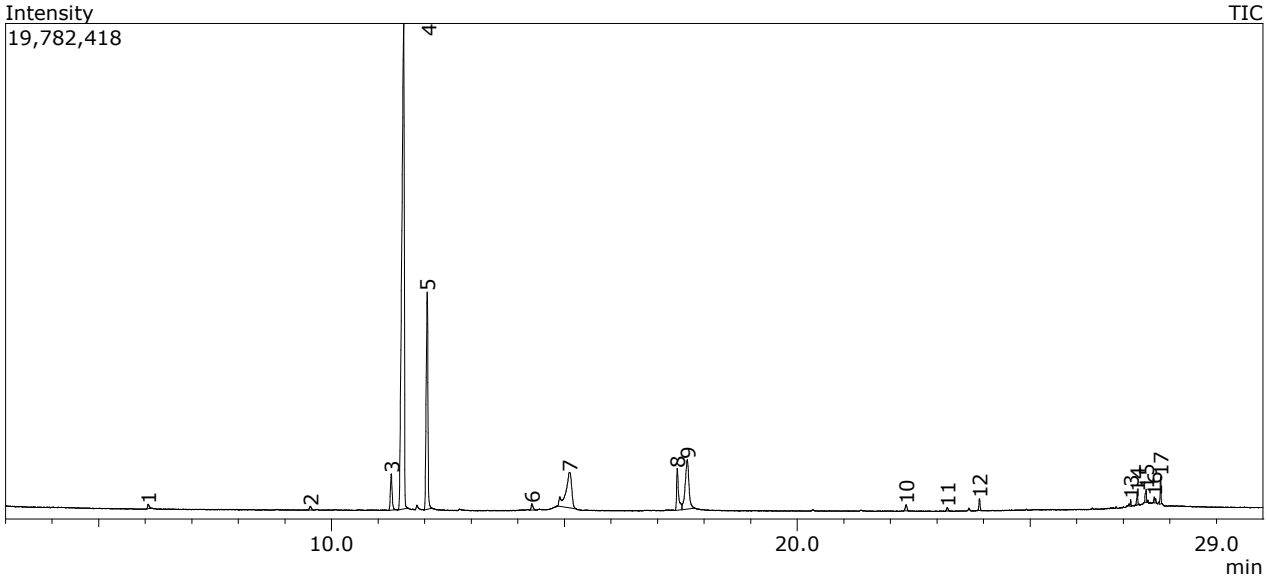
CSIR-INDIAN INSTITUTE OF INTEGRATIVE MEDICINE
Quality Management and Instrumentation Division
GCMS ANALYSIS REPORT

Sample Information

Analyzed by : Dr. Nagaraju Nekkala
Analyzed : 05-05-2026 16:00:44
Sample Name : TM
Sample ID : TM
Vial # : 25
Injection Volume : 1.00
Data File : D:\GCMS-2026\Dr. Suphla Gupta\DATA\MAY-2026\05.05.2026-18.qgd
Batch File : D:\GCMS-2026\BATCH\MAY-2026\05.05.2026-01.qgb
Method File : D:\GCMS-2026\Dr. Suphla Gupta\METHODS\GCMS_LIQ_1_5ms_EO_07.qgm
Tuning File : D:\GCMS-2026\Tuning\F1-15-04-2026.qgt
Modified : 05-05-2026 16:47:59



Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Name
1	6.064	445848	0.33	97	Butanoic acid, 2-methyl-, ethyl ester
2	9.546	410116	0.31	89	Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-
3	11.283	3811863	2.84	94	Limonene
4	11.549	72538847	53.96	95	trans-.beta.-Ocimene
5	12.055	22633912	16.84	93	7-Octen-4-one, 2,6-dimethyl-
6	14.302	679746	0.51	94	1,4-Hexadiene, 5-methyl-3-(1-methylethylidene)-
7	15.113	12557551	9.34	93	5,7-Octadien-4-one, 2,6-dimethyl-, (Z)-
8	17.425	5043772	3.75	90	(Z)-2,6-Dimethylocta-2,5,7-trien-4-one
9	17.640	10903853	8.11	90	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-
10	22.337	631224	0.47	94	Caryophyllene
11	23.223	313911	0.23	92	Humulene
12	23.912	829301	0.62	92	.gamma.-Elemene
13	27.158	292321	0.22	79	(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)h
14	27.300	715223	0.53	90	(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)h
15	27.490	893818	0.66	91	(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)h
16	27.665	347094	0.26	68	(Z)-.alpha.-Atlantone
17	27.801	1385517	1.03	85	1,5-Heptadien-4-one, 3,3,6-trimethyl-
		134433917	100.00		

Qualitative Analysis Report

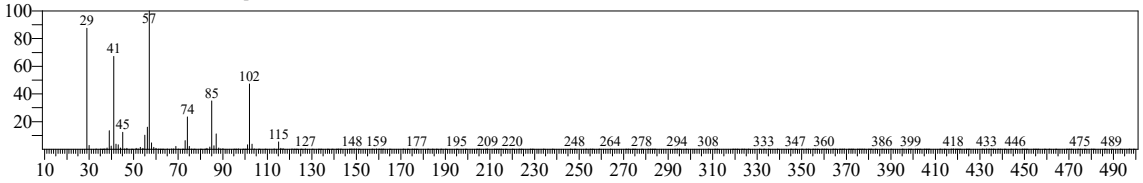
Library

<< Target >>

Line#:1 R.Time:6.065(Scan#:614) MassPeaks:229

RawMode:Averaged 6.060-6.070(613-615) BasePeak:57.05(37913)

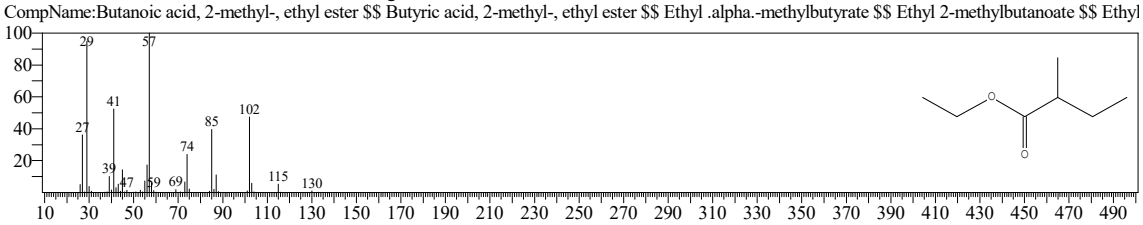
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:6633 Library:NIST17R.lib

SI:97 Formula:C7H14O2 CAS:7452-79-1 MolWeight:130 RetIndex:820

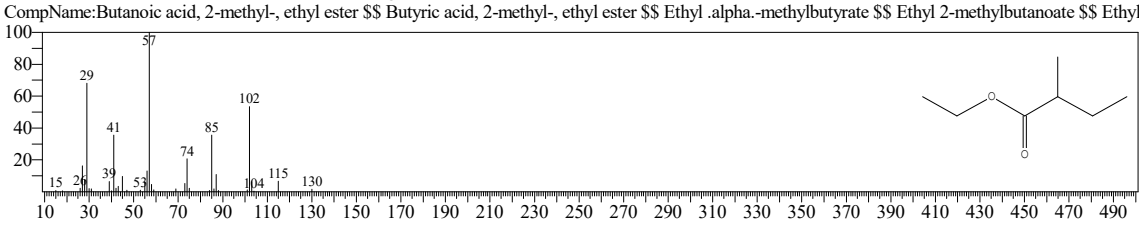
CompName:Butanoic acid, 2-methyl-, ethyl ester $$ Butyric acid, 2-methyl-, ethyl ester $$ Ethyl .alpha.-methylbutyrate $$ Ethyl 2-methylbutanoate $$ Ethyl



Hit#:2 Entry:8386 Library:NIST17M1.lib

SI:94 Formula:C7H14O2 CAS:7452-79-1 MolWeight:130 RetIndex:820

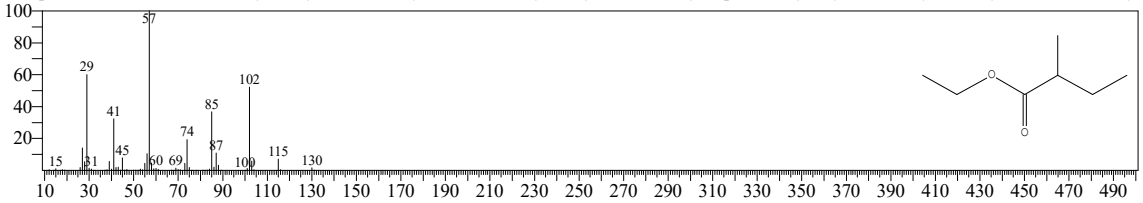
CompName:Butanoic acid, 2-methyl-, ethyl ester $$ Butyric acid, 2-methyl-, ethyl ester $$ Ethyl .alpha.-methylbutyrate $$ Ethyl 2-methylbutanoate $$ Ethyl



