



CASE STUDY

Perfume: Generic vs. Name Brand

PROBLEM

A personal care products formulation lab was trying to understand how their version of a popular designer perfume compared to the “real thing”. Sensory tests demonstrated that the scent of their version faded more quickly, and that their product dried the skin. Jordi’s role was to determine the source of the unfavorable effects to aid them in improving their formula.

ANALYTICAL STRATEGY

After an initial consultation call to understand the customer’s ultimate goals for the investigative analysis, Jordi Labs prepared a thorough technical proposal detailing a tailored series of recommended analytical techniques and their applicability to solving the customer’s problem. The final analytical approach agreed to by both parties is outlined below.

GC-FID was used to screen for the relative quantity of alcohol between the two products and to screen for other potential volatiles. A greater alcohol concentration can affect drying of the skin.

DMS was used to compare the chemistry of the oils and fragrance package in the two materials. This technique is not strictly quantitative, but an estimation of relative quantities between the products was achieved by comparing peak areas.

TGA was used to compare the percentage residuals, relating to inorganic sample components.

CONCLUSIONS

We found that the customer’s product had a notably higher alcohol content and different fragrance package as compared to the competitive product.

Read the following report to see the full analysis.

MATERIAL SOLUTIONS. UNCOMPROMISING INTEGRITY.
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Final Report

Jordi Labs Perfume Analysis

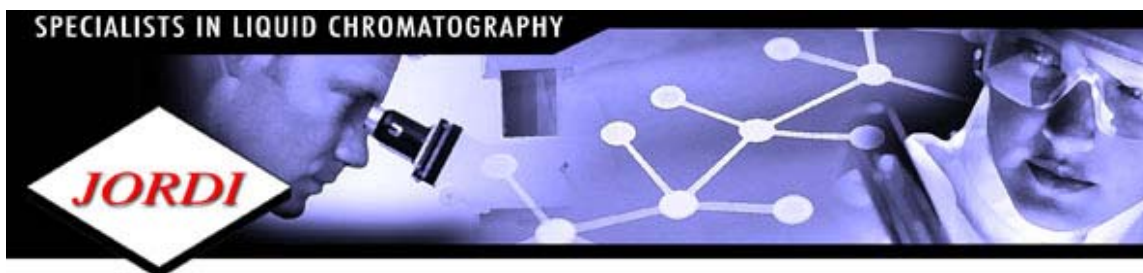
Date: 06/30/10

Prepared by:
Dr. Mark Jordi
President
Jordi Labs LLC

Report Number: J4916

Jordi Labs Confidential





June 30, 2010

Your Name Here
Your Company Name Here

P: xxx-xxx-xxx
E: xxxxx@xxxx.com

Dear Client,

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

1. Designer – Original Designer Product
2. Imitation – Imitation Product

The following tests were performed:

1. Desorption Mass Spectroscopy (DMS)
2. Thermogravimetric Analysis (TGA)
3. Gas Chromatography - Flame Ionization Detector (GC-FID)

Objective

The objective of this work is to compare a designer and an imitation perfume. Special attention is paid to sources of fragrance longevity and materials which may cause drying of the skin.

Summary of Results

The perfumes were found to contain similar components by DMS. The *Designer* sample was found to contain some additional fragrance components and a UV-B absorber. The *Imitation* sample was found to contain isopropyl myristate, which is reported to be an emollient. GC-FID and TGA were able to show the composition differences in the samples. The *Designer* sample was found to contain larger fragrance content, and correspondingly a lower amount of ethanol.

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.

DMS: – The fragrance mixture and other volatile sample components were investigated by DMS. The samples were analyzed using an injection port temperature of 310°C. Identifications are based on comparison with the NIST spectral library of over 147,350 compounds. Match quality is based on a 1000 scale with a perfect match indicated by a score of 1000. **Table I** contains a list of the components that were detected in each sample.

Table I DMS Results				
Component	<i>Designer</i>	<i>Imitation</i>	Retention Time (minutes)	Apparent Purpose
Ethanol	X	X	3.2	Solvent
Propylene glycol		X	4.3	Carrier
Pinene	X	X	5.6 (α), 6.0 (β)	Fragrance
Myrcene	X		6.1	Fragrance
Limonene	X	X	6.6	Fragrance
3,7-dimethyl-1,6-Octadien-3-ol (Linalool)	X	X	7.3	Fragrance
Laevo-camphor	X		7.8	Fragrance
Benzyl Acetate	X	X	7.9	Fragrance
Estragole	X		8.4	Fragrance
Turpineol		X	8.2	Fragrance
Benzene propanol		X	8.6	Fragrance
Citronellol	X	X	8.7	Fragrance
3,7-dimethyl-2-aminobenzoate-1,6-octadien-3-ol	X	X	8.9	Fragrance
(E)-citral	X		9.1	Fragrance
2,6-dimethyl-2,6-octadiene	X	X	9.8	Fragrance
Neryl Acetate	X	X	9.9	Fragrance
Geranyl Acetate	X	X	10.1	Fragrance
Vanillin	X	X	10.8	Fragrance
Coumarin	X	X	11.0	Fragrance
Diethyl phthalate	X	X	12.3	
Cedrol		X	12.3	Fragrance
Methyl dihydrojasmonate	X	X	12.9	Fragrance
Cubenol		X	12.6	Fragrance
Nuciferol	X		13.4	Fragrance
Benzyl Benzoate		X	13.5	Stabilizer

Component	<i>Designer</i>	<i>Imitation</i>	Retention Time (minutes)	Apparent Purpose
Cedryl acetate	X	X	13.8	Fragrance
Isopropyl Myristate		X	13.8	Emollient
6,7-diethyl-1,2,3,4-tetrahydro-1,1,4,4-tetramethyl-naphthalene	X		14.0	Fragrance
Versalide	X	X	14.4	Fragrance
Isophytol	X		14.8	Fragrance
Musk ketone	X	X	15.3	Fragrance
Ethylene brassylate	X	X	15.5	Fragrance
Octyl methoxycinnamate	X		17.3	UV-B absorber
Cinnamyl cinnamate	X		17.9	Fragrance

* X indicates that a particular compound was detected in the sample.

TGA

The sample was subjected to TGA analysis over the temperature range from ambient to 1000°C. The samples were analyzed under nitrogen. Analysis results are shown in **Table II**. The decomposition of the *Designer* sample took place in three steps. The large initial weight loss is most likely due to loss of the ethanol solvent which accounted for approximately 85% of the total sample. The remaining two losses can be attributed to evaporation and thermal degradation of the fragrance components.

The thermogram for the *Imitation* sample only exhibited two recognizable weight losses. Again the first can be attributed to the loss of ethanol, and the second to the loss of fragrance components. The major difference between the two samples is the relative amount of loss observed in each portion. The *Imitation* sample lost 94% at low temperature as compared to 84% for the *Designer* sample. This observation agrees with data from GC-FID, confirming that the *Imitation* sample contains more ethanol and less of the fragrance components. The *Imitation* sample was also observed to contain slightly more (~0.3%) residual inorganic material.

Table II TGA Weight Loss				
Sample	Weight Loss Step	Weight Loss %	Total % Weight Loss	% Residual
<i>Designer</i>	1	84.97	99.49	0.51
	2	10.40		
	3	4.123		
<i>Imitation</i>	1	93.82	99.15	0.85
	2	5.333		

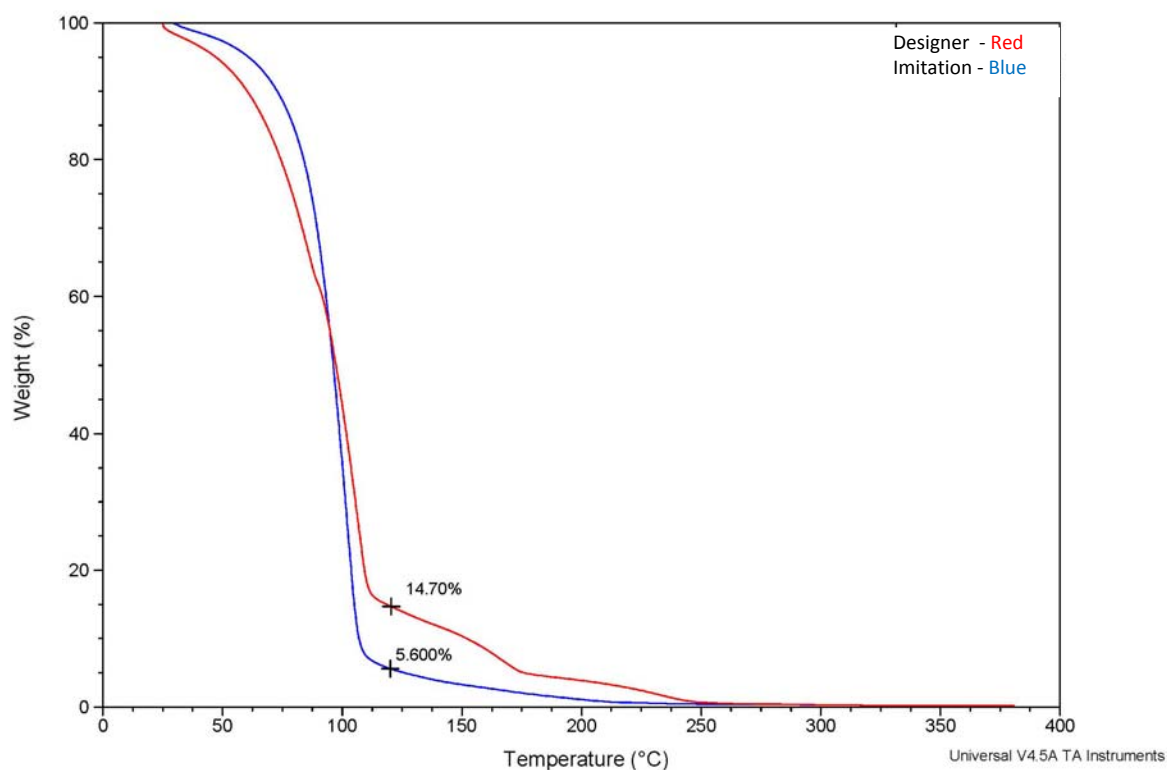


Figure I – Overlay of TGA thermograms.

GC-FID

GC-FID was used to screen the samples for the relative quantity of the solvent and other volatile materials. The *Imitation* sample was observed to contain a larger amount of ethanol than was observed for the *Designer* sample. This conclusion is based on the observed peak area of the peak at 2.5 minutes retention time. **Figure II** contains an overlay of the GC-FID chromatograms in this region.

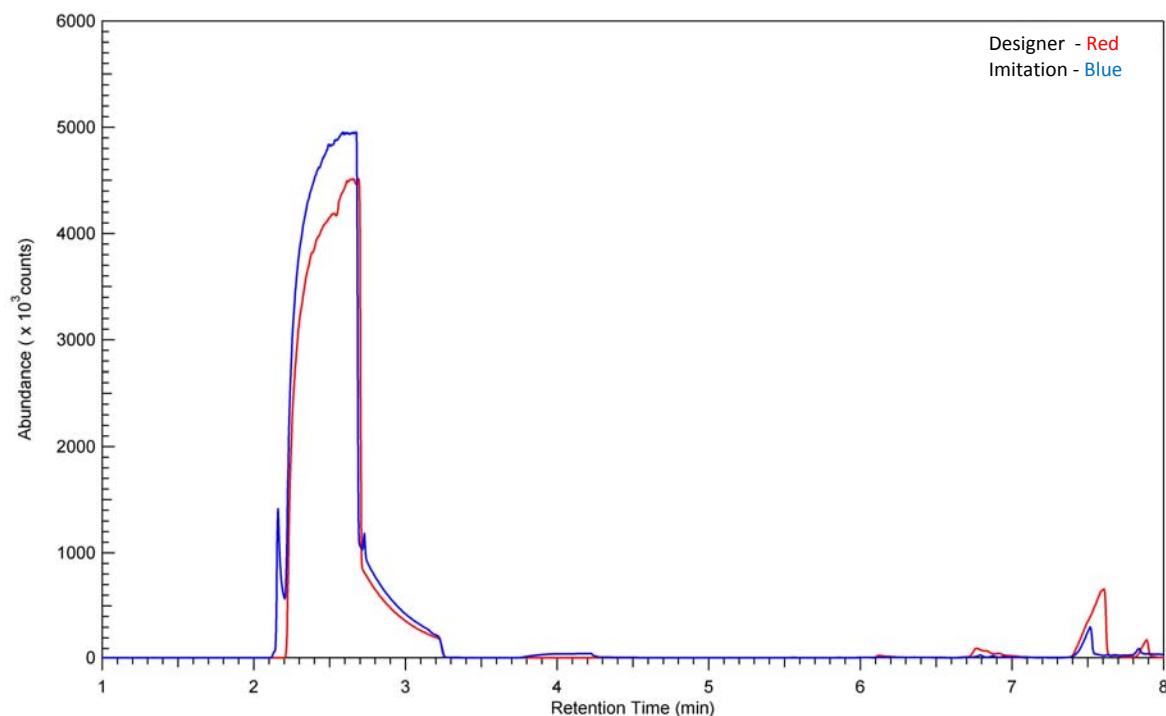


Figure II – Overlay of GC-FID chromatograms in the solvent region.

Additional components, including the fragrances detected, were observed between 6 and 20 minutes retention time. All components observed in the *Imitation* sample appear at lower concentration than those observed in the *Designer* sample. **Figure III** contains an overlay of sample chromatograms in this region.

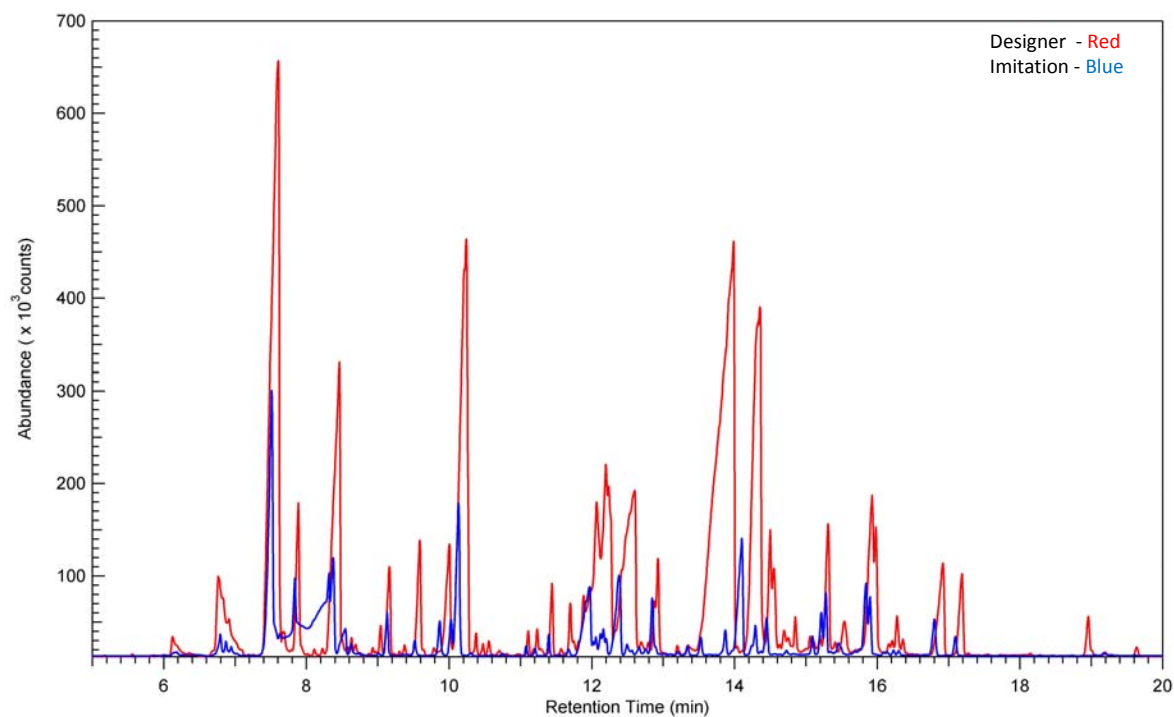


Figure III – Overlay of GC-FID chromatograms in the fragrance region.

Analysis Conditions

DMS

The samples were analyzed using a Hewlet 5890 gas chromatograph in conjunction with a 5972 mass selective detector and a thermal desorption attachment. Data acquisition was accomplished using chemstation software. Sample peaks were compared with over 147,350 reference compounds using the NIST/EPA/NIH mass spectral search program.

A blank run was used immediately before analysis of the samples to ensure the absence of contaminants. The sample was analyzed in duplicate to confirm the repeatability of the results.

Sample Size = 0.1 μ L
Initial Delay = 2.0 minutes
Initial Temperature: 50°C
Final Temperature: 320°C
Temperature Ramp Rate 1: 15°C per minute
Injector Port Temperature: 310°C
Detector Temperature: 310°C
Injector Split = NA
Mass Range: Low Mass = 29, High Mass = 550

TGA

Analysis of samples was accomplished using a TA 500 Thermogravimetric Analyzer in combination with TA Universal Analysis software. Approximately 30mg of the sample was weighed into a platinum weigh boat for each analysis. Samples were run under a nitrogen atmosphere and heated from ambient to 1000°C at a rate of 20°C per minute.

GC-FID

The samples were analyzed directly using an HP 5890a gas chromatograph in conjunction with a flame ionization detector. Data acquisition was accomplished using chemstation software. A blank run was used immediately before analysis of the samples to insure the absence of contaminants.

The following run conditions were applied for Gas Chromatographic analysis:

Injection Size = 1 μ L
Initial Temperature: 50°C
Final Temperature: 320°C
Temperature Ramp Rate 1: 15°C per minute
Injector Port Temperature: 310°C
Detector Temperature: 320°C

Injector Split = NA
Column = RTX-5MS 30m x .25mm

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 25 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

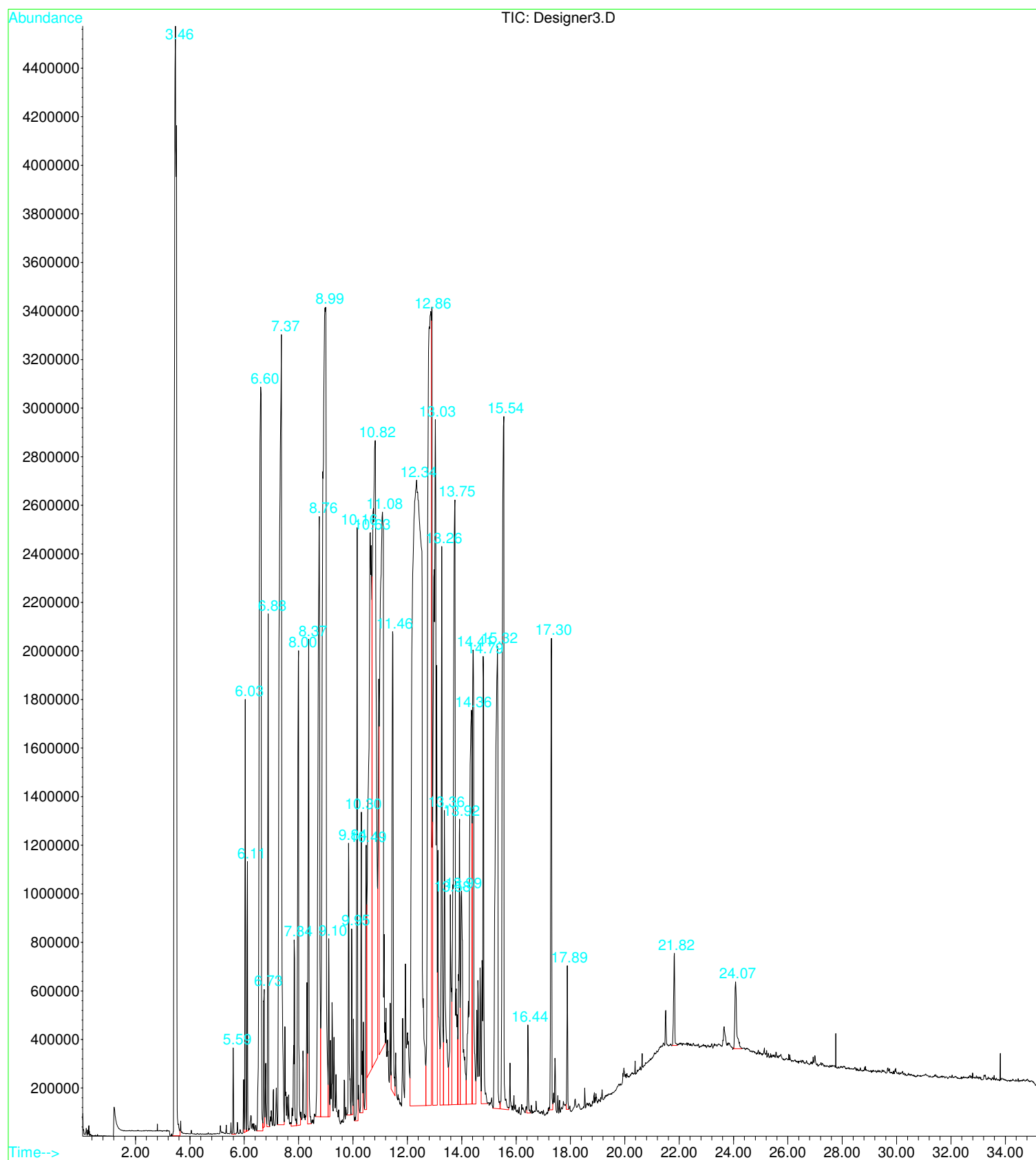
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- Page 96-100 – TGA Data
- Page 101-103 – GC-FID Data

DMS RESULTS

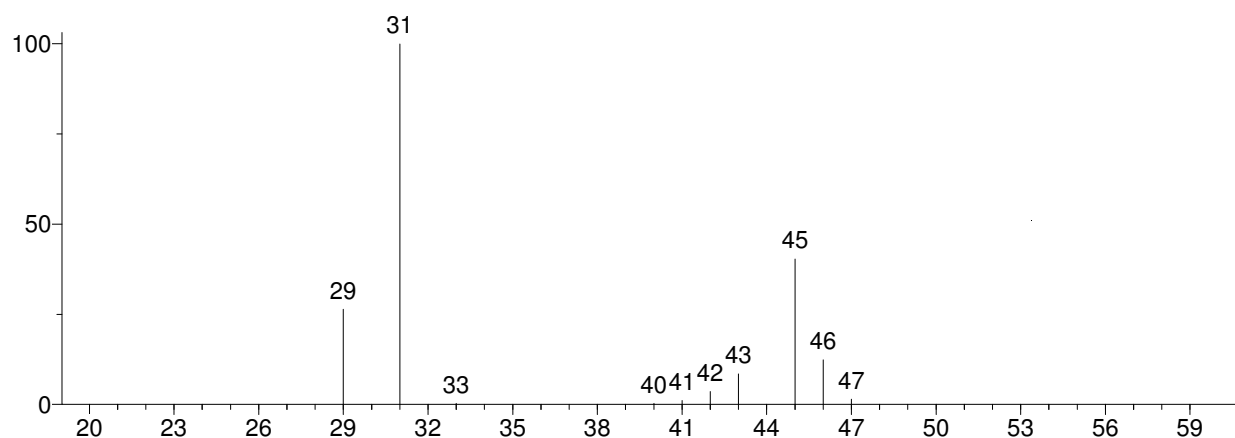
Designer

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Operator : KR
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Instrument : DMS Instr
Sample Name: Designer .1ul
Misc Info : desorp2 inj 310 ramp 50-320 15C/min
Vial Number: 100

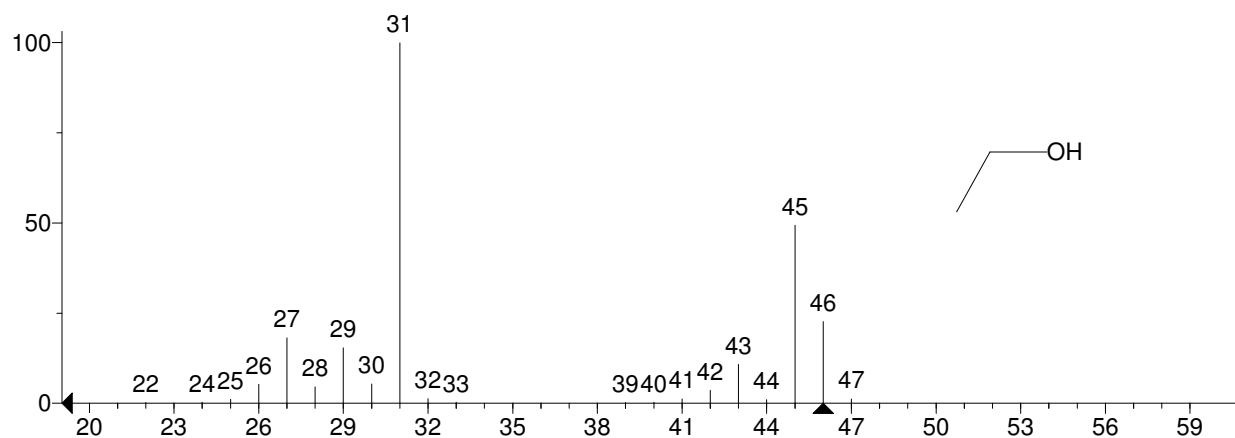


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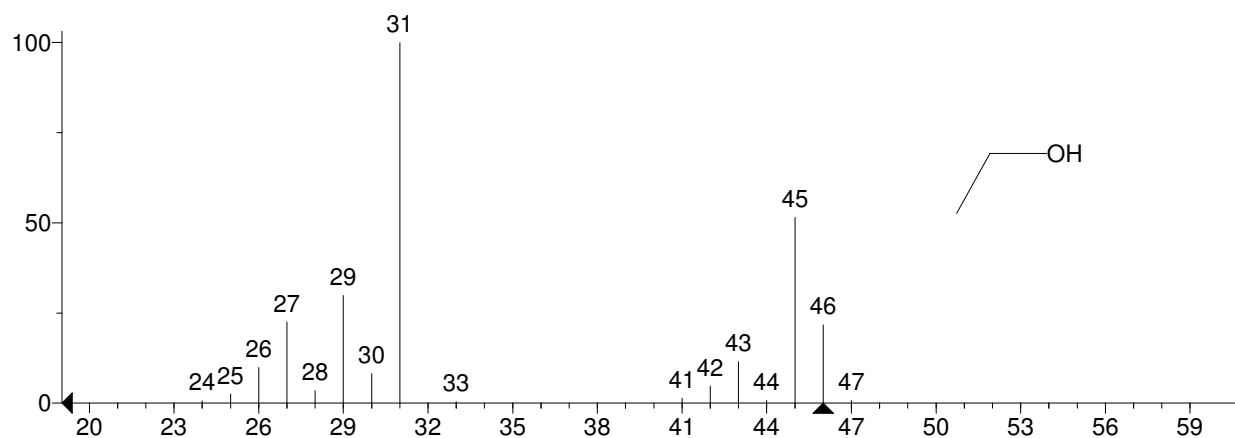
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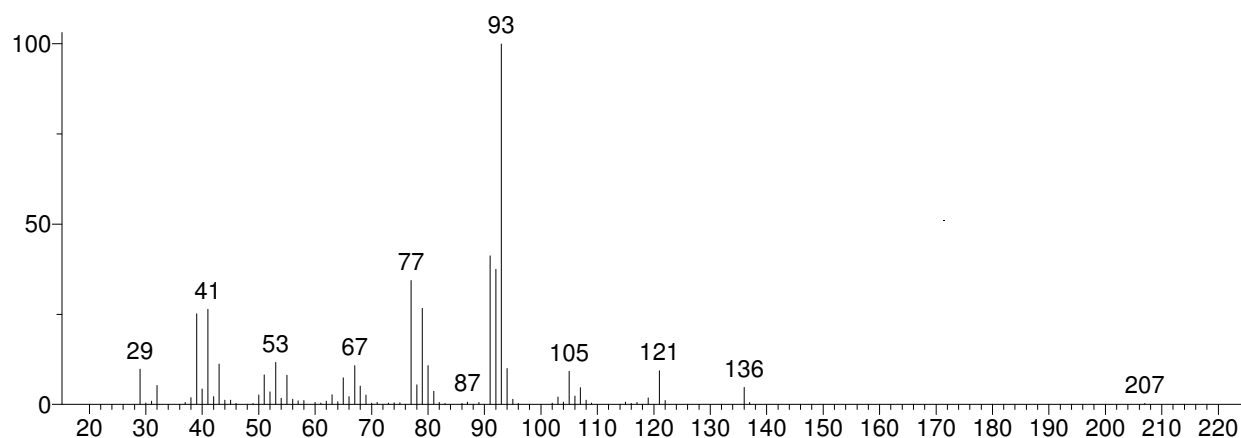


Hit 2 : Ethyl alcohol
C2H6O; MF: 912; RMF: 913; Prob 94.3%; CAS: 64-17-5; Lib: mainlib; ID: 1334.

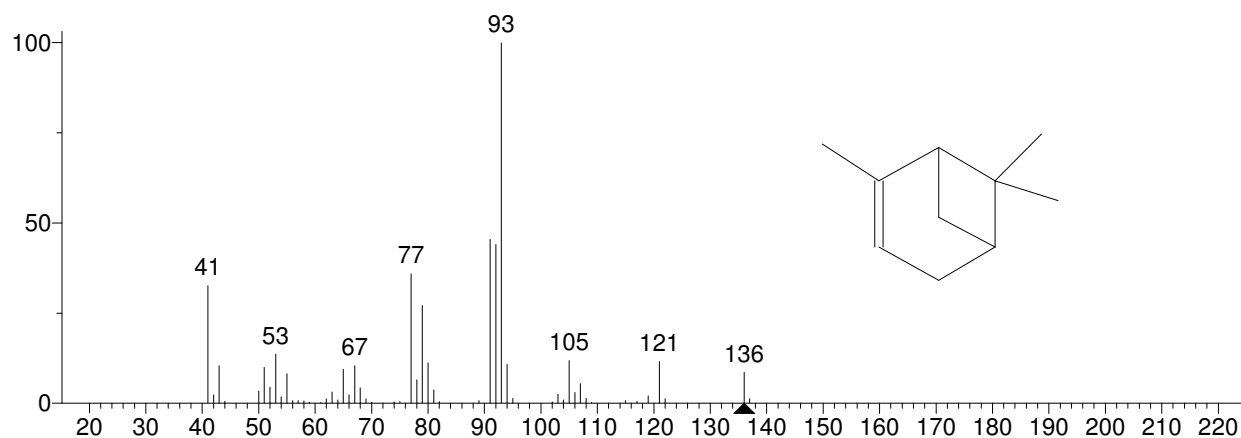


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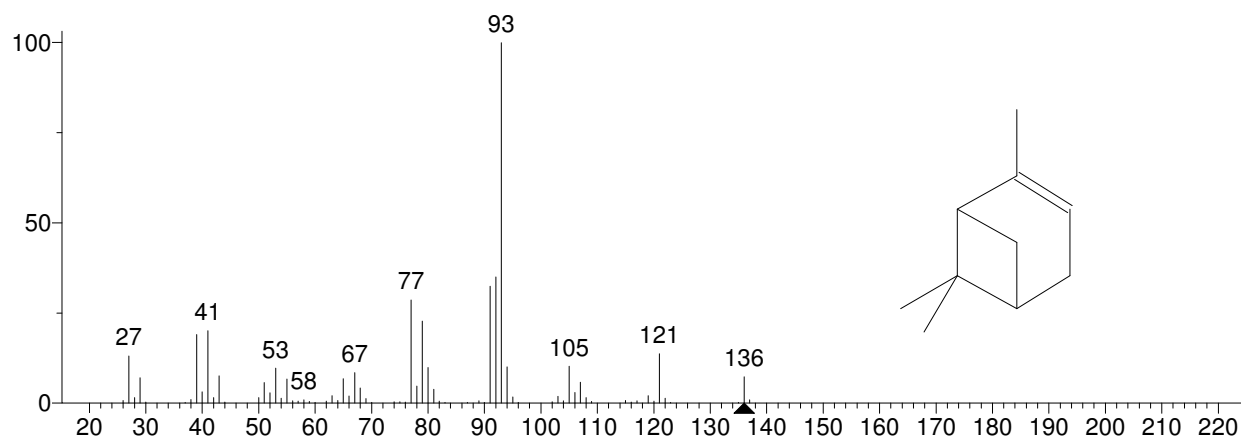
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Hit 1 : 1R-.alpha.-Pinene
C₁₀H₁₆; MF: 947; RMF: 952; Prob 17.0%; CAS: 7785-70-8; Lib: replib; ID: 12053.

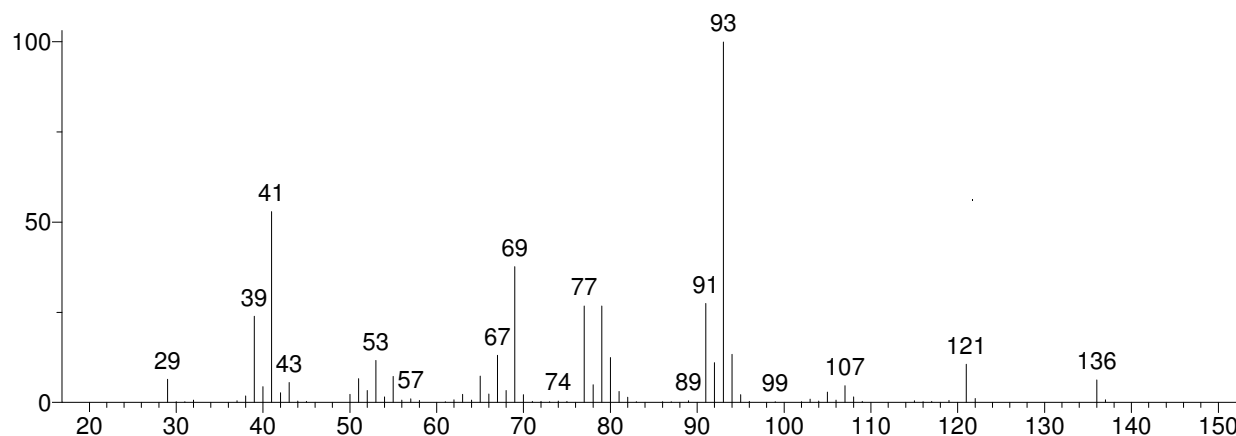


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C₁₀H₁₆; MF: 946; RMF: 953; Prob 16.3%; CAS: 80-56-8; Lib: mainlib; ID: 51652.

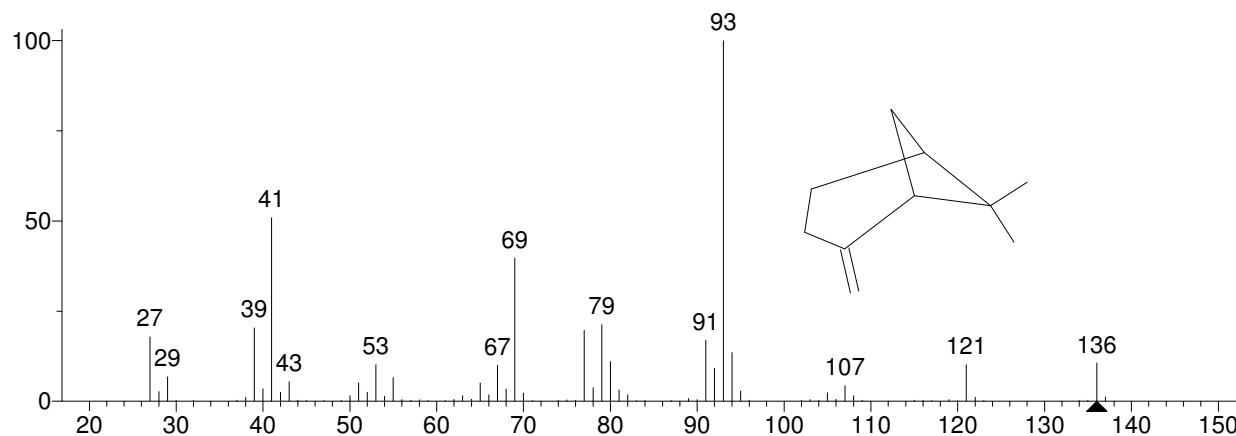


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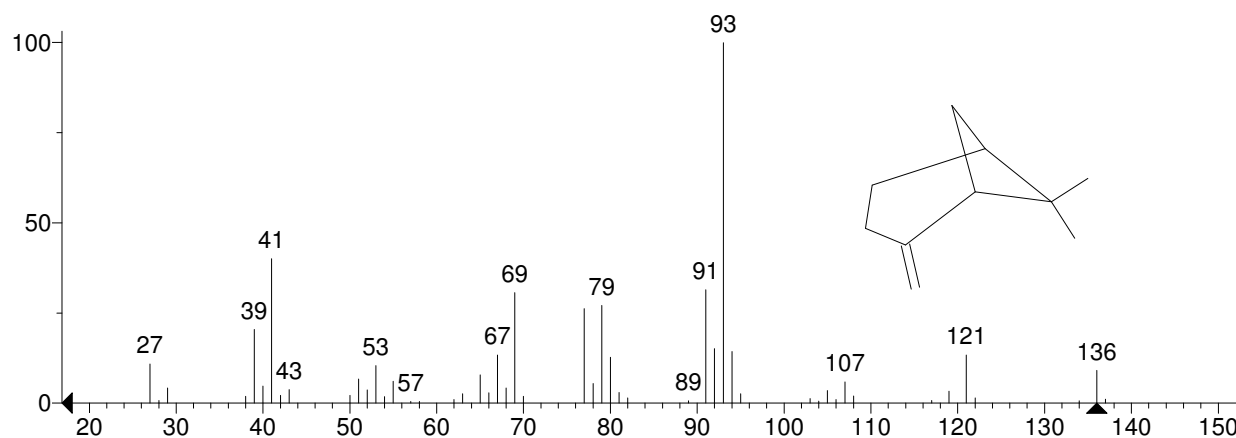
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Hit 1 : .beta.-Pinene
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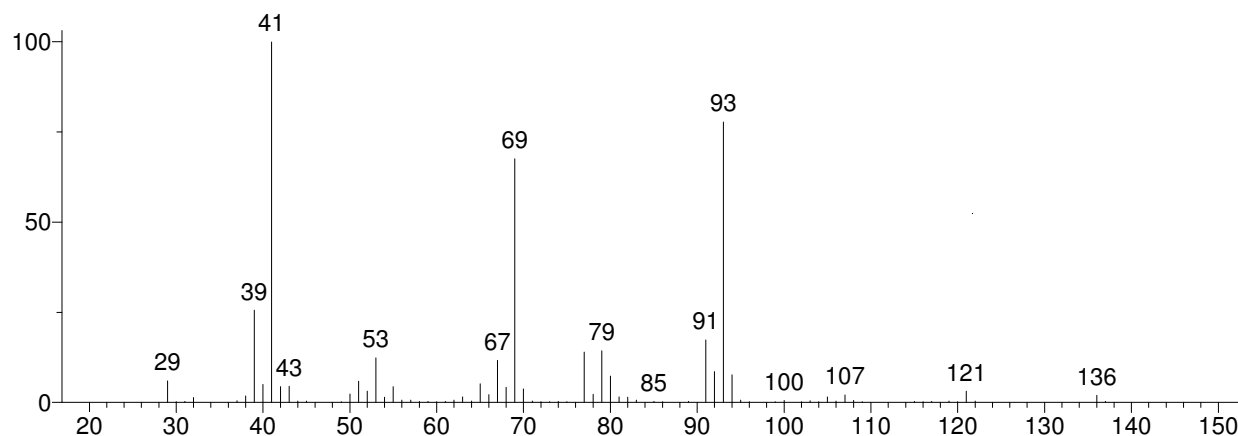


Hit 2 : Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-
C₁₀H₁₆; MF: 939; RMF: 944; Prob 29.4%; CAS: 18172-67-3; Lib: replib; ID: 11958.

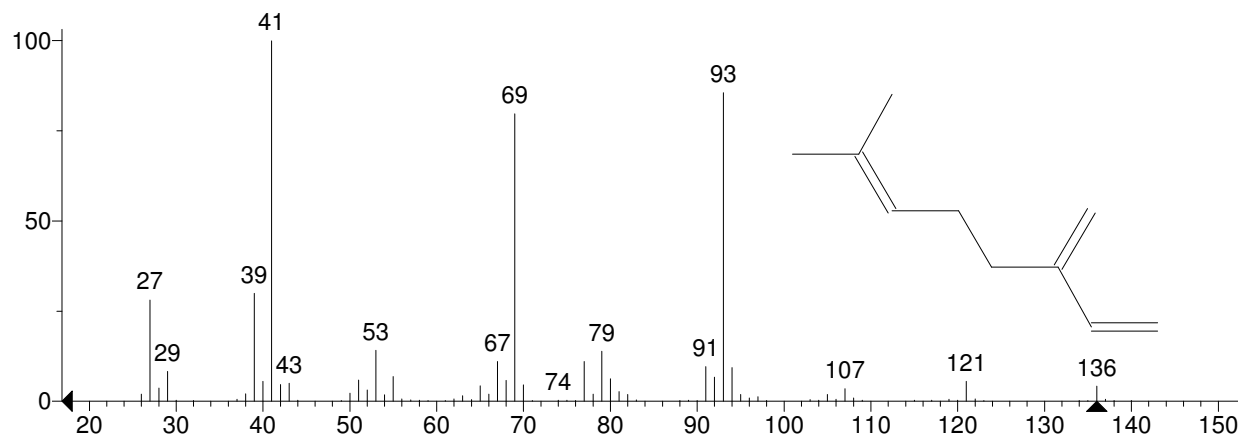


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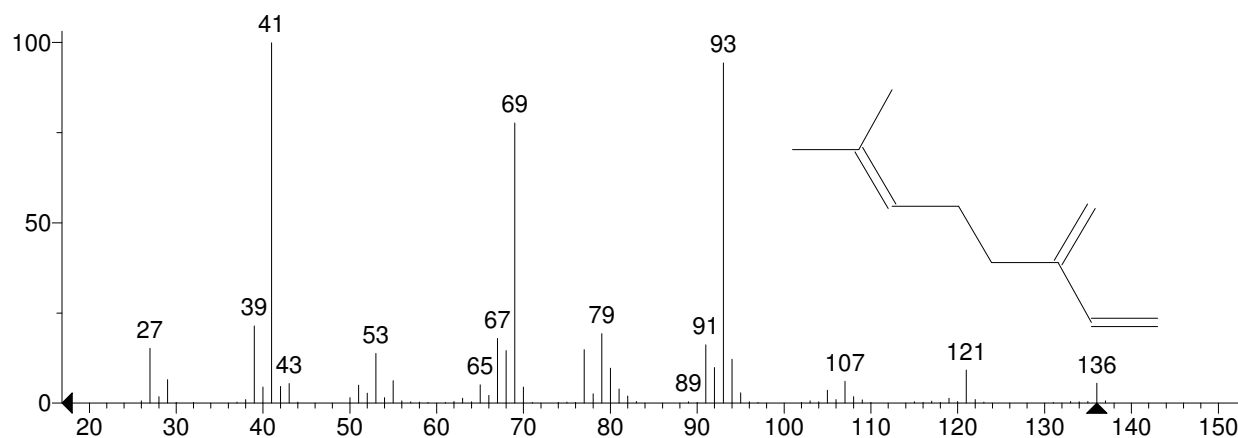
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Hit 1 : .beta.-Myrcene
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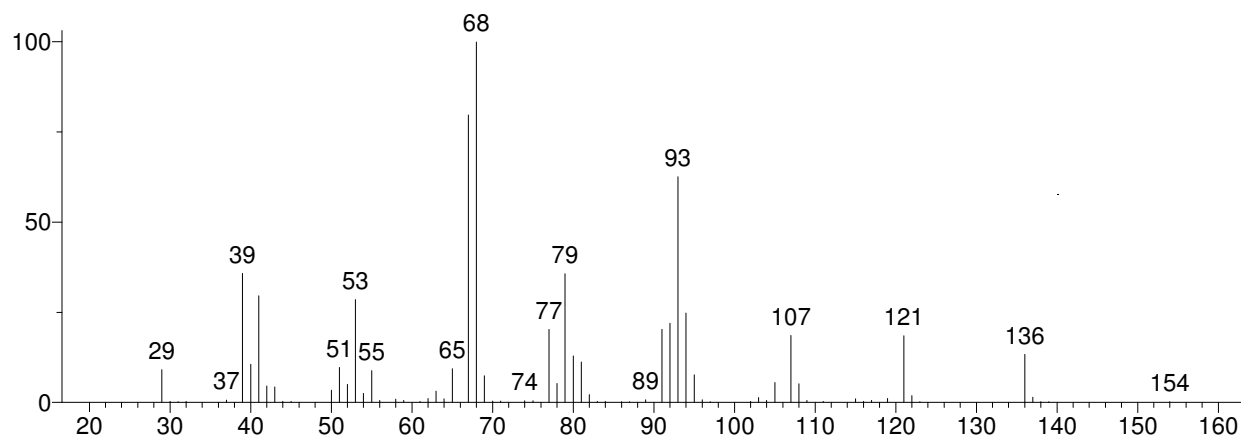


Hit 2 : .beta.-Myrcene
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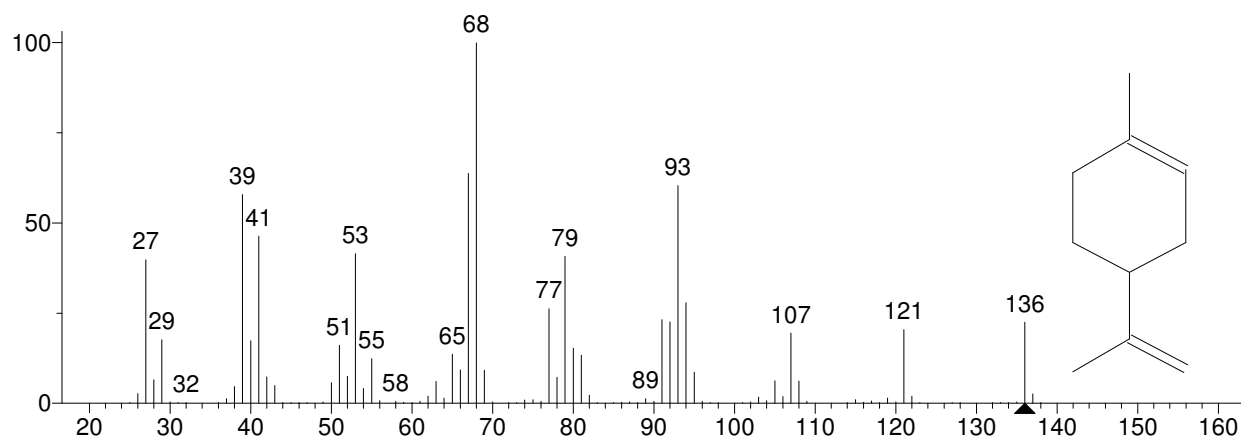


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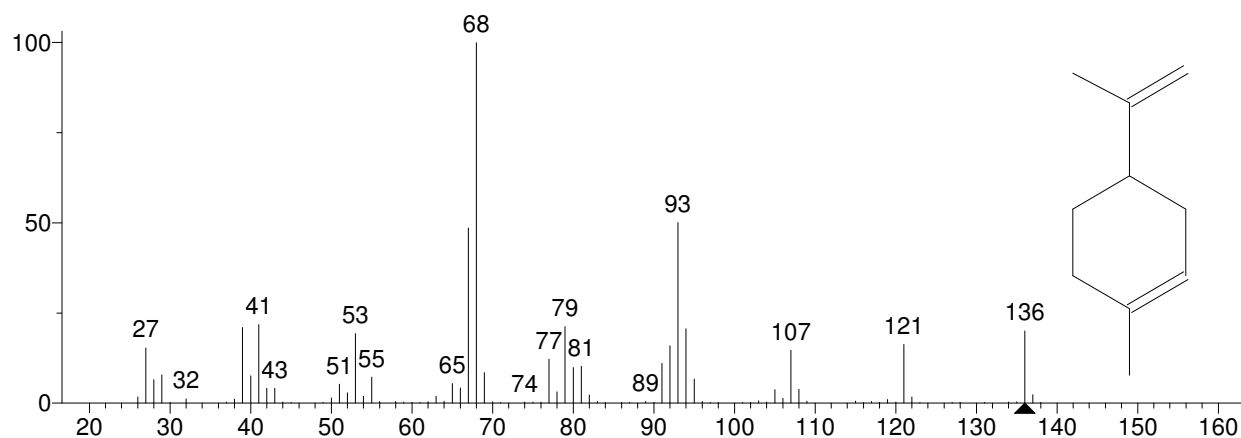
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Hit 1 : Limonene
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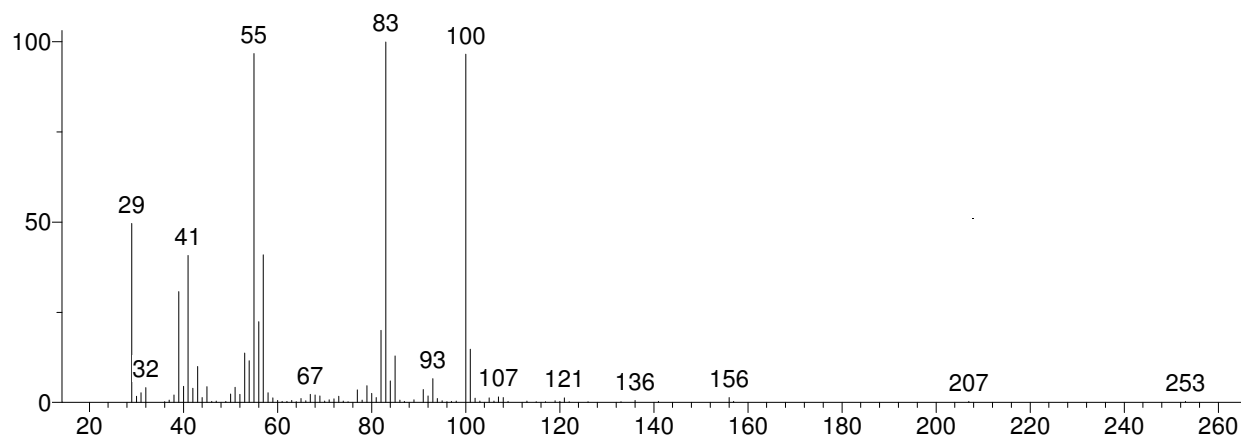


Hit 2 : D-Limonene
C₁₀H₁₆; MF: 931; RMF: 931; Prob 18.5%; CAS: 5989-27-5; Lib: replib; ID: 7415.

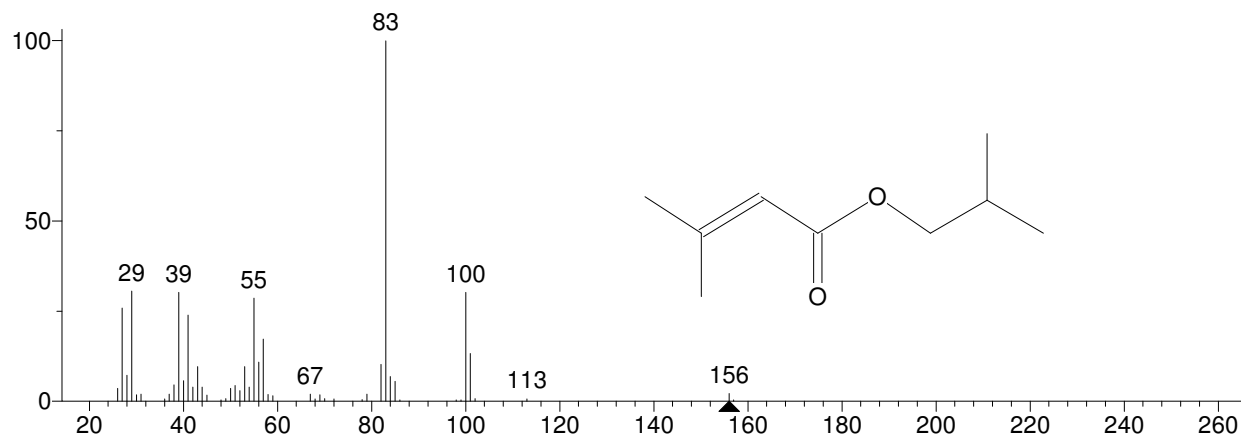


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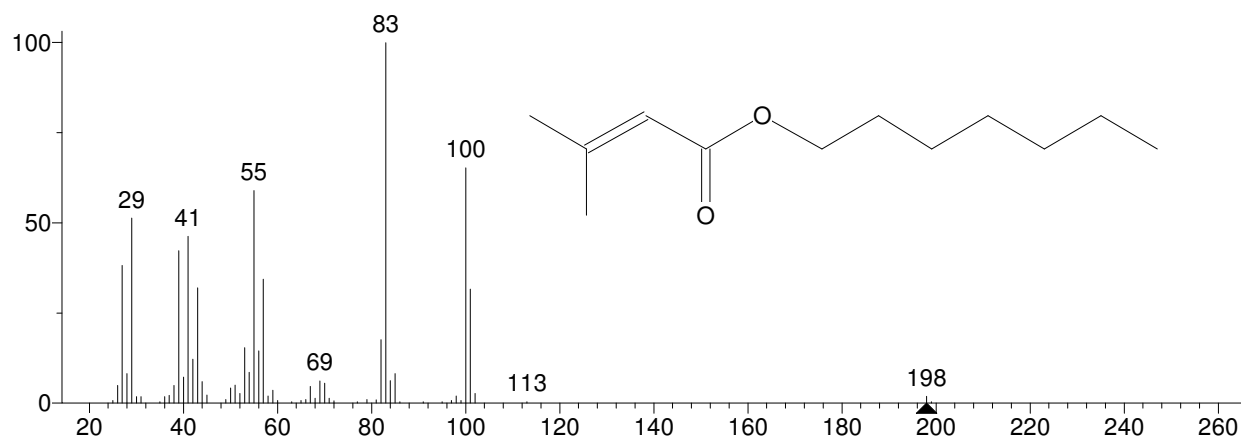
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Hit 1 : 2-Butenoic acid, 3-methyl-, 2-methylpropyl ester
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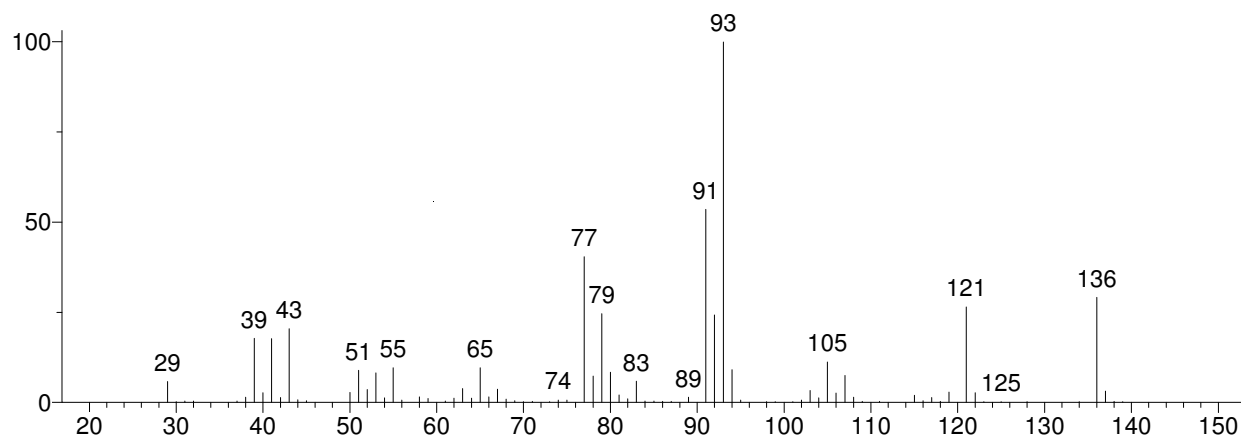


Hit 2 : 3-Methyl-2-butenoic acid, heptyl ester
C₁₂H₂₂O₂; MF: 815; RMF: 846; Prob 18.7%; Lib: mainlib; ID: 41622.

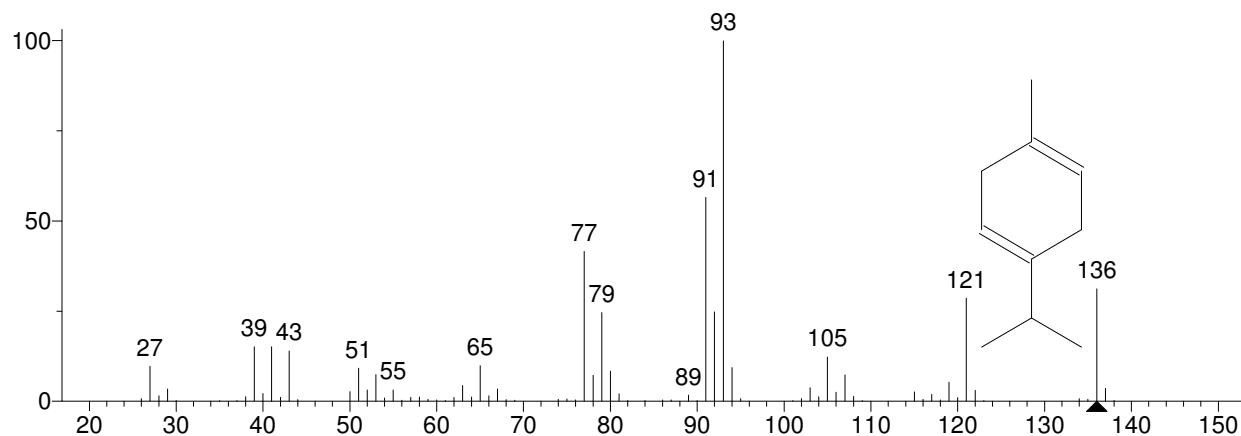


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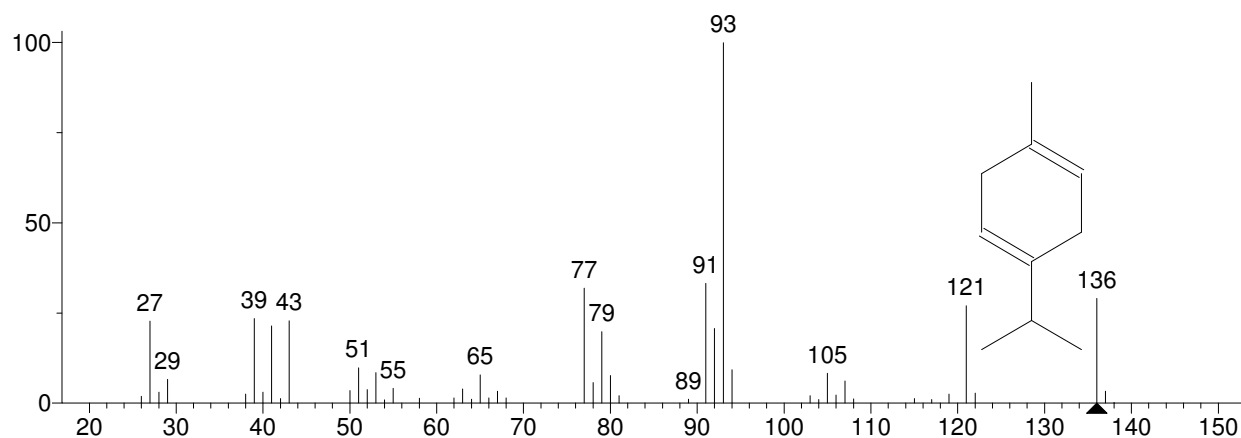
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Hit 1 : 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
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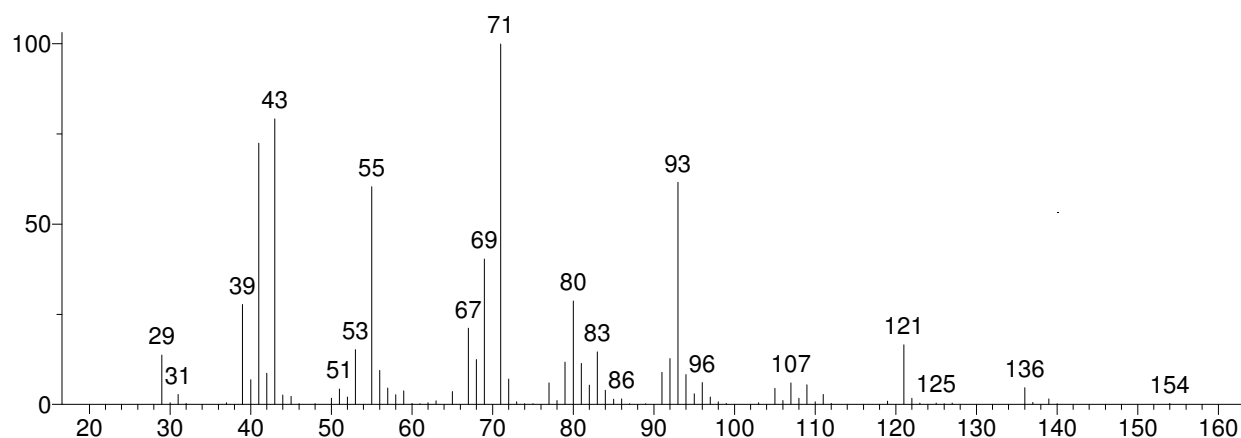


Hit 2 : 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
C₁₀H₁₆; MF: 946; RMF: 962; Prob 28.7%; CAS: 99-85-4; Lib: replib; ID: 12040.

