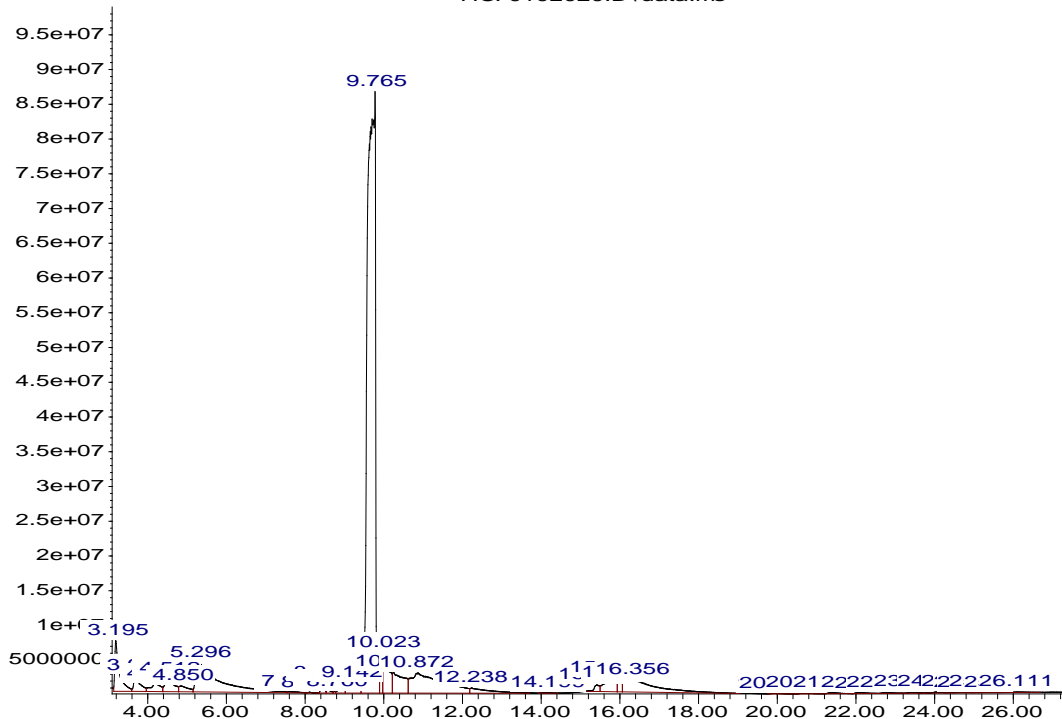


Abundance

TIC: 0102020.D\data.ms



Time-->

Chemistry Lab

Library Search Report

Data Path : C:\Users\chemistrylab\Desktop\1\DATA\0101677.D\

Data File : 0102020.D

Acq On : 25 Sep 2019 17:35

Operator :

Sample : L

Misc :

ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\Database\NIST11.L Minimum Quality: 50

C:\Database\NIST14.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
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1	3.194	2.77	C:\Database\NIST11.L		
			(1R)-2,6,6-Trimethylbicyclo[3.1.1]	15854	007785-70-8 96
			hept-2-ene		
			.alpha.-Pinene	15699	000080-56-8 95
			(1R)-2,6,6-Trimethylbicyclo[3.1.1]	15852	007785-70-8 94
			hept-2-ene		
2	3.686	1.19	C:\Database\NIST11.L		
			1,3,7-Octatriene, 3,7-dimethyl-	15769	000502-99-8 91
			(1R)-2,6,6-Trimethylbicyclo[3.1.1]	15854	007785-70-8 91
			hept-2-ene		
			Cyclohexene, 4-methylene-1-(1-meth	15844	000099-84-3 90
			ylethyl)-		
3	4.193	0.94	C:\Database\NIST11.L		
			.alpha.-Phellandrene	15728	000099-83-2 91
			.alpha.-Phellandrene	15730	000099-83-2 91
			Bicyclo[3.1.0]hex-2-ene, 2-methyl-	15898	002867-05-2 90
			5-(1-methylethyl)-		
4	4.511	1.38	C:\Database\NIST11.L		
			4-Carene, (1S,3R,6R)-(-)-	15741	005208-49-1 64
			D-Limonene	15682	005989-27-5 64
			Bicyclo[3.1.1]hept-2-ene, 3,6,6-tr	15837	004889-83-2 64
			imethyl-		
5	4.851	0.64	C:\Database\NIST11.L		
			.gamma.-Terpinene	15711	000099-85-4 94
			3-Carene	15664	013466-78-9 91
			(1S)-2,6,6-Trimethylbicyclo[3.1.1]	15851	007785-26-4 87
			hept-2-ene		

6 5.298 8.13 C:\Database\NIST11.L
Cyclohexene, 1-methyl-4-(1-methyle 15862 000586-62-9 95
thylidene)-
Cyclohexene, 1-methyl-4-(1-methyle 15863 000586-62-9 95
thylidene)-
Cyclohexene, 1-methyl-4-(1-methyle 15858 000586-62-9 94
thylidene)-

7 7.614 0.14 C:\Database\NIST11.L
Cyclohexene, 1-methyl-4-(1-methyle 15858 000586-62-9 96
thylidene)-
2-Carene 15666 000554-61-0 87
(+)-4-Carene 15688 029050-33-7 87

8 8.121 0.03 C:\Database\NIST11.L
Cyclohexene, 1-methyl-4-(1-methyle 15858 000586-62-9 95
thylidene)-
2-Carene 15666 000554-61-0 76
1,3-Cyclohexadiene, 1-methyl-4-(1- 15877 000099-86-5 76
methylethyl)-

9 8.431 0.37 C:\Database\NIST11.L
Cyclohexene, 4-ethenyl-4-methyl-3- 64501 020307-84-0 98
(1-methylethenyl)-1-(1-methylethyl
)-, (3R-trans)-
2-Carene 15666 000554-61-0 91
Cyclohexene, 1-methyl-4-(1-methyle 15863 000586-62-9 90
thylidene)-

10 8.583 0.16 C:\Database\NIST14.L
1-Methyl-4-(6-methylhept-5-en-2-yl 68678 000451-55-8 89
)cyclohexa-1,3-diene
Cyclohexene, 1-methyl-4-(1-methyle 16238 000586-62-9 64

			thylidene)-		
			Spiro[5.5]undeca-1,8-diene, 1,5,5,	68681	019912-83-5 52
			9-tetramethyl-, (R)-		
11	8.757	0.04	C:\Database\NIST11.L		
			.gamma.-Muurolene	64338	030021-74-0 62
			.gamma.-Muurolene	64337	030021-74-0 58
			Cyclohexene, 1-methyl-4-(1-methyle	15858	000586-62-9 52
			thylidene)-		
12	8.938	0.72	C:\Database\NIST11.L		
			Copaene	64250	003856-25-5 94
			Copaene	64252	003856-25-5 93
			.alpha.-ylangene	64307	1000374-19-0 64
13	9.143	1.30	C:\Database\NIST11.L		
			1,3,6-Octatriene, 3,7-dimethyl-, (15808	003338-55-4 50
			Z)-		
			.beta.-Ocimene	15698	013877-91-3 49
			1H-Pyrrole, 1-butyl-	10219	000589-33-3 46
14	9.763	58.14	C:\Database\NIST11.L		
			Caryophyllene	64272	000087-44-5 99
			Caryophyllene	64275	000087-44-5 97
			Bicyclo[5.2.0]nonane, 2-methylene-	64421	242794-76-9 95
			4,8,8-trimethyl-4-vinyl-		
15	9.937	0.94	C:\Database\NIST11.L		
			Isocaryophyllene	64304	1000140-07-2 86
			Bicyclo[7.2.0]undec-4-ene, 4,11,11	64479	000118-65-0 83
			-trimethyl-8-methylene-, [1R-(1R*,4		
			Z,9S*)]-		
			.alpha.-ylangene	64307	1000374-19-0 78

16	10.021	2.67	C:\Database\NIST11.L			
				Bicyclo[3.1.1]hept-2-ene, 2,6-dime	64434	017699-05-7 83
				thyl-6-(4-methyl-3-pentenyl)-		
				cis-.alpha.-Bisabolene	64361	029837-07-8 72
				Humulene	64256	006753-98-6 70
17	10.248	2.82	C:\Database\NIST11.L			
				Santolina triene	15707	002153-66-4 83
				Bicyclo[7.2.0]undec-4-ene, 4,11,11	64477	000118-65-0 62
				-trimethyl-8-methylene-, [1R-(1R*,4		
				Z,9S*)]-		
				1,7-Octadiene, 2,7-dimethyl-3,6-bi	32335	016714-60-6 62
				s(methylene)-		
18	10.868	7.76	C:\Database\NIST11.L			
				Naphthalene, 1,2,4a,5,6,8a-hexahyd	64456	000483-75-0 97
				ro-4,7-dimethyl-1-(1-methylethyl)-		
				.gamma.-Muurolene	64337	030021-74-0 96
				.gamma.-Muurolene	64324	030021-74-0 91
19	12.238	1.24	C:\Database\NIST11.L			
				Cedrene	64249	011028-42-5 83
				Tricyclo[5.4.0.0(2,8)]undec-9-ene,	64464	005989-08-2 81
				2,6,6,9-tetramethyl-, (1R,2S,7R,8		
				R)-		
				1H-Benzocycloheptene, 2,4a,5,6,7,8	64507	003853-83-6 78
				,9,9a-octahydro-3,5,5-trimethyl-9-		
				methylene-, (4aS-cis)-		
20	14.199	0.06	C:\Database\NIST11.L			
				(E,Z)-.alpha.-Farnesene	64366	1000293-03-2 58
				cis-.alpha.-Bisabolene	64361	029837-07-8 58

2,5-Cyclooctadiene-1-carboxamide, 83637 1000159-75-2 50
N-phenyl-

21 15.425 0.41 C:\Database\NIST11.L

1,3,6,10-Cyclotetradecatetraene, 3 121356 001898-13-1 96
,7,11-trimethyl-14-(1-methylethyl)
-, [S-(E,Z,E,E)]-
Alloaromadendrene 64332 025246-27-9 70
1,5-Cycloundecadiene, 8,8-dimethyl 53193 062338-54-9 64
-9-methylene-

22 15.705 1.69 C:\Database\NIST11.L

1-Cyclohexene-1-methanol, 4-(1-met 25281 000536-59-4 50
hylethenyl)-
1-Nitro-bicyclo[6.1.0]nonan-2-one 48257 1000282-07-3 46
2,3-Hexadiene, 2-methyl- 2886 029212-09-7 43

23 16.015 0.46 C:\Database\NIST11.L

1,3,6,10-Cyclotetradecatetraene, 3 121356 001898-13-1 91
,7,11-trimethyl-14-(1-methylethyl)
-, [S-(E,Z,E,E)]-
Cyclohexane, 1-ethenyl-1-methyl-2, 64415 110823-68-2 78
4-bis(1-methylethenyl)-
Camphene 15676 000079-92-5 38

24 16.356 4.81 C:\Database\NIST11.L

Cyclopropane, trimethyl(2-methyl-1 15889 014803-30-6 64
-propenylidene)-
1,3,6,10-Cyclotetradecatetraene, 3 121356 001898-13-1 56
,7,11-trimethyl-14-(1-methylethyl)
-, [S-(E,Z,E,E)]-
Bicyclo[4.1.0]heptane, 7-(1-methyl 15866 053282-47-6 46
ethylidene)-

25	19.951	0.03	C:\Database\NIST11.L		
			Dodecane, 1,2-dibromo-	165284	055334-42-4 64
			Decane, 1-iodo-	116706	002050-77-3 55
			Tritetracontane	241174	007098-21-7 52
26	20.019	0.03	C:\Database\NIST14.L		
			Octadecane, 1-chloro-	148106	003386-33-2 49
			1-Octadecanesulphonyl chloride	206960	1000342-70-4 49
			Tritetracontane	273205	007098-21-7 46
27	20.693	0.10	C:\Database\NIST11.L		
			Nonadecane	117636	000629-92-5 90
			Octacosane	209566	000630-02-4 83
			Methoxyacetic acid, 2-tetradecyl ester	132964	1000282-04-8 83
28	21.396	0.13	C:\Database\NIST11.L		
			Eicosane	129493	000112-95-8 89
			Heneicosane, 11-pentyl-	194505	014739-72-1 87
			Tricosane, 2-methyl-	175565	001928-30-9 83
29	22.108	0.13	C:\Database\NIST11.L		
			Hexatriacontane	235974	000630-06-8 87
			Tricosane, 2-methyl-	175564	001928-30-9 87
			Docosane, 9-octyl-	219832	055319-83-0 87
30	22.456	0.01	C:\Database\NIST11.L		
			Octadecane, 1-chloro-	134595	003386-33-2 55
			Octadecane	105884	000593-45-3 55
			Nonadecane	117638	000629-92-5 55
31	22.751	0.12	C:\Database\NIST11.L		

