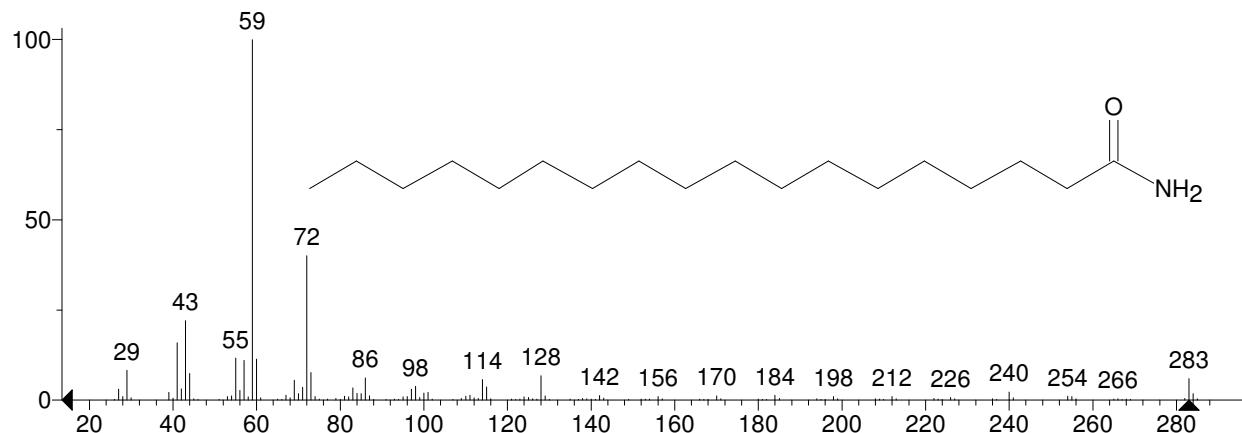
Unknown: Scan 1587 (18.144 min): J5169JO2.D
 Compound in Library Factor = -138



Hit 1 : Tetradeccanamide
 C14H29NO; MF: 873; RMF: 899; Prob 60.3%; CAS: 638-58-4; Lib: mainlib; ID: 24922.

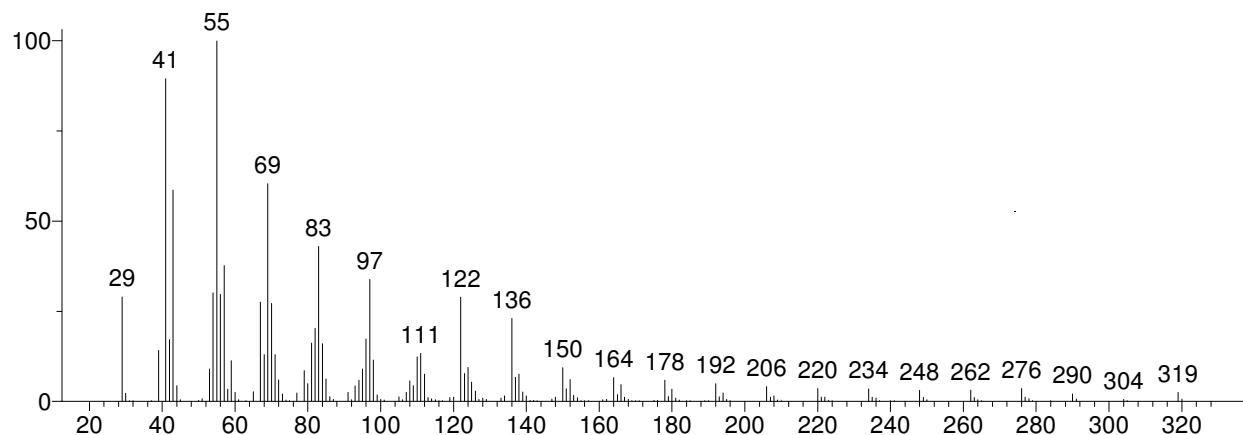


Hit 2 : Octadecanamide
 C18H37NO; MF: 833; RMF: 833; Prob 14.0%; CAS: 124-26-5; Lib: mainlib; ID: 24926.

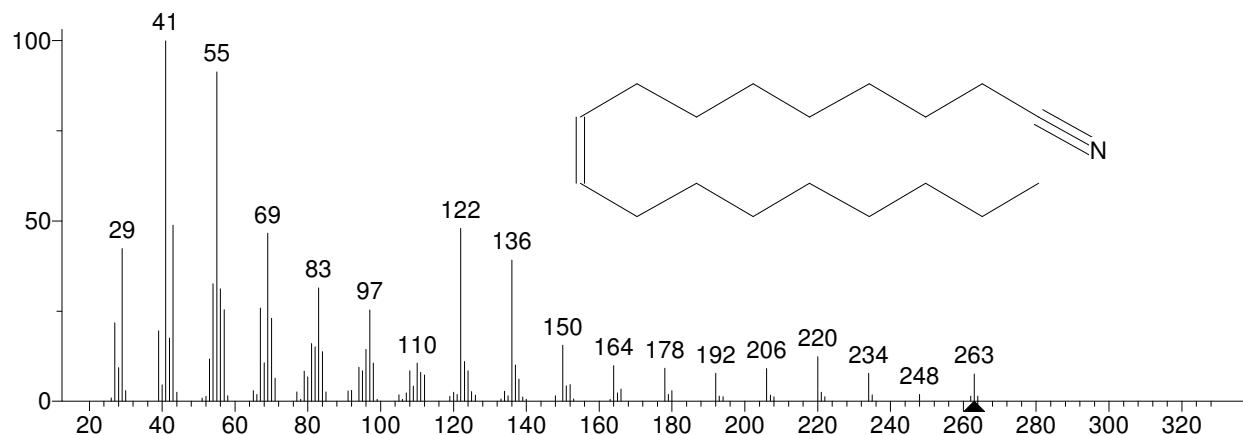


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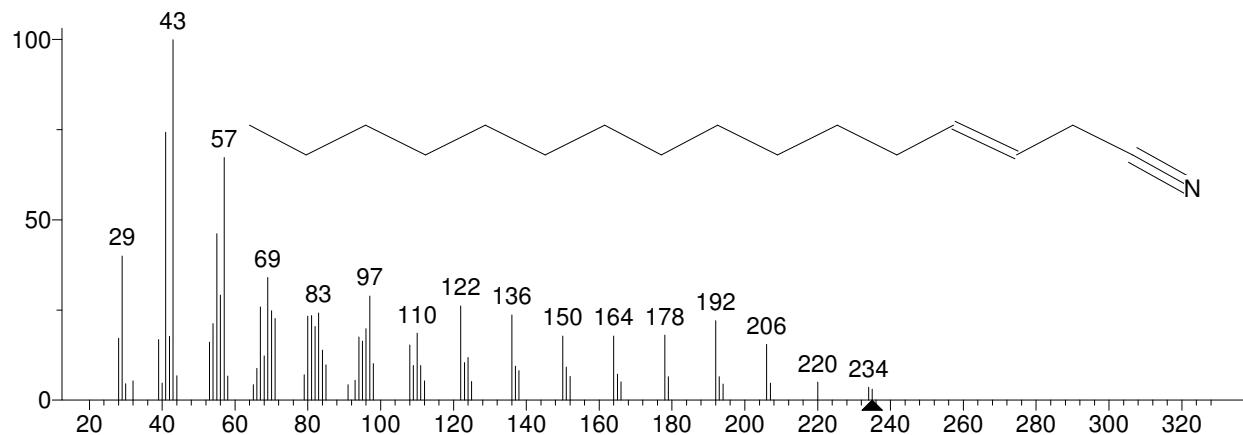
Unknown: Scan 1644 (18.795 min): J5169JO2.D
 Compound in Library Factor = -197



Hit 1 : Oleanitrile
 C18H33N; MF: 831; RMF: 878; Prob 59.2%; Lib: mainlib; ID: 2385.

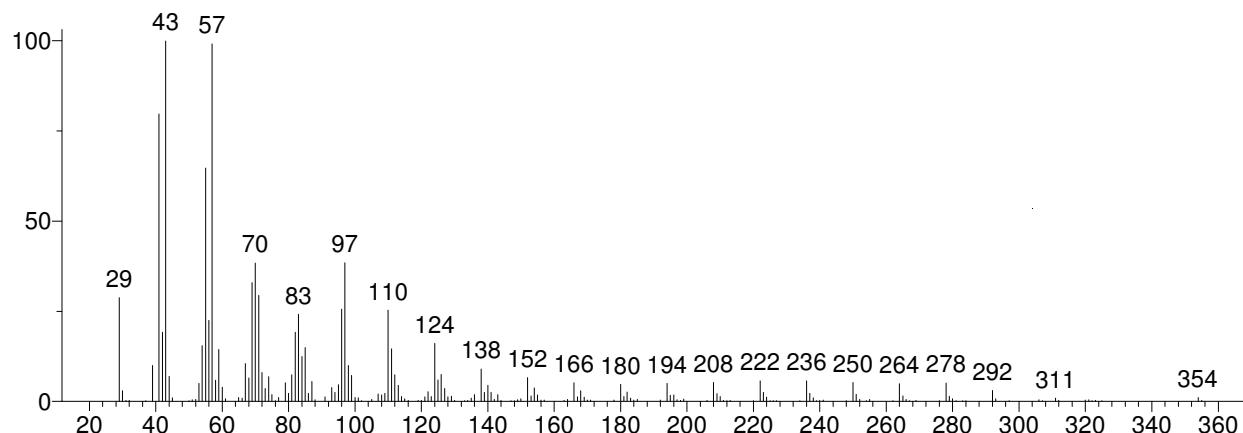


Hit 2 : Hexadecenenitrile
 C16H29N; MF: 773; RMF: 853; Prob 10.9%; CAS: 88592-11-4; Lib: mainlib; ID: 5511.

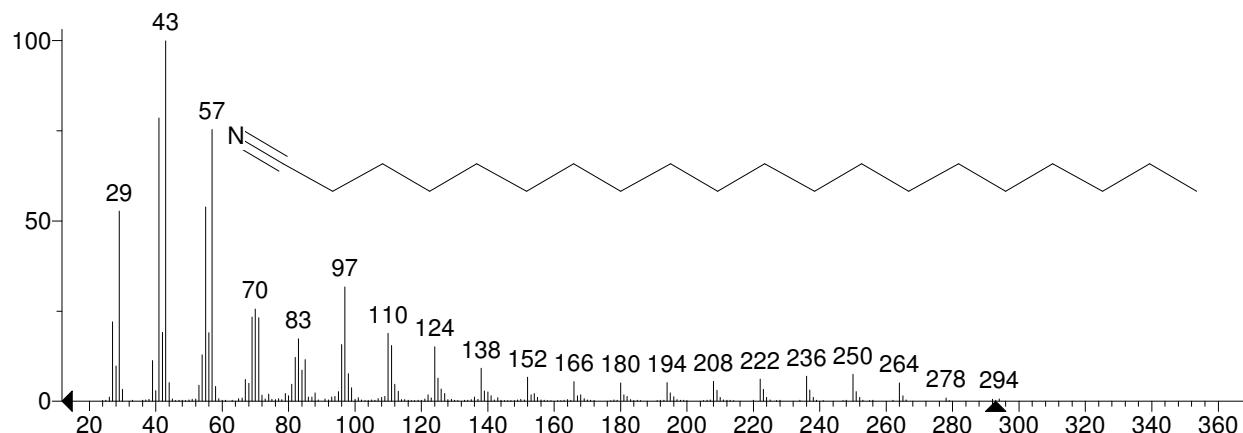


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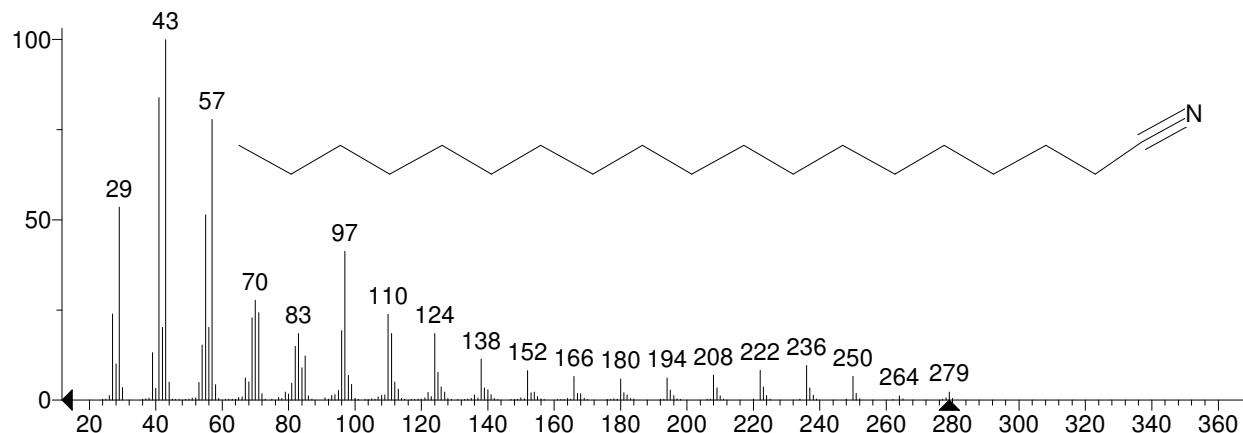
Unknown: Scan 1651 (18.875 min): J5169JO2.D
 Compound in Library Factor = -168



Hit 1 : Eicosanenitrile
 C₂₀H₃₉N; MF: 871; RMF: 879; Prob 49.4%; CAS: 4616-73-3; Lib: mainlib; ID: 5477.

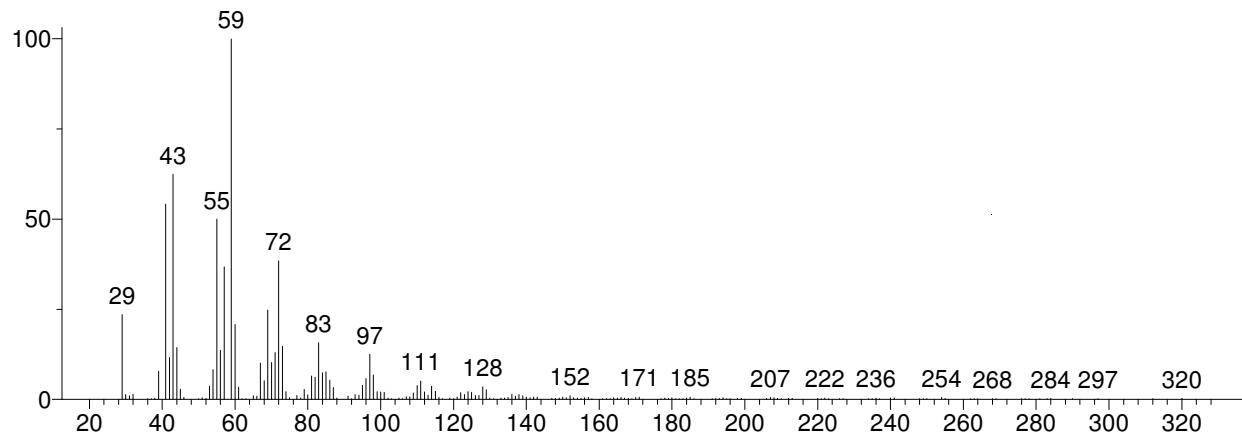


Hit 2 : Nonadecanenitrile
 C₁₉H₃₇N; MF: 854; RMF: 877; Prob 27.0%; CAS: 28623-46-3; Lib: replib; ID: 1685.

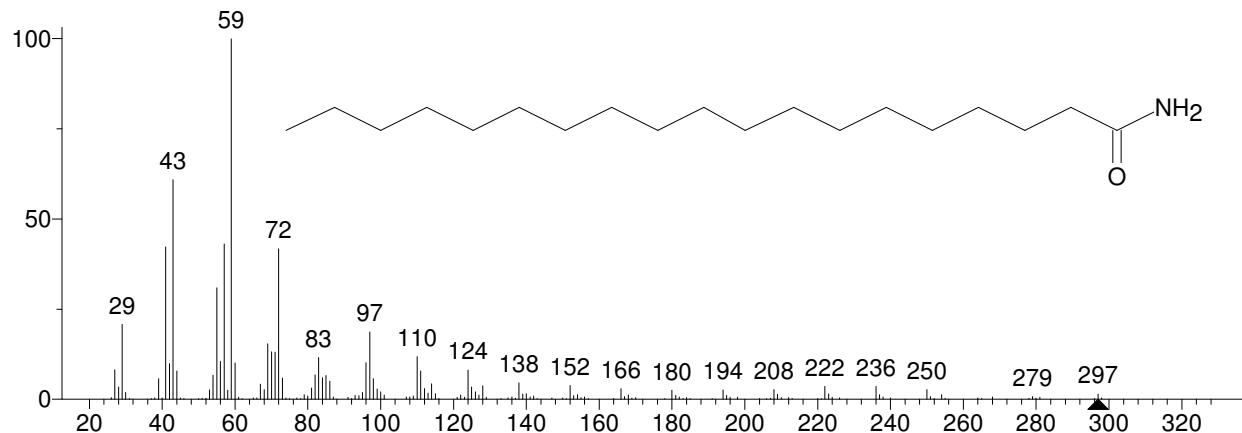


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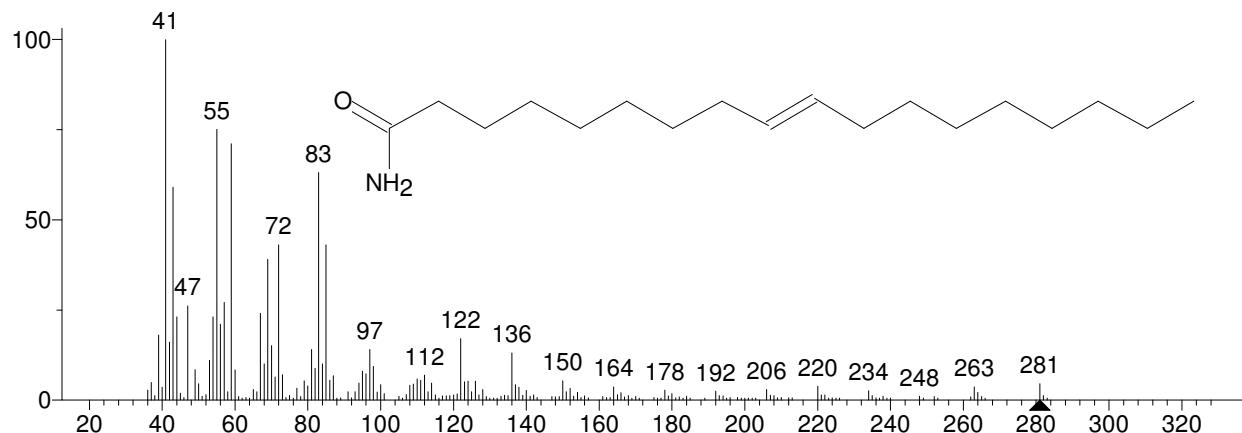
Unknown: Scan 1661 (18.989 min): J5169JO2.D
 Compound in Library Factor = -402



Hit 1 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 787; RMF: 799; Prob 35.1%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

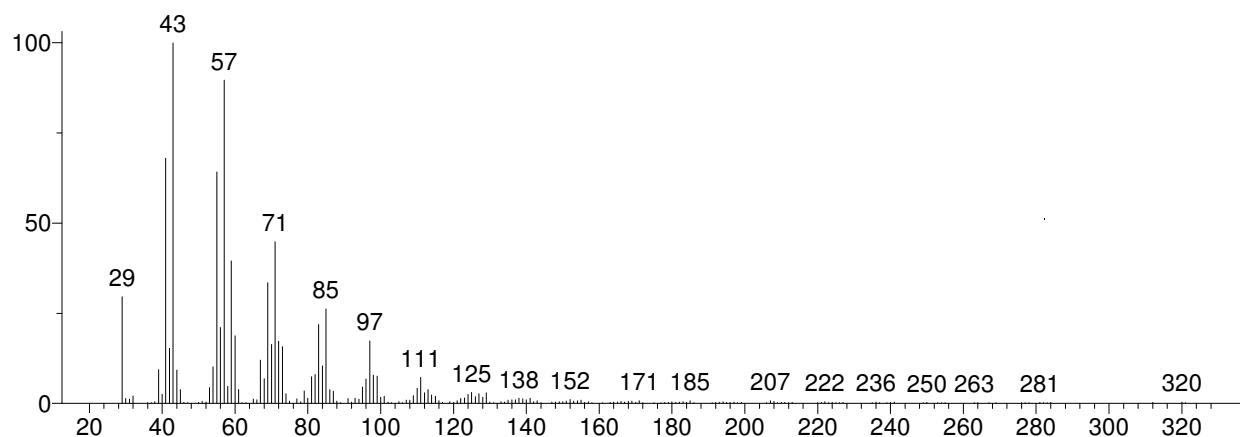


Hit 2 : 9-Octadecenamide
 $C_{18}H_{35}NO$; MF: 754; RMF: 758; Prob 9.17%; CAS: 3322-62-1; Lib: mainlib; ID: 2451.

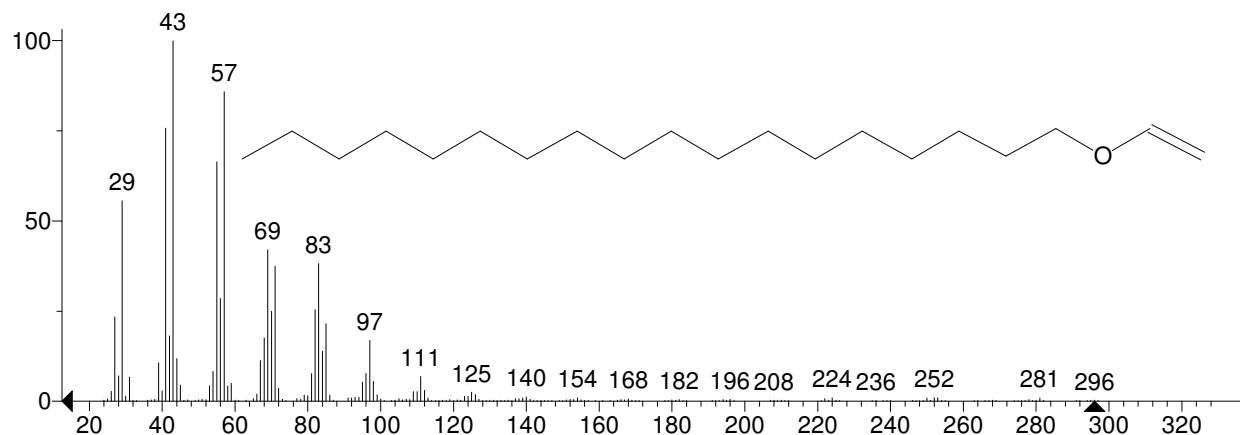


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Unknown: Scan 1675 (19.149 min): J5169JO2.D
 Compound in Library Factor = -509



Hit 1 : Octadecane, 1-(ethenylloxy)-
 C₂₀H₄₀O; MF: 792; RMF: 798; Prob 8.41%; CAS: 930-02-9; Lib: replib; ID: 2069.