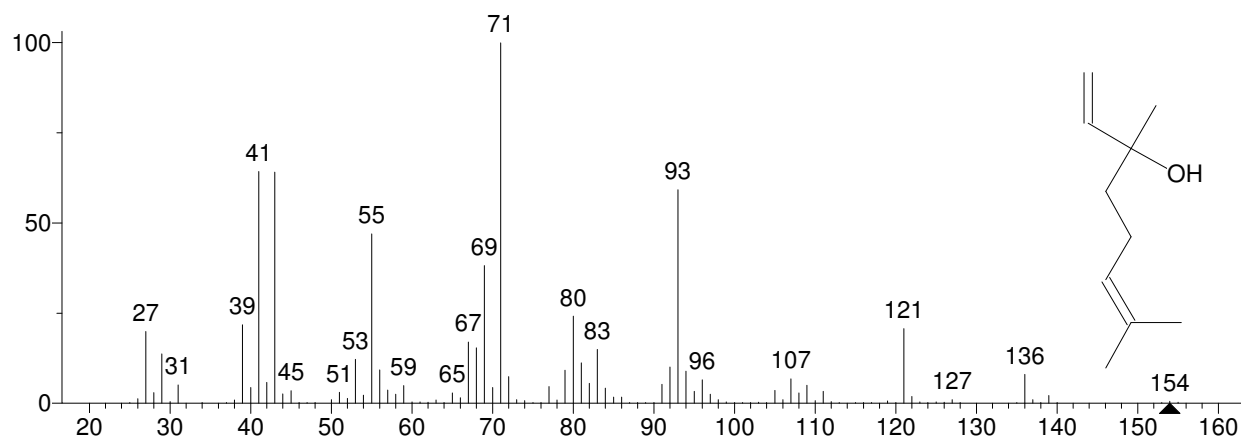


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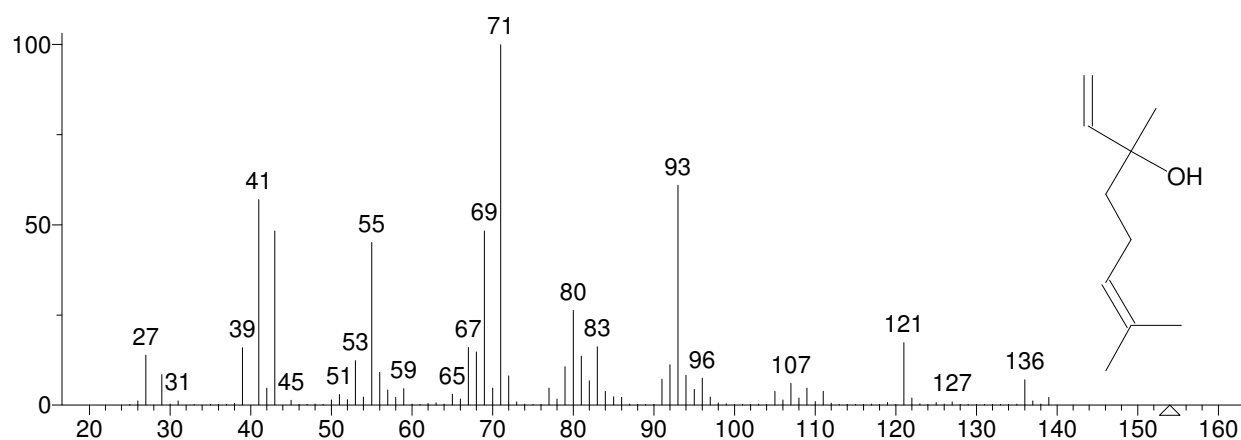
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Hit 1 : 1,6-Octadien-3-ol, 3,7-dimethyl-
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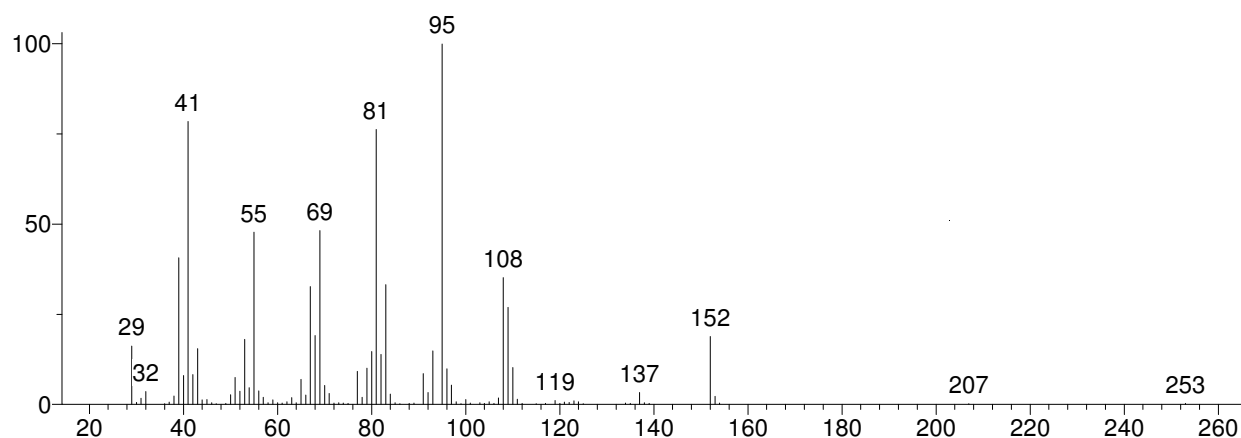


Hit 2 : 1,6-Octadien-3-ol, 3,7-dimethyl-
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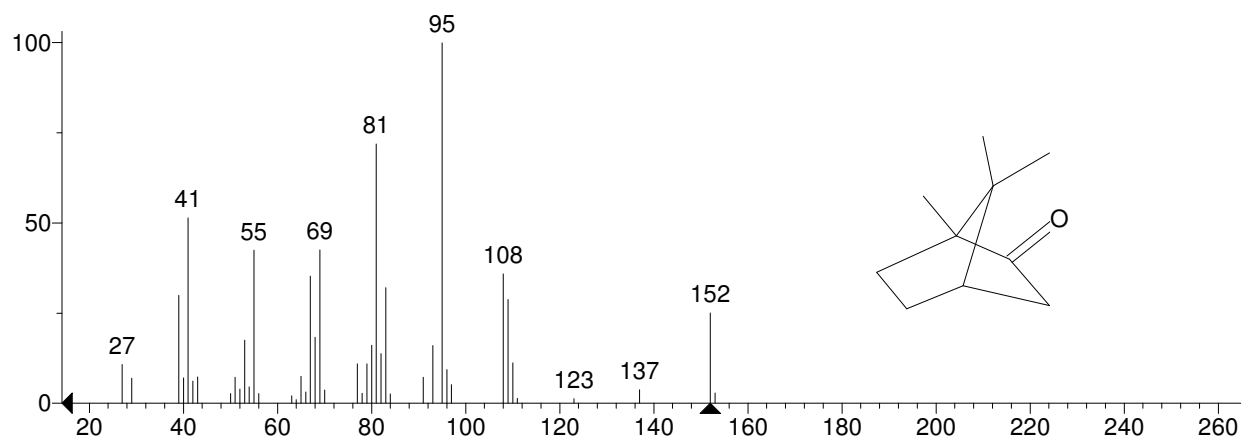


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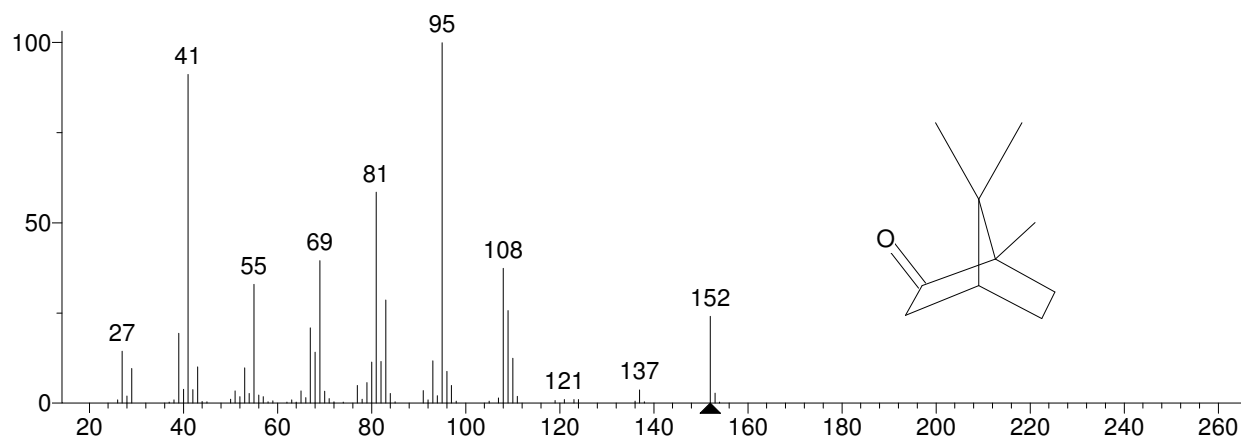
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Hit 1 : Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)-
C₁₀H₁₆O; MF: 942; RMF: 967; Prob 43.8%; CAS: 464-48-2; Lib: mainlib; ID: 53149.

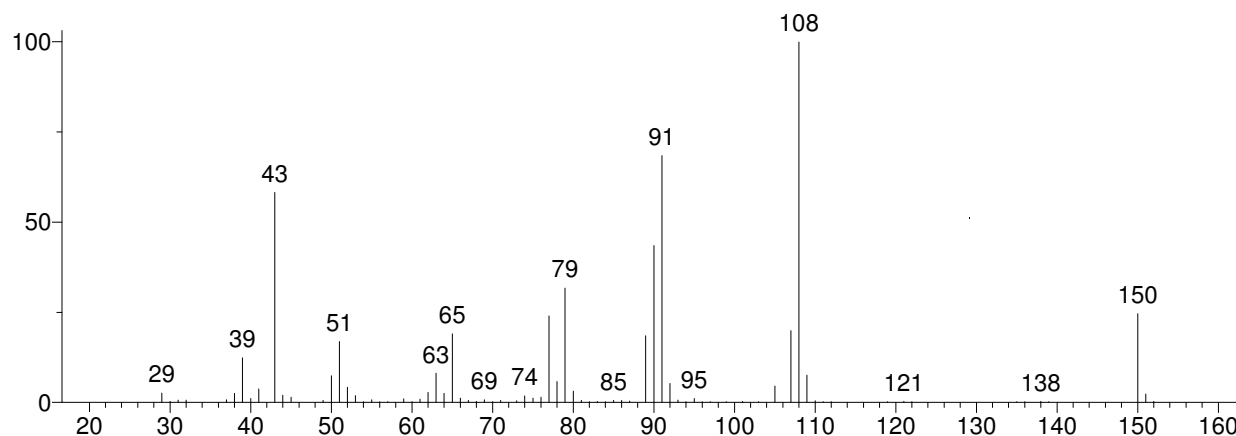


Hit 2 : Camphor
C₁₀H₁₆O; MF: 928; RMF: 936; Prob 27.4%; CAS: 76-22-2; Lib: replib; ID: 12335.

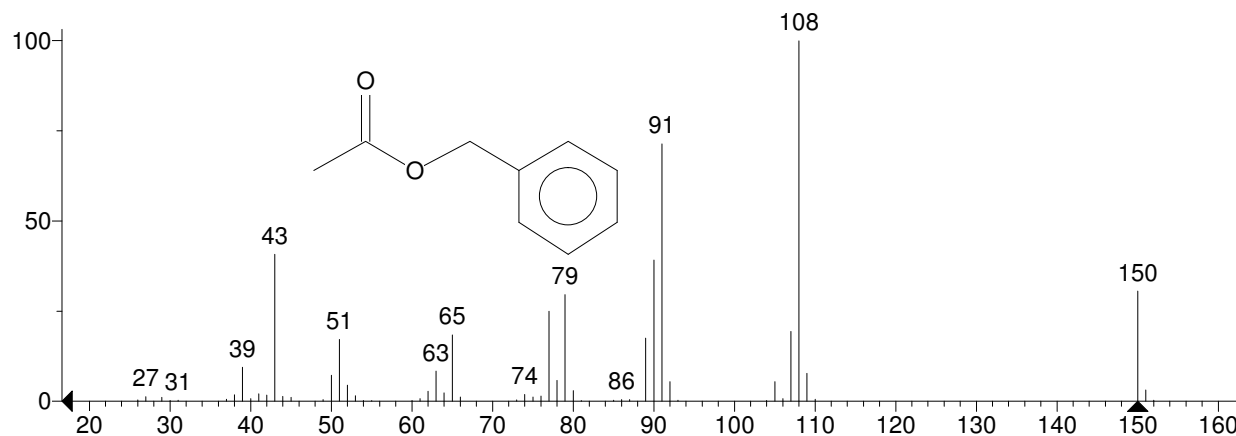


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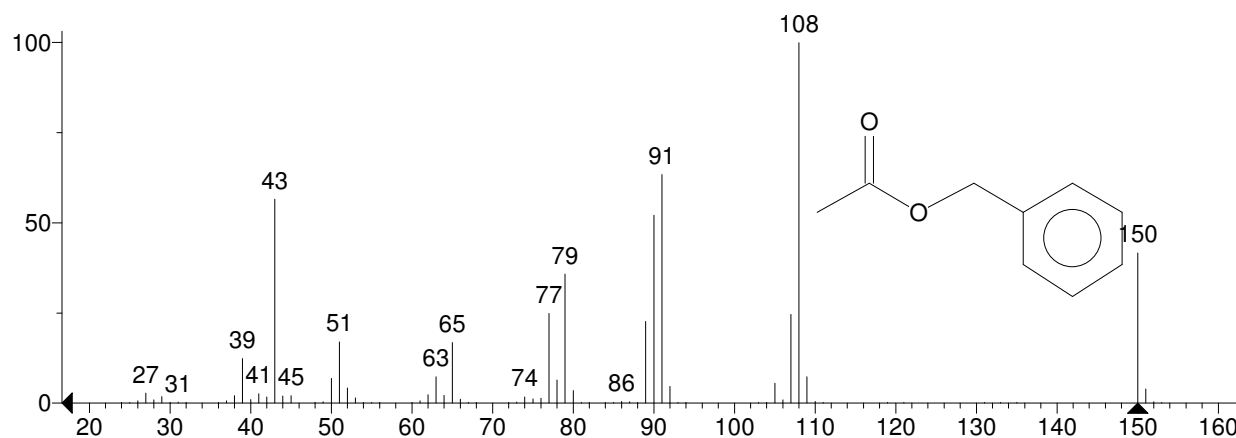
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Hit 1 : Acetic acid, phenylmethyl ester
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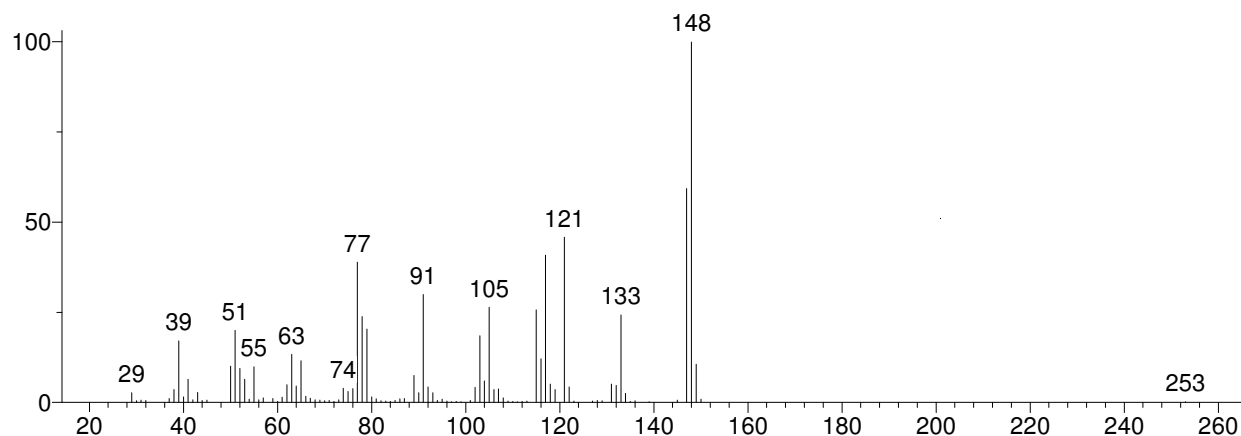


Hit 2 : Acetic acid, phenylmethyl ester
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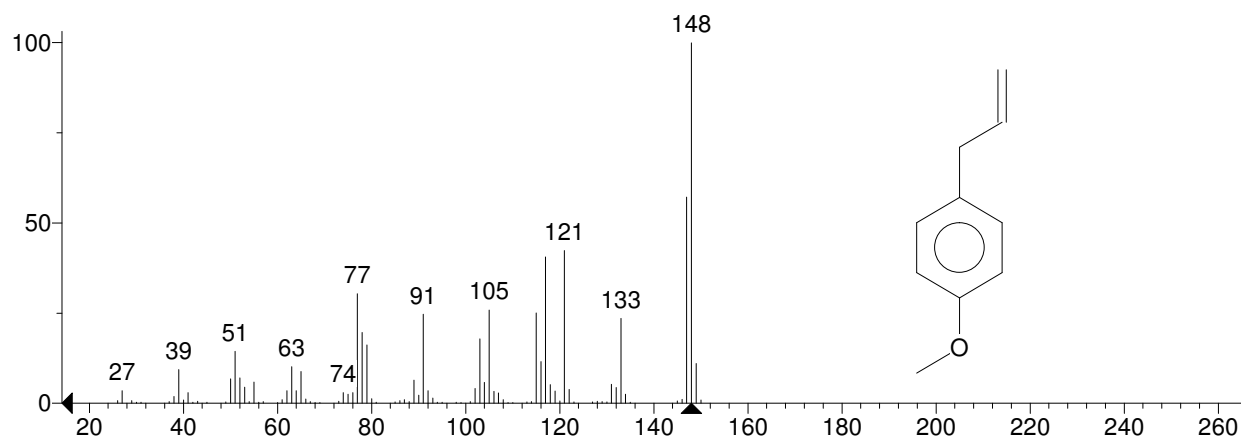


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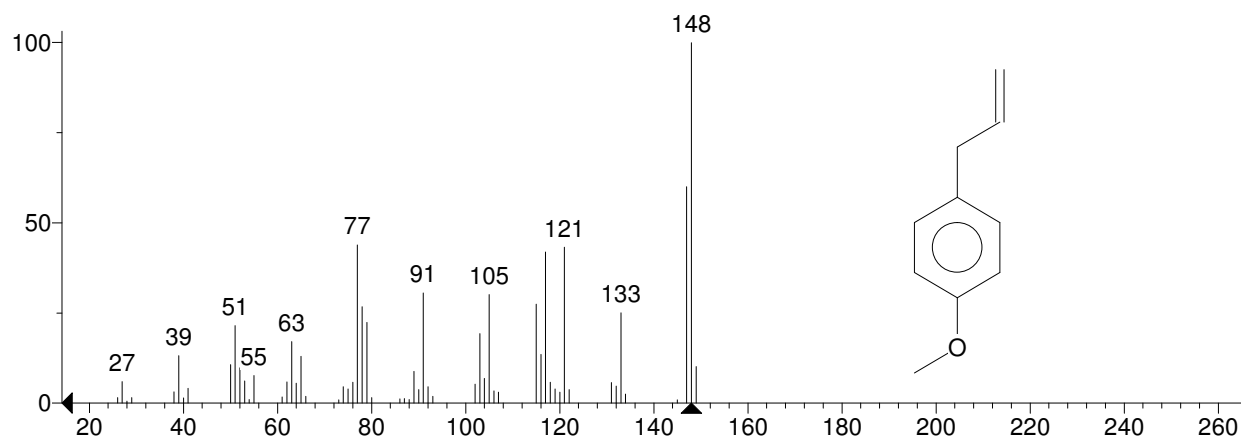
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Hit 1 : Estragole
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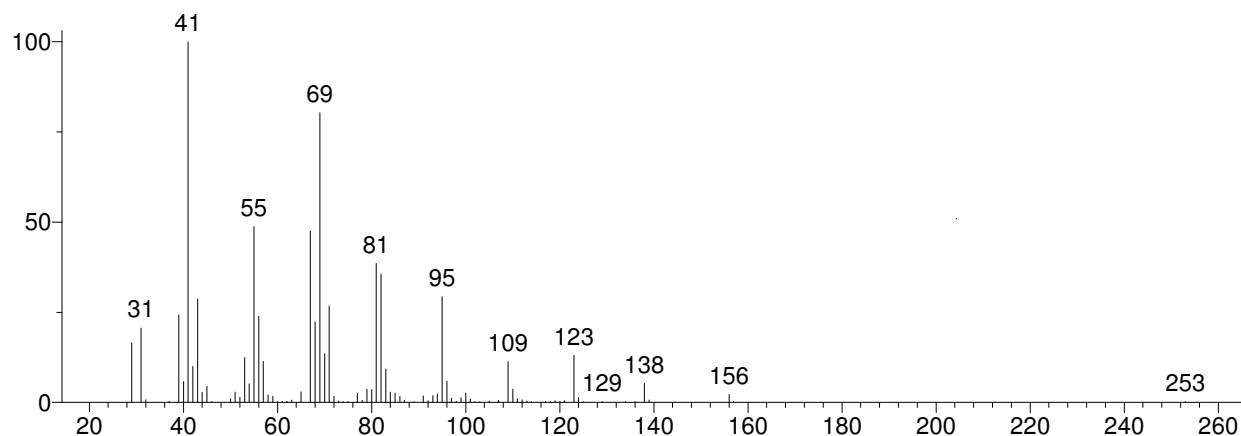


Hit 2 : Estragole
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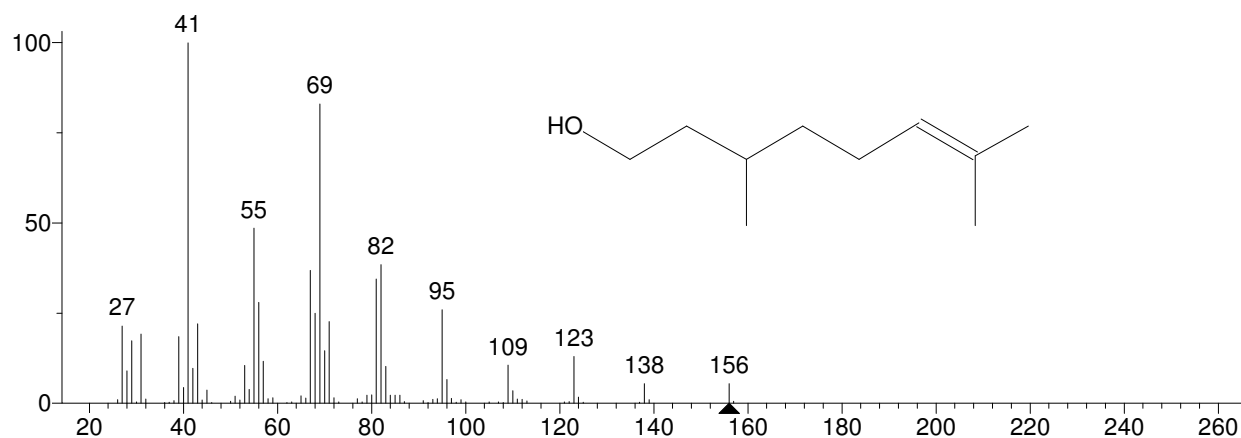


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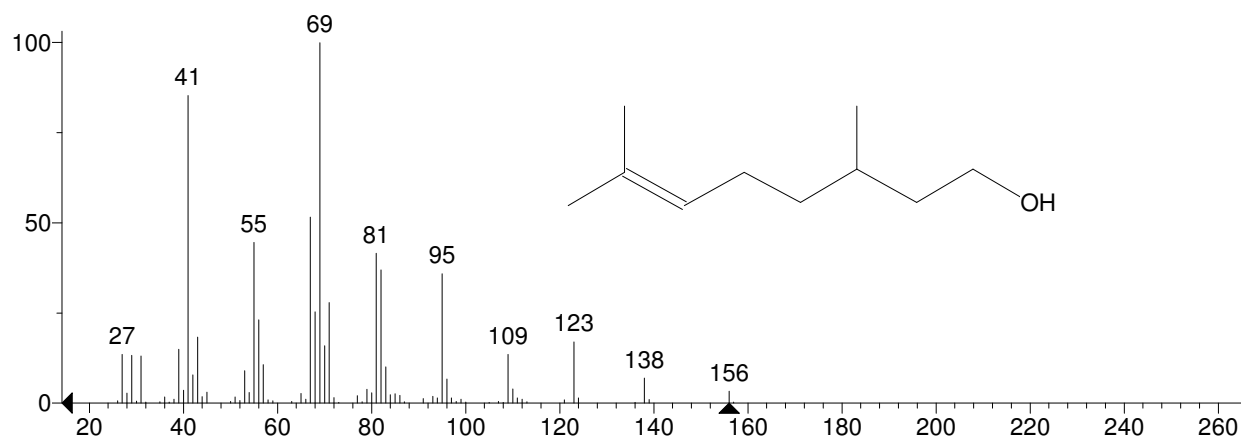
Unknown: Scan 764 (8.762 min): Designer3.D
Compound in Library Factor = -107



Hit 1 : 6-Octen-1-ol, 3,7-dimethyl-
C₁₀H₂₀O; MF: 922; RMF: 924; Prob 31.9%; CAS: 106-22-9; Lib: mainlib; ID: 3042.

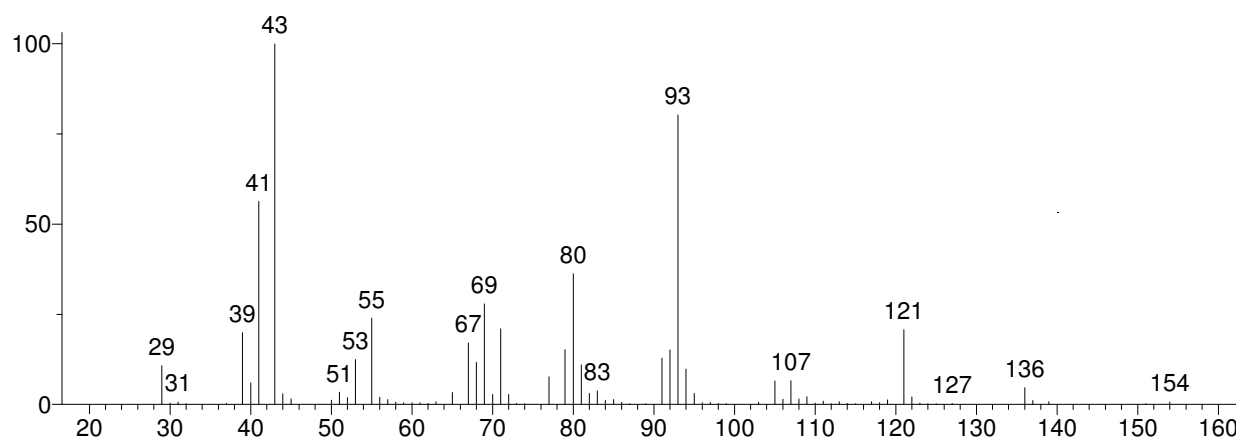


Hit 2 : 6-Octen-1-ol, 3,7-dimethyl-, (R)-
C₁₀H₂₀O; MF: 918; RMF: 921; Prob 26.9%; CAS: 1117-61-9; Lib: mainlib; ID: 28138.

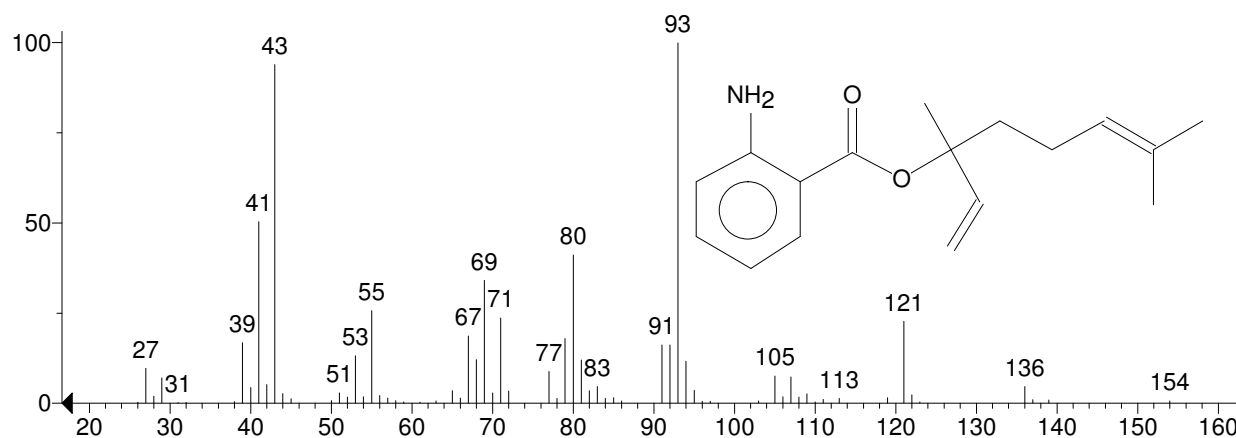


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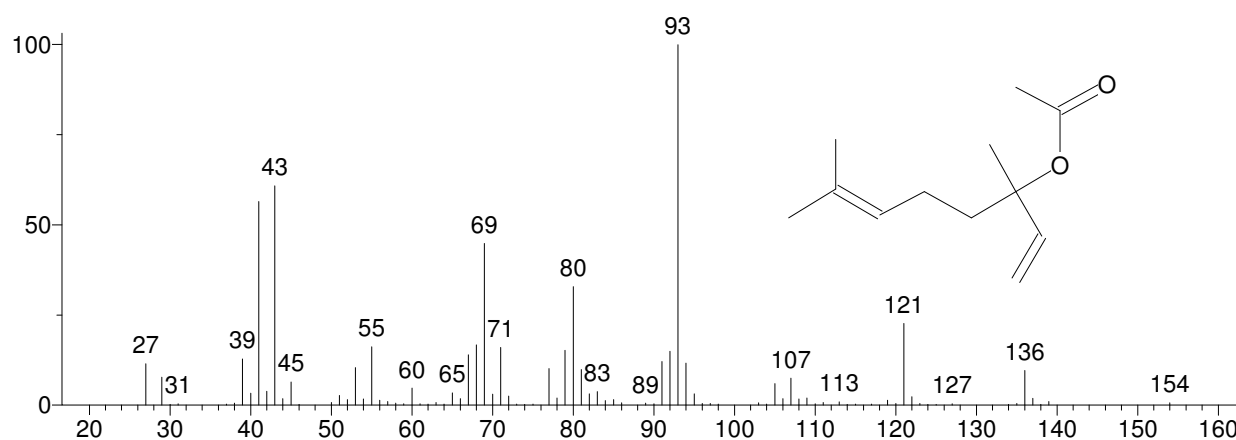
Unknown: Scan 784 (8.991 min): Designer3.D
Compound in Library Factor = 170



Hit 1 : 1,6-Octadien-3-ol, 3,7-dimethyl-, 2-aminobenzoate
C₁₇H₂₃NO₂; MF: 962; RMF: 966; Prob 76.1%; CAS: 7149-26-0; Lib: mainlib; ID: 51289.

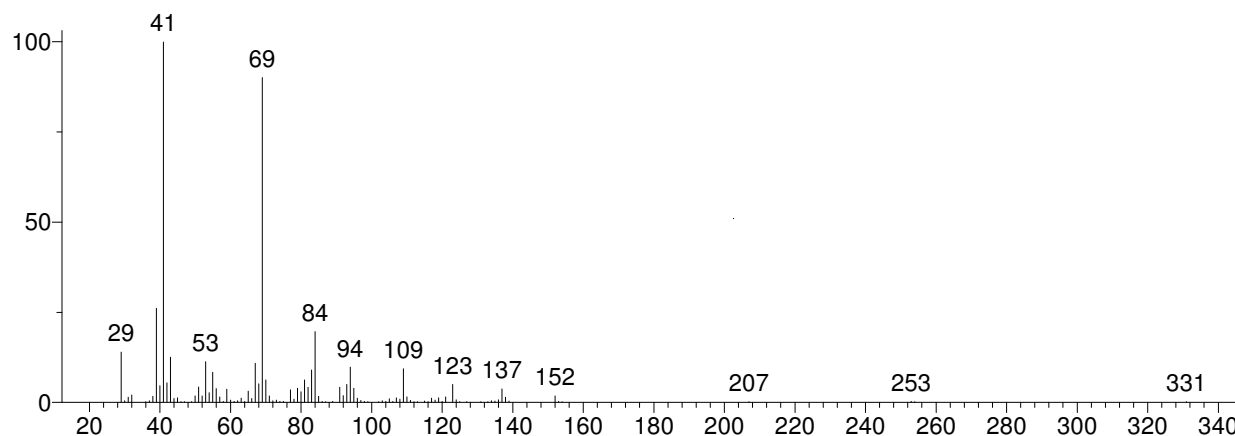


Hit 2 : 1,6-Octadien-3-ol, 3,7-dimethyl-, acetate
C₁₂H₂₀O₂; MF: 912; RMF: 912; Prob 15.5%; CAS: 115-95-7; Lib: mainlib; ID: 51290.

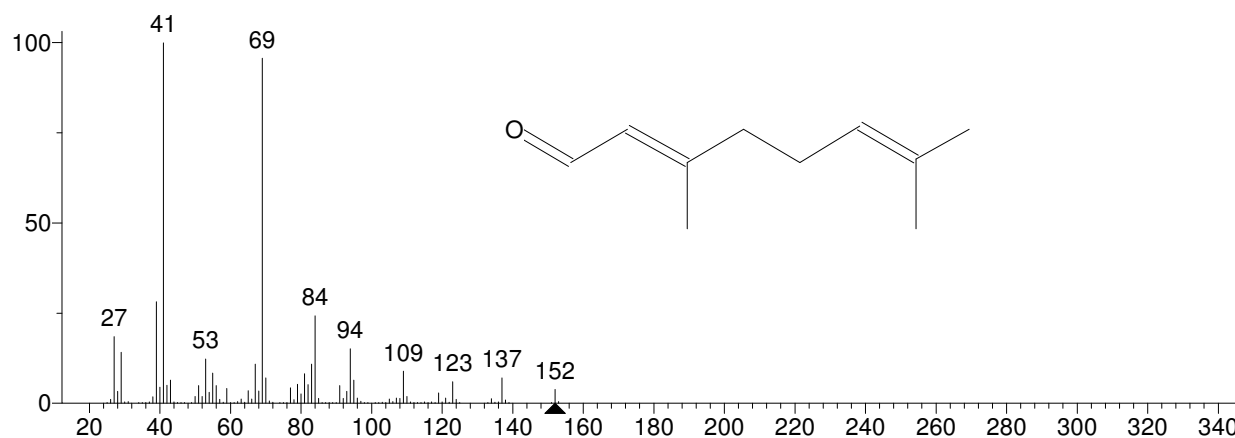


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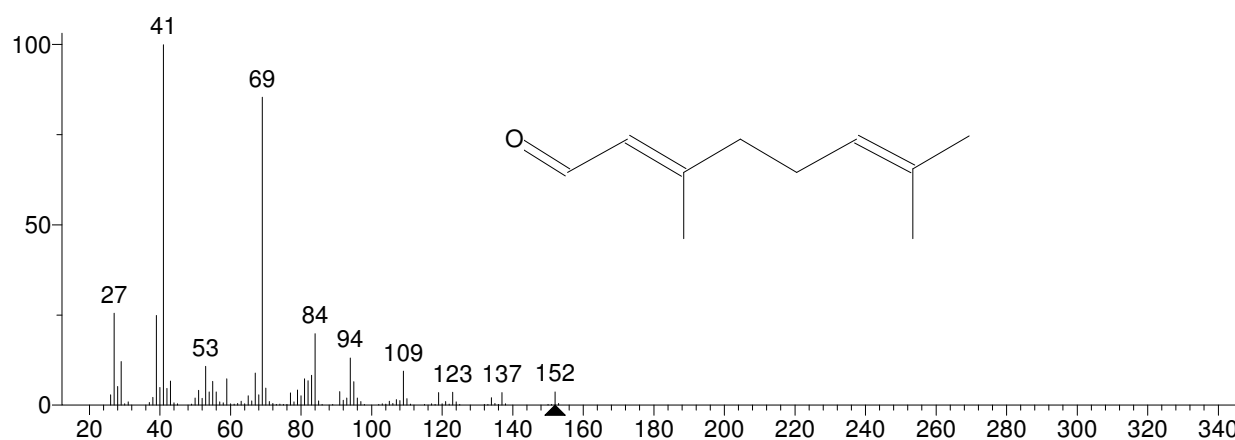
Unknown: Scan 794 (9.105 min): Designer3.D
Compound in Library Factor = 112



Hit 1 : 2,6-Octadienal, 3,7-dimethyl-, (E)-
C₁₀H₁₆O; MF: 885; RMF: 889; Prob 39.1%; CAS: 141-27-5; Lib: mainlib; ID: 2980.

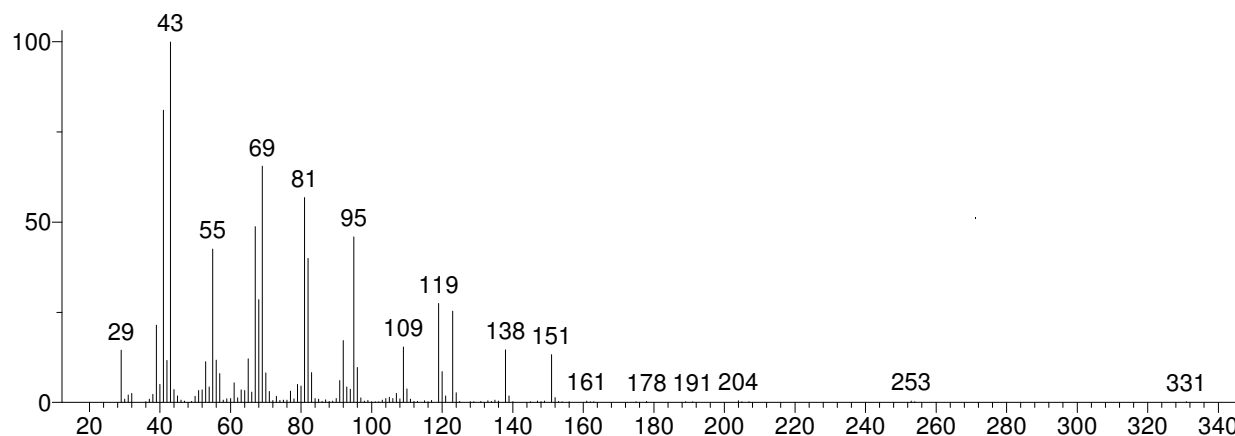


Hit 2 : 2,6-Octadienal, 3,7-dimethyl-, (Z)-
C₁₀H₁₆O; MF: 873; RMF: 878; Prob 26.0%; CAS: 106-26-3; Lib: mainlib; ID: 2942.

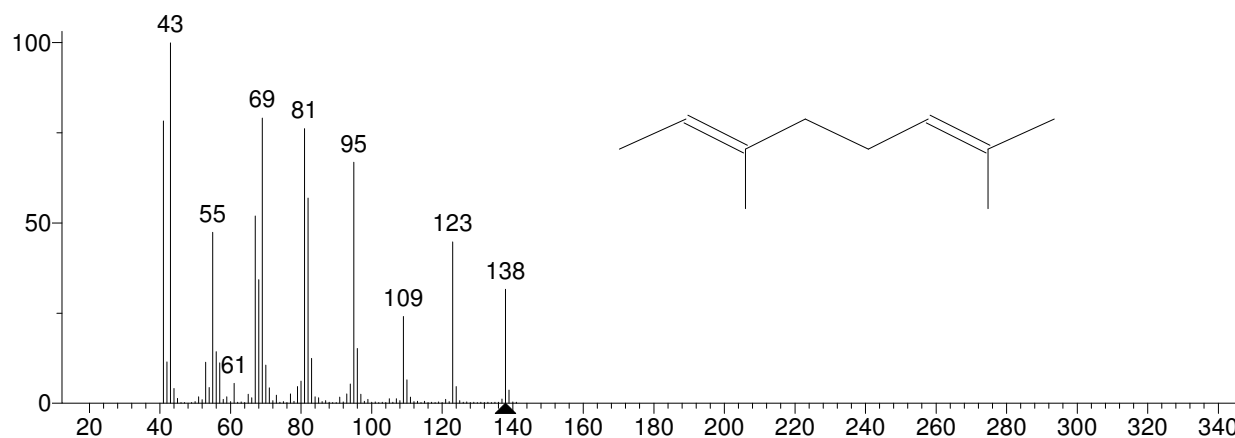


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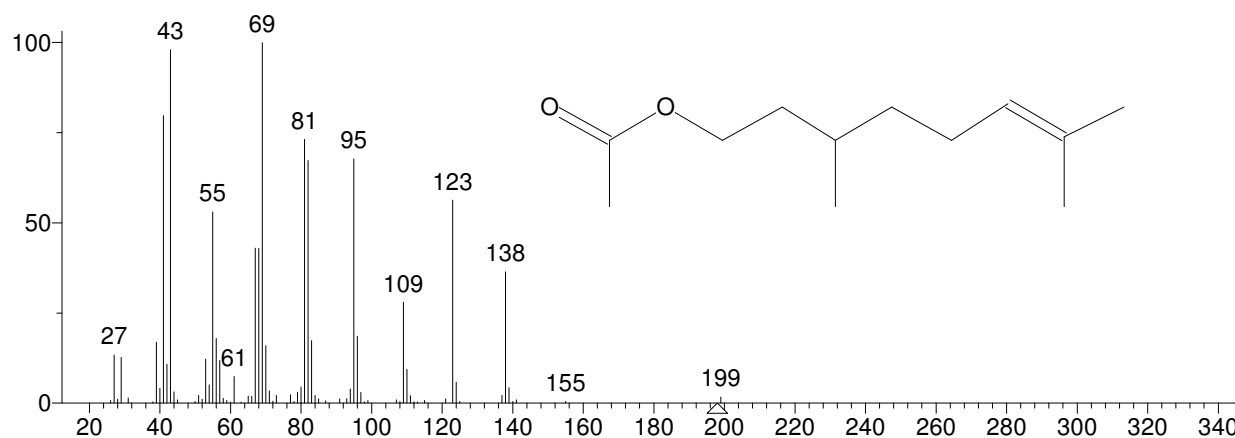
Unknown: Scan 858 (9.836 min): Designer3.D
Compound in Library Factor = -388



Hit 1 : 2,6-Octadiene, 2,6-dimethyl-
C₁₀H₁₈; MF: 801; RMF: 822; Prob 14.3%; CAS: 2792-39-4; Lib: replib; ID: 2290.

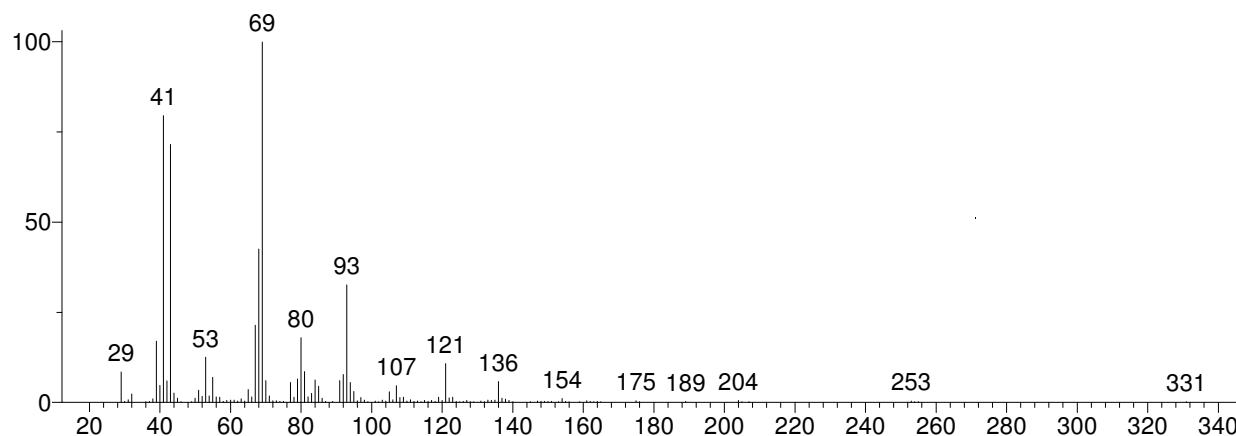


Hit 2 : 6-Octen-1-ol, 3,7-dimethyl-, acetate
C₁₂H₂₂O₂; MF: 799; RMF: 882; Prob 13.2%; CAS: 150-84-5; Lib: replib; ID: 7605.

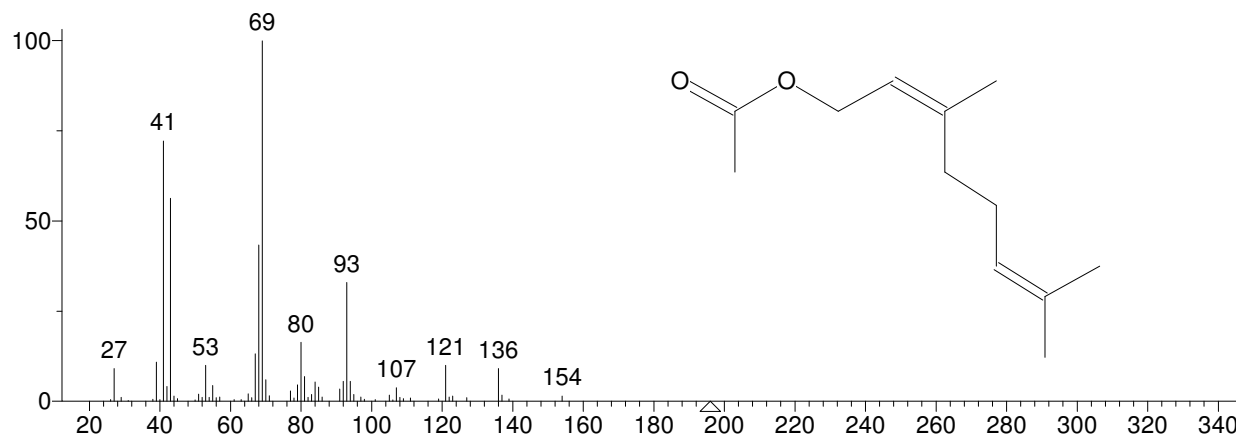


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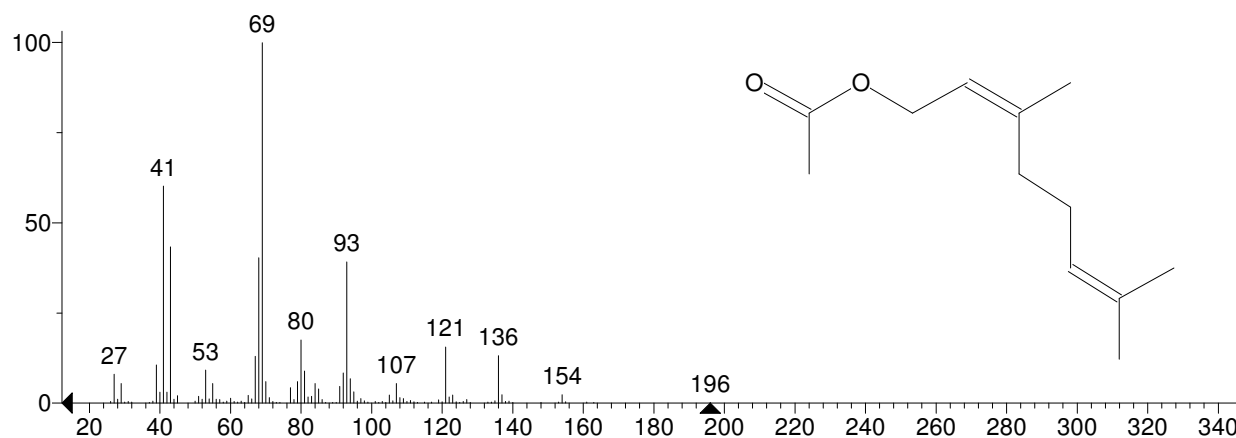
Unknown: Scan 868 (9.950 min): Designer3.D
Compound in Library Factor = 103



Hit 1 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-
C₁₂H₂₀O₂; MF: 916; RMF: 944; Prob 44.9%; CAS: 141-12-8; Lib: replib; ID: 7487.

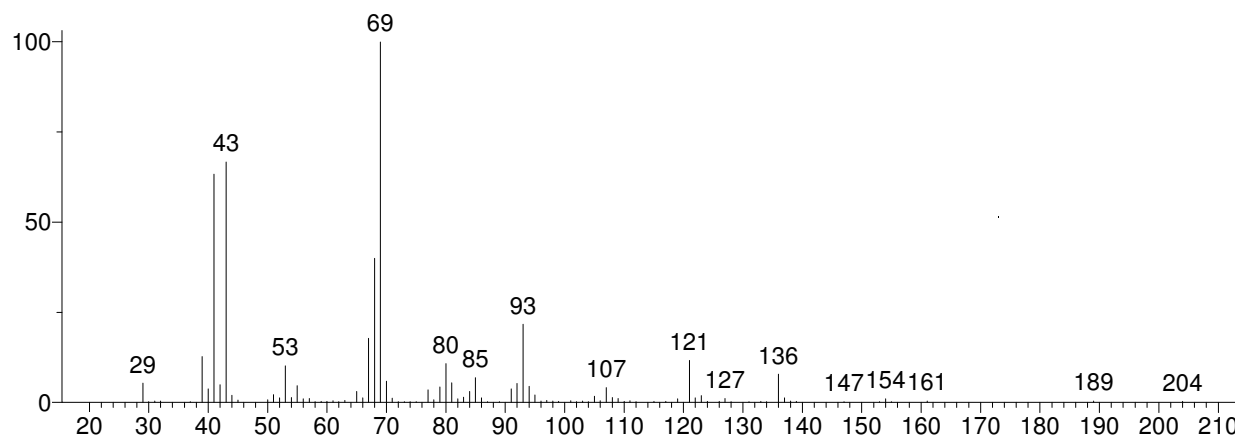


Hit 2 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-
C₁₂H₂₀O₂; MF: 898; RMF: 906; Prob 44.9%; CAS: 141-12-8; Lib: mainlib; ID: 28008.

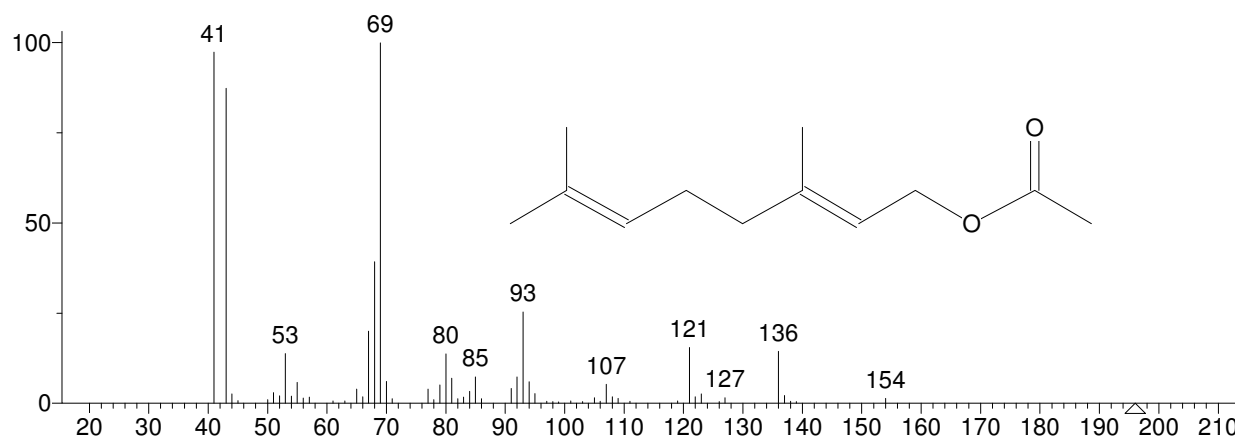


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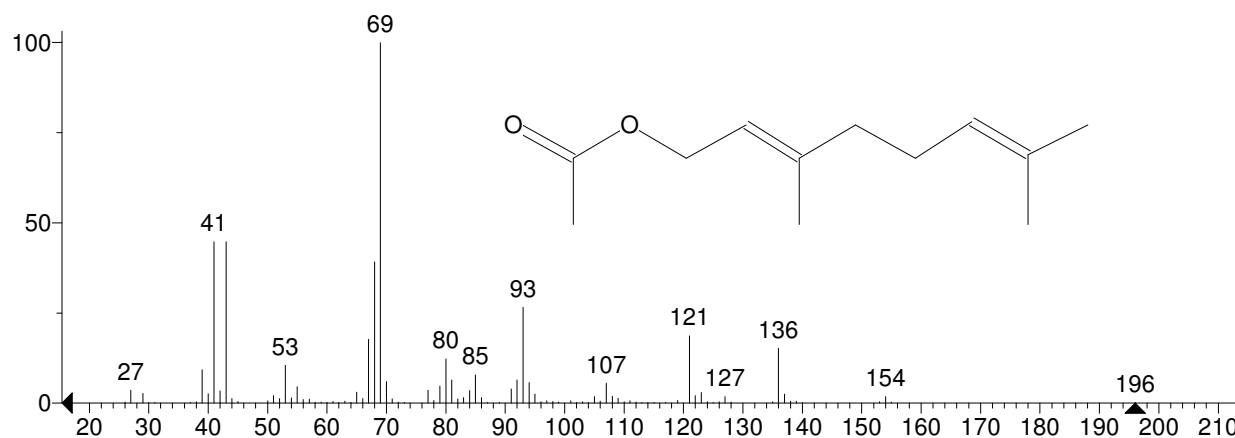
Unknown: Scan 886 (10.155 min): Designer3.D
Compound in Library Factor = 168



Hit 1 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate
C₁₂H₂₀O₂; MF: 957; RMF: 966; Prob 47.4%; CAS: 16409-44-2; Lib: replib; ID: 7488.

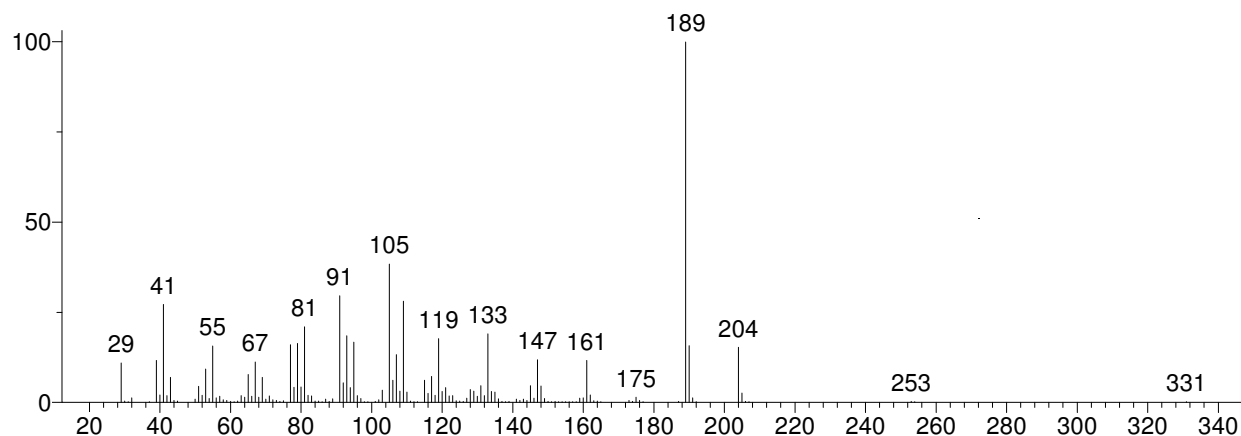


Hit 2 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (E)-
C₁₂H₂₀O₂; MF: 947; RMF: 950; Prob 33.5%; CAS: 105-87-3; Lib: replib; ID: 7492.

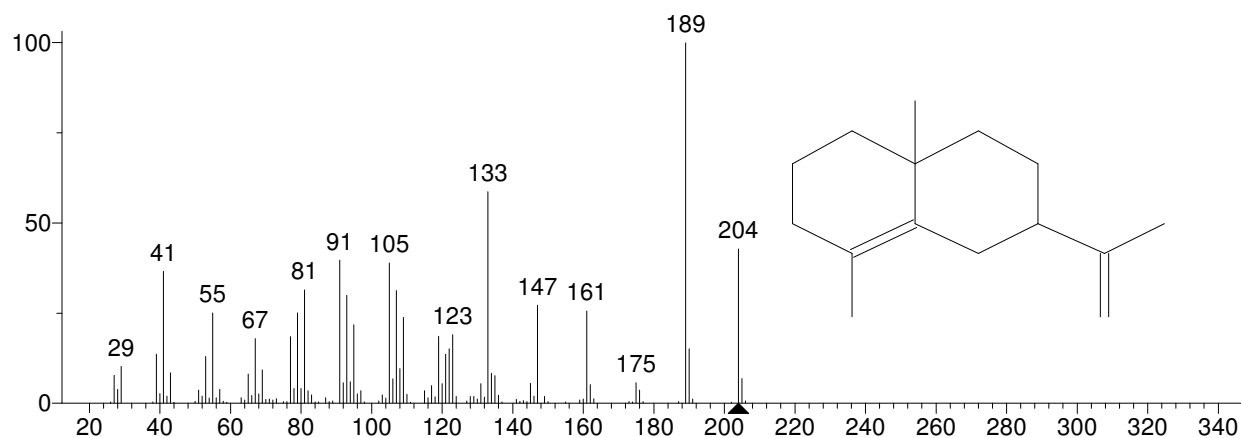


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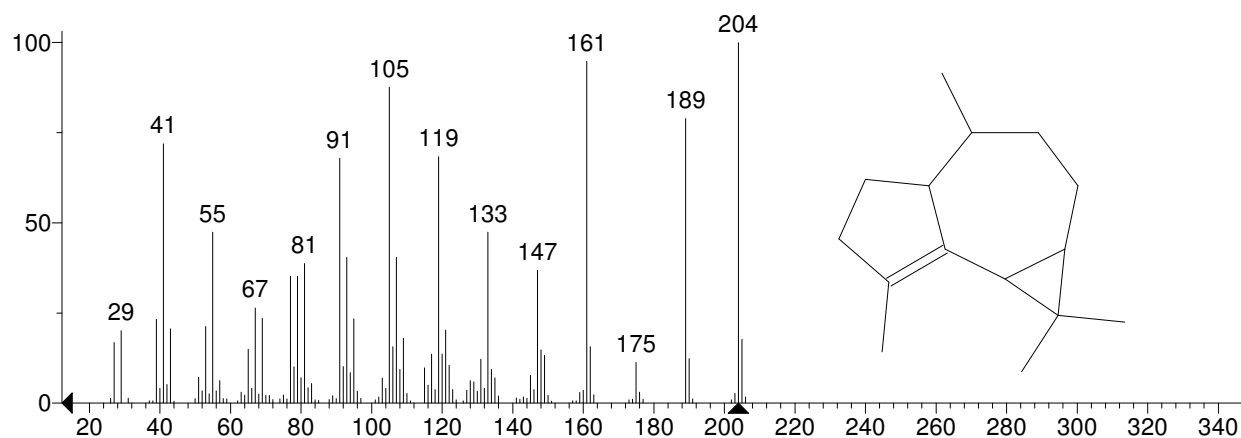
Unknown: Scan 899 (10.304 min): Designer3.D
Compound in Library Factor = -185



Hit 1 : 2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene
C₁₅H₂₄; MF: 881; RMF: 888; Prob 16.0%; Lib: mainlib; ID: 118910.

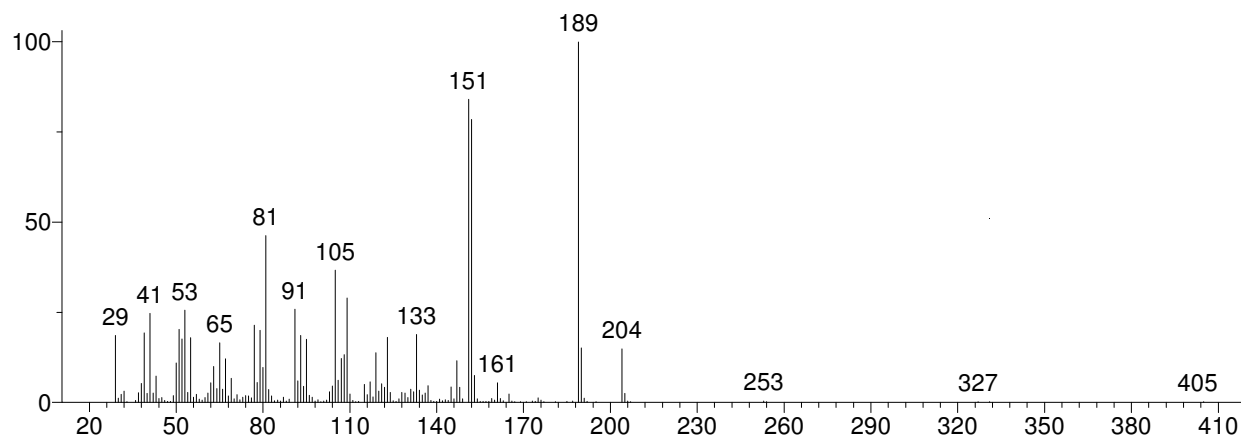


Hit 2 : 1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.alpha.,4a.beta.,7
C₁₅H₂₄; MF: 862; RMF: 865; Prob 7.74%; CAS: 489-40-7; Lib: mainlib; ID: 125451.

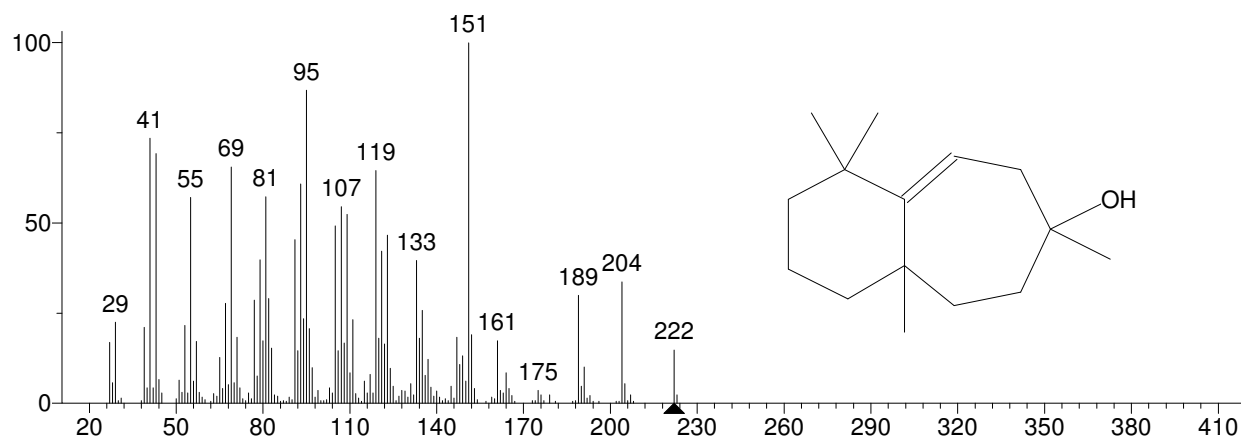


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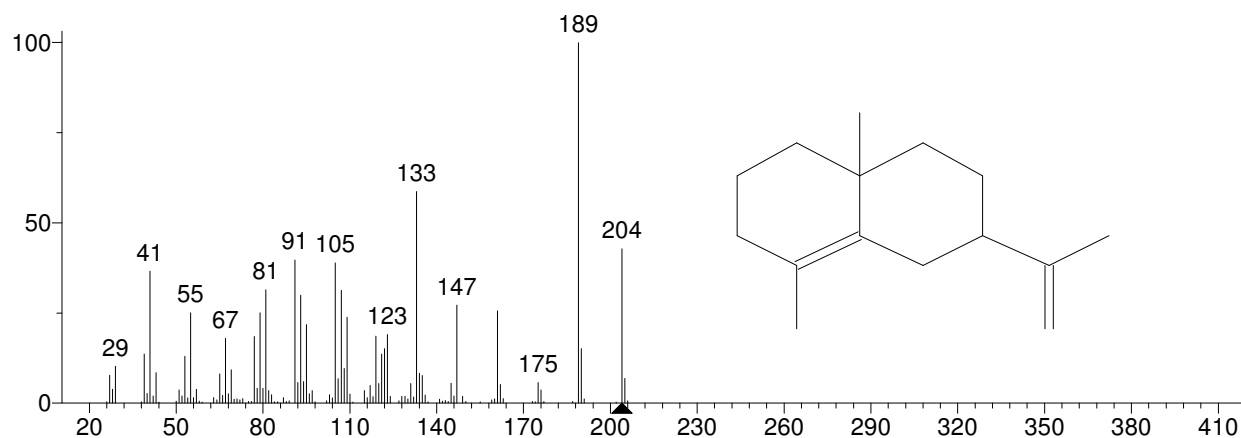
Unknown: Scan 915 (10.486 min): Designer3.D
Compound in Library Factor = -733



Hit 1 : 1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-
C₁₅H₂₆O; MF: 742; RMF: 745; Prob 20.8%; CAS: 6892-80-4; Lib: replib; ID: 19977.