		Octadecane	105885 000593-45-3 97
		Octadecane	105884 000593-45-3 96
		Octadecane	105883 000593-45-3 95
32	23.440	0.11 C:\Database\NIST11.L	
		Tridecane, 2-methyl-	59889 001560-96-9 87
		1-Iodo-2-methylundecane	140553 073105-67-6 78
		Octadecane, 2-methyl-	117649 001560-88-9 70
33	24.046	0.12 C:\Database\NIST11.L	
		Eicosane, 2-methyl-	141430 001560-84-5 90
		Octadecane	105883 000593-45-3 90
		1-Chloroeicosane	158254 042217-02-7 90
34	24.651	0.16 C:\Database\NIST11.L	
		Eicosane	129492 000112-95-8 87
		Hexadecane, 1-chloro-	110906 004860-03-1 86
		Tricosane, 2-methyl-	175566 001928-30-9 70
35	24.969	0.01 C:\Database\NIST11.L	
		.alpha.-Ketostearic acid	143037 004468-17-1 83
		2-Piperidinone, N-[4-bromo-n-butyl	88460 195194-80-0 50
]-	
		Vinyl lauryl ether	71313 000765-14-0 50
36	25.052	0.02 C:\Database\NIST11.L	
		3-Eicosene, (E)-	127771 074685-33-9 90
		Octacosane	209565 000630-02-4 83
		1-Docosene	151537 001599-67-3 78
37	25.355	0.12 C:\Database\NIST11.L	
		Octadecane, 1-chloro-	134595 003386-33-2 89
		Octadecane	105884 000593-45-3 83

2-Piperidinone, N-[4-bromo-n-butyl 88460 195194-80-0 64
]-

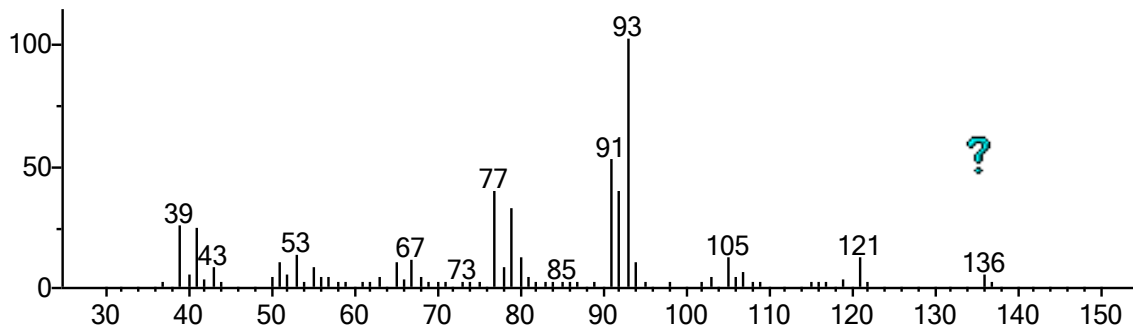
38 25.741 0.03 C:\Database\NIST11.L

Octadecane 105886 000593-45-3 60
17-Pentatriacontene 234187 006971-40-0 53
2-Piperidinone, N-[4-bromo-n-butyl 88460 195194-80-0 50
]-

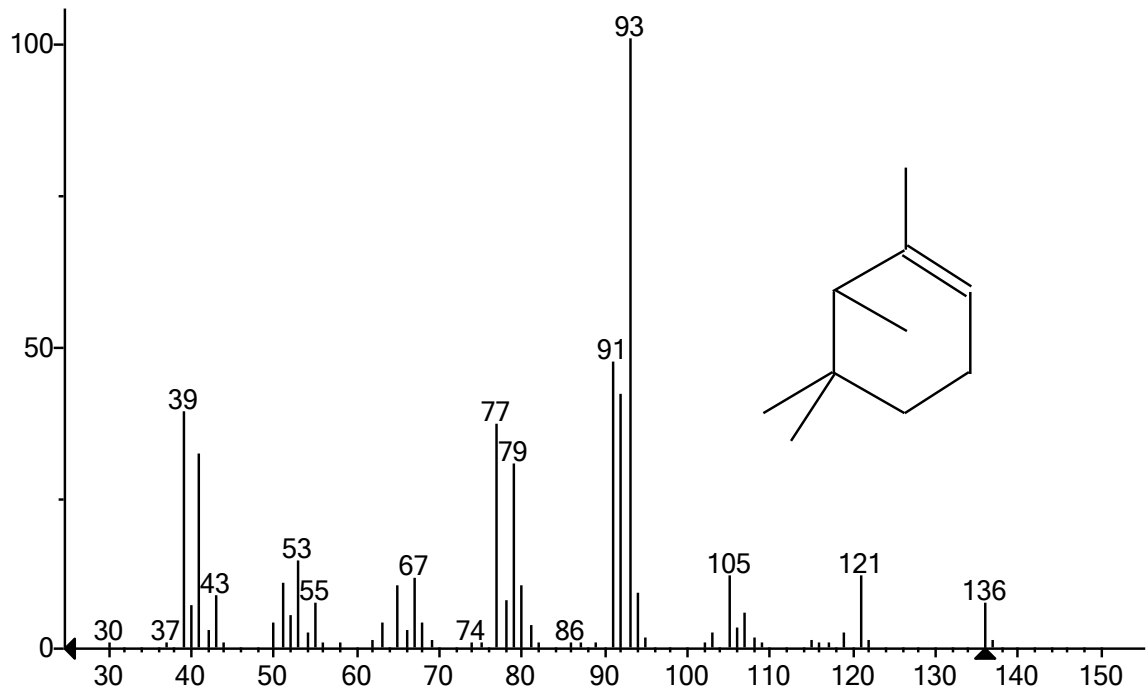
39 26.112 0.07 C:\Database\NIST11.L

Octadecane 105886 000593-45-3 86
Eicosane 129490 000112-95-8 86
Hentriacontane 223851 000630-04-6 83

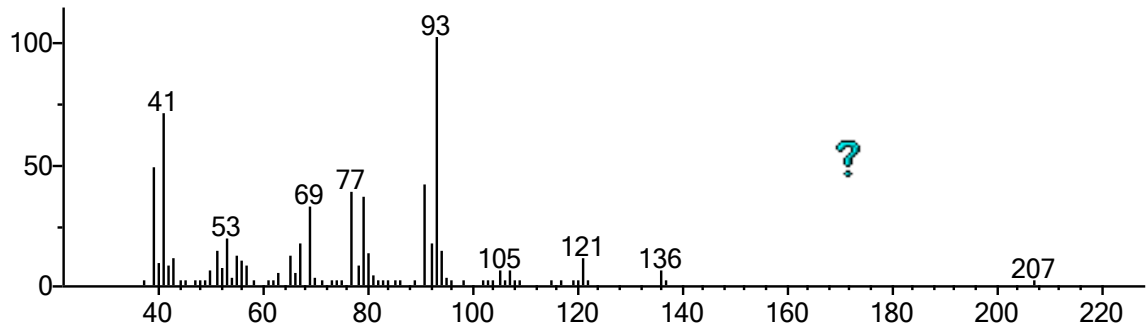
Thu Sep 26 19:18:53 2019



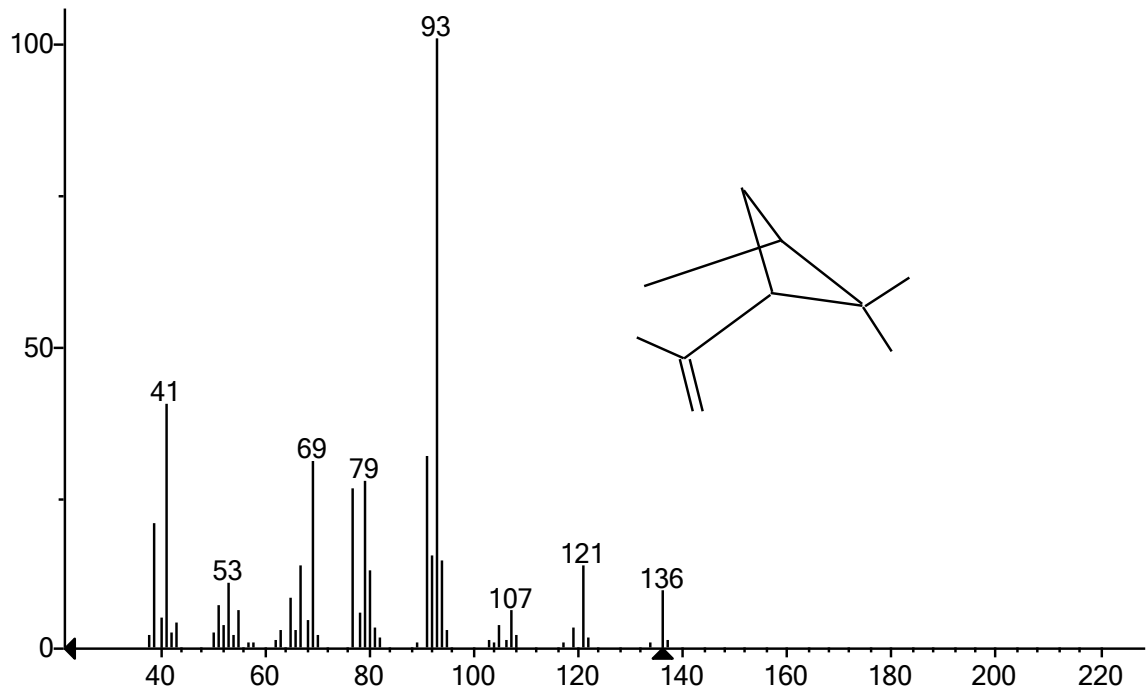
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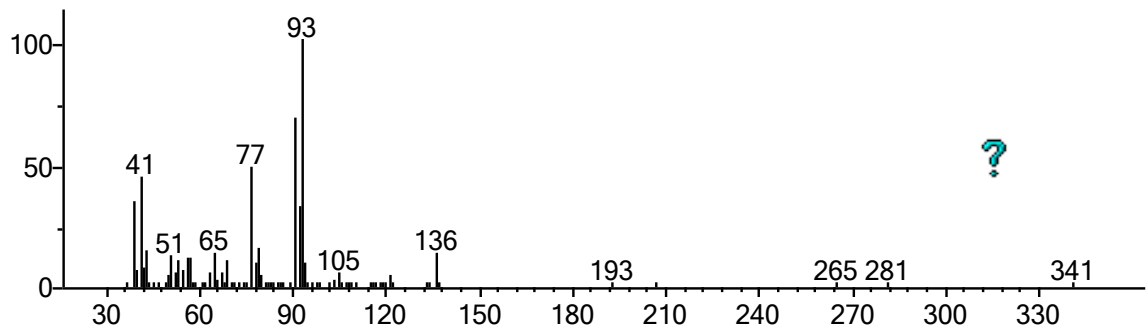
(mainlib) α -Pinene