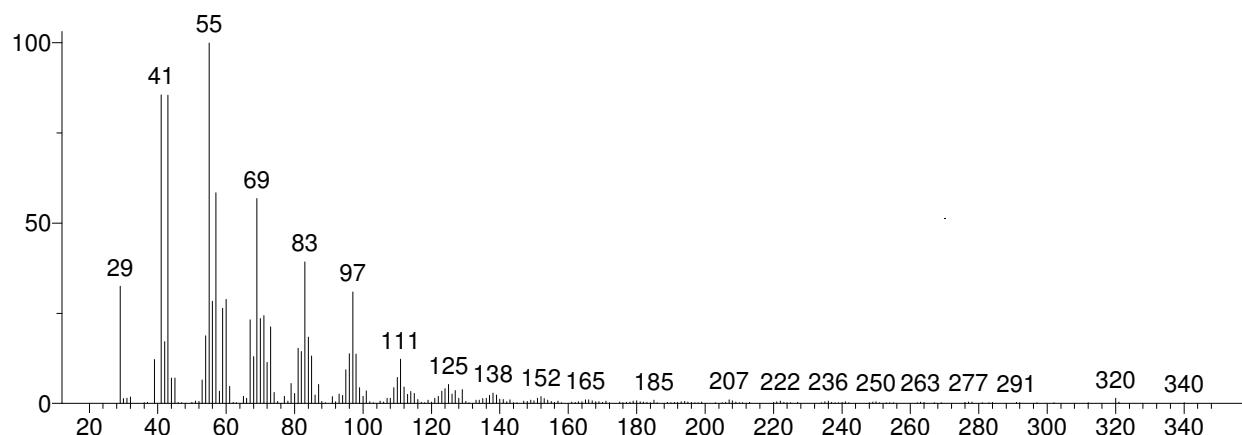


Hit 2 : 10-Undecenoic acid, octyl ester
 C₁₉H₃₆O₂; MF: 790; RMF: 804; Prob 7.76%; CAS: 28080-85-5; Lib: mainlib; ID: 2418.

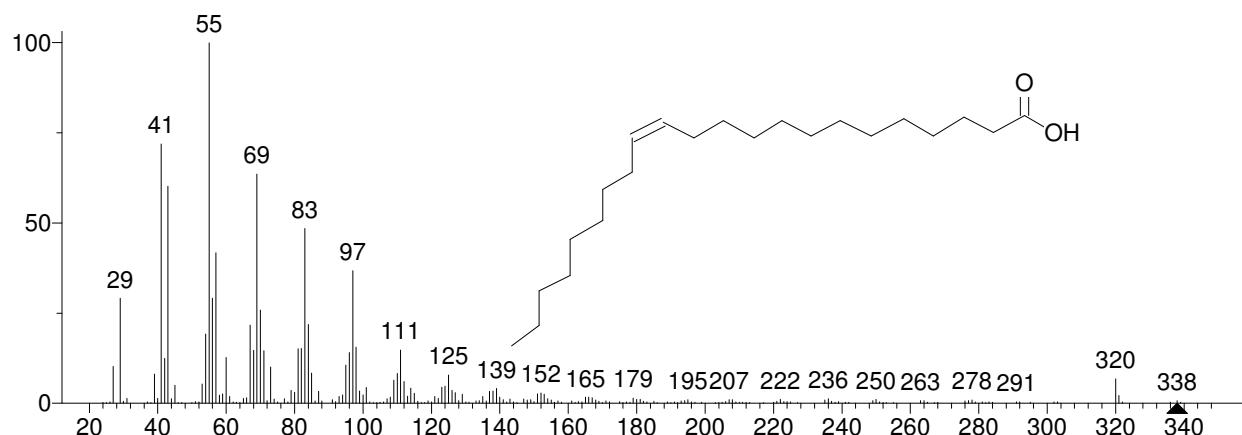


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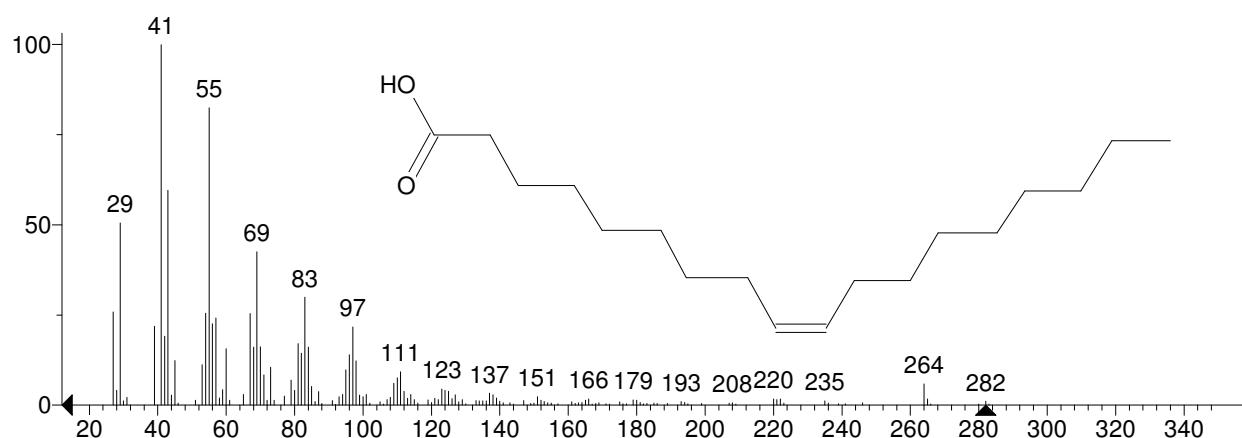
Unknown: Scan 1684 (19.252 min): J5169JO2.D
 Compound in Library Factor = -246



Hit 1 : Erucic acid
 $C_{22}H_{42}O_2$; MF: 864; RMF: 864; Prob 20.7%; CAS: 112-86-7; Lib: mainlib; ID: 16740.

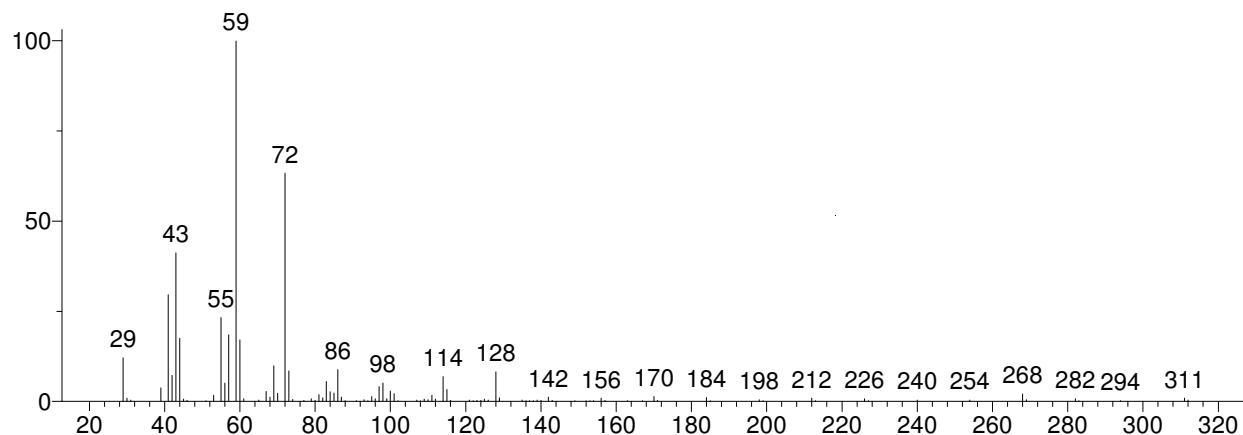


Hit 2 : Oleic Acid
 $C_{18}H_{34}O_2$; MF: 850; RMF: 865; Prob 13.0%; CAS: 112-80-1; Lib: replib; ID: 856.

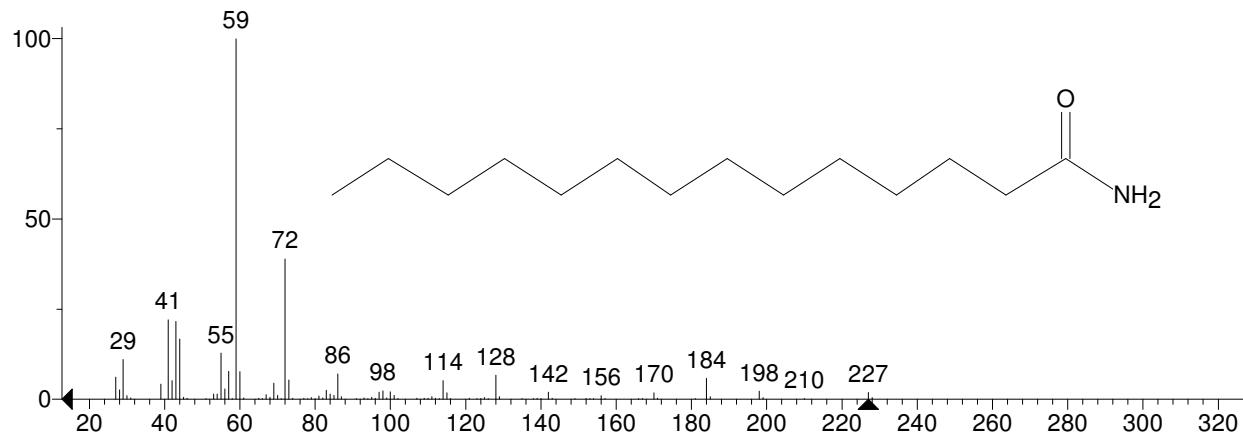


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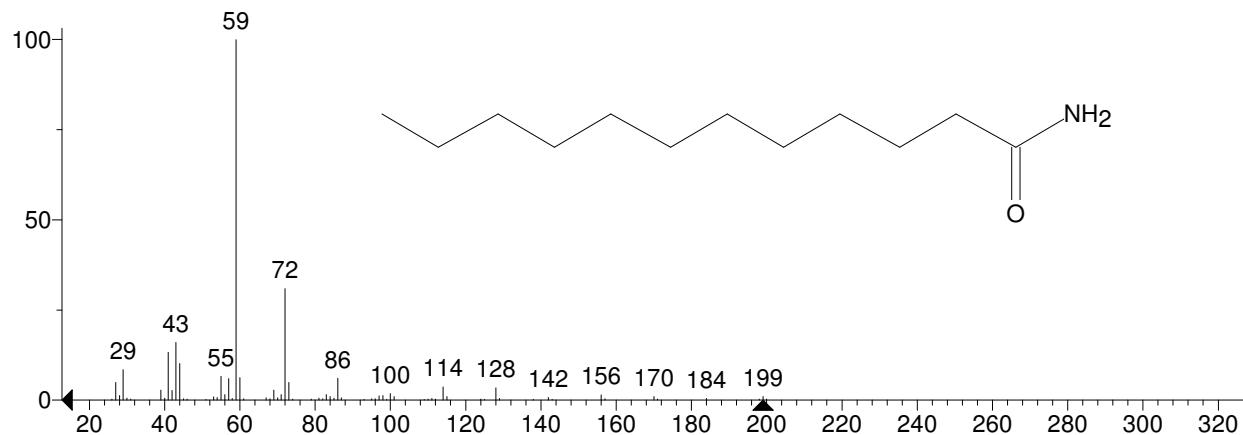
Unknown: Scan 1713 (19.583 min): J5169JO2.D
 Compound in Library Factor = -301



Hit 1 : Tetradecanamide
 $C_{14}H_{29}NO$; MF: 844; RMF: 871; Prob 60.4%; CAS: 638-58-4; Lib: mainlib; ID: 24922.

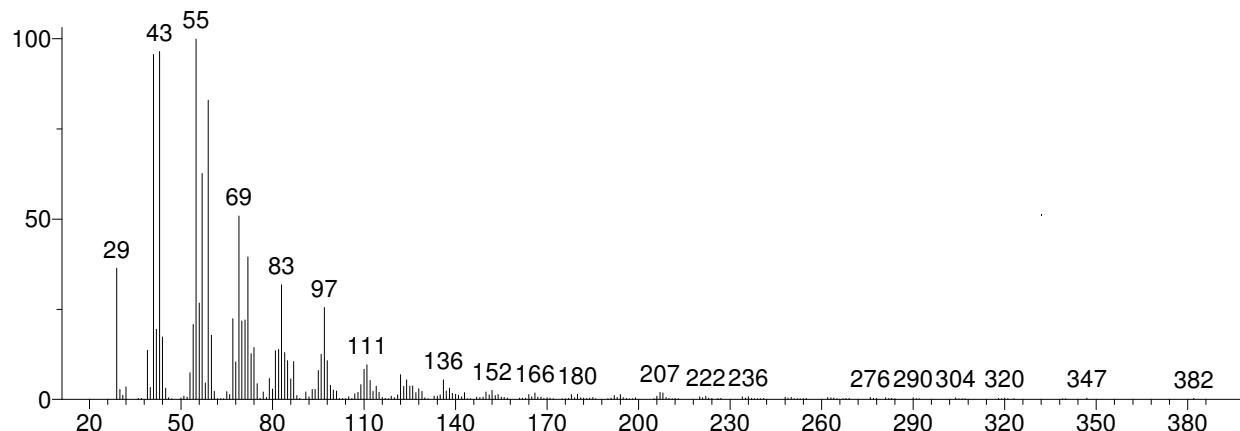


Hit 2 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 821; RMF: 855; Prob 22.0%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

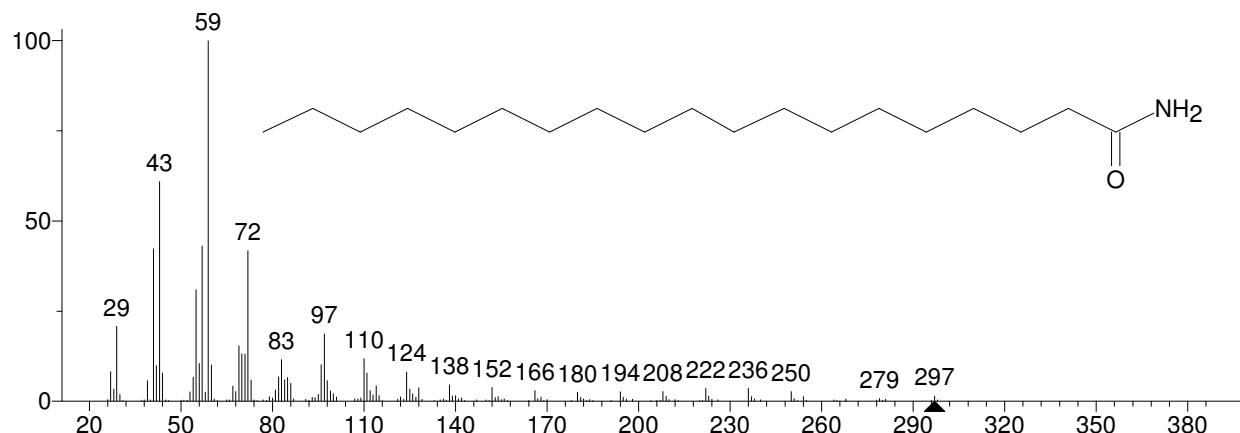


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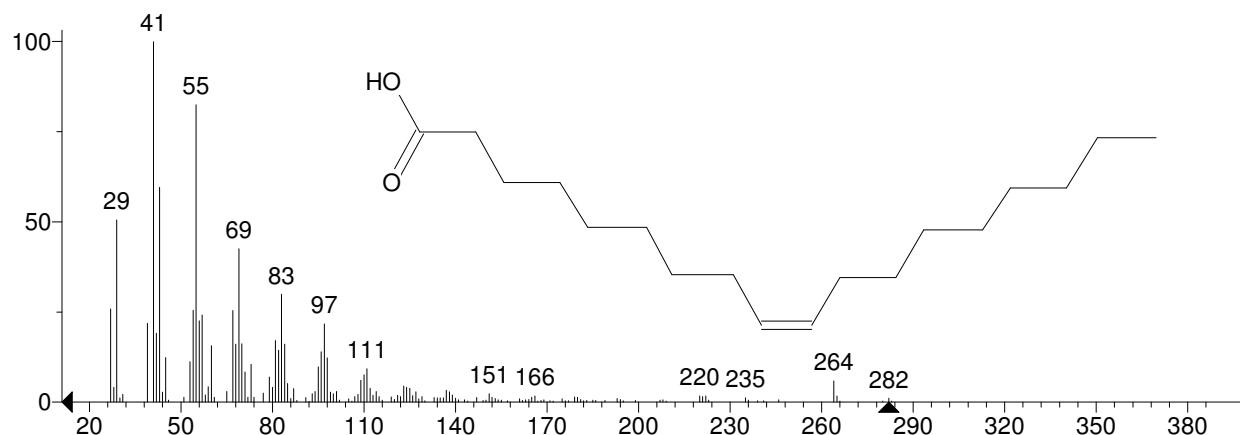
Unknown: Scan 1742 (19.914 min): J5169JO2.D
 Compound in Library Factor = -591



Hit 1 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 779; RMF: 808; Prob 13.0%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

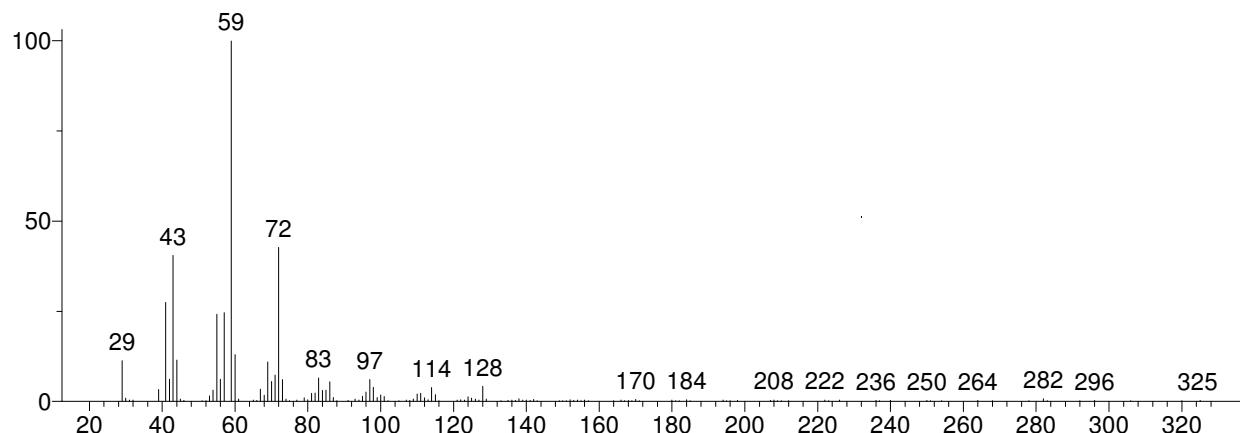


Hit 2 : Oleic Acid
 $C_{18}H_{34}O_2$; MF: 772; RMF: 796; Prob 9.98%; CAS: 112-80-1; Lib: replib; ID: 856.

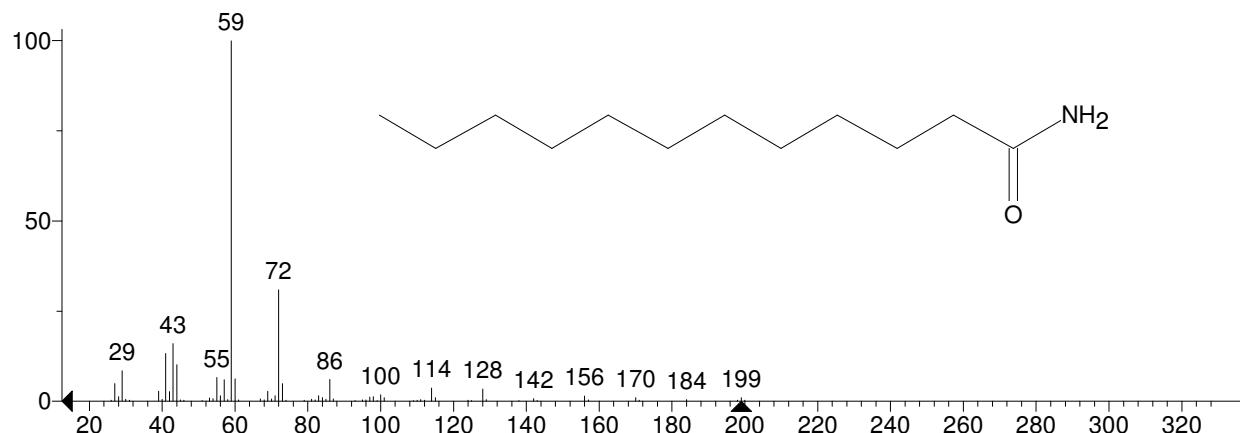


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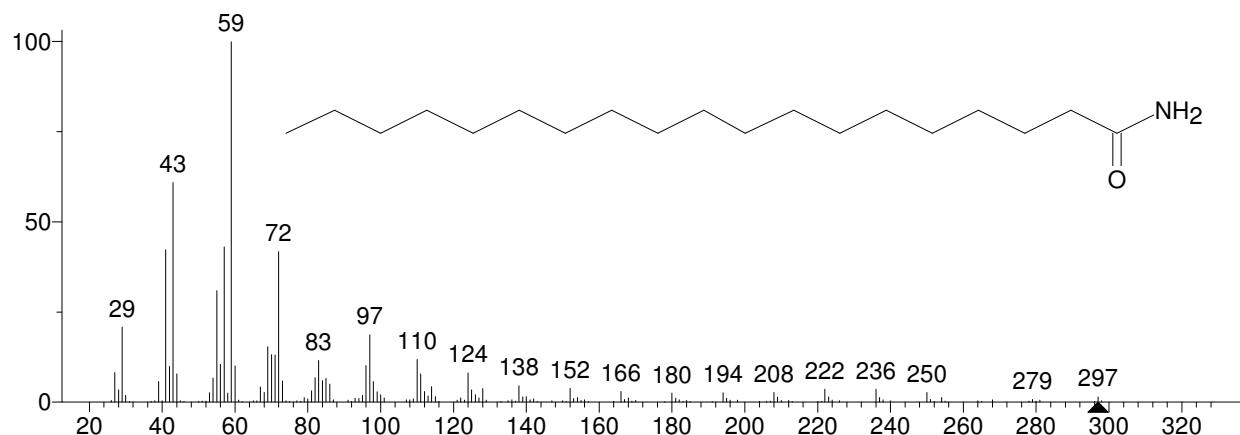
Unknown: Scan 1748 (19.982 min): J5169JO2.D
 Compound in Library Factor = -457



Hit 1 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 809; RMF: 843; Prob 38.2%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