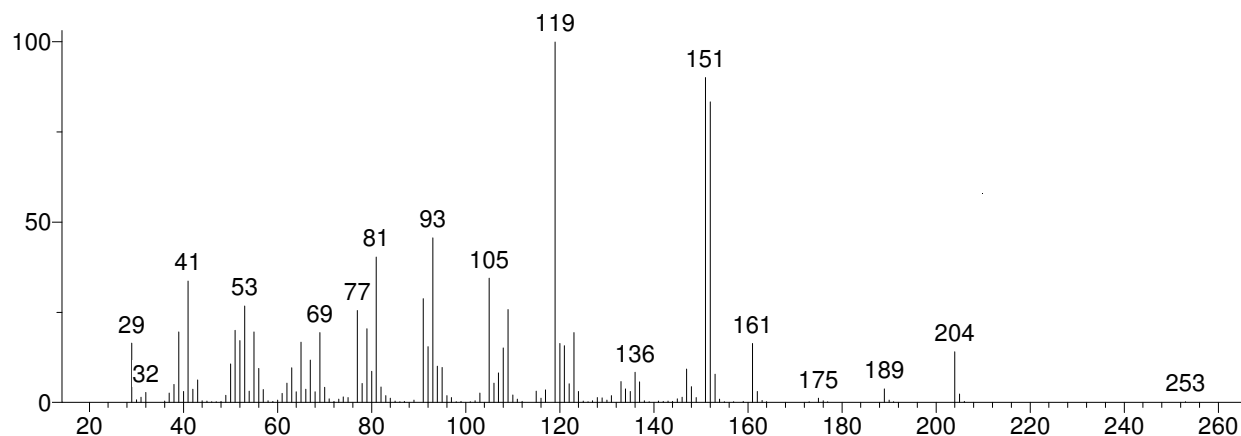


Hit 2 : 2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene
C₁₅H₂₄; MF: 728; RMF: 853; Prob 13.0%; Lib: mainlib; ID: 118910.

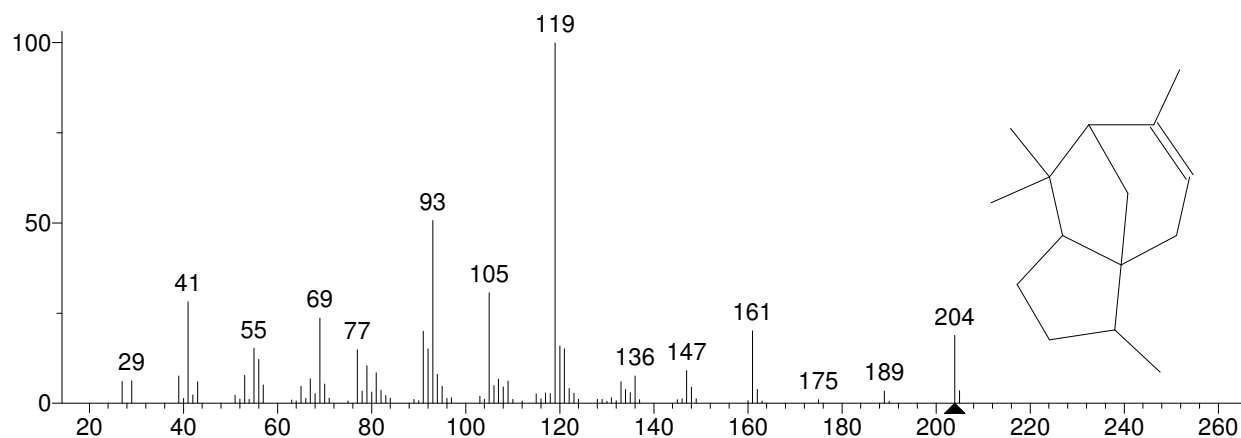


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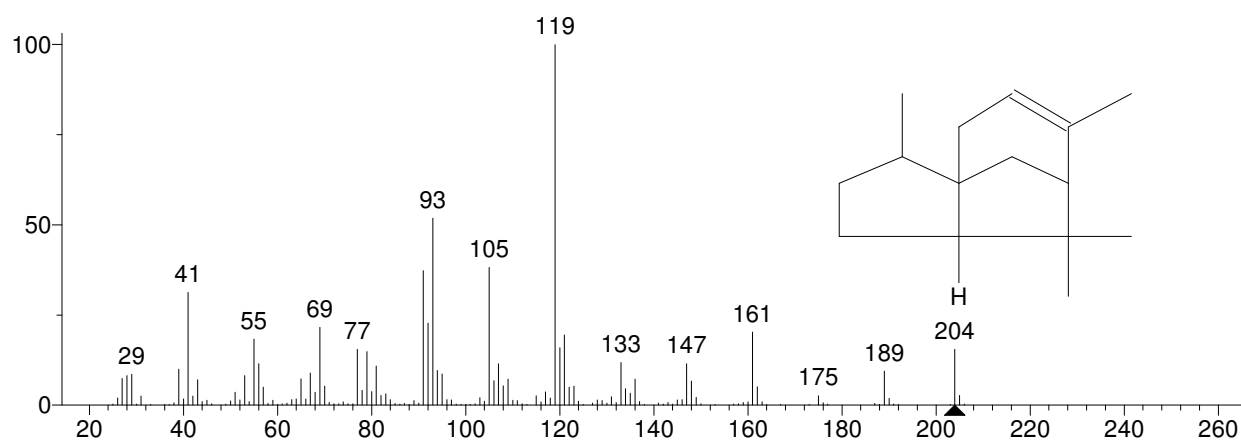
Unknown: Scan 928 (10.635 min): Designer3.D
Compound in Library Factor = -804



Hit 1 : 1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)] C₁₅H₂₄; MF: 743; RMF: 887; Prob 13.3%; CAS: 469-61-4; Lib: replib; ID: 15877.

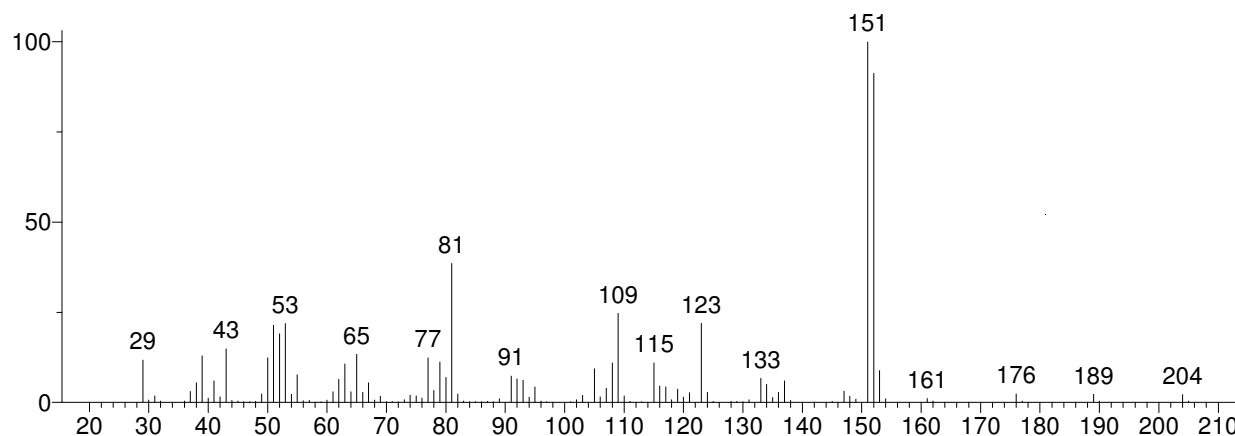


Hit 2 : Di-epi-alpha-cedrene
C₁₅H₂₄; MF: 740; RMF: 859; Prob 11.8%; Lib: mainlib; ID: 72092.

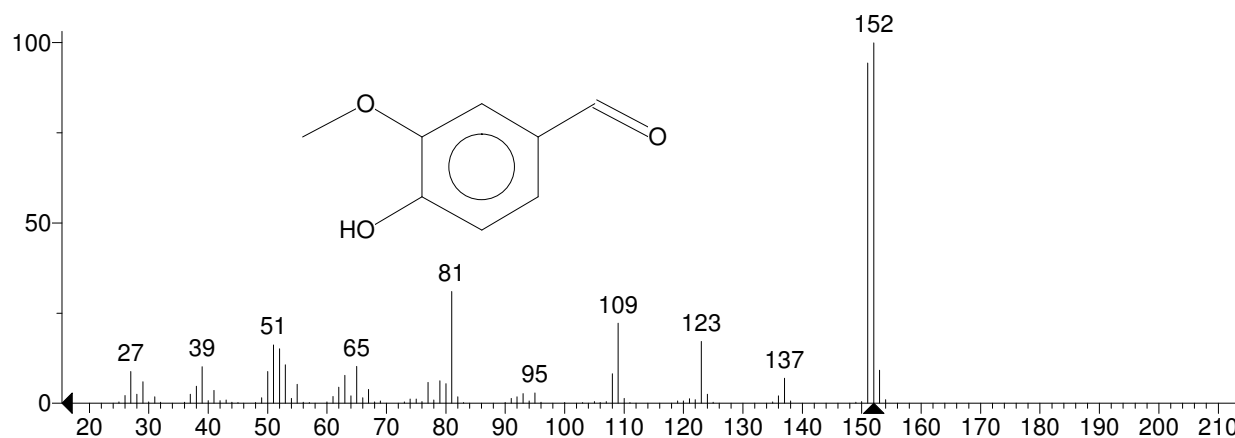


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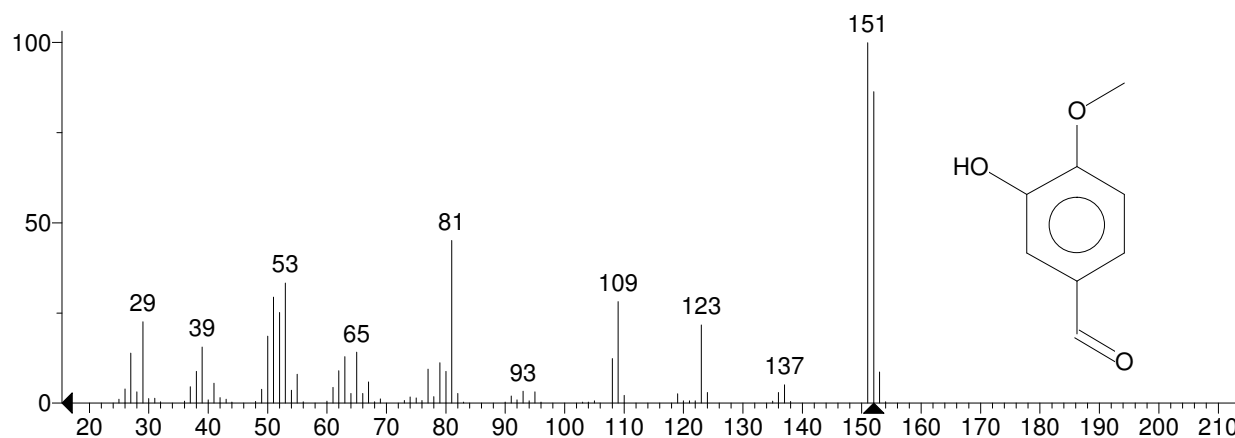
Unknown: Scan 944 (10.818 min): Designer3.D
Compound in Library Factor = -181



Hit 1 : Vanillin
C₈H₈O₃; MF: 855; RMF: 905; Prob 37.2%; CAS: 121-33-5; Lib: mainlib; ID: 98716.

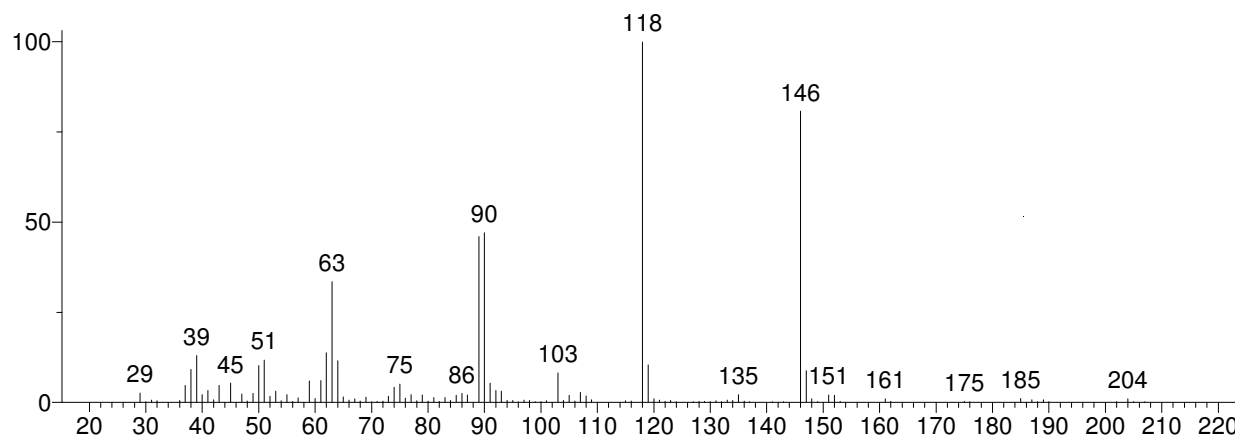


Hit 2 : Benzaldehyde, 3-hydroxy-4-methoxy-
C₈H₈O₃; MF: 854; RMF: 912; Prob 35.8%; CAS: 621-59-0; Lib: replib; ID: 20012.

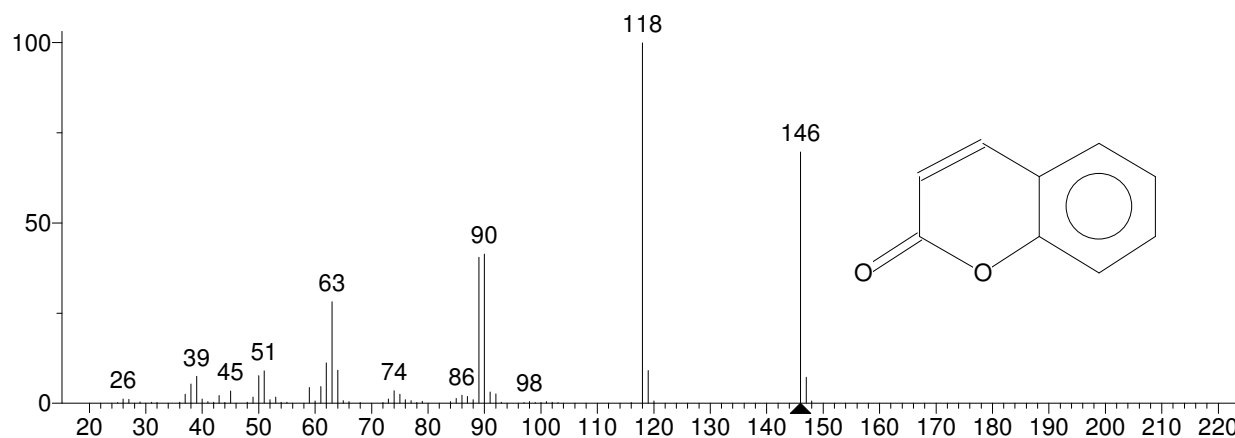


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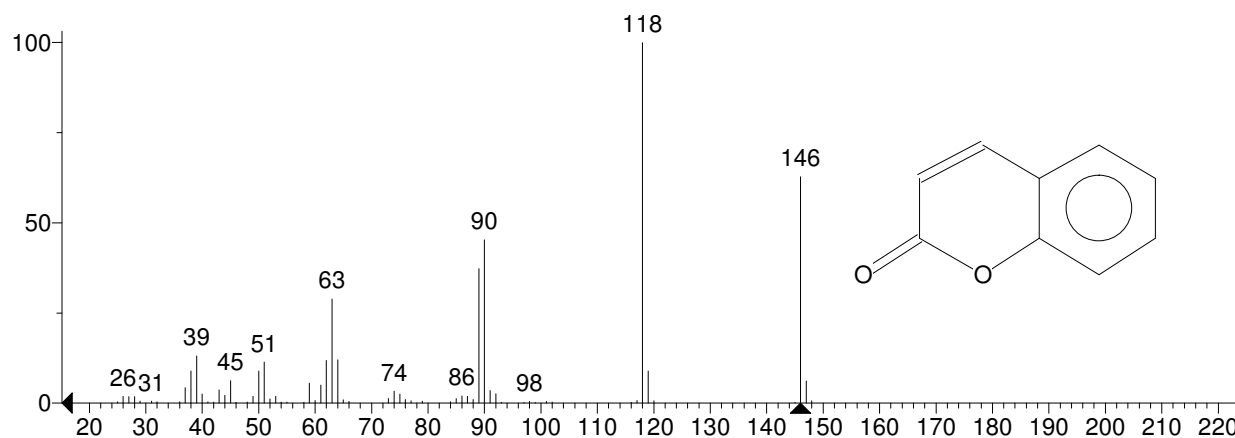
Unknown: Scan 967 (11.080 min): Designer3.D
Compound in Library Factor = 143



Hit 1 : 2H-1-Benzopyran-2-one
C₉H₆O₂; MF: 868; RMF: 908; Prob 77.2%; CAS: 91-64-5; Lib: replib; ID: 15749.

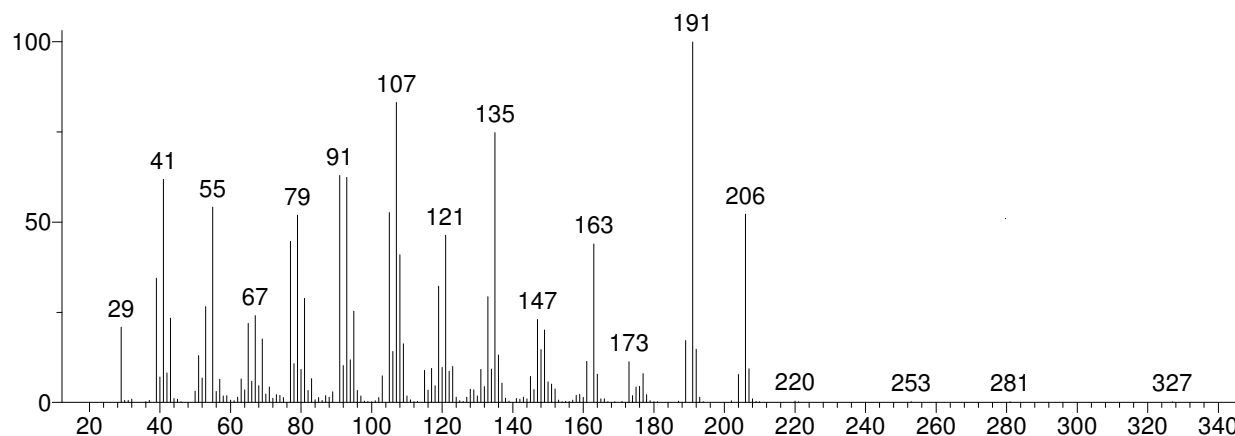


Hit 2 : 2H-1-Benzopyran-2-one
C₉H₆O₂; MF: 862; RMF: 913; Prob 77.2%; CAS: 91-64-5; Lib: replib; ID: 15748.

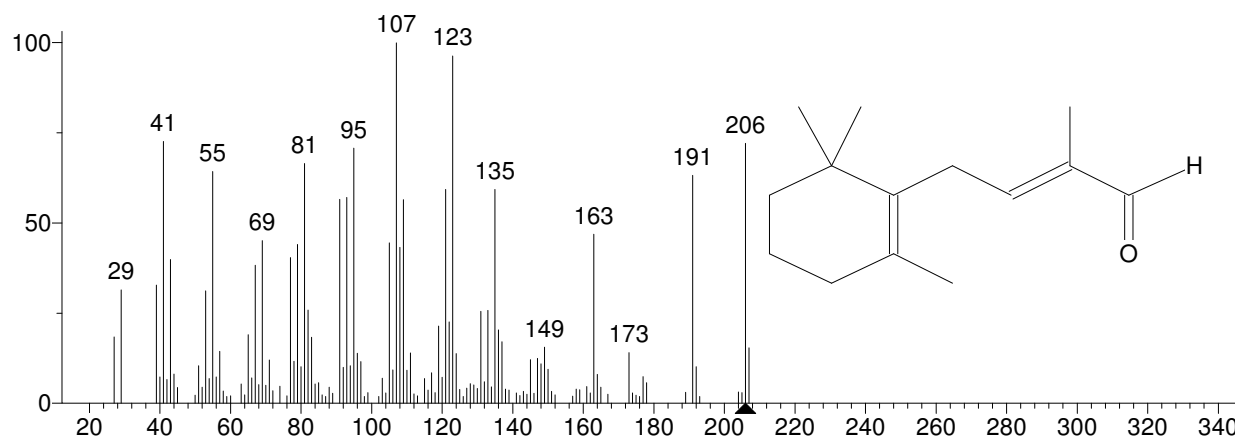


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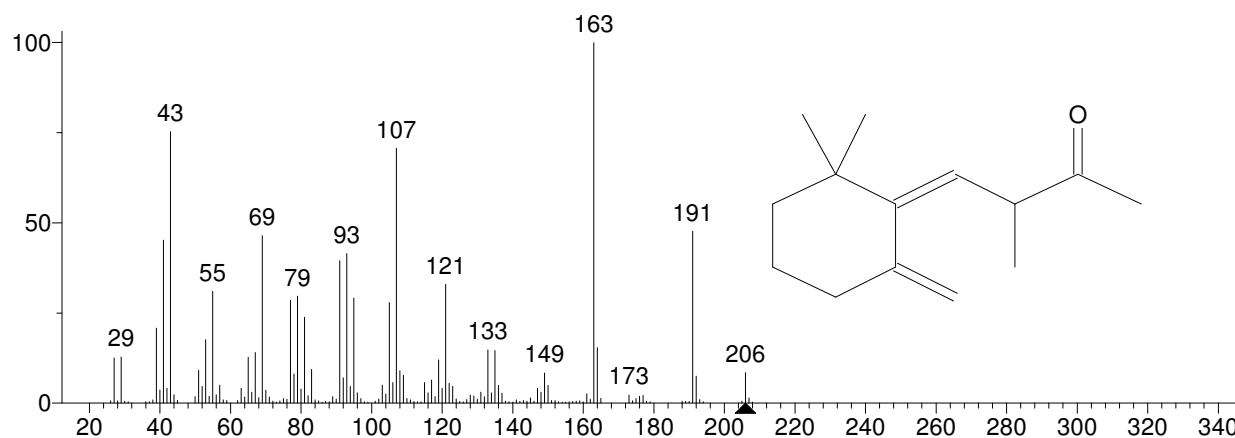
Unknown: Scan 1000 (11.457 min): Designer3.D
Compound in Library Factor = -328



Hit 1 : 2-Butenal, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
C₁₄H₂₂O; MF: 834; RMF: 838; Prob 22.1%; CAS: 3155-71-3; Lib: mainlib; ID: 64185.

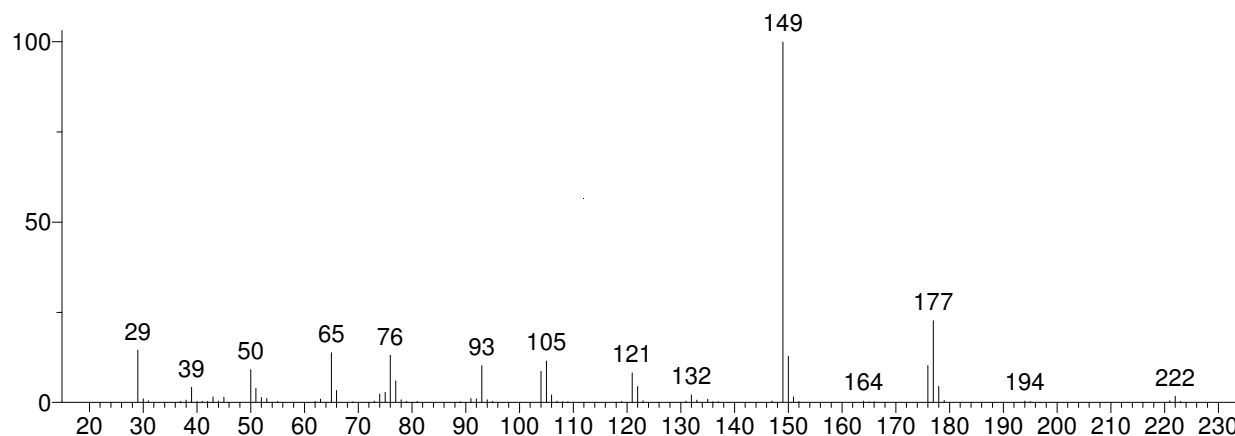


Hit 2 : 4-(2,2-Dimethyl-6-methylenecyclohexylidene)-3-methylbutan-2-one
C₁₄H₂₂O; MF: 829; RMF: 834; Prob 17.8%; CAS: 93175-74-7; Lib: mainlib; ID: 104424.

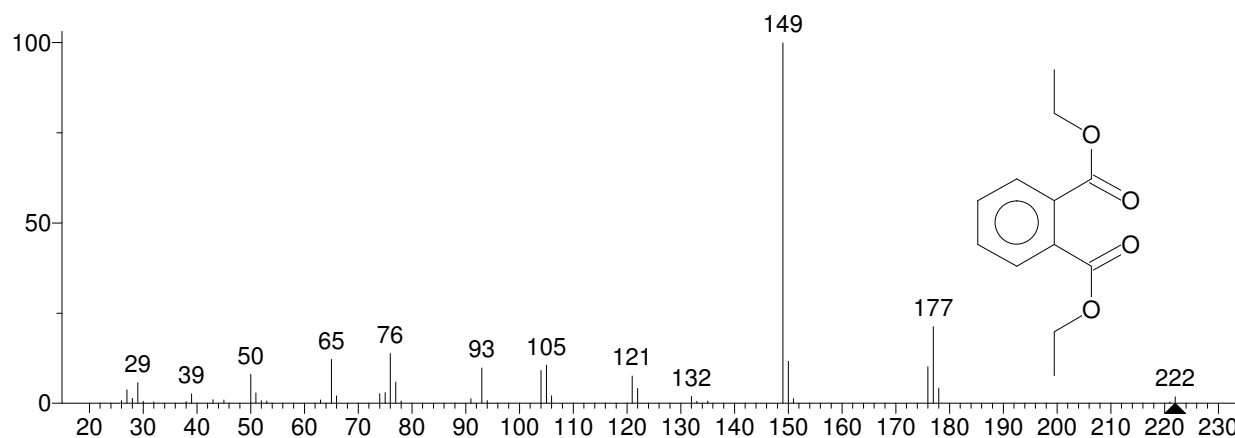


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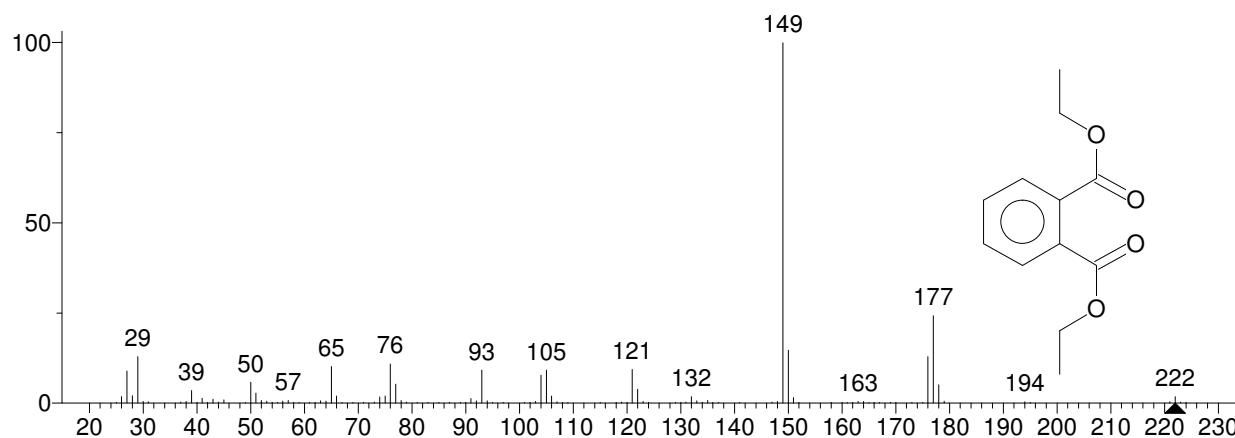
Unknown: Scan 1077 (12.336 min): Designer3.D
Compound in Library Factor = 513



Hit 1 : Diethyl Phthalate
C₁₂H₁₄O₄; MF: 961; RMF: 974; Prob 90.7%; CAS: 84-66-2; Lib: replib; ID: 19810.

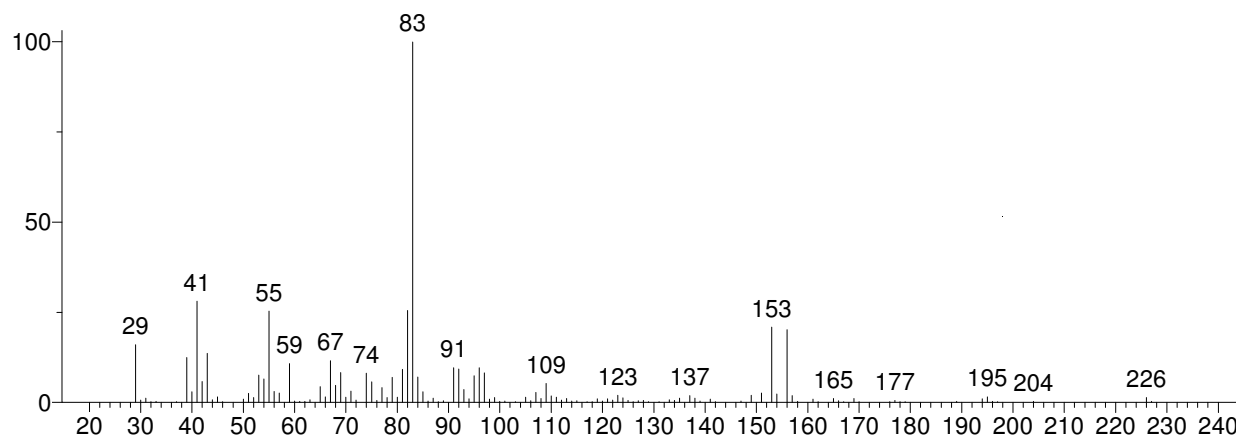


Hit 2 : Diethyl Phthalate
C₁₂H₁₄O₄; MF: 947; RMF: 948; Prob 90.7%; CAS: 84-66-2; Lib: replib; ID: 19812.

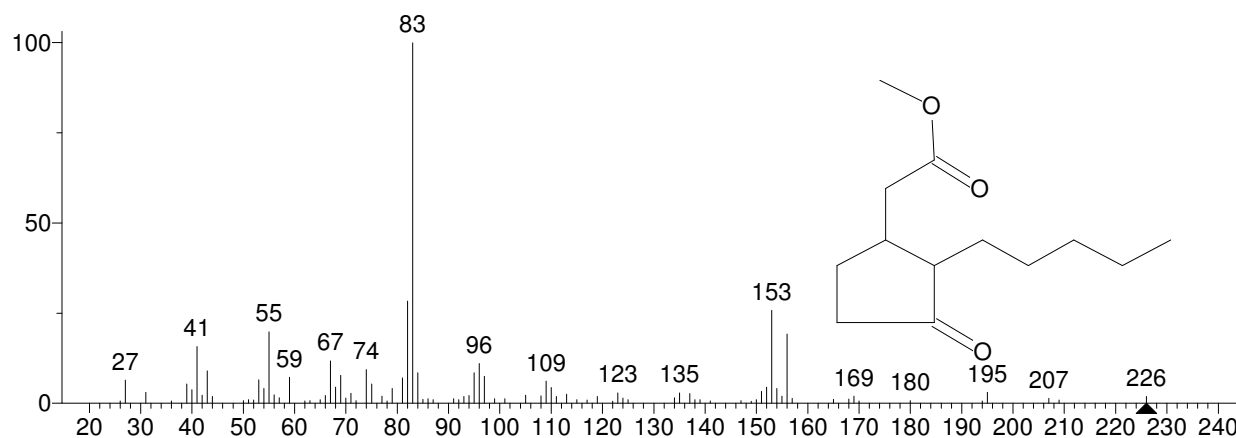


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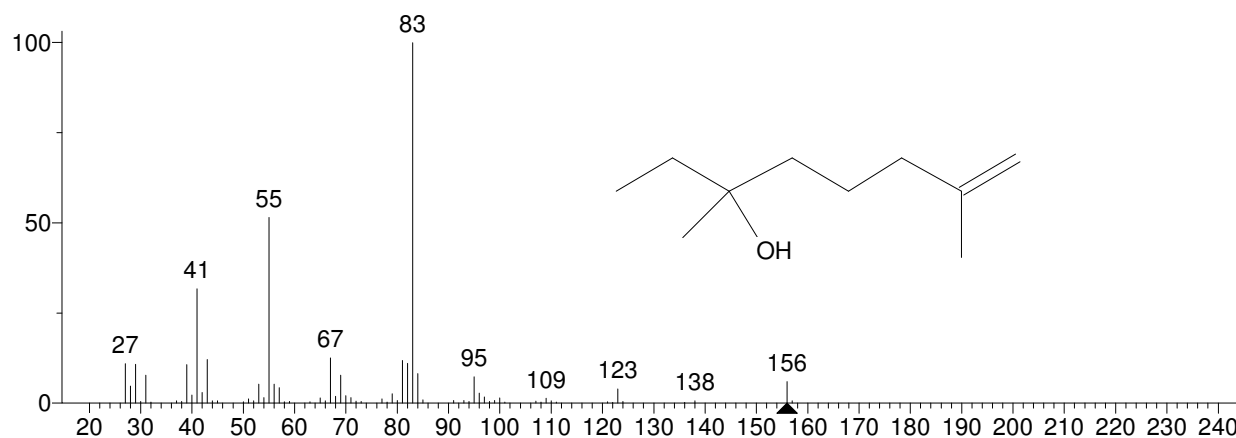
Unknown: Scan 1123 (12.861 min): Designer3.D
Compound in Library Factor = -137



Hit 1 : Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester
C₁₃H₂₂O₃; MF: 797; RMF: 825; Prob 70.7%; CAS: 24851-98-7; Lib: mainlib; ID: 41498.

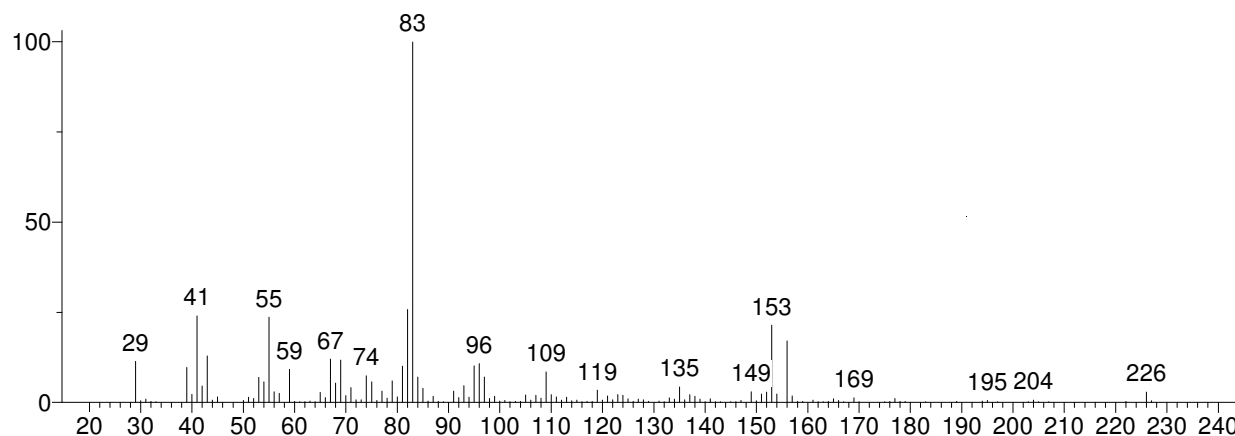


Hit 2 : Isocitronellol
C₁₀H₂₀O; MF: 687; RMF: 799; Prob 4.52%; CAS: 18479-52-2; Lib: mainlib; ID: 41109.

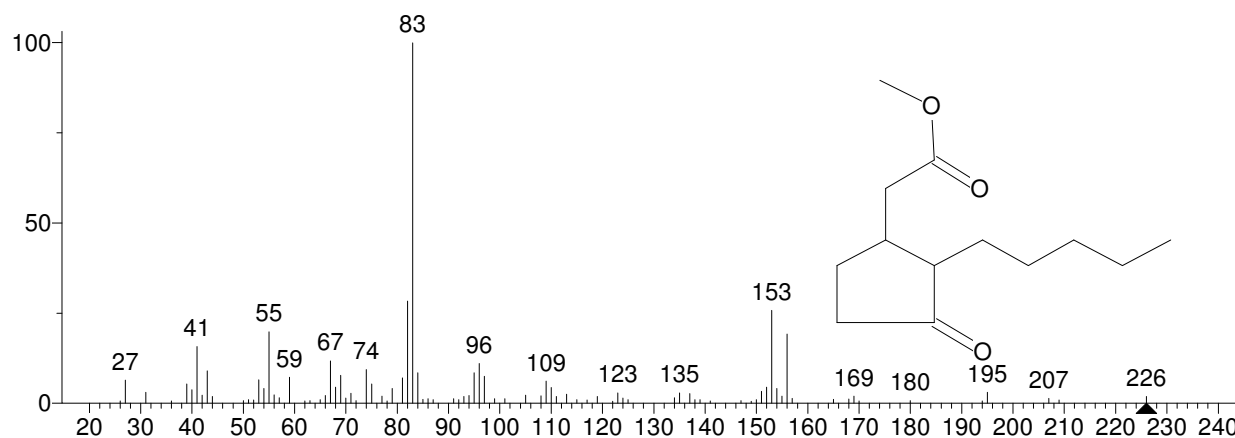


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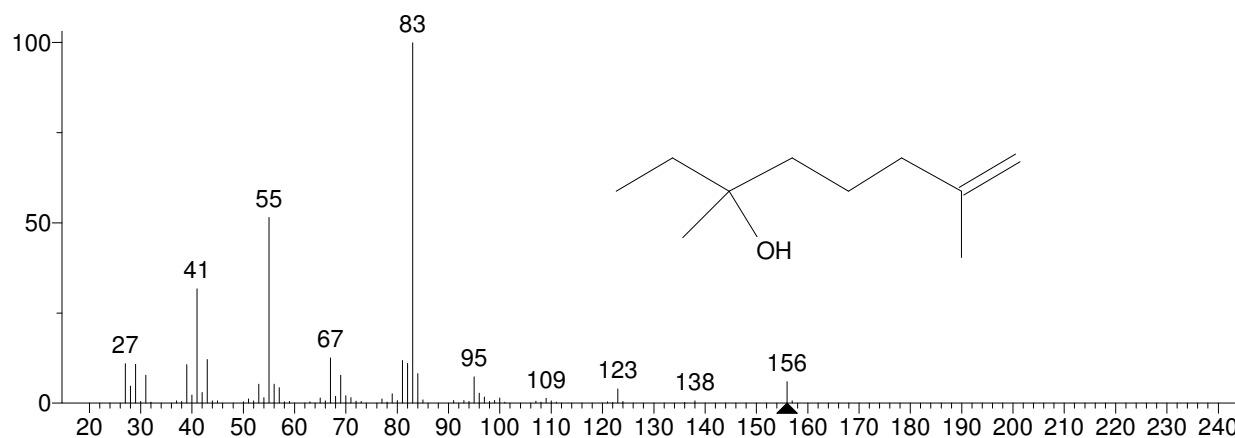
Unknown: Scan 1138 (13.033 min): Designer3.D
Compound in Library Factor = 123



Hit 1 : Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester
C₁₃H₂₂O₃; MF: 811; RMF: 849; Prob 66.3%; CAS: 24851-98-7; Lib: mainlib; ID: 41498.

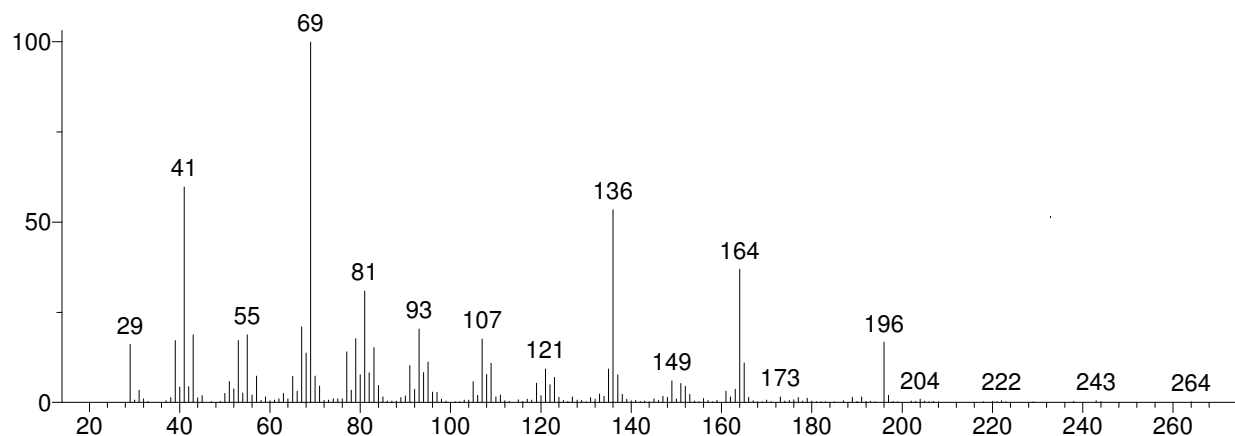


Hit 2 : Isocitronellol
C₁₀H₂₀O; MF: 676; RMF: 806; Prob 2.51%; CAS: 18479-52-2; Lib: mainlib; ID: 41109.

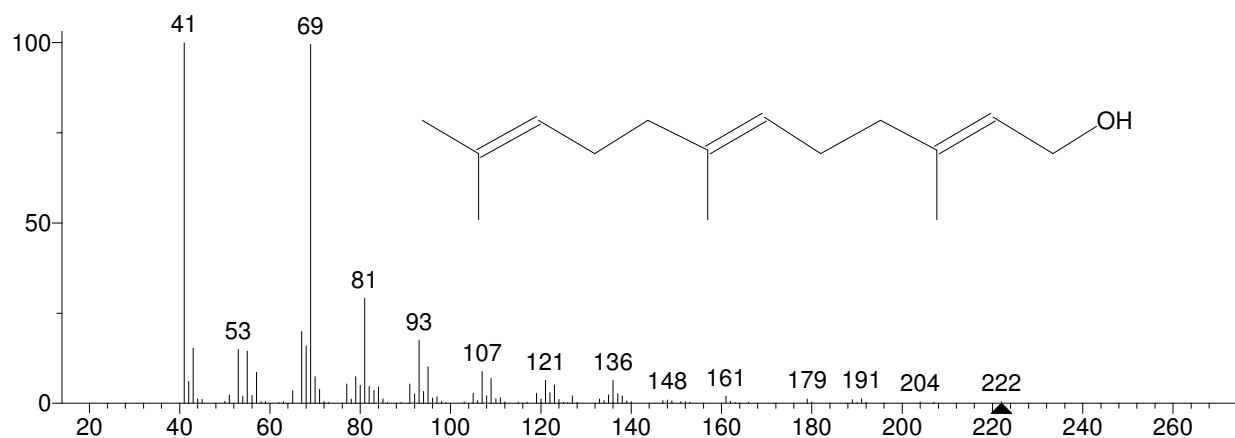


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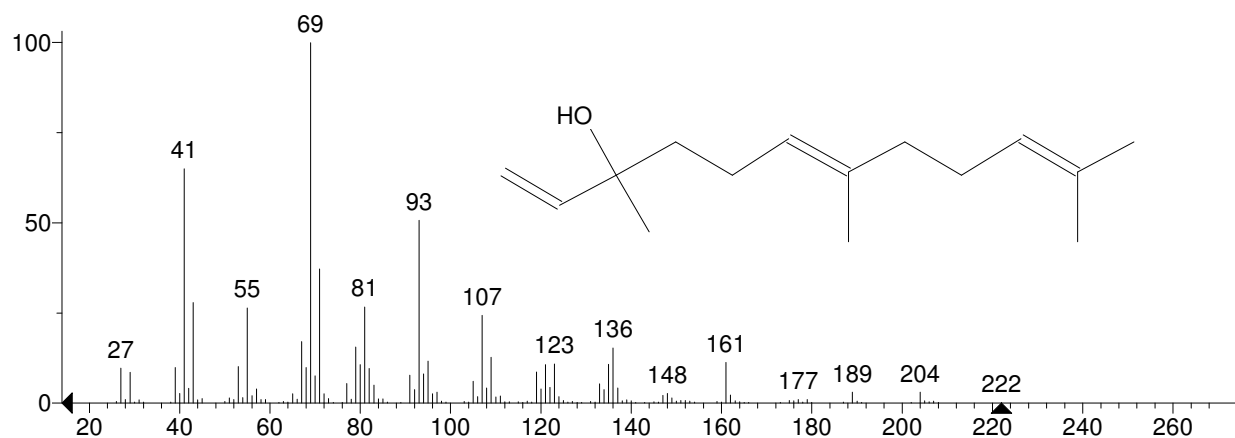
Unknown: Scan 1158 (13.261 min): Designer3.D
Compound in Library Factor = -1120



Hit 1 : 2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (E,E)-
C₁₅H₂₆O; MF: 740; RMF: 846; Prob 7.52%; CAS: 106-28-5; Lib: mainlib; ID: 3080.

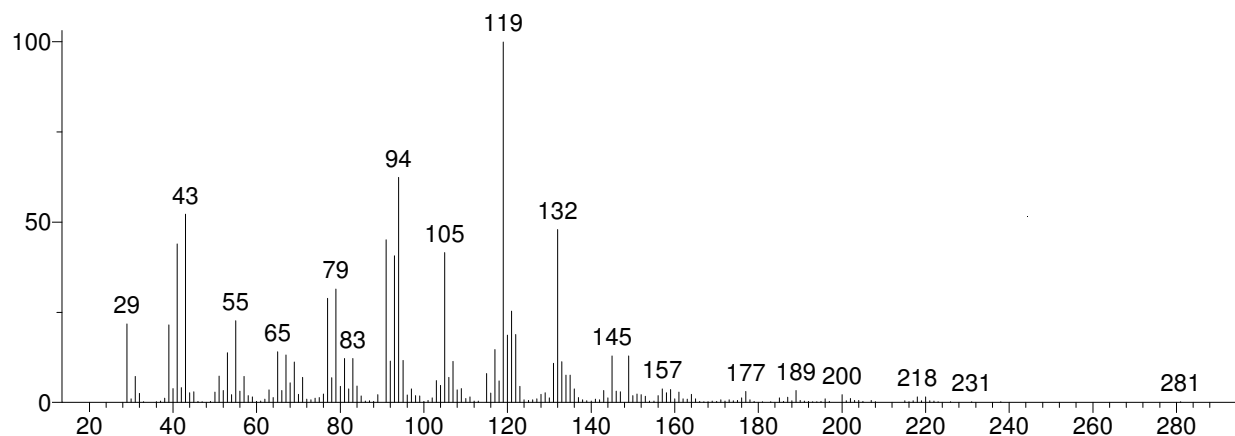


Hit 2 : 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-
C₁₅H₂₆O; MF: 736; RMF: 763; Prob 6.35%; CAS: 7212-44-4; Lib: replib; ID: 7568.

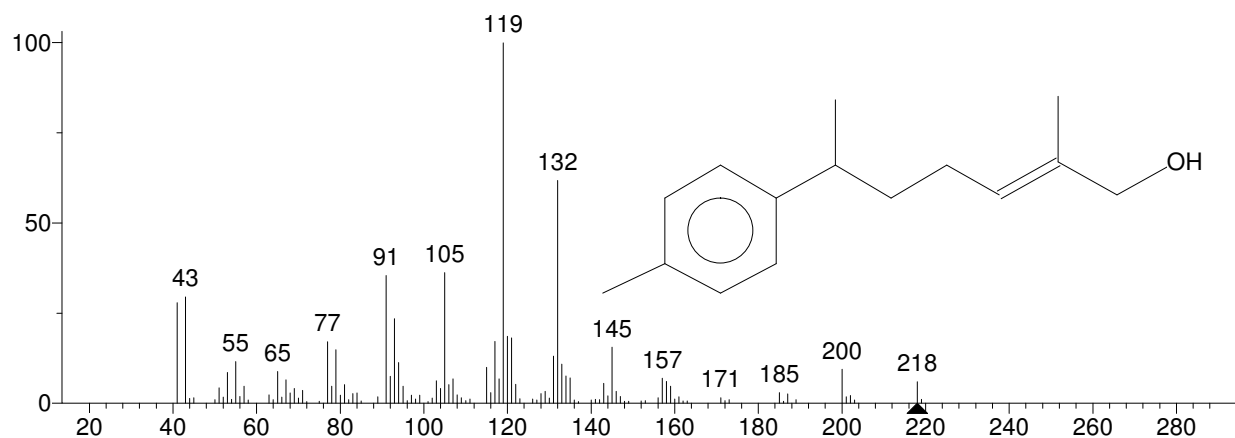


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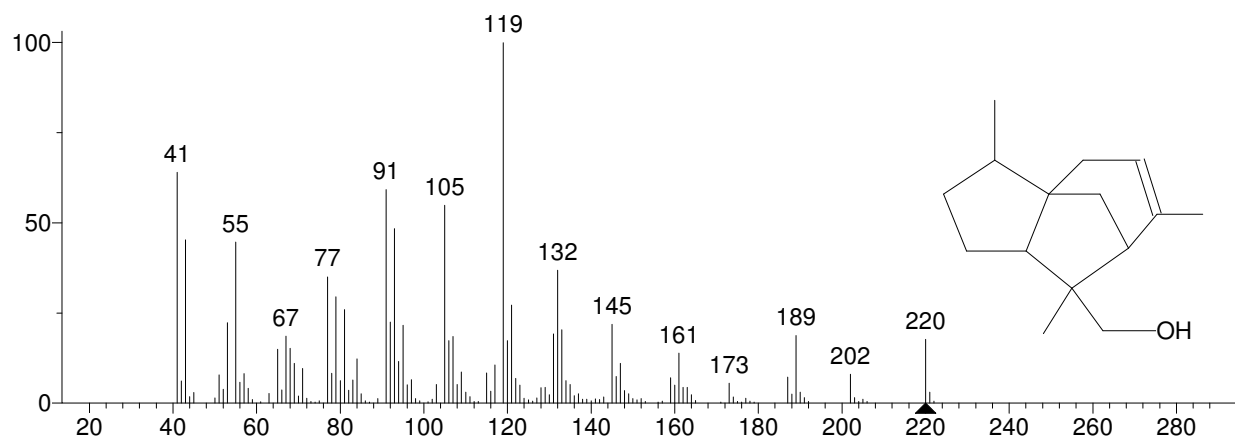
Unknown: Scan 1167 (13.364 min): Designer3.D
Compound in Library Factor = -117



Hit 1 : 6-(p-Tolyl)-2-methyl-2-heptenol
C₁₅H₂₂O; MF: 867; RMF: 892; Prob 60.9%; CAS: 39599-18-3; Lib: mainlib; ID: 72280.

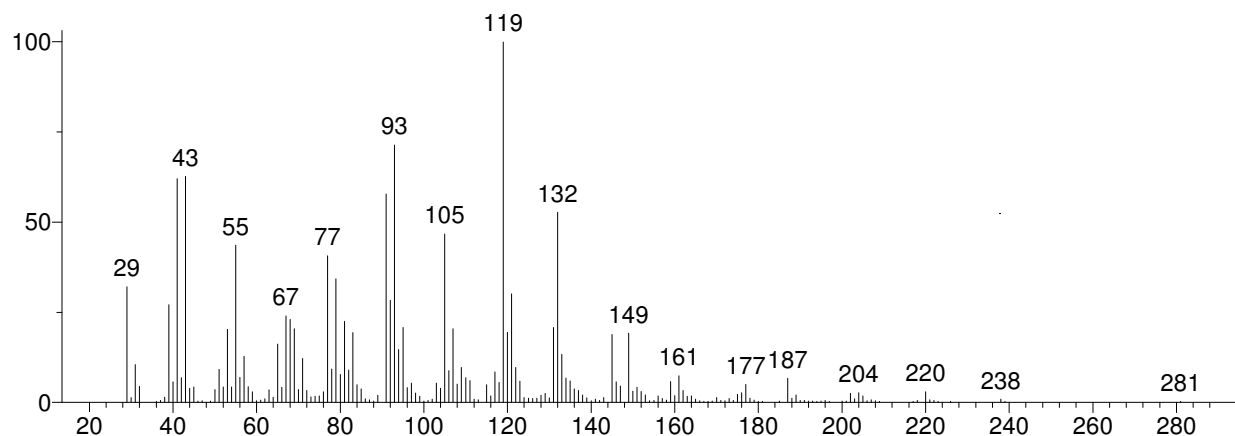


Hit 2 : Cedren-13-ol, 8-
C₁₅H₂₄O; MF: 802; RMF: 822; Prob 9.80%; CAS: 18319-35-2; Lib: mainlib; ID: 71326.

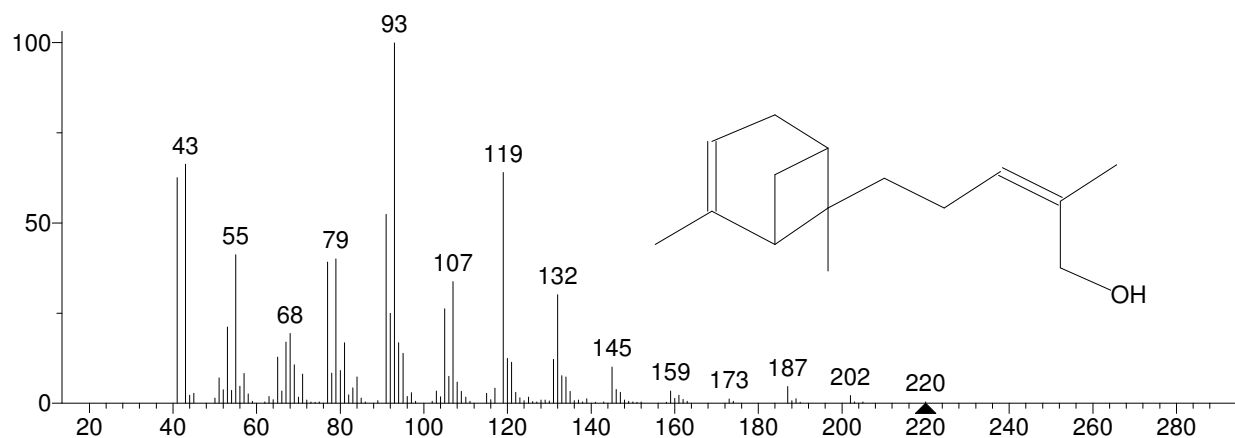


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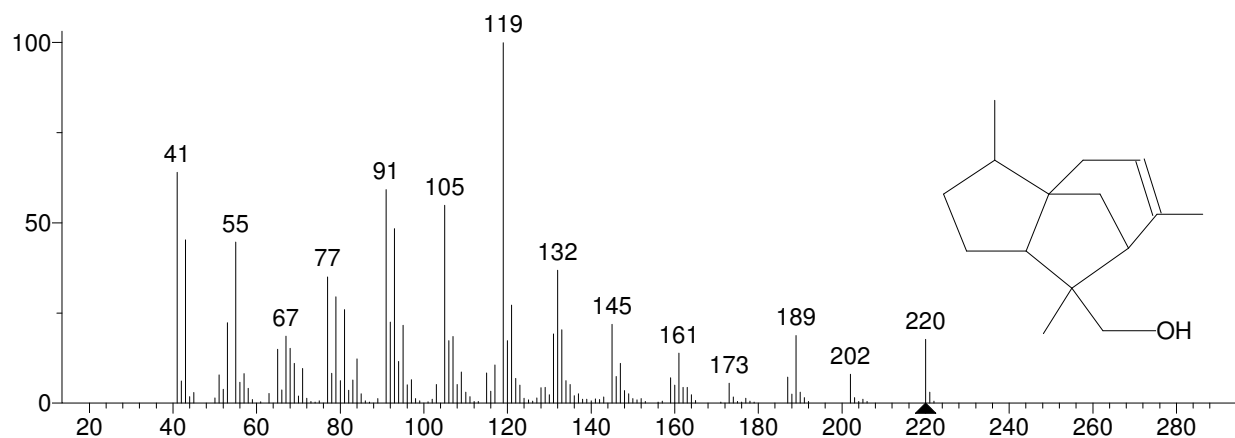
Unknown: Scan 1186 (13.581 min): Designer3.D
Compound in Library Factor = -278



Hit 1 : Bergamotol, Z-.alpha.-trans-
C₁₅H₂₄O; MF: 839; RMF: 873; Prob 34.9%; CAS: 88034-74-6; Lib: mainlib; ID: 51309.

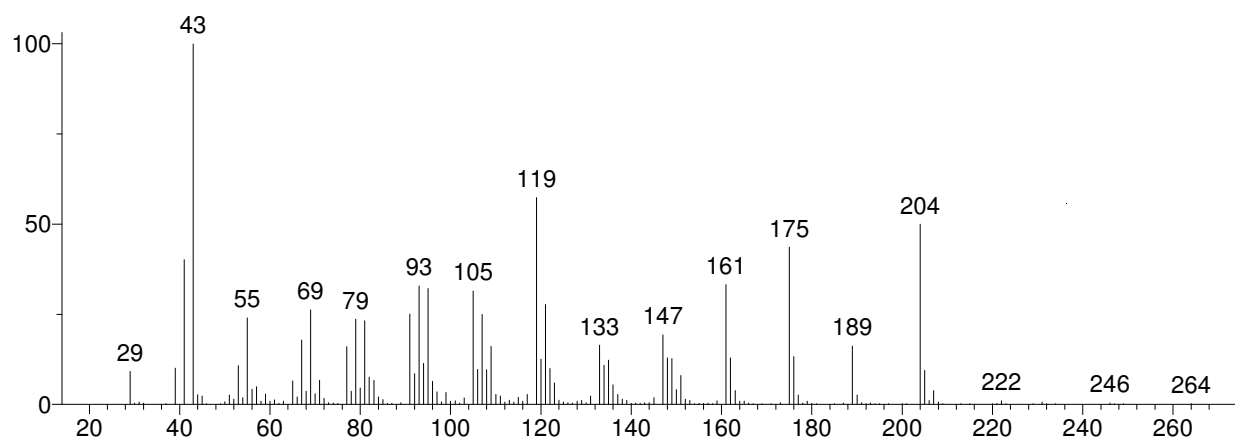


Hit 2 : Cedren-13-ol, 8-
C₁₅H₂₄O; MF: 830; RMF: 845; Prob 25.4%; CAS: 18319-35-2; Lib: mainlib; ID: 71326.

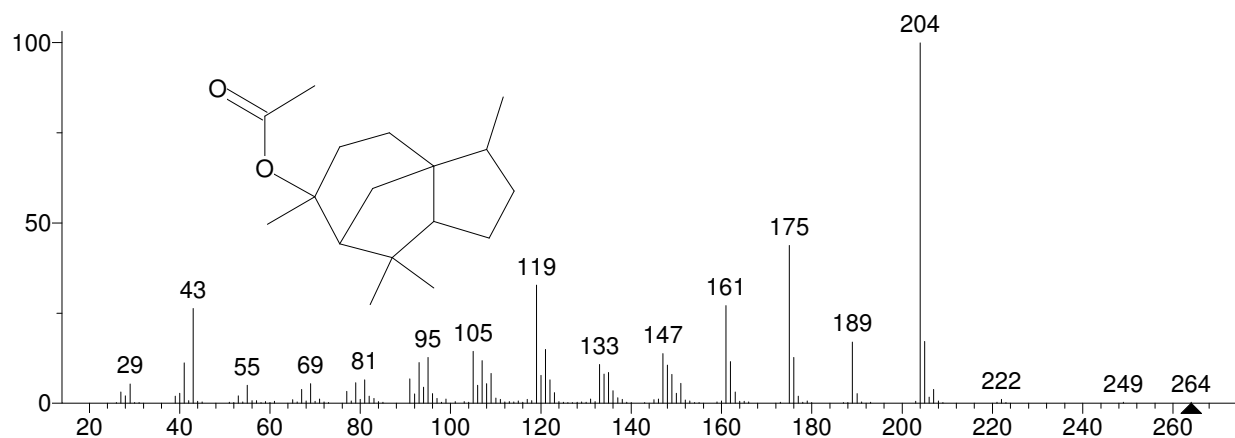


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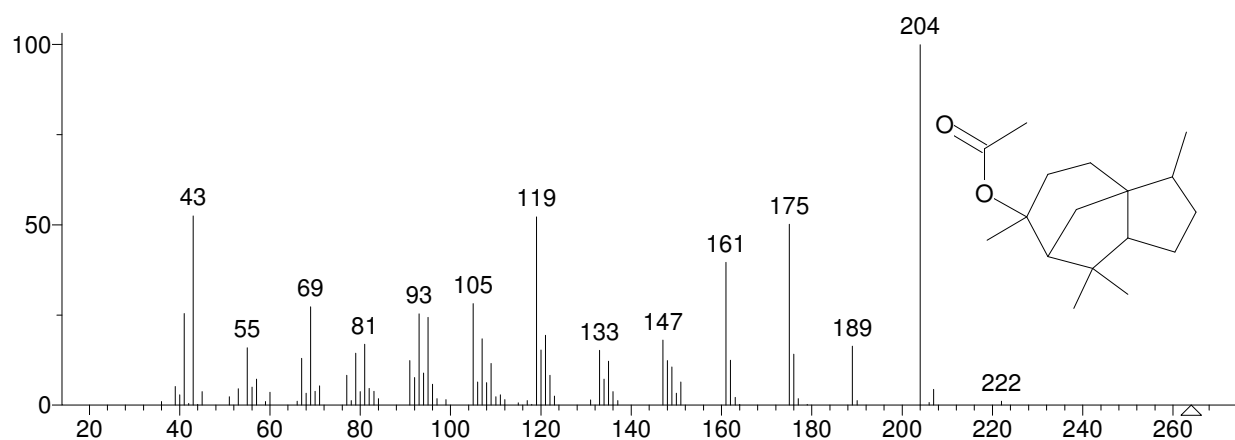
Unknown: Scan 1201 (13.752 min): Designer3.D
Compound in Library Factor = 120



Hit 1 : 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate, [3R-(3.alpha.,3a.beta.,6.alpha.,7.beta.,8 C17H28O2; MF: 892; RMF: 897; Prob 20.7%; CAS: 77-54-3; Lib: mainlib; ID: 125471.

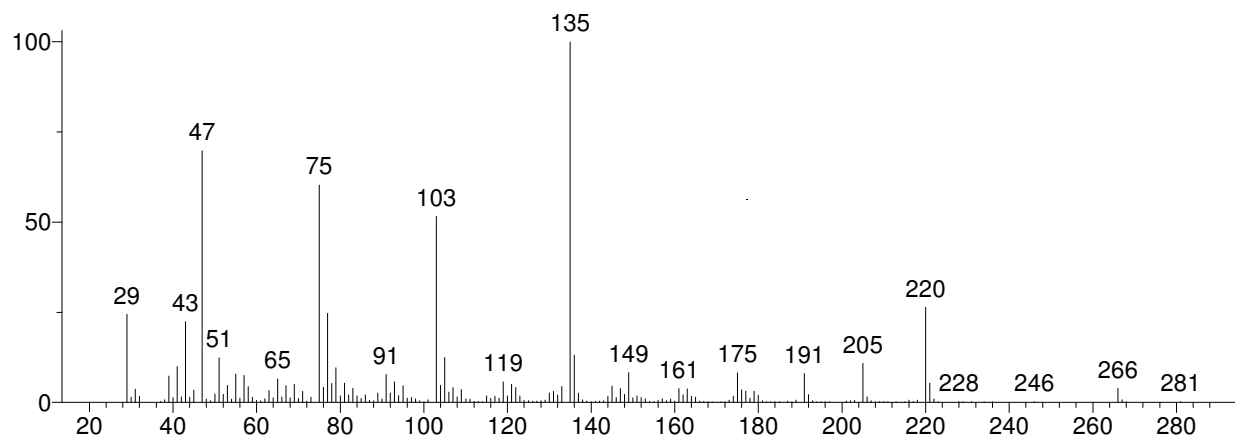


Hit 2 : 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate, [3R-(3.alpha.,3a.beta.,6.alpha.,7.beta.,8 C17H28O2; MF: 870; RMF: 904; Prob 20.7%; CAS: 77-54-3; Lib: replib; ID: 24049.