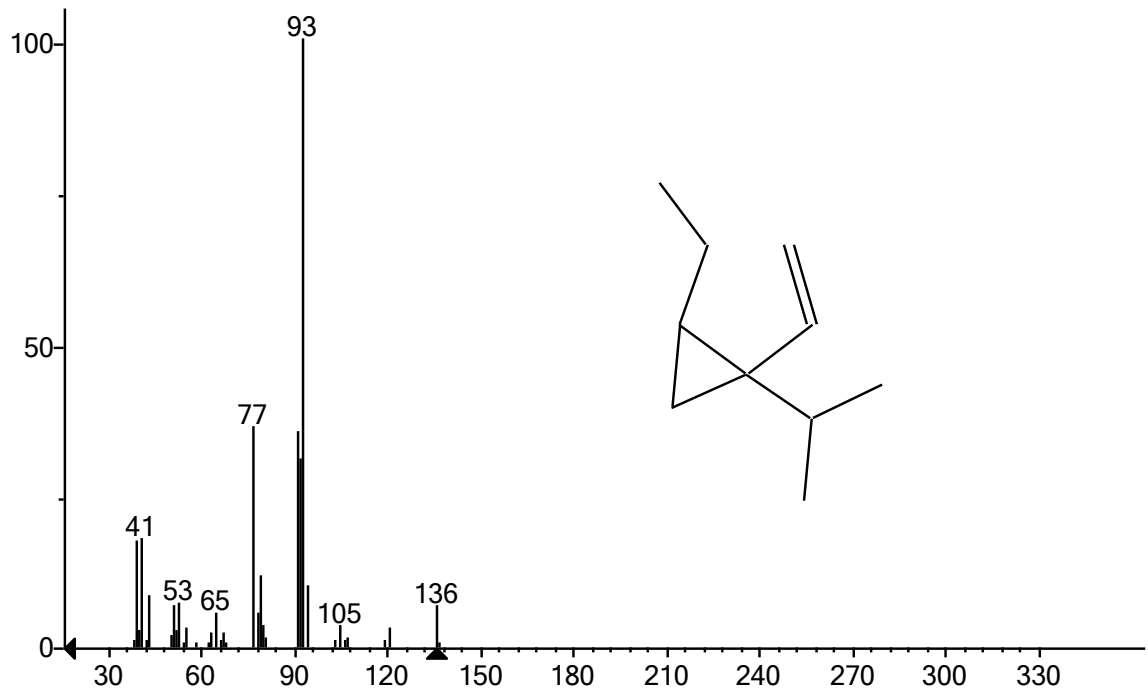
(Text File) Scan 78 (3.678 min): 0102020.D\data.ms



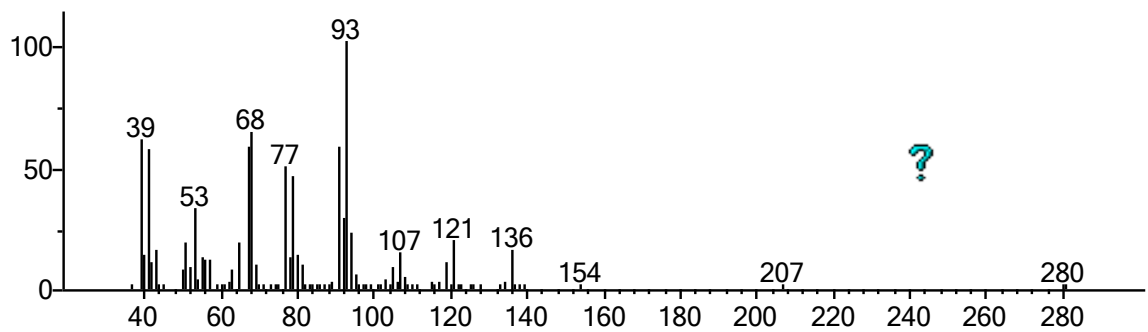
(replib) Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-



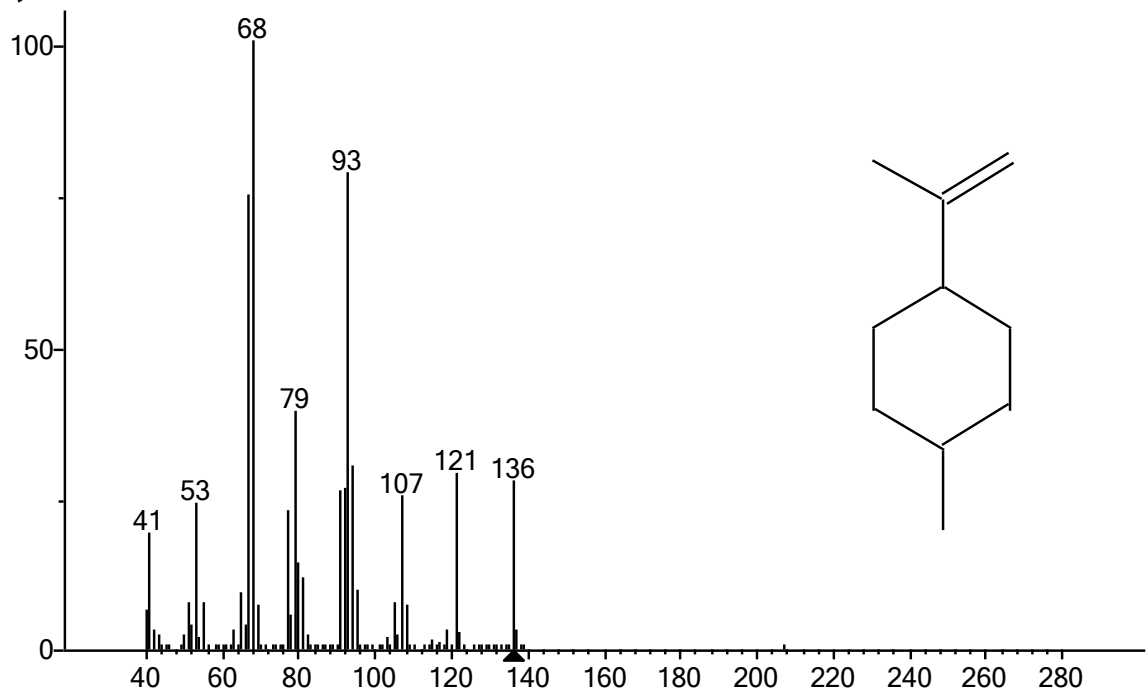
(Text File) Scan 146 (4.193 min): 0102020.D\data.ms



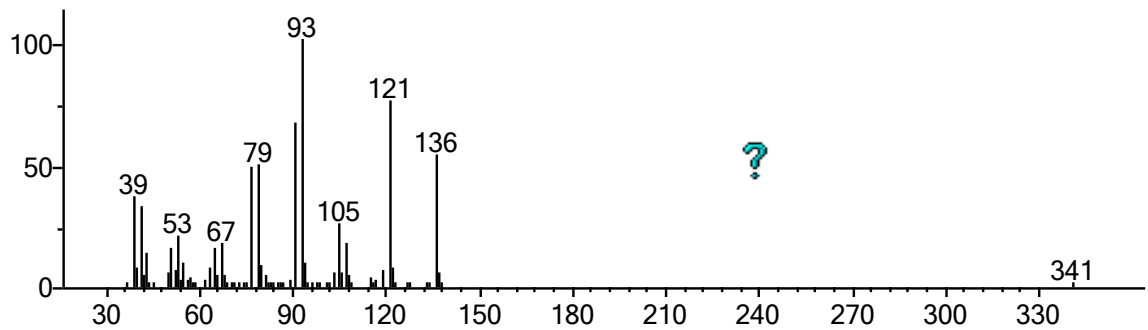
(mainlib) Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-



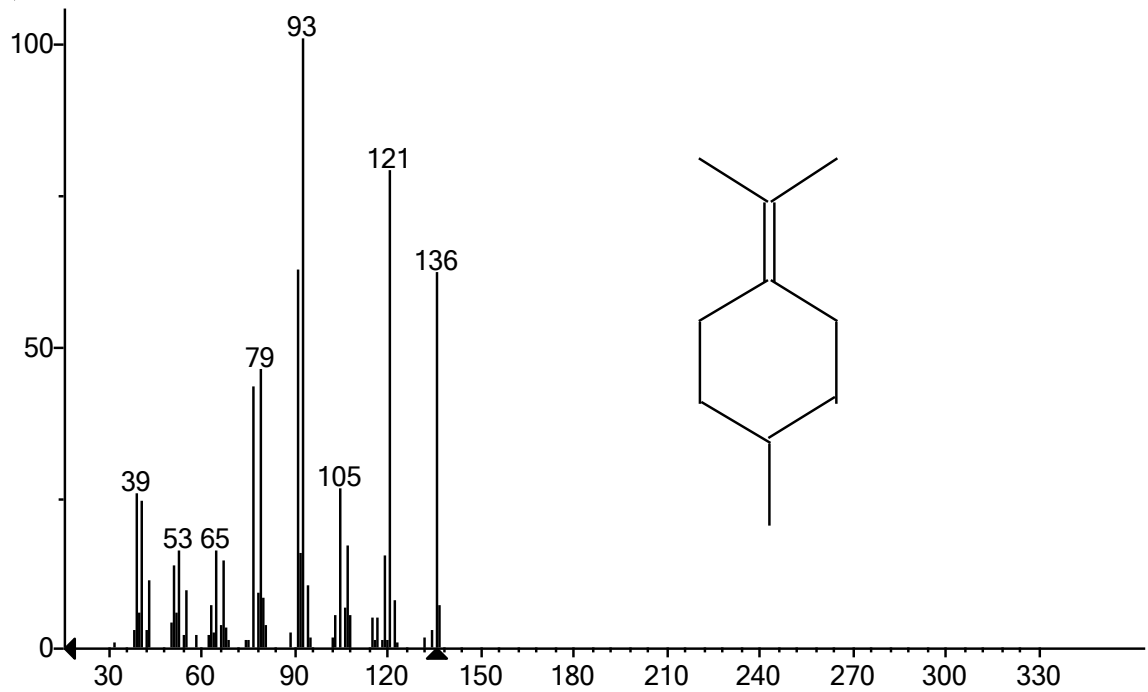
(Text File) Scan 188 (4.511 min): 0102020.D\data.ms



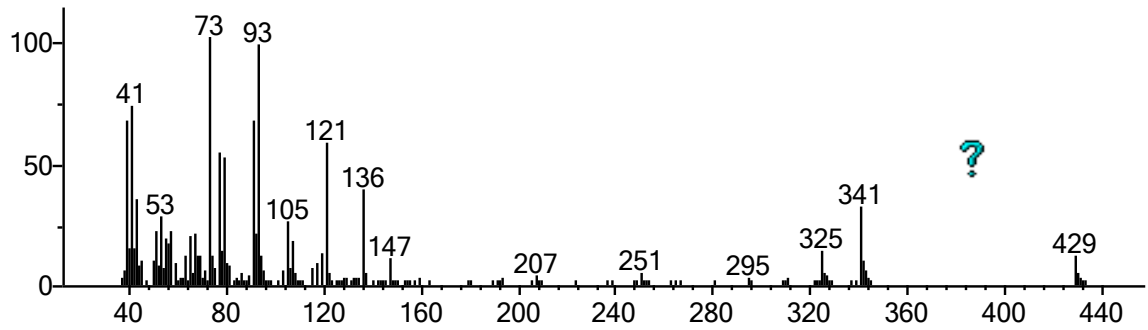
(replib) D-Limonene



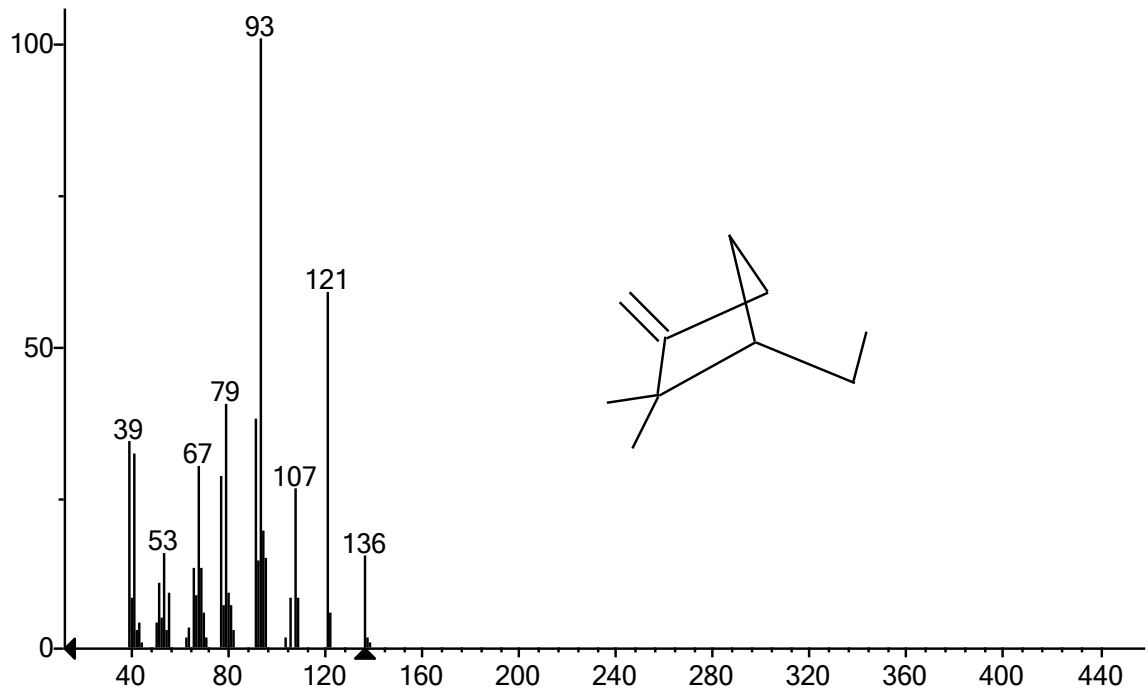
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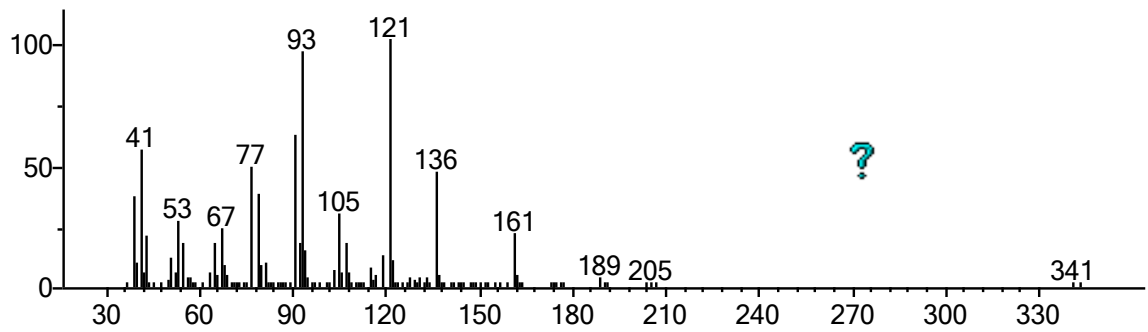
(mainlib) Cyclohexene, 1-methyl-4-(1-methylethylidene)-