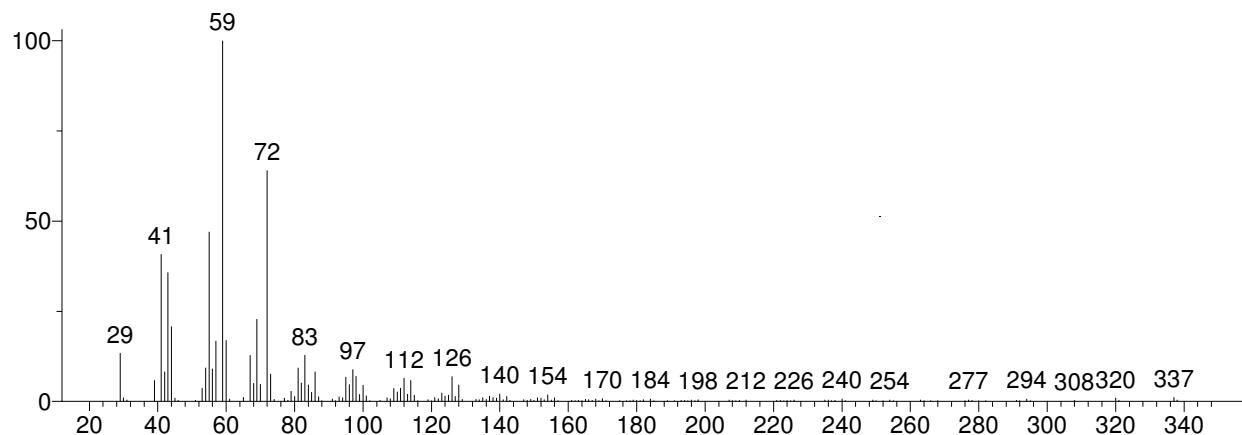


Hit 2 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 788; RMF: 792; Prob 16.3%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

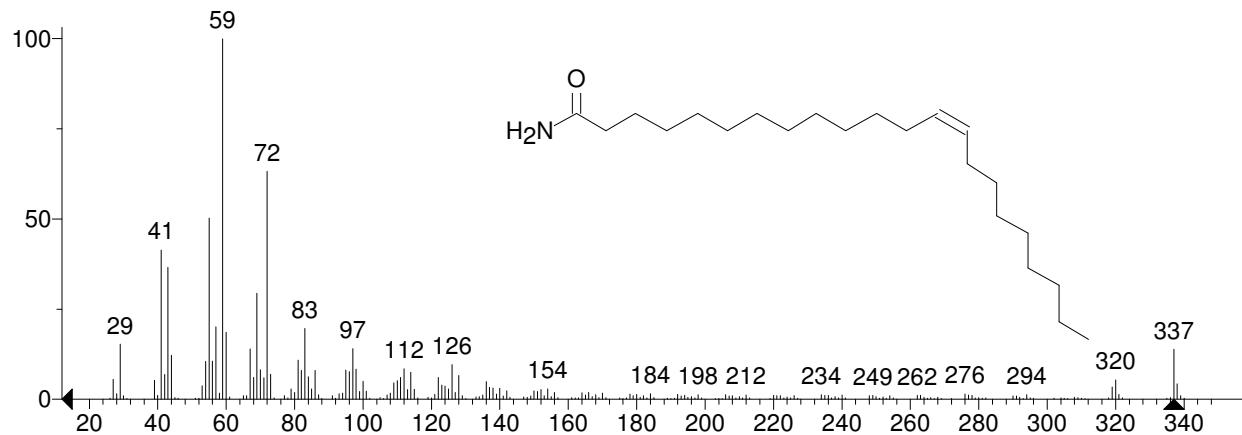


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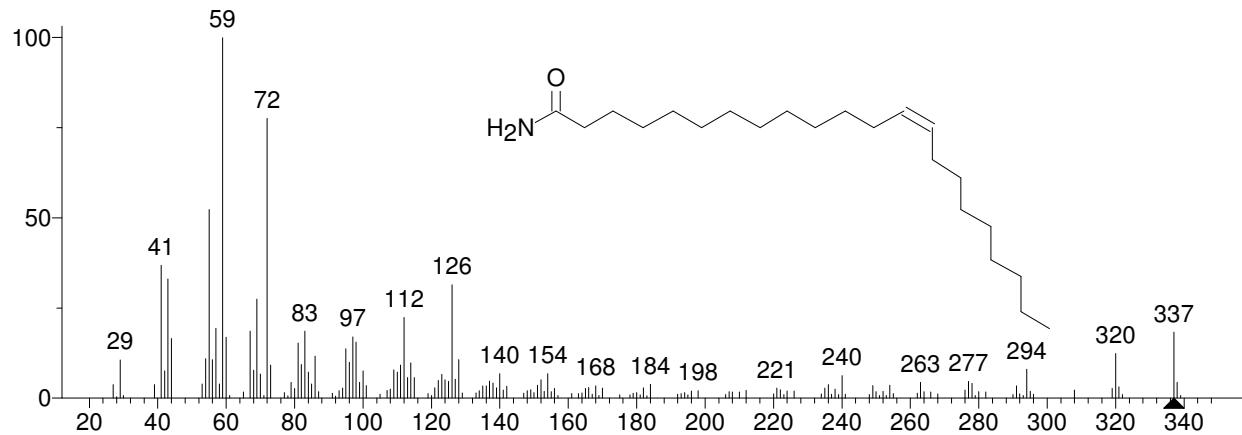
Unknown: Scan 1791 (20.473 min): J5169JO2.D
 Compound in Library Factor = -175



Hit 1 : 13-Docosenamide, (Z)-
 C₂₂H₄₃NO; MF: 826; RMF: 826; Prob 48.1%; CAS: 112-84-5; Lib: replib; ID: 6556.

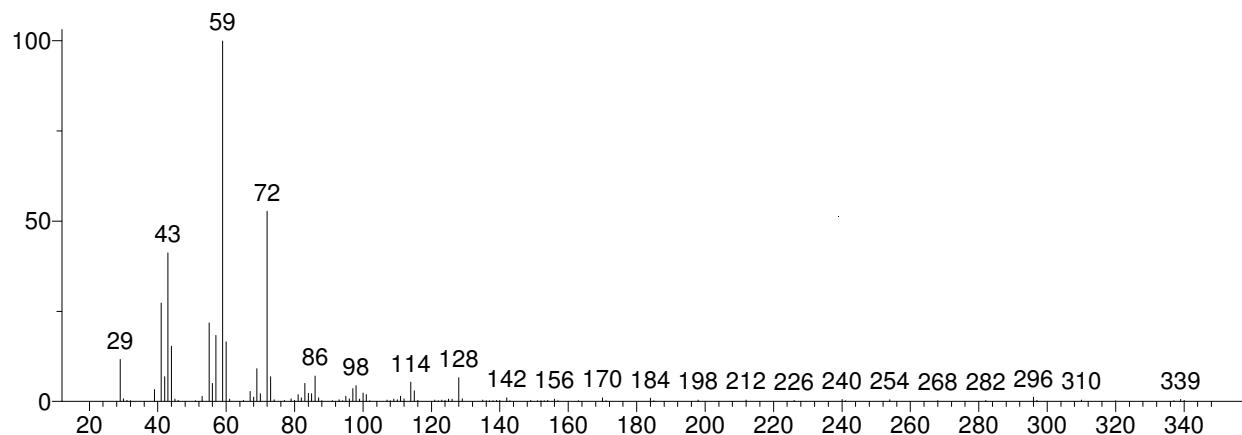


Hit 2 : 13-Docosenamide, (Z)-
 C₂₂H₄₃NO; MF: 812; RMF: 814; Prob 48.1%; CAS: 112-84-5; Lib: mainlib; ID: 24934.

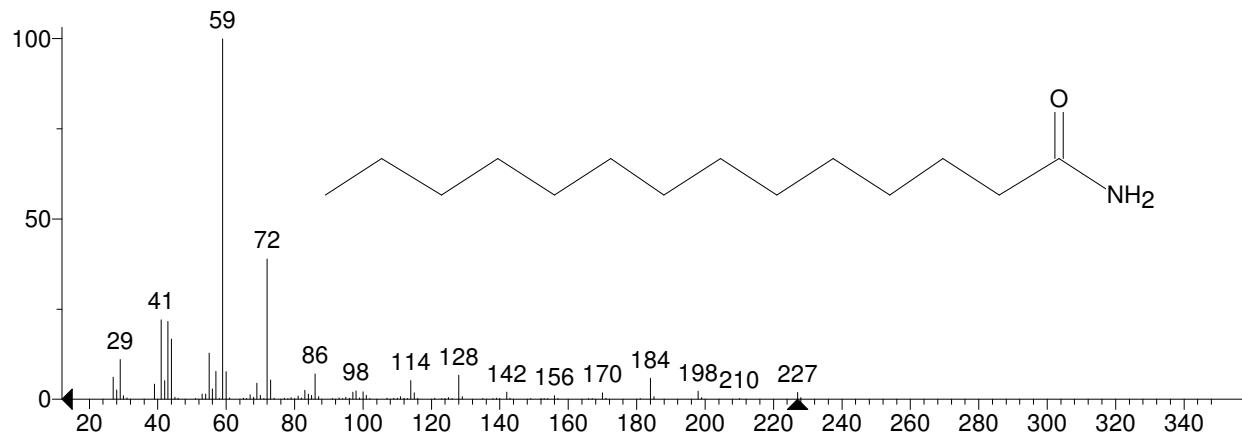


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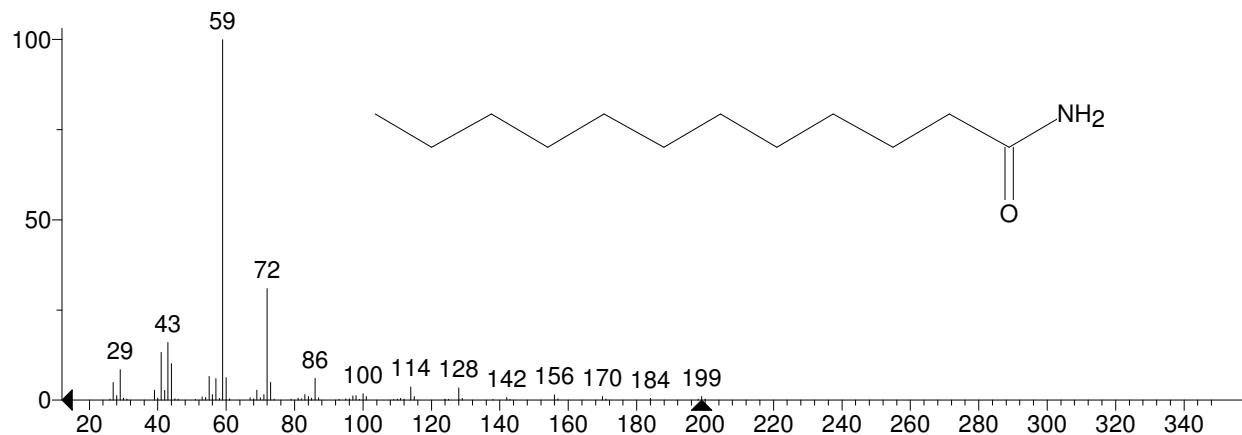
Unknown: Scan 1816 (20.759 min): J5169JO2.D
 Compound in Library Factor = -229



Hit 1 : Tetradecanamide
 $C_{14}H_{29}NO$; MF: 835; RMF: 855; Prob 42.7%; CAS: 638-58-4; Lib: mainlib; ID: 24922.

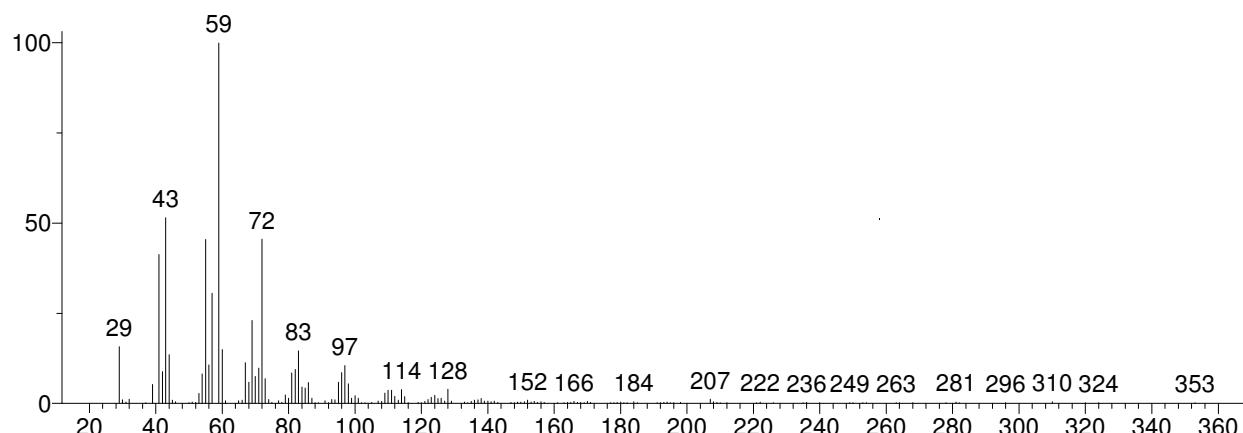


Hit 2 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 828; RMF: 857; Prob 32.7%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

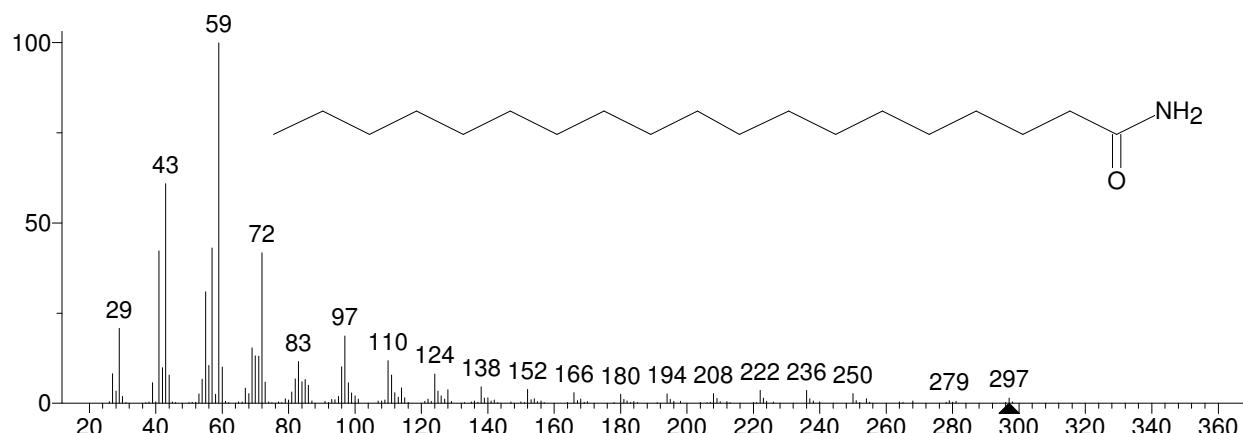


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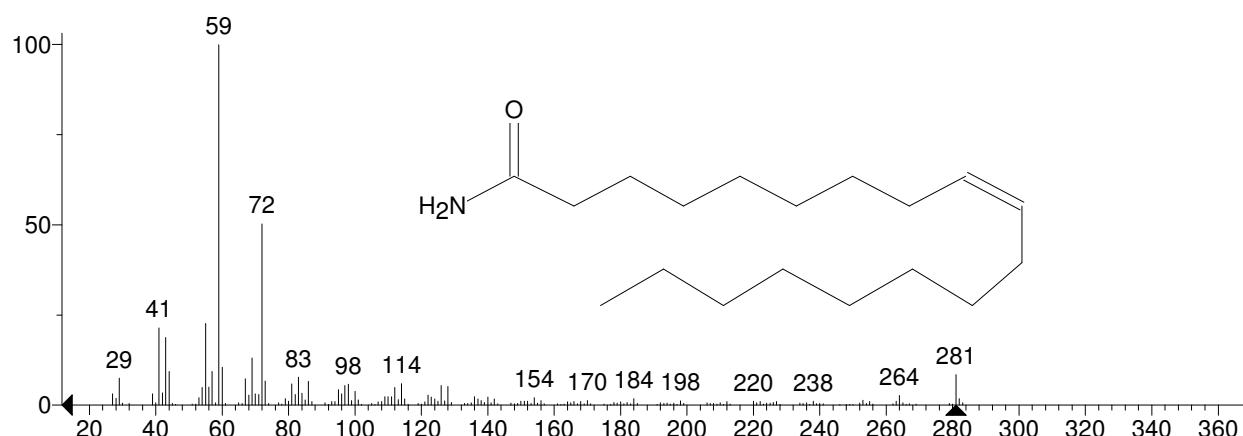
Unknown: Scan 1849 (21.135 min): J5169JO2.D
 Compound in Library Factor = -394



Hit 1 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 791; RMF: 797; Prob 31.2%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

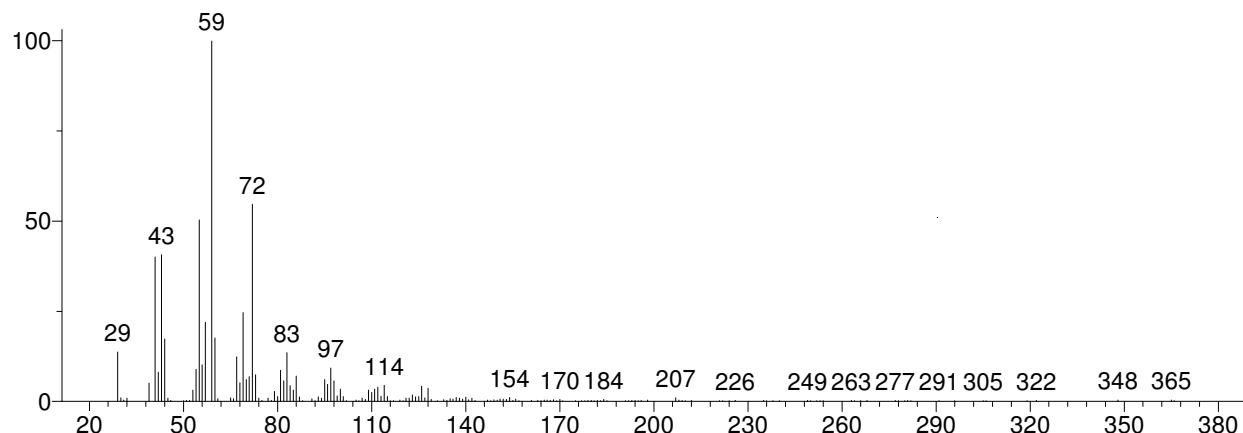


Hit 2 : 9-Octadecenamide, (Z)-
 $C_{18}H_{35}NO$; MF: 781; RMF: 782; Prob 22.0%; CAS: 301-02-0; Lib: mainlib; ID: 24937.

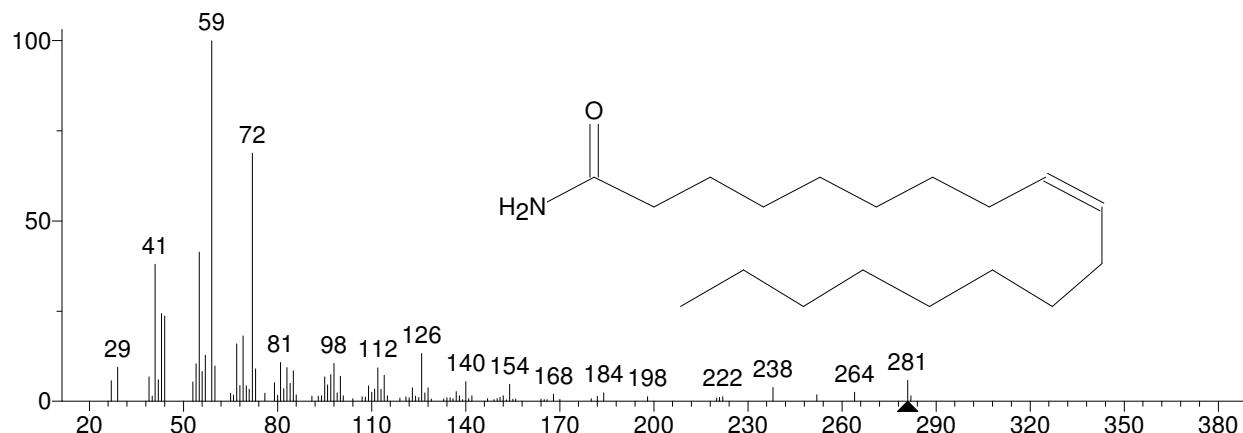


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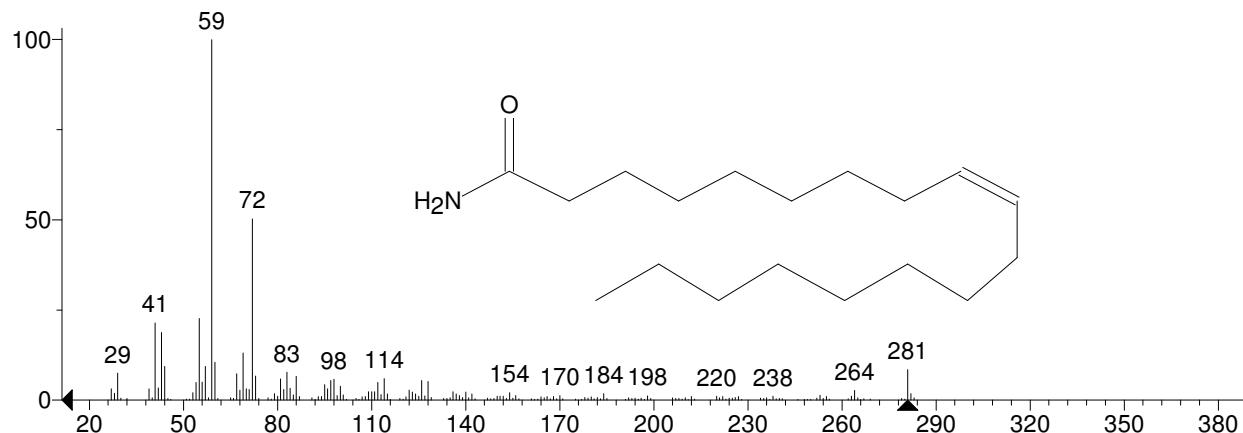
Unknown: Scan 1889 (21.592 min): J5169JO2.D
 Compound in Library Factor = -388



Hit 1 : 9-Octadecenamide, (Z)-
 C18H35NO; MF: 803; RMF: 823; Prob 42.4%; CAS: 301-02-0; Lib: replib; ID: 6559.