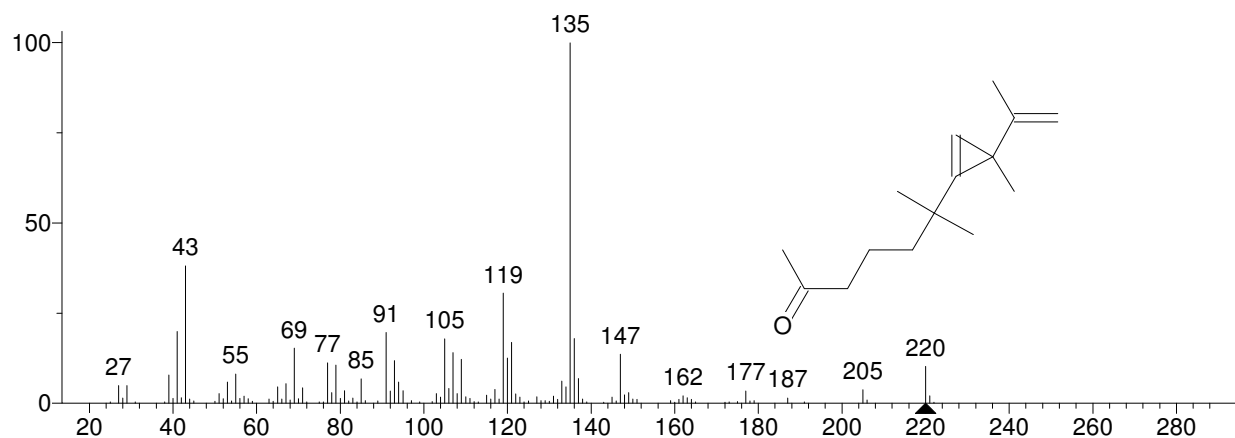


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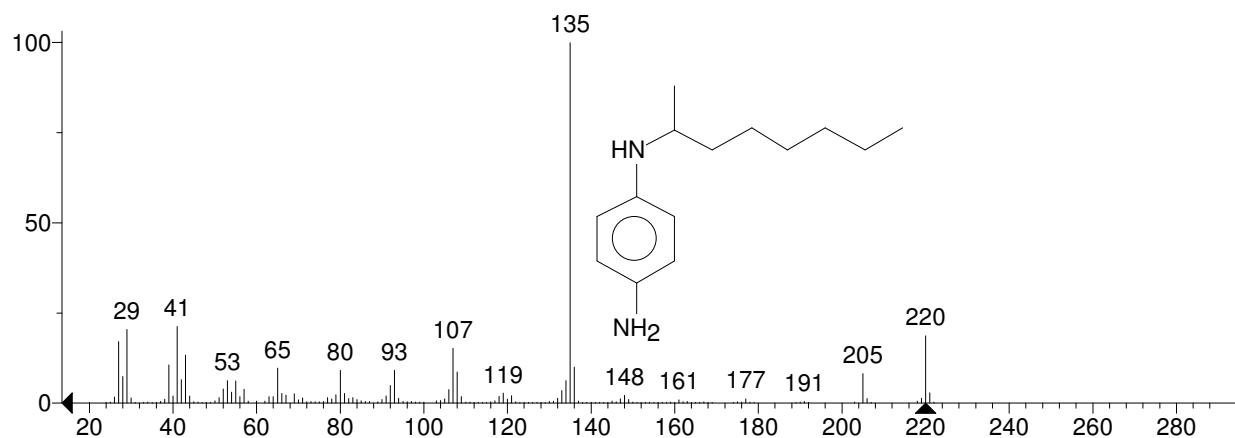
Unknown: Scan 1216 (13.923 min): Designer3.D
Compound in Library Factor = -1149



Hit 1 : 2-Heptanone, 6-methyl-6-[3-methyl-3-(1-methylethenyl)-1-cyclopropen-1-yl]-
C₁₅H₂₄O; MF: 672; RMF: 719; Prob 17.4%; CAS: 69296-87-3; Lib: mainlib; ID: 84618.

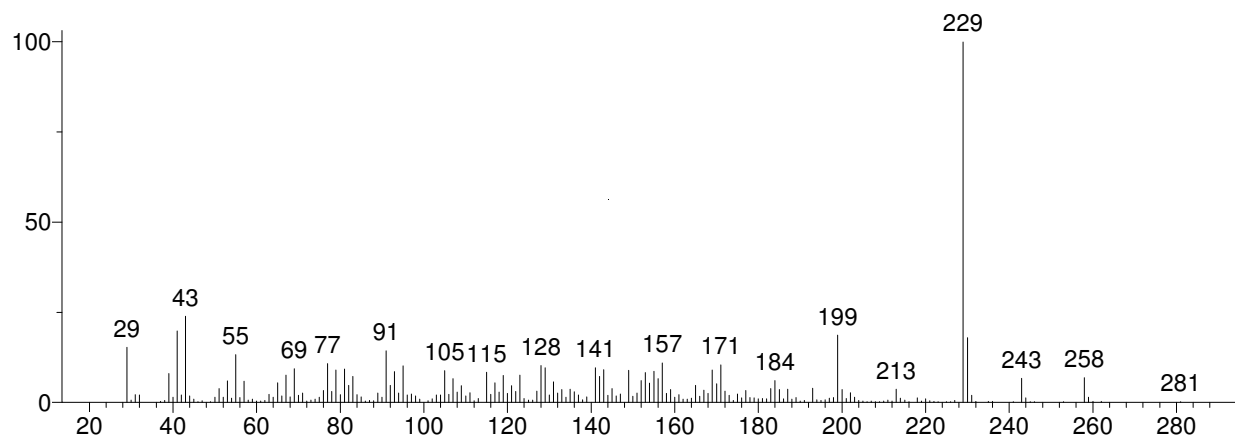


Hit 2 : 1,4-Benzenediamine, N-(1-methylheptyl)-
C₁₄H₂₄N₂; MF: 670; RMF: 682; Prob 16.1%; CAS: 39563-50-3; Lib: mainlib; ID: 84554.

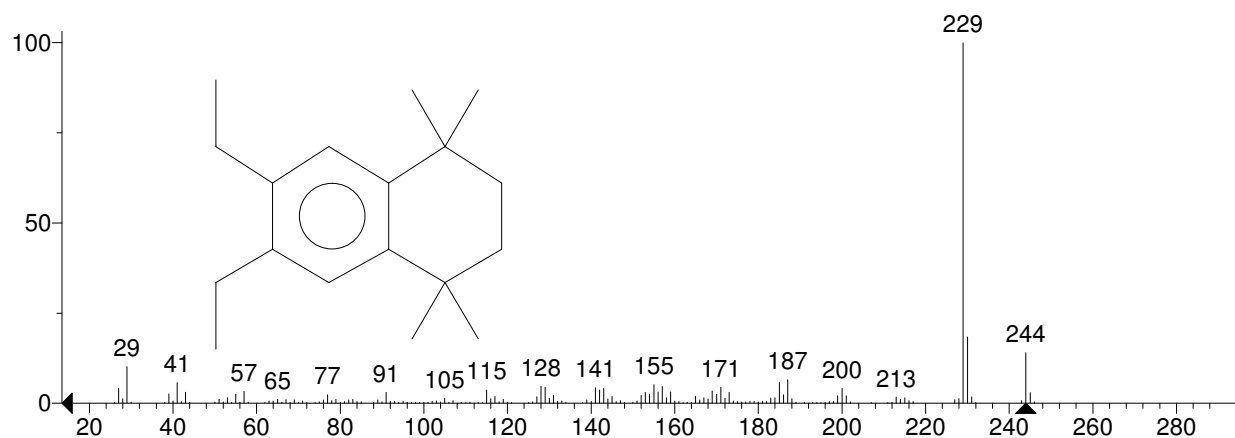


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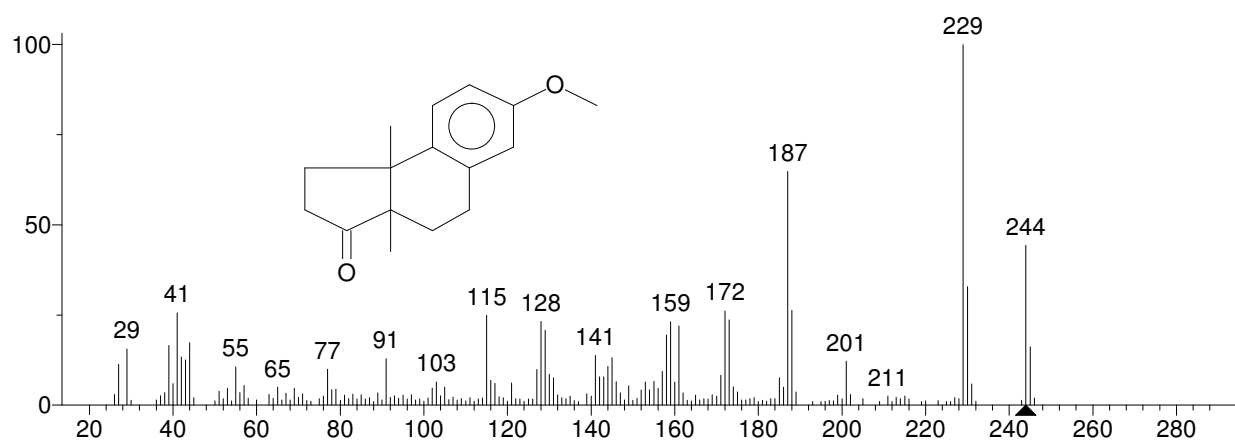
Unknown: Scan 1222 (13.992 min): Designer3.D
Compound in Library Factor = -513



Hit 1 : Naphthalene, 6,7-diethyl-1,2,3,4-tetrahydro-1,1,4,4-tetramethyl-
C₁₈H₂₈; MF: 746; RMF: 780; Prob 56.5%; CAS: 55741-10-1; Lib: mainlib; ID: 134407.

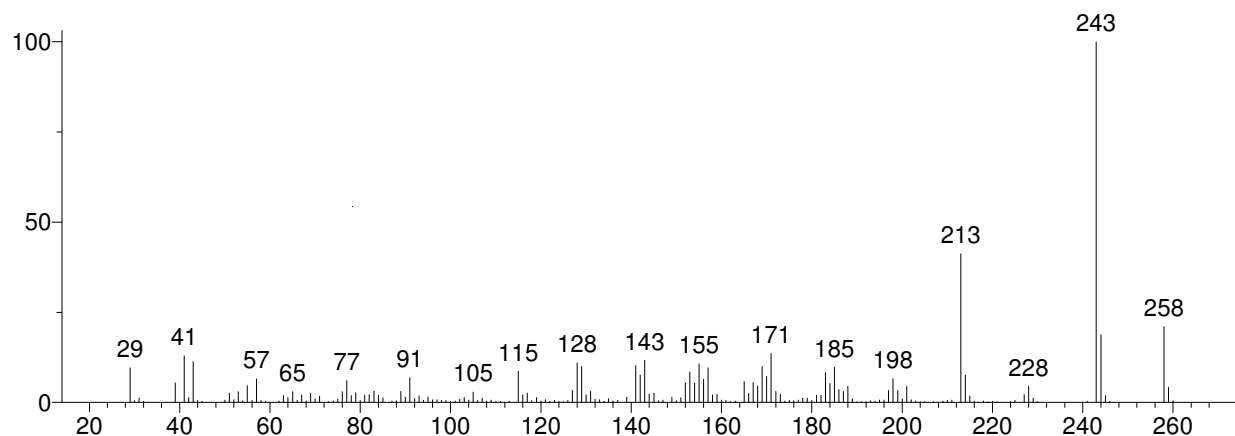


Hit 2 : Benzo[e](1H)indene, 1,2,3a,4,5,9b-hexahydro-7-methoxy-3-oxo-3a,9b-dimethyl-
C₁₆H₂₀O₂; MF: 698; RMF: 712; Prob 11.7%; Lib: mainlib; ID: 134337.

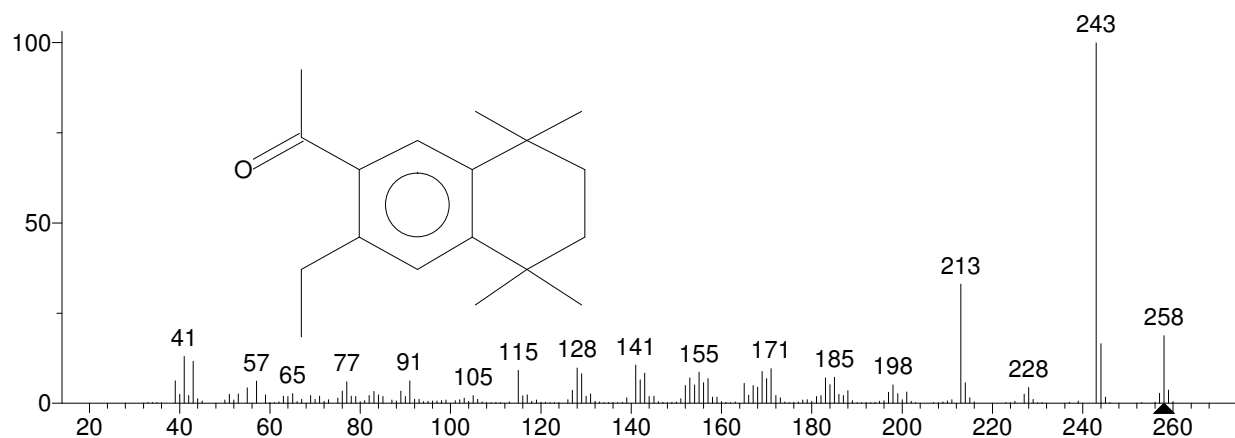


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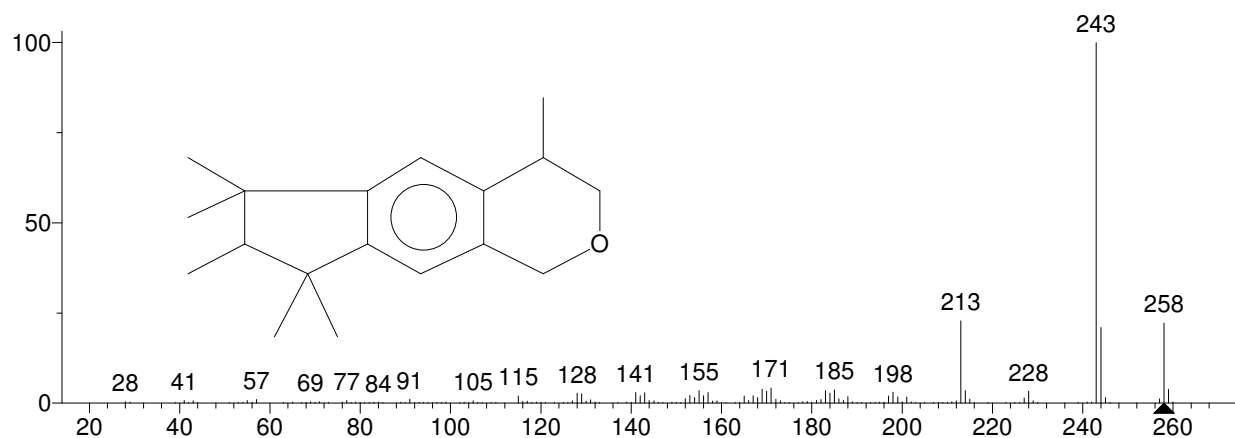
Unknown: Scan 1254 (14.357 min): Designer3.D
Compound in Library Factor = 316



Hit 1 : 7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
C₁₈H₂₆O; MF: 925; RMF: 928; Prob 81.8%; CAS: 88-29-9; Lib: replib; ID: 25619.

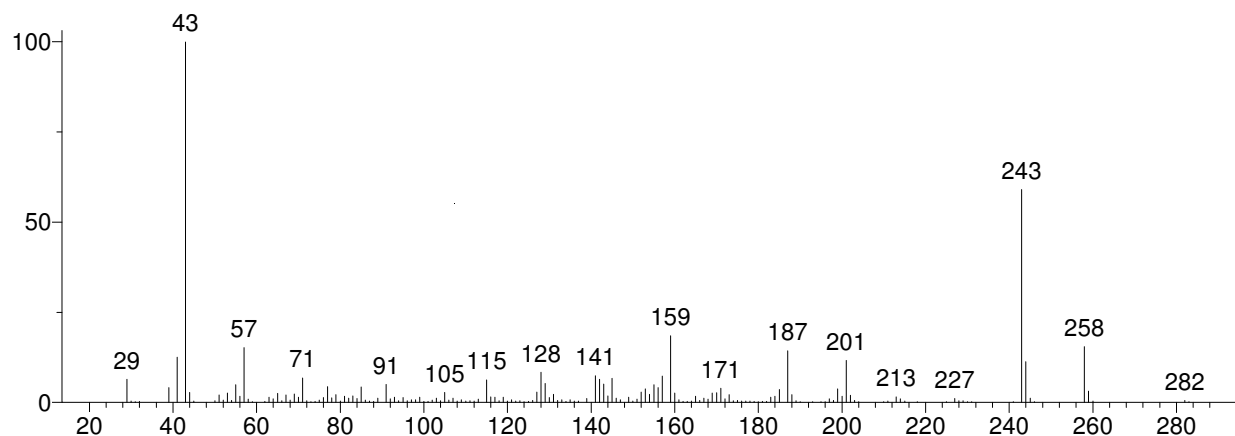


Hit 2 : Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-
C₁₈H₂₆O; MF: 872; RMF: 886; Prob 16.2%; CAS: 1222-05-5; Lib: mainlib; ID: 138703.

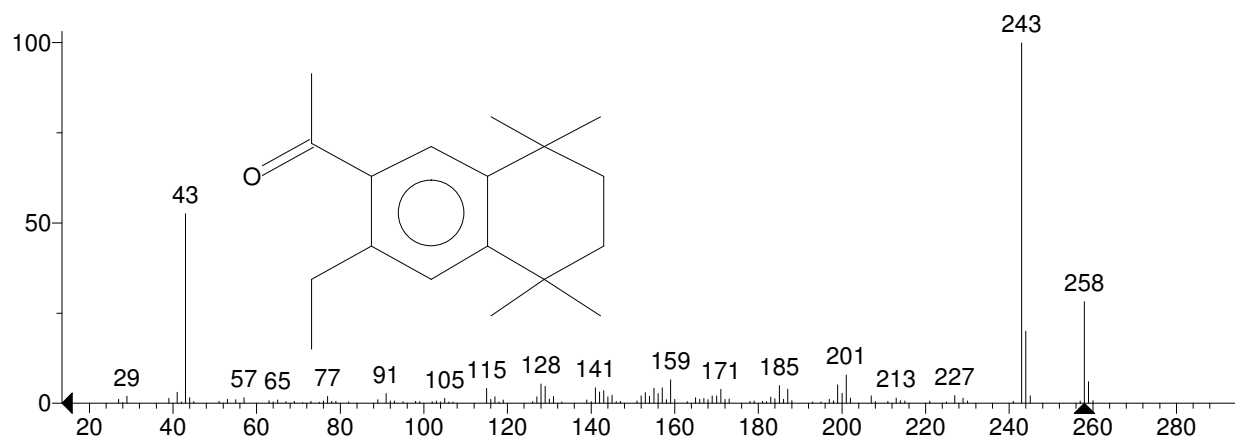


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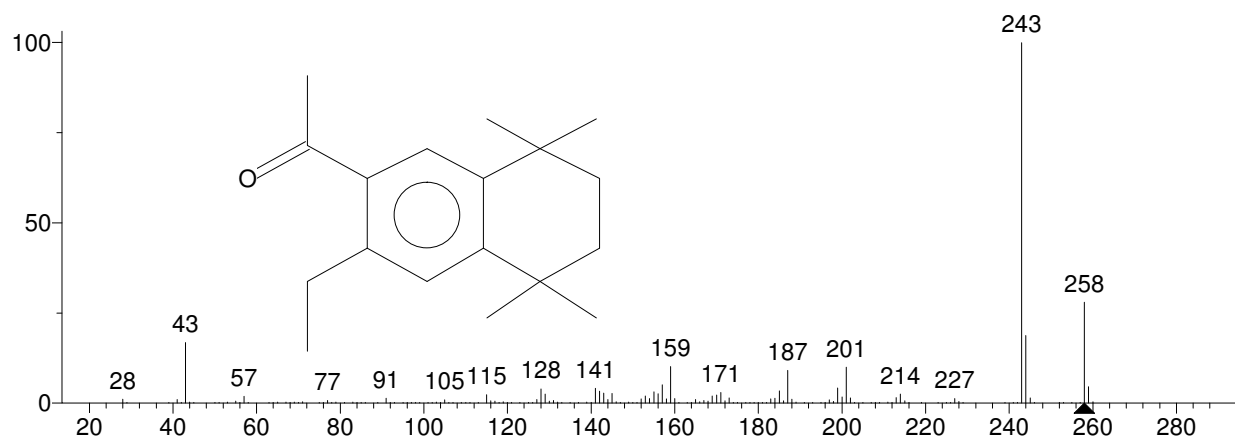
Unknown: Scan 1259 (14.414 min): Designer3.D
Compound in Library Factor = -109



Hit 1 : 7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
C₁₈H₂₆O; MF: 841; RMF: 873; Prob 75.2%; CAS: 88-29-9; Lib: replib; ID: 25601.

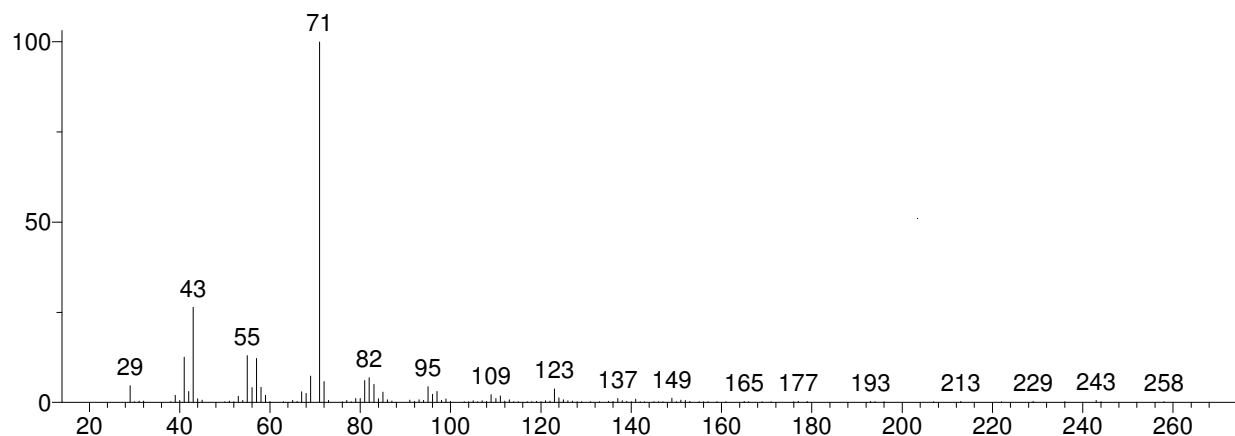


Hit 2 : 7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
C₁₈H₂₆O; MF: 827; RMF: 850; Prob 75.2%; CAS: 88-29-9; Lib: mainlib; ID: 138812.

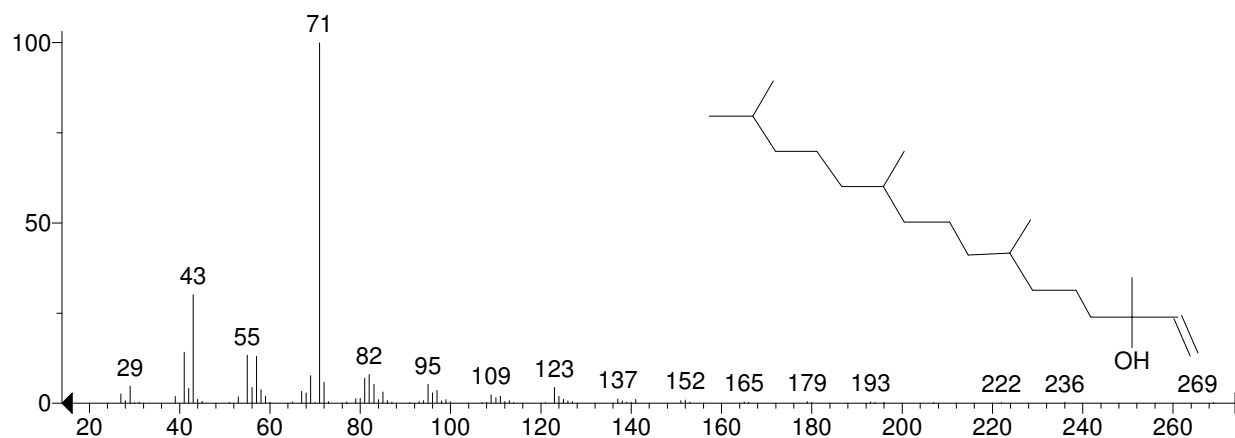


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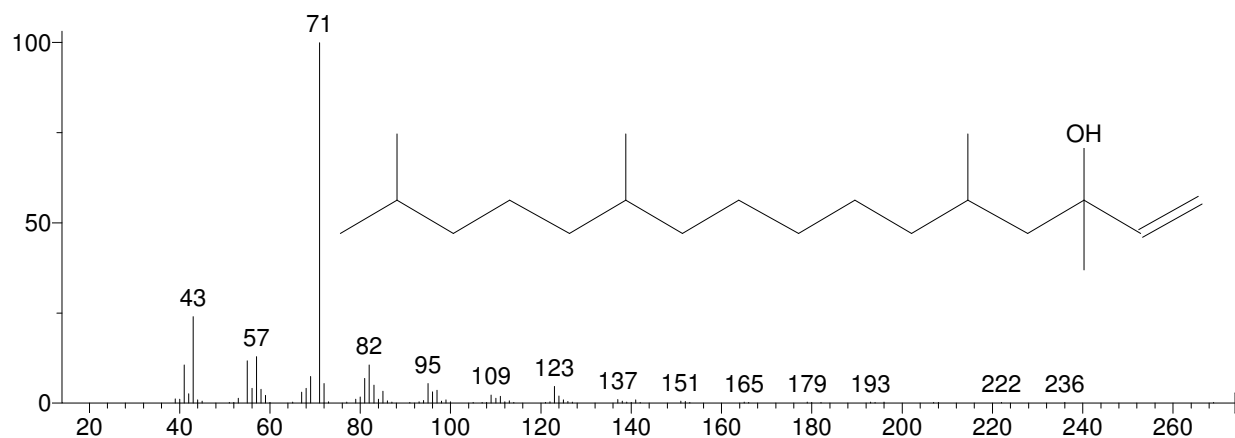
Unknown: Scan 1292 (14.791 min): Designer3.D
Compound in Library Factor = 298



Hit 1 : Isophytol
C₂₀H₄₀O; MF: 914; RMF: 933; Prob 54.4%; CAS: 505-32-8; Lib: replib; ID: 8047.

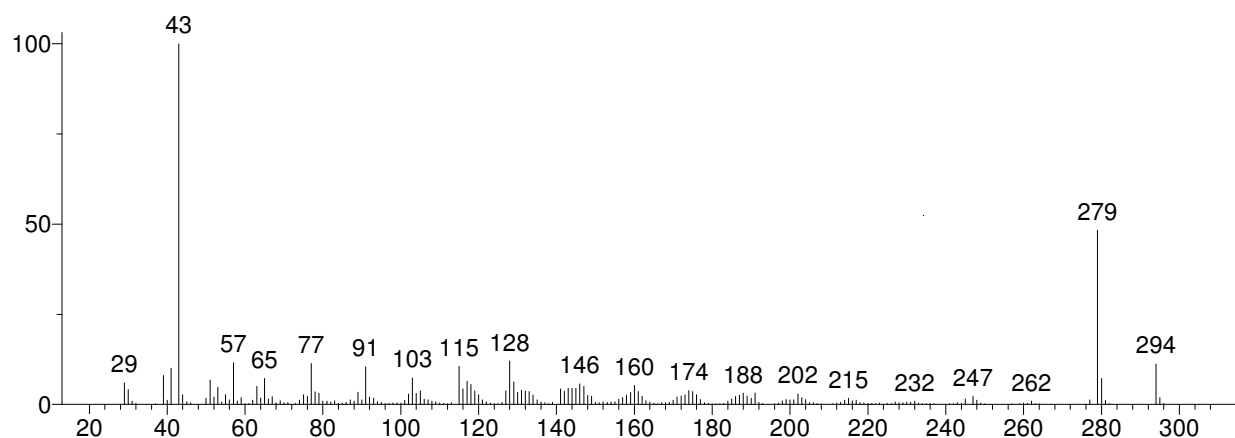


Hit 2 : 1-Hexadecen-3-ol, 3,5,11,15-tetramethyl-
C₂₀H₄₀O; MF: 902; RMF: 920; Prob 36.3%; Lib: mainlib; ID: 30894.

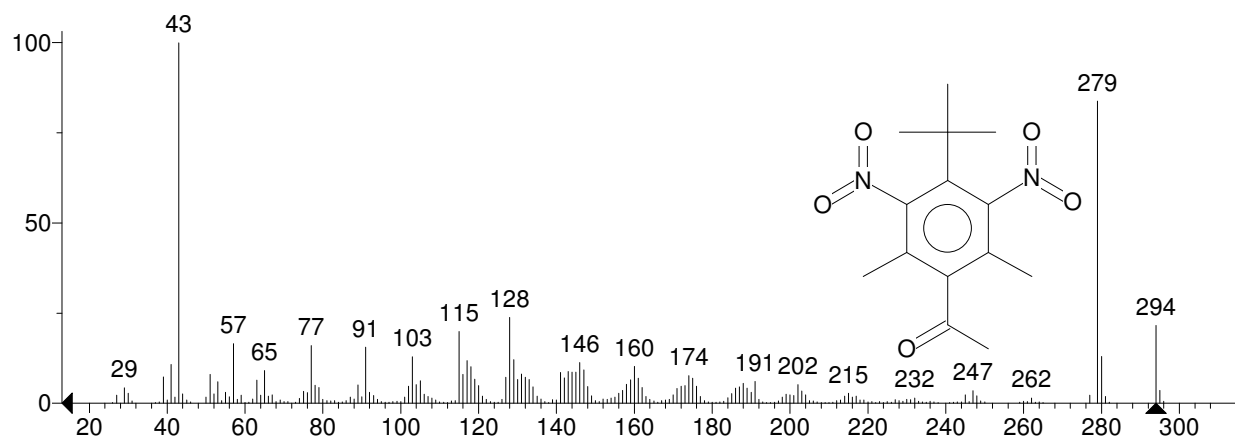


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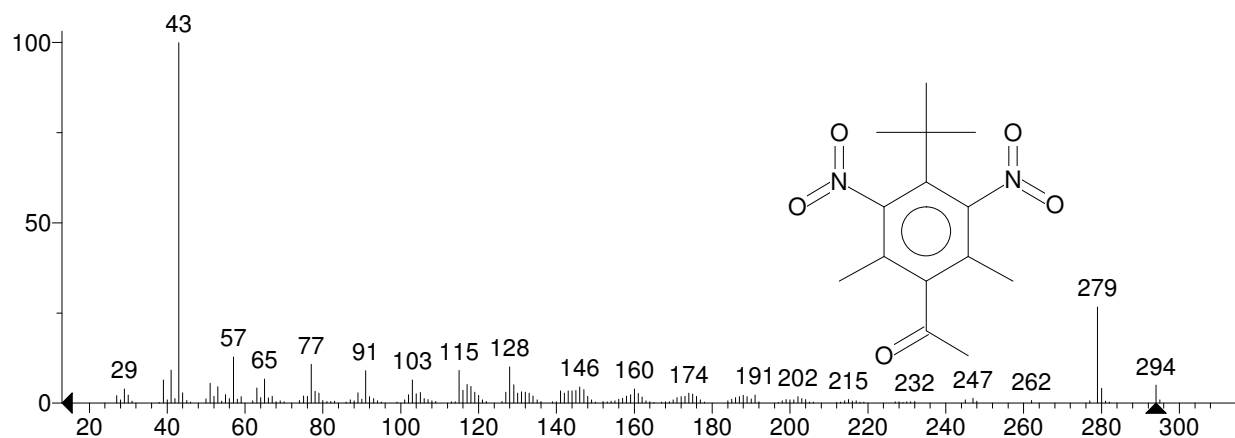
Unknown: Scan 1338 (15.316 min): Designer3.D
Compound in Library Factor = 993



Hit 1 : Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-
C₁₄H₁₈N₂O₅; MF: 958; RMF: 958; Prob 93.1%; CAS: 81-14-1; Lib: replib; ID: 3079.

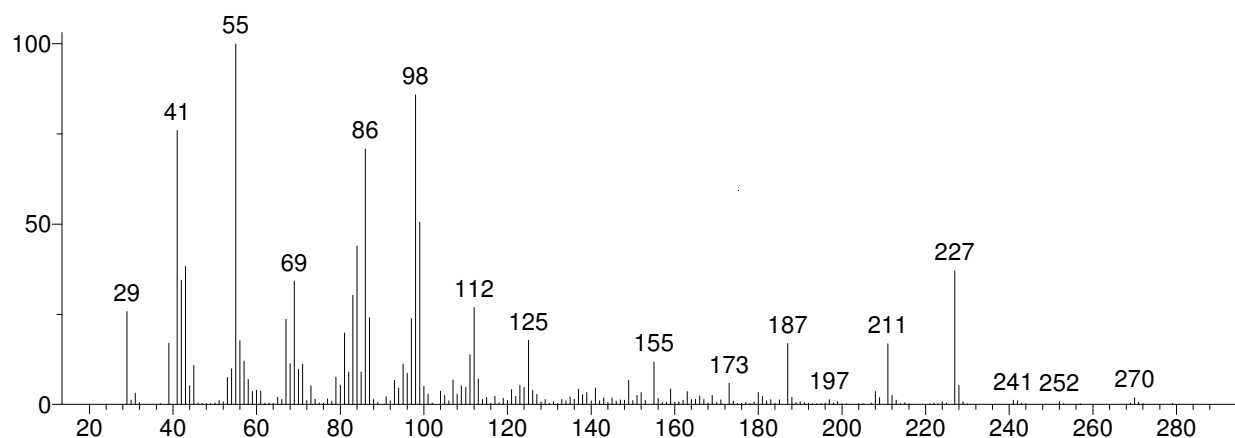


Hit 2 : Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-
C₁₄H₁₈N₂O₅; MF: 943; RMF: 953; Prob 93.1%; CAS: 81-14-1; Lib: replib; ID: 3078.

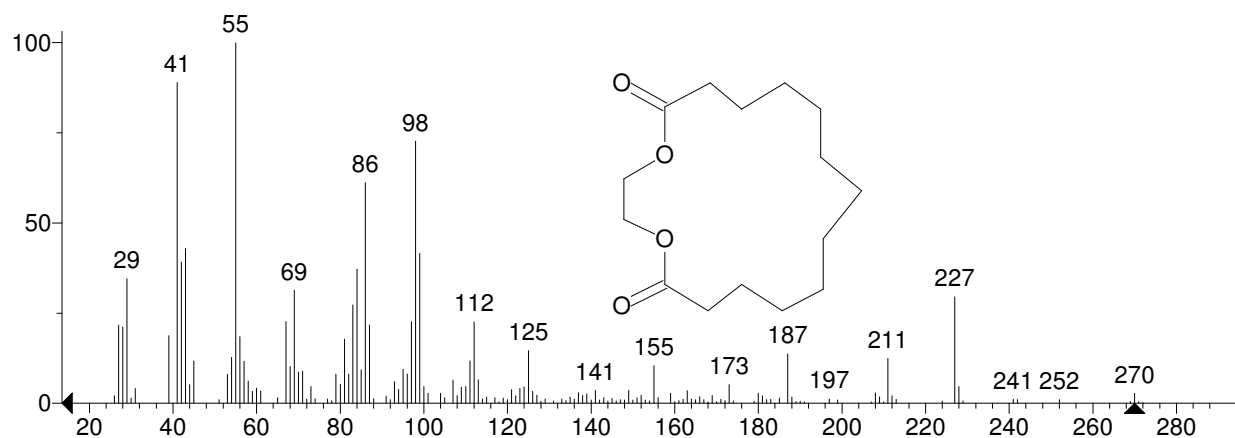


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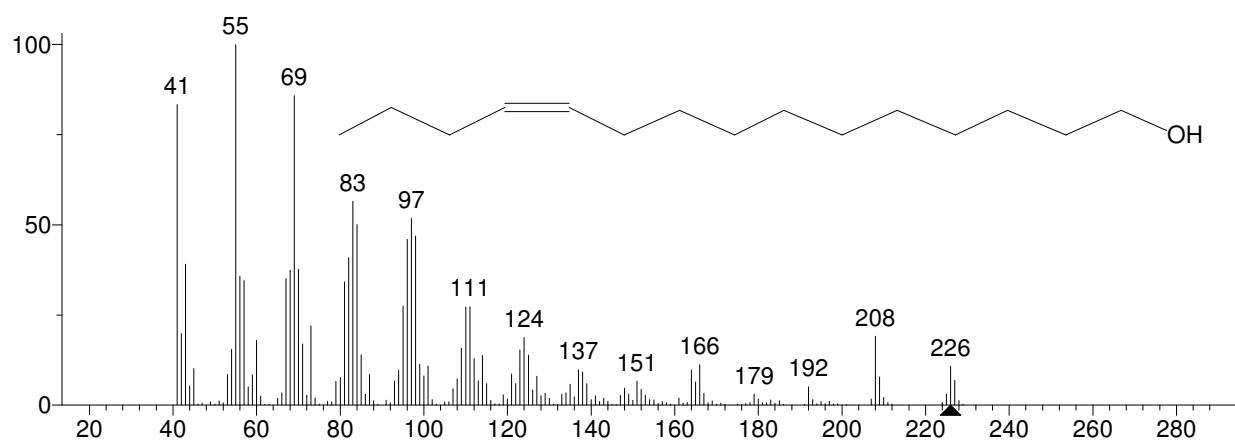
Unknown: Scan 1358 (15.545 min): Designer3.D
Compound in Library Factor = 885



Hit 1 : Ethylene brassylate
C₁₅H₂₆O₄; MF: 960; RMF: 967; Prob 92.0%; CAS: 105-95-3; Lib: mainlib; ID: 16894.

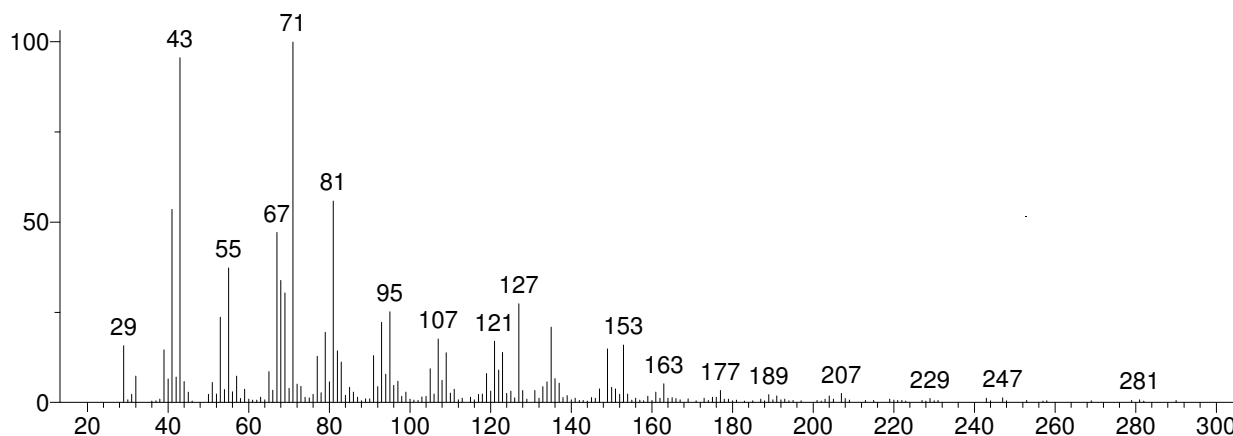


Hit 2 : Z-11-Pentadecenol
C₁₅H₃₀O; MF: 684; RMF: 709; Prob 0.91%; Lib: mainlib; ID: 17391.

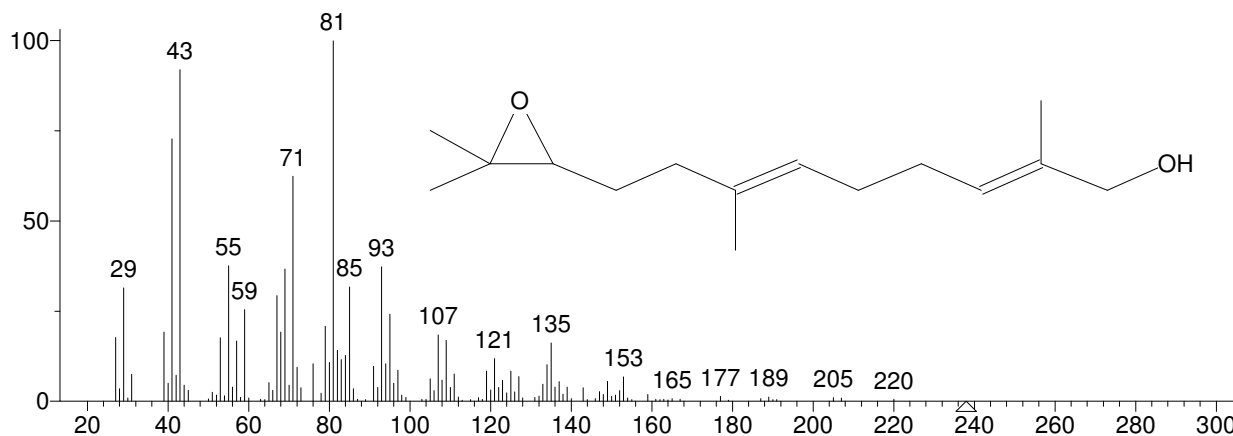


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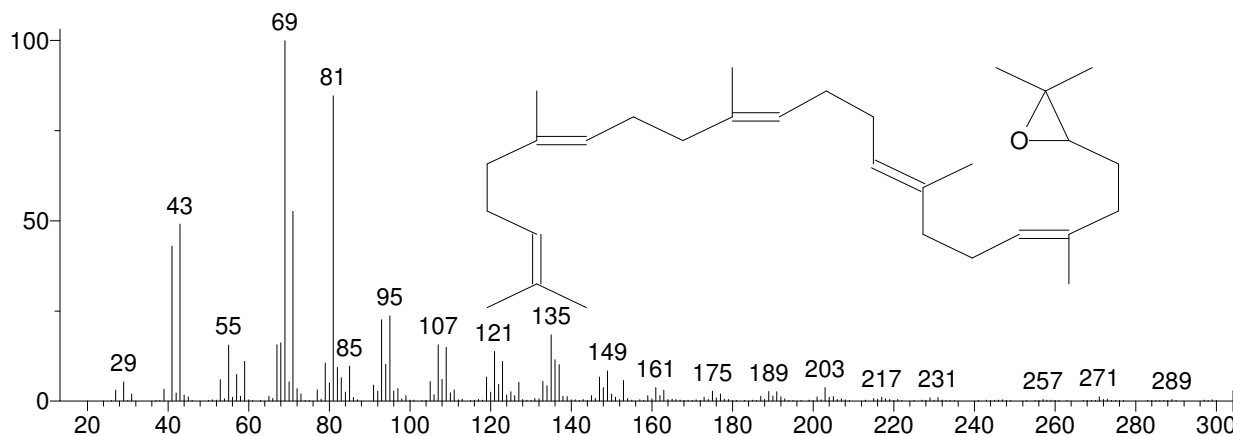
Unknown: Scan 1436 (16.435 min): Designer3.D
Compound in Library Factor = -520



Hit 1 : 9-(3,3-Dimethyloxiran-2-yl)-2,7-dimethylnona-2,6-dien-1-ol
C₁₅H₂₆O₂; MF: 783; RMF: 832; Prob 12.5%; Lib: mainlib; ID: 39428.

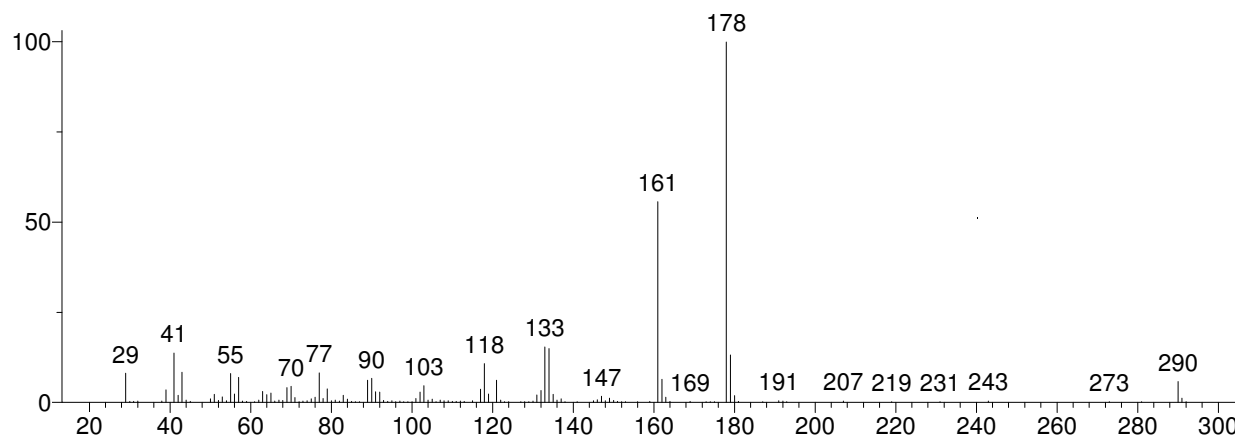


Hit 2 : Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-, (all-E)-
C₃₀H₅₀O; MF: 781; RMF: 798; Prob 11.5%; CAS: 7200-26-2; Lib: mainlib; ID: 28997.

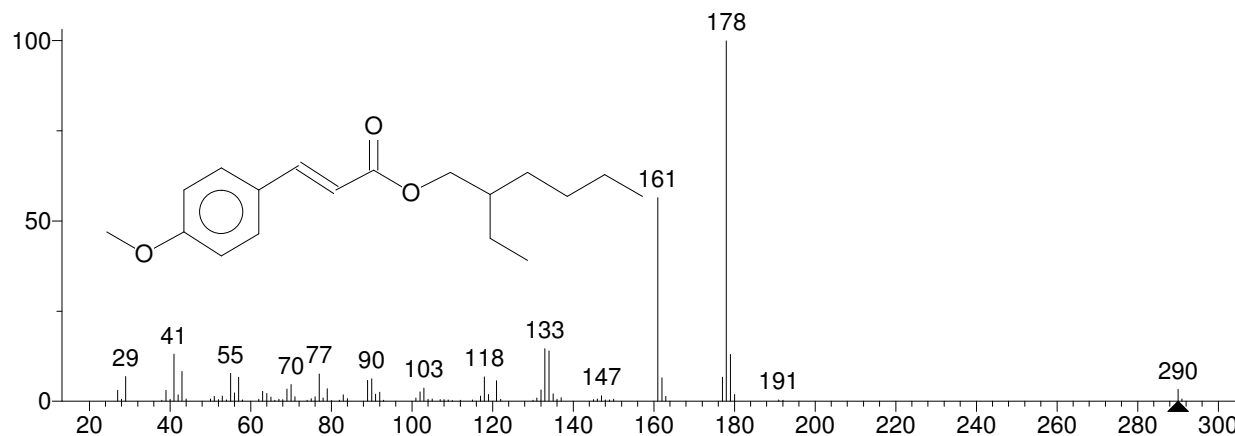


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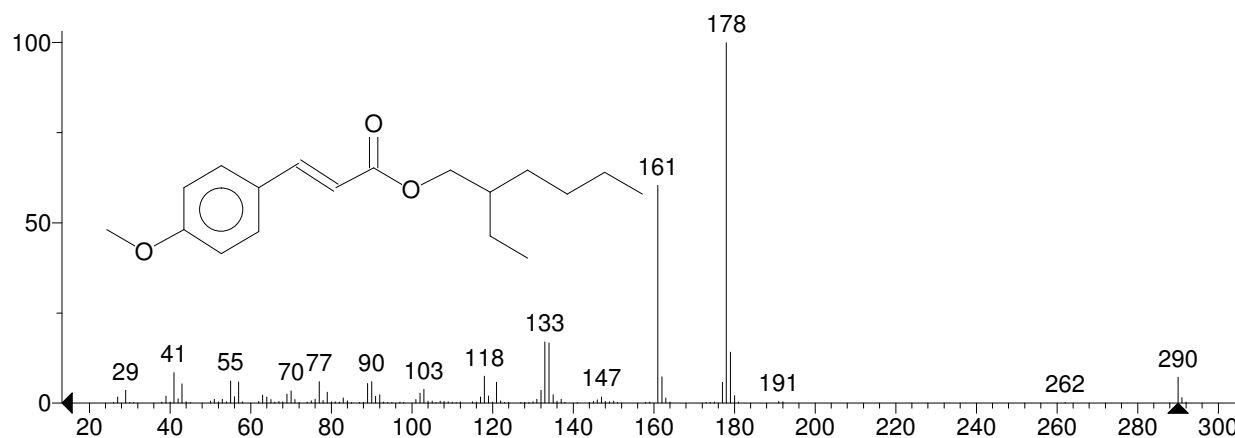
Unknown: Scan 1512 (17.303 min): Designer3.D
Compound in Library Factor = 256



Hit 1 : 2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester
C₁₈H₂₆O₃; MF: 929; RMF: 935; Prob 82.4%; CAS: 5466-77-3; Lib: mainlib; ID: 113107.

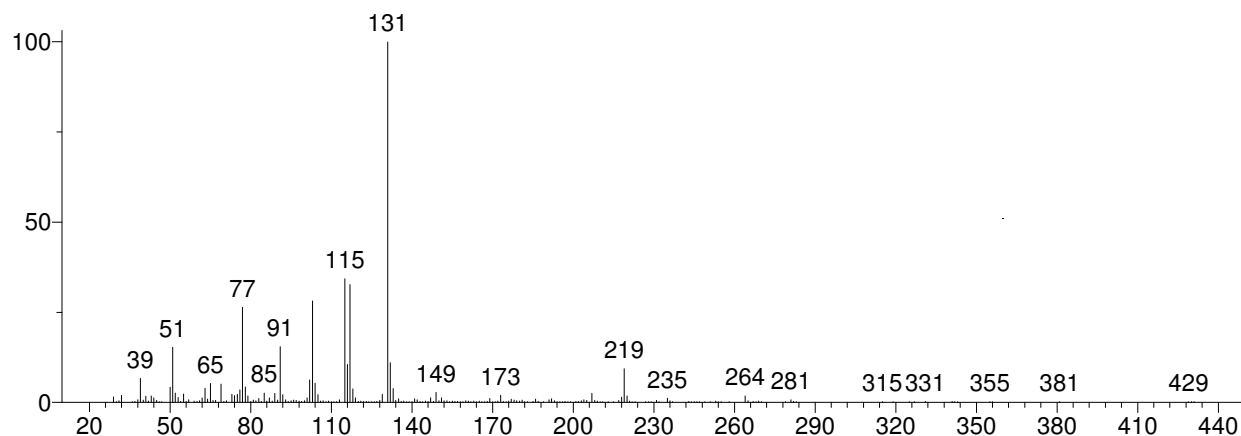


Hit 2 : 2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester
C₁₈H₂₆O₃; MF: 928; RMF: 931; Prob 82.4%; CAS: 5466-77-3; Lib: replib; ID: 22337.

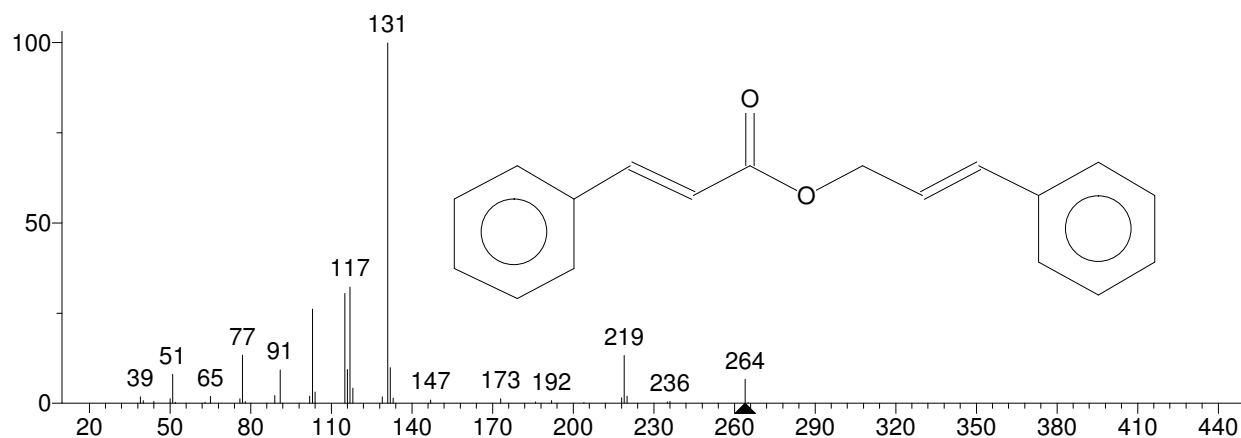


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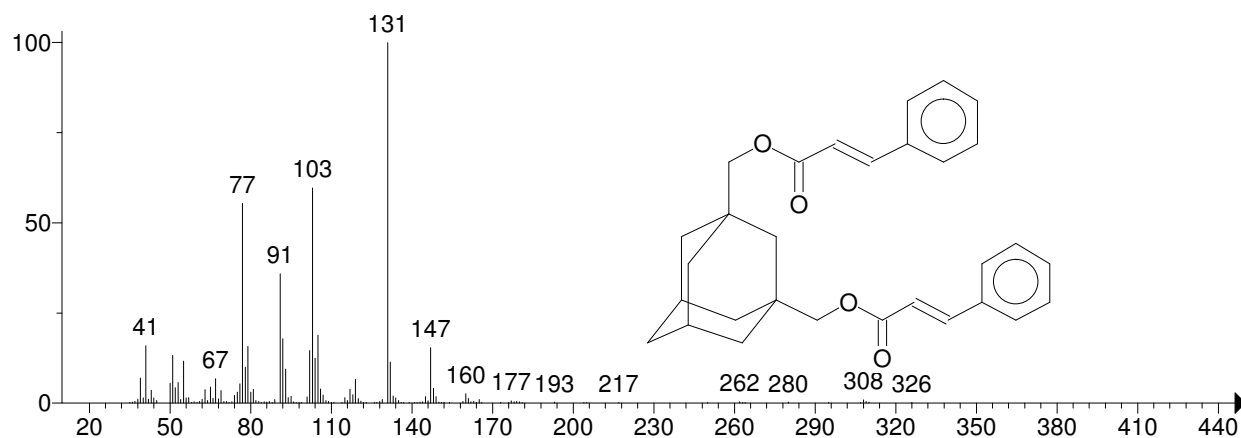
Unknown: Scan 1563 (17.885 min): Designer3.D
Compound in Library Factor = -207



Hit 1 : Cinnamyl cinnamate
C₁₈H₁₆O₂; MF: 761; RMF: 874; Prob 45.6%; CAS: 122-69-0; Lib: mainlib; ID: 82160.

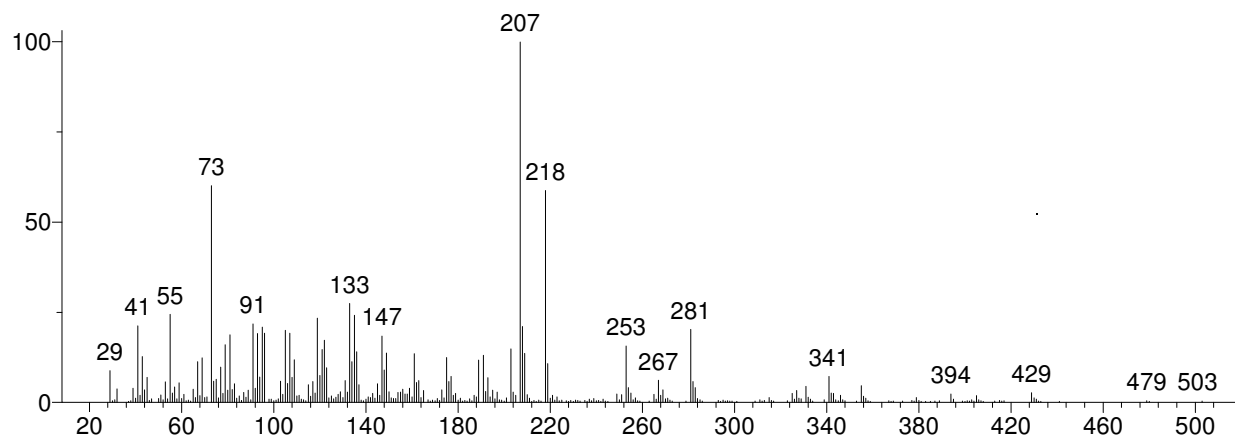


Hit 2 : 1,3-Bis(cinnamoyloxymethyl)adamantane
C₃₀H₃₂O₄; MF: 667; RMF: 715; Prob 3.73%; CAS: 303797-58-2; Lib: mainlib; ID: 82083.

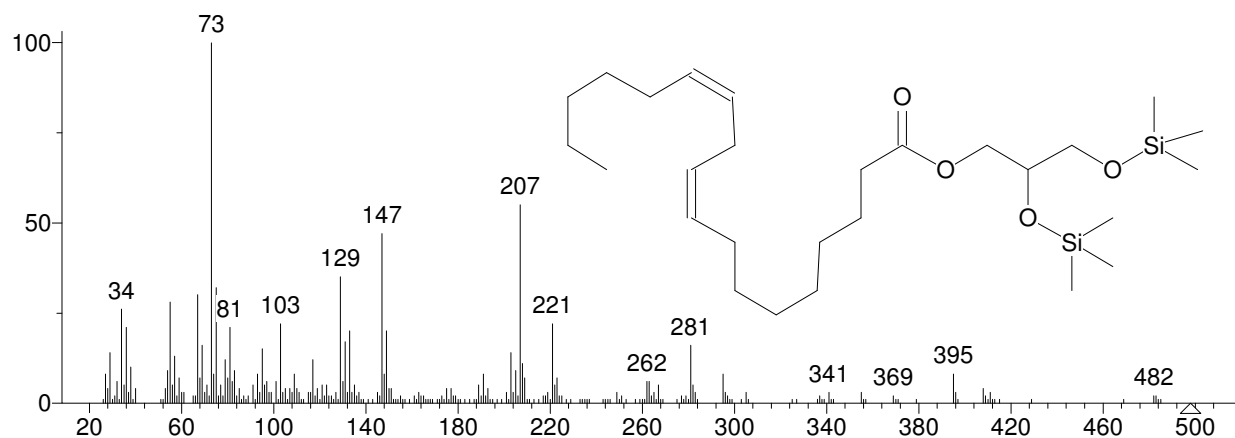


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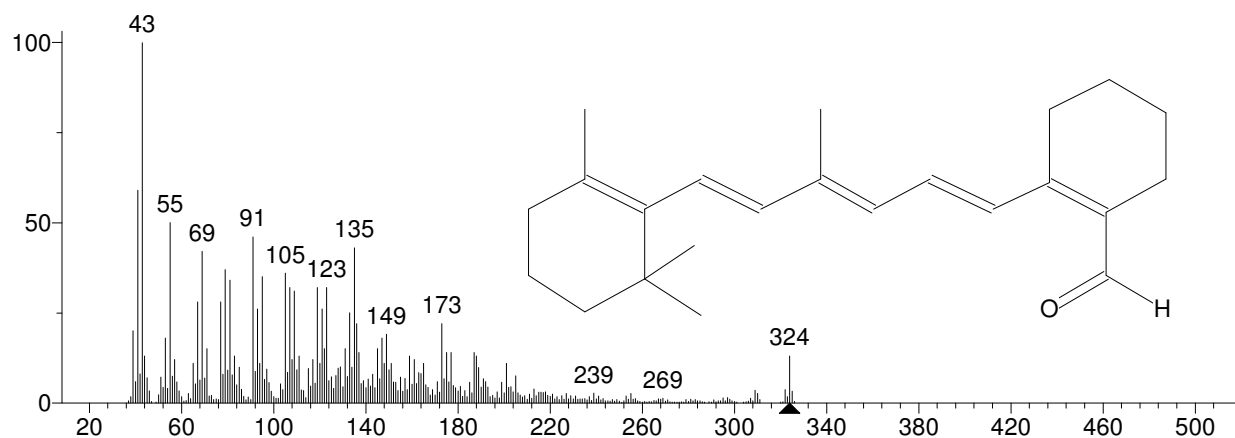
Unknown: Scan 1908 (21.825 min): Designer3.D
Compound in Library Factor = -1210



Hit 1 : 1-Monolinoleoylglycerol trimethylsilyl ether
C₂₇H₅₄O₄Si₂; MF: 653; RMF: 693; Prob 11.3%; CAS: 54284-45-6; Lib: mainlib; ID: 34242.

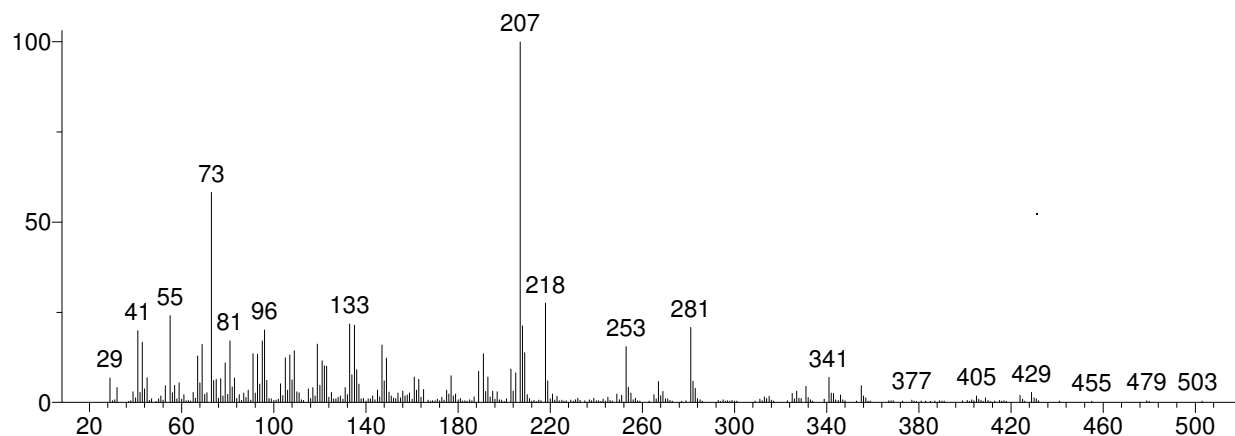


Hit 2 : 2-[4-methyl-6-(2,6,6-trimethylcyclohex-1-enyl)hexa-1,3,5-trienyl]cyclohex-1-en-1-carboxaldehyde
C₂₃H₃₂O; MF: 652; RMF: 689; Prob 10.9%; Lib: mainlib; ID: 5319.