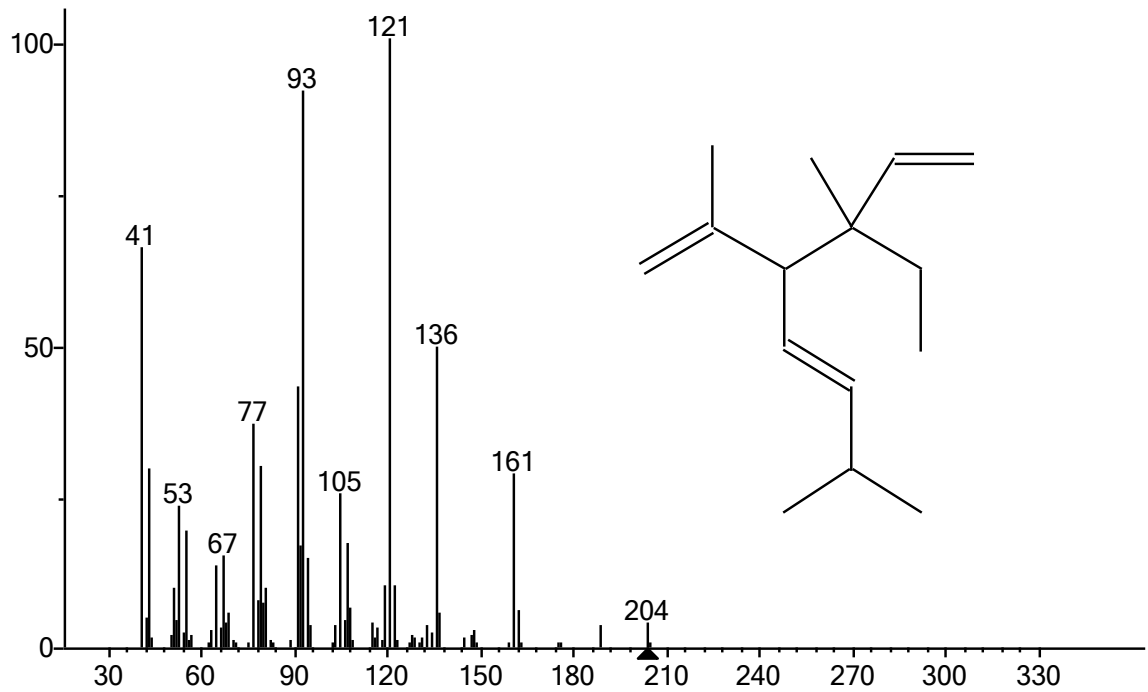
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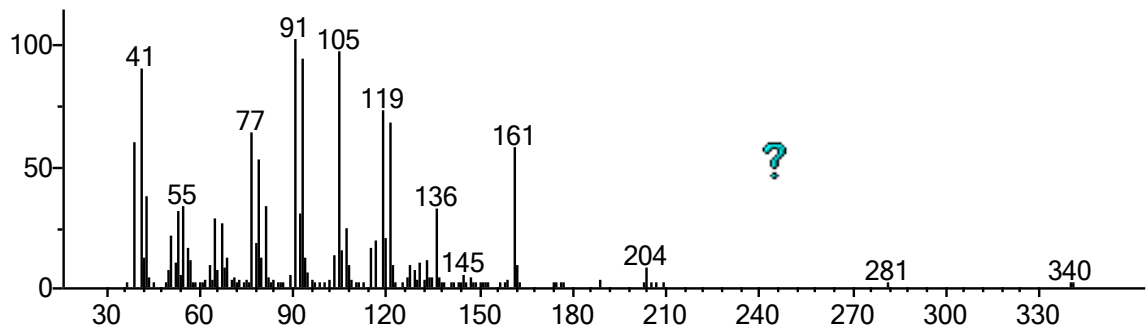
(mainlib) Camphene



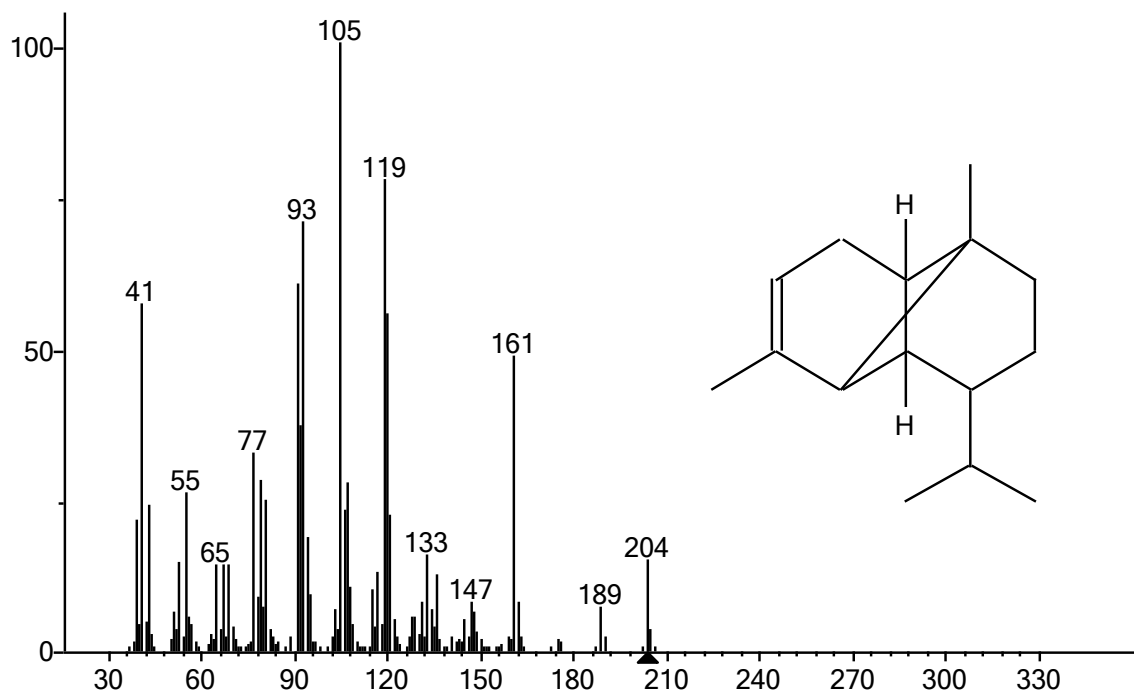
(Text File) Scan 705 (8.424 min): 0102020.D\data.ms



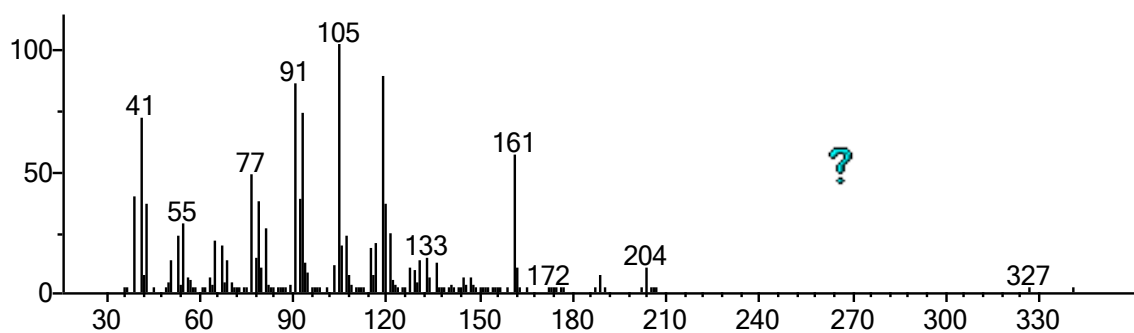
(replib) Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-, (3R-trans)-



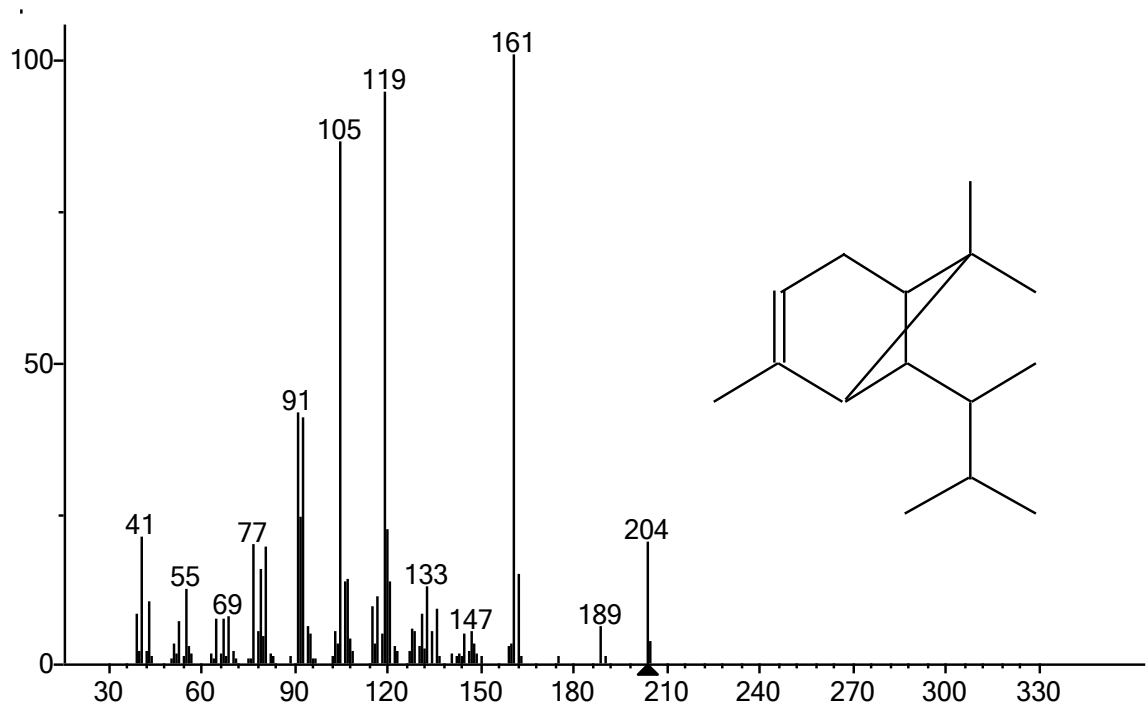
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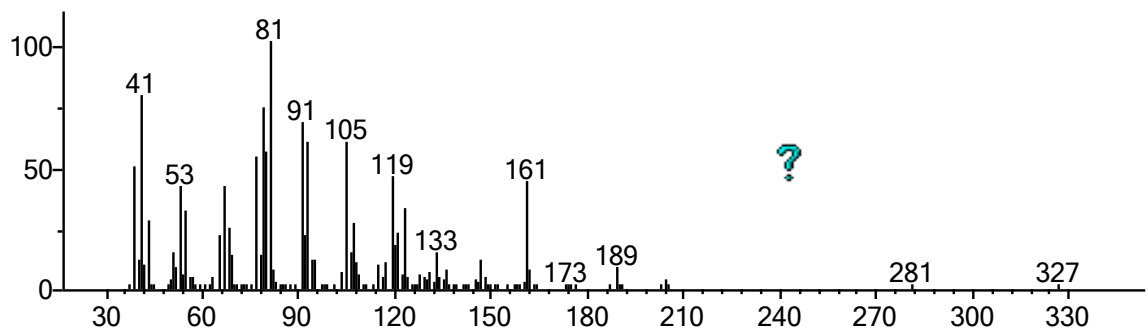
(mainlib) α-ylangene