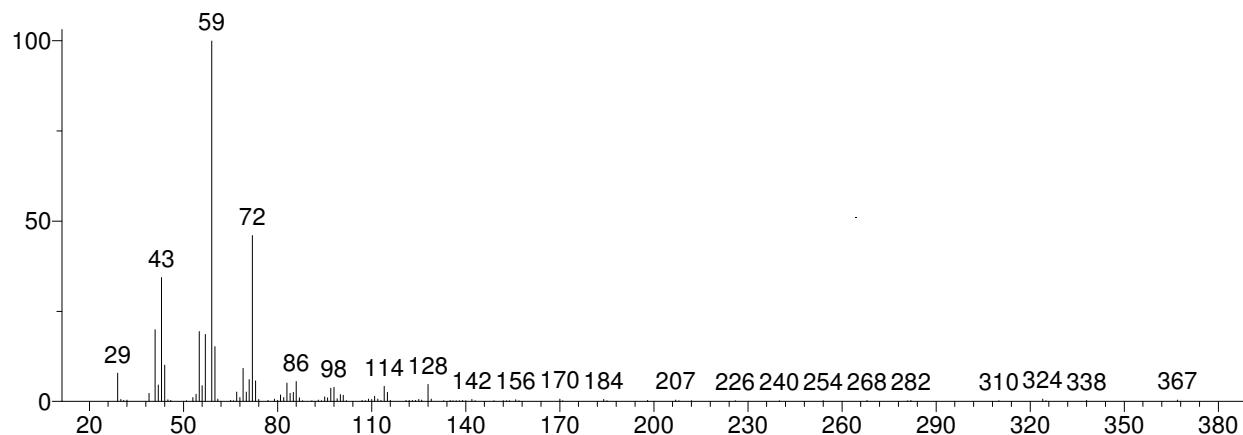


Hit 2 : 9-Octadecenamide, (Z)-
 C18H35NO; MF: 792; RMF: 796; Prob 42.4%; CAS: 301-02-0; Lib: mainlib; ID: 24937.

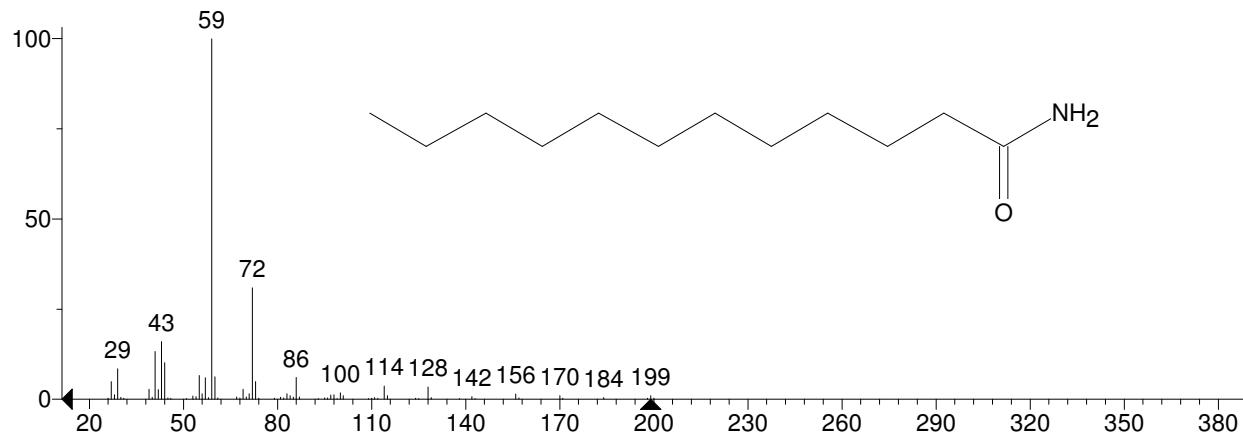


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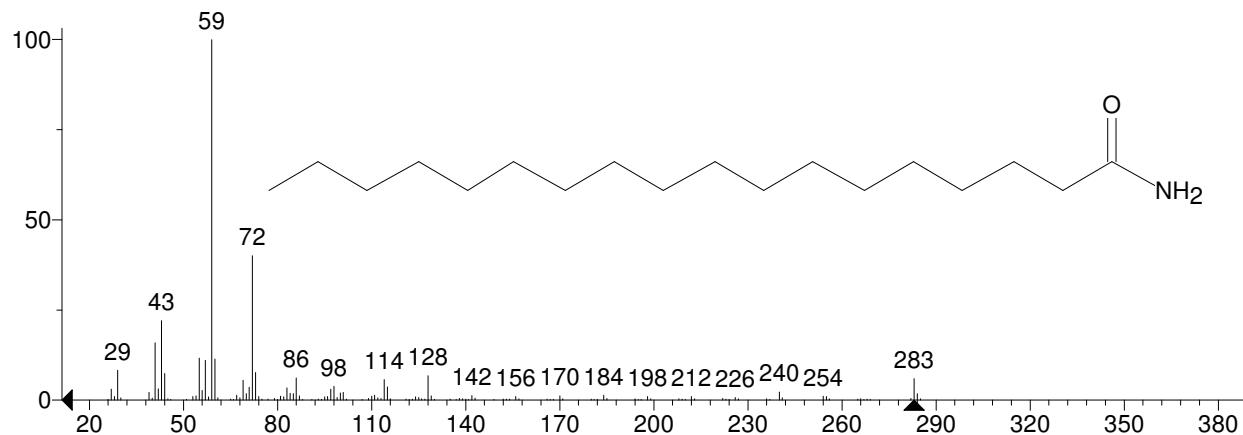
Unknown: Scan 1896 (21.672 min): J5169JO2.D
 Compound in Library Factor = -211



Hit 1 : Dodecanamide
 $C_{12}H_{25}NO$; MF: 850; RMF: 868; Prob 55.8%; CAS: 1120-16-7; Lib: mainlib; ID: 24927.

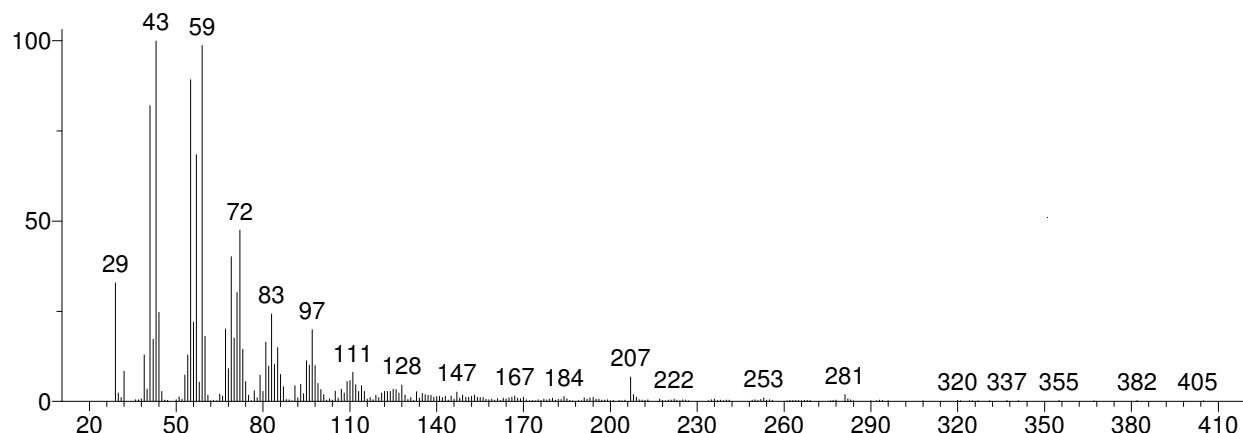


Hit 2 : Octadecanamide
 $C_{18}H_{37}NO$; MF: 813; RMF: 822; Prob 13.6%; CAS: 124-26-5; Lib: mainlib; ID: 24926.

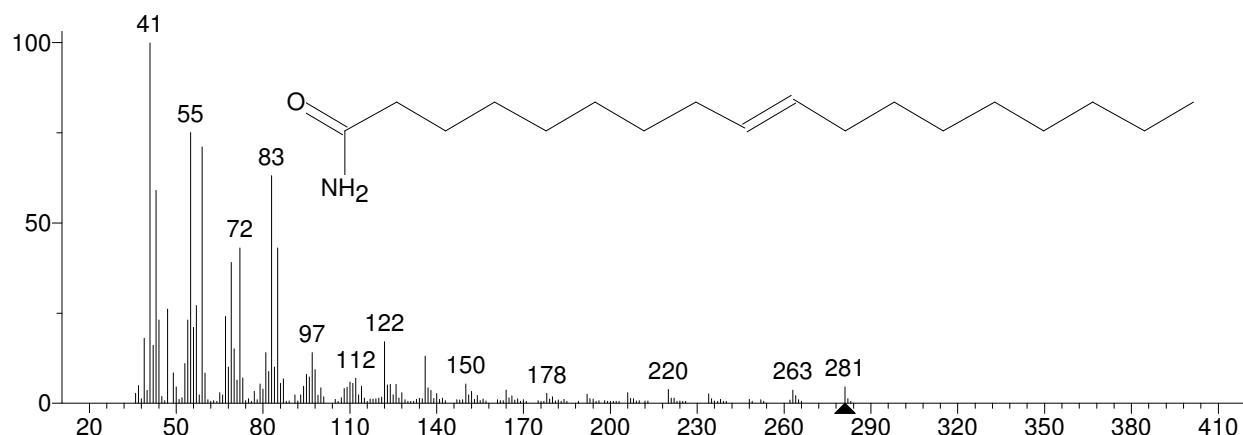


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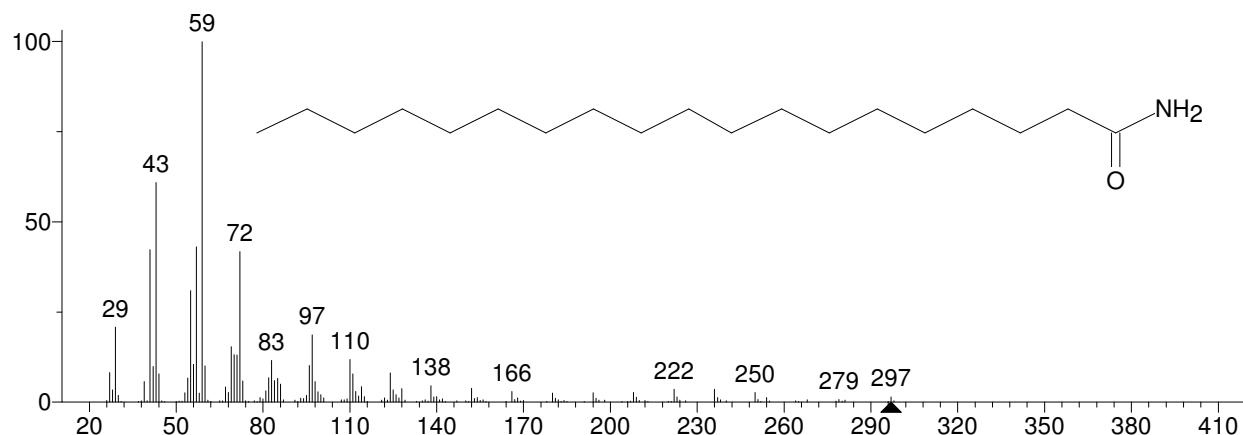
Unknown: Scan 1918 (21.923 min): J5169JO2.D
 Compound in Library Factor = -570



Hit 1 : 9-Octadecenamide
 $C_{18}H_{35}NO$; MF: 764; RMF: 778; Prob 32.2%; CAS: 3322-62-1; Lib: mainlib; ID: 2451.

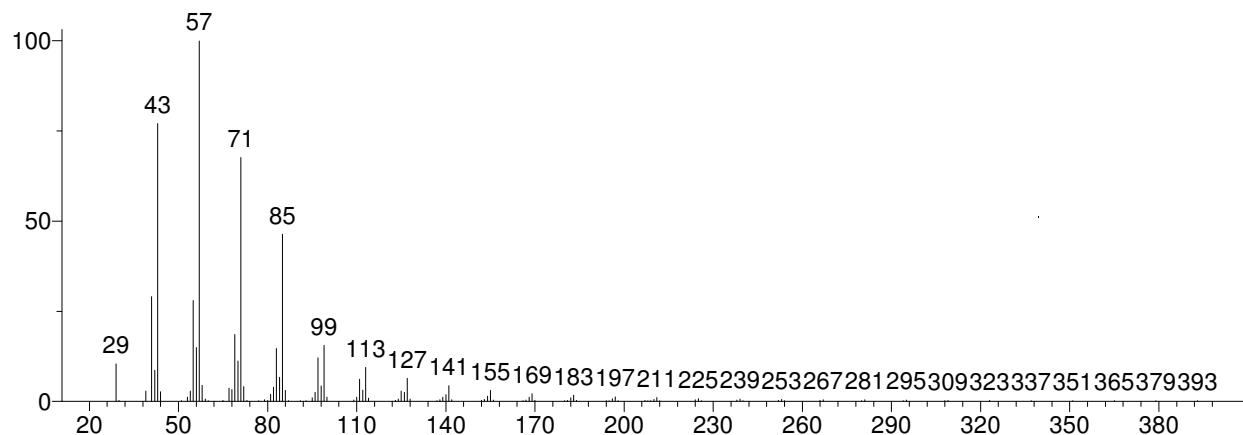


Hit 2 : Nonadecanamide
 $C_{19}H_{39}NO$; MF: 744; RMF: 785; Prob 14.7%; CAS: 58185-32-3; Lib: mainlib; ID: 24635.

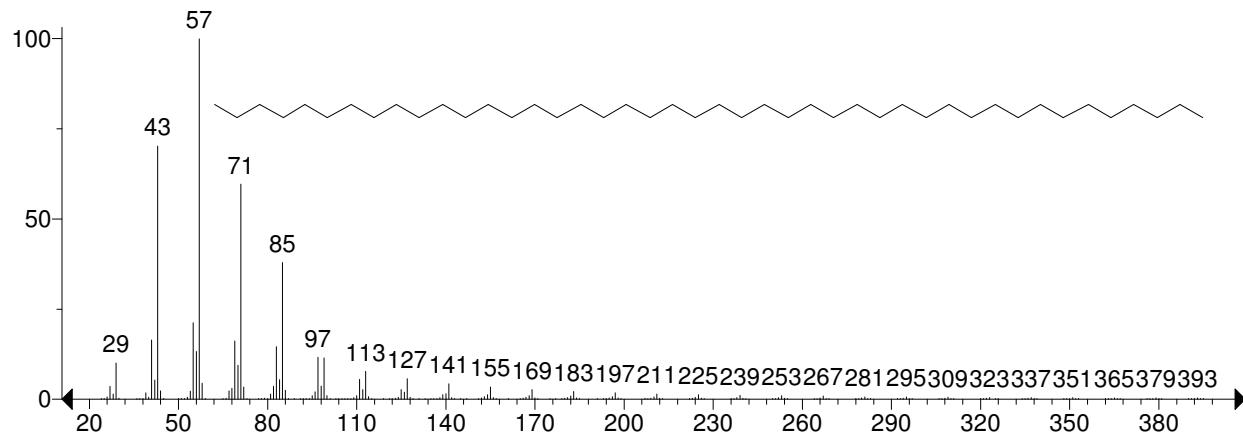


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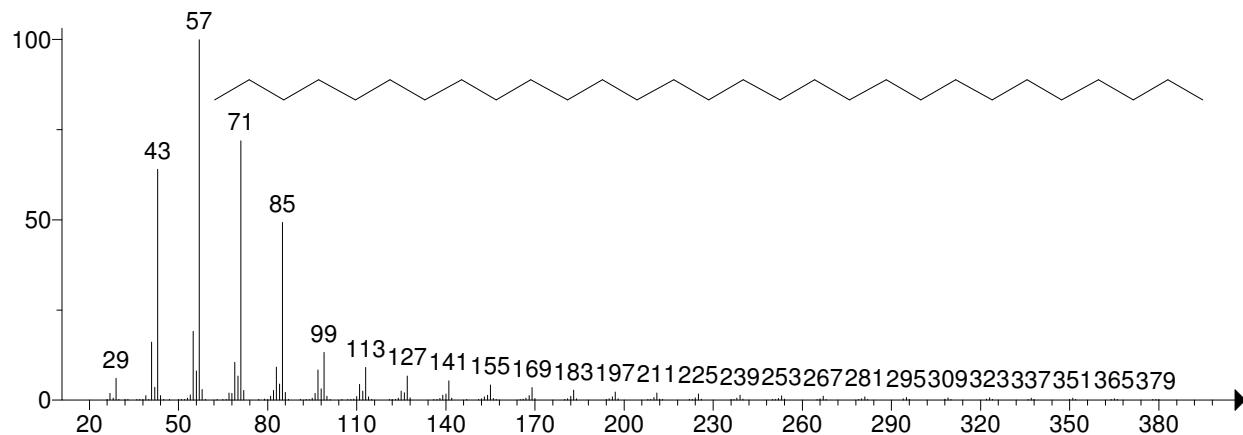
Unknown: Scan 1985 (22.688 min): J5169JO2.D
 Compound in Library Factor = -117



Hit 1 : Tetratetracontane
 C44H90; MF: 922; RMF: 922; Prob 9.61%; CAS: 7098-22-8; Lib: mainlib; ID: 20872.

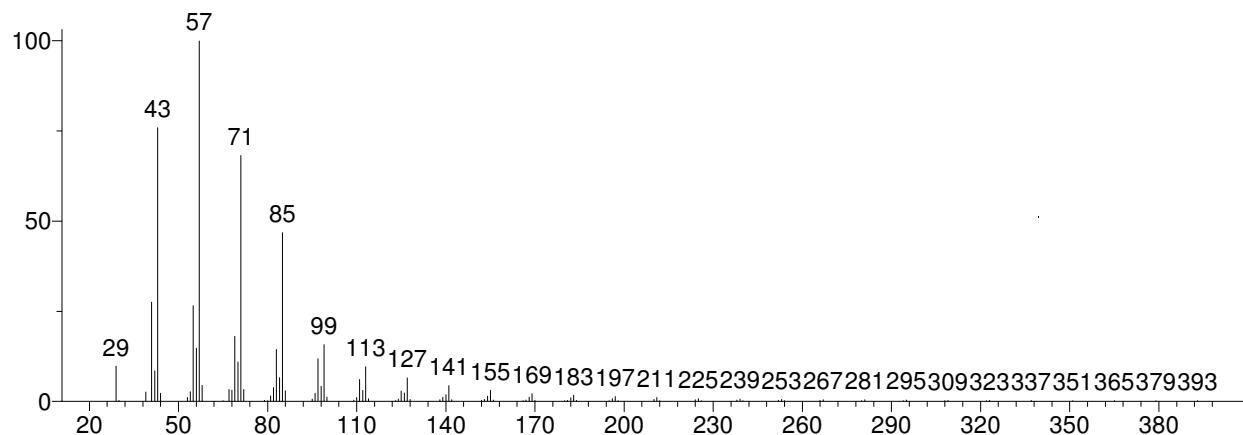


Hit 2 : Nonacosane
 C29H60; MF: 916; RMF: 917; Prob 7.55%; CAS: 630-03-5; Lib: replib; ID: 5696.

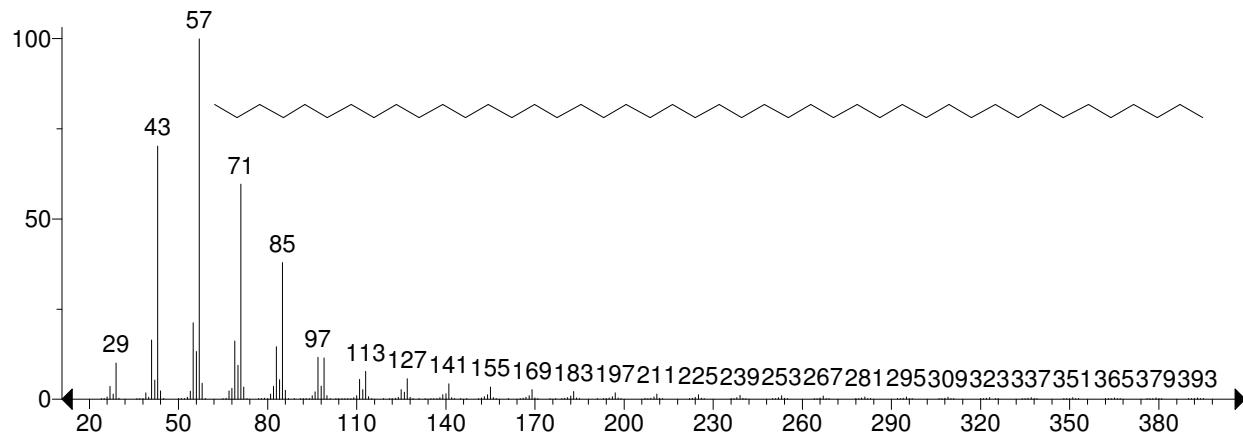


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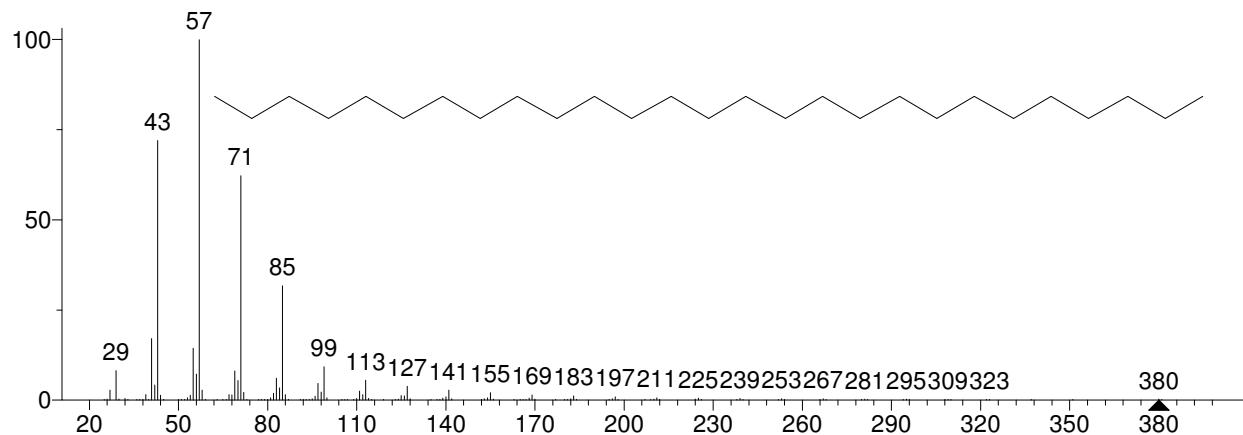
Unknown: Scan 1985 (22.688 min): J5169JO2.D
Compound in Library Factor = -161



Hit 1 : Tetratetracontane
C44H90; MF: 923; RMF: 923; Prob 9.79%; CAS: 7098-22-8; Lib: mainlib; ID: 20872.