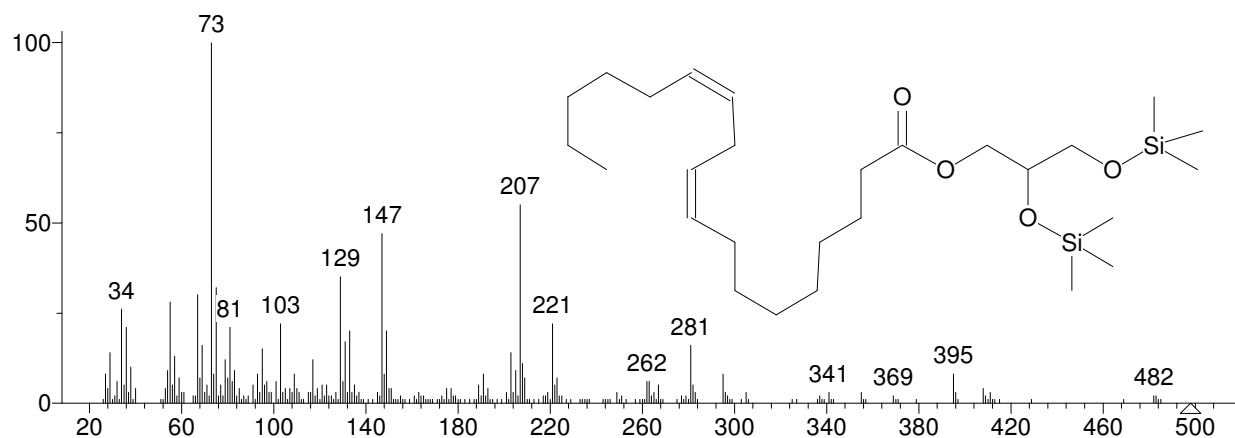


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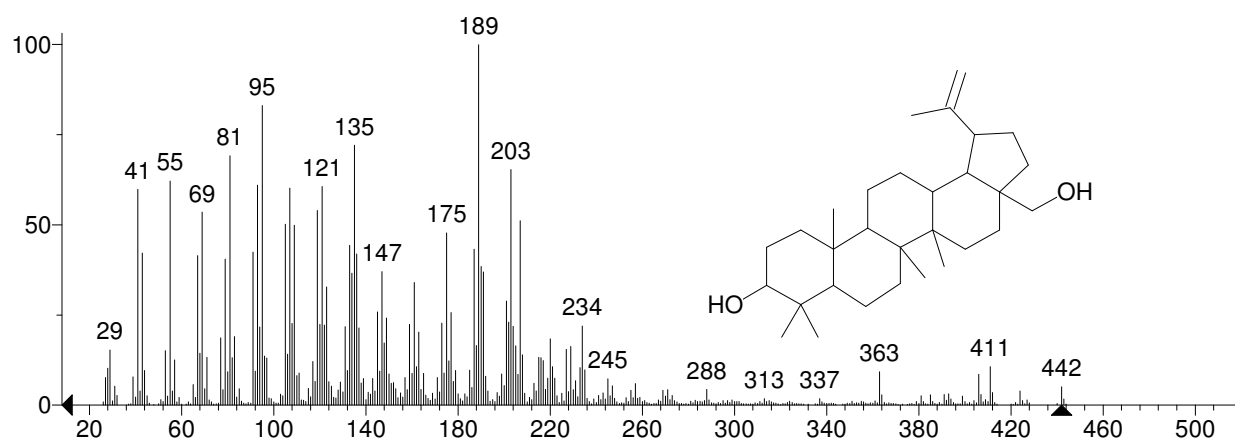
Unknown: Scan 2105 (24.074 min): Designer3.D
Compound in Library Factor = -1169



Hit 1 : 1-Monolinoleoylglycerol trimethylsilyl ether
C₂₇H₅₄O₄Si₂; MF: 665; RMF: 718; Prob 16.3%; CAS: 54284-45-6; Lib: mainlib; ID: 34242.

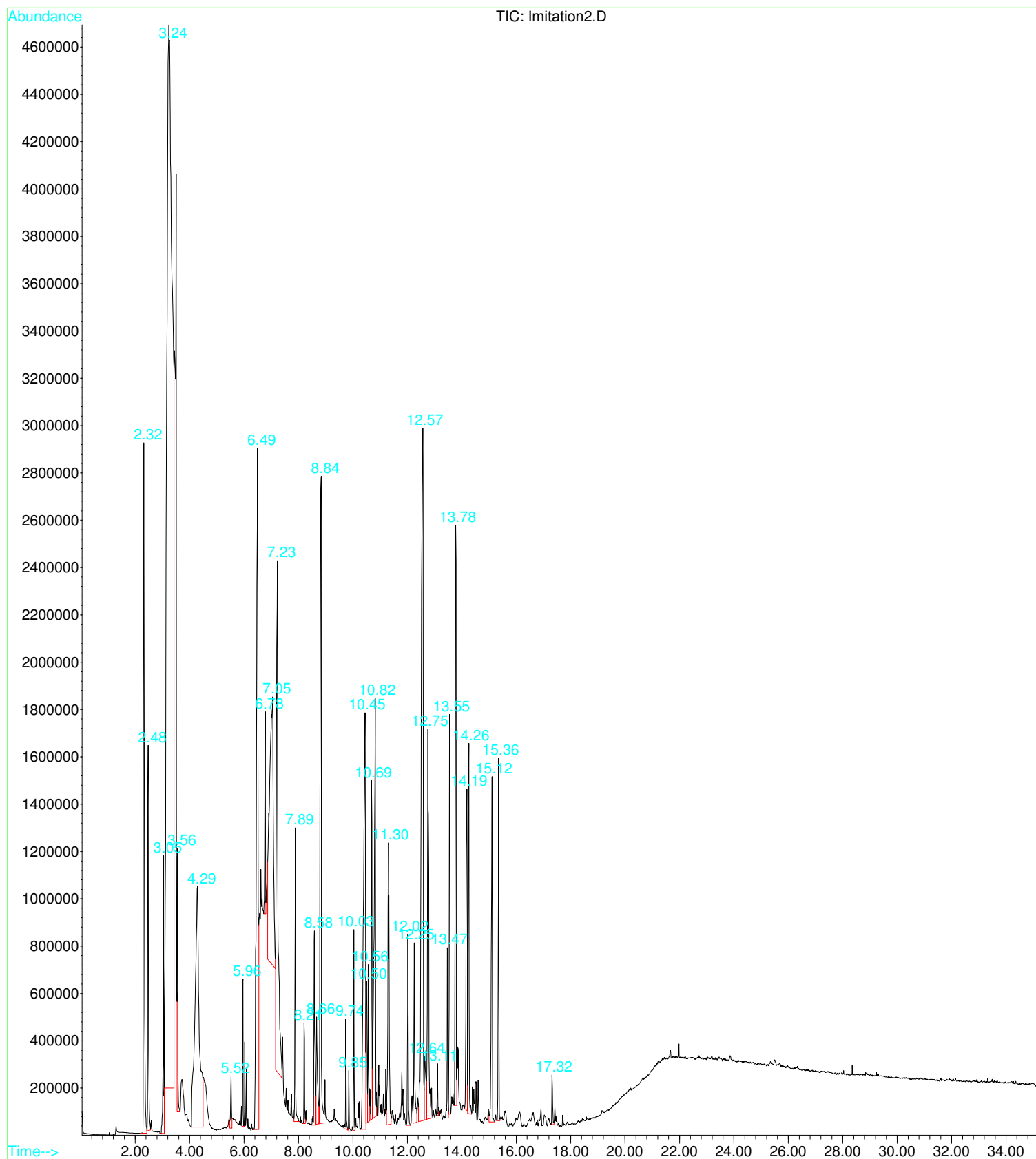


Hit 2 : Betulin
C₃₀H₅₀O₂; MF: 648; RMF: 660; Prob 8.87%; CAS: 473-98-3; Lib: replib; ID: 23168.



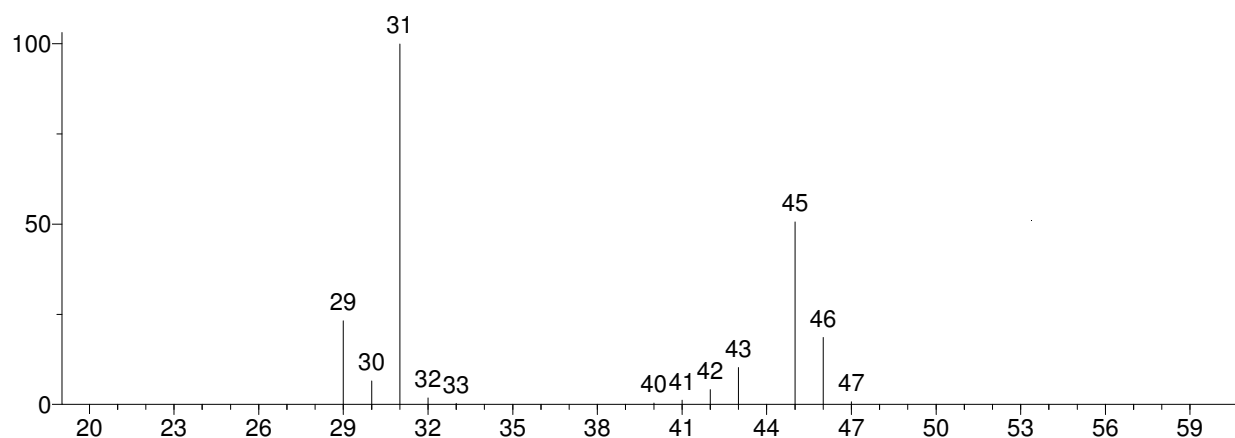
DMS RESULTS

Imitation

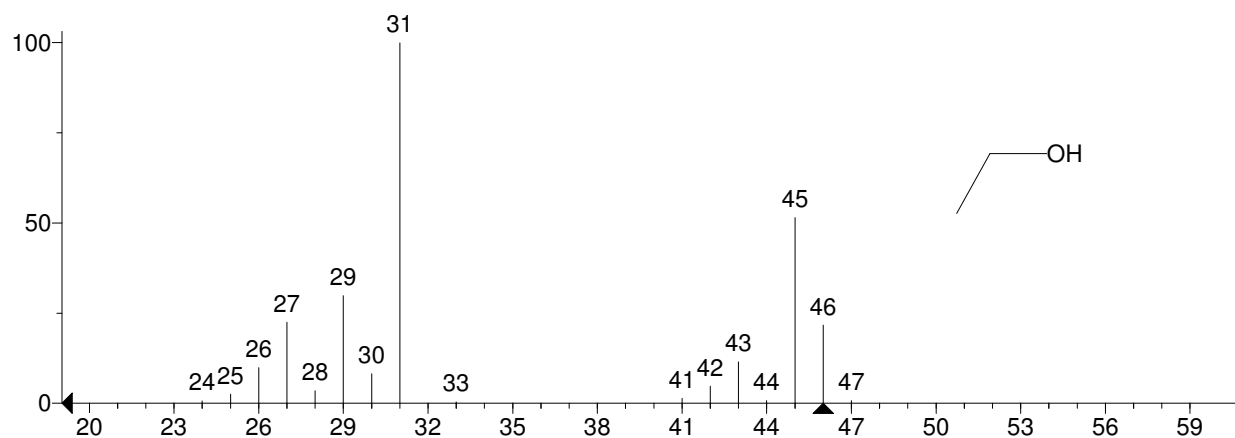


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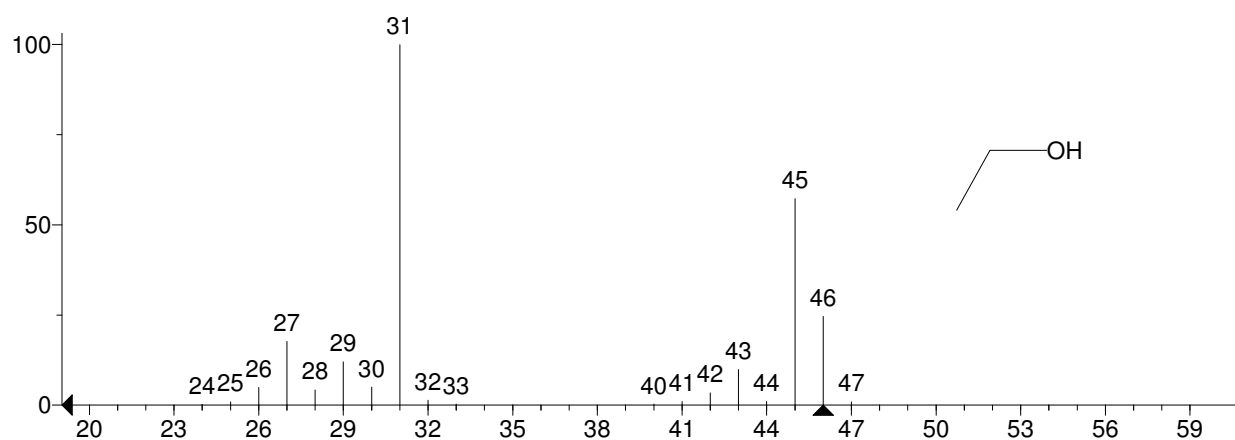
Unknown: Scan 200 (2.316 min): Imitation2.D
Compound in Library Factor = 614



Hit 1 : Ethyl alcohol
C2H6O; MF: 973; RMF: 978; Prob 98.1%; CAS: 64-17-5; Lib: mainlib; ID: 1334.

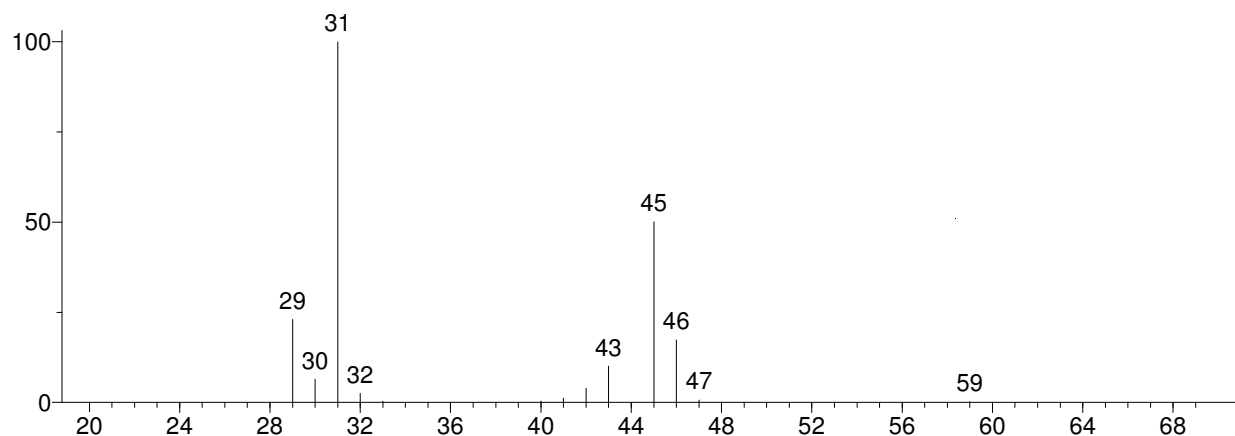


Hit 2 : Ethyl alcohol
C2H6O; MF: 945; RMF: 945; Prob 98.1%; CAS: 64-17-5; Lib: replib; ID: 552.

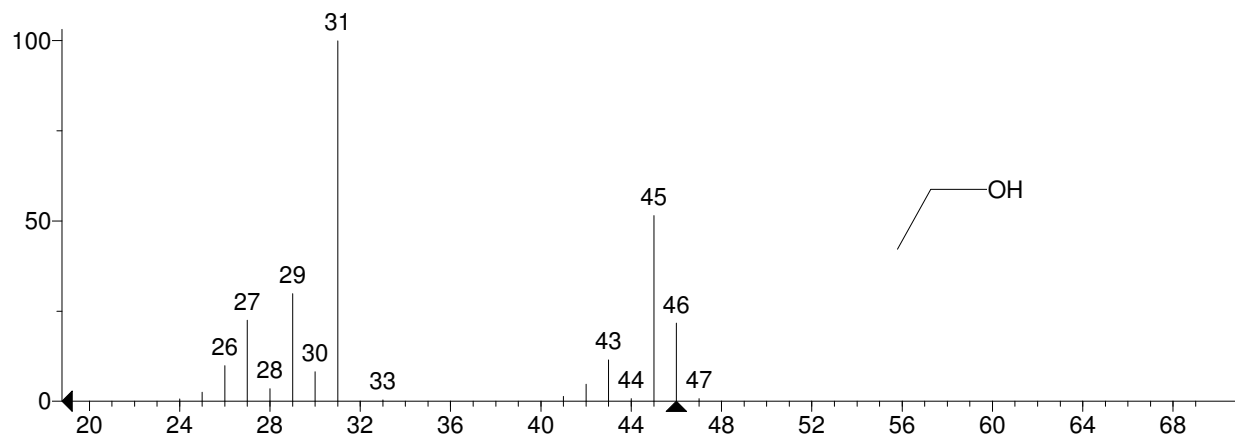


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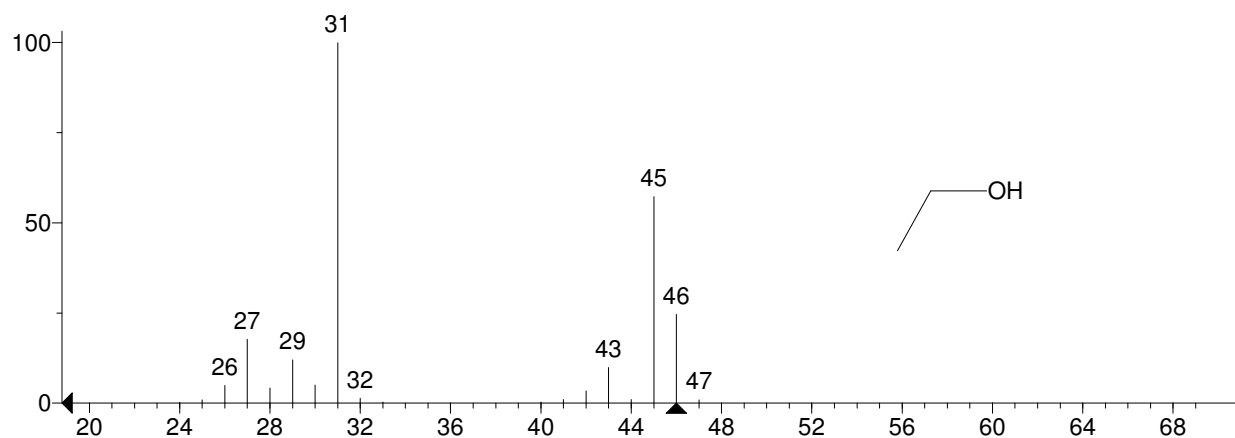
Unknown: Scan 214 (2.475 min): Imitation2.D
Compound in Library Factor = 614



Hit 1 : Ethyl alcohol
C2H6O; MF: 971; RMF: 978; Prob 97.7%; CAS: 64-17-5; Lib: mainlib; ID: 1334.

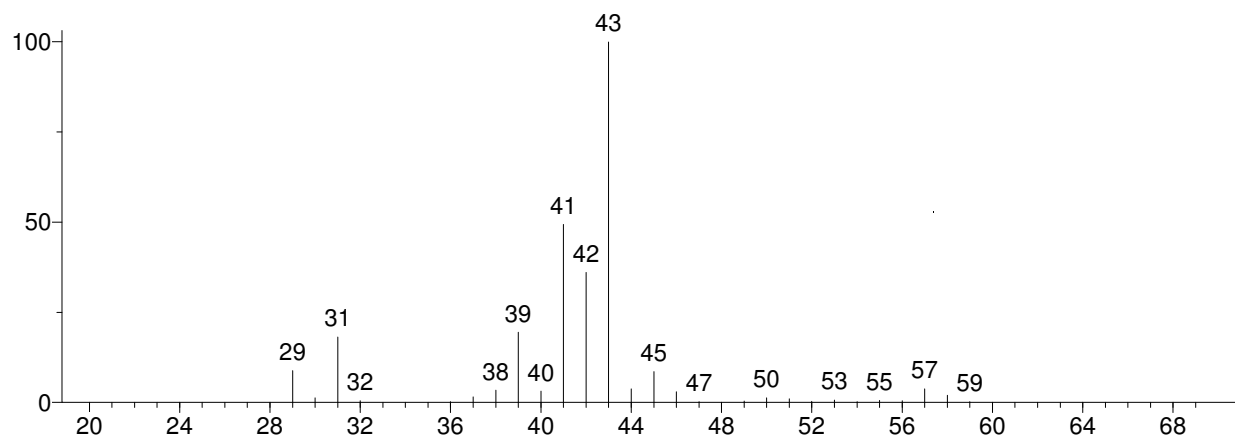


Hit 2 : Ethyl alcohol
C2H6O; MF: 934; RMF: 934; Prob 97.7%; CAS: 64-17-5; Lib: replib; ID: 552.

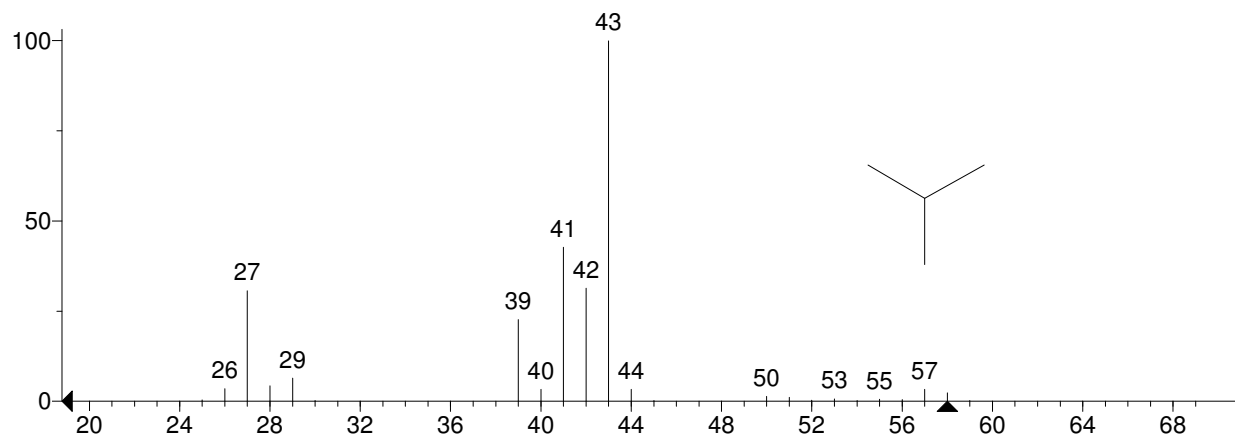


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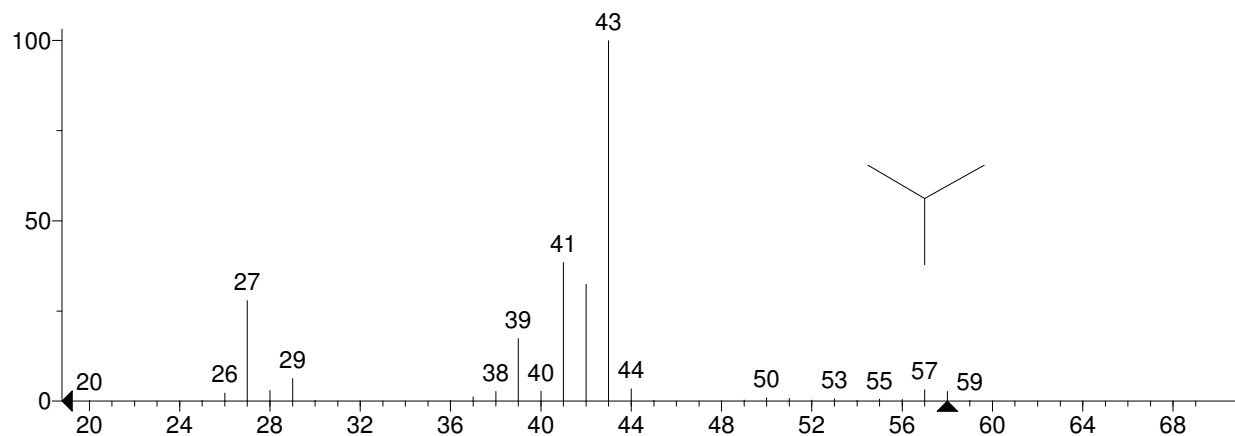
Unknown: Scan 264 (3.046 min): Imitation2.D
Compound in Library Factor = 199



Hit 1 : Isobutane
C₄H₁₀; MF: 898; RMF: 962; Prob 83.5%; CAS: 75-28-5; Lib: replib; ID: 1629.

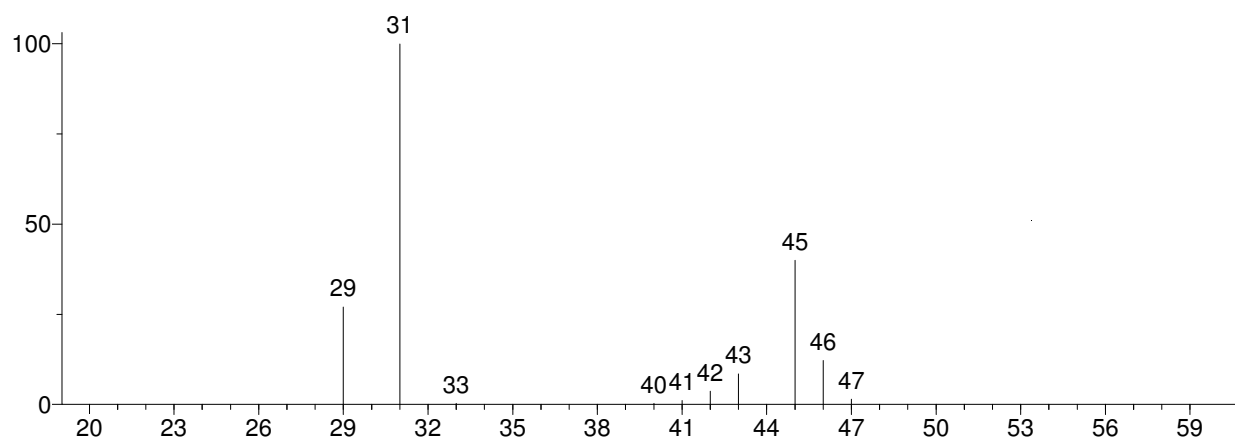


Hit 2 : Isobutane
C₄H₁₀; MF: 889; RMF: 923; Prob 83.5%; CAS: 75-28-5; Lib: mainlib; ID: 5254.

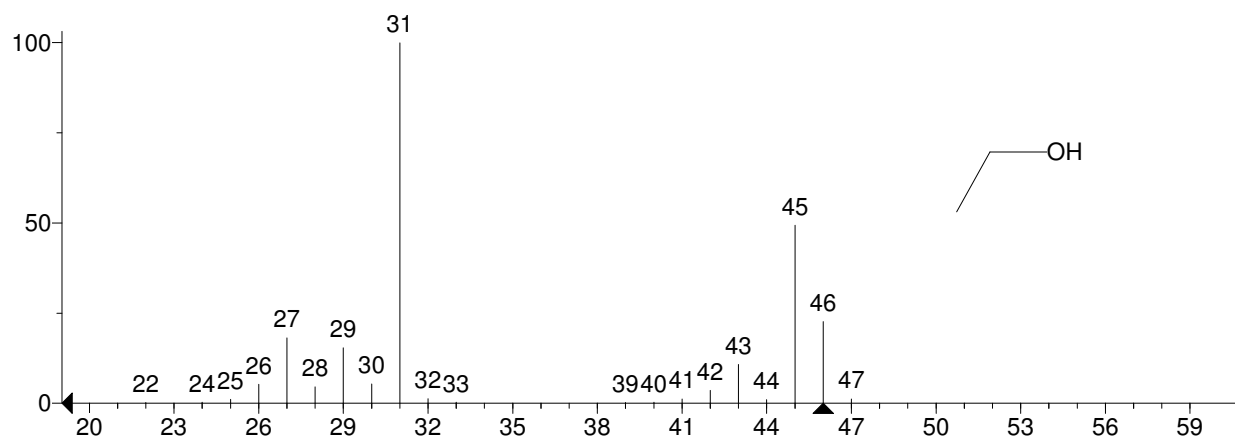


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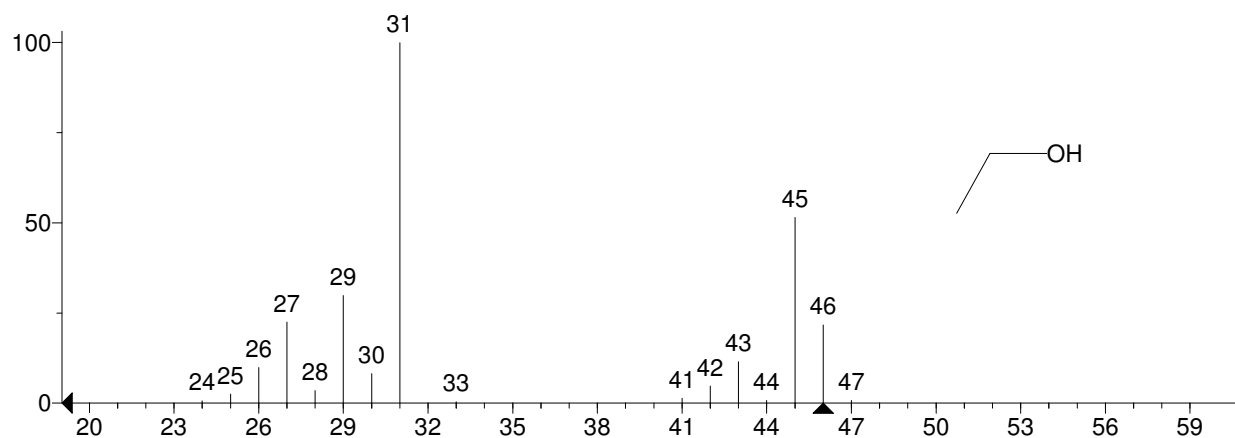
Unknown: Scan 281 (3.240 min): Imitation.D
Compound in Library Factor = 449



Hit 1 : Ethyl alcohol
C₂H₆O; MF: 918; RMF: 918; Prob 93.9%; CAS: 64-17-5; Lib: replib; ID: 551.

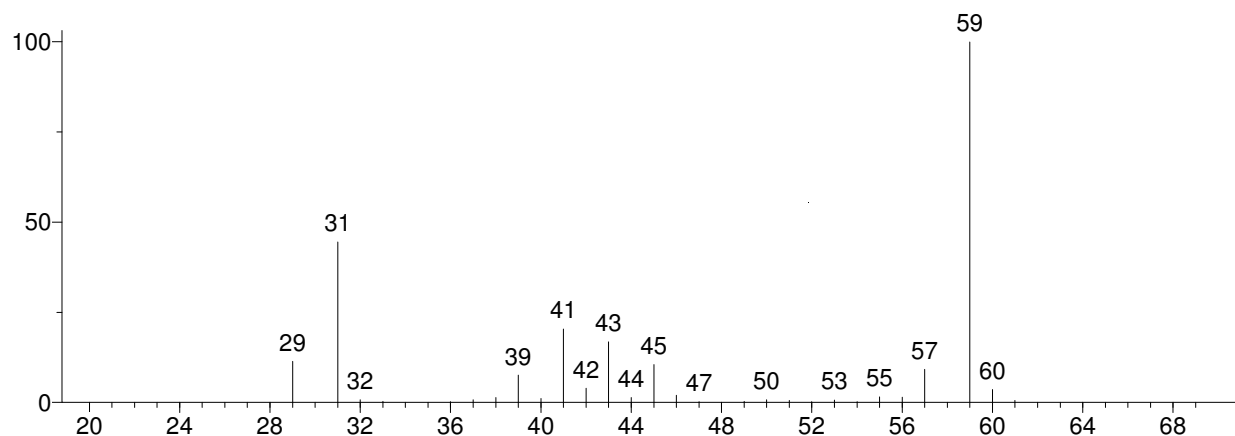


Hit 2 : Ethyl alcohol
C₂H₆O; MF: 911; RMF: 912; Prob 93.9%; CAS: 64-17-5; Lib: mainlib; ID: 1334.

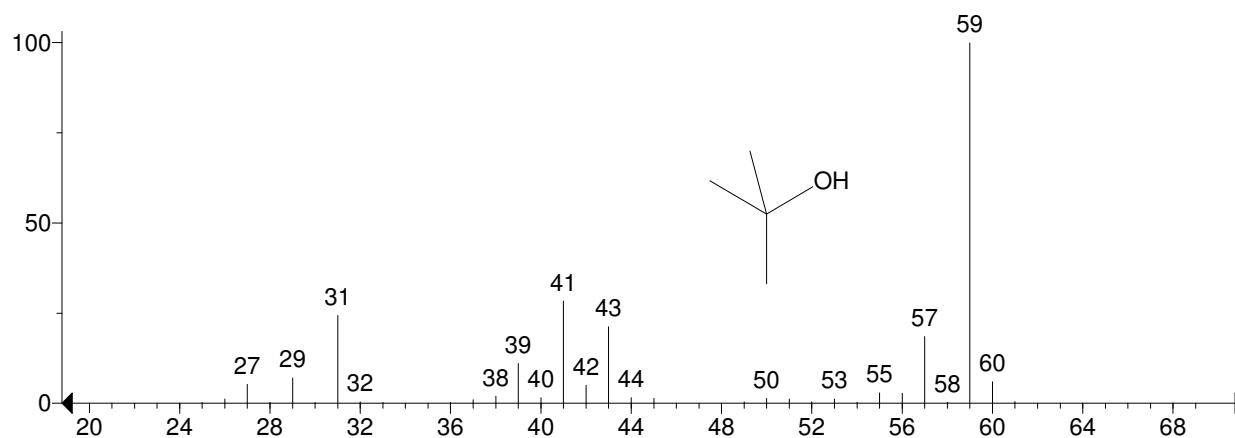


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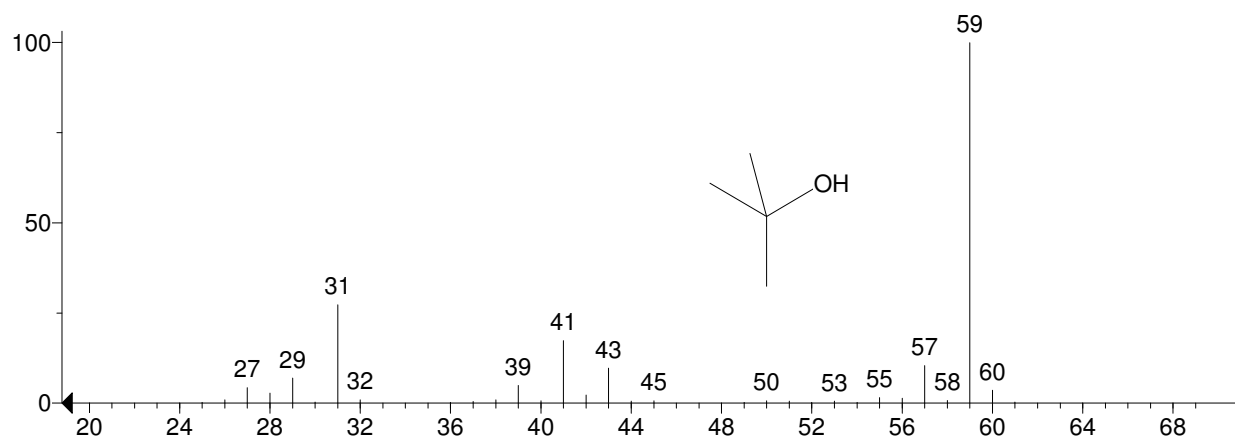
Unknown: Scan 309 (3.560 min): Imitation.D
Compound in Library Factor = 178



Hit 1 : 2-Propanol, 2-methyl-
C₄H₁₀O; MF: 913; RMF: 916; Prob 61.7%; CAS: 75-65-0; Lib: replib; ID: 6416.

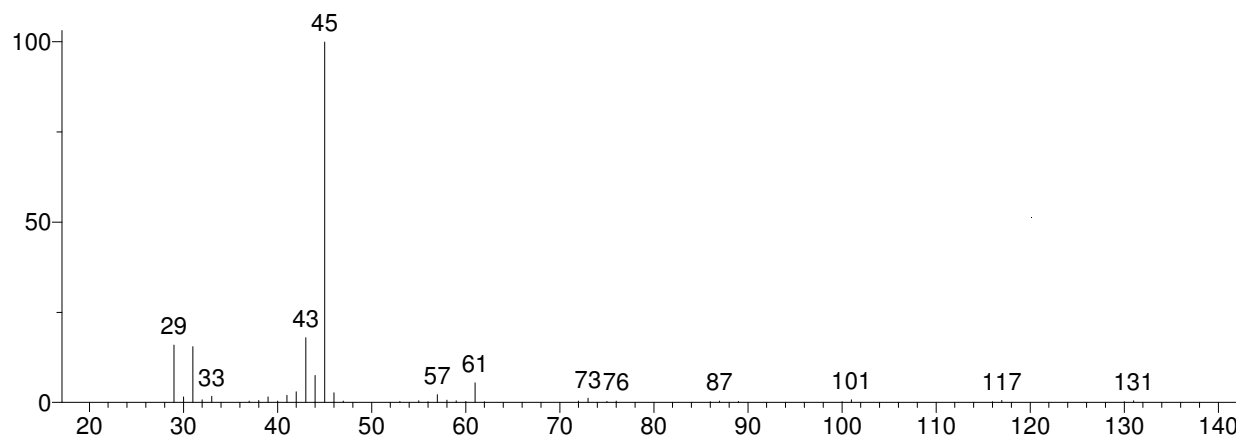


Hit 2 : 2-Propanol, 2-methyl-
C₄H₁₀O; MF: 909; RMF: 914; Prob 61.7%; CAS: 75-65-0; Lib: replib; ID: 6395.

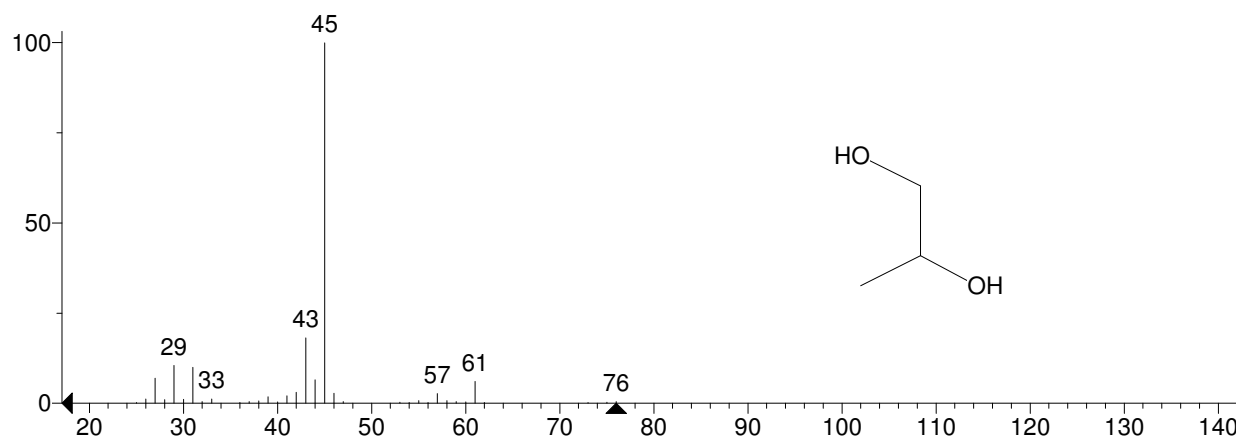


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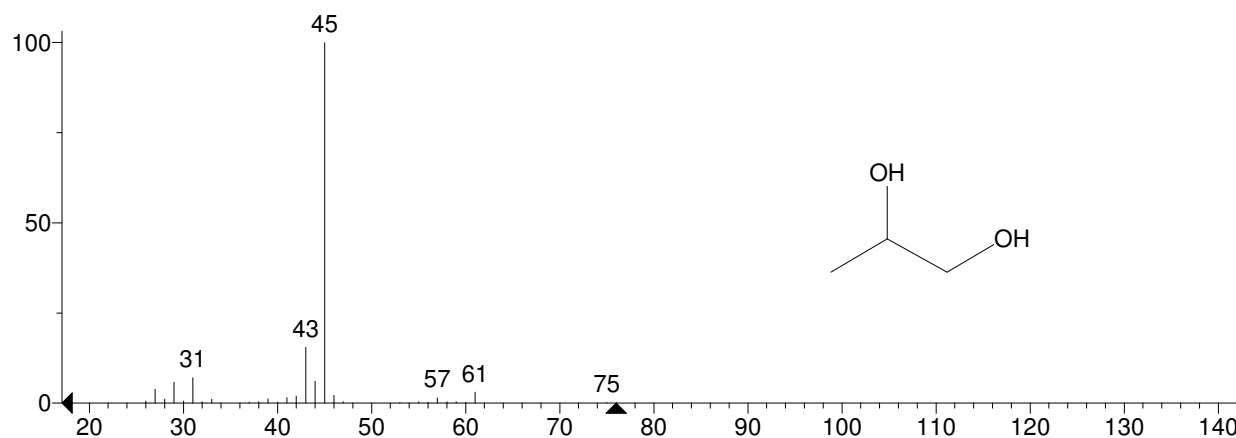
Unknown: Scan 373 (4.291 min): Imitation2.D
Compound in Library Factor = 242



Hit 1 : Propylene Glycol
C3H8O2; MF: 913; RMF: 929; Prob 39.3%; CAS: 57-55-6; Lib: replib; ID: 3553.

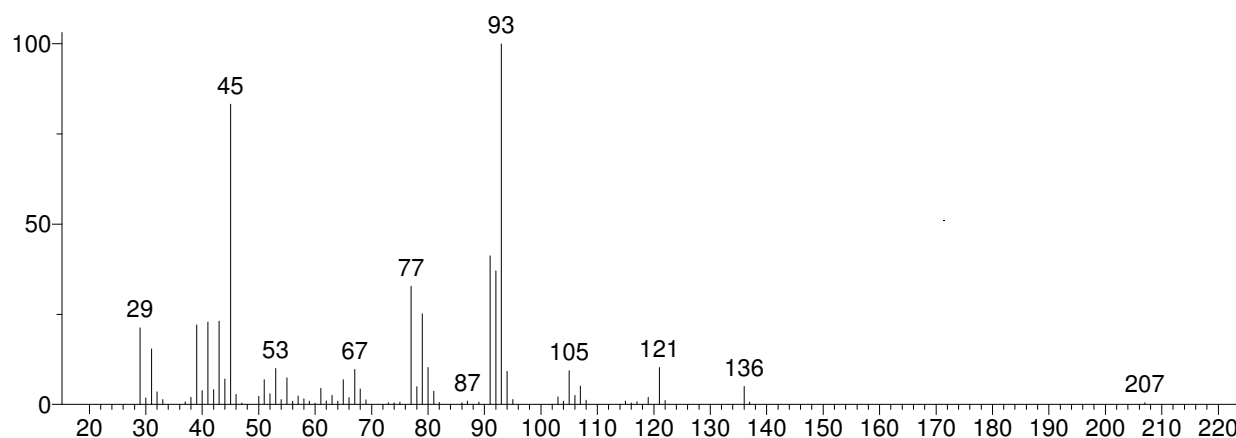


Hit 2 : (S)-(+)-1,2-Propanediol
C3H8O2; MF: 912; RMF: 933; Prob 37.8%; CAS: 4254-15-3; Lib: replib; ID: 3557.

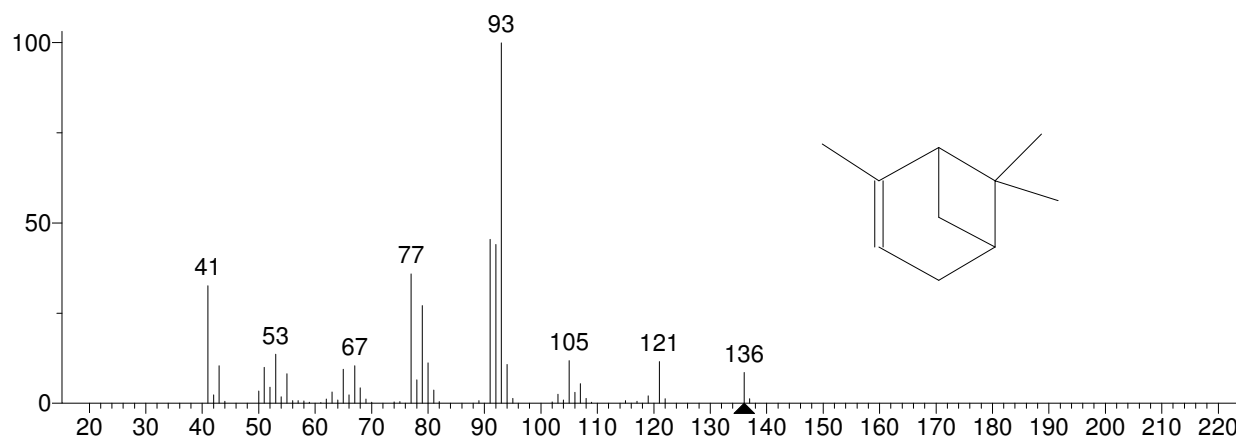


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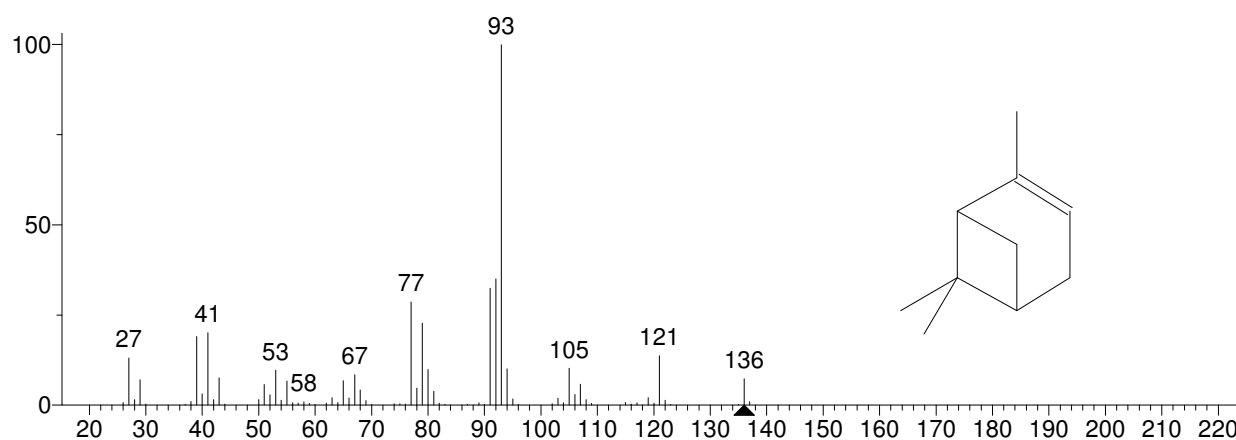
Unknown: Scan 481 (5.524 min): Imitation.D
Compound in Library Factor = -217



Hit 1 : 1R-.alpha.-Pinene
C₁₀H₁₆; MF: 880; RMF: 937; Prob 17.6%; CAS: 7785-70-8; Lib: replib; ID: 12053.

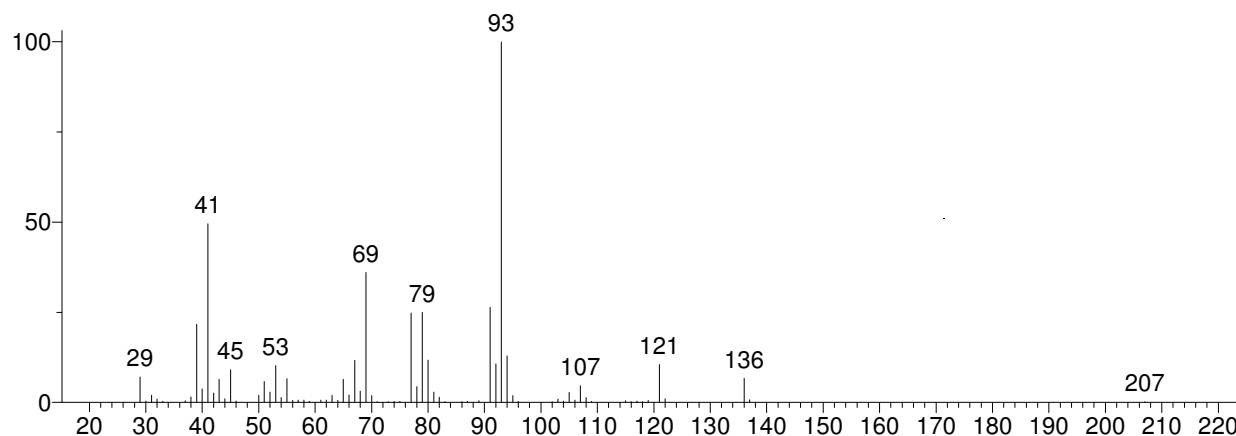


Hit 2 : .alpha.-Pinene
C₁₀H₁₆; MF: 876; RMF: 941; Prob 14.9%; CAS: 80-56-8; Lib: mainlib; ID: 51652.

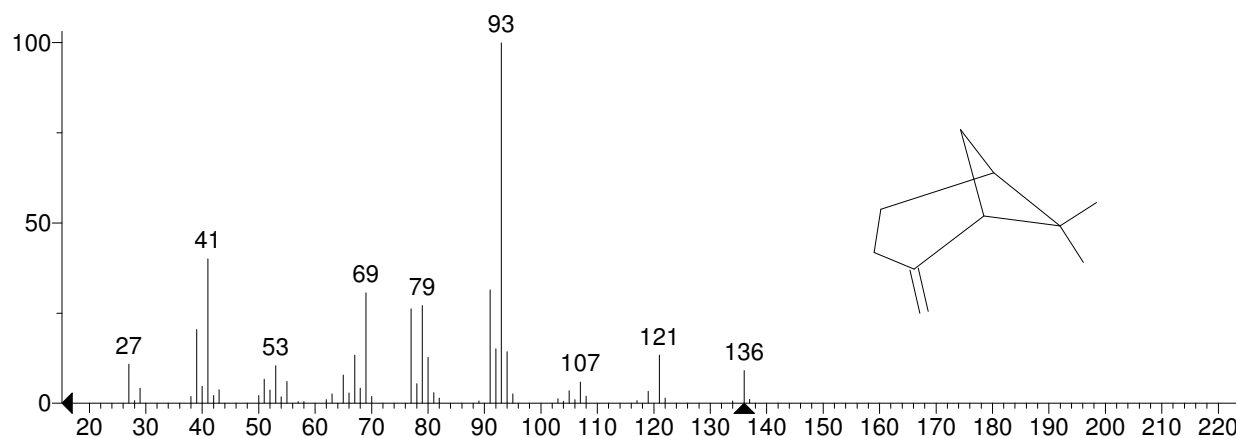


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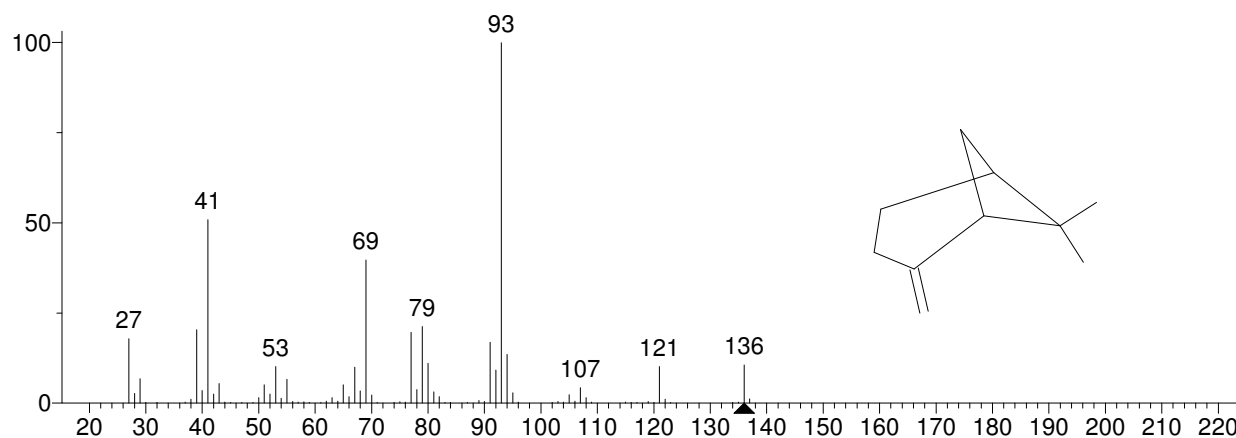
Unknown: Scan 519 (5.958 min): Imitation2.D
Compound in Library Factor = -107



Hit 1 : Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-
C₁₀H₁₆; MF: 929; RMF: 942; Prob 28.4%; CAS: 18172-67-3; Lib: replib; ID: 11958.

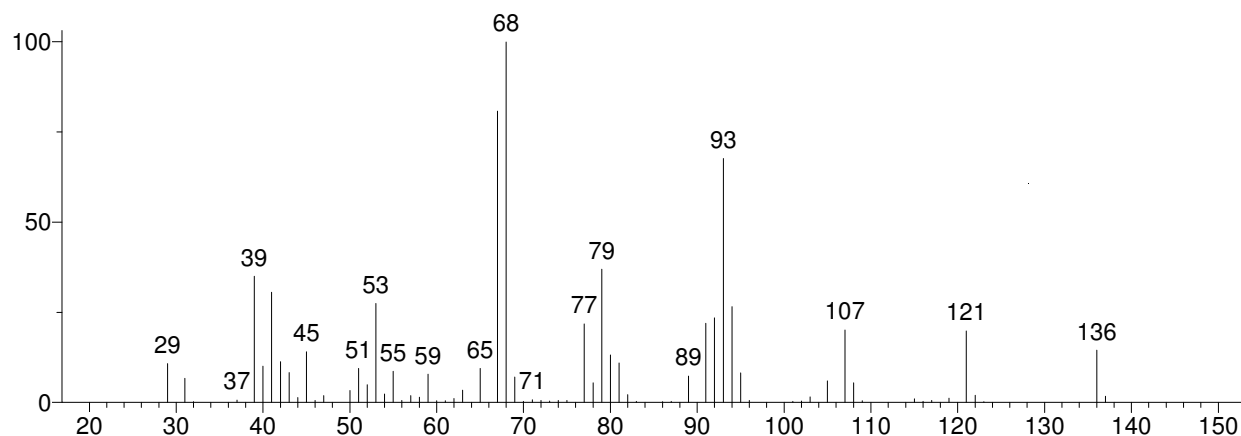


Hit 2 : .beta.-Pinene
C₁₀H₁₆; MF: 927; RMF: 929; Prob 26.2%; CAS: 127-91-3; Lib: replib; ID: 11947.

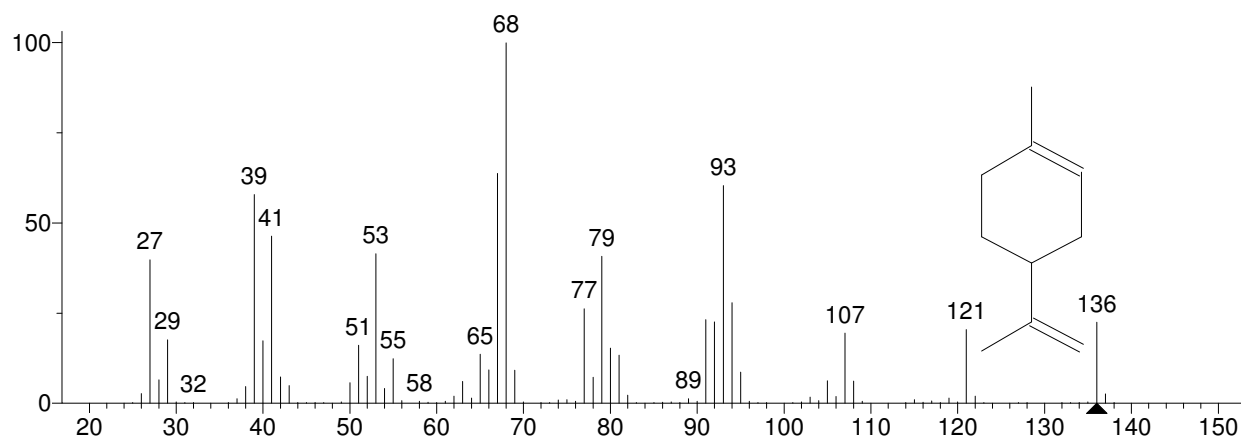


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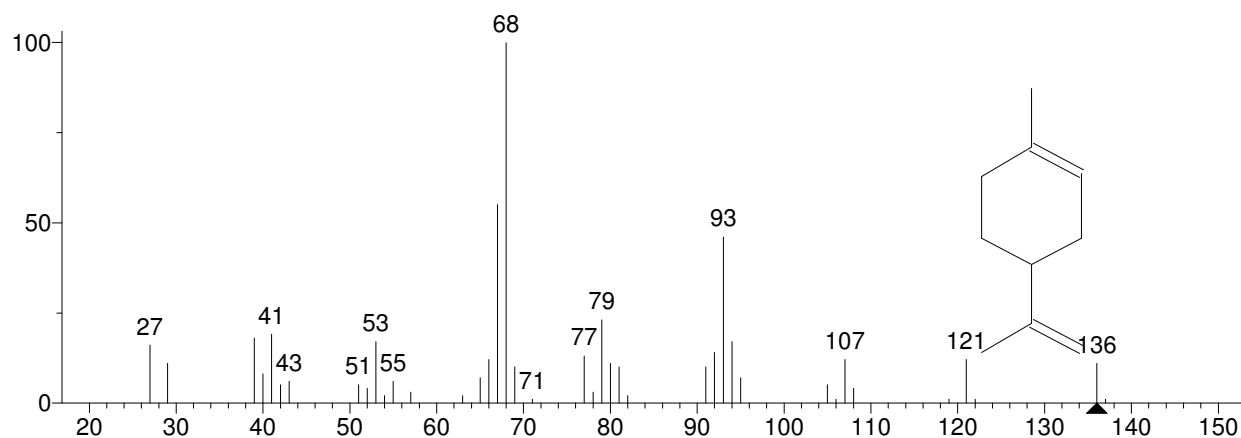
Unknown: Scan 566 (6.495 min): Imitation2.D
Compound in Library Factor = -113



Hit 1 : Limonene
C₁₀H₁₆; MF: 912; RMF: 919; Prob 25.0%; CAS: 138-86-3; Lib: replib; ID: 7399.

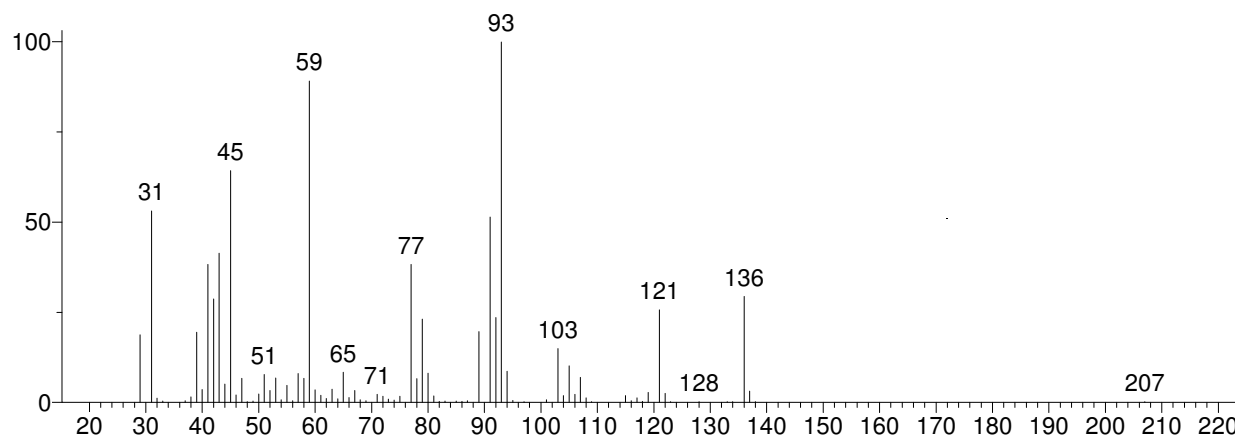


Hit 2 : Limonene
C₁₀H₁₆; MF: 897; RMF: 932; Prob 25.0%; CAS: 138-86-3; Lib: replib; ID: 7398.

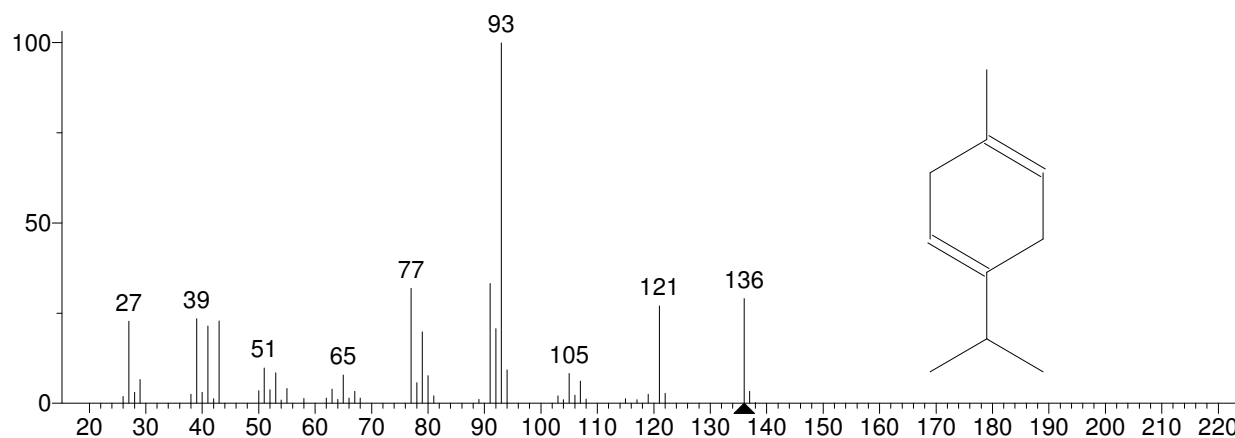


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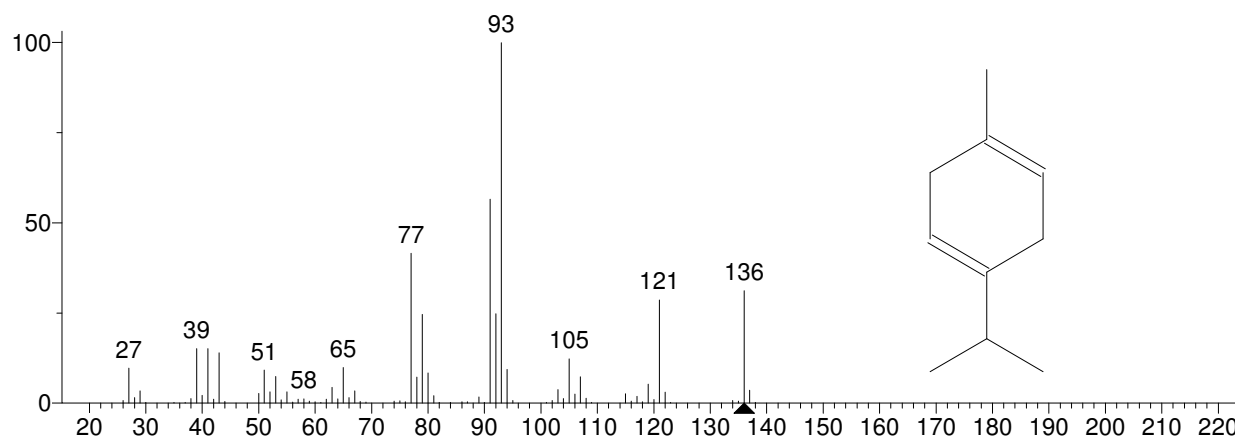
Unknown: Scan 591 (6.780 min): Imitation2.D
Compound in Library Factor = -394



Hit 1 : 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
C₁₀H₁₆; MF: 793; RMF: 903; Prob 22.6%; CAS: 99-85-4; Lib: replib; ID: 12040.