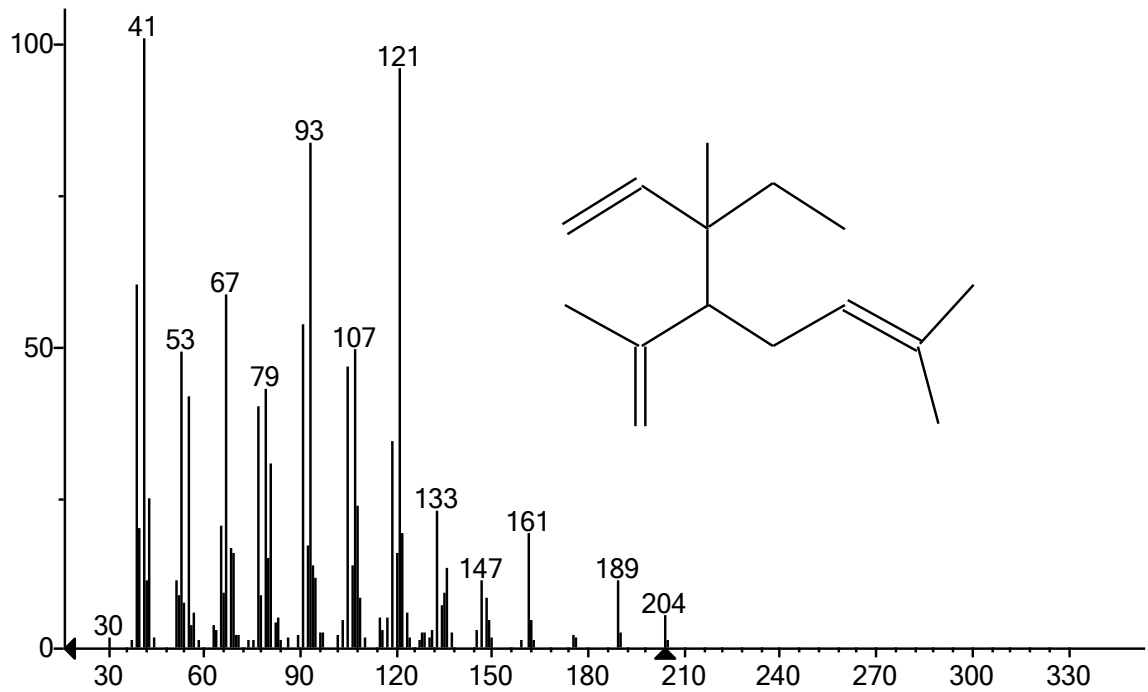
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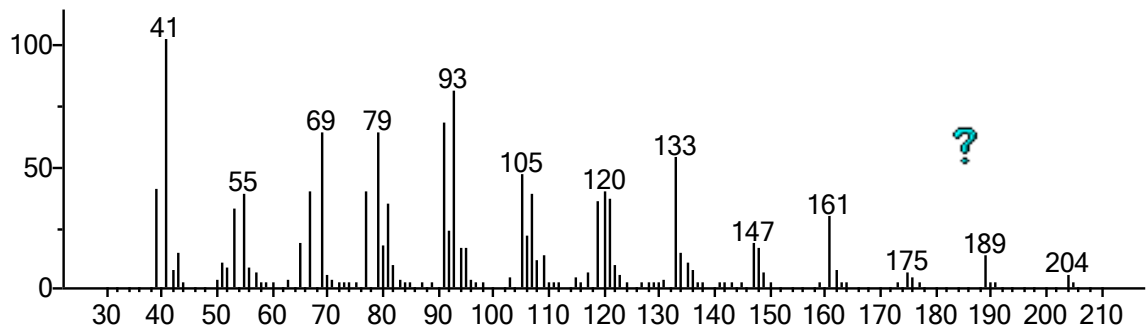
(mainlib) .alfa.-Copaene



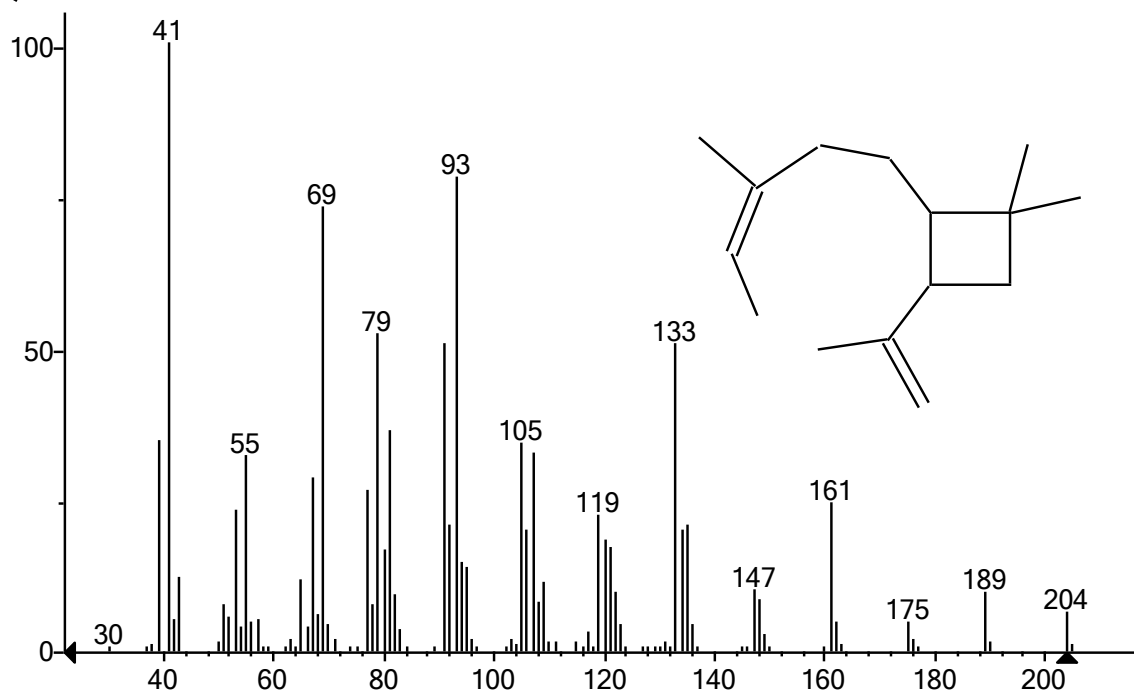
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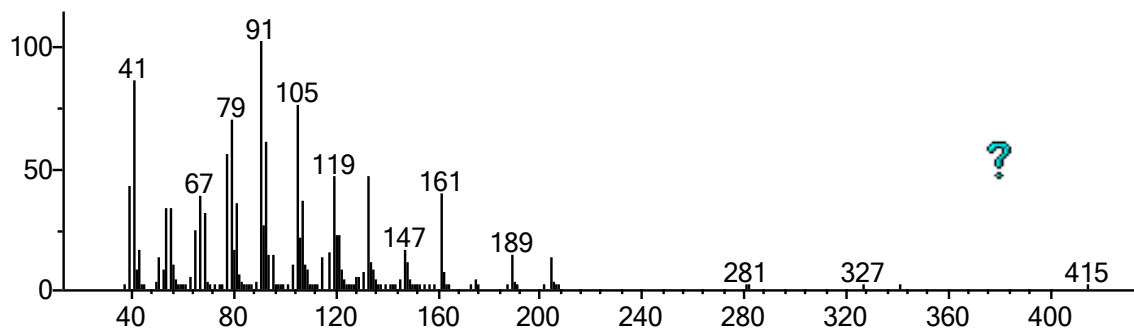
(replib) γ -Elemene



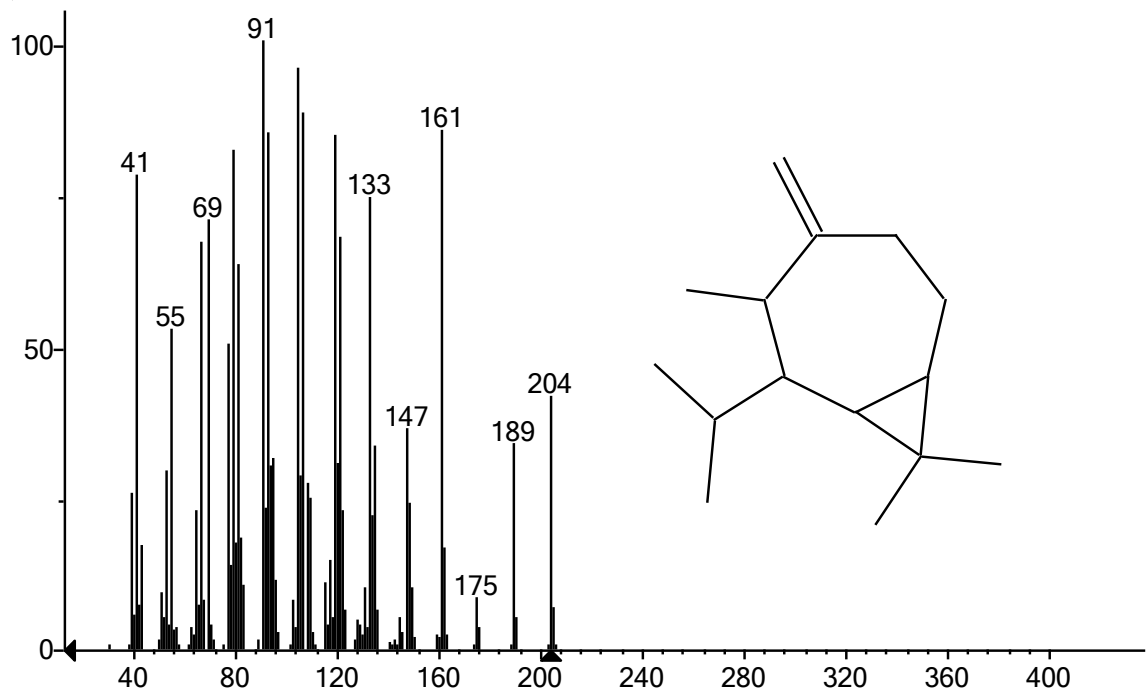
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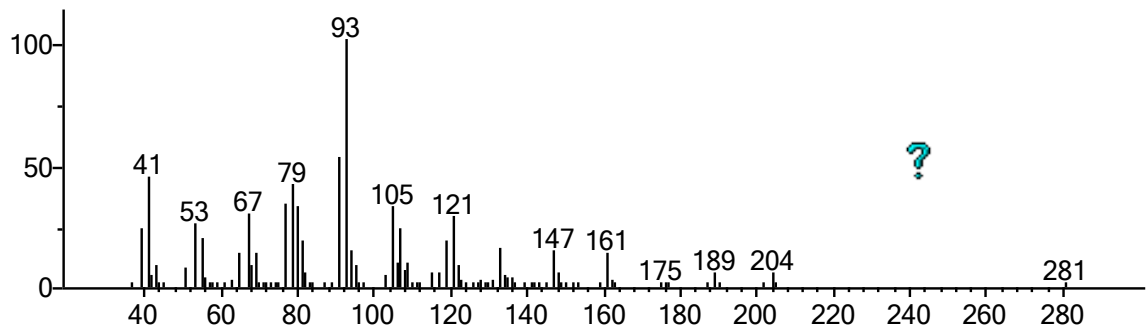
(mainlib) Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-