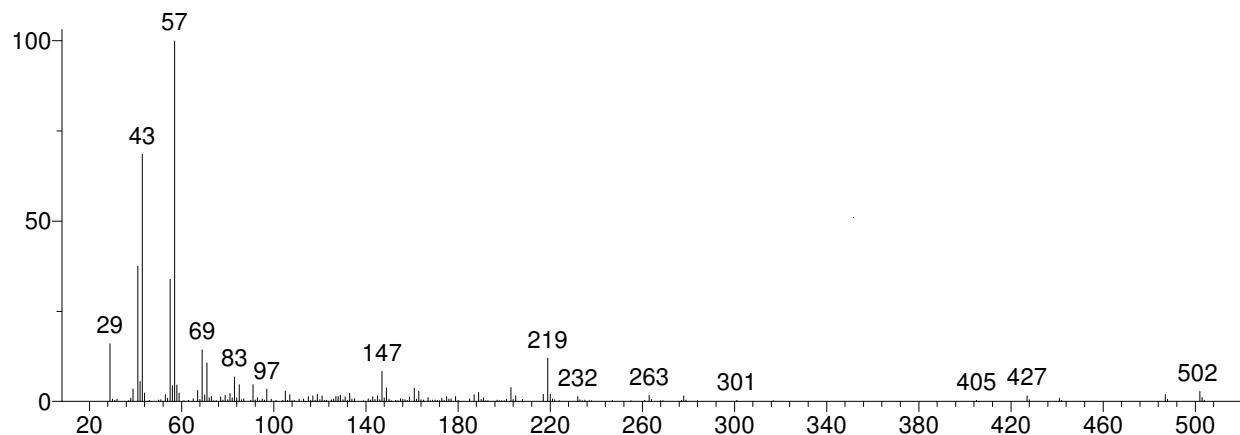


Hit 2 : Heptacosane
C27H56; MF: 917; RMF: 918; Prob 7.69%; CAS: 593-49-7; Lib: replib; ID: 5462.

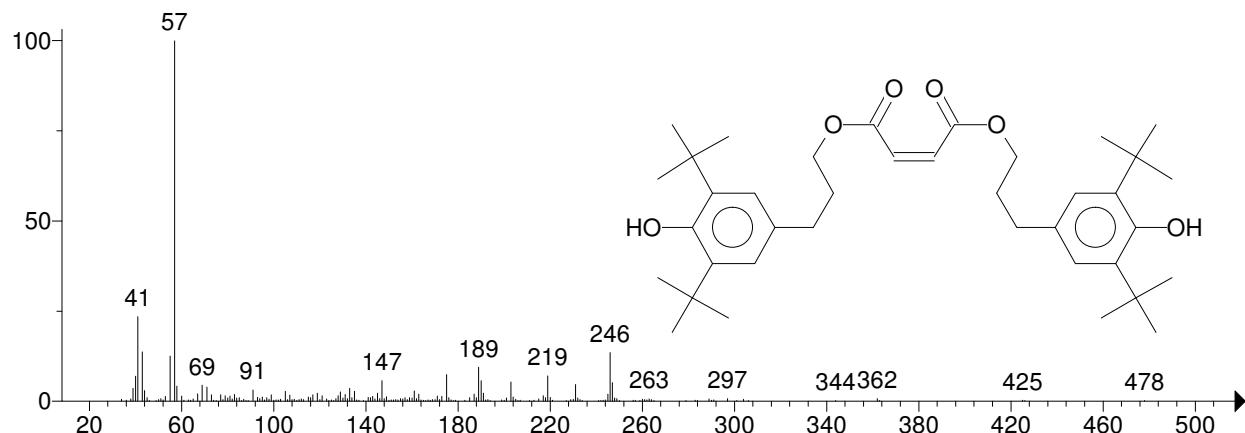


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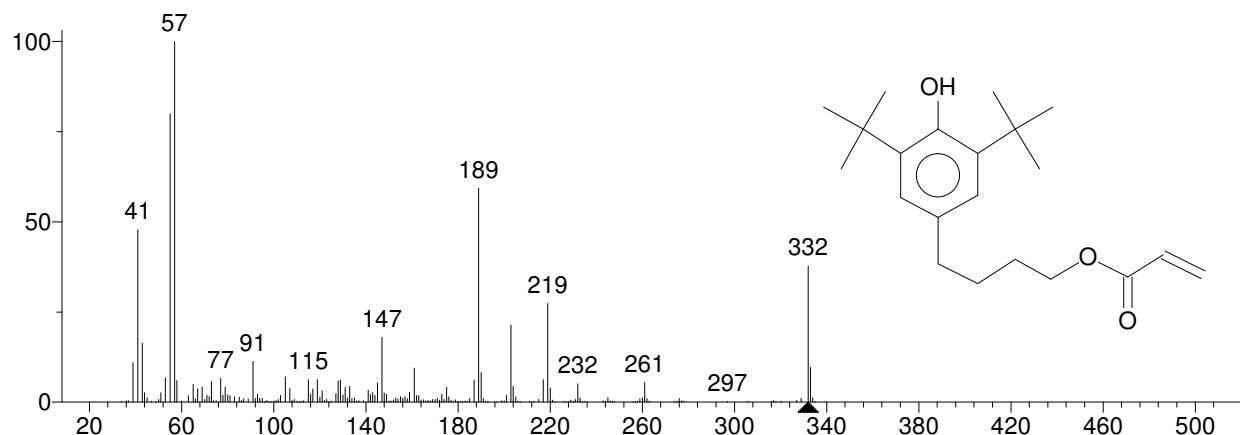
Unknown: Scan 2139 (24.446 min): J5169JO2.D
 Compound in Library Factor = -1187



Hit 1 : Bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propyl] maleate
 C₃₈H₅₆O₆; MF: 616; RMF: 675; Prob 20.6%; Lib: mainlib; ID: 20093.

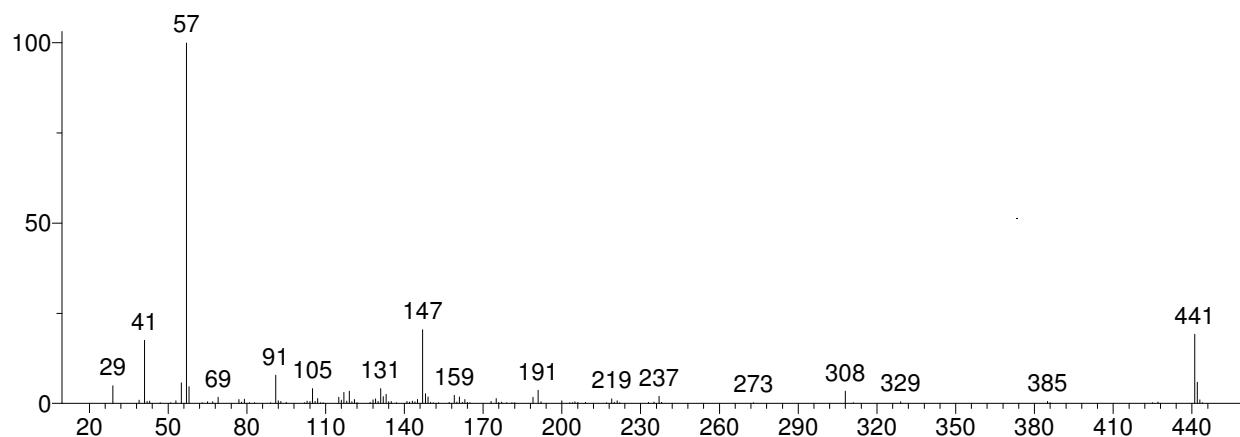


Hit 2 : 4-(3,5-Di-tert-butyl-4-hydroxyphenyl)butyl acrylate
 C₂₁H₃₂O₃; MF: 593; RMF: 643; Prob 7.53%; CAS: 87033-84-9; Lib: mainlib; ID: 21235.

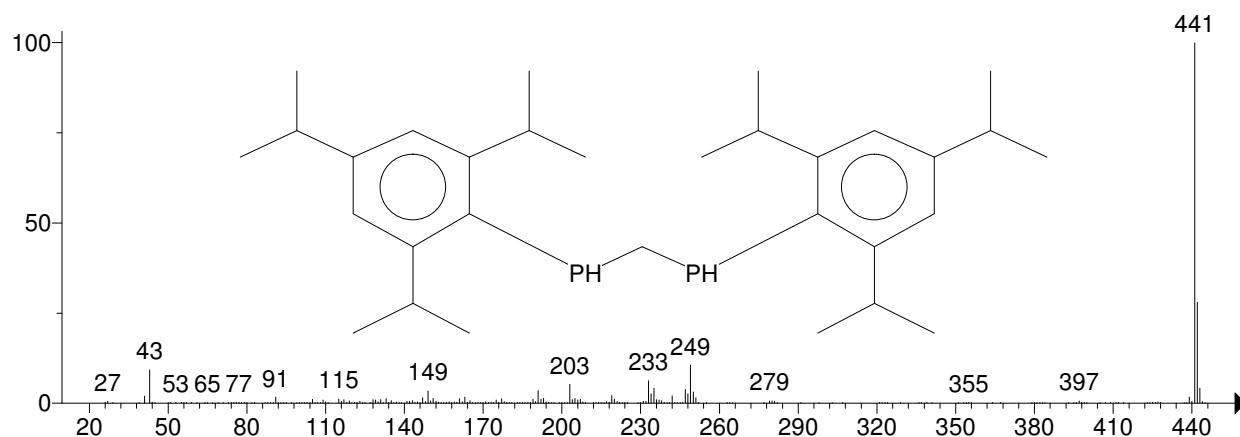


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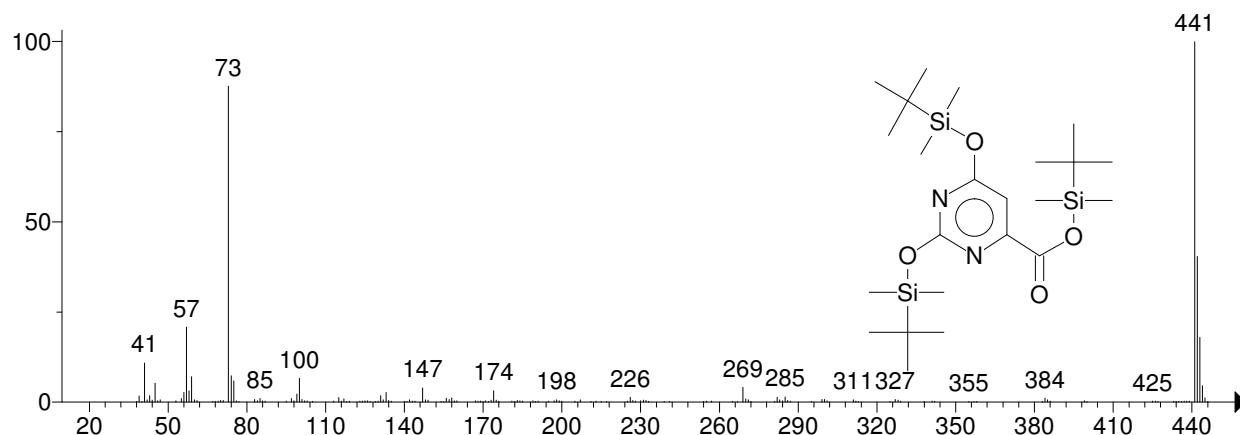
Unknown: Scan 2170 (24.800 min): J5169JO2.D
 Compound in Library Factor = -1275



Hit 1 : Methylenebis(2,4,6-triisopropylphenylphosphine)
 C₃₁H₅₀P₂; MF: 545; RMF: 626; Prob 45.7%; Lib: mainlib; ID: 161561.

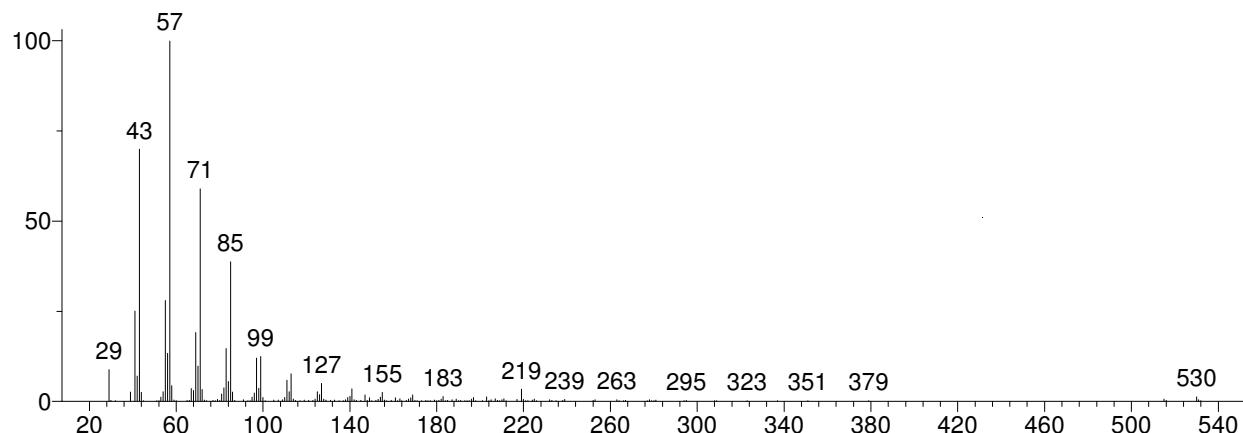


Hit 2 : 4-Pyrimidinecarboxylic acid, 2,6-bis[(tert-butyldimethylsilyl)oxy]-, tert-butyldimethylsilyl ester
 C₂₃H₄₆N₂O₄Si₃; MF: 510; RMF: 552; Prob 11.5%; Lib: mainlib; ID: 161552.

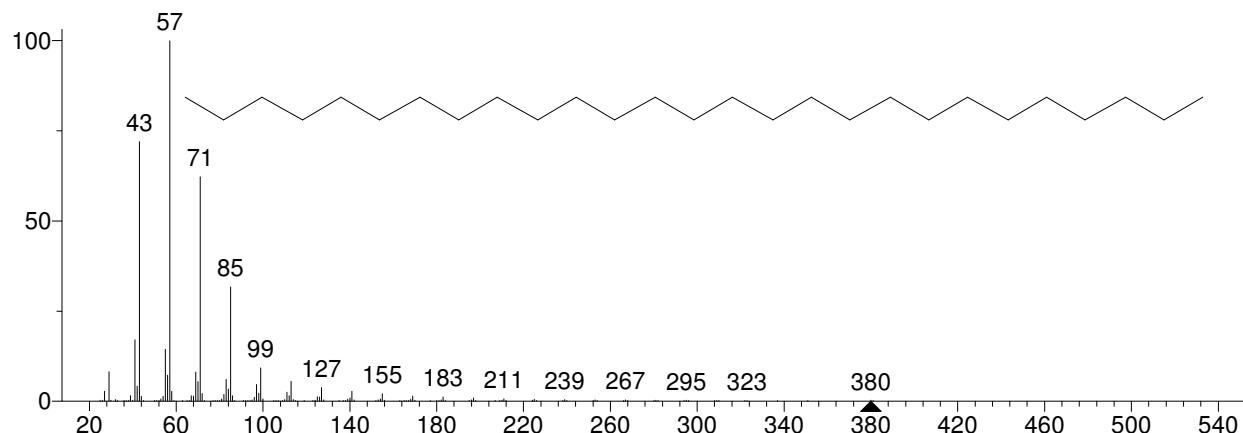


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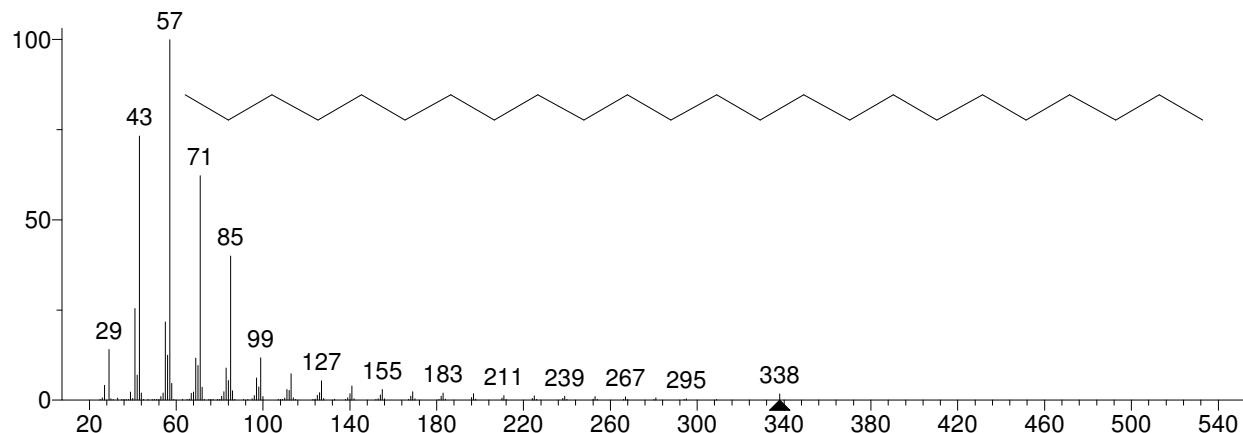
Unknown: Scan 2349 (26.844 min): J5169JO2.D
Compound in Library Factor = -389



Hit 1 : Heptacosane
C₂₇H₅₆; MF: 853; RMF: 915; Prob 6.90%; CAS: 593-49-7; Lib: replib; ID: 5462.

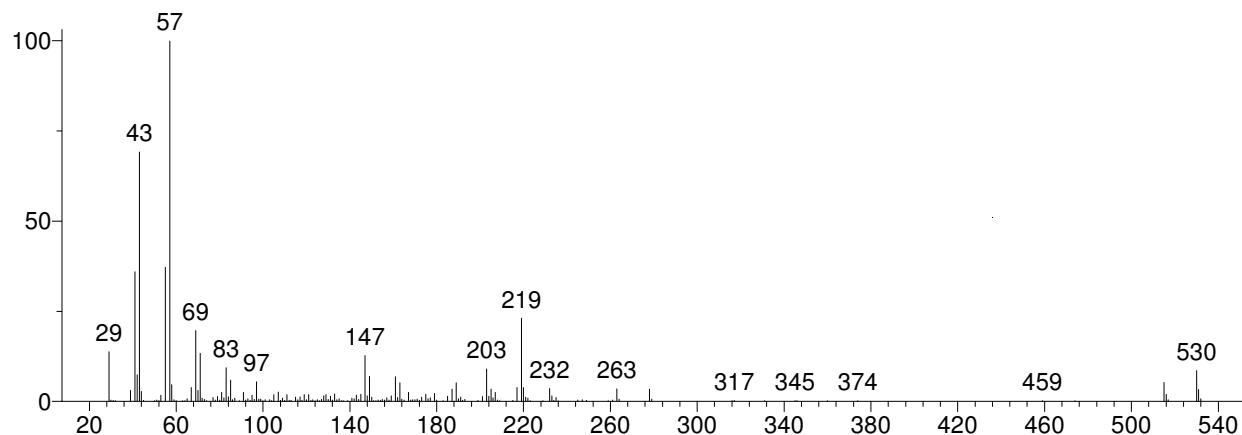


Hit 2 : Tetracosane
C₂₄H₅₀; MF: 851; RMF: 912; Prob 6.36%; CAS: 646-31-1; Lib: replib; ID: 5493.

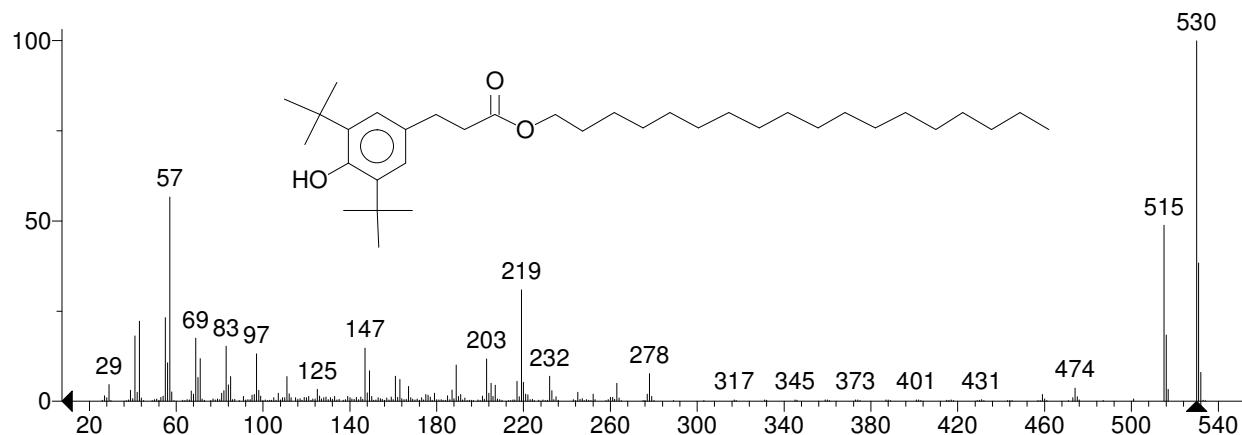


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Unknown: Scan 2386 (27.266 min): J5169JO2.D
 Compound in Library Factor = -159



Hit 1 : Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester
 C35H62O3; MF: 744; RMF: 744; Prob 87.1%; CAS: 2082-79-3; Lib: mainlib; ID: 162602.

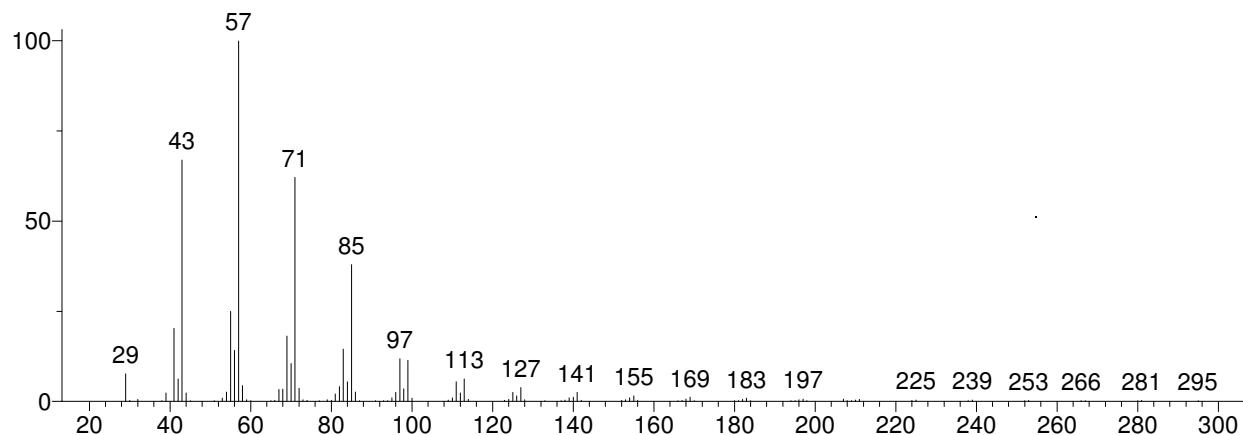


Hit 2 : Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester
 C35H62O3; MF: 690; RMF: 694; Prob 87.1%; CAS: 2082-79-3; Lib: replib; ID: 27601.