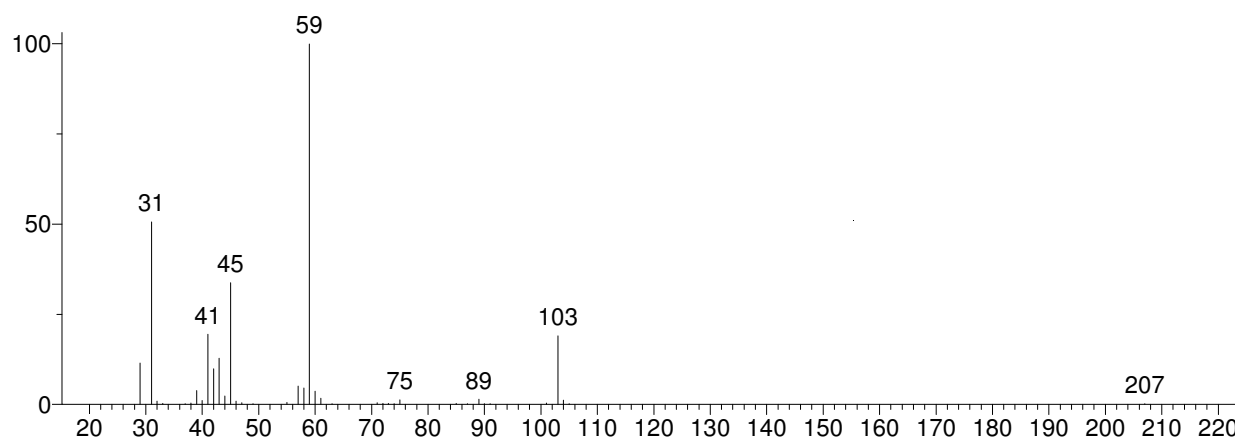


Hit 2 : 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
C₁₀H₁₆; MF: 785; RMF: 829; Prob 22.6%; CAS: 99-85-4; Lib: replib; ID: 12042.

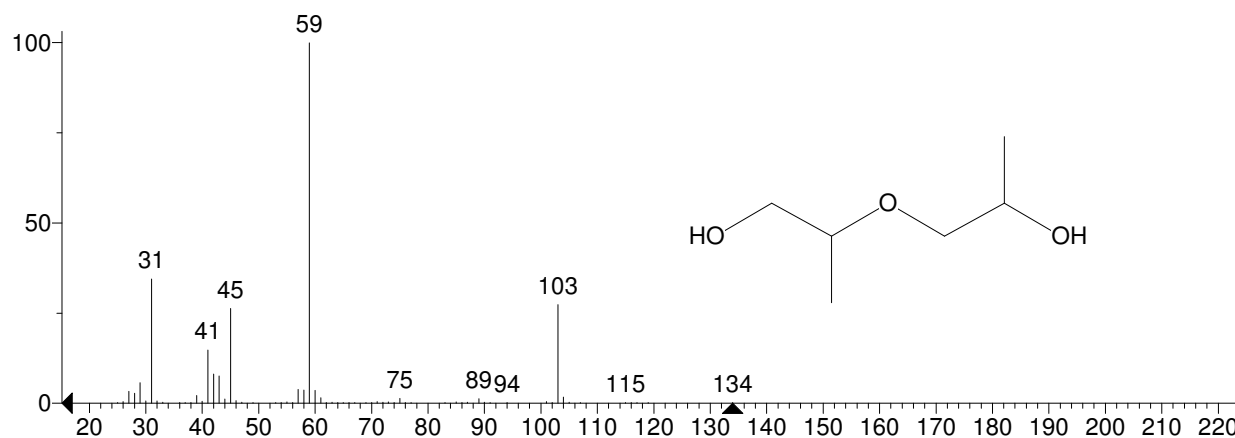


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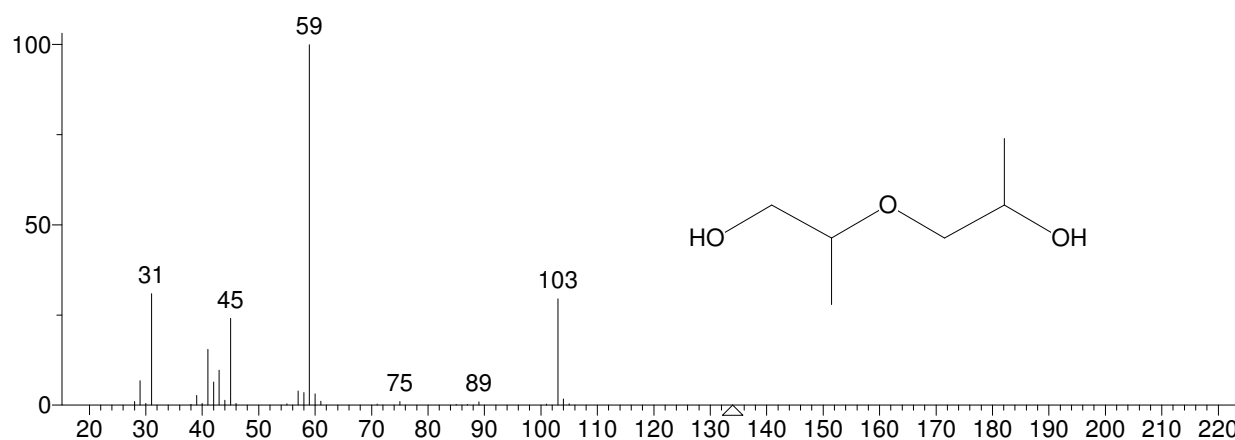
Unknown: Scan 615 (7.054 min): Imitation2.D
Compound in Library Factor = 125



Hit 1 : 1-Propanol, 2-(2-hydroxypropoxy)-
C₆H₁₄O₃; MF: 918; RMF: 918; Prob 38.3%; CAS: 106-62-7; Lib: mainlib; ID: 24523.

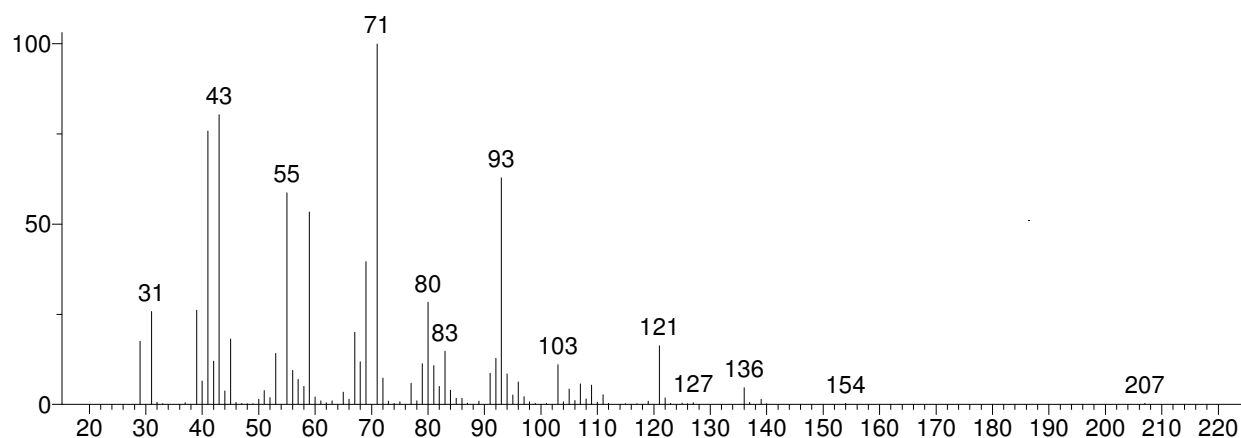


Hit 2 : 1-Propanol, 2-(2-hydroxypropoxy)-
C₆H₁₄O₃; MF: 916; RMF: 919; Prob 38.3%; CAS: 106-62-7; Lib: replib; ID: 6407.

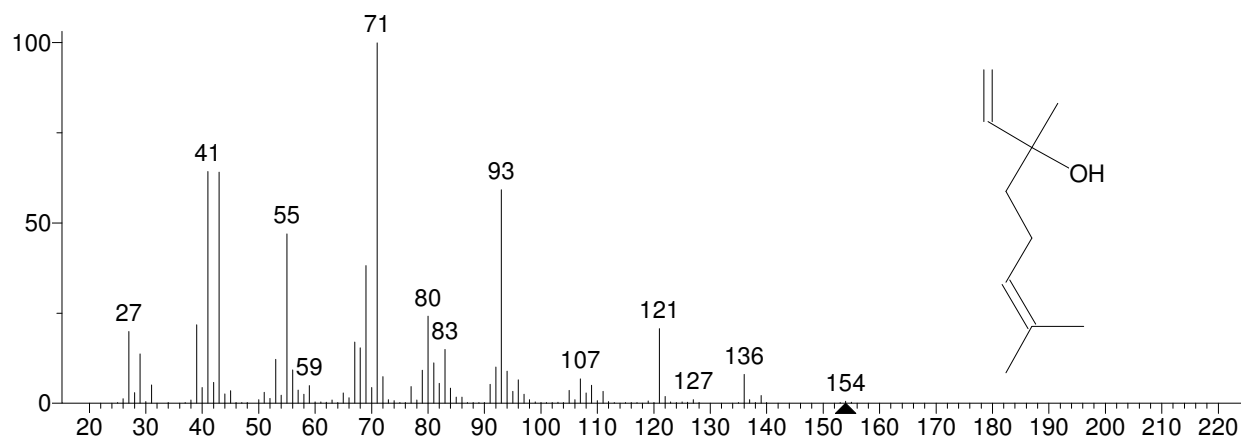


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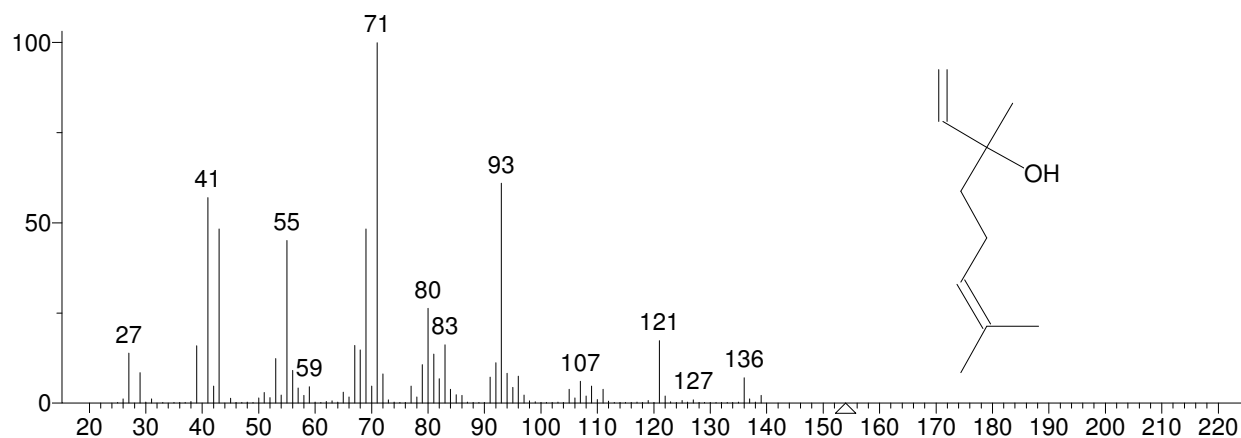
Unknown: Scan 630 (7.225 min): Imitation2.D
Compound in Library Factor = 102



Hit 1 : 1,6-Octadien-3-ol, 3,7-dimethyl-
C₁₀H₁₈O; MF: 875; RMF: 876; Prob 64.7%; CAS: 78-70-6; Lib: mainlib; ID: 30690.

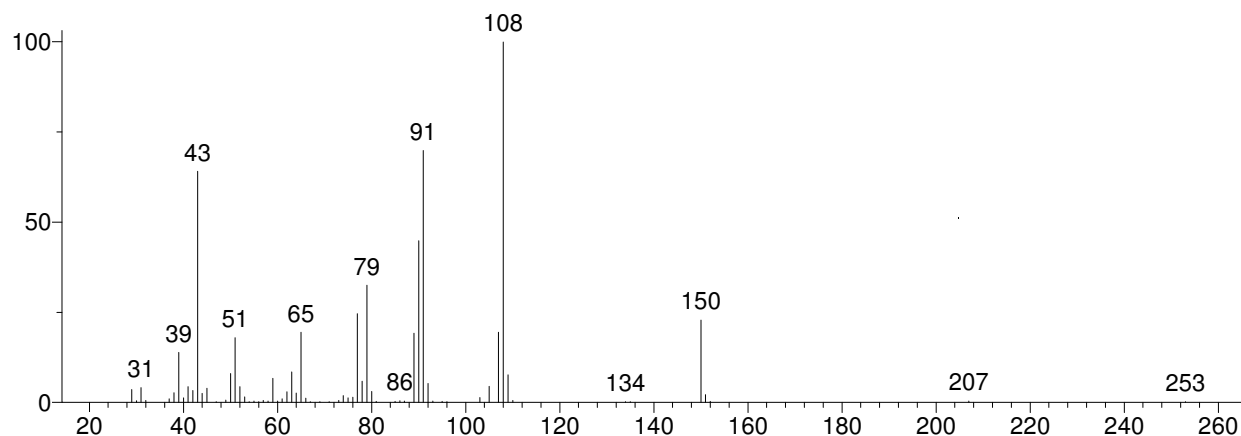


Hit 2 : 1,6-Octadien-3-ol, 3,7-dimethyl-
C₁₀H₁₈O; MF: 868; RMF: 874; Prob 64.7%; CAS: 78-70-6; Lib: replib; ID: 8161.

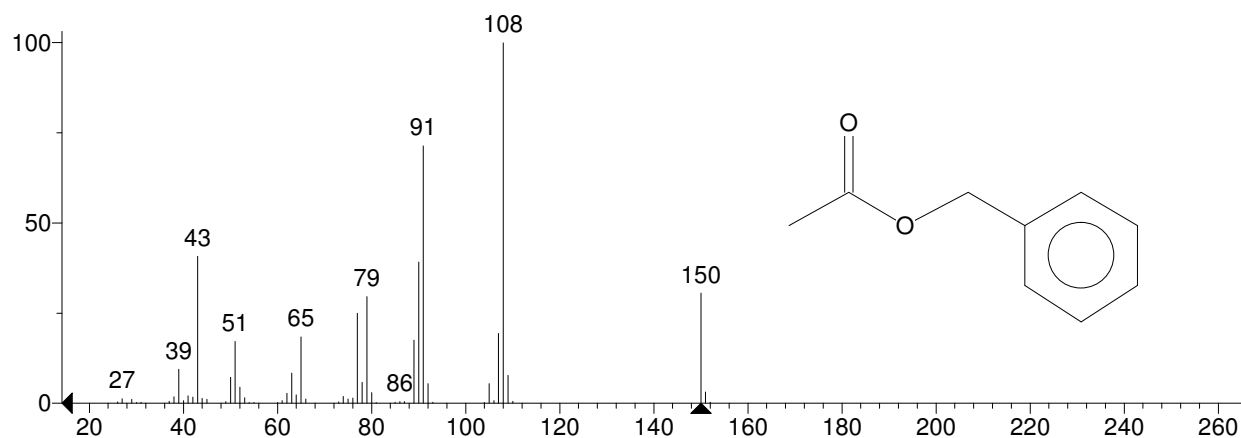


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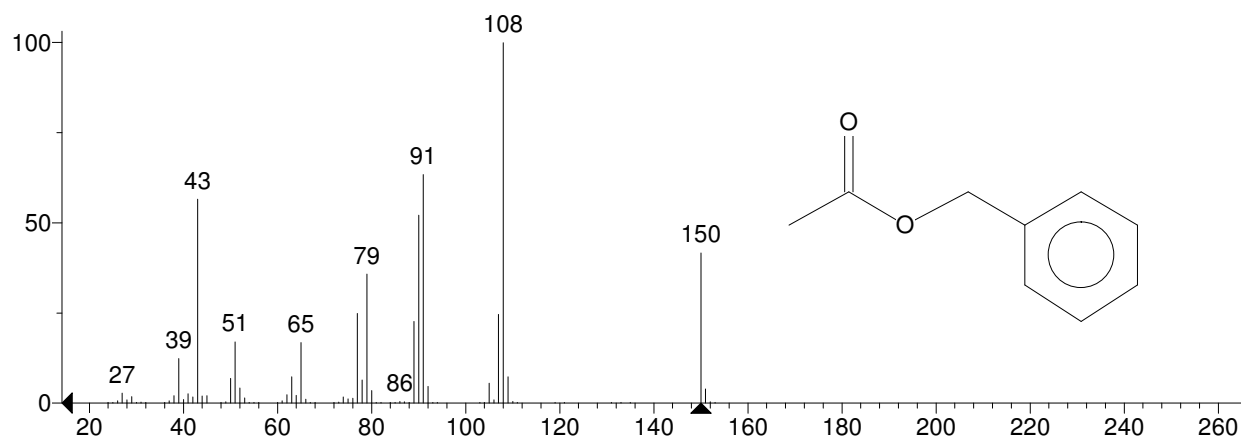
Unknown: Scan 688 (7.888 min): Imitation2.D
Compound in Library Factor = 265



Hit 1 : Acetic acid, phenylmethyl ester
C₉H₁₀O₂; MF: 935; RMF: 943; Prob 85.6%; CAS: 140-11-4; Lib: replib; ID: 14560.

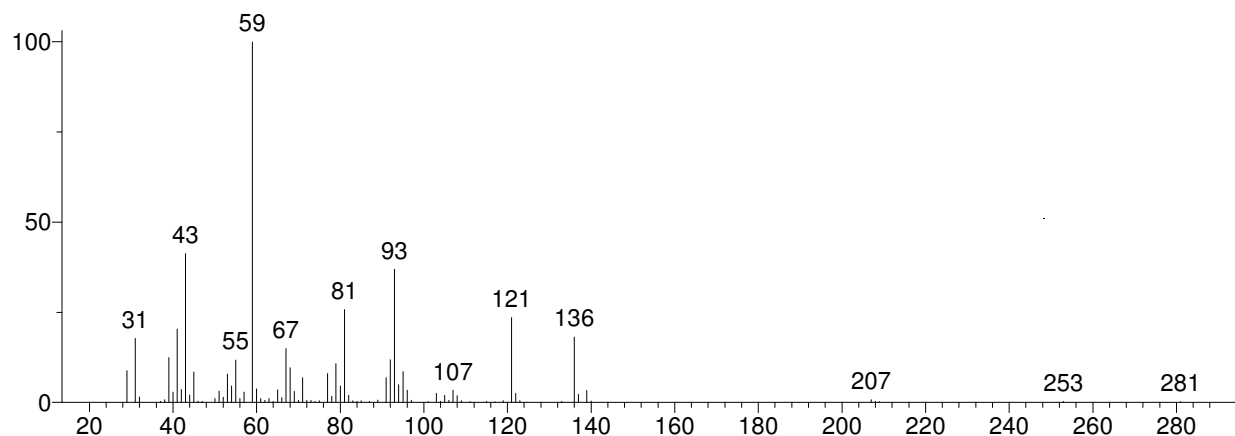


Hit 2 : Acetic acid, phenylmethyl ester
C₉H₁₀O₂; MF: 928; RMF: 936; Prob 85.6%; CAS: 140-11-4; Lib: mainlib; ID: 64787.

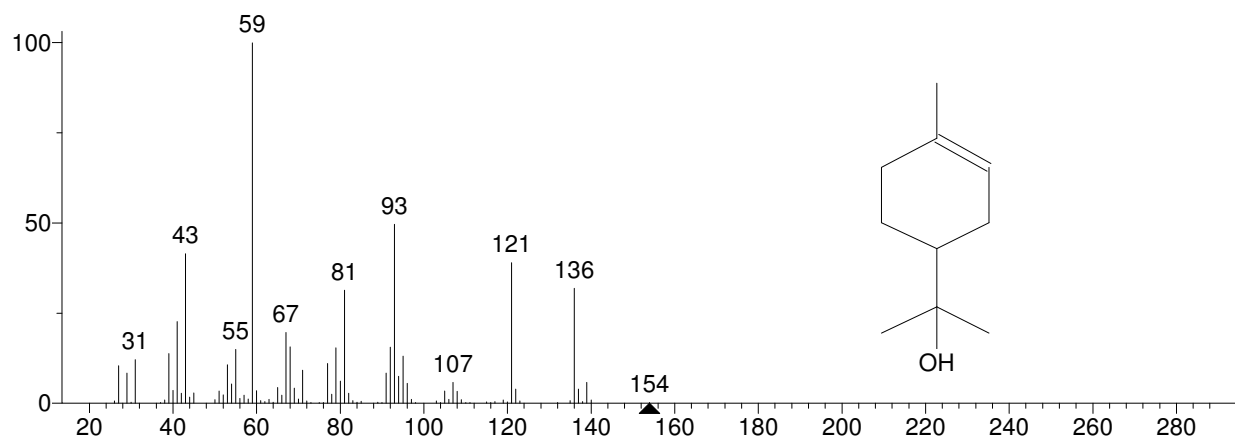


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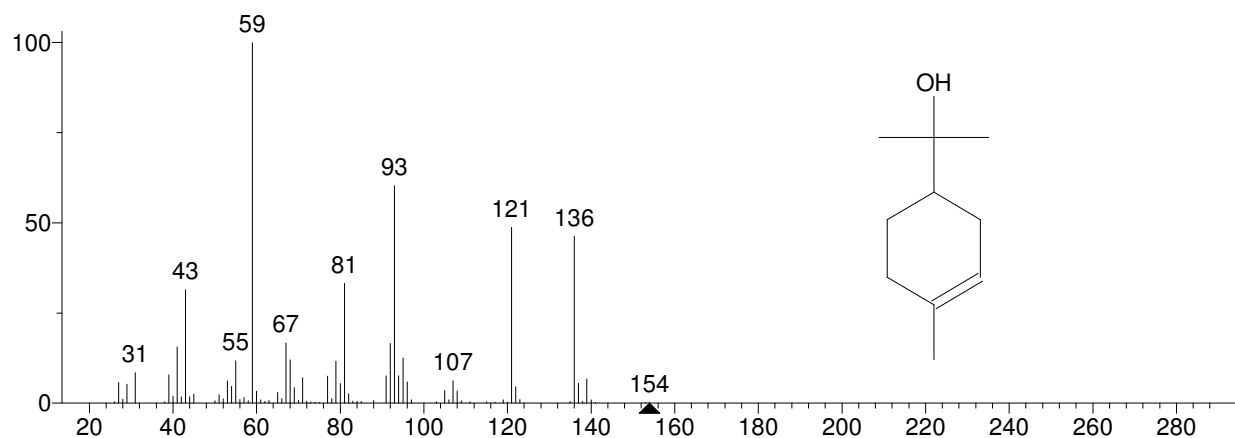
Unknown: Scan 716 (8.207 min): Imitation2.D
Compound in Library Factor = 242



Hit 1 : p-menth-1-en-8-ol
C₁₀H₁₈O; MF: 918; RMF: 925; Prob 44.4%; Lib: mainlib; ID: 25072.

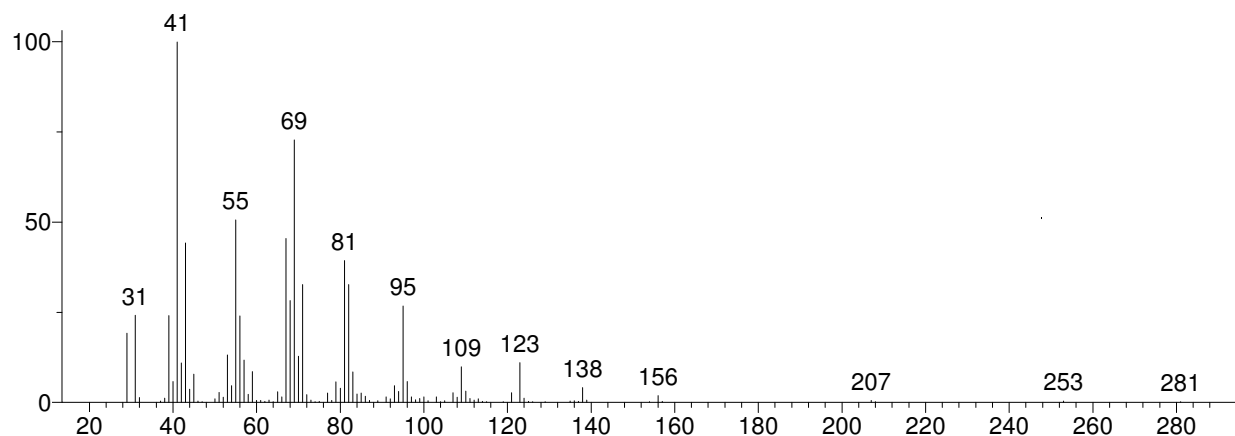


Hit 2 : 3-Cyclohexene-1-methanol, .alpha.,.alpha.4-trimethyl-
C₁₀H₁₈O; MF: 906; RMF: 912; Prob 29.6%; CAS: 98-55-5; Lib: replib; ID: 6602.



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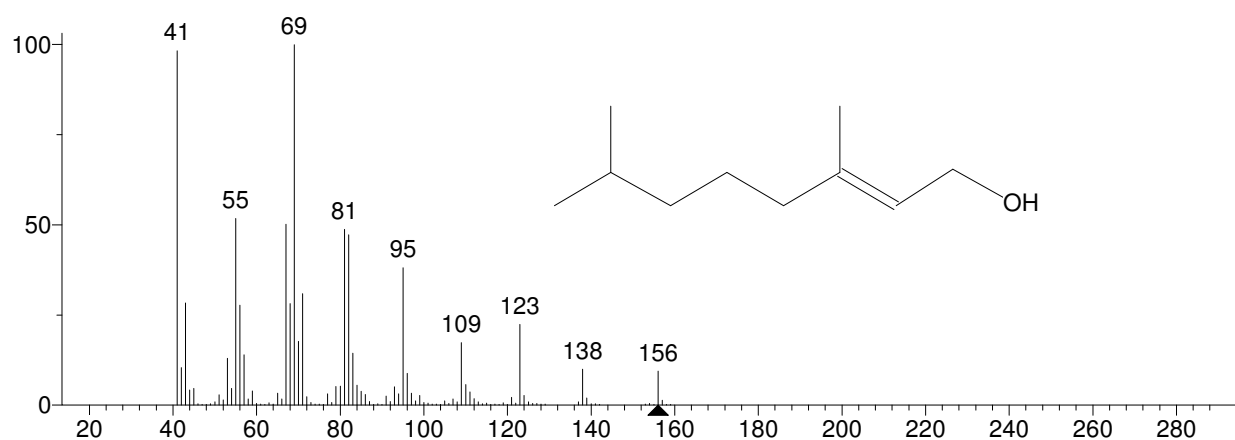
Unknown: Scan 749 (8.584 min): Imitation2.D
Compound in Library Factor = -168



Hit 1 : 6-Octen-1-ol, 3,7-dimethyl-, (R)-
C₁₀H₂₀O; MF: 888; RMF: 898; Prob 24.4%; CAS: 1117-61-9; Lib: mainlib; ID: 28138.

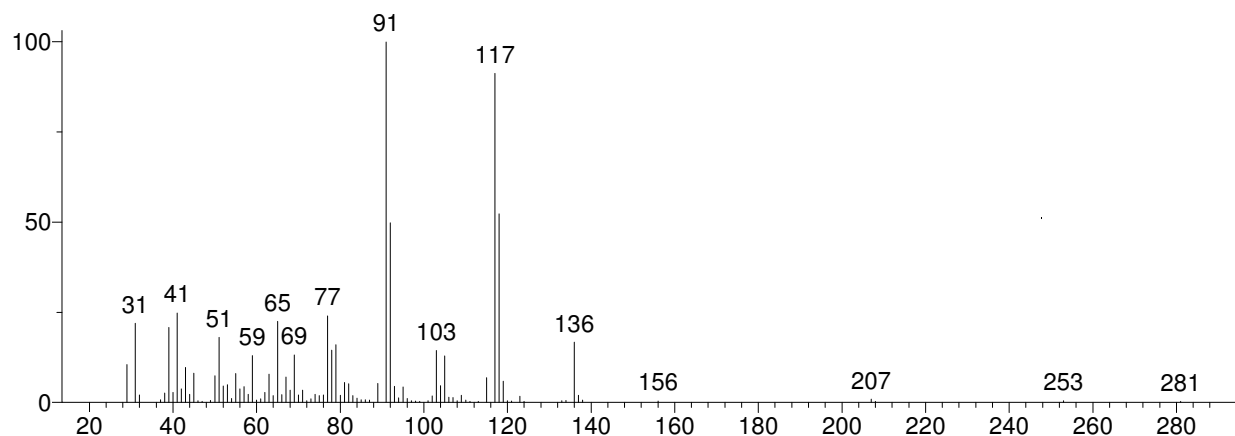


Hit 2 : 2-Octen-1-ol, 3,7-dimethyl-
C₁₀H₂₀O; MF: 888; RMF: 891; Prob 24.4%; CAS: 40607-48-5; Lib: mainlib; ID: 28107.

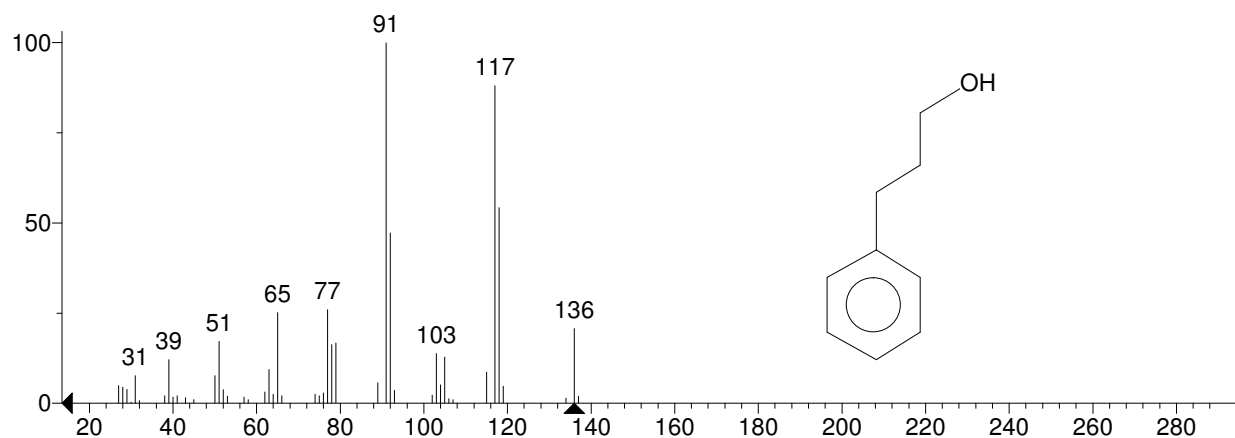


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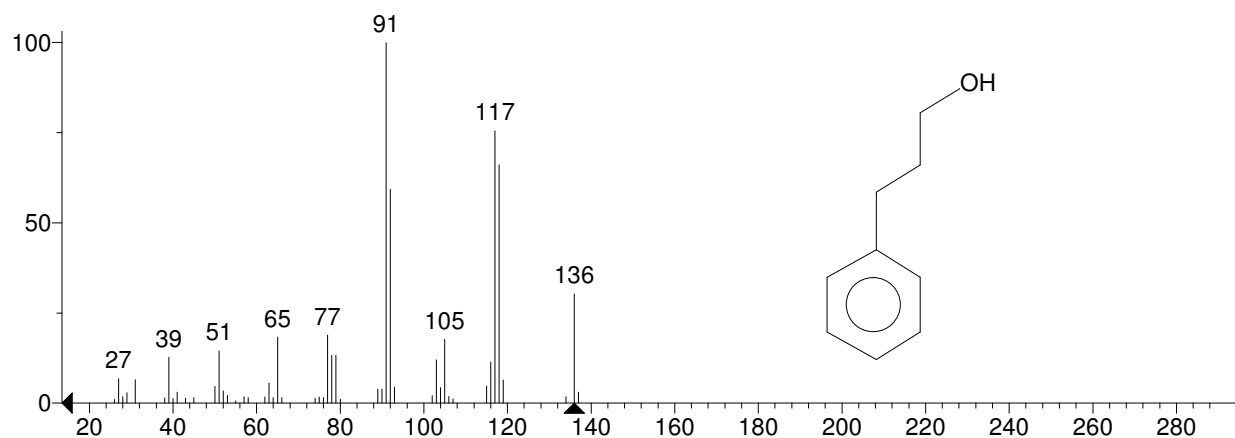
Unknown: Scan 756 (8.664 min): Imitation2.D
Compound in Library Factor = -103



Hit 1 : Benzenepropanol
C₉H₁₂O; MF: 873; RMF: 944; Prob 68.4%; CAS: 122-97-4; Lib: replib; ID: 11463.

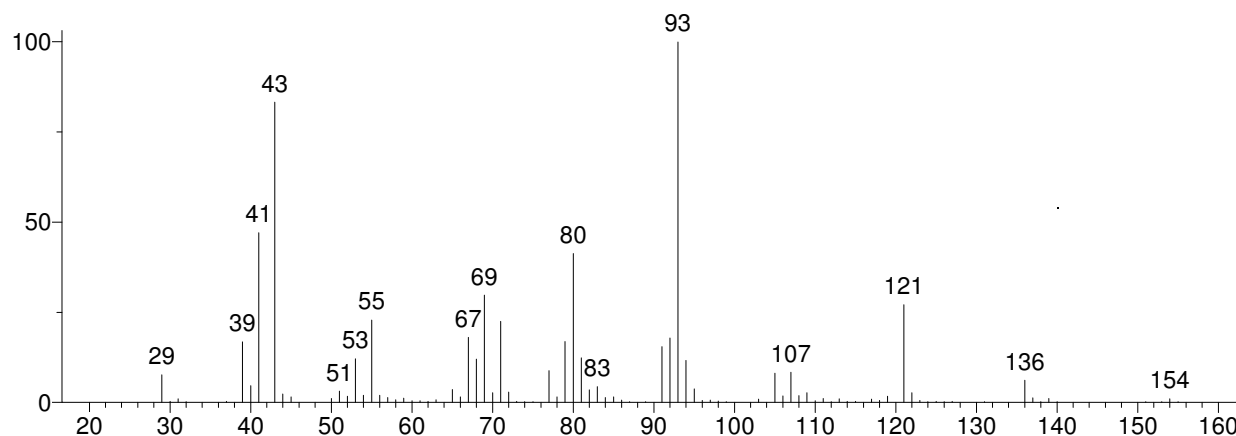


Hit 2 : Benzenepropanol
C₉H₁₂O; MF: 845; RMF: 909; Prob 68.4%; CAS: 122-97-4; Lib: mainlib; ID: 48216.

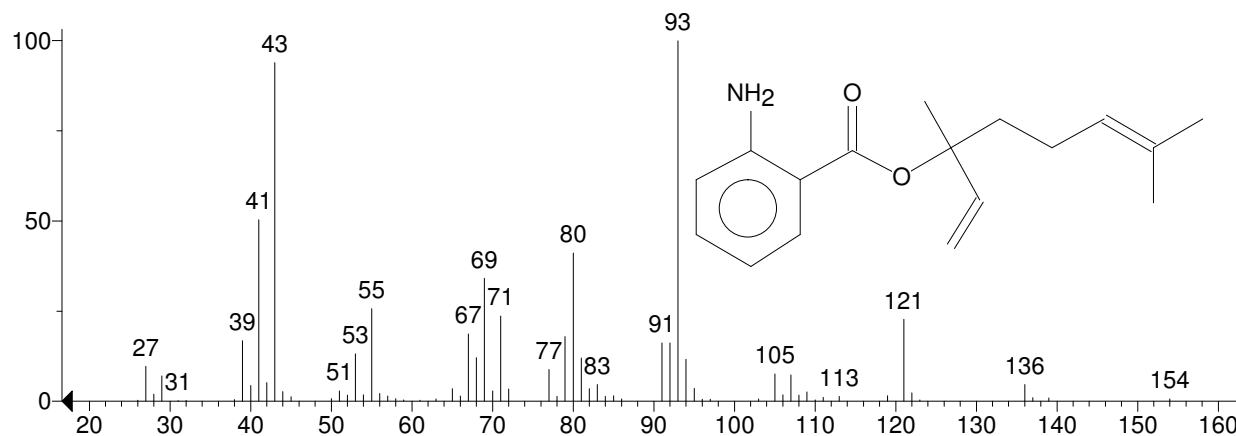


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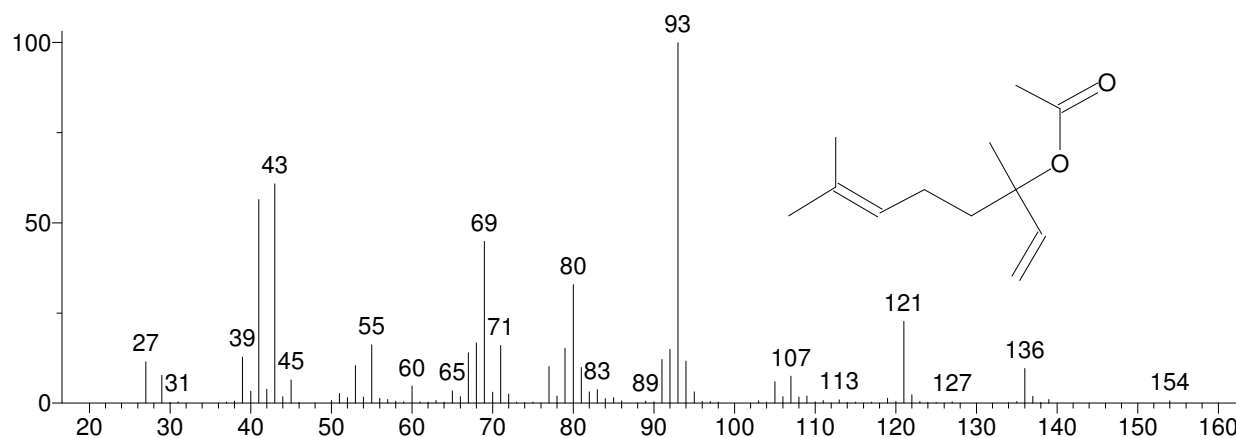
Unknown: Scan 771 (8.835 min): Imitation2.D
Compound in Library Factor = 146



Hit 1 : 1,6-Octadien-3-ol, 3,7-dimethyl-, 2-aminobenzoate
C₁₇H₂₃NO₂; MF: 963; RMF: 967; Prob 72.7%; CAS: 7149-26-0; Lib: mainlib; ID: 51289.

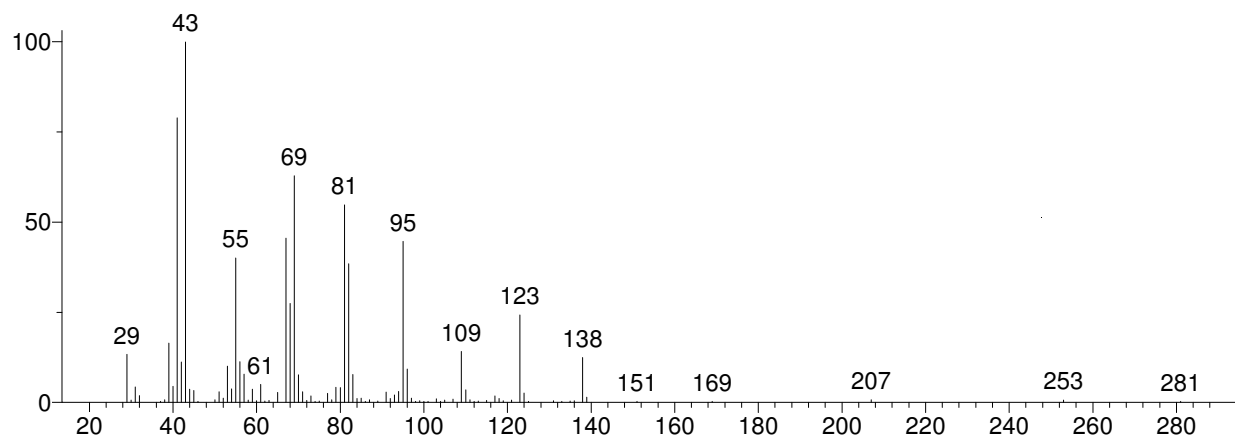


Hit 2 : 1,6-Octadien-3-ol, 3,7-dimethyl-, acetate
C₁₂H₂₀O₂; MF: 916; RMF: 917; Prob 15.2%; CAS: 115-95-7; Lib: mainlib; ID: 51290.

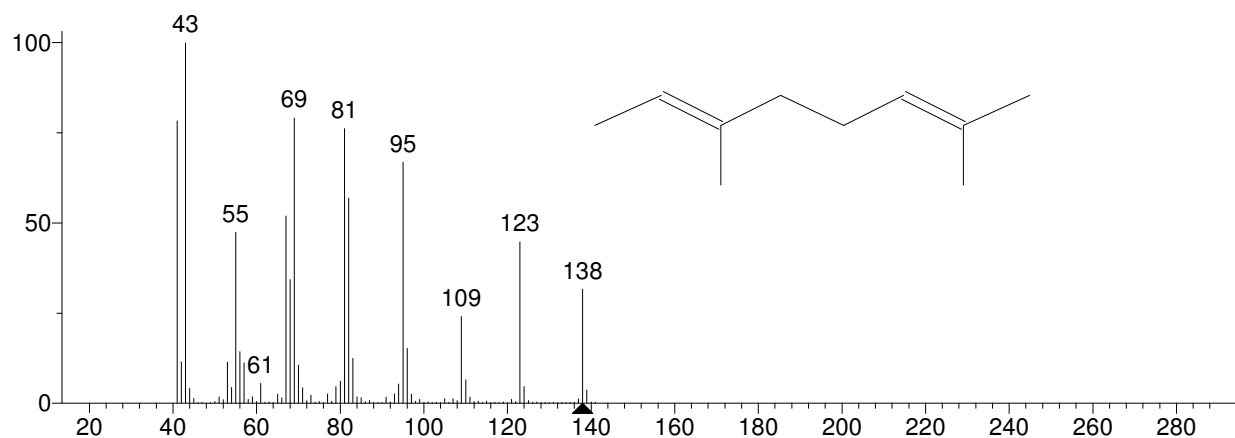


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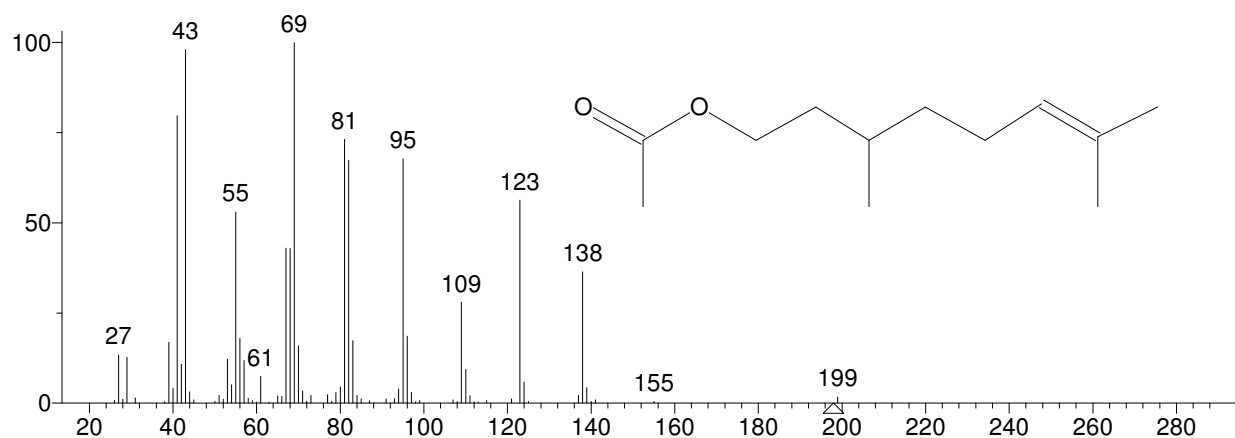
Unknown: Scan 850 (9.737 min): Imitation2.D
Compound in Library Factor = -151



Hit 1 : 2,6-Octadiene, 2,6-dimethyl-
C₁₀H₁₈; MF: 896; RMF: 901; Prob 24.6%; CAS: 2792-39-4; Lib: replib; ID: 2290.

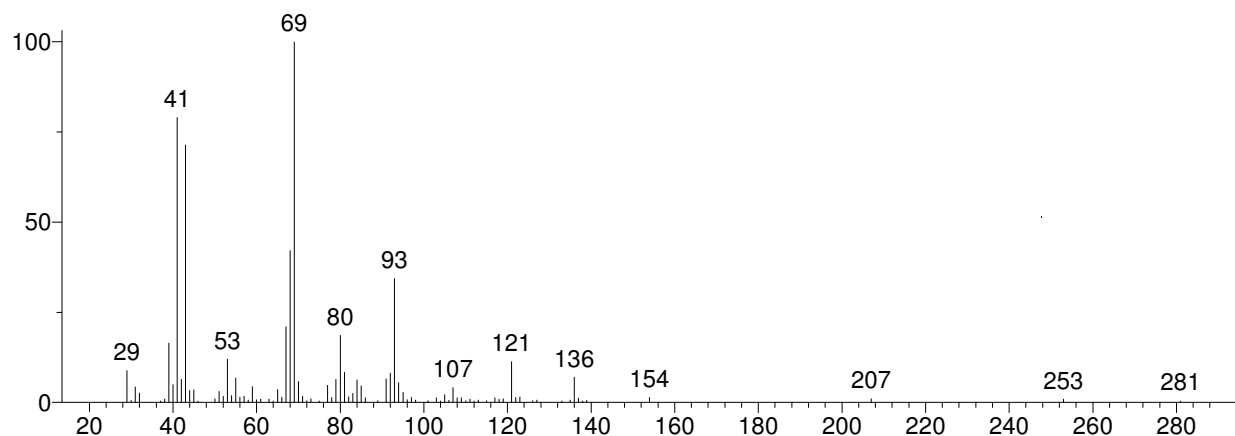


Hit 2 : 6-Octen-1-ol, 3,7-dimethyl-, acetate
C₁₂H₂₂O₂; MF: 889; RMF: 905; Prob 18.8%; CAS: 150-84-5; Lib: replib; ID: 7605.

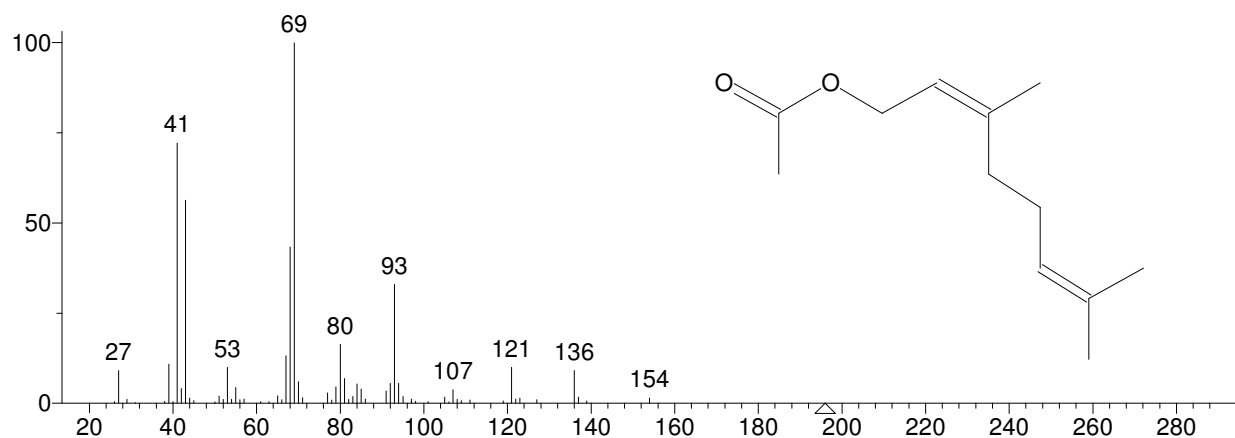


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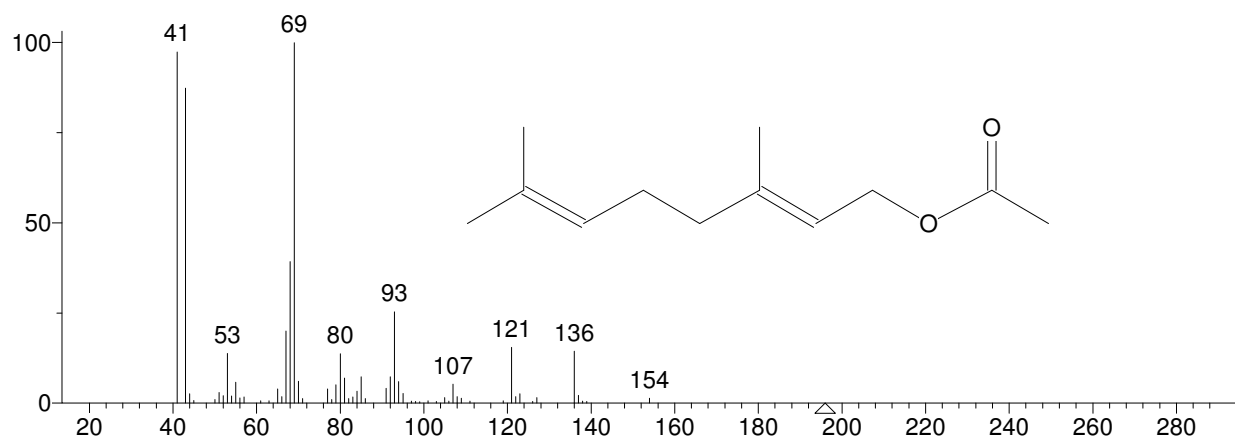
Unknown: Scan 860 (9.852 min): Imitation2.D
Compound in Library Factor = 103



Hit 1 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-
C₁₂H₂₀O₂; MF: 918; RMF: 947; Prob 51.8%; CAS: 141-12-8; Lib: replib; ID: 7487.

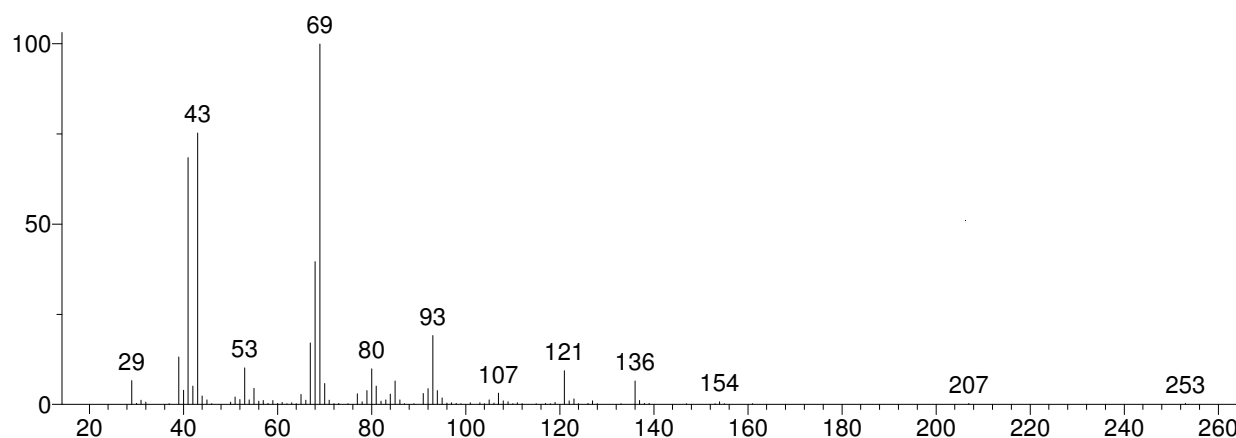


Hit 2 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate
C₁₂H₂₀O₂; MF: 897; RMF: 926; Prob 22.1%; CAS: 16409-44-2; Lib: replib; ID: 7488.

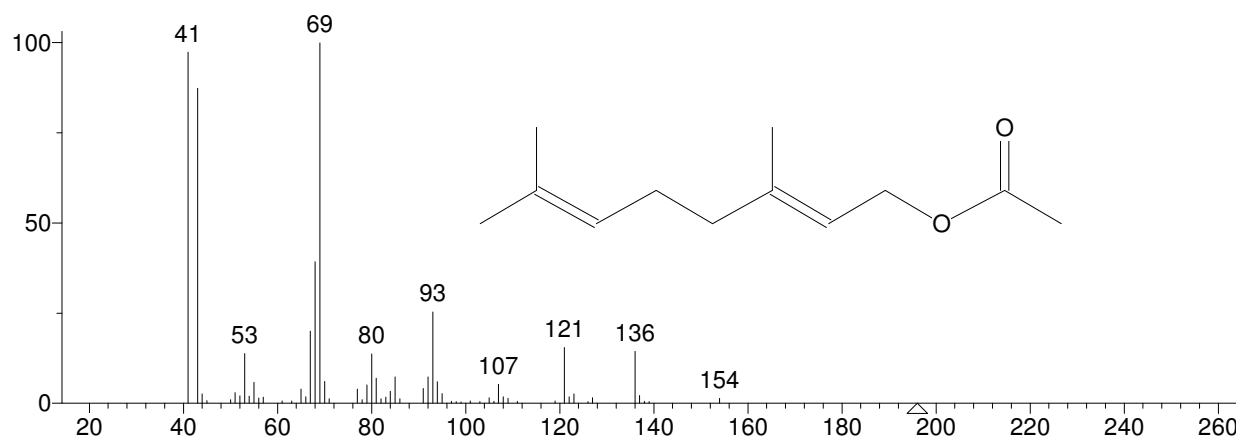


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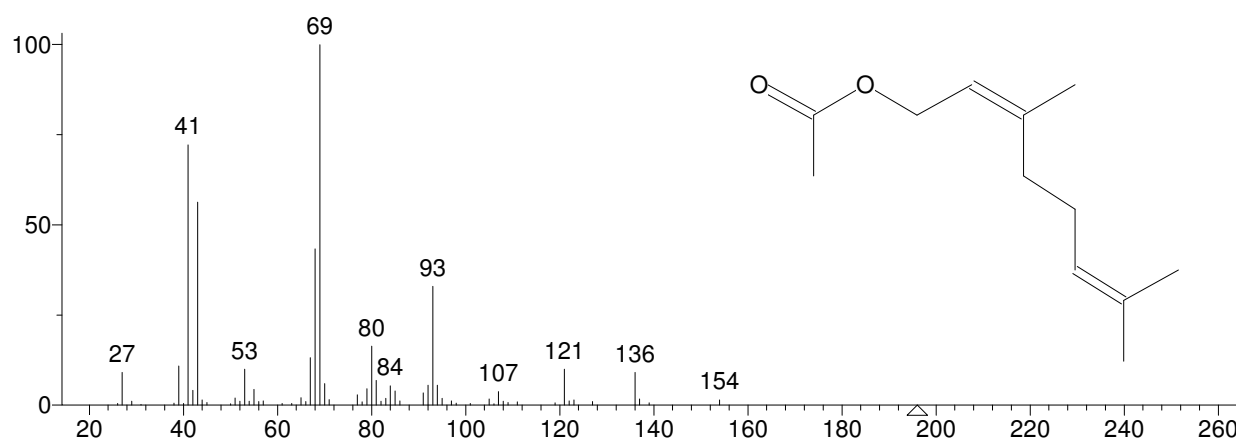
Unknown: Scan 876 (10.034 min): Imitation2.D
Compound in Library Factor = 141



Hit 1 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate
C₁₂H₂₀O₂; MF: 944; RMF: 952; Prob 50.6%; CAS: 16409-44-2; Lib: replib; ID: 7488.

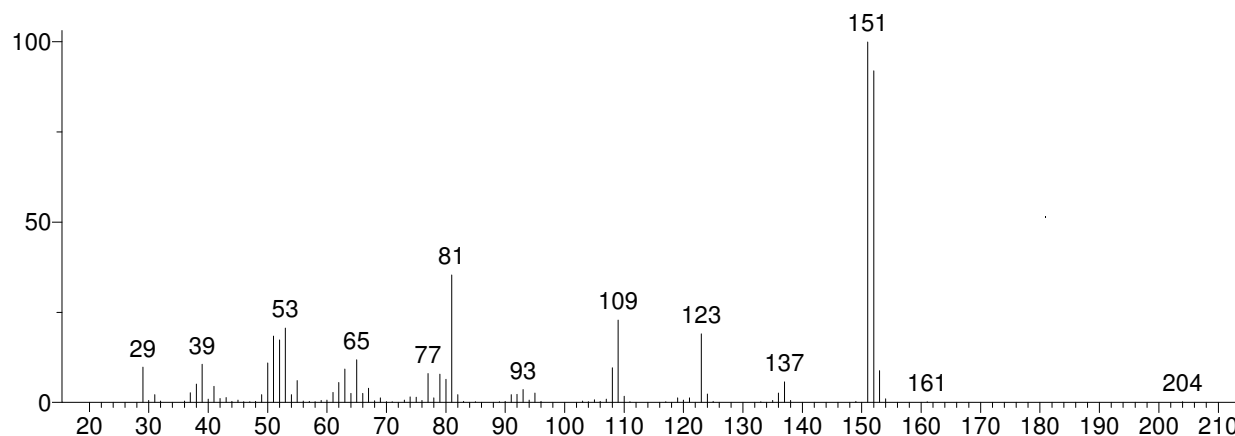


Hit 2 : 2,6-Octadien-1-ol, 3,7-dimethyl-, acetate, (Z)-
C₁₂H₂₀O₂; MF: 923; RMF: 930; Prob 21.5%; CAS: 141-12-8; Lib: replib; ID: 7487.

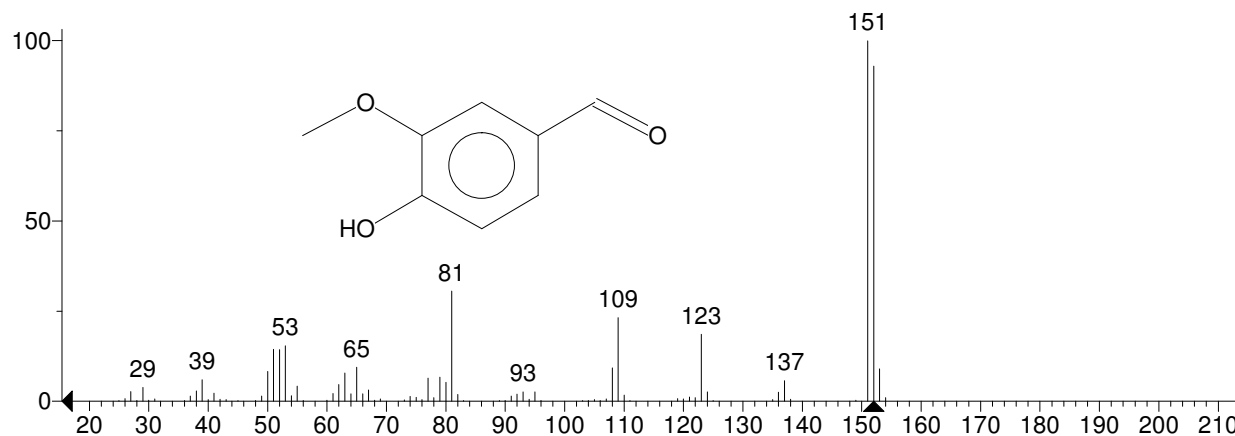


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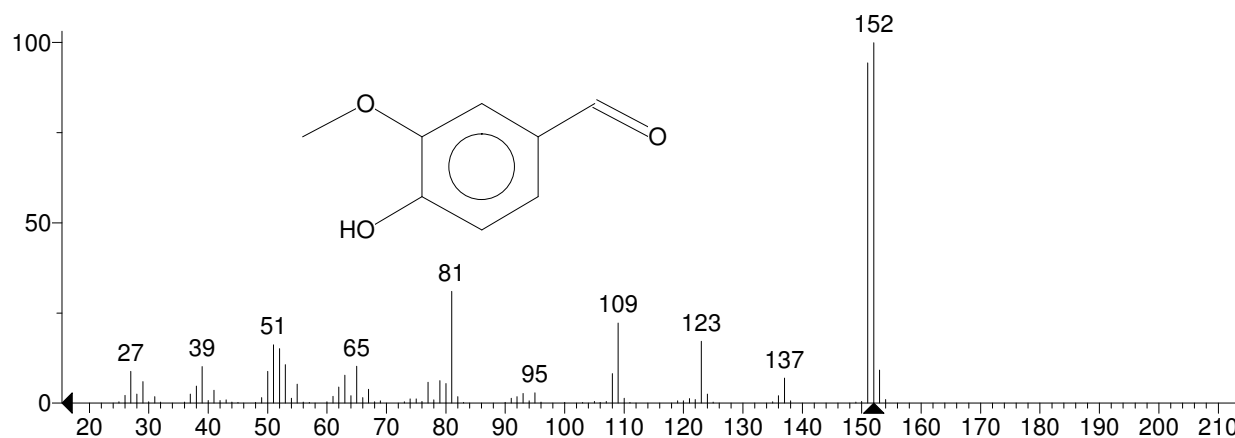
Unknown: Scan 912 (10.445 min): Imitation2.D
Compound in Library Factor = 144



Hit 1 : Vanillin
C₈H₈O₃; MF: 952; RMF: 952; Prob 59.4%; CAS: 121-33-5; Lib: replib; ID: 20015.

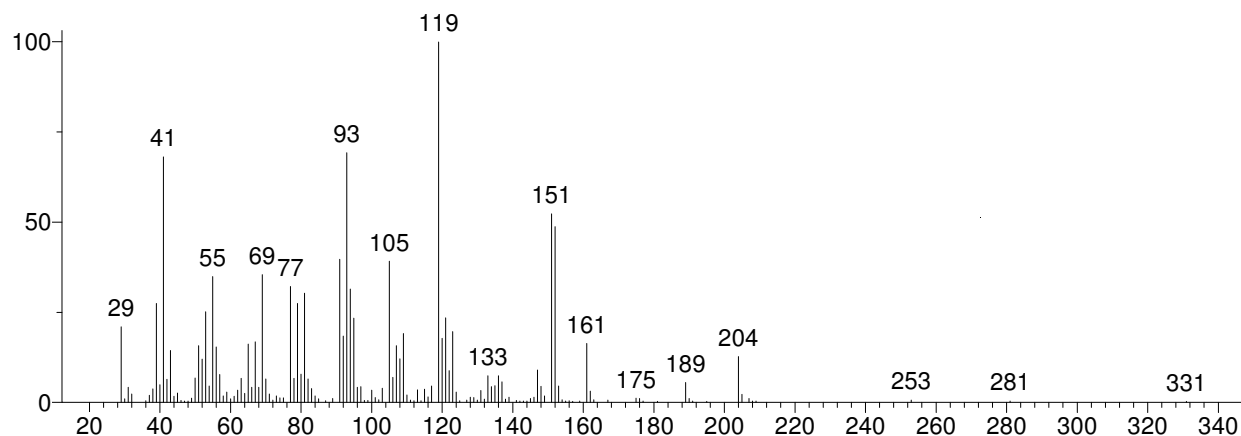


Hit 2 : Vanillin
C₈H₈O₃; MF: 944; RMF: 944; Prob 59.4%; CAS: 121-33-5; Lib: mainlib; ID: 98716.