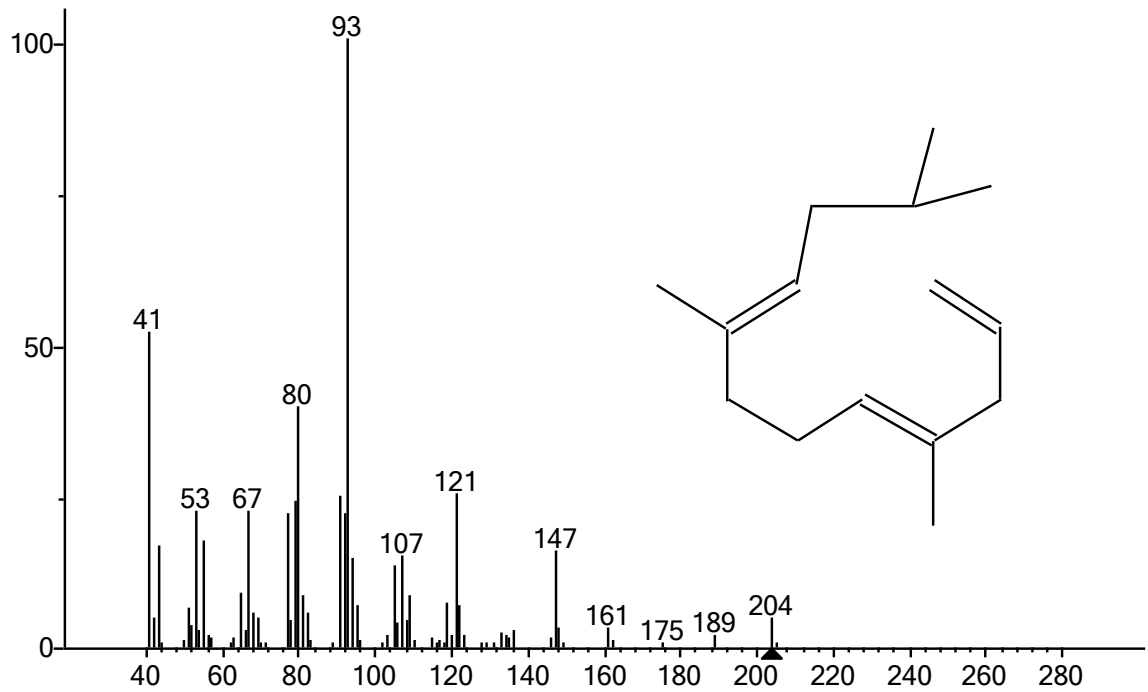
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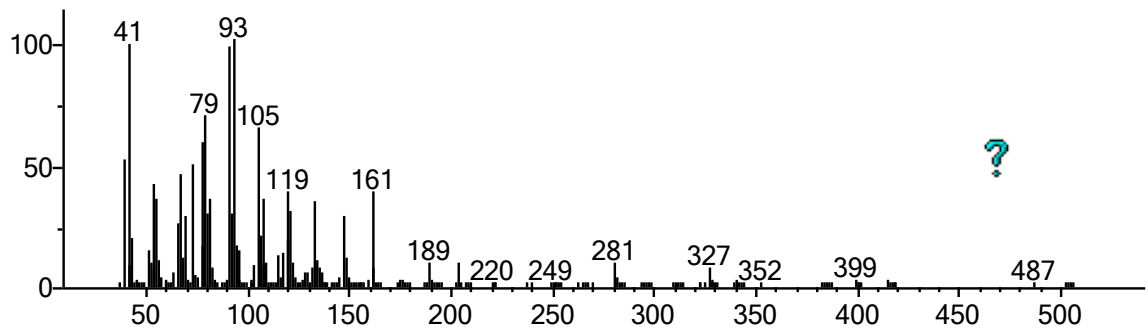
(replib) Aromandendrene



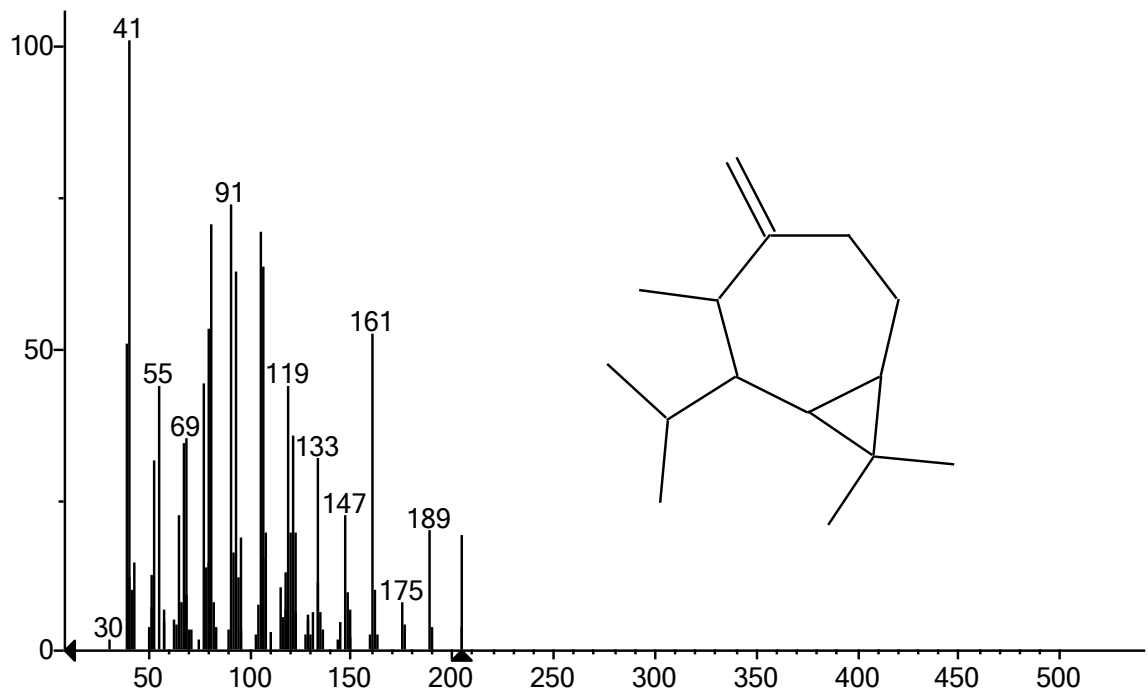
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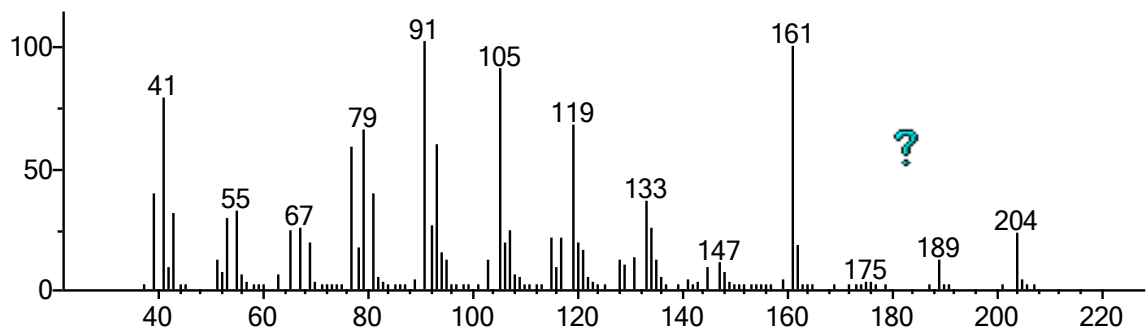
(replib) Humulene



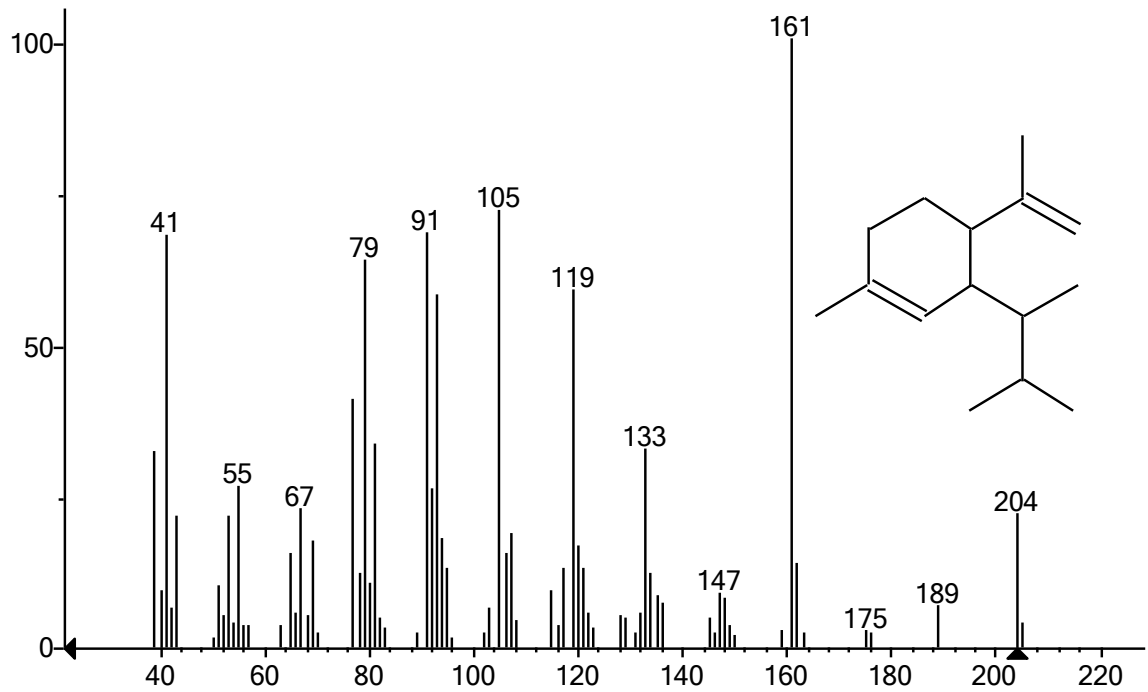
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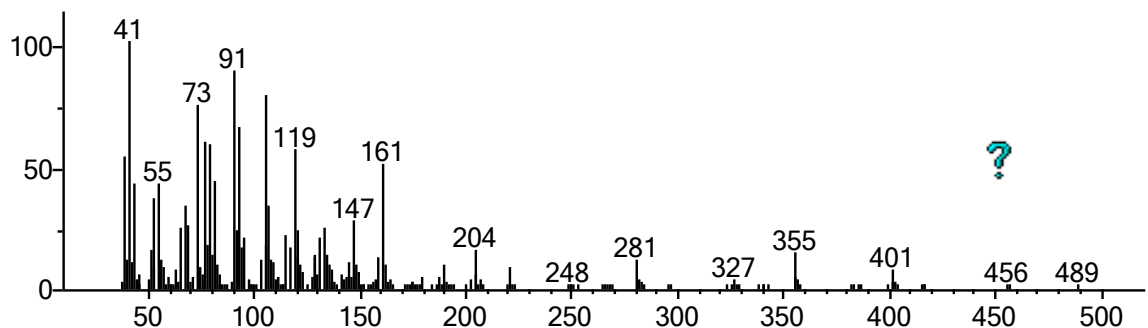
(replib) Alloaromadendrene