Hit#:3 Entry:6641 Library:NIST17R.lib

SI:92 Formula:C7H14O2 CAS:7452-79-1 MolWeight:130 RetIndex:820

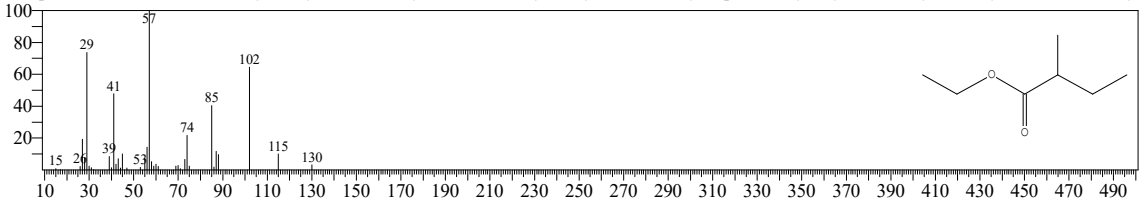
CompName:Butanoic acid, 2-methyl-, ethyl ester $$ Butyric acid, 2-methyl-, ethyl ester $$ Ethyl .alpha.-methylbutyrate $$ Ethyl 2-methylbutanoate $$ Ethyl



Hit#:4 Entry:6640 Library:NIST17R.lib

SI:92 Formula:C7H14O2 CAS:7452-79-1 MolWeight:130 RetIndex:820

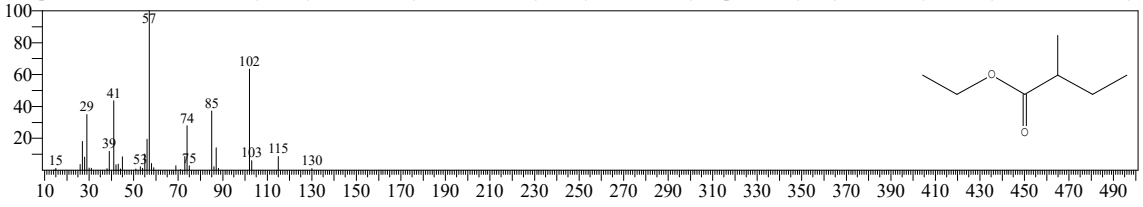
CompName:Butanoic acid, 2-methyl-, ethyl ester $$ Butyric acid, 2-methyl-, ethyl ester $$ Ethyl .alpha.-methylbutyrate $$ Ethyl 2-methylbutanoate $$ Ethyl



Hit#:5 Entry:6650 Library:NIST17R.lib

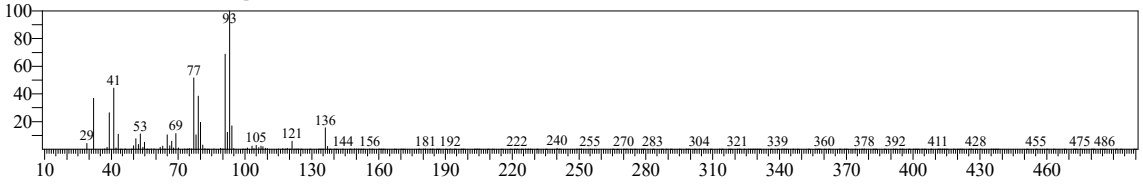
SI:91 Formula:C7H14O2 CAS:7452-79-1 MolWeight:130 RetIndex:820

CompName:Butanoic acid, 2-methyl-, ethyl ester $$ Butyric acid, 2-methyl-, ethyl ester $$ Ethyl .alpha.-methylbutyrate $$ Ethyl 2-methylbutanoate $$ Ethyl

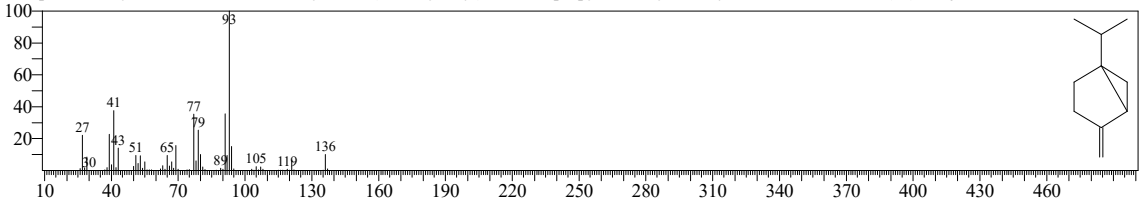


Qualitative Analysis Report

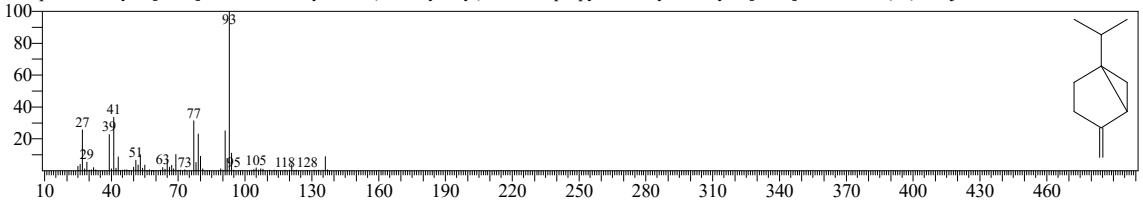
<< Target >>
Line#:2 R.Time:9.545(Scan#:1310) MassPeaks:225
RawMode:Averaged 9.540-9.550(1309-1311) BasePeak:93.05(26593)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



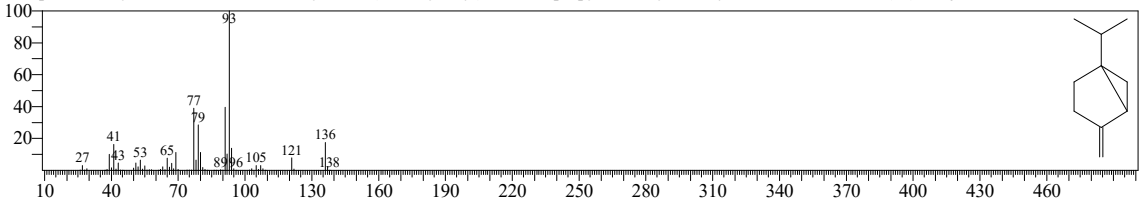
Hit#:1 Entry:7930 Library:NIST17R.lib
SI:89 Formula:C10H16 CAS:3387-41-5 MolWeight:136 RetIndex:897
CompName:Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- $$ 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane $$ 4(10)-Thujene $$ Sabinen $$ Sabine



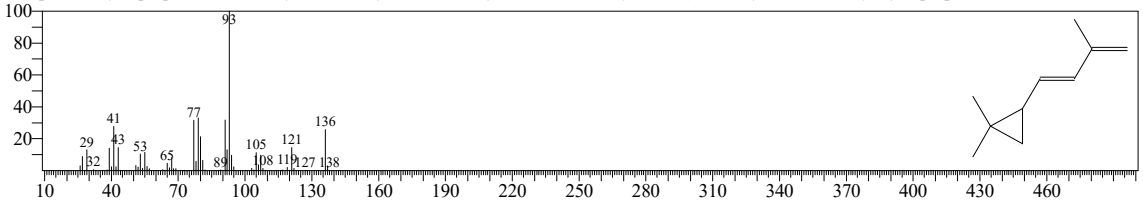
Hit#:2 Entry:7925 Library:NIST17R.lib
SI:88 Formula:C10H16 CAS:3387-41-5 MolWeight:136 RetIndex:897
CompName:Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- $$ 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane $$ 4(10)-Thujene $$ Sabinen $$ Sabine



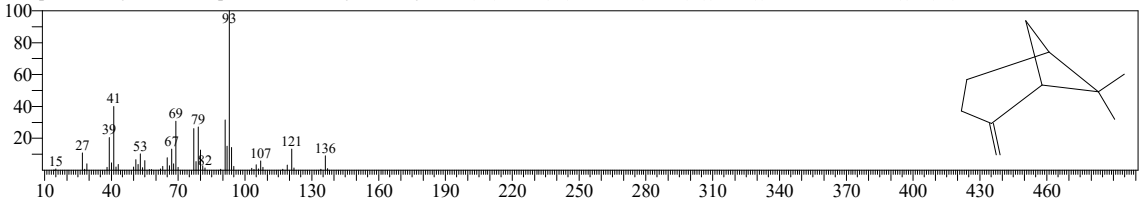
Hit#:3 Entry:10383 Library:NIST17M1.lib
SI:87 Formula:C10H16 CAS:3387-41-5 MolWeight:136 RetIndex:897
CompName:Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)- $$ 1-Isopropyl-4-methylenebicyclo[3.1.0]hexane $$ 4(10)-Thujene $$ Sabinen $$ Sabine