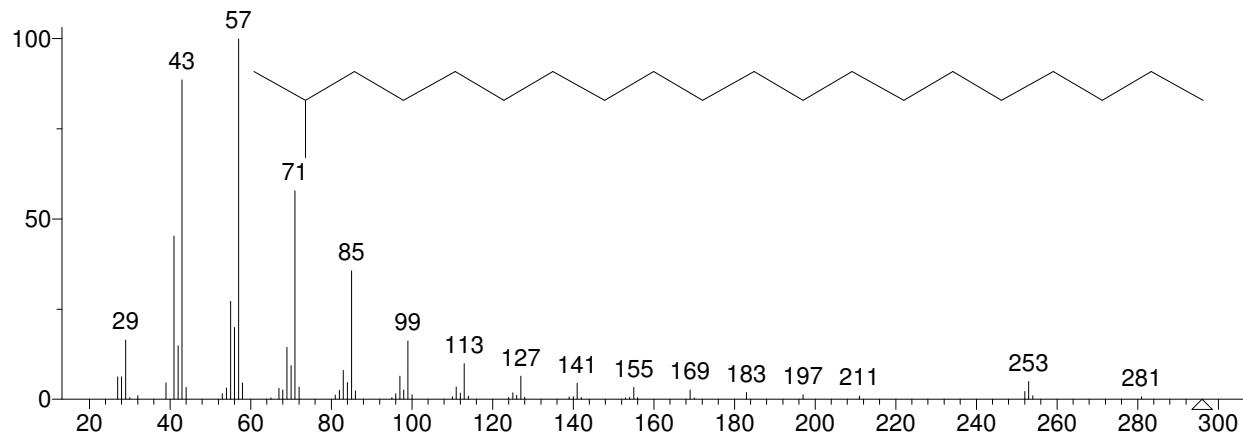


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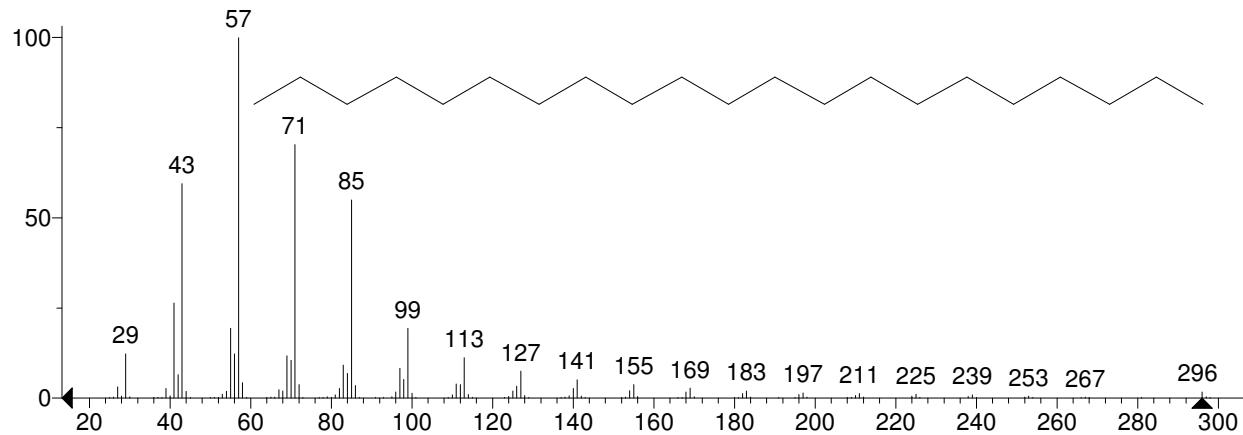
Unknown: Scan 2979 (34.036 min): J5169JO2.D
Compound in Library Factor = -207



Hit 1 : Eicosane, 2-methyl-
C₂₁H₄₄; MF: 893; RMF: 907; Prob 6.45%; CAS: 1560-84-5; Lib: replib; ID: 5423.

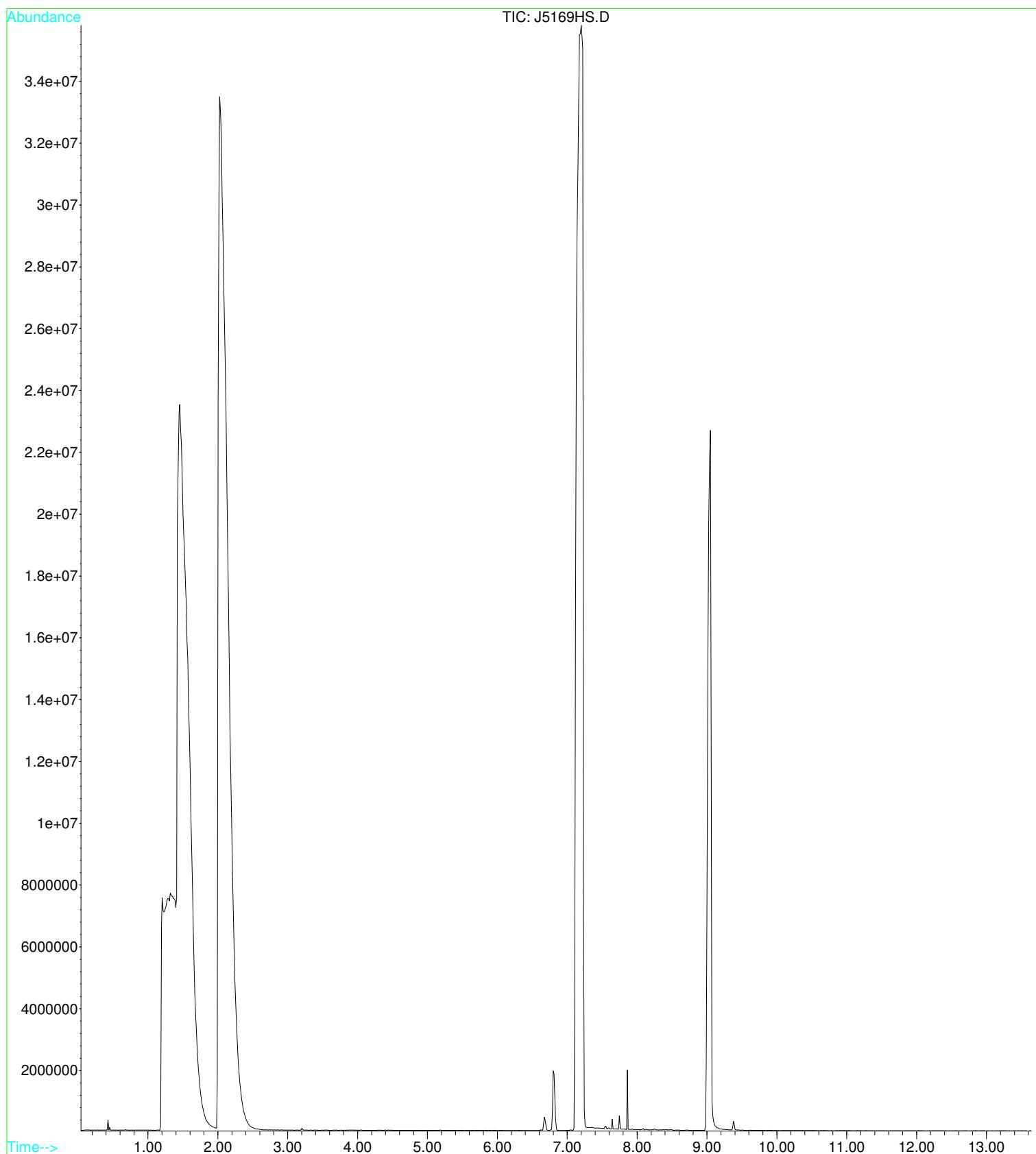


Hit 2 : Heneicosane
C₂₁H₄₄; MF: 891; RMF: 895; Prob 5.95%; CAS: 629-94-7; Lib: replib; ID: 5723.



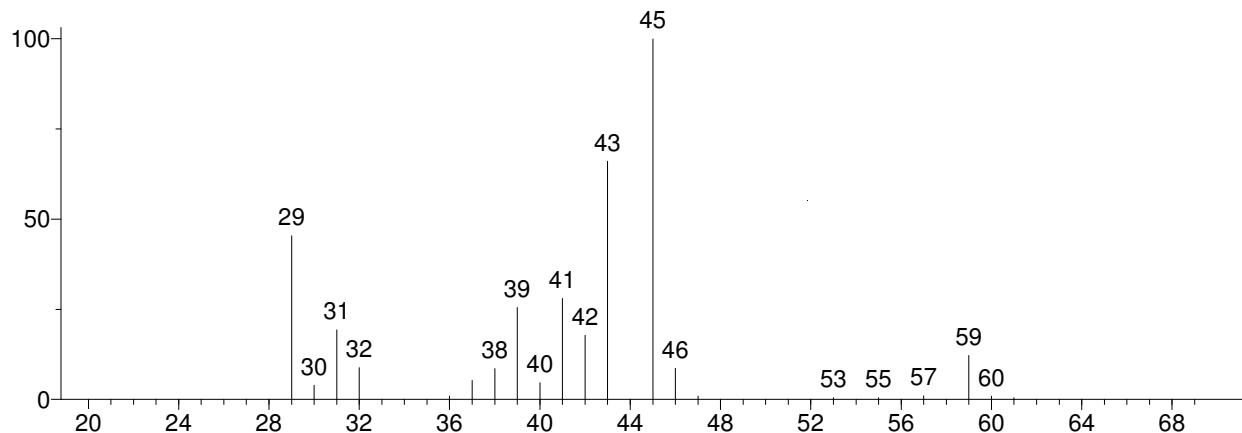
HEADSPACE GCMS RESULTS

File : C:\HPCHEM\1\DATA\2010\JOB2010\J5169JOR\J5169HS.D
Operator :
Acquired : 21 Oct 2010 11:44 using AcqMethod HEADSTD2
Instrument : DMS Instr
Sample Name: J5169 Jordi Unknown
Misc Info :
Vial Number: 1

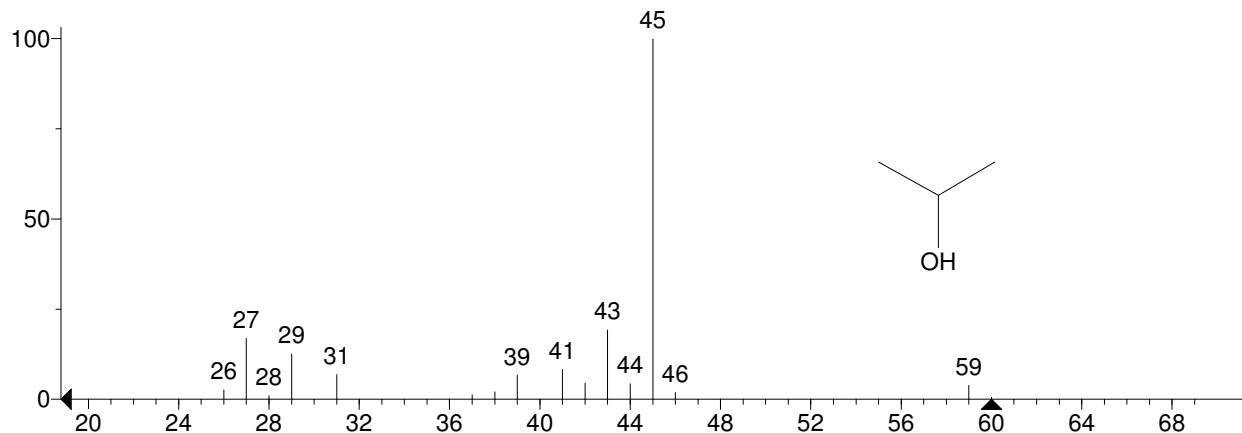


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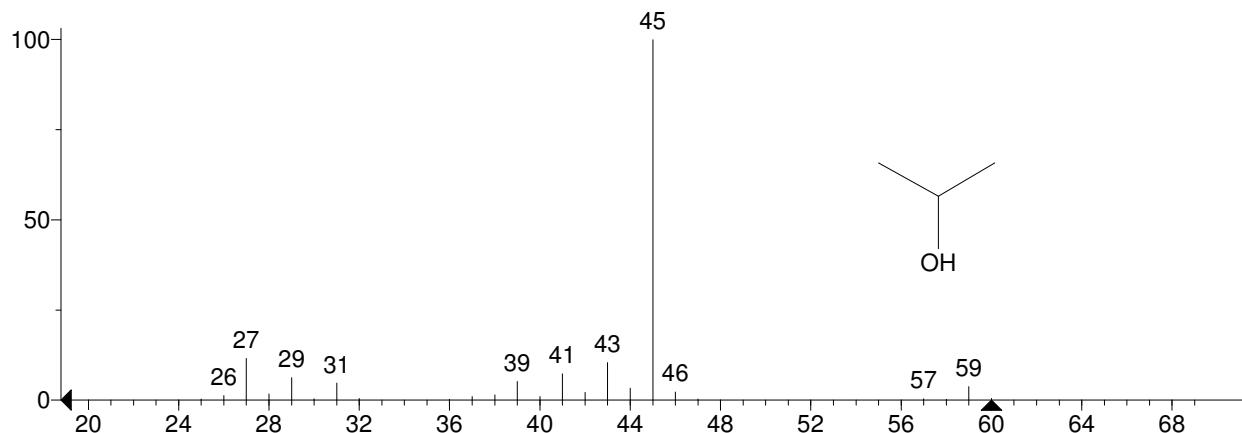
Unknown: Scan 125 (1.455 min): J5169HS.D
Compound in Library Factor = -136



Hit 1 : Isopropyl Alcohol
C₃H₈O; MF: 826; RMF: 857; Prob 55.5%; CAS: 67-63-0; Lib: replib; ID: 3548.

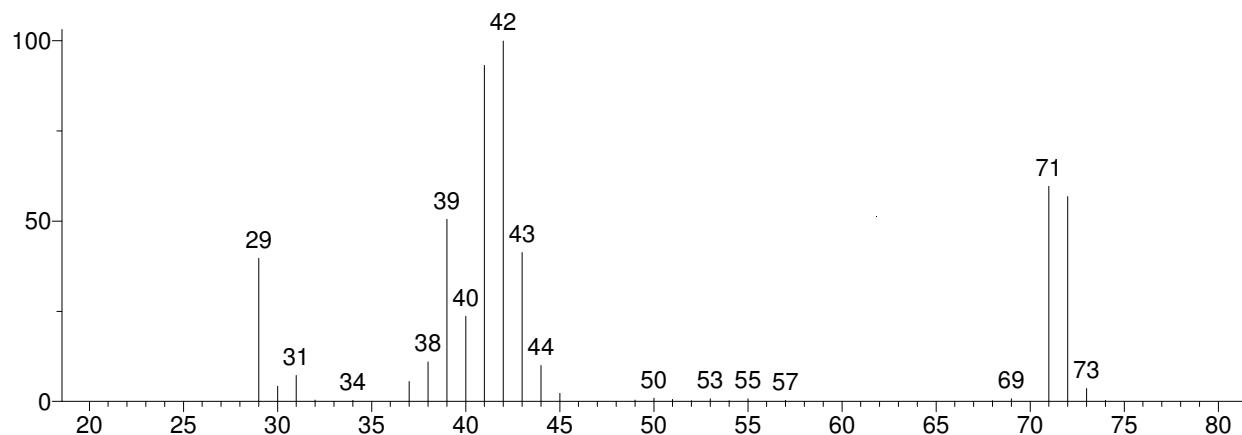


Hit 2 : Isopropyl Alcohol
C₃H₈O; MF: 802; RMF: 804; Prob 55.5%; CAS: 67-63-0; Lib: mainlib; ID: 14532.

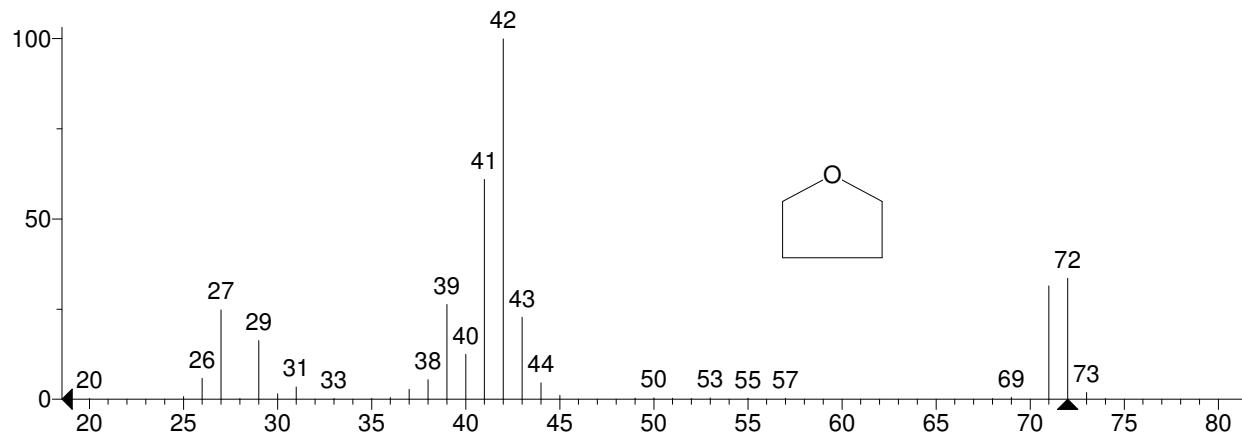


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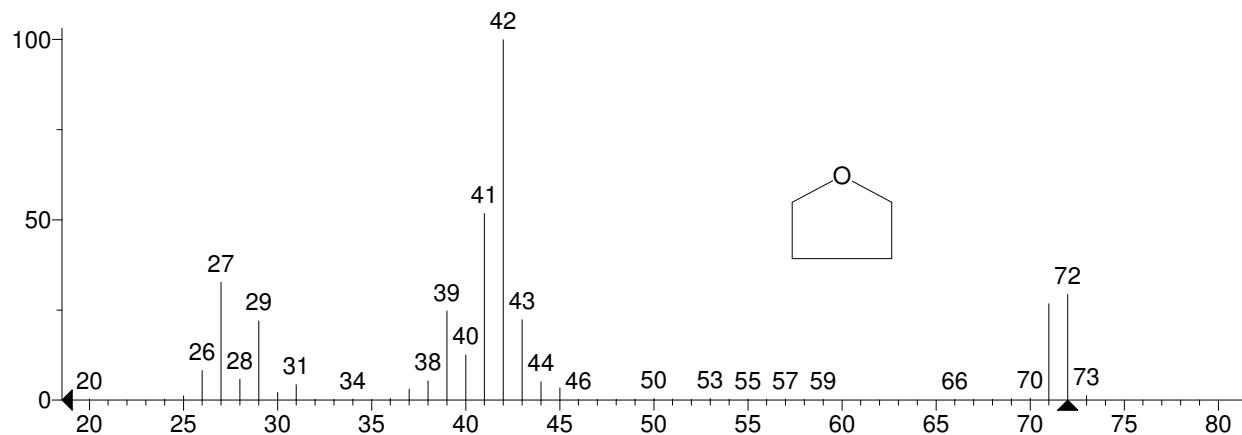
Unknown: Scan 175 (2.026 min): J5169HS.D
 Compound in Library Factor = 237



Hit 1 : Furan, tetrahydro-
 C4H8O; MF: 933; RMF: 933; Prob 87.4%; CAS: 109-99-9; Lib: replib; ID: 1325.

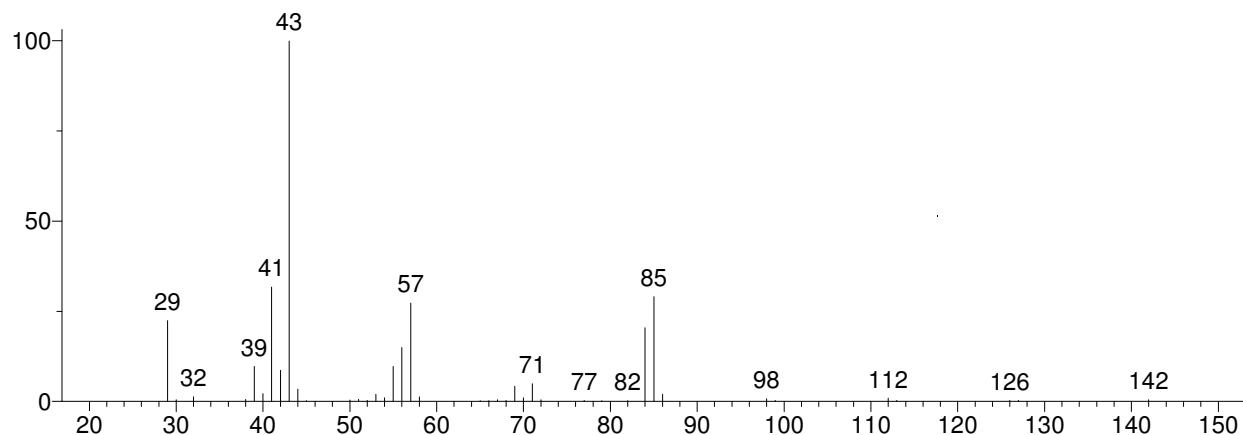


Hit 2 : Furan, tetrahydro-
 C4H8O; MF: 893; RMF: 894; Prob 87.4%; CAS: 109-99-9; Lib: replib; ID: 1305.

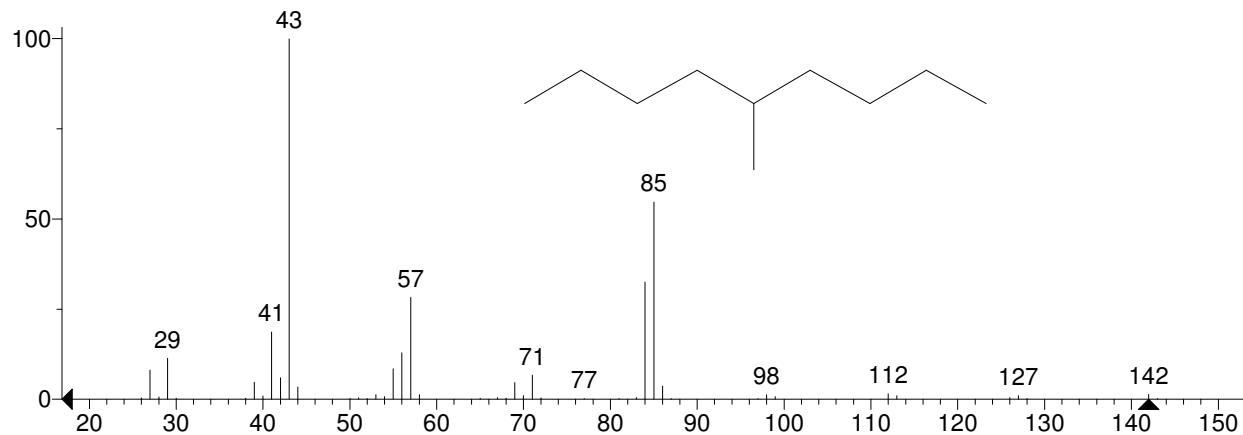


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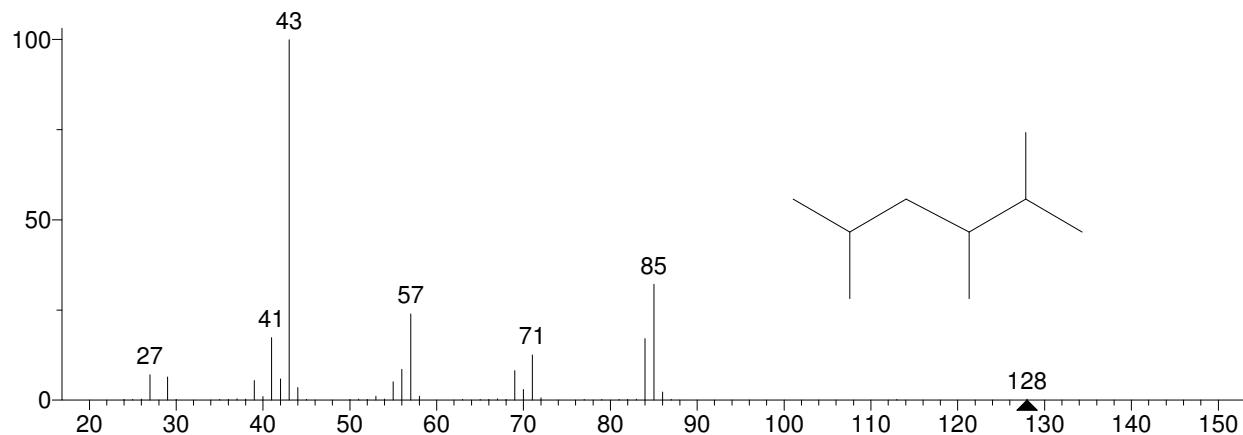
Unknown: Scan 582 (6.673 min): J5169HS.D
Compound in Library Factor = -151



Hit 1 : Nonane, 5-methyl-
C10H22; MF: 894; RMF: 895; Prob 15.0%; CAS: 15869-85-9; Lib: mainlib; ID: 8816.