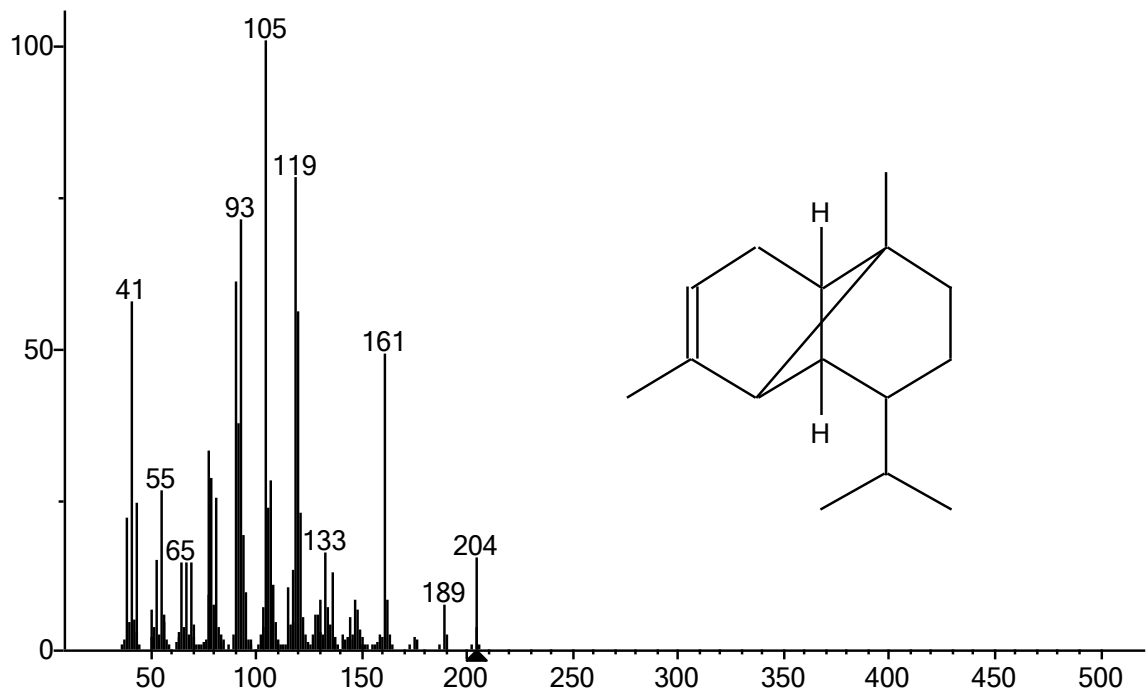
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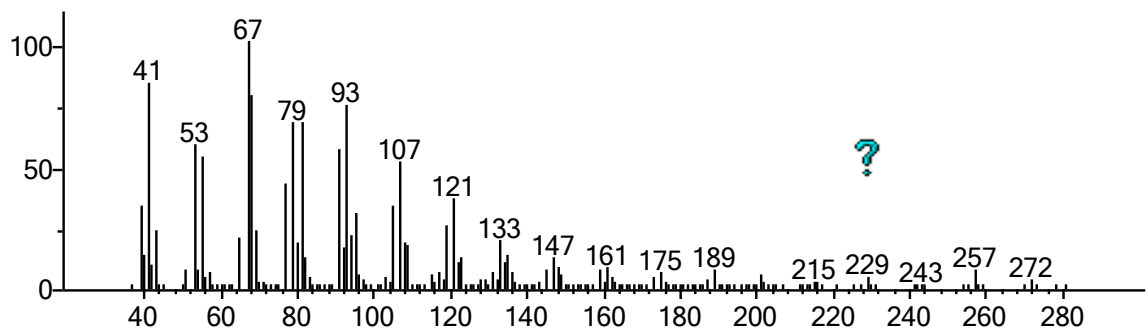
(replib) Naphthalene, 1,2,4a,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-



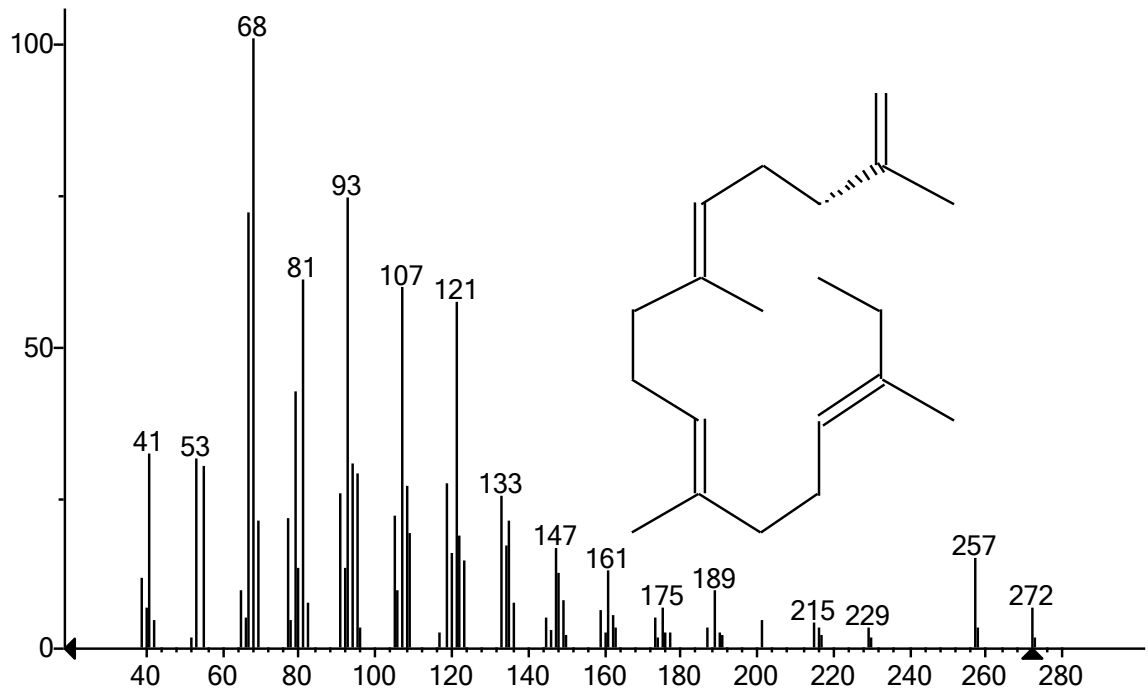
(Text File) Scan 1209 (12.238 min): 0102020.D\data.ms



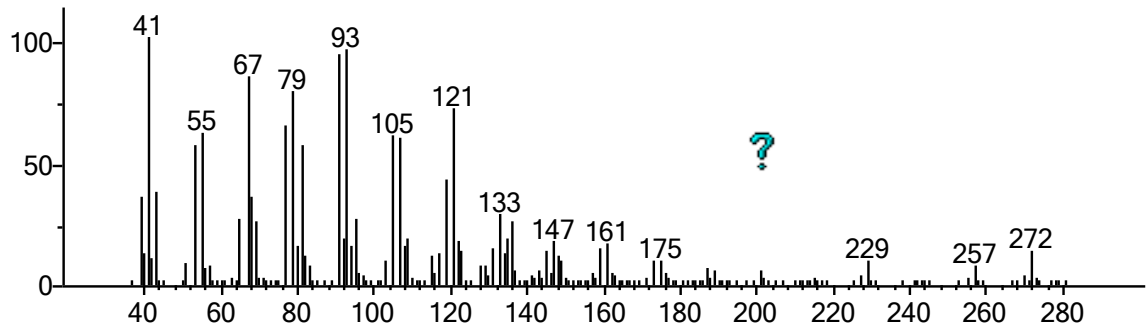
(mainlib) α -ylangene



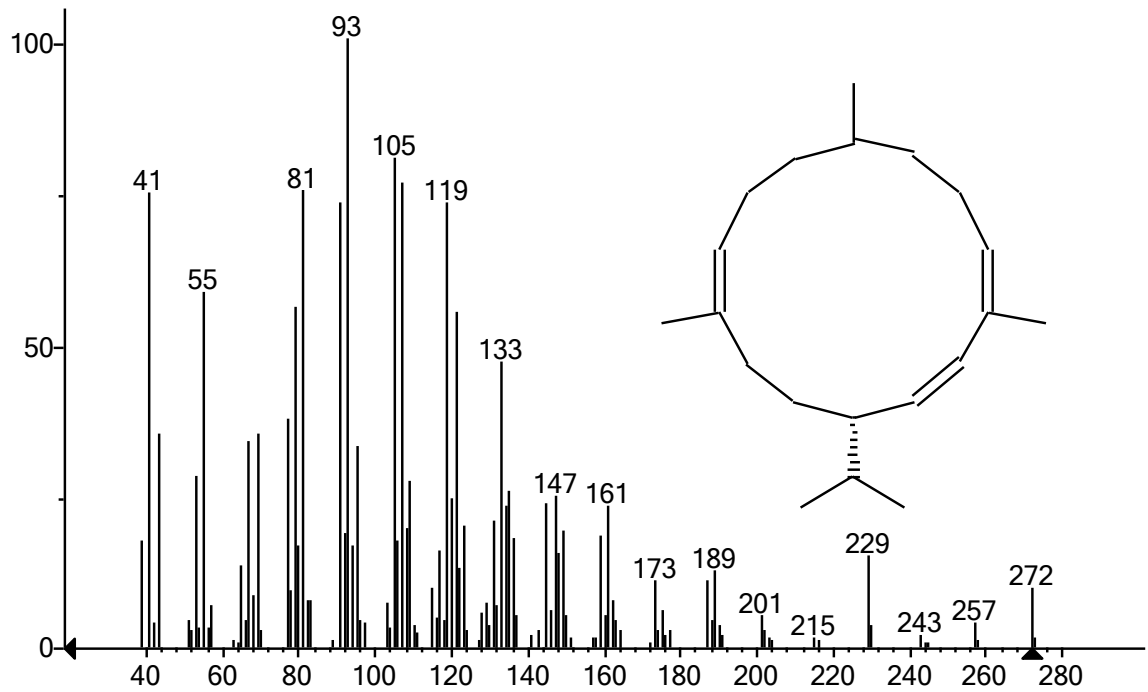
(Text File) Scan 1666 (15.697 min): 0102020.D\data.ms



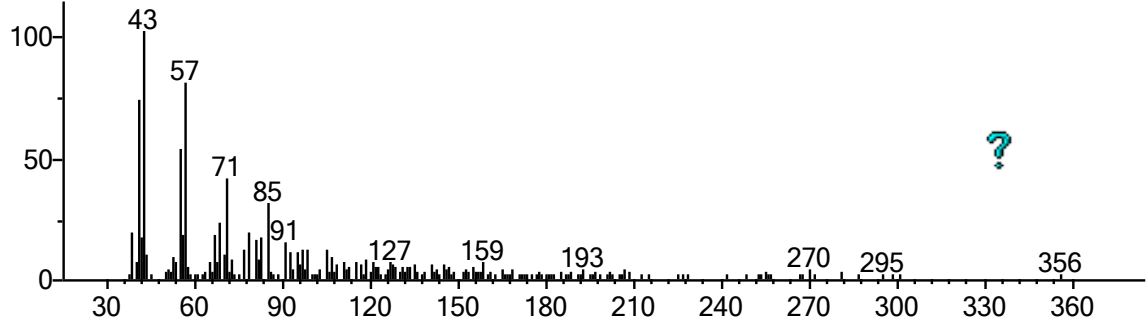
(mainlib) (R,1E,5E,9E)-1,5,9-Trimethyl-12-(prop-1-en-2-yl)cyclotetradeca-1,5,9-triene



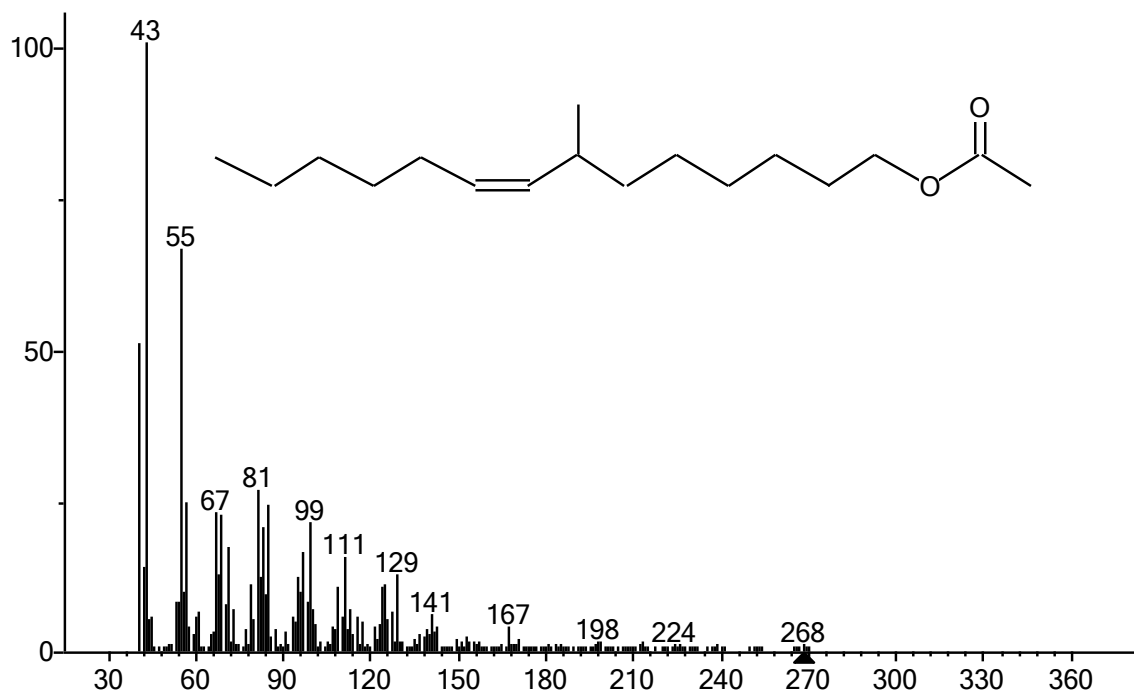
(Text File) Scan 1753 (16.356 min): 0102020.D\data.ms