Hit#:4 Entry:10374 Library:NIST17M1.lib
SI:87 Formula:C10H16 CAS:68998-21-0 MolWeight:136 RetIndex:928
CompName:Cyclopropane, 1,1-dimethyl-2-(3-methyl-1,3-butadienyl)- $$ 1,1-Dimethyl-2-[(1E)-3-methyl-1,3-butadienyl]cyclopropane #

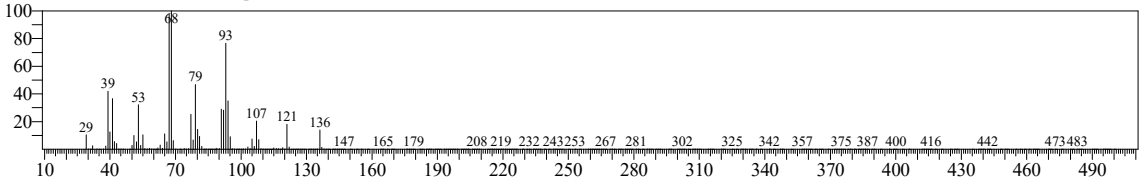


Hit#:5 Entry:7929 Library:NIST17R.lib
SI:87 Formula:C10H16 CAS:18172-67-3 MolWeight:136 RetIndex:943
CompName:Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)- $$ 2(10)-Pinene, (1S,5S)-(-)- $$ (-)-.beta.-Pinene $$ (-)-2(10)-Pinene $$ L-.beta.-Piner

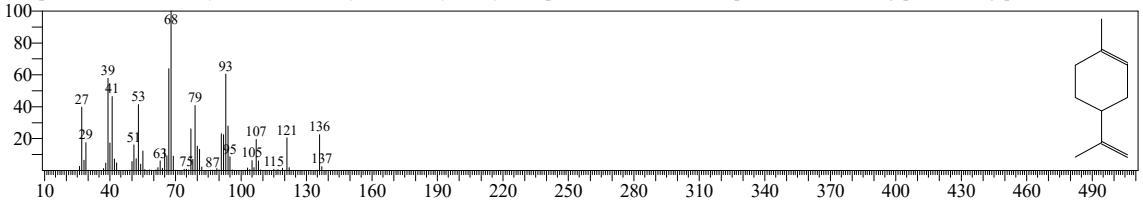


Qualitative Analysis Report

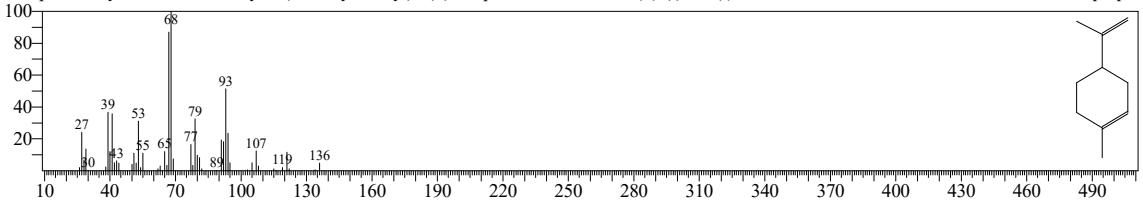
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Line#:3 R.Time:11.285(Scan#:1658) MassPeaks:308
RawMode:Averaged 11.280-11.290(1657-1659) BasePeak:68.05(184840)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



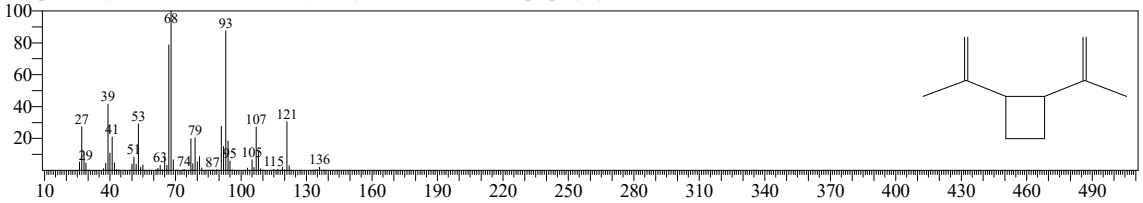
Hit#:1 Entry:7897 Library:NIST17R.lib
SI:94 Formula:C10H16 CAS:138-86-3 MolWeight:136 RetIndex:1018
CompName:Limonene $$ Cyclohexene, 1-methyl-4-(1-methylethenyl)- $$ p-Mentha-1,8-diene $$ .alpha.-Limonene $$ Cajeputen $$ Cajeputene $$ Cinen $



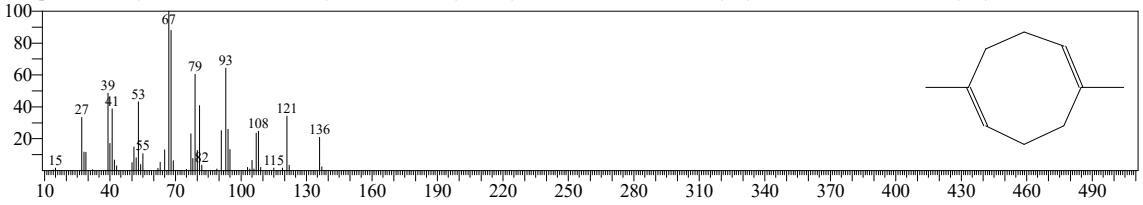
Hit#:2 Entry:7898 Library:NIST17R.lib
SI:93 Formula:C10H16 CAS:5989-54-8 MolWeight:136 RetIndex:1018
CompName:Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (S)- $$ p-Mentha-1,8-diene, (S)-(-)- $$ (-)-Limonene $$ L-Limonene $$ Limonene $$ 4-Isoproper



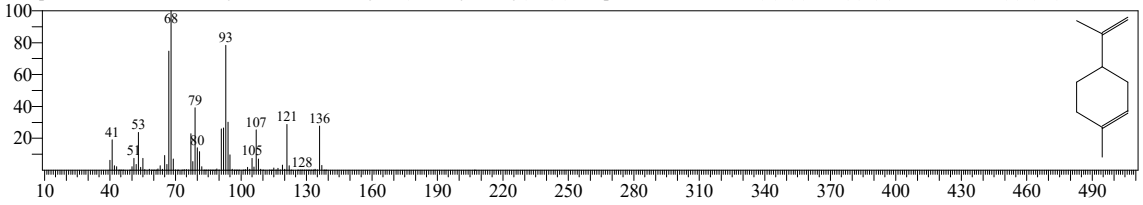
Hit#:3 Entry:10324 Library:NIST17M1.lib
SI:92 Formula:C10H16 CAS:19465-02-2 MolWeight:136 RetIndex:934
CompName:Cyclobutane, 1,2-bis(1-methylethenyl)-, trans- $$ 1,2-Diisopropenylcyclobutane #



Hit#:4 Entry:10306 Library:NIST17M1.lib
SI:91 Formula:C10H16 CAS:3760-14-3 MolWeight:136 RetIndex:1103
CompName:1,5-Cyclooctadiene, 1,5-dimethyl- $$ 1,5-Dimethyl-1,5-cyclooctadiene $$ 1,5-Dimethyl cyclooctadiene $$ 1,5-Dimethyl-cycloocta-1,5-diene

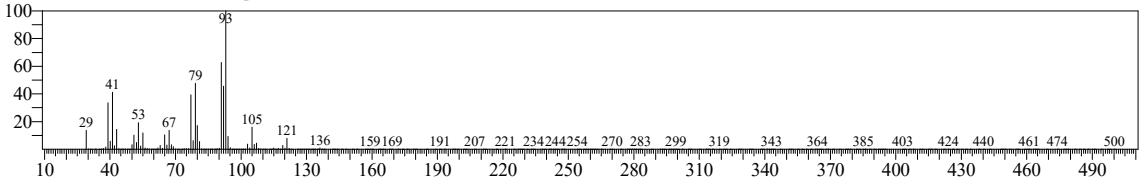


Hit#:5 Entry:7903 Library:NIST17R.lib
SI:91 Formula:C10H16 CAS:5989-27-5 MolWeight:136 RetIndex:1018
CompName:D-Limonene $$ Cyclohexene, 1-methyl-4-(1-methylethenyl)-, (R)- $$ p-Mentha-1,8-diene, (R)-(+)- $$ (+)-(R)-Limonene $$ (+)-(4R)-Limonene