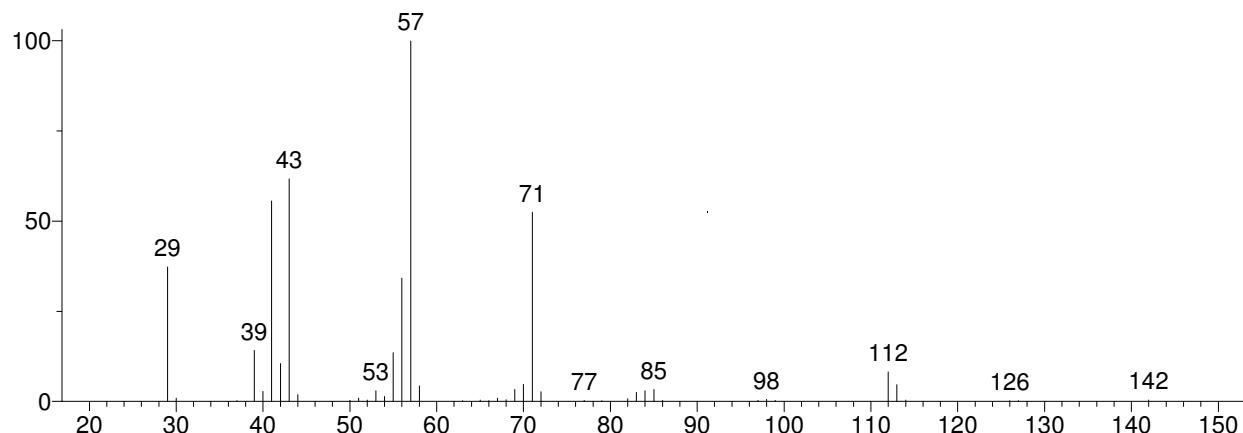


Hit 2 : Hexane, 2,3,5-trimethyl-
C9H20; MF: 890; RMF: 903; Prob 12.7%; CAS: 1069-53-0; Lib: replib; ID: 2635.

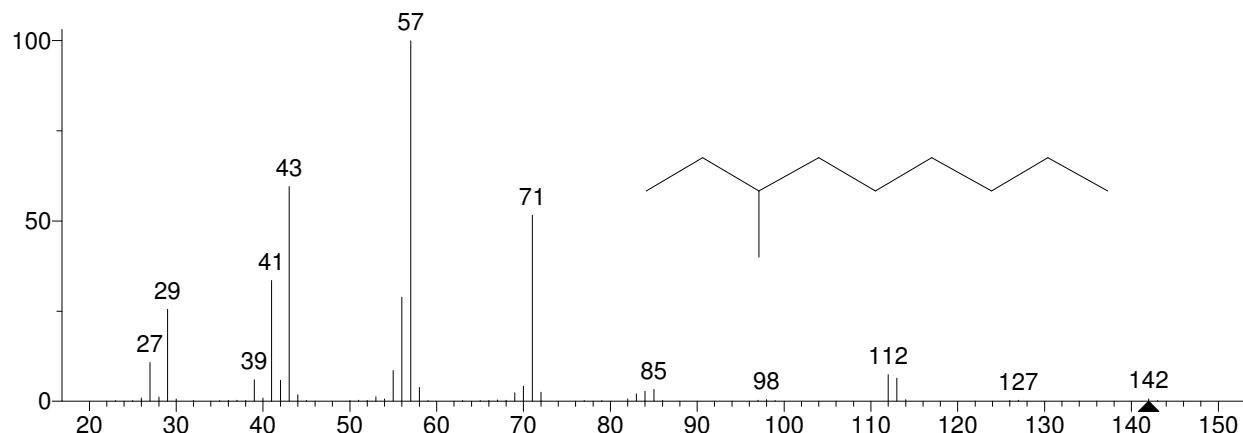


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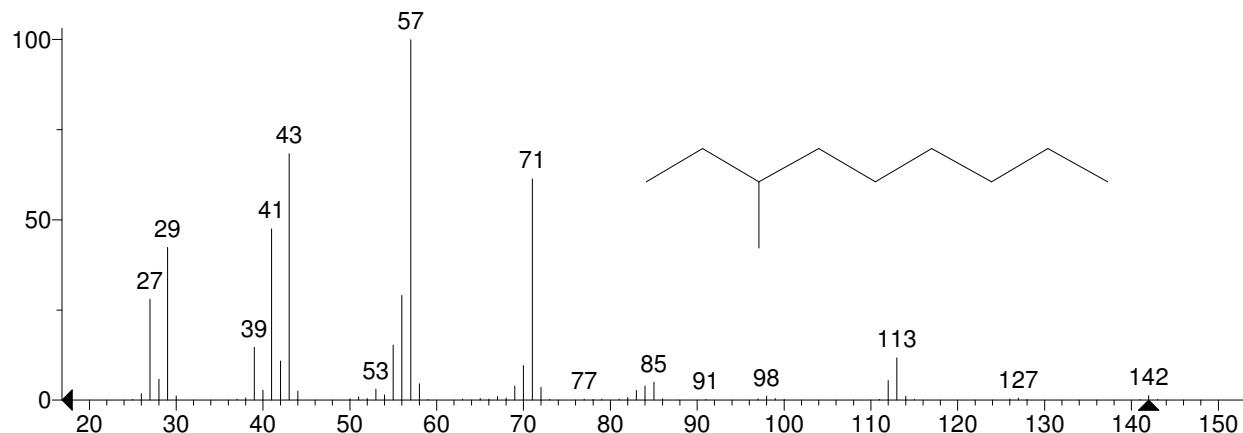
Unknown: Scan 594 (6.810 min): J5169HS.D
Compound in Library Factor = 109



Hit 1 : Nonane, 3-methyl-
C10H22; MF: 925; RMF: 925; Prob 32.1%; CAS: 5911-04-6; Lib: replib; ID: 5419.

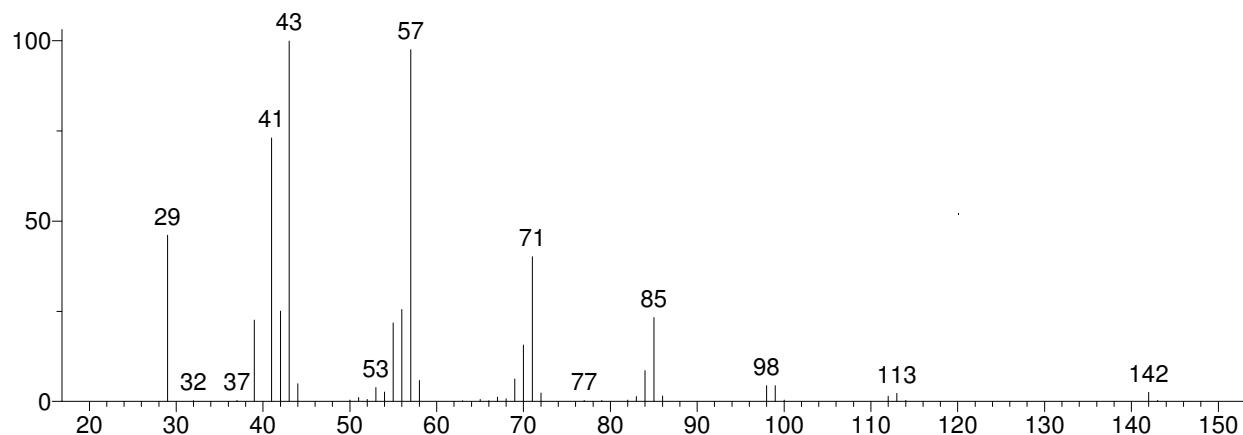


Hit 2 : Nonane, 3-methyl-
C10H22; MF: 917; RMF: 917; Prob 32.1%; CAS: 5911-04-6; Lib: replib; ID: 5418.

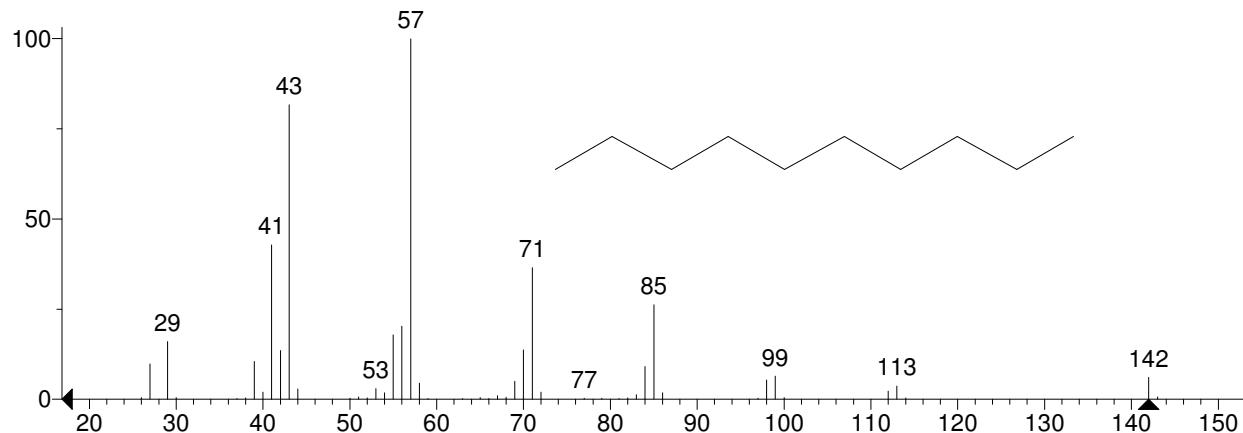


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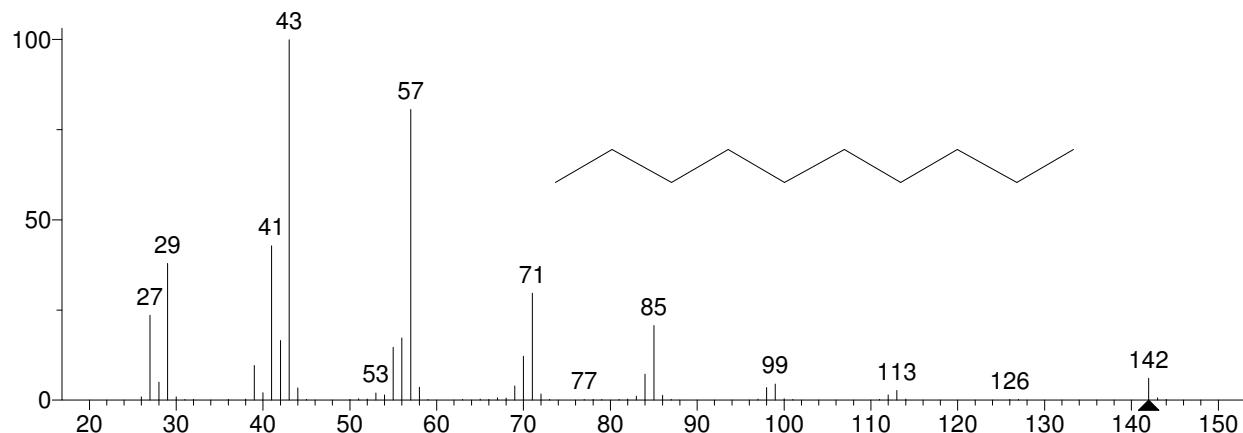
Unknown: Scan 627 (7.187 min): J5169HS.D
Compound in Library Factor = 144



Hit 1 : Decane
C10H22; MF: 952; RMF: 952; Prob 39.6%; CAS: 124-18-5; Lib: replib; ID: 5329.

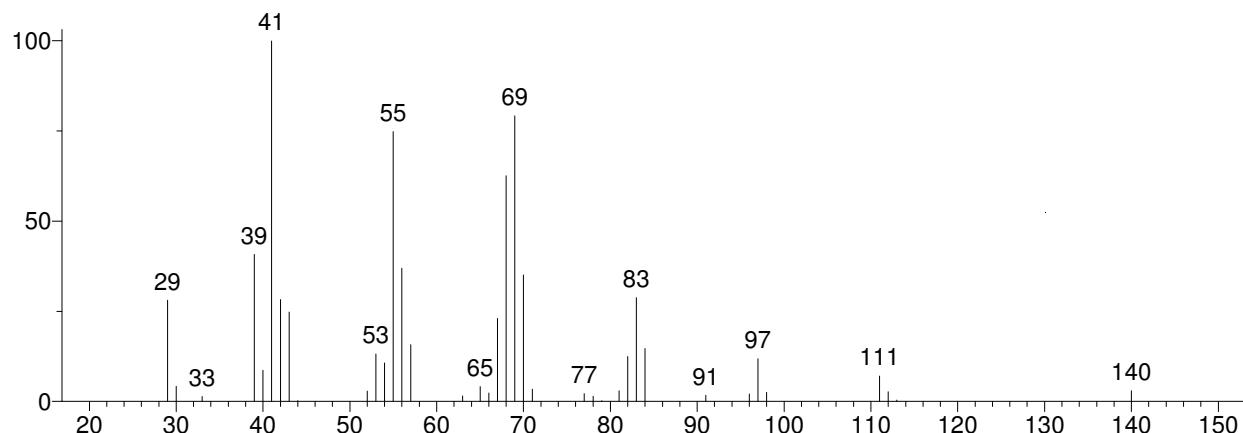


Hit 2 : Decane
C10H22; MF: 940; RMF: 941; Prob 39.6%; CAS: 124-18-5; Lib: mainlib; ID: 6868.

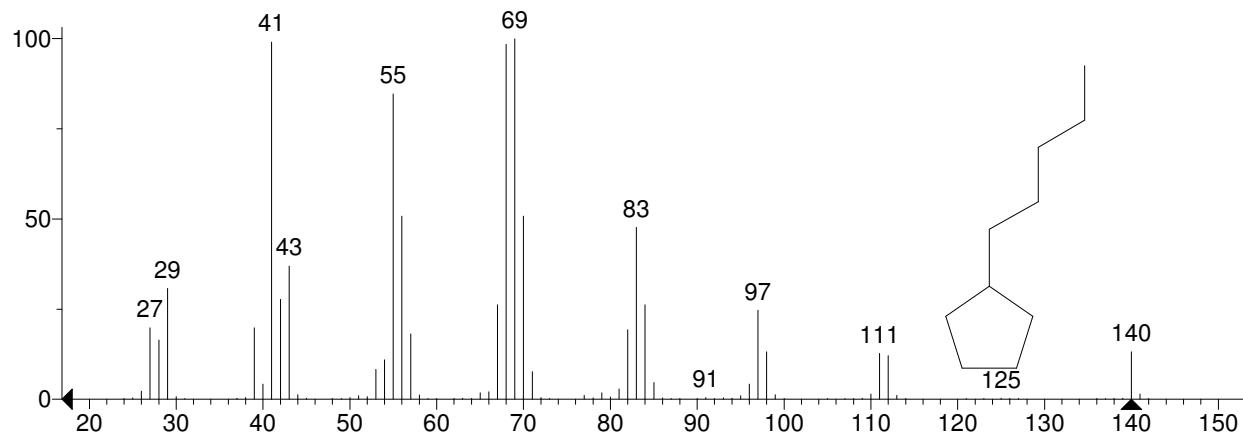


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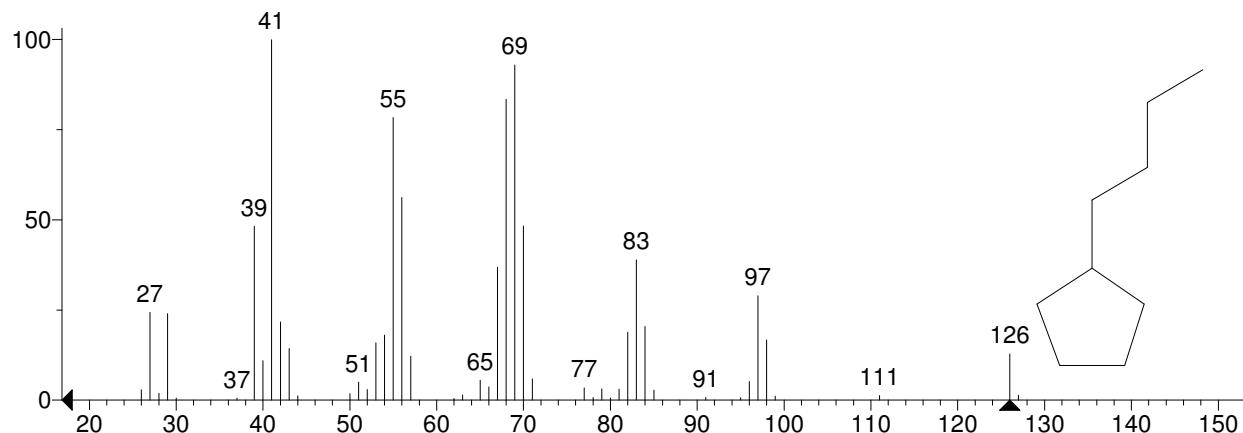
Unknown: Scan 658 (7.541 min): J5169HS.D
 Compound in Library Factor = -246



Hit 1 : Cyclopentane, pentyl-
 C10H20; MF: 861; RMF: 862; Prob 13.8%; CAS: 3741-00-2; Lib: mainlib; ID: 28159.

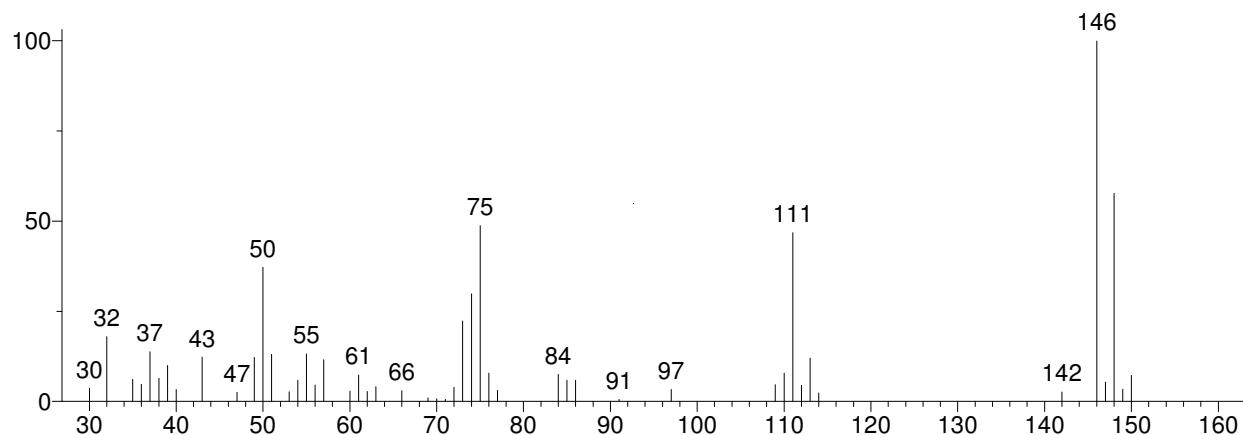


Hit 2 : Cyclopentane, butyl-
 C9H18; MF: 855; RMF: 865; Prob 10.9%; CAS: 2040-95-1; Lib: mainlib; ID: 3070.

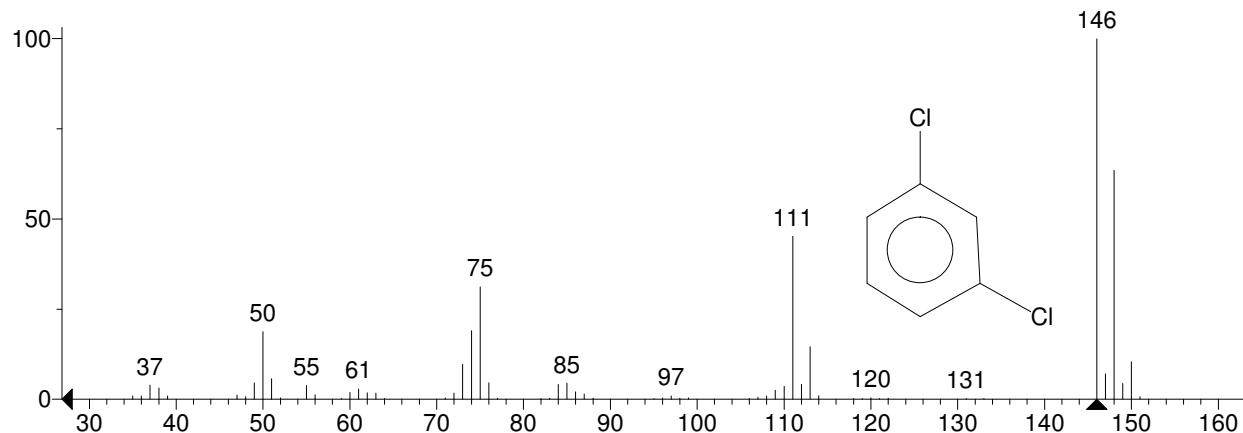


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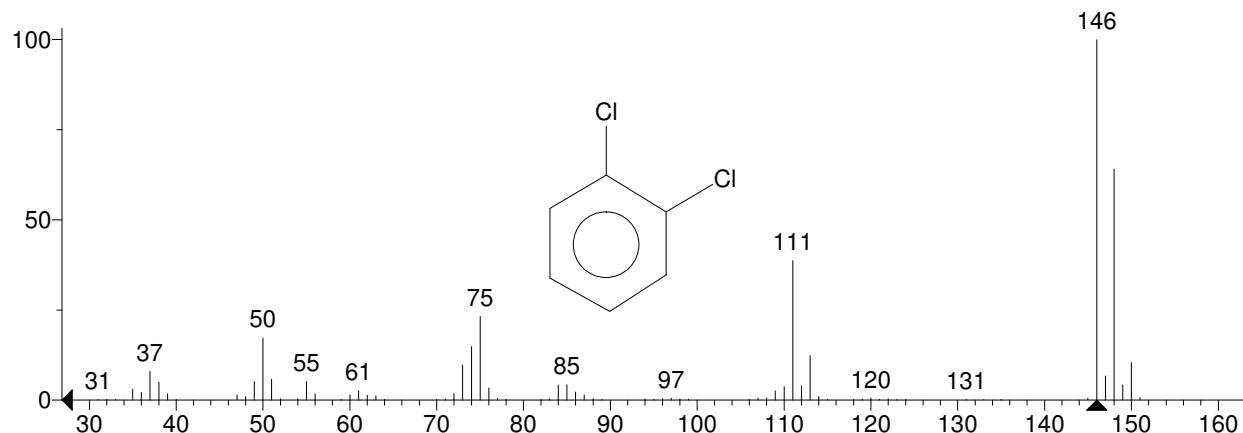
Unknown: Scan 663 (7.598 min): J5169HS.D
 Compound in Library Factor = 226



Hit 1 : Benzene, 1,3-dichloro-
 C₆H₄Cl₂; MF: 866; RMF: 897; Prob 35.9%; CAS: 541-73-1; Lib: replib; ID: 19431.