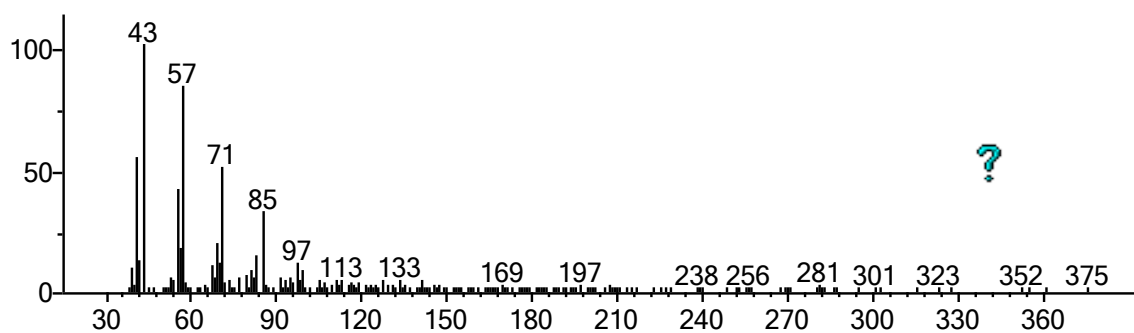
(replib) 1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E,Z,E,E)]-



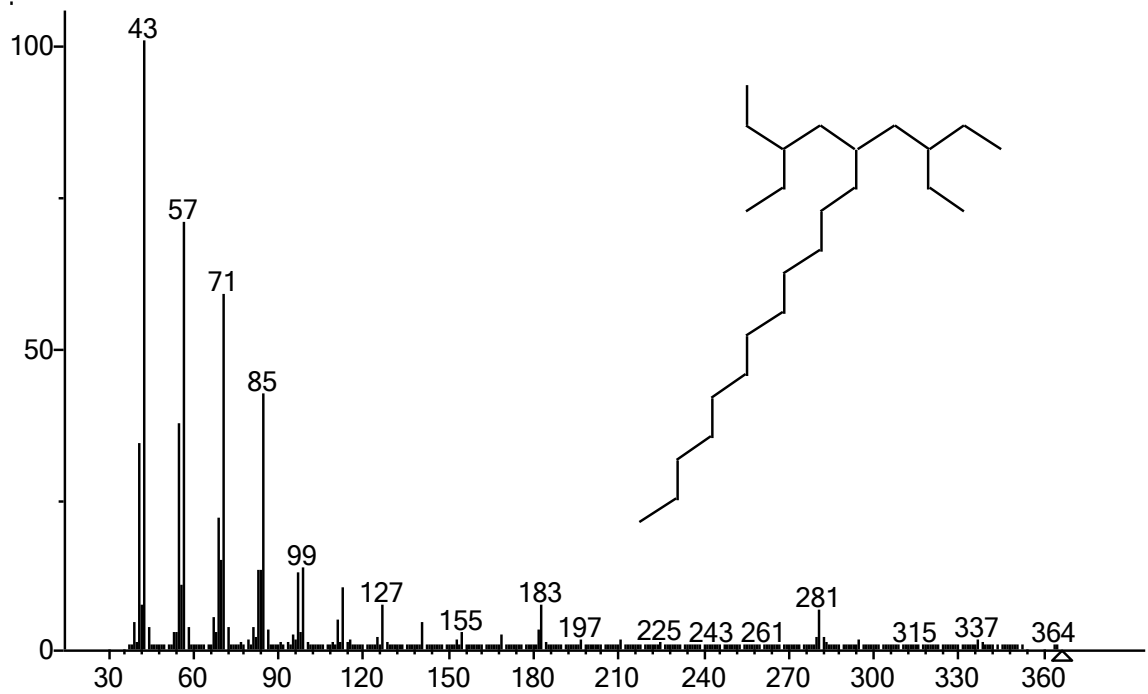
(Text File) Scan 2228 (19.951 min): 0102020.D\data.ms



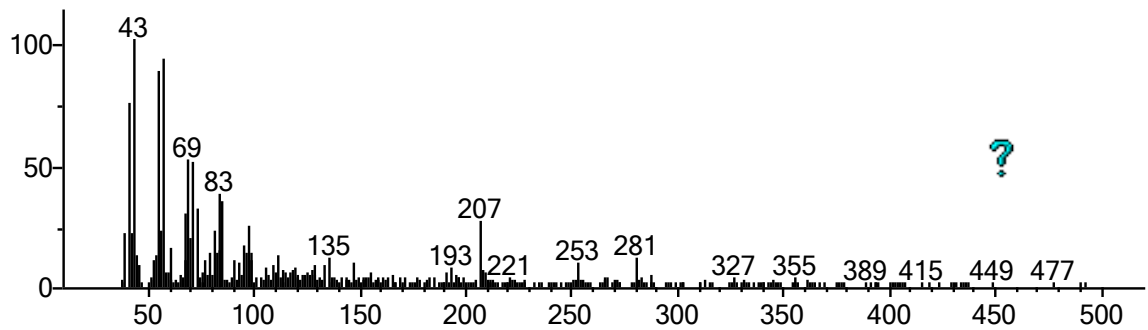
(mainlib) 7-Methyl-Z-tetradecen-1-ol acetate



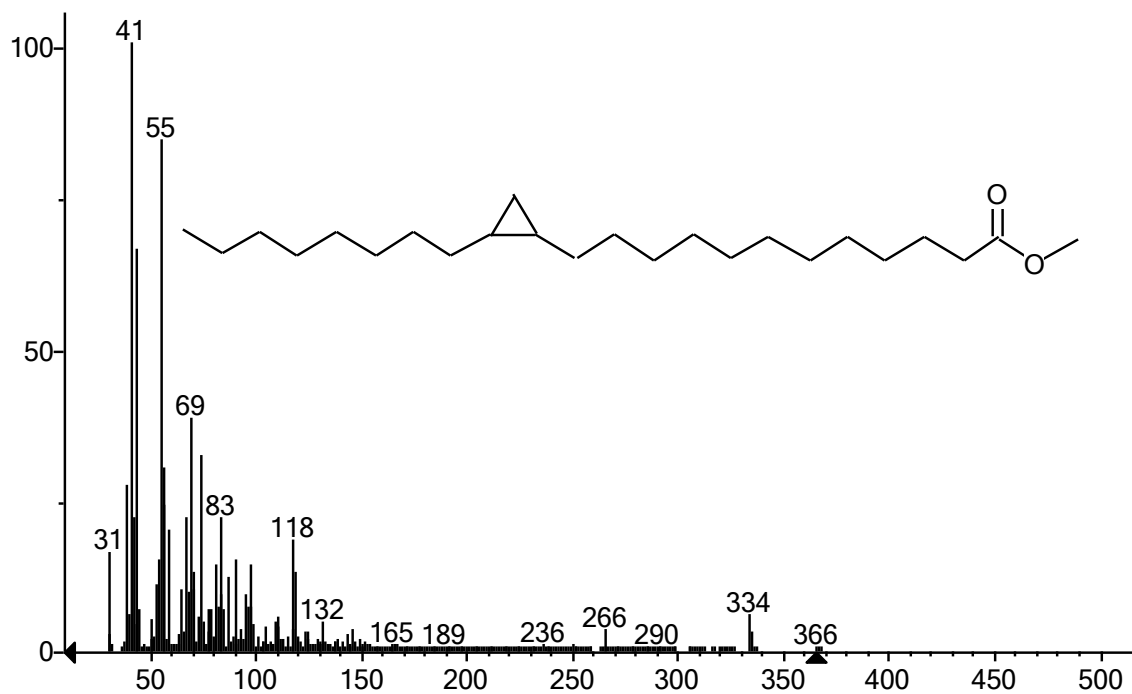
(Text File) Scan 2324 (20.677 min): 0102020.D\data.ms



(mainlib) Octadecane, 3-ethyl-5-(2-ethylbutyl)-



(Text File) Scan 3042 (26.112 min): 0102020.D\data.ms



(mainlib) Cyclopropanedodecanoic acid, 2-octyl-, methyl ester

INSTRUMENT CONTROL PARAMETERS: GC-MSD

C:\MSDCHEM\1\METHODS\Plant ext .M

Wed Sep 25 18:02:35 2019

Control Information

Sample Inlet : GC
Injection Source : GC ALS
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

Oven

Equilibration Time 8 min

Max Temperature	310 degrees C
Slow Fan	Disabled
Oven Program	On
60 °C for 0.5 min	
then 10 °C/min to 300 °C for 3 min	
Run Time	27.5 min

Front Injector

Syringe Size	10 µL
Injection Volume	0.2 µL
Injection Repetitions	1
Injection Delay	0 sec
Solvent A Washes (PreInj)	1
Solvent A Washes (PostInj)	2
Solvent A Volume	8 µL
Solvent B Washes (PreInj)	1
Solvent B Washes (PostInj)	1
Solvent B Volume	8 µL
Sample Washes	2
Sample Wash Volume	5 µL
Sample Pumps	1
Dwell Time (PreInj)	0 min
Dwell Time (PostInj)	0 min
Solvent Wash Draw Speed	300 µL/min
Solvent Wash Dispense Speed	6000 µL/min
Sample Wash Draw Speed	300 µL/min
Sample Wash Dispense Speed	6000 µL/min
Injection Dispense Speed	6000 µL/min
Viscosity Delay	7 sec
Sample Depth	Disabled

Sample Overlap

Sample overlap is not enabled

Front SS Inlet He

Mode	Split
Heater	On 270 °C
Pressure	On 10.983 psi
Total Flow	On 3.6407 mL/min
Septum Purge Flow	On 1 mL/min
Gas Saver	On 20 mL/min After 2 min
Split Ratio	1 :1
Split Flow	1.3203 mL/min

Thermal Aux 2 (MSD Transfer Line)

Heater	On
Temperature Program	On
300 °C for 0 min	
Run Time	27.5 min

Column #1

Agilent 19091S-433: 469.56509
HP-5MS 5% Phenyl Methyl Silox
325 °C: 30 m x 250 µm x 0.25 µm
In: Front SS Inlet He
Out: Vacuum

(Initial) 60 °C

Pressure	11.649 psi
Flow	1.3203 mL/min
Average Velocity	42.082 cm/sec
Holdup Time	1.1882 min
Flow Program	Off
1.3203 mL/min for 0 min	
Run Time	27.5 min

Signals

Signal #1: Test Plot	Save Off
	50 Hz
Signal #2: Test Plot	Save Off
	50 Hz
Signal #3: Test Plot	Save Off
	50 Hz
Signal #4: Test Plot	Save Off
	50 Hz

MS ACQUISITION PARAMETERS

General Information

Tune File	: atune.u
Acquisition Mode	: Scan/SIM

MS Information

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Solvent Delay : 3.00 min

EMV Mode : Gain Factor

Gain Factor : 2.00

Resulting EM Voltage : 2459

[Scan Parameters]

Low Mass : 35.0

High Mass : 550.0

Threshold : 150

Sample # : 2 A/D Samples 4

Plot 1 low mass : 50.0

Plot 1 high mass : 550.0

[Sim Parameters]

GROUP 1

Group ID : 1

Resolution : Low

Plot 1 Ion : 74.10

Ions/Dwell In Group (Mass, Dwell)
(74.10, 100)

[MSZones]

MS Source : 250 C maximum 280 C

MS Quad : 150 C maximum 200 C

END OF MS ACQUISITION PARAMETERS

TUNE PARAMETERS for SN: us73226898

Trace Ion Detection is OFF.

EMISSION : 34.610
ENERGY : 69.922
REPELLER : 34.814
IONFOCUS : 90.157
ENTRANCE_LE : 0.000
EMVOLTS : 2988.235

Actual EMV : 2458.82

GAIN FACTOR : 2.02

AMUGAIN : 2066.000
AMUOFFSET : 118.750
FILAMENT : 1.000
DCPOLARITY : 0.000
ENTLENSOFFS : 16.063
MASSGAIN : -504.000
MASSOFFSET : -40.000

END OF TUNE PARAMETERS

END OF INSTRUMENT CONTROL

PARAMETERS