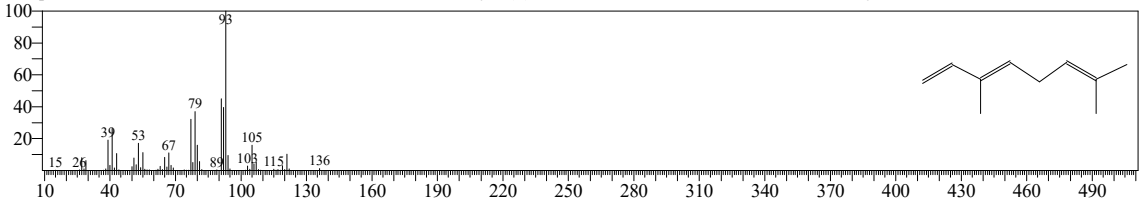


Qualitative Analysis Report

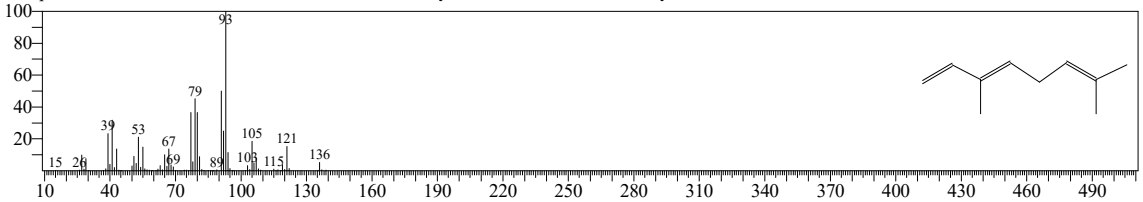
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Line#:4 R.Time:11.550(Scan#:1711) MassPeaks:279
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BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



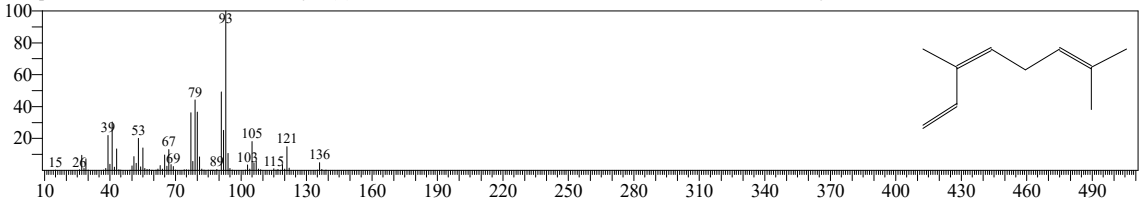
Hit#:1 Entry:7958 Library:NIST17R.lib
SI:95 Formula:C10H16 CAS:3779-61-1 MolWeight:136 RetIndex:976
CompName:trans-.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl-, (E)- $$ .beta.-trans-Ocimene $$ trans-3,7-Dimethyl-1,3,6-Octatriene $$ Ocimene, trans



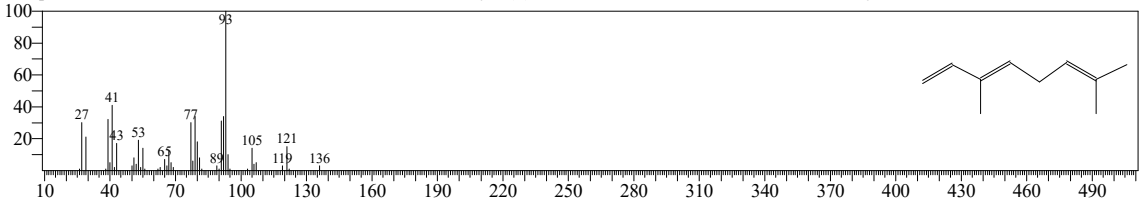
Hit#:2 Entry:10386 Library:NIST17M1.lib
SI:94 Formula:C10H16 CAS:13877-91-3 MolWeight:136 RetIndex:976
CompName:.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl- $$ Ocimene $$ 3,7-Dimethyl-1,3,6-octatriene $$ beta-Ocimene



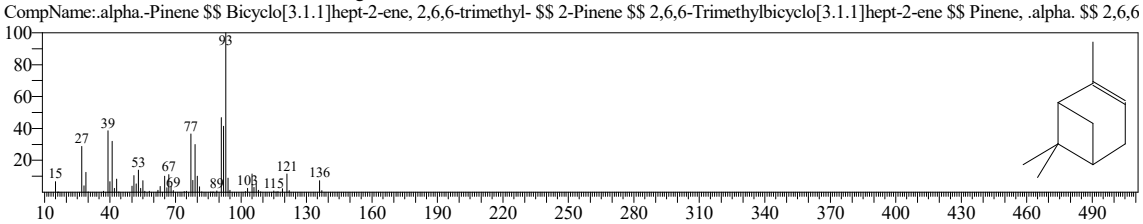
Hit#:3 Entry:7956 Library:NIST17R.lib
SI:94 Formula:C10H16 CAS:3338-55-4 MolWeight:136 RetIndex:976
CompName:1,3,6-Octatriene, 3,7-dimethyl-, (Z)- $$ .beta.-cis-Ocimene $$ cis-.beta.-Ocimene $$ cis-3,7-Dimethyl-1,3,6-octatriene $$ Ocimene, cis-.beta.- $



Hit#:4 Entry:7926 Library:NIST17R.lib
SI:94 Formula:C10H16 CAS:3779-61-1 MolWeight:136 RetIndex:976
CompName:trans-.beta.-Ocimene $$ 1,3,6-Octatriene, 3,7-dimethyl-, (E)- $$ .beta.-trans-Ocimene $$ trans-3,7-Dimethyl-1,3,6-Octatriene $$ Ocimene, trans

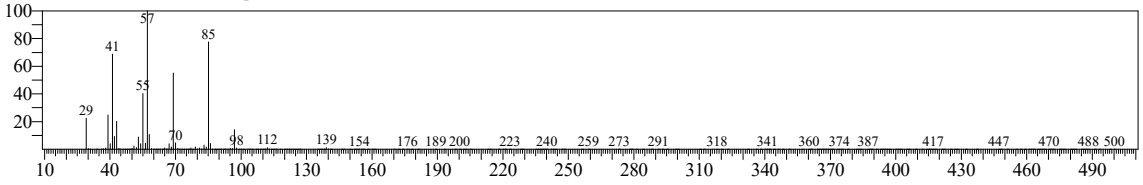


Hit#:5 Entry:10389 Library:NIST17M1.lib
SI:94 Formula:C10H16 CAS:80-56-8 MolWeight:136 RetIndex:948
CompName:.alpha.-Pinene $$ Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- $$ 2-Pinene $$ 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene $$ Pinene, .alpha. $$ 2,6,6

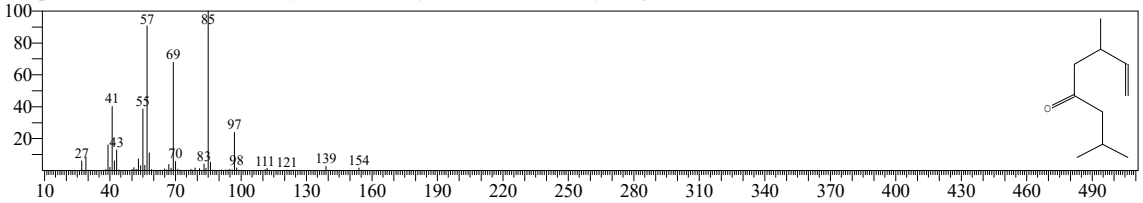


Qualitative Analysis Report

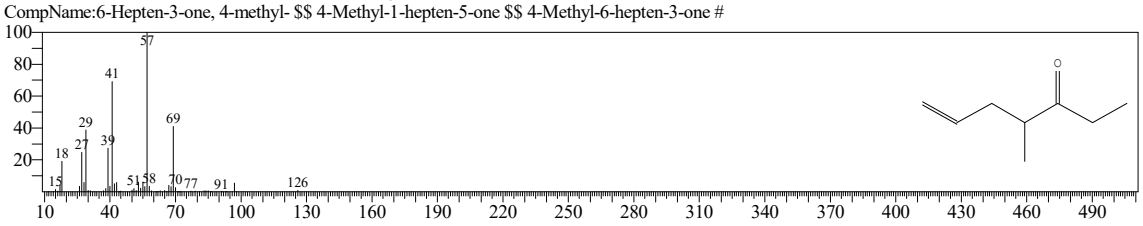
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Line#:5 R.Time:12.055(Scan#:1812) MassPeaks:246
RawMode:Averaged 12.050-12.060(1811-1813) BasePeak:57.05(1700503)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