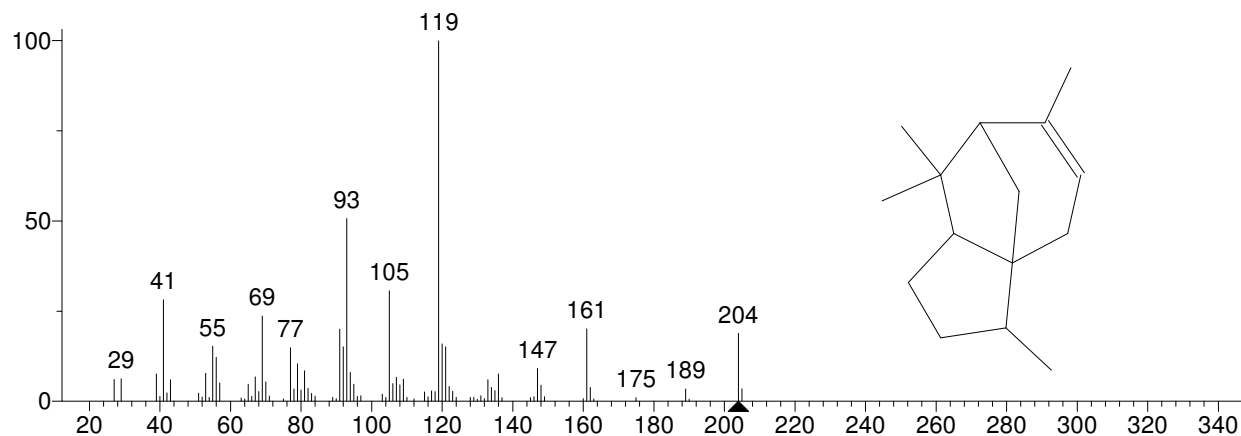


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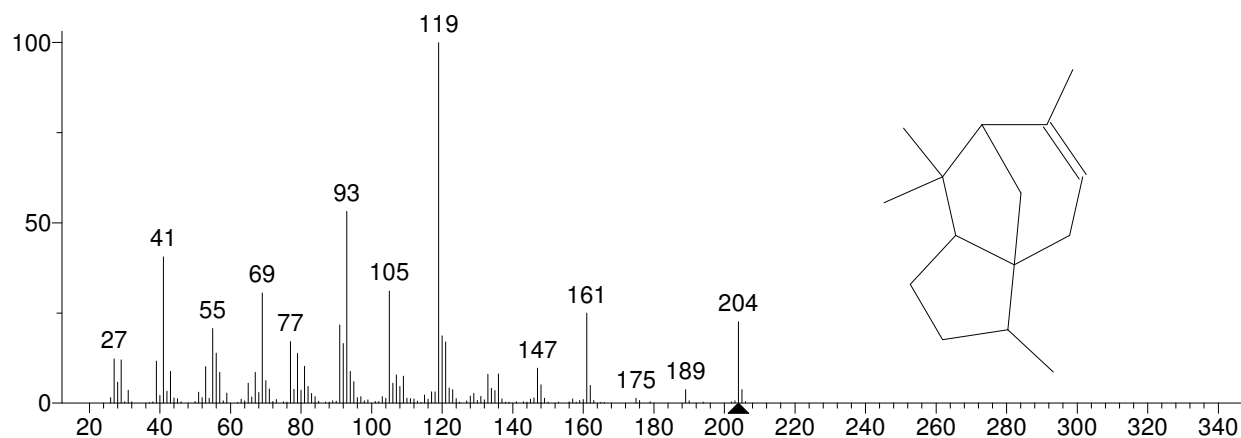
Unknown: Scan 917 (10.502 min): Imitation2.D
Compound in Library Factor = -509



Hit 1 : 1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)] C₁₅H₂₄; MF: 796; RMF: 893; Prob 11.2%; CAS: 469-61-4; Lib: replib; ID: 15877.

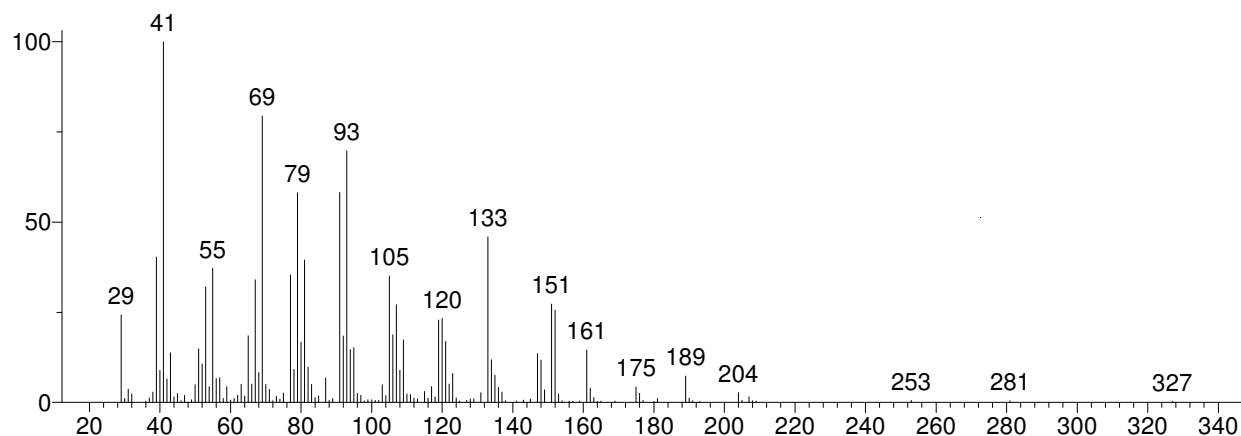


Hit 2 : 1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3.alpha.,3a.beta.,7.beta.,8a.alpha.)] C₁₅H₂₄; MF: 788; RMF: 862; Prob 11.2%; CAS: 469-61-4; Lib: replib; ID: 15876.

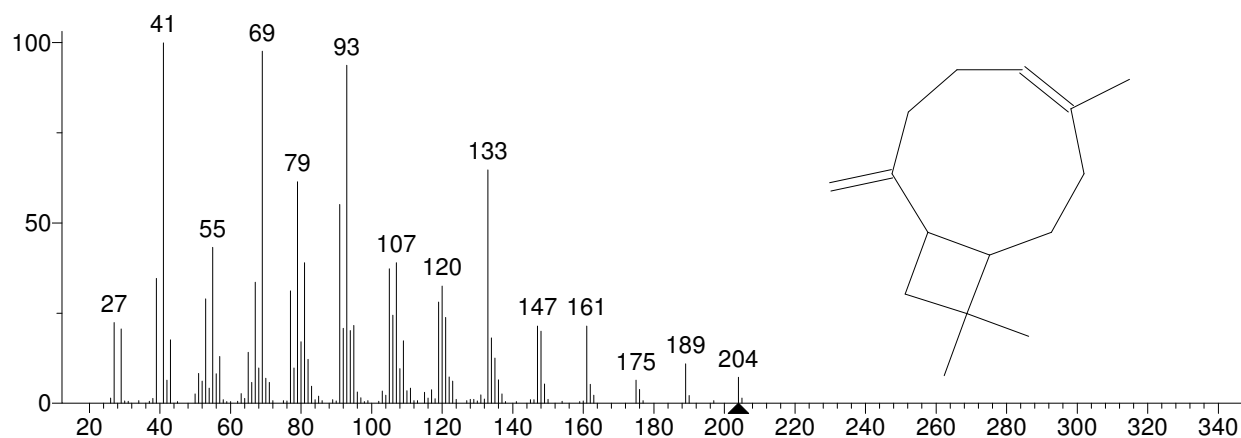


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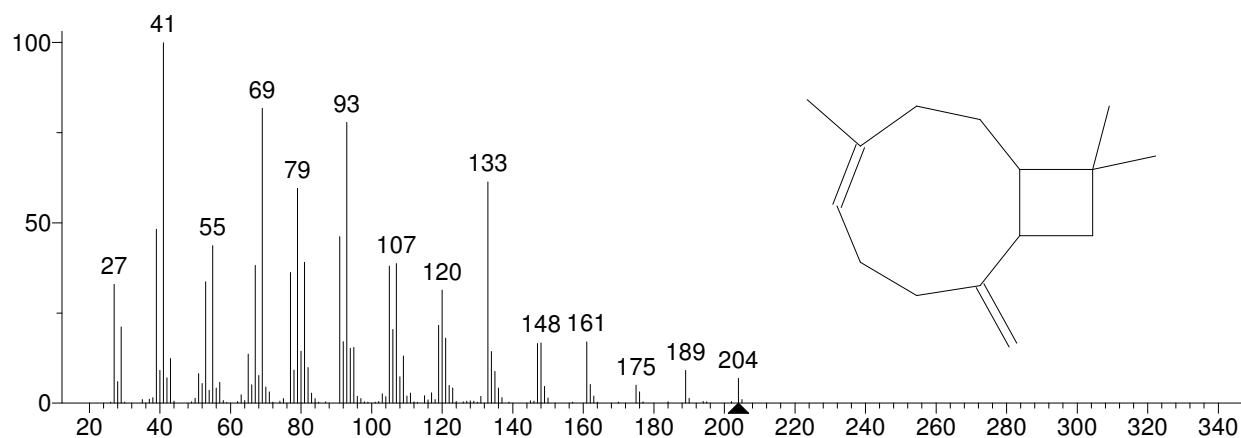
Unknown: Scan 922 (10.559 min): Imitation2.D
Compound in Library Factor = -168



Hit 1 : Caryophyllene
C₁₅H₂₄; MF: 883; RMF: 938; Prob 32.9%; CAS: 87-44-5; Lib: replib; ID: 1122.

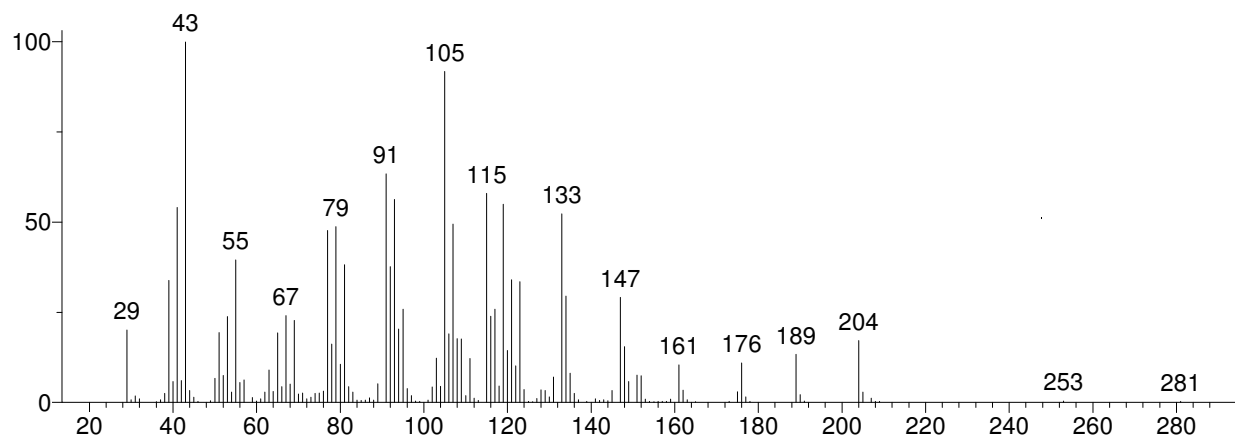


Hit 2 : Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-
C₁₅H₂₄; MF: 860; RMF: 910; Prob 12.0%; CAS: 118-65-0; Lib: replib; ID: 1121.

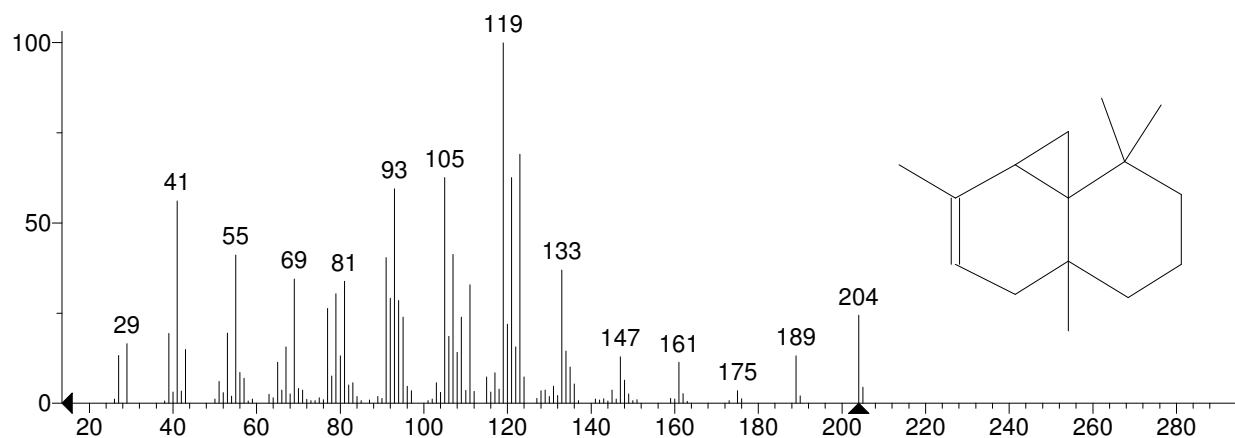


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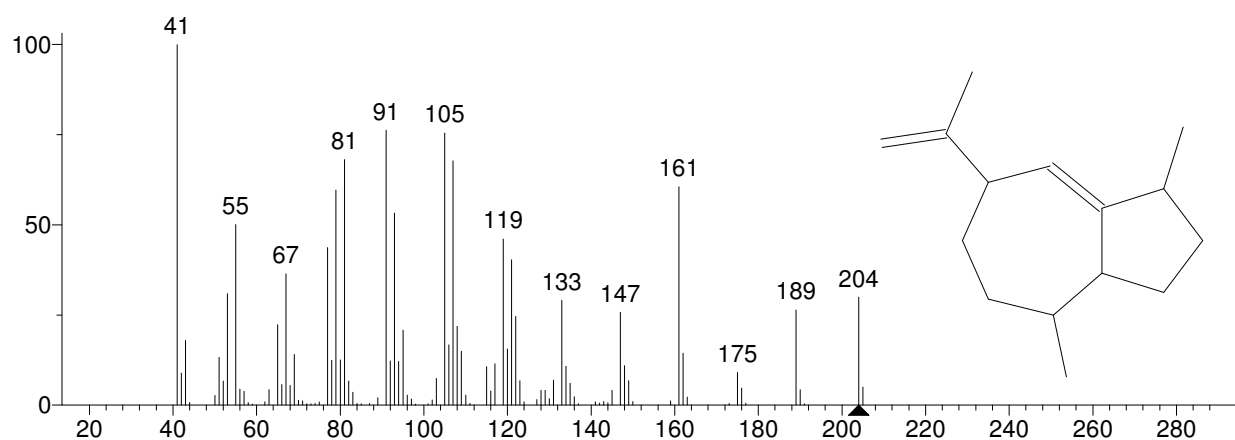
Unknown: Scan 933 (10.685 min): Imitation2.D
Compound in Library Factor = -331



Hit 1 : Thujopsene
C₁₅H₂₄; MF: 847; RMF: 857; Prob 9.31%; CAS: 470-40-6; Lib: mainlib; ID: 72266.

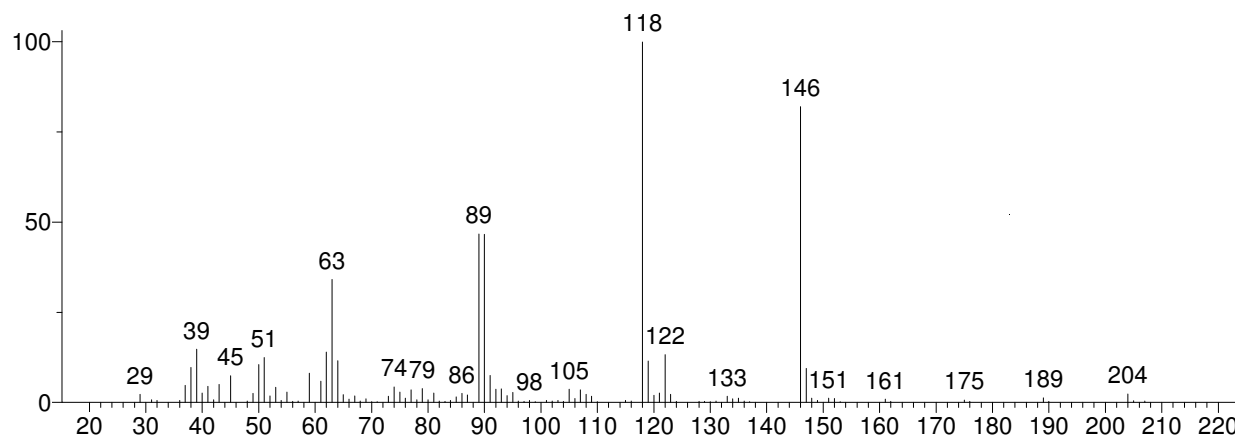


Hit 2 : Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methylethenyl)-, [1R-(1.alpha.,3a.beta.,4.alpha.,7.beta.)]
C₁₅H₂₄; MF: 830; RMF: 846; Prob 5.08%; CAS: 22567-17-5; Lib: replib; ID: 1192.

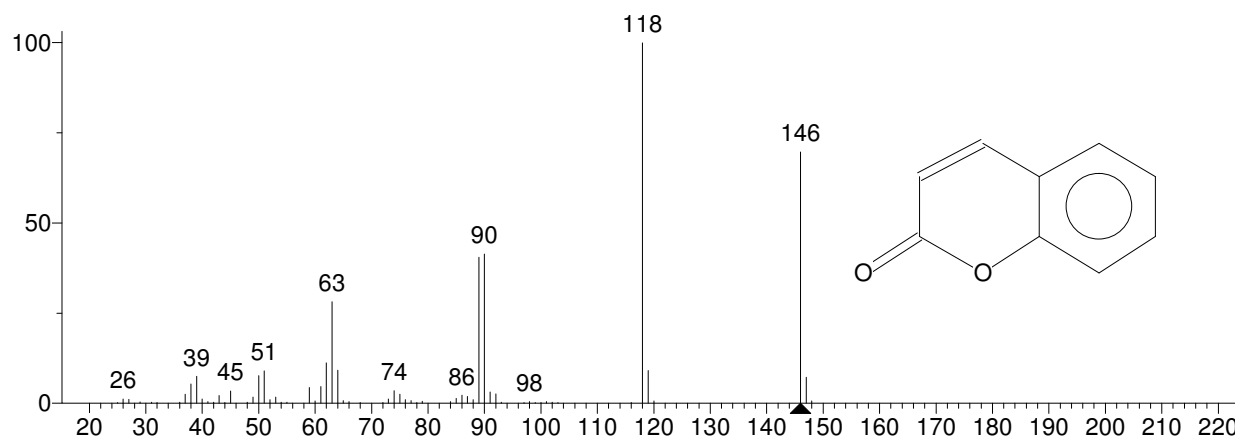


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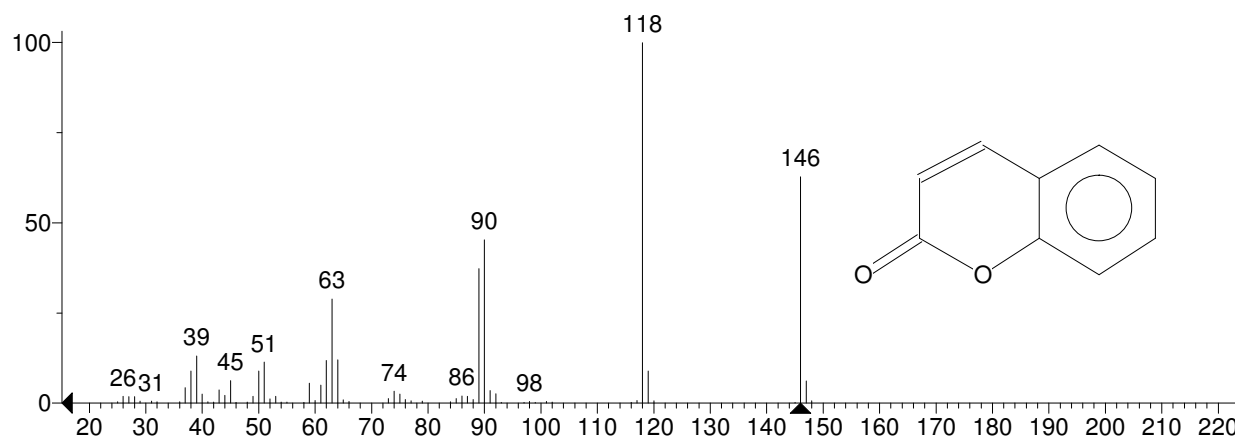
Unknown: Scan 945 (10.822 min): Imitation.D
Compound in Library Factor = -119



Hit 1 : 2H-1-Benzopyran-2-one
C₉H₆O₂; MF: 840; RMF: 907; Prob 73.3%; CAS: 91-64-5; Lib: replib; ID: 15749.

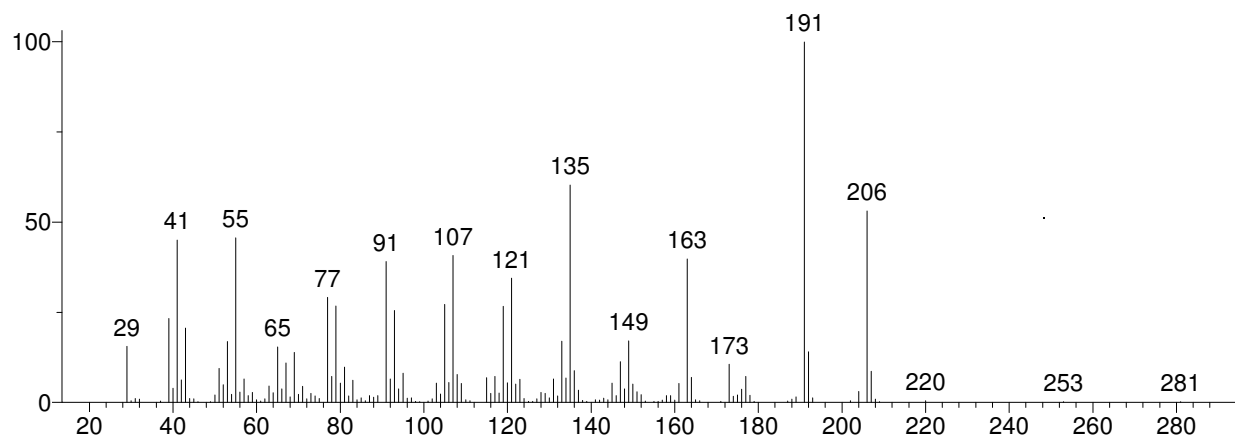


Hit 2 : 2H-1-Benzopyran-2-one
C₉H₆O₂; MF: 839; RMF: 908; Prob 73.3%; CAS: 91-64-5; Lib: replib; ID: 15748.

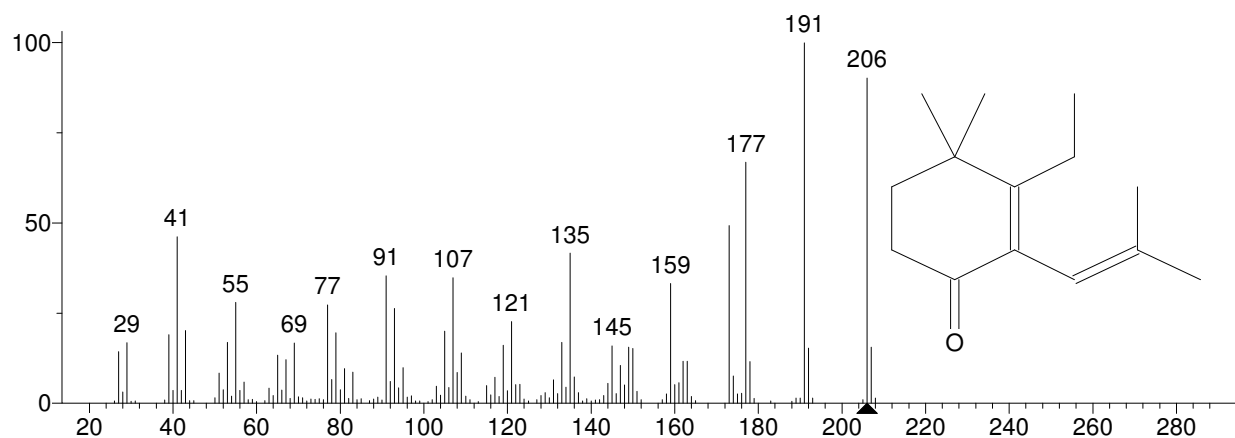


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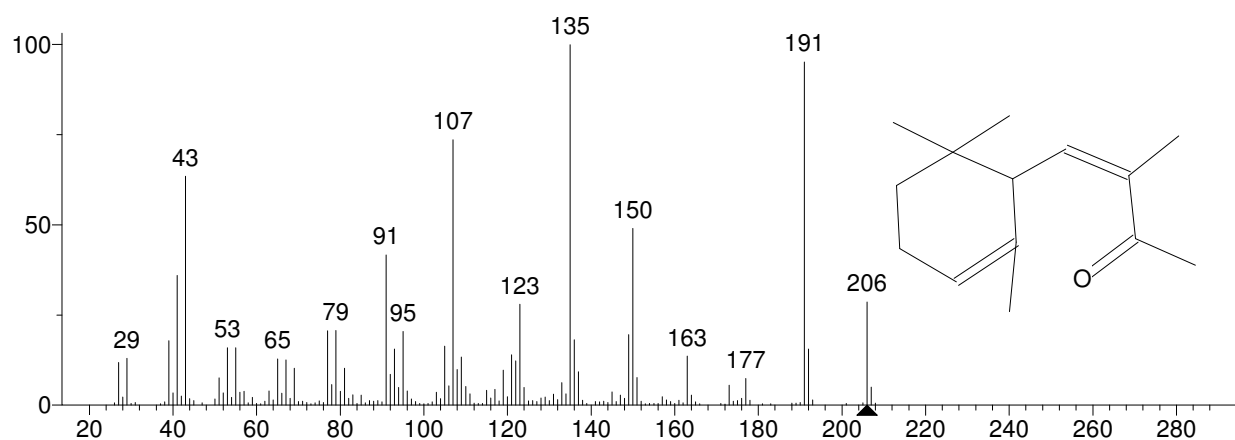
Unknown: Scan 987 (11.302 min): Imitation2.D
Compound in Library Factor = -328



Hit 1 : 3-Ethyl-4,4-dimethyl-2-(2-methylpropenyl)cyclohex-2-enone
C₁₄H₂₂O; MF: 836; RMF: 840; Prob 17.0%; CAS: 97452-08-9; Lib: mainlib; ID: 120006.

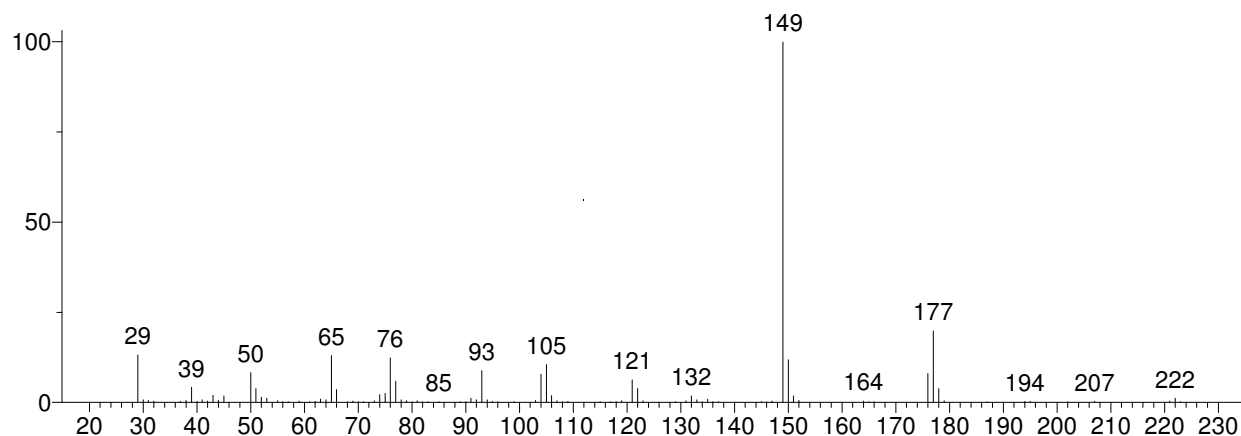


Hit 2 : 3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
C₁₄H₂₂O; MF: 833; RMF: 836; Prob 15.0%; CAS: 13743-21-0; Lib: mainlib; ID: 86213.

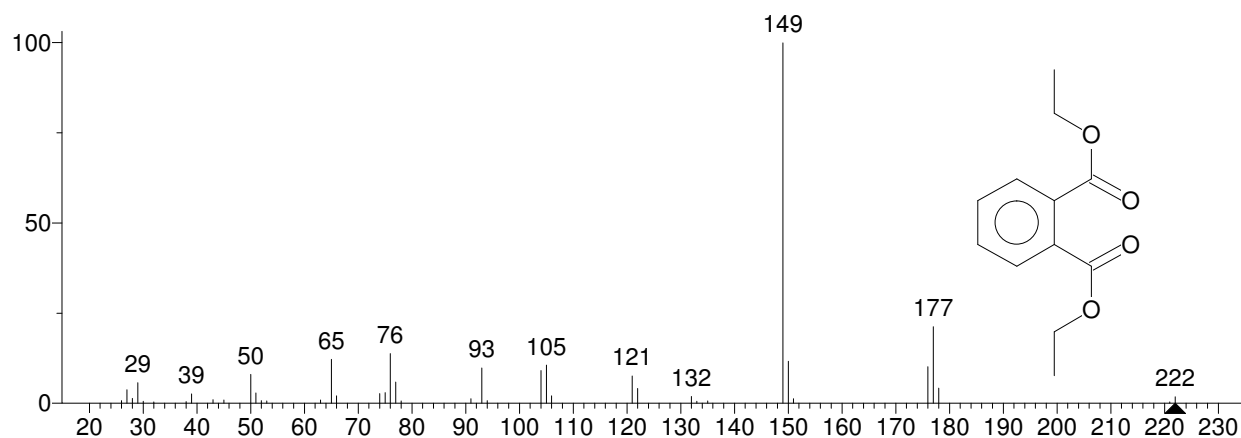


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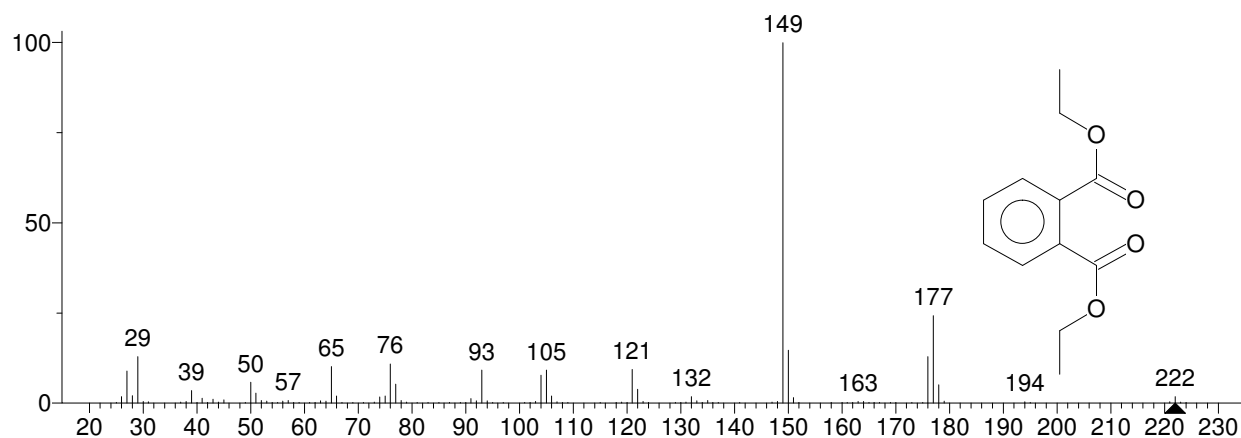
Unknown: Scan 1050 (12.021 min): Imitation2.D
Compound in Library Factor = 398



Hit 1 : Diethyl Phthalate
C₁₂H₁₄O₄; MF: 942; RMF: 962; Prob 85.9%; CAS: 84-66-2; Lib: replib; ID: 19810.

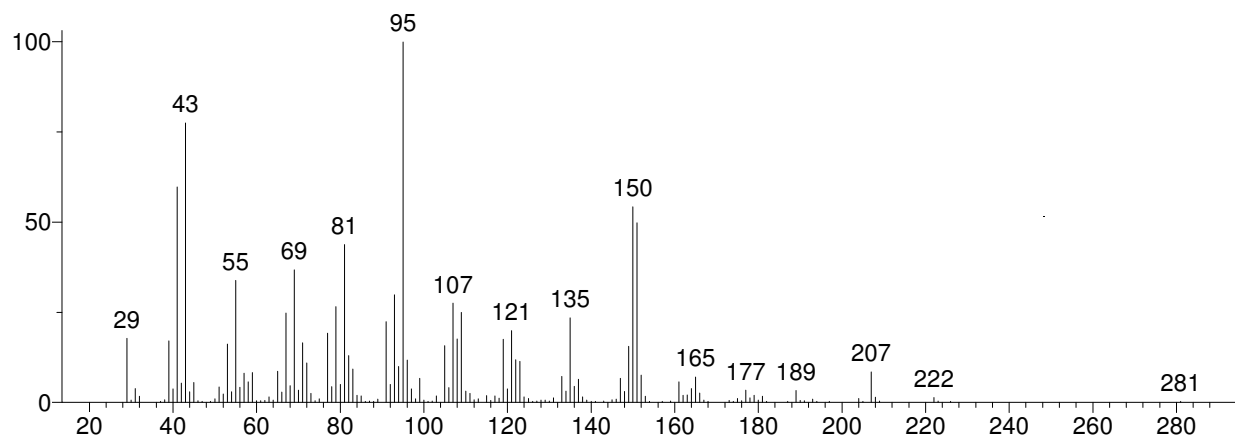


Hit 2 : Diethyl Phthalate
C₁₂H₁₄O₄; MF: 920; RMF: 923; Prob 85.9%; CAS: 84-66-2; Lib: replib; ID: 19812.

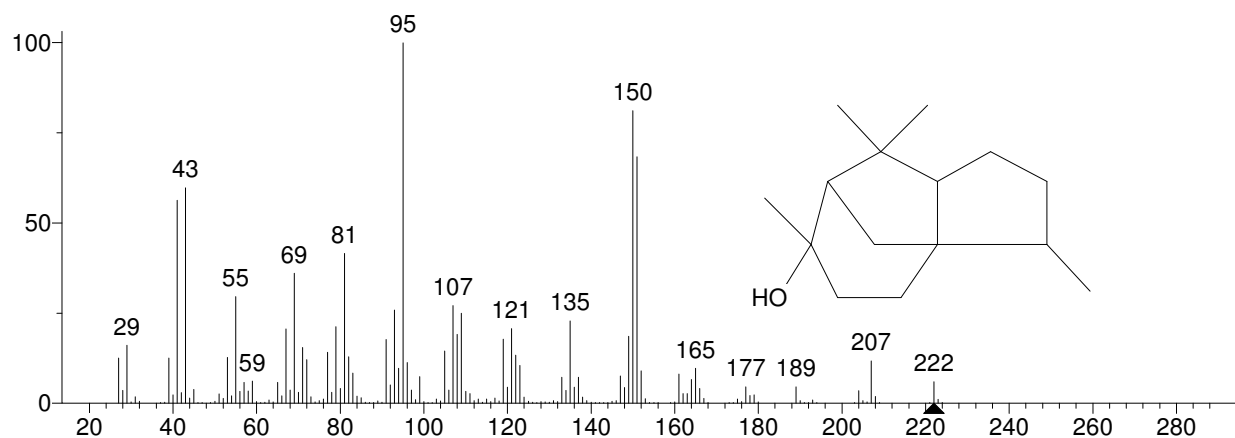


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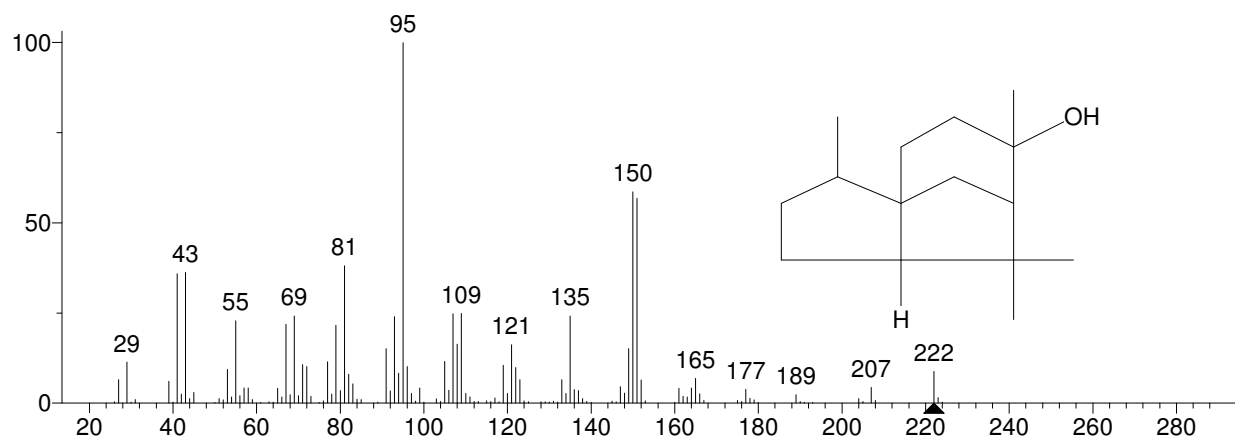
Unknown: Scan 1070 (12.249 min): Imitation2.D
Compound in Library Factor = -104



Hit 1 : Cedrol
C₁₅H₂₆O; MF: 910; RMF: 913; Prob 39.8%; CAS: 77-53-2; Lib: mainlib; ID: 53559.

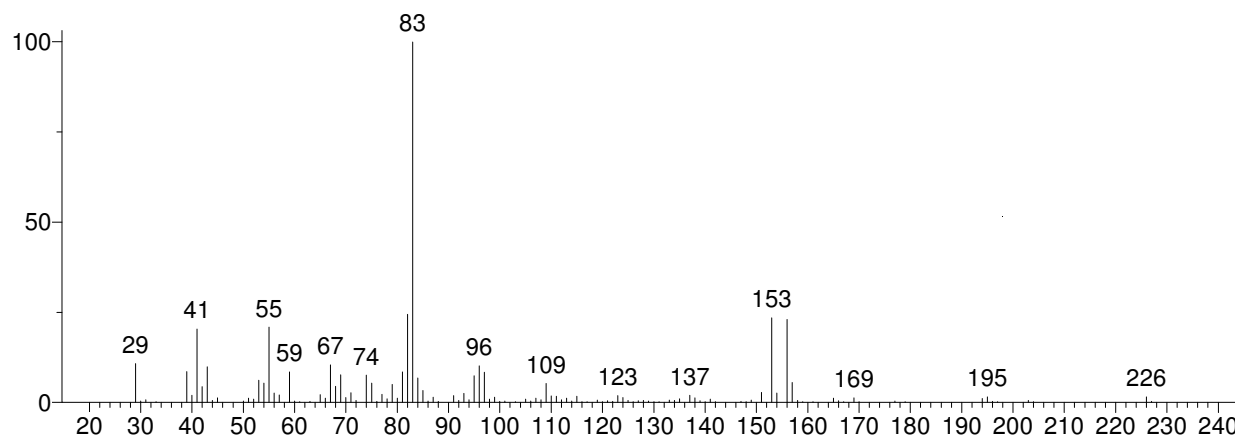


Hit 2 : Epicedrol
C₁₅H₂₆O; MF: 906; RMF: 912; Prob 33.7%; Lib: mainlib; ID: 53558.

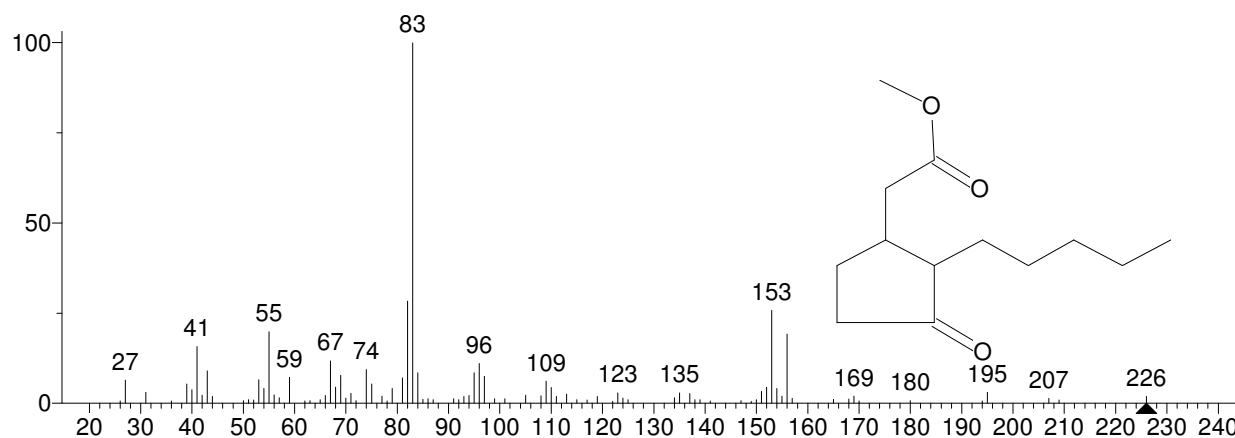


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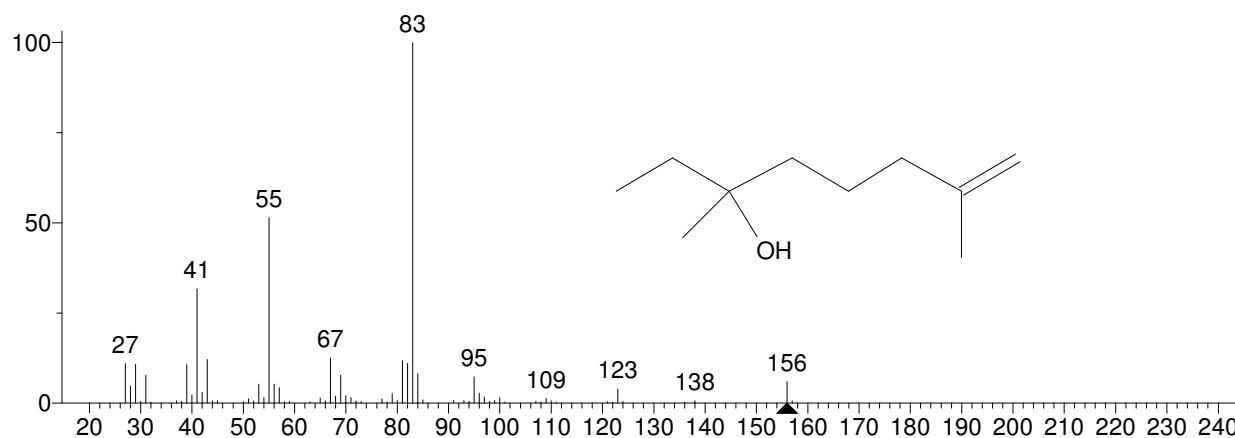
Unknown: Scan 1098 (12.569 min): Imitation.D
Compound in Library Factor = -113



Hit 1 : Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester
C₁₃H₂₂O₃; MF: 806; RMF: 828; Prob 75.3%; CAS: 24851-98-7; Lib: mainlib; ID: 41498.

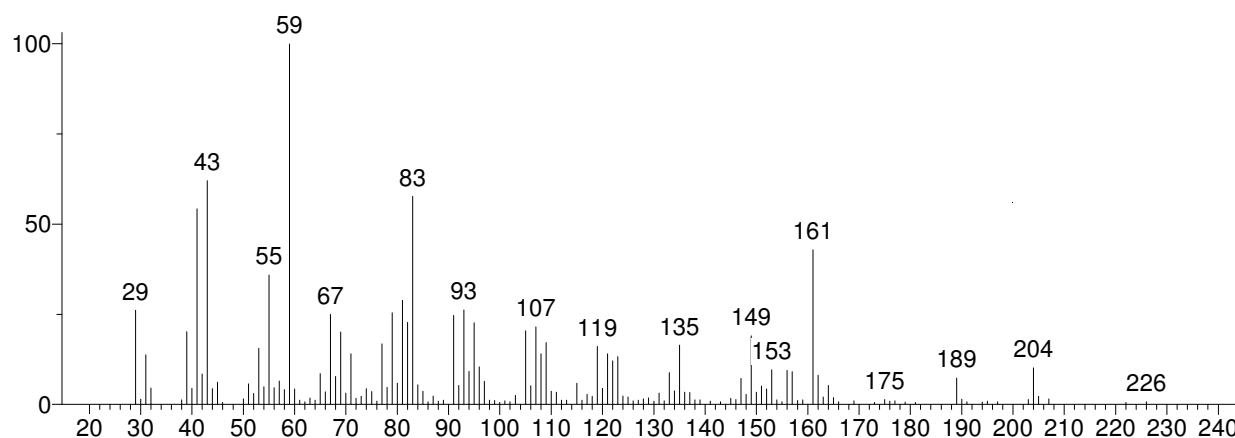


Hit 2 : Isocitronellol
C₁₀H₂₀O; MF: 678; RMF: 790; Prob 3.23%; CAS: 18479-52-2; Lib: mainlib; ID: 41109.

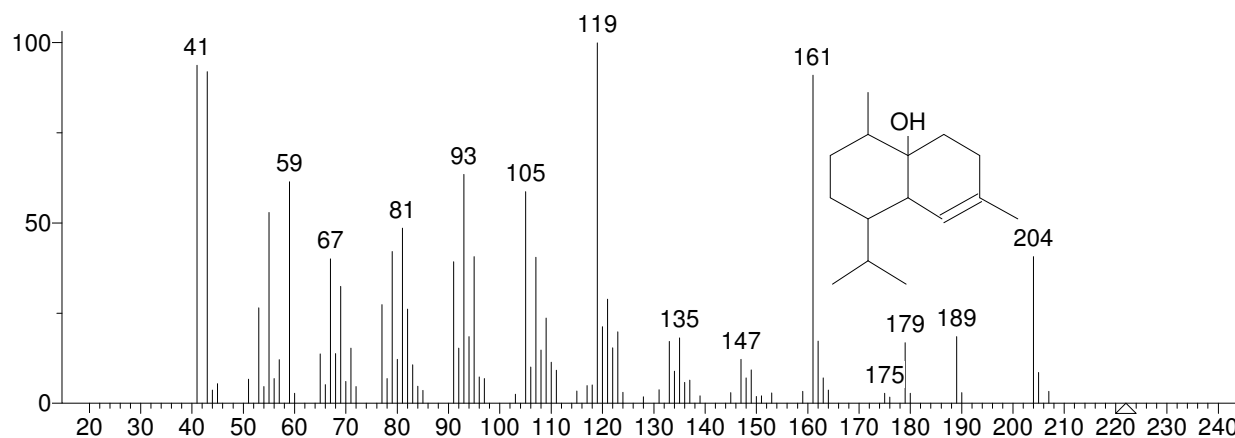


** Search Report Page 1 of 1 **

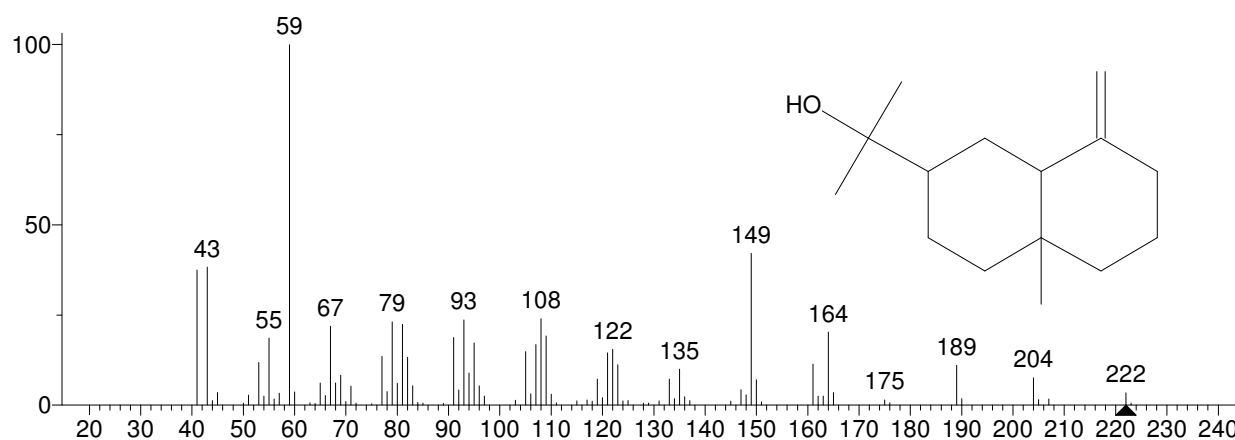
Unknown: Scan 1104 (12.638 min): Imitation2.D
Compound in Library Factor = -688



Hit 1 : Cubenol
C₁₅H₂₆O; MF: 807; RMF: 862; Prob 15.2%; CAS: 21284-22-0; Lib: mainlib; ID: 71320.

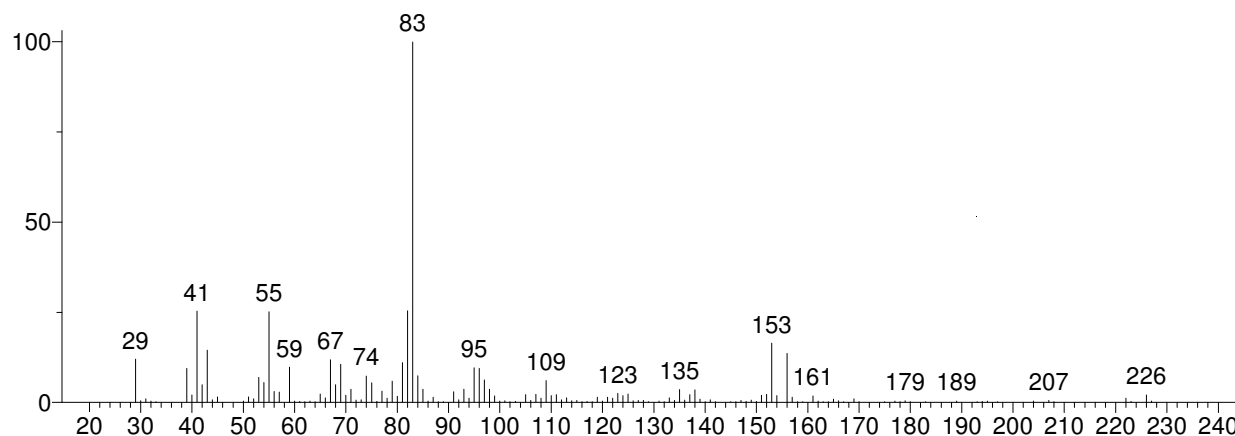


Hit 2 : 2-Naphthalenemethanol, decahydro-.alpha.,.alpha.,4a-trimethyl-8-methylene-, [2R-(2.alpha.,4a.alpha.,8a.beta.
C₁₅H₂₆O; MF: 798; RMF: 854; Prob 11.0%; CAS: 473-15-4; Lib: mainlib; ID: 25231.

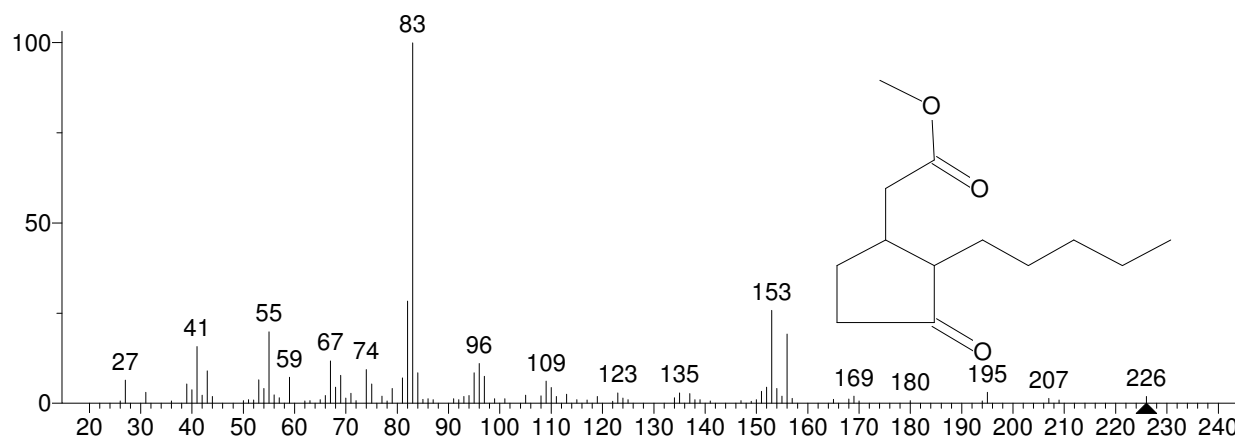


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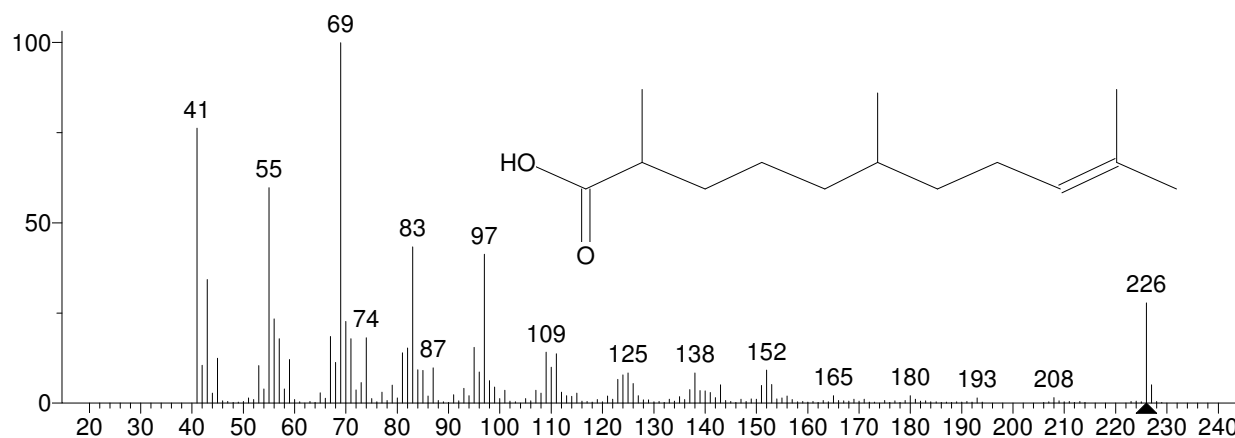
Unknown: Scan 1114 (12.752 min): Imitation2.D
Compound in Library Factor = -143



Hit 1 : Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester
C₁₃H₂₂O₃; MF: 799; RMF: 843; Prob 46.2%; CAS: 24851-98-7; Lib: mainlib; ID: 41498.

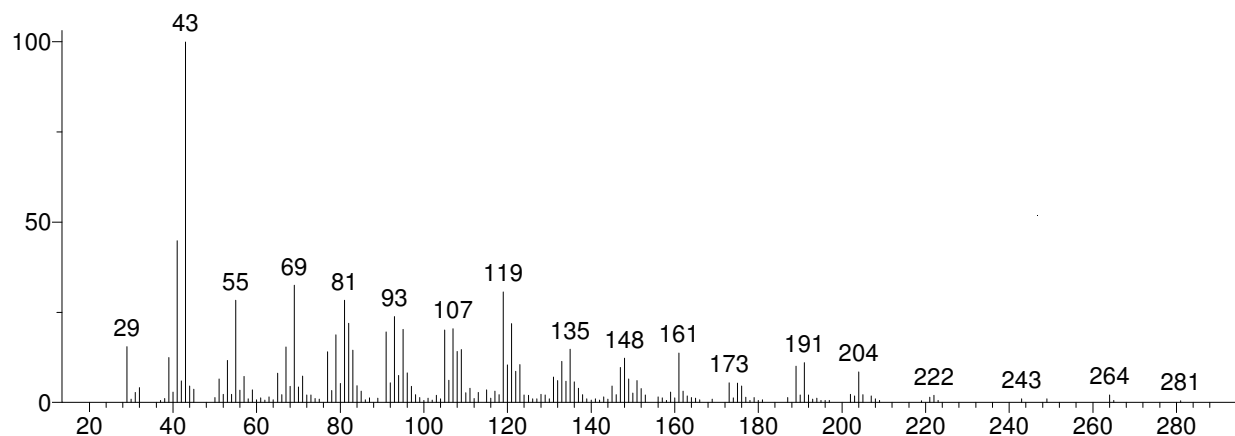


Hit 2 : 9-Undecenoic acid, 2,6,10-trimethyl-
C₁₄H₂₆O₂; MF: 696; RMF: 700; Prob 3.26%; Lib: mainlib; ID: 28039.

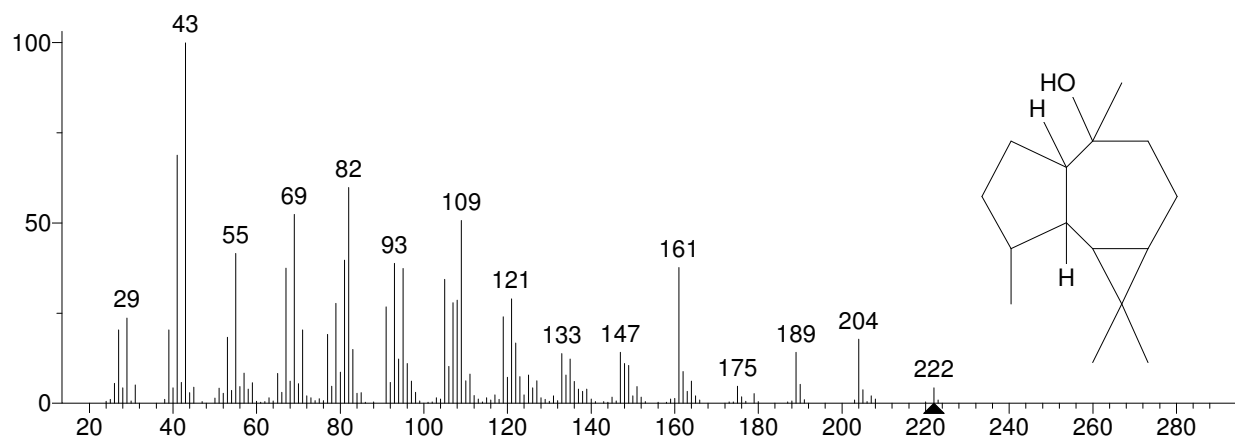


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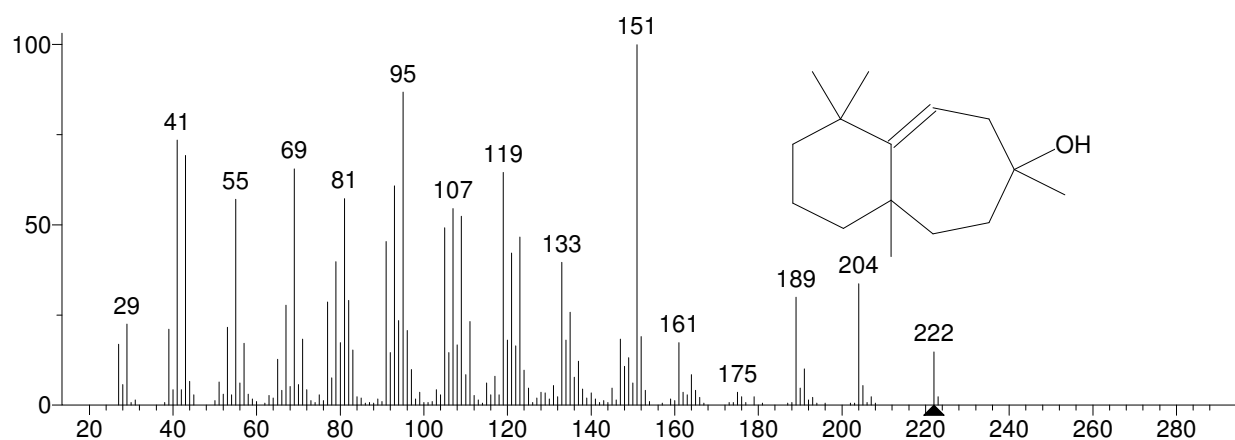
Unknown: Scan 1145 (13.106 min): Imitation2.D
Compound in Library Factor = -407



Hit 1 : Epiglobulol
C₁₅H₂₆O; MF: 819; RMF: 841; Prob 10.8%; Lib: mainlib; ID: 5651.

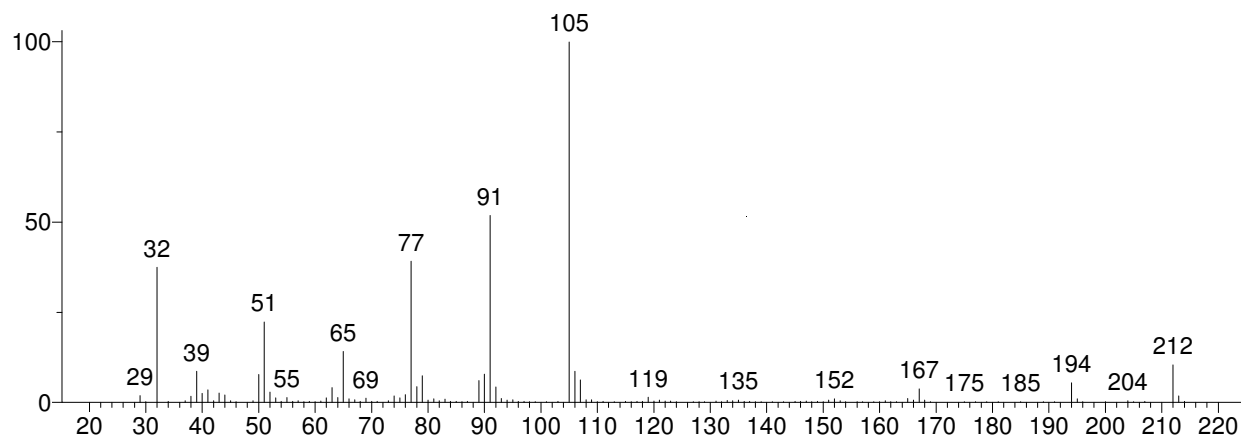


Hit 2 : 1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-
C₁₅H₂₆O; MF: 815; RMF: 829; Prob 9.12%; CAS: 6892-80-4; Lib: replib; ID: 19977.