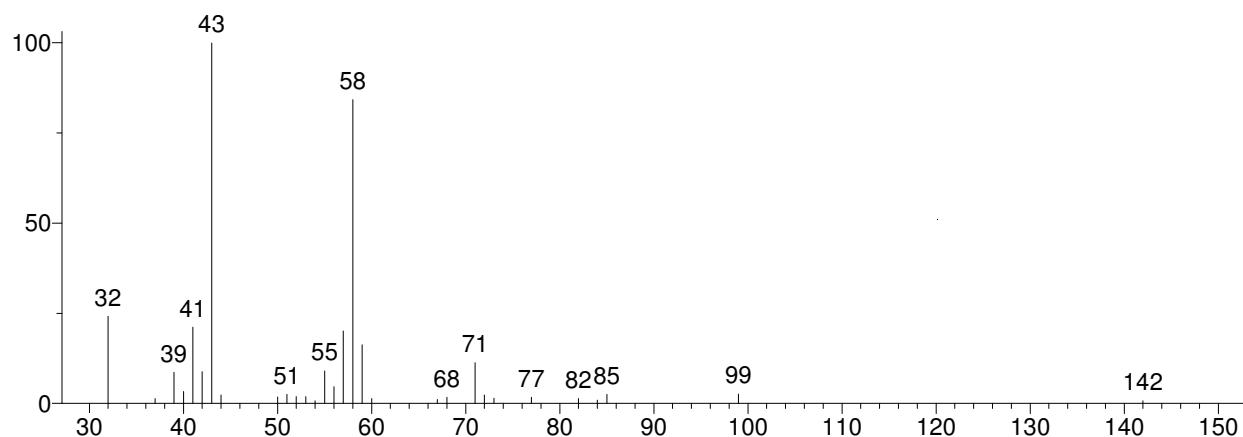


Hit 2 : Benzene, 1,2-dichloro-
 C₆H₄Cl₂; MF: 866; RMF: 886; Prob 35.9%; CAS: 95-50-1; Lib: replib; ID: 19426.

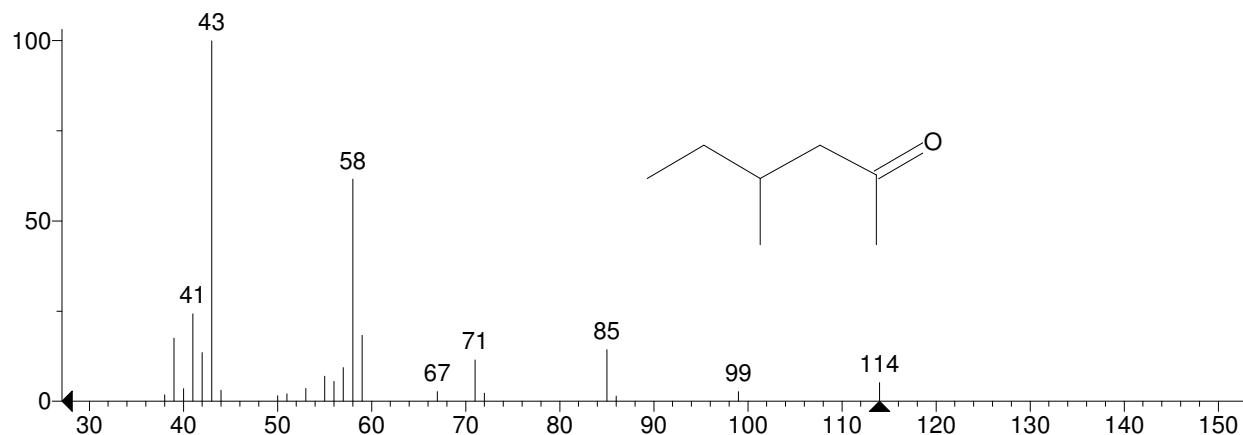


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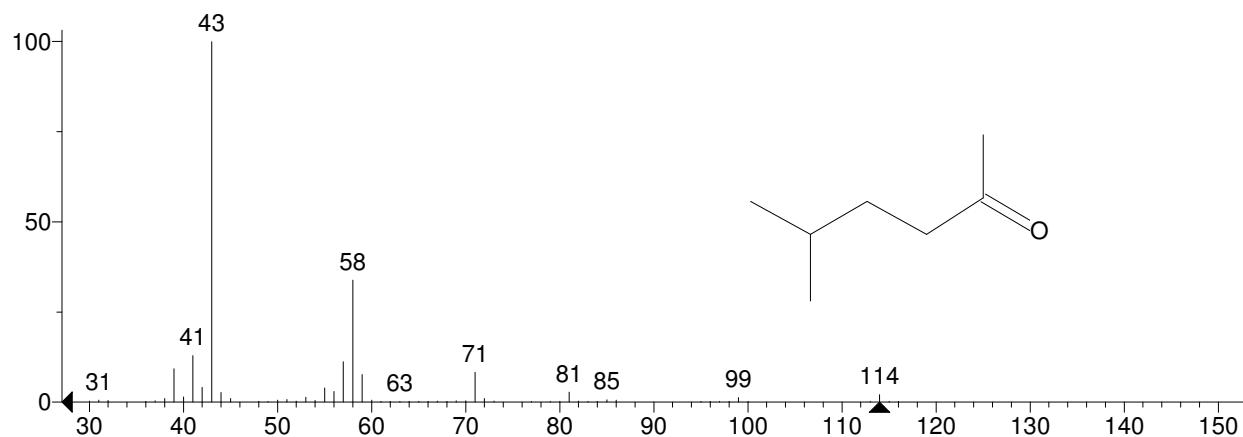
Unknown: Scan 705 (8.077 min): J5169HS.D
 Compound in Library Factor = -367



Hit 1 : 2-Hexanone, 4-methyl-
 C7H14O; MF: 826; RMF: 879; Prob 24.0%; CAS: 105-42-0; Lib: replib; ID: 2188.

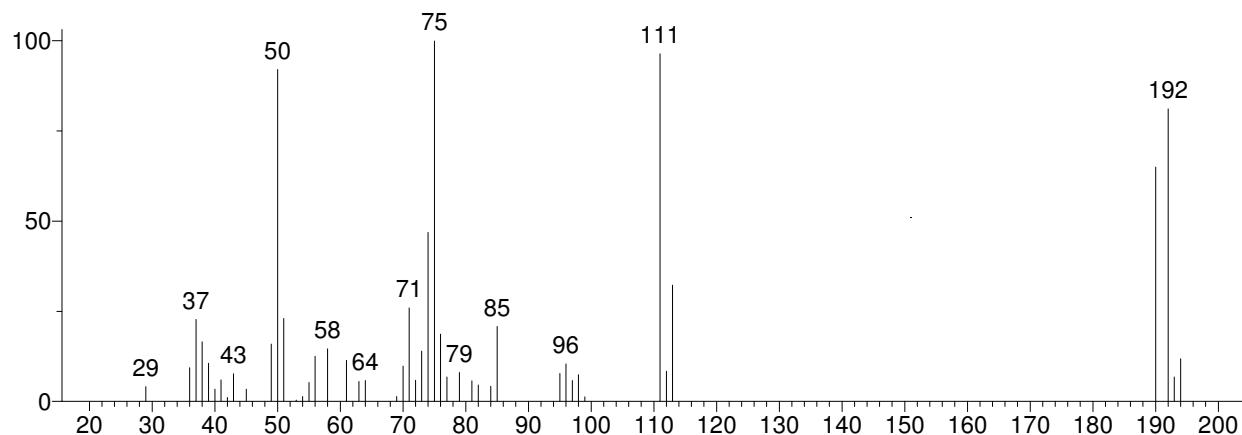


Hit 2 : 2-Hexanone, 5-methyl-
 C7H14O; MF: 816; RMF: 828; Prob 16.9%; CAS: 110-12-3; Lib: mainlib; ID: 7217.

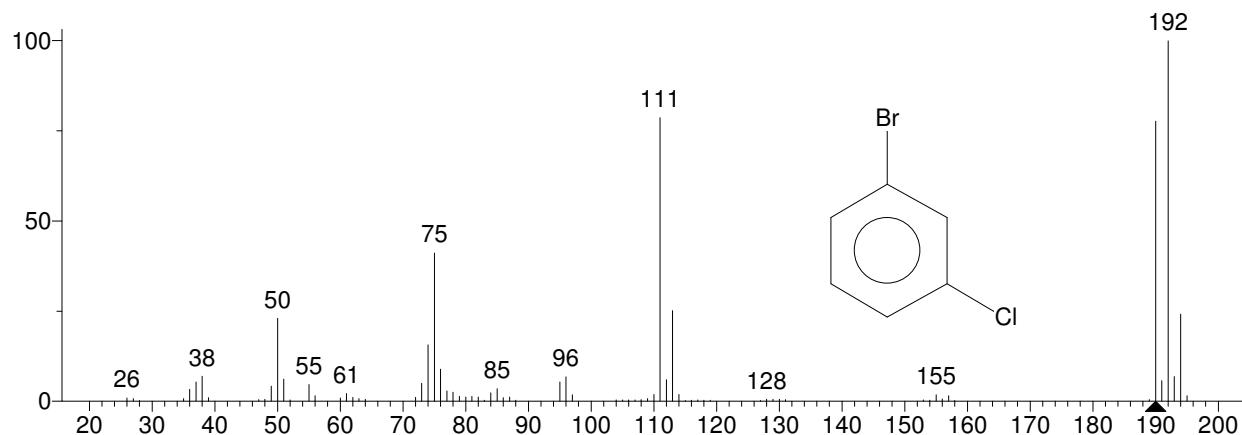


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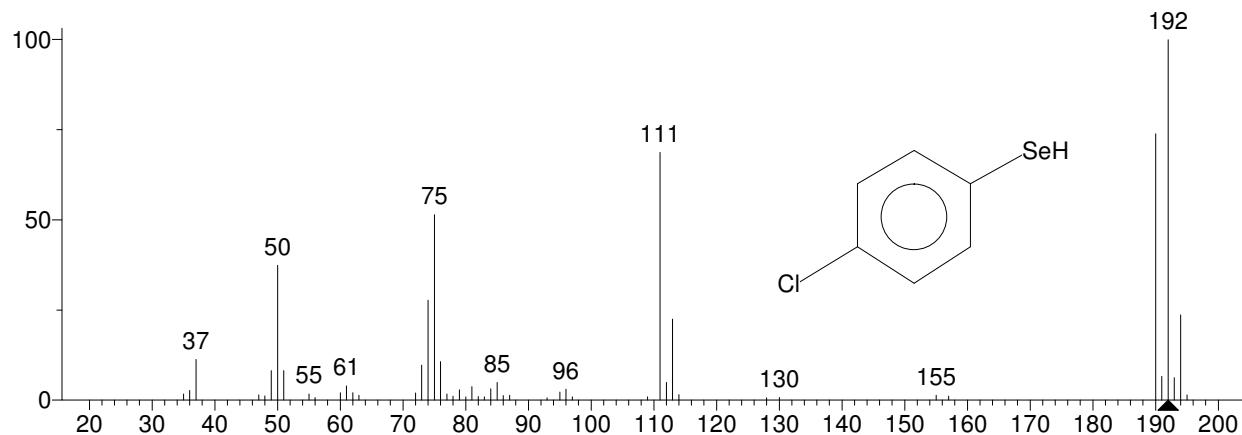
Unknown: Scan 720 (8.249 min): J5169HS.D
 Compound in Library Factor = 177



Hit 1 : Benzene, 1-bromo-3-chloro-
 C6H4BrCl; MF: 812; RMF: 846; Prob 33.6%; CAS: 108-37-2; Lib: replib; ID: 23330.

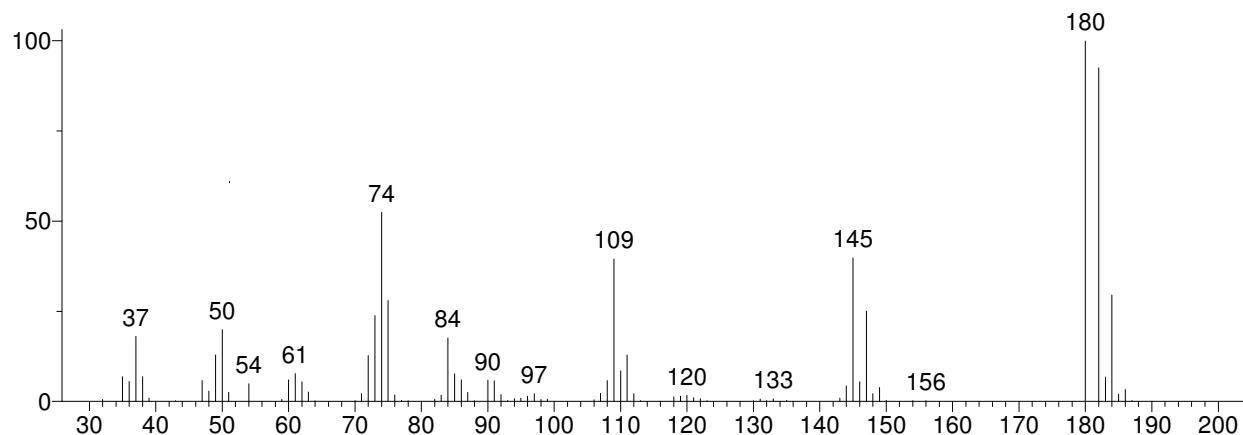


Hit 2 : 4-Chlorophenylselenol
 C6H5ClSe; MF: 808; RMF: 853; Prob 28.4%; CAS: 16645-10-6; Lib: mainlib; ID: 120419.

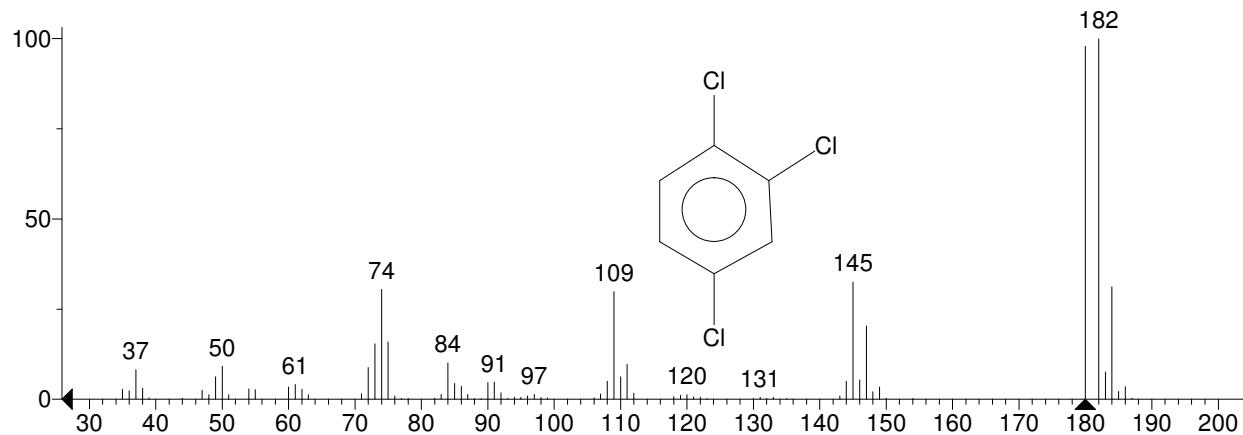


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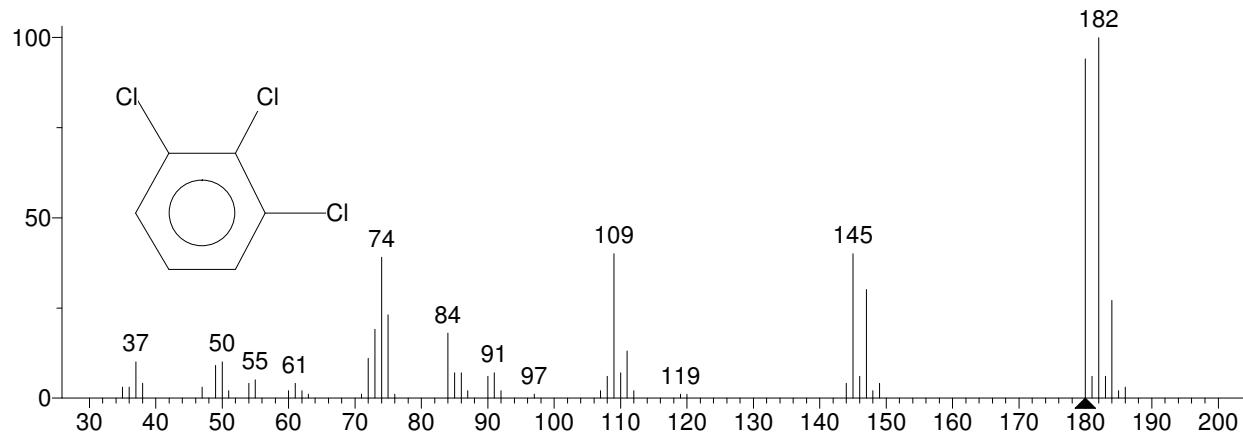
Unknown: Scan 788 (9.025 min): J5169HS.D
 Compound in Library Factor = 1033



Hit 1 : Benzene, 1,2,4-trichloro-
 C6H3Cl3; MF: 954; RMF: 954; Prob 45.7%; CAS: 120-82-1; Lib: replib; ID: 22722.

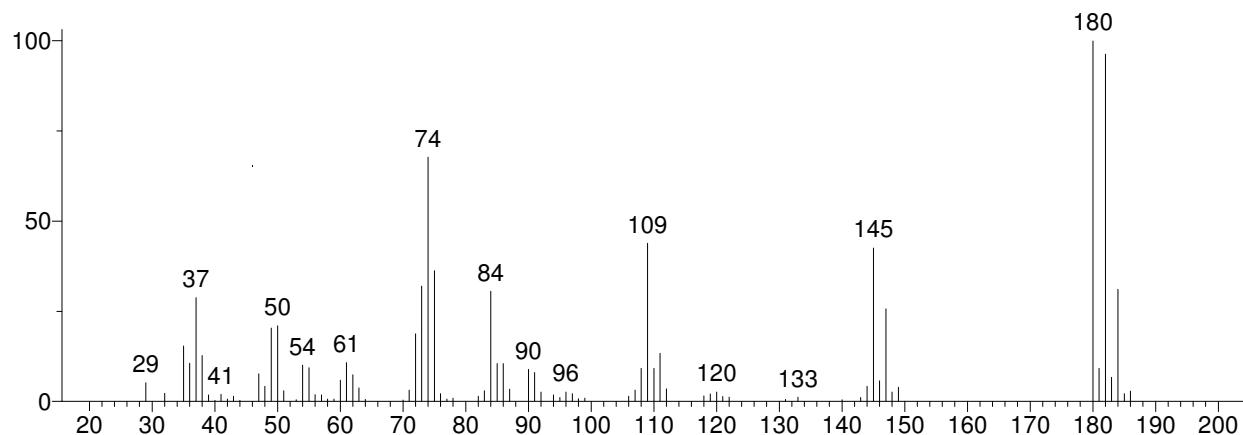


Hit 2 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 942; RMF: 953; Prob 30.4%; CAS: 87-61-6; Lib: replib; ID: 22721.

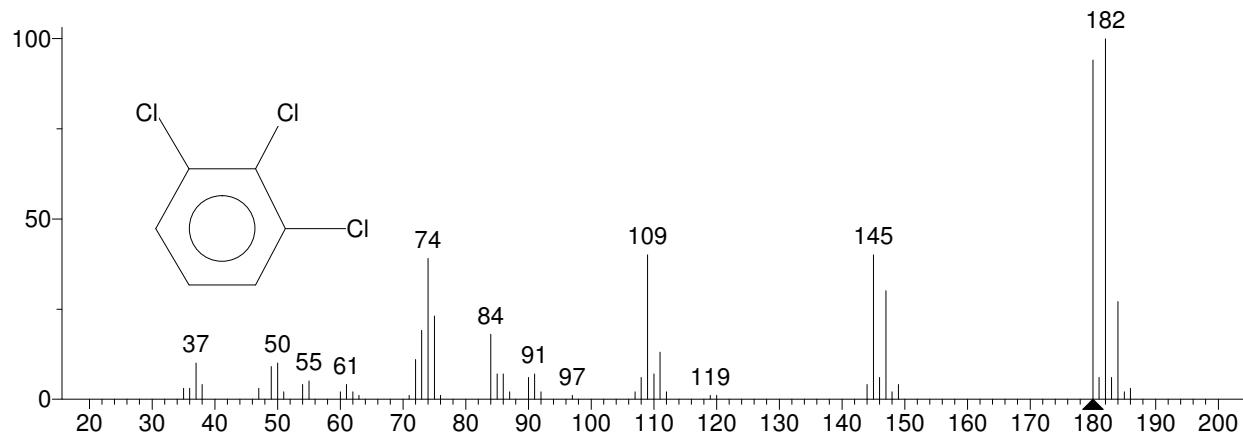


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Unknown: Scan 819 (9.379 min): J5169HS.D
 Compound in Library Factor = 889



Hit 1 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 933; RMF: 950; Prob 57.1%; CAS: 87-61-6; Lib: replib; ID: 22721.



Hit 2 : Benzene, 1,2,3-trichloro-
 C6H3Cl3; MF: 933; RMF: 936; Prob 57.1%; CAS: 87-61-6; Lib: replib; ID: 22558.