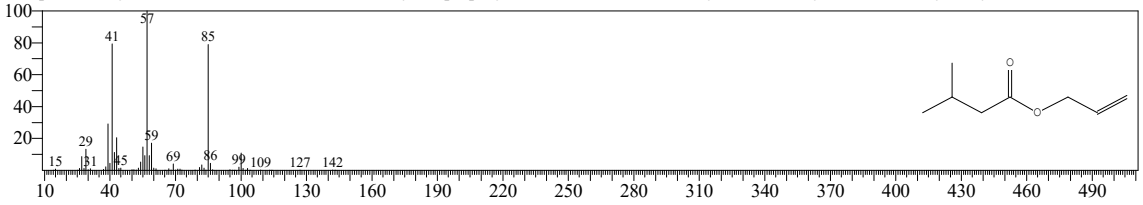
Hit#:1 Entry:18843 Library:NIST17M1.lib
SI:93 Formula:C10H18O CAS:1879-00-1 MolWeight:154 RetIndex:1013
CompName:7-Octen-4-one, 2,6-dimethyl- $$ 2,6-Dimethyloct-7-en-4-one $$ Dihydrotagetone



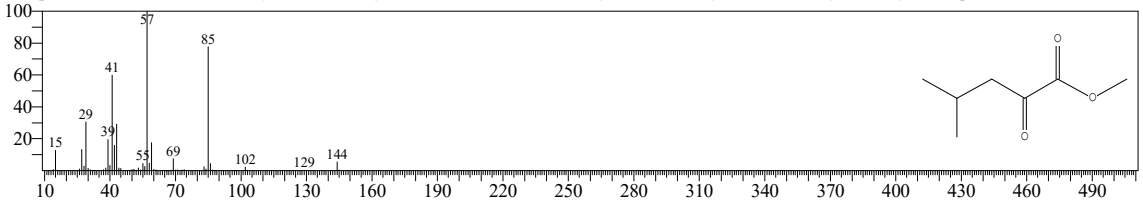
Hit#:2 Entry:6915 Library:NIST17M1.lib
SI:87 Formula:C8H14O CAS:26118-97-8 MolWeight:126 RetIndex:878
CompName:6-Hepten-3-one, 4-methyl- $$ 4-Methyl-1-hepten-5-one $$ 4-Methyl-6-hepten-3-one #



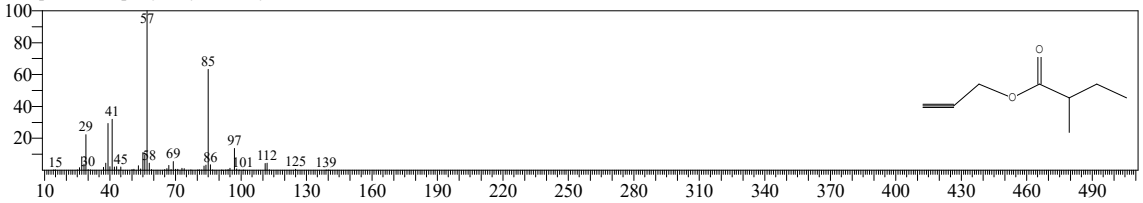
Hit#:3 Entry:12838 Library:NIST17M1.lib
SI:87 Formula:C8H14O2 CAS:2835-39-4 MolWeight:142 RetIndex:910
CompName:Allyl isovalerate $$ Butanoic acid, 3-methyl-, 2-propenyl ester $$ Isovaleric acid, allyl ester $$ Butyric acid, 3-methyl-, allyl ester $$ NCI-C547



Hit#:4 Entry:13682 Library:NIST17M1.lib
SI:87 Formula:C7H12O3 CAS:3682-43-7 MolWeight:144 RetIndex:956
CompName:Pentanoic acid, 4-methyl-2-oxo-, methyl ester $$ Valeric acid, 4-methyl-2-oxo-, methyl ester $$ Methyl 4-methyl-2-oxopentanoate #

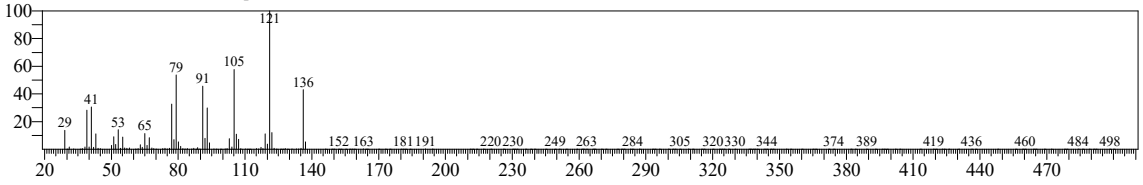


Hit#:5 Entry:11768 Library:NIST17M1.lib
SI:87 Formula:C8H12O2 CAS:0-00-0 MolWeight:140 RetIndex:917
CompName:Prop-2-yn-1-yl 2-methylbutanoate

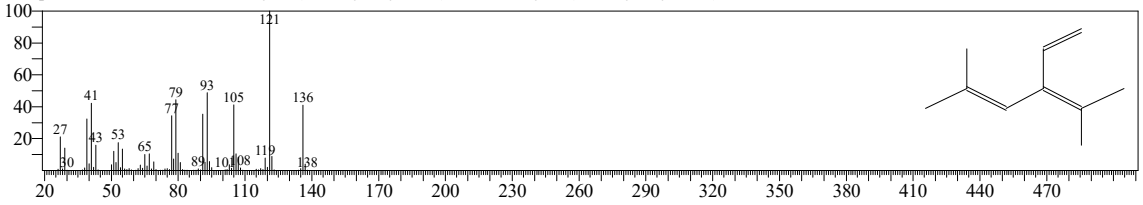


Qualitative Analysis Report

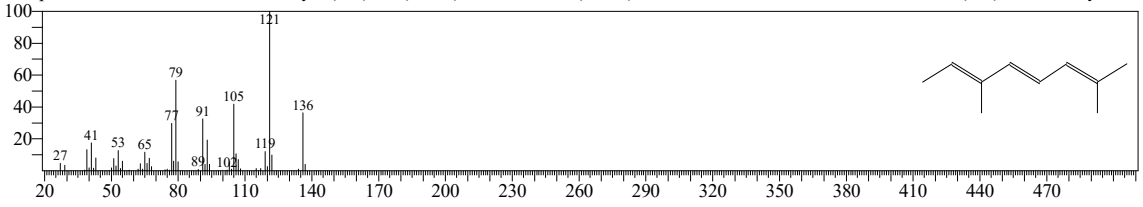
<< Target >>
Line#:6 R.Time:14.300(Scan#:2261) MassPeaks:207
RawMode:Averaged 14.295-14.305(2260-2262) BasePeak:121.10(40754)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



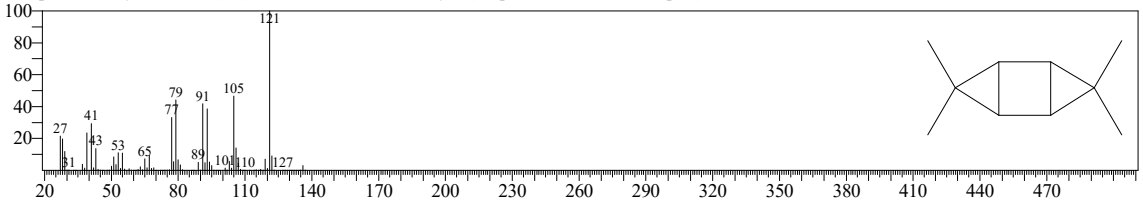
Hit#:1 Entry:10429 Library:NIST17M1.lib
SI:94 Formula:C10H16 CAS:113687-24-4 MolWeight:136 RetIndex:953
CompName:1,4-Hexadiene, 5-methyl-3-(1-methylethylidene)- $$ 5-Methyl-3-(1-methylethylidene)-1,4-hexadiene #



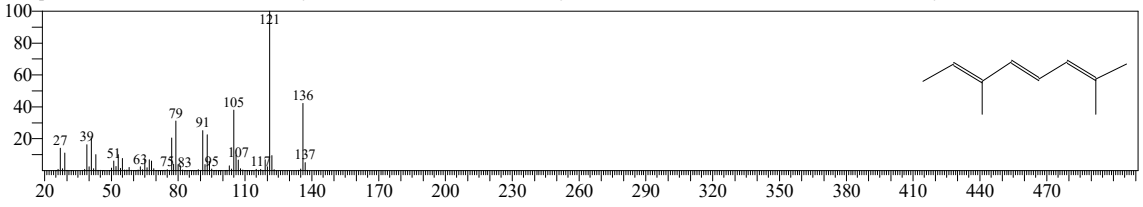
Hit#:2 Entry:10426 Library:NIST17M1.lib
SI:93 Formula:C10H16 CAS:3016-19-1 MolWeight:136 RetIndex:993
CompName:2,4,6-Octatriene, 2,6-dimethyl-, (E,E)- $$ (4E,6E)-Allocimene $$ (4E,6E)-Alloocimene $$ trans,trans-Alloocimene $$ (E,E)-2,6-Dimethyl-2,4,(