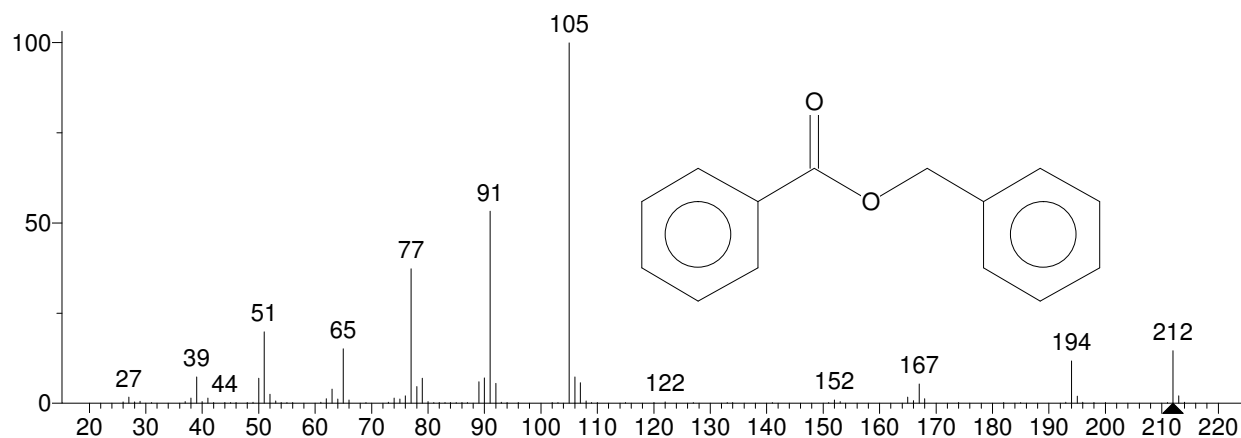


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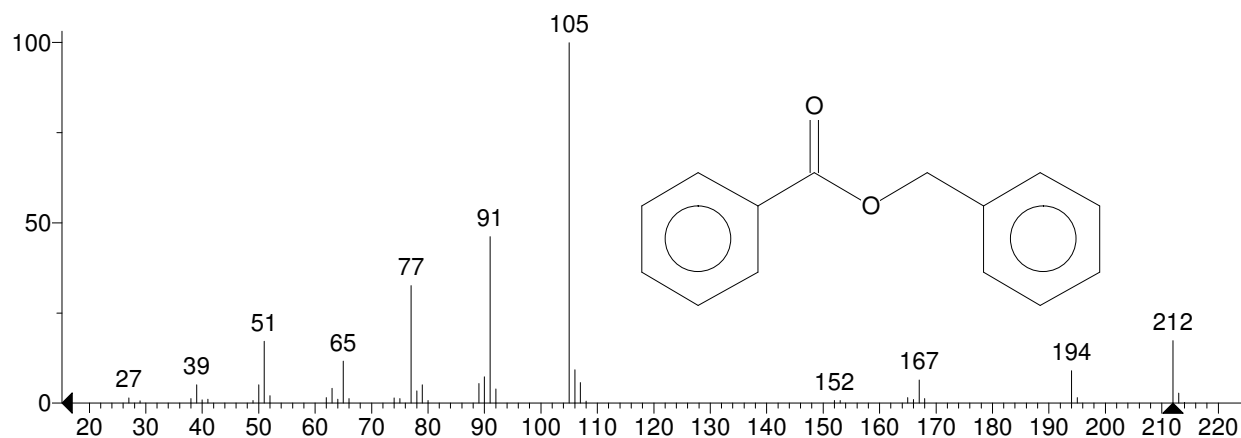
Unknown: Scan 1177 (13.471 min): Imitation.D
Compound in Library Factor = 278



Hit 1 : Benzyl Benzoate
C₁₄H₁₂O₂; MF: 888; RMF: 938; Prob 88.8%; CAS: 120-51-4; Lib: replib; ID: 13845.

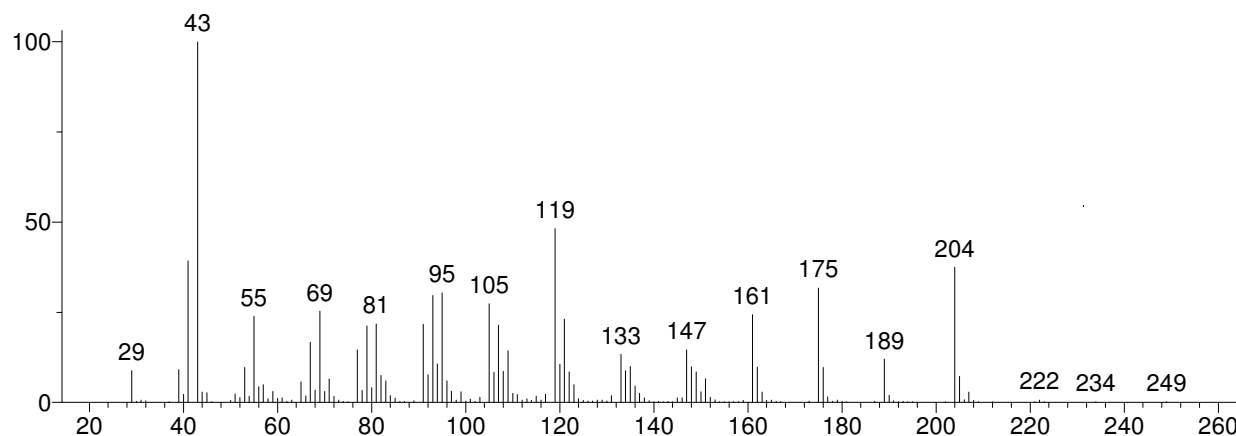


Hit 2 : Benzyl Benzoate
C₁₄H₁₂O₂; MF: 881; RMF: 941; Prob 88.8%; CAS: 120-51-4; Lib: mainlib; ID: 61201.

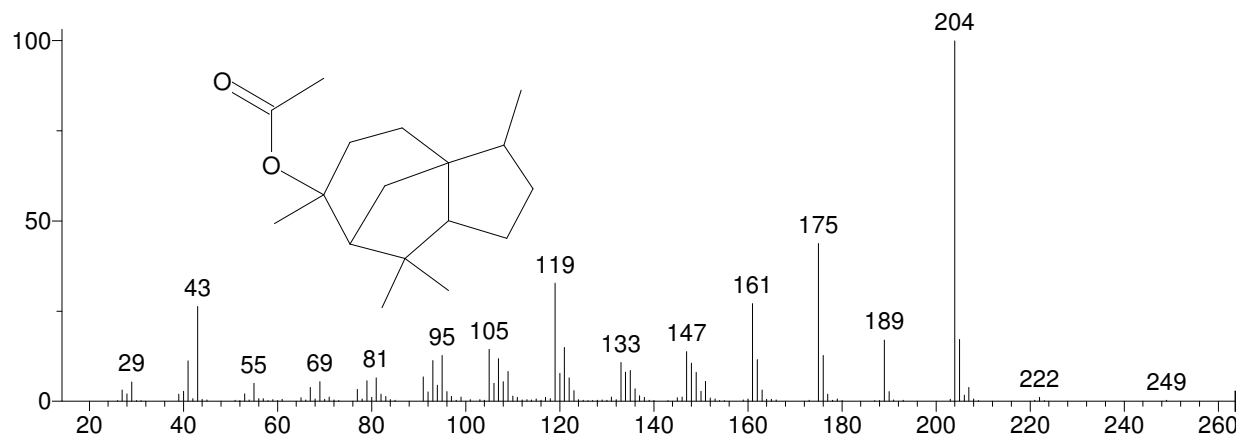


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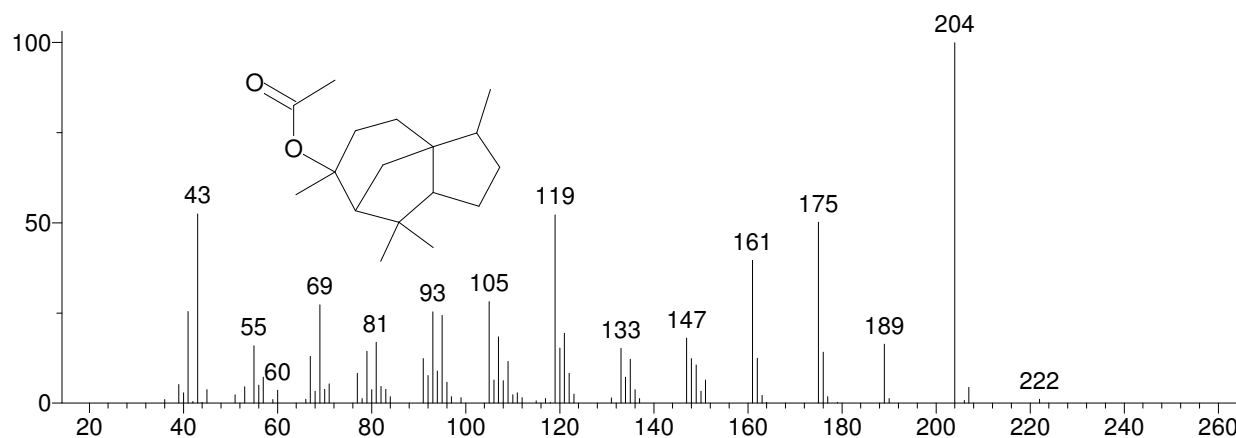
Unknown: Scan 1184 (13.551 min): Imitation2.D
Compound in Library Factor = -197



Hit 1 : 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate, [3R-(3.alpha.,3a.beta.,6.alpha.,7.beta.,8 C17H28O2; MF: 876; RMF: 878; Prob 17.8%; CAS: 77-54-3; Lib: mainlib; ID: 125471.

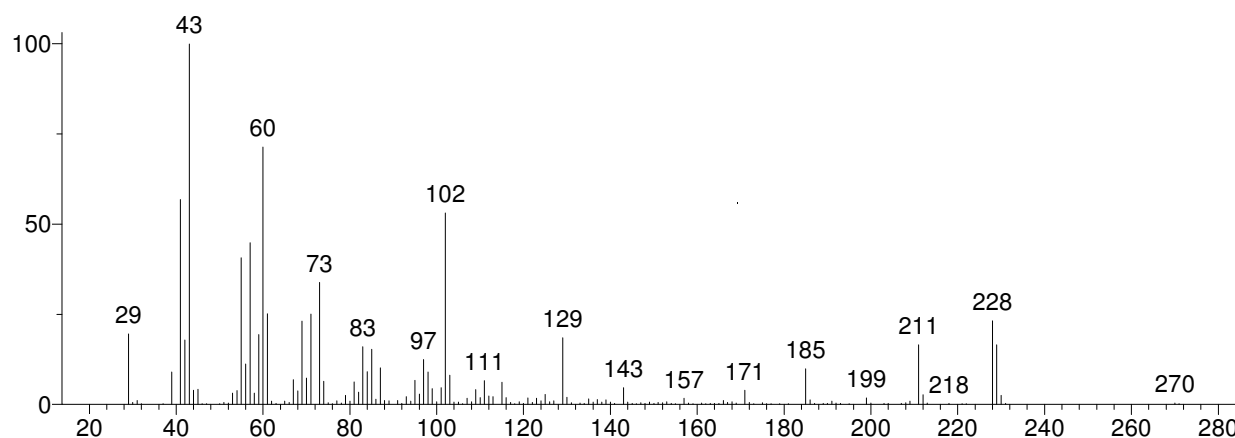


Hit 2 : 1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate, [3R-(3.alpha.,3a.beta.,6.alpha.,7.beta.,8 C17H28O2; MF: 867; RMF: 897; Prob 17.8%; CAS: 77-54-3; Lib: replib; ID: 24049.

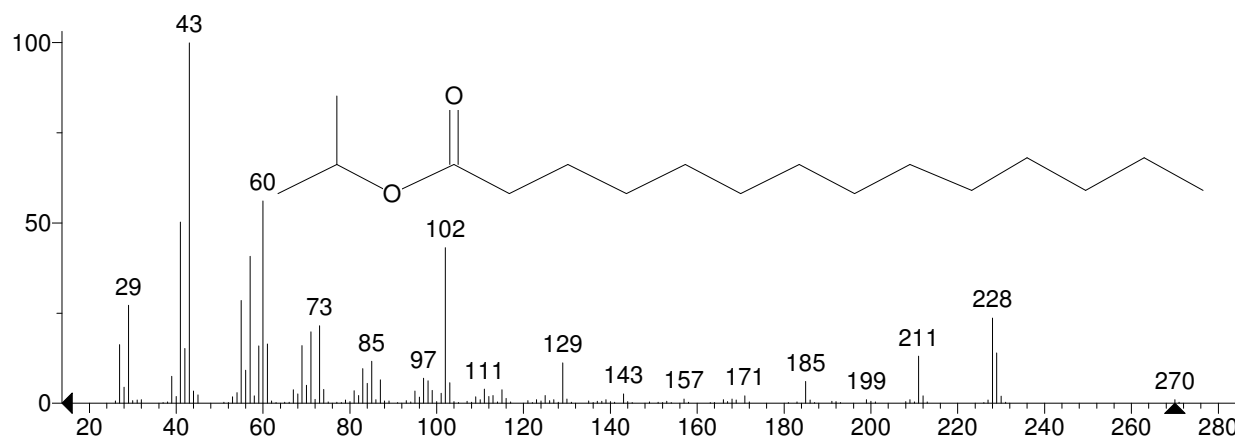


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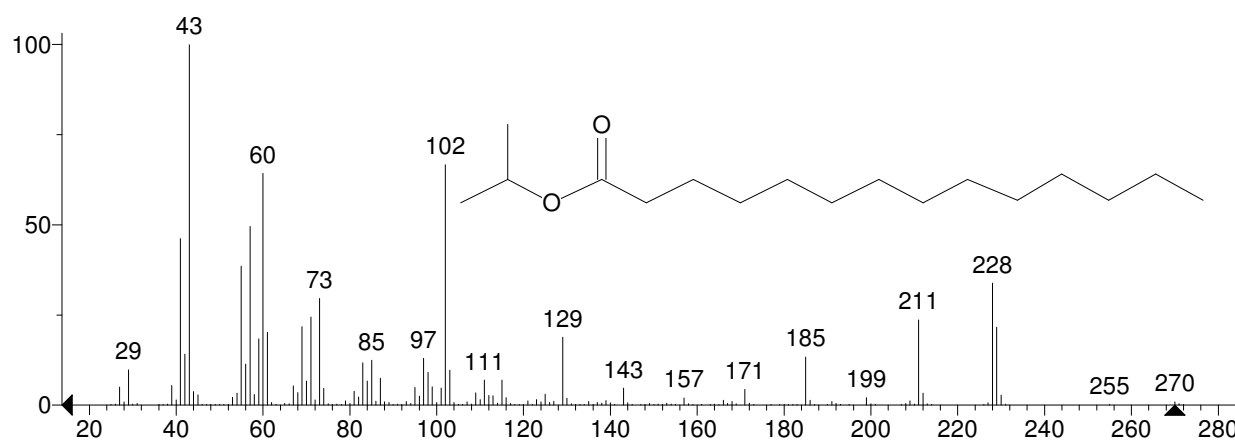
Unknown: Scan 1204 (13.779 min): Imitation2.D
Compound in Library Factor = 224



Hit 1 : Isopropyl Myristate
C₁₇H₃₄O₂; MF: 909; RMF: 914; Prob 77.4%; CAS: 110-27-0; Lib: replib; ID: 2233.

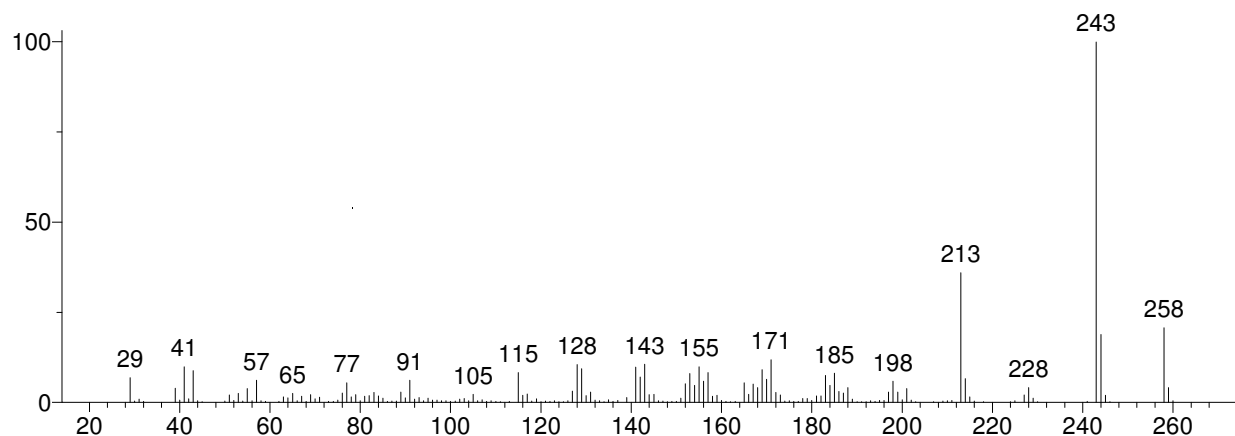


Hit 2 : Isopropyl Myristate
C₁₇H₃₄O₂; MF: 908; RMF: 912; Prob 77.4%; CAS: 110-27-0; Lib: mainlib; ID: 9582.

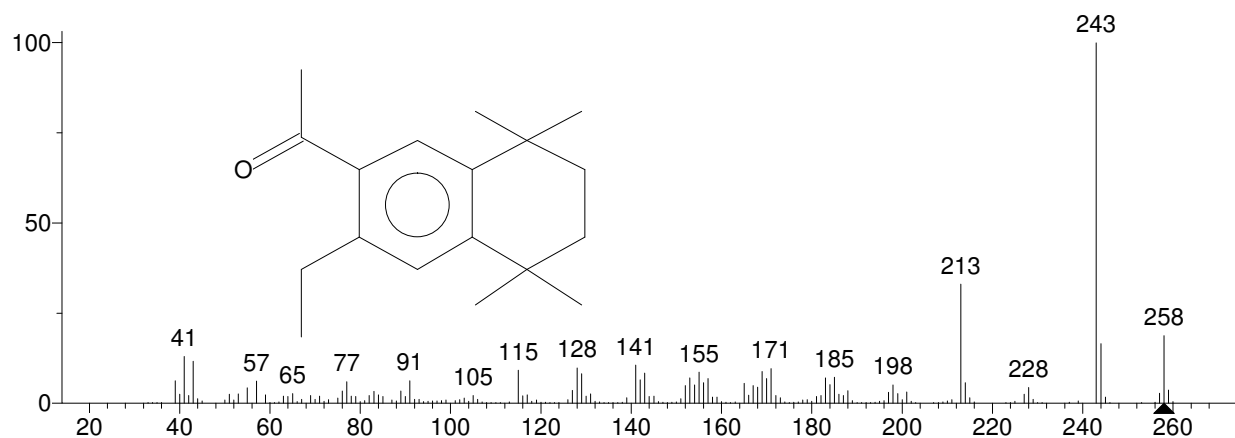


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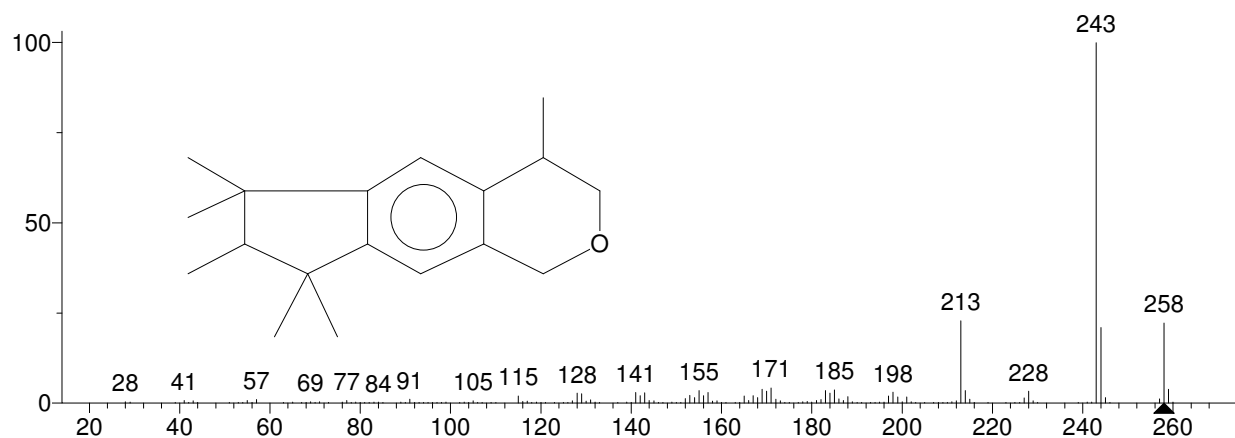
Unknown: Scan 1240 (14.190 min): Imitation2.D
Compound in Library Factor = 473



Hit 1 : 7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
C₁₈H₂₆O; MF: 926; RMF: 928; Prob 80.2%; CAS: 88-29-9; Lib: replib; ID: 25619.

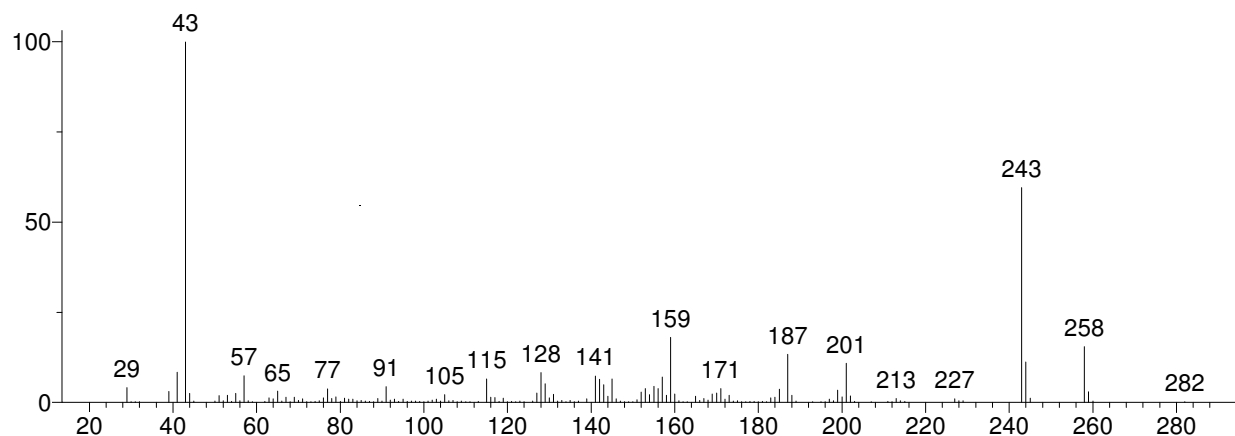


Hit 2 : Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-
C₁₈H₂₆O; MF: 884; RMF: 895; Prob 18.0%; CAS: 1222-05-5; Lib: mainlib; ID: 138703.

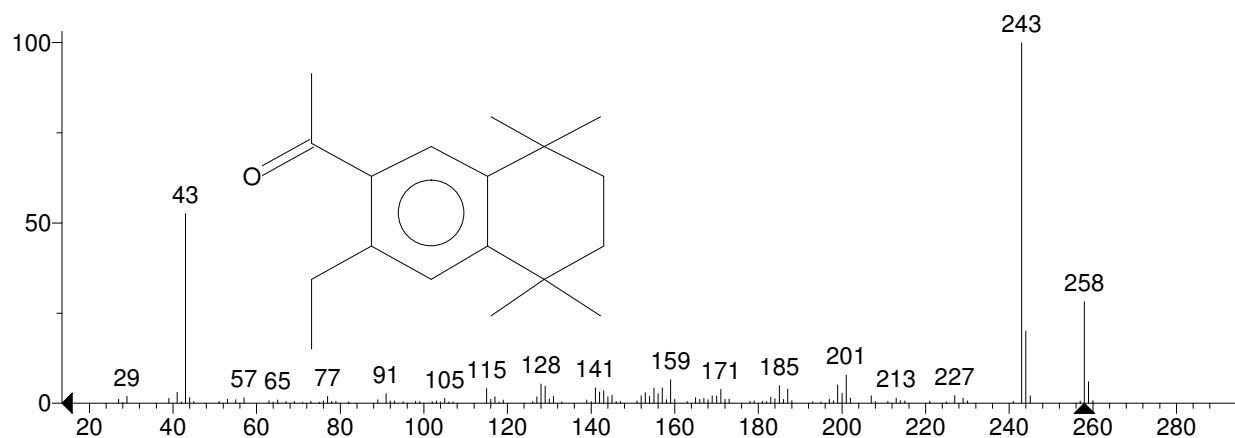


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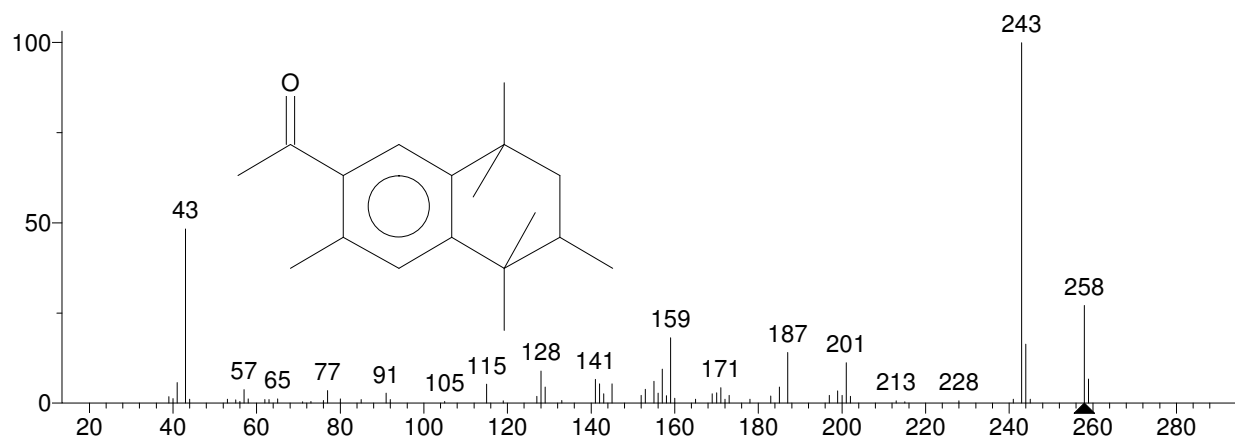
Unknown: Scan 1246 (14.259 min): Imitation2.D
Compound in Library Factor = 204



Hit 1 : 7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin
C₁₈H₂₆O; MF: 867; RMF: 879; Prob 59.2%; CAS: 88-29-9; Lib: replib; ID: 25601.

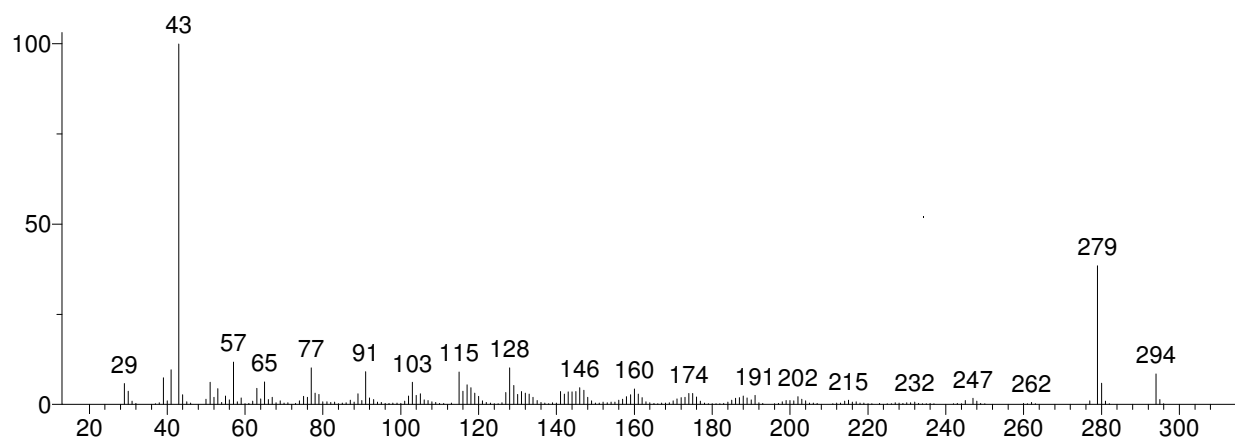


Hit 2 : Ethanone, 1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthalenyl)-
C₁₈H₂₆O; MF: 853; RMF: 914; Prob 37.1%; CAS: 1506-02-1; Lib: mainlib; ID: 138466.

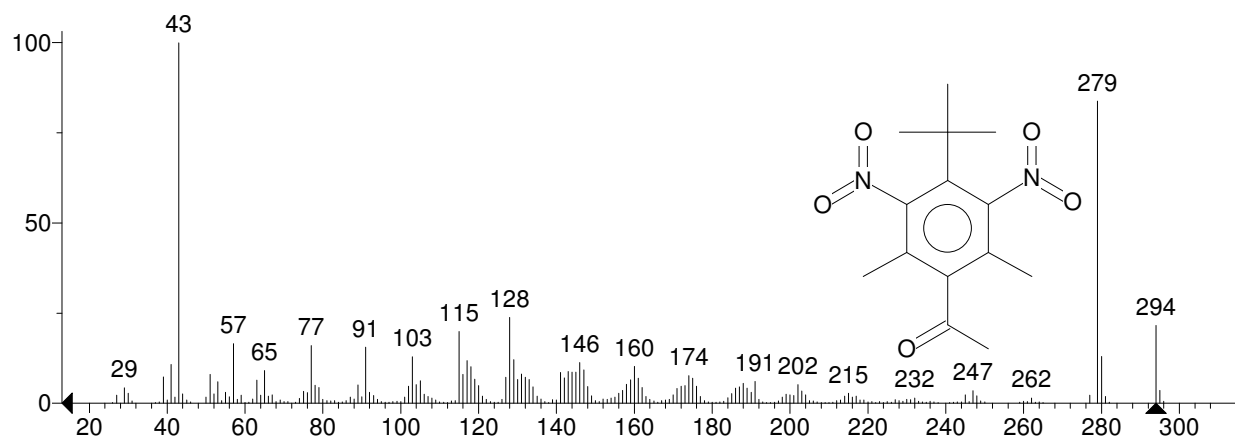


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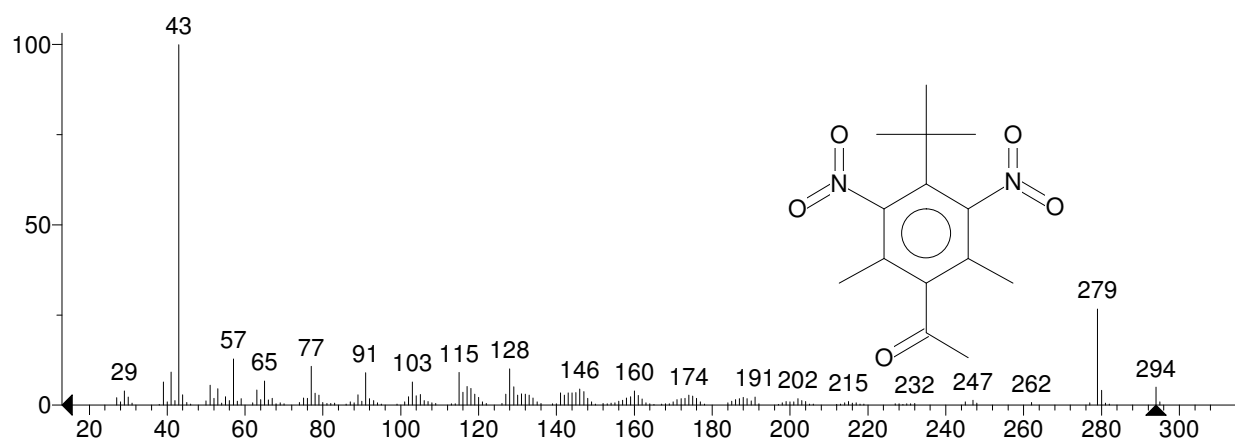
Unknown: Scan 1321 (15.115 min): Imitation2.D
Compound in Library Factor = 993



Hit 1 : Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-
C₁₄H₁₈N₂O₅; MF: 954; RMF: 954; Prob 93.2%; CAS: 81-14-1; Lib: replib; ID: 3079.

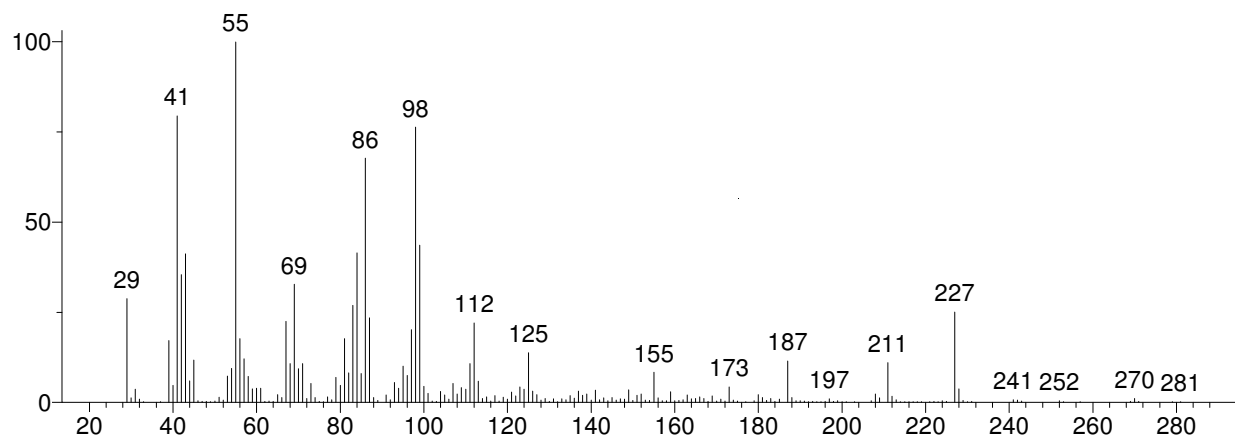


Hit 2 : Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethyl-3,5-dinitrophenyl]-
C₁₄H₁₈N₂O₅; MF: 952; RMF: 960; Prob 93.2%; CAS: 81-14-1; Lib: replib; ID: 3078.

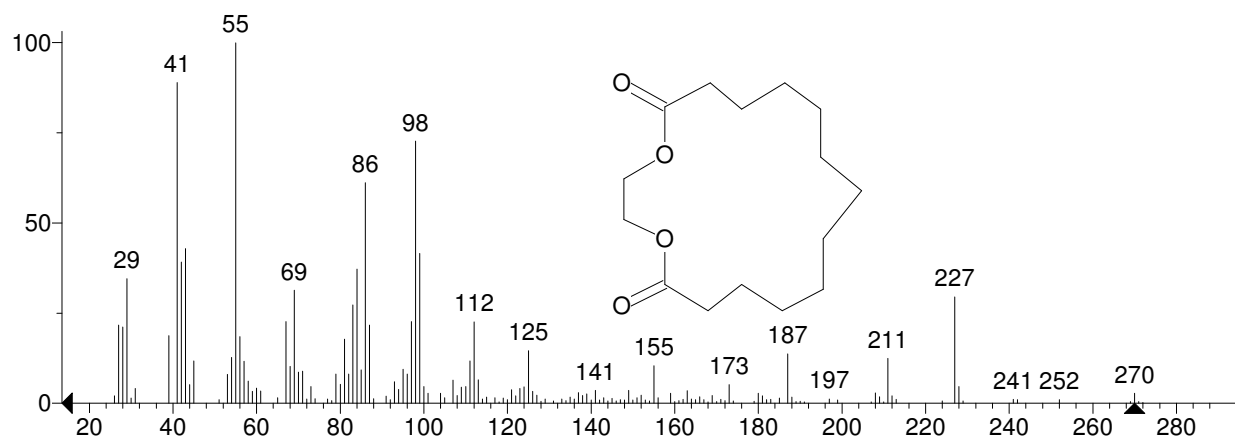


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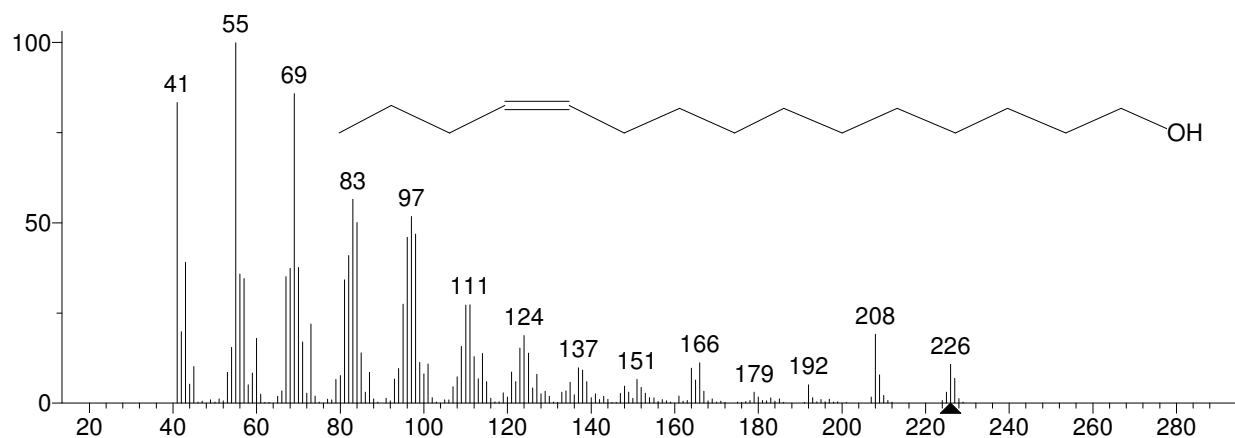
Unknown: Scan 1342 (15.355 min): Imitation.D
Compound in Library Factor = 797



Hit 1 : Ethylene brassylate
C₁₅H₂₆O₄; MF: 949; RMF: 956; Prob 90.4%; CAS: 105-95-3; Lib: mainlib; ID: 16894.

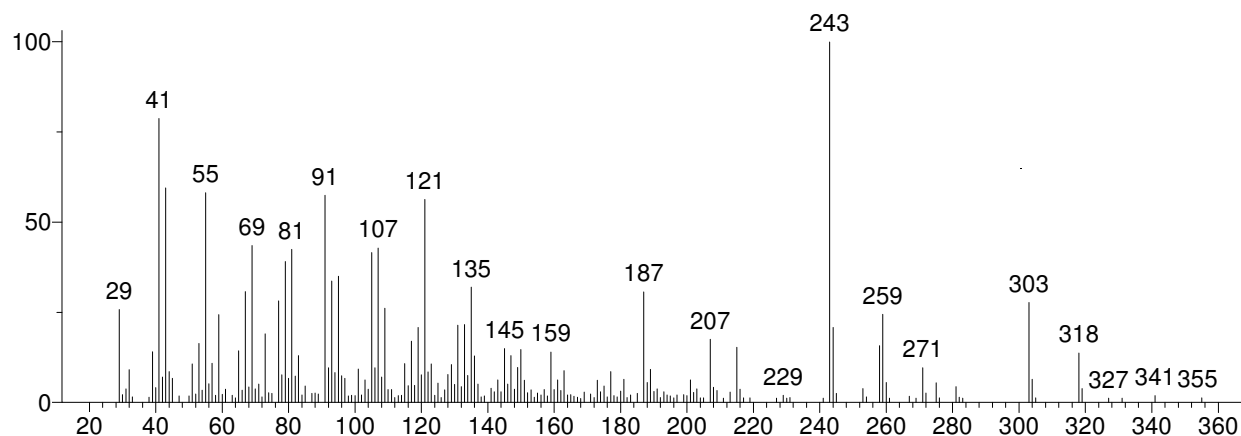


Hit 2 : Z-11-Pentadecenol
C₁₅H₃₀O; MF: 690; RMF: 710; Prob 0.90%; Lib: mainlib; ID: 17391.

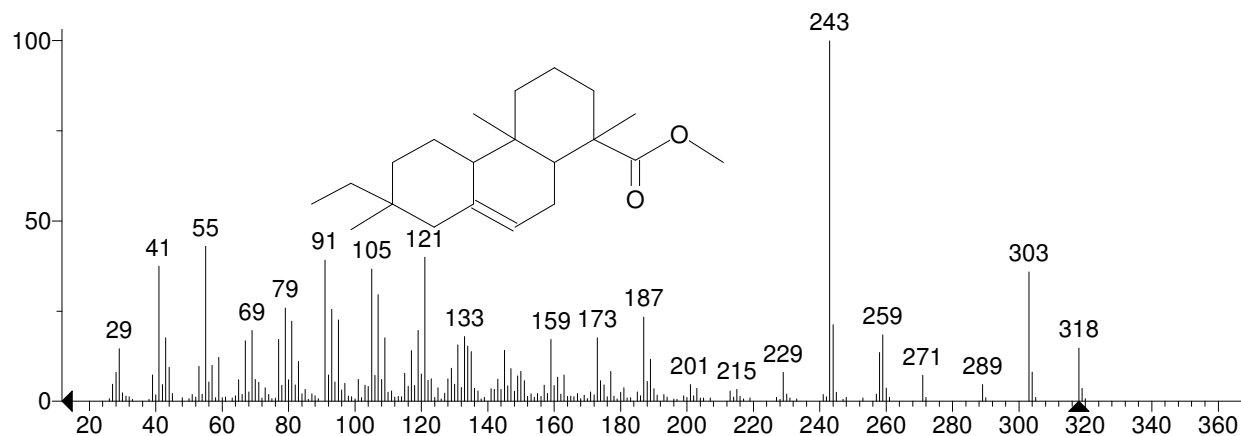


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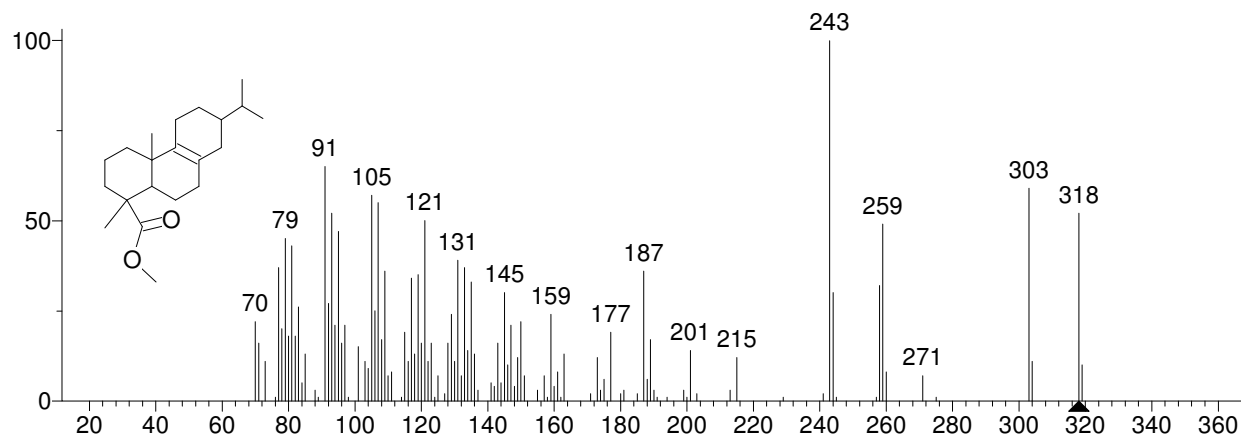
Unknown: Scan 1514 (17.319 min): Imitation.D
Compound in Library Factor = -119



Hit 1 : 1-Phenanthrenecarboxylic acid, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl ester
C₂₁H₃₄O₂; MF: 871; RMF: 890; Prob 71.9%; CAS: 72088-13-2; Lib: mainlib; ID: 138475.



Hit 2 : 1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester
C₂₁H₃₄O₂; MF: 815; RMF: 879; Prob 13.7%; CAS: 33892-15-8; Lib: mainlib; ID: 138505.



TGA RESULTS

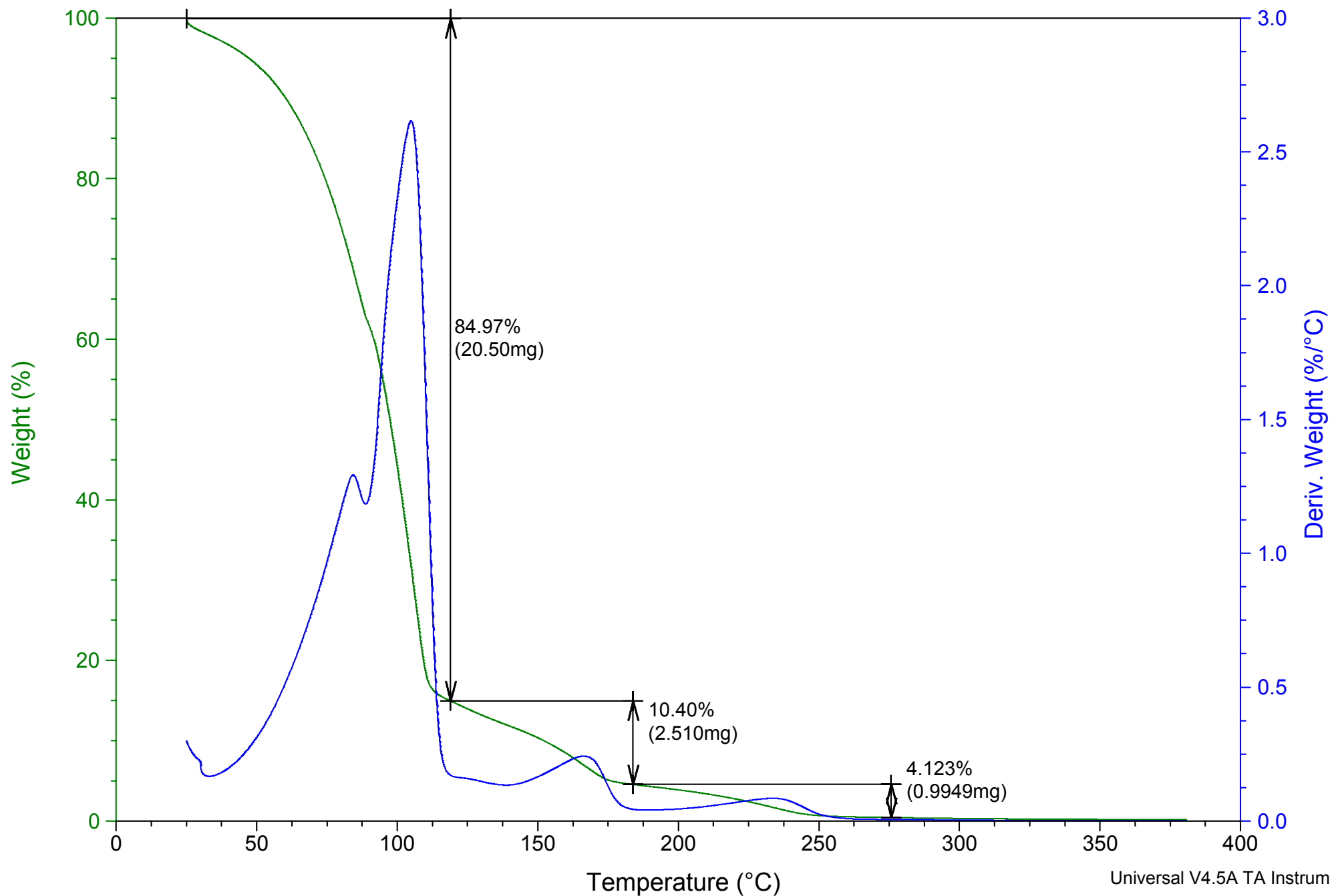
Sample: Designer
Size: 24.1320 mg
Method: Ramp

TGA

File: I:\...\dsc pan Designer.001 Page 97 of 103

Run Date: 09-Jun-2010 15:52

Instrument: TGA Q500 V20.8 Build 34



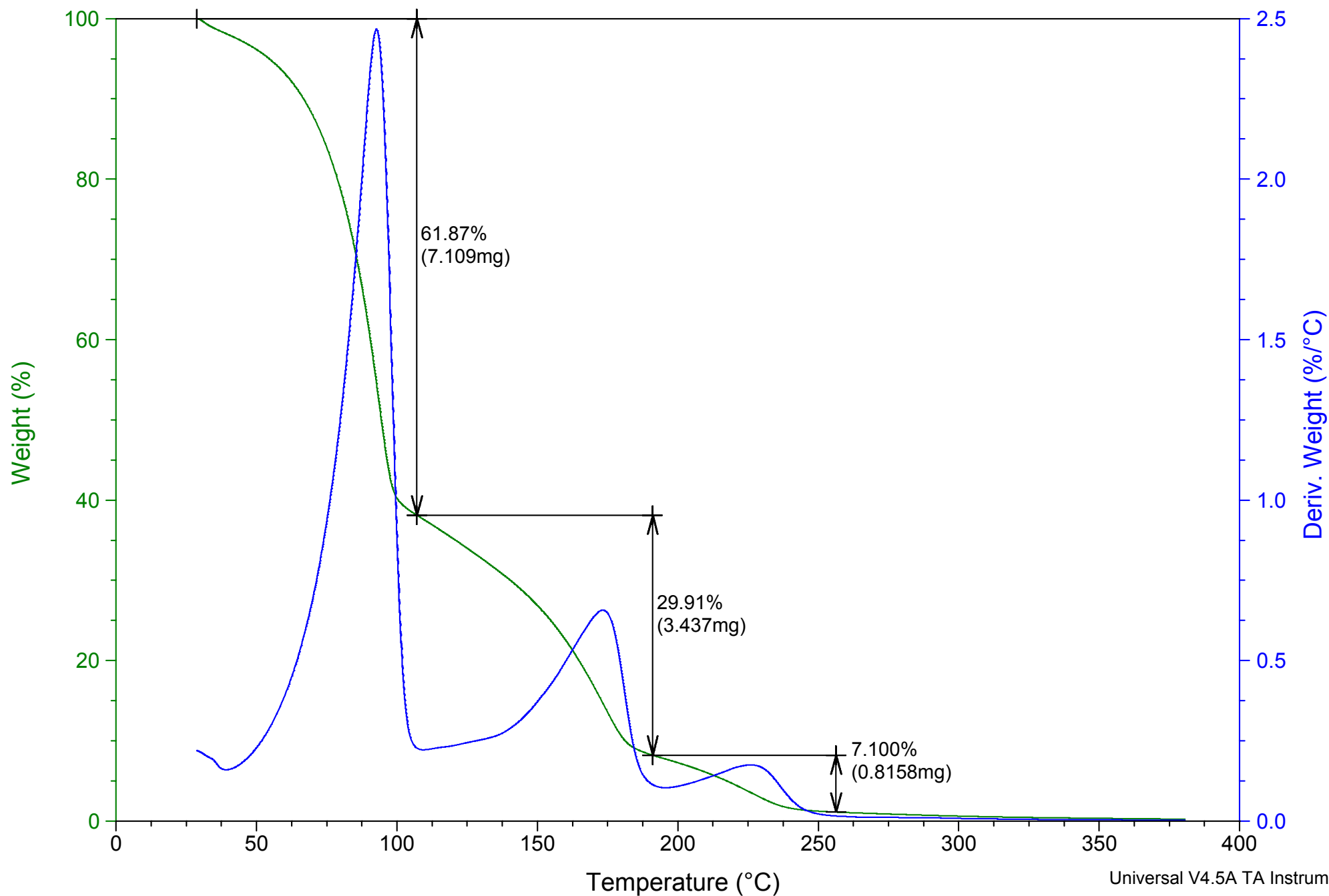
Sample: Designer
Size: 11.4910 mg
Method: Ramp

TGA

File: I:\...\dsc pan Designer.002 Page 98 of 103

Run Date: 09-Jun-2010 19:24

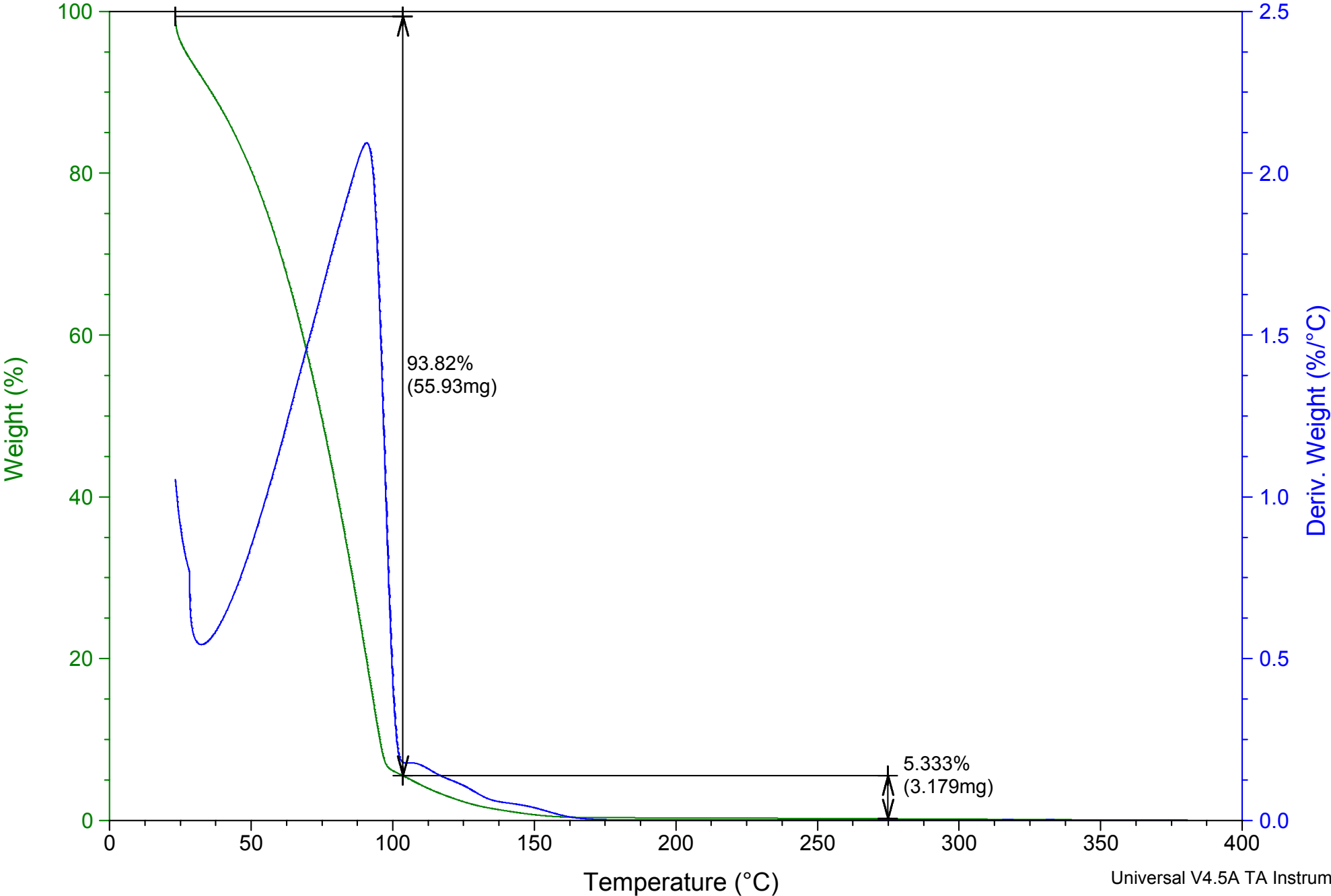
Instrument: TGA Q500 V20.8 Build 34



Sample: Imitation
Size: 59.6190 mg
Method: Ramp

TGA

File: I:\...\manual Imitation.001
Run Date: 08-Jun-2010 15:44
Instrument: TGA Q500 V20.8 Build 34



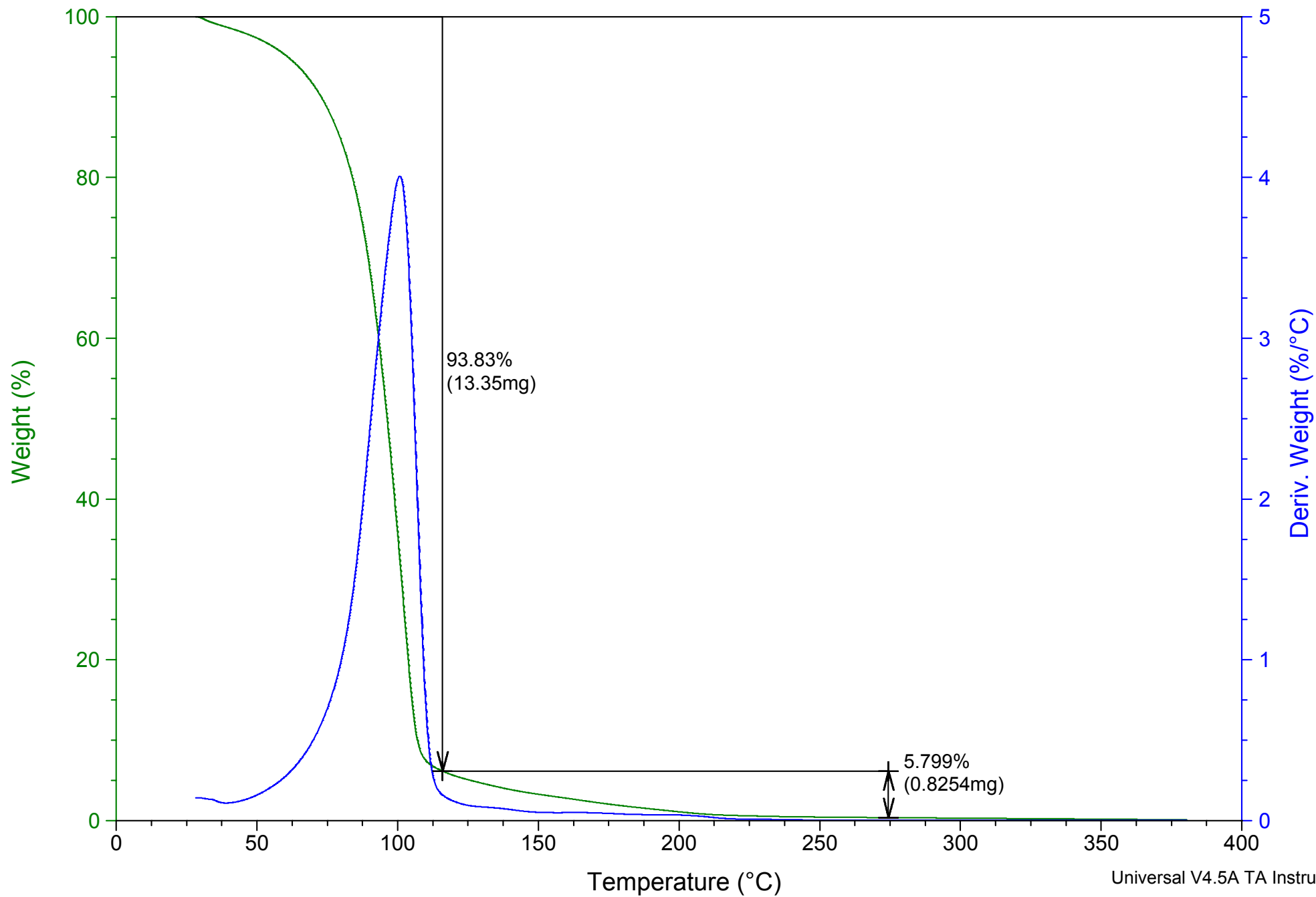
Sample: Imitation
Size: 14.2320 mg
Method: Ramp

TGA

File: I:\...\dsc pan Imitation.002 Page 100 of 103

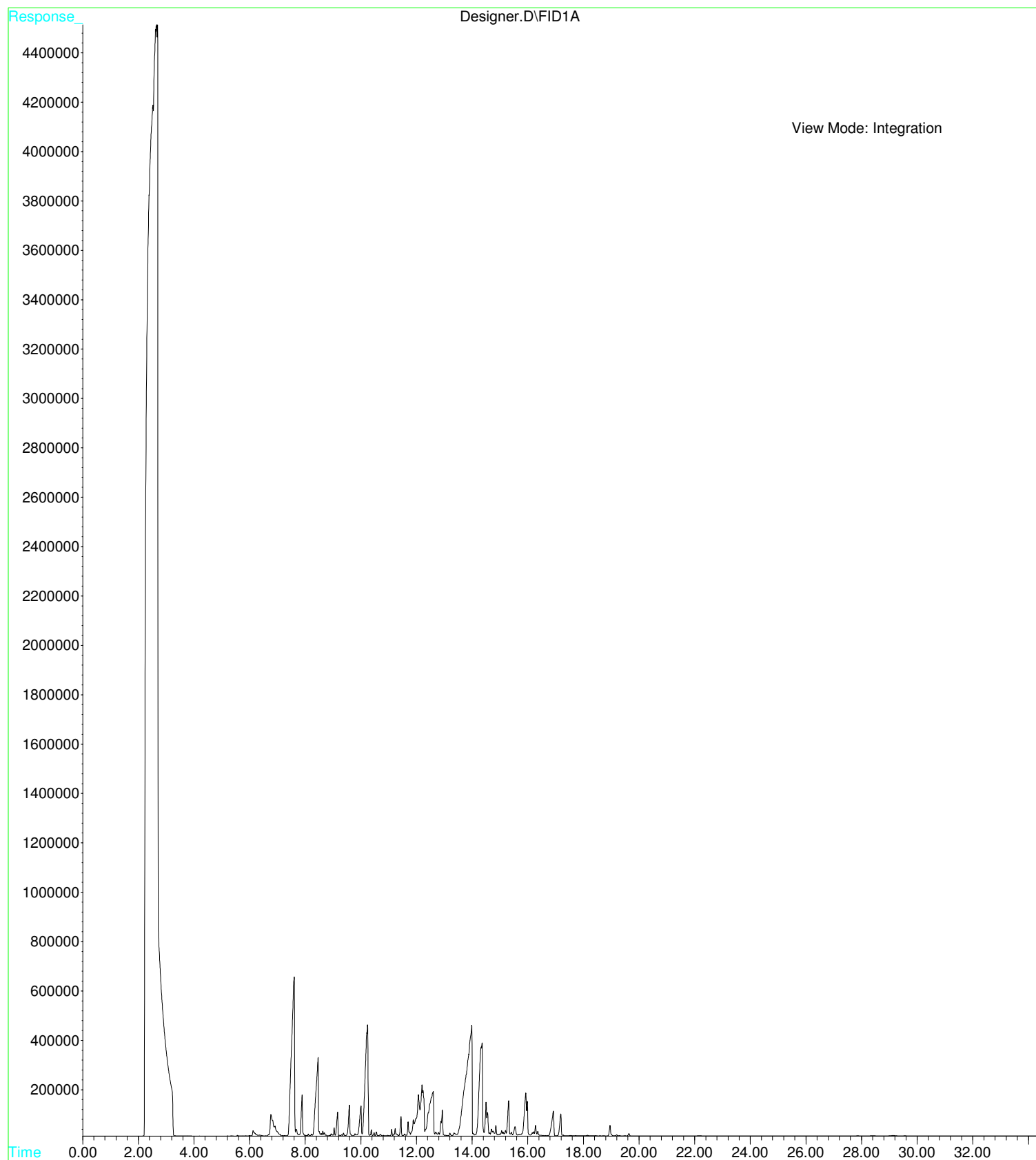
Run Date: 09-Jun-2010 18:24

Instrument: TGA Q500 V20.8 Build 34



GC-FID RESULTS

File : C:\HPCHEM\1\DATA\2010\JOB2010\EXPDEF\GC-FID DATA\Designer.D
Operator : KV
Acquired : 8 Jun 2010 11:06 using AcqMethod JORDIGEL.M
Instrument : HP5890
Sample Name: Designer Perfume
Misc Info :
Vial Number: 10



File : C:\HPCHEM\1\DATA\2010\JOB2010\EXPDEF\GC-FID DATA\Imitation.D
Operator : KV
Acquired : 8 Jun 2010 13:09 using AcqMethod JORDIGEL.M
Instrument : HP5890
Sample Name: Imitation Perfume
Misc Info :
Vial Number: 11