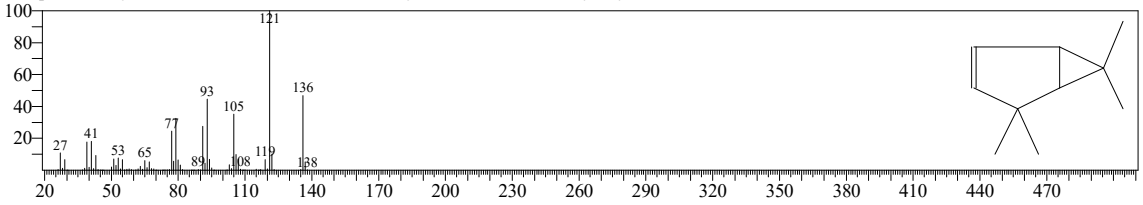
Hit#:3 Entry:10436 Library:NIST17M1.lib
SI:92 Formula:C10H16 CAS:58987-01-2 MolWeight:136 RetIndex:670
CompName:Tricyclo[3.1.0.0(2,4)]hexane, 3,3,6,6-tetramethyl-, (1.alpha.,2.beta.,4.beta.,5.alpha.)-



Hit#:4 Entry:7993 Library:NIST17R.lib
SI:92 Formula:C10H16 CAS:673-84-7 MolWeight:136 RetIndex:993
CompName:2,4,6-Octatriene, 2,6-dimethyl- $$ Allo-Ocimene $$ 2,6-Dimethyl-2,4,6-octatriene $$ Ocimene, allo- $$ 2,6-dimethyl-octa-2,4,6-triene $$ Alloo

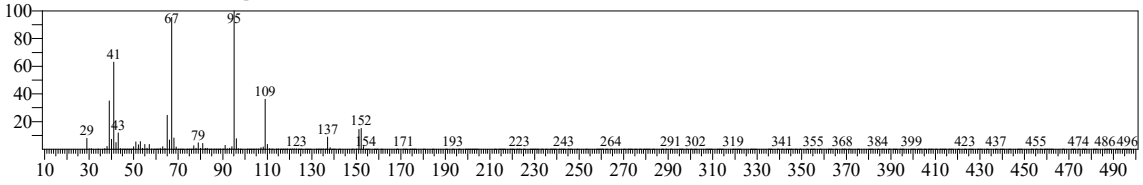


Hit#:5 Entry:10442 Library:NIST17M1.lib
SI:91 Formula:C10H16 CAS:19487-09-3 MolWeight:136 RetIndex:873
CompName:Bicyclo[3.1.0]hex-2-ene, 4,4,6,6-tetramethyl- $$ 4,4,6,6-Tetramethylbicyclo[3.1.0]hex-2-ene #

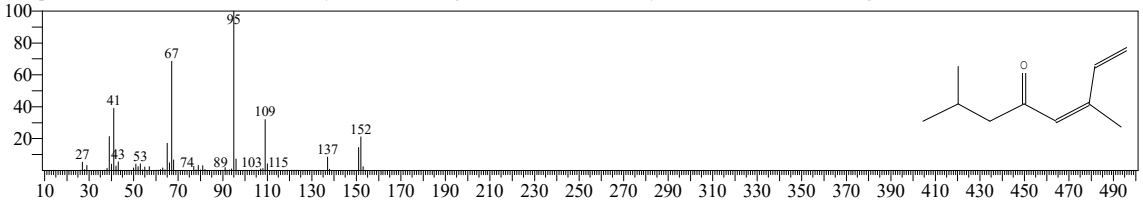


Qualitative Analysis Report

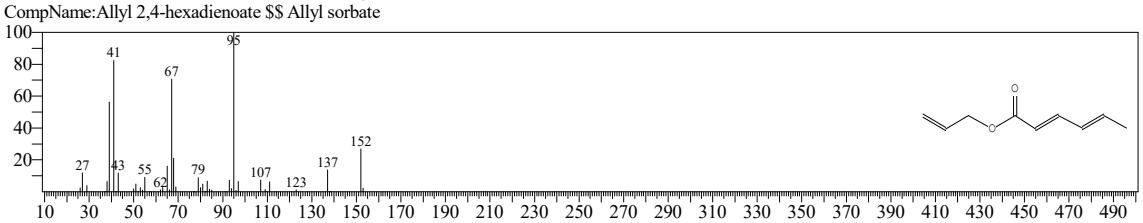
<< Target >>
Line#:7 R.Time:15.115(Scan#:2424) MassPeaks:268
RawMode:Averaged 15.110-15.120(2423-2425) BasePeak:95.05(276250)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



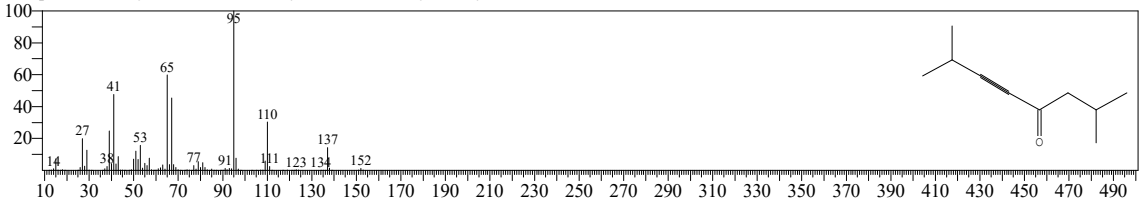
Hit#:1 Entry:17573 Library:NIST17M1.lib
SI:93 Formula:C10H16O CAS:3588-18-9 MolWeight:152 RetIndex:1062
CompName:5,7-Octadien-4-one, 2,6-dimethyl-, (Z)- $$ cis-Tagetone $$ (5Z)-2,6-Dimethyl-5,7-octadien-4-one # $$ Tagetone (Z) $$ (Z)-5,7-Octadien-4-one



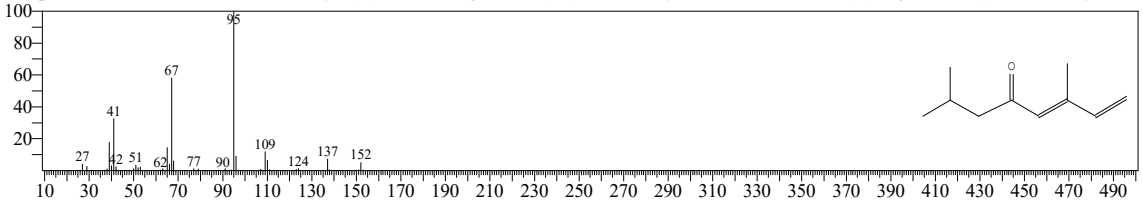
Hit#:2 Entry:17306 Library:NIST17M1.lib
SI:86 Formula:C9H12O2 CAS:0-00-0 MolWeight:152 RetIndex:1089
CompName:Allyl 2,4-hexadienoate $$ Allyl sorbate



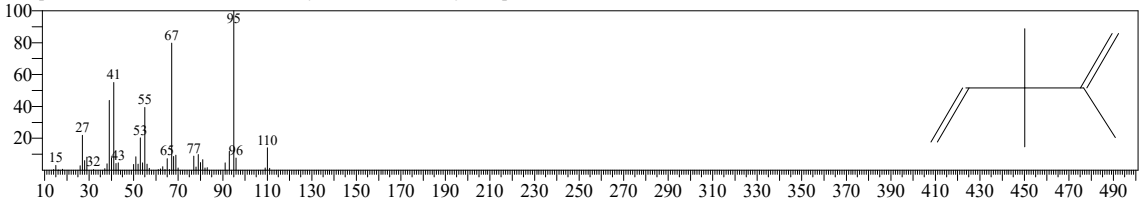
Hit#:3 Entry:17569 Library:NIST17M1.lib
SI:85 Formula:C10H16O CAS:29030-74-8 MolWeight:152 RetIndex:1040
CompName:5-Octyn-4-one, 2,7-dimethyl- $$ 2,7-Dimethyl-5-octyn-4-one #



Hit#:4 Entry:17570 Library:NIST17M1.lib
SI:85 Formula:C10H16O CAS:6752-80-3 MolWeight:152 RetIndex:1062
CompName:5,7-Octadien-4-one, 2,6-dimethyl-, (E)- $$ trans-Tagetone $$ (5E)-2,6-Dimethyl-5,7-octadien-4-one $$ (E)-Tagetone $$ (E)-2,6-Dimethylocta-5

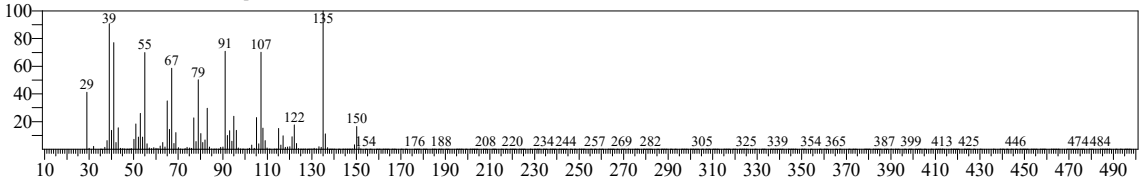


Hit#:5 Entry:3295 Library:NIST17R.lib
SI:84 Formula:C8H14 CAS:756-02-5 MolWeight:110 RetIndex:689
CompName:1,4-Pentadiene, 2,3,3-trimethyl- $$ 2,3,3-Trimethyl-1,4-pentadiene

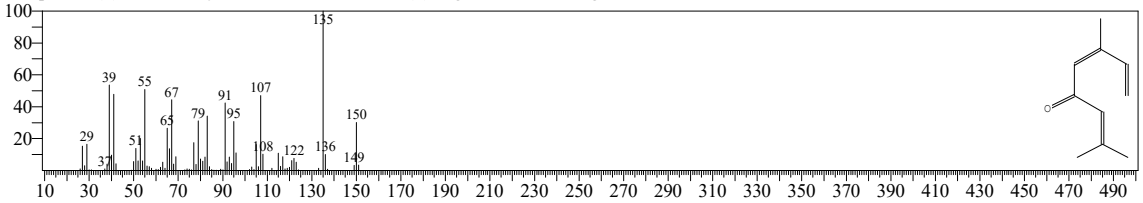


Qualitative Analysis Report

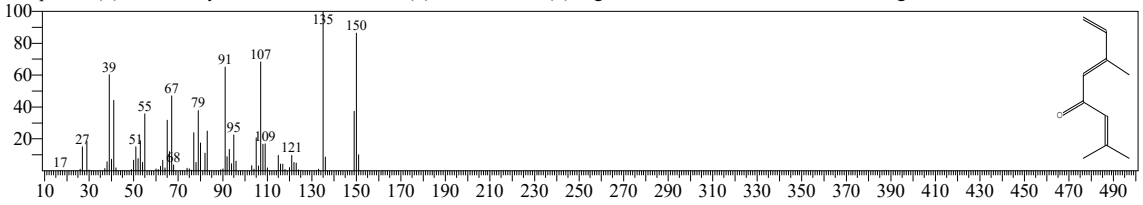
<< Target >>
Line#:8 R.Time:17.425(Scan#:2886) MassPeaks:317
RawMode:Averaged 17.420-17.430(2885-2887) BasePeak:135.10(138603)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



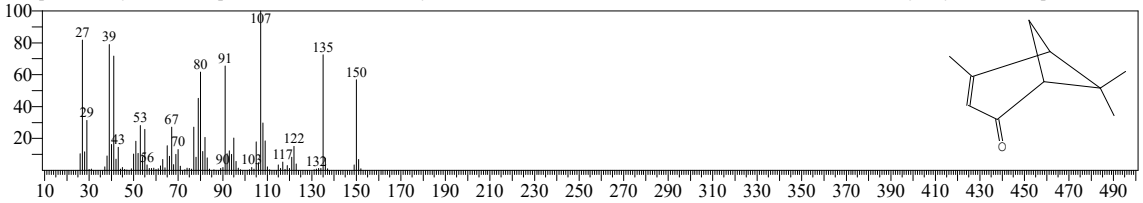
Hit#:1 Entry:16494 Library:NIST17M1.lib
SI:90 Formula:C10H14O CAS:33746-71-3 MolWeight:150 RetIndex:1112
CompName:(Z)-2,6-Dimethylocta-2,5,7-trien-4-one $$ (Z)-Tagetenone $$ cis-Tagetenone $$ cis-Ocimenone



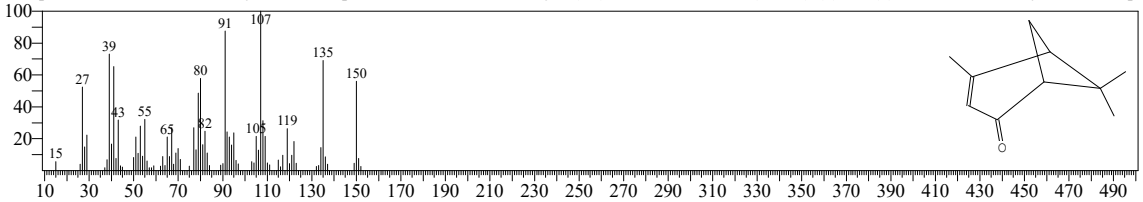
Hit#:2 Entry:16519 Library:NIST17M1.lib
SI:89 Formula:C10H14O CAS:33746-72-4 MolWeight:150 RetIndex:1112
CompName:(E)-2,6-Dimethylocta-2,5,7-trien-4-one $$ (E)-Ocimenone $$ (E)-Tagetenone $$ trans-Ocimenone $$ trans-Tagetenone



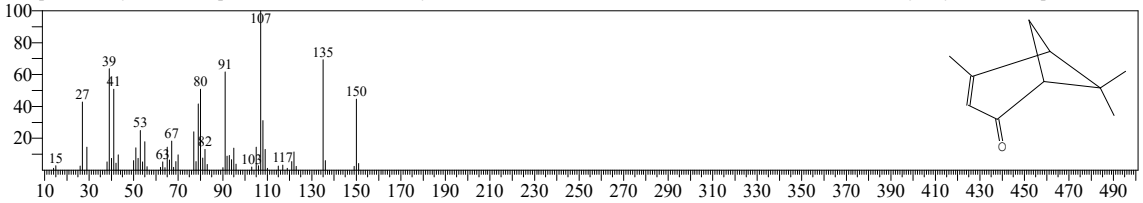
Hit#:3 Entry:10821 Library:NIST17R.lib
SI:88 Formula:C10H14O CAS:80-57-9 MolWeight:150 RetIndex:1119
CompName:Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl- $$ 2-Pinen-4-one $$ Berbenone $$ Verbenone $$ 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one



Hit#:4 Entry:16445 Library:NIST17M1.lib
SI:86 Formula:C10H14O CAS:18309-32-5 MolWeight:150 RetIndex:1119
CompName:D-Verbenone $$ Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1R)- $$ 2-Pinen-4-one, (1R,5R)-(+)- $$ (+)-Verbenone $$ Bicyclo[3.1.1]hept

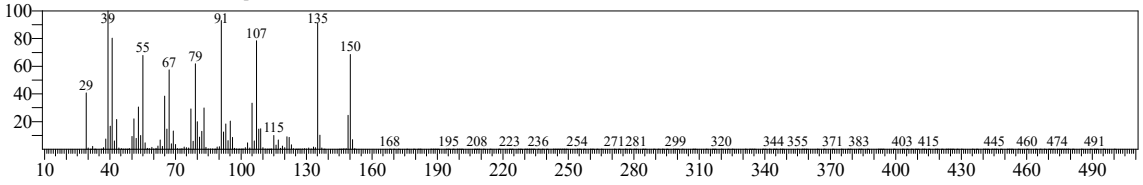


Hit#:5 Entry:10830 Library:NIST17R.lib
SI:86 Formula:C10H14O CAS:80-57-9 MolWeight:150 RetIndex:1119
CompName:Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl- $$ 2-Pinen-4-one $$ Berbenone $$ Verbenone $$ 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one

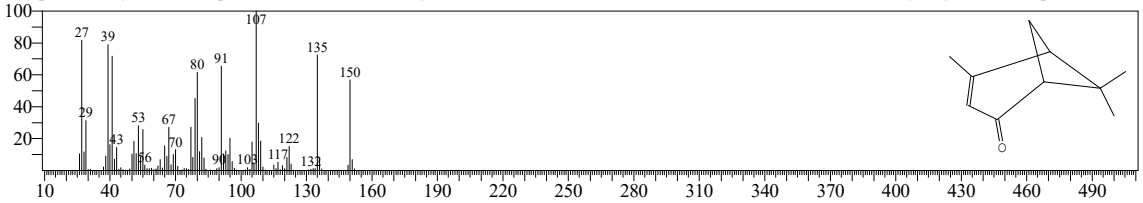


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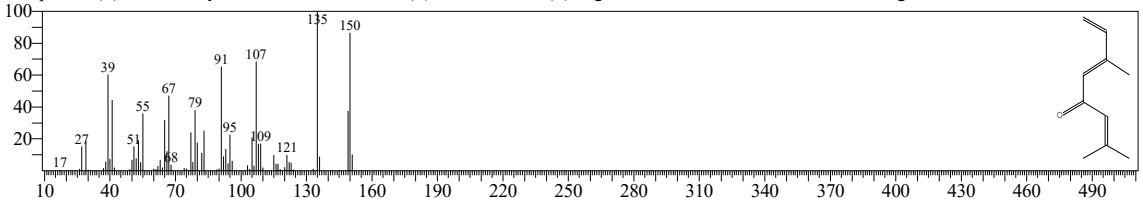
<< Target >>
Line#:9 R.Time:17.640(Scan#:2929) MassPeaks:267
RawMode:Averaged 17.635-17.645(2928-2930) BasePeak:39.05(139522)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



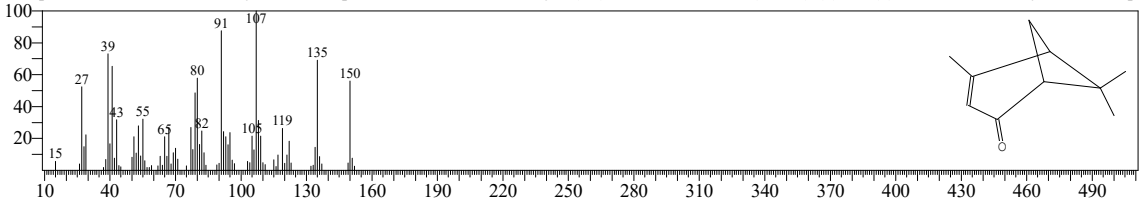
Hit#:1 Entry:10821 Library:NIST17R.lib
SI:90 Formula:C10H14O CAS:80-57-9 MolWeight:150 RetIndex:1119
CompName:Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl- $$ 2-Pinen-4-one $$ Berbenone $$ Verbenone $$ 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one



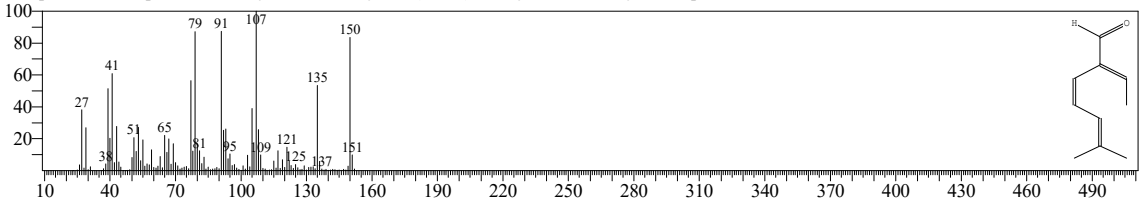
Hit#:2 Entry:16519 Library:NIST17M1.lib
SI:89 Formula:C10H14O CAS:33746-72-4 MolWeight:150 RetIndex:1112
CompName:(E)-2,6-Dimethylocta-2,5,7-trien-4-one $$ (E)-Ocimenone $$ (E)-Tagetenone $$ trans-Ocimenone $$ trans-Tagetenone



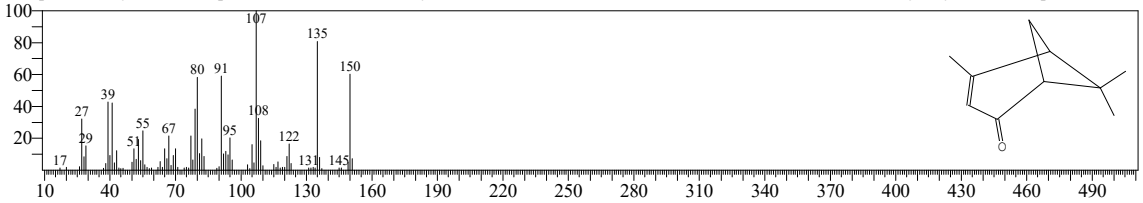
Hit#:3 Entry:16445 Library:NIST17M1.lib
SI:88 Formula:C10H14O CAS:18309-32-5 MolWeight:150 RetIndex:1119
CompName:D-Verbenone $$ Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1R)- $$ 2-Pinen-4-one, (1R,5R)-(+)- $$ (+)-Verbenone $$ Bicyclo[3.1.1]hep



Hit#:4 Entry:16447 Library:NIST17M1.lib
SI:87 Formula:C10H14O CAS:99172-18-6 MolWeight:150 RetIndex:1182
CompName:3,5-Heptadienal, 2-ethylidene-6-methyl- $$ (2E,3Z)-2-Ethylidene-6-methyl-3,5-heptadienal #

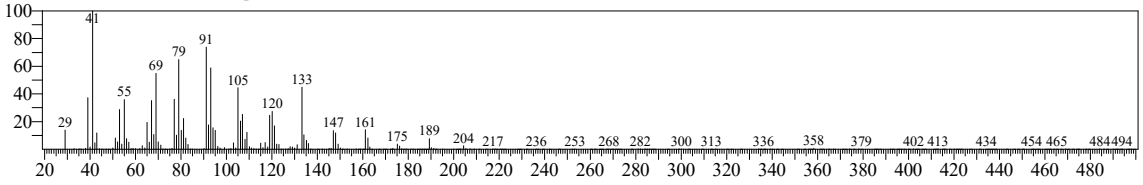


Hit#:5 Entry:10833 Library:NIST17R.lib
SI:87 Formula:C10H14O CAS:80-57-9 MolWeight:150 RetIndex:1119
CompName:Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl- $$ 2-Pinen-4-one $$ Berbenone $$ Verbenone $$ 4,6,6-Trimethylbicyclo[3.1.1]hept-3-en-2-one

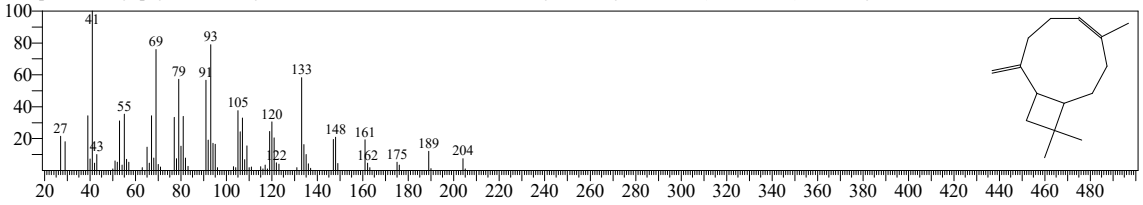


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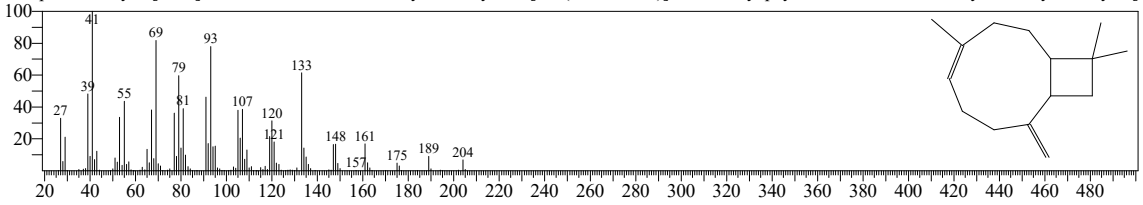
<< Target >>
Line#:10 R.Time:22.335(Scan#:3868) MassPeaks:275
RawMode:Averaged 22.330-22.340(3867-3869) BasePeak:41.05(22198)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



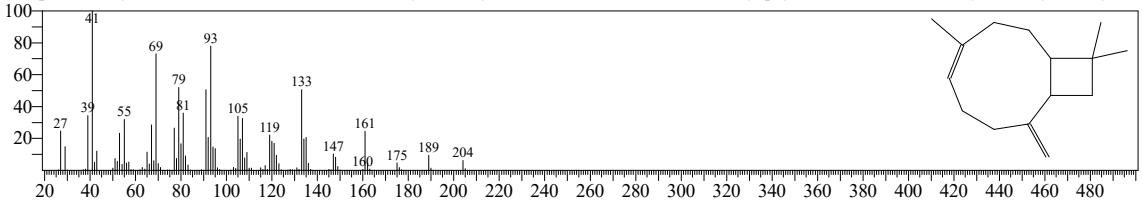
Hit#:1 Entry:22265 Library:NIST17R.lib
SI:94 Formula:C15H24 CAS:87-44-5 MolWeight:204 RetIndex:1494
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime



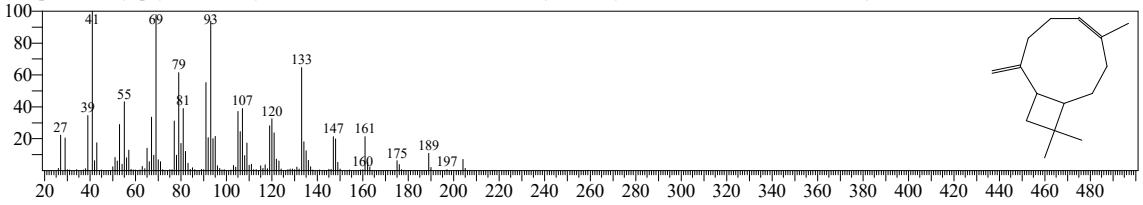
Hit#:2 Entry:22252 Library:NIST17R.lib
SI:93 Formula:C15H24 CAS:118-65-0 MolWeight:204 RetIndex:1494
CompName:Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-,[1R-(1R*,4Z,9S*)]- $$ Isocaryophyllene $$ 4,11,11-Trimethyl-8-methylenebicyclo[



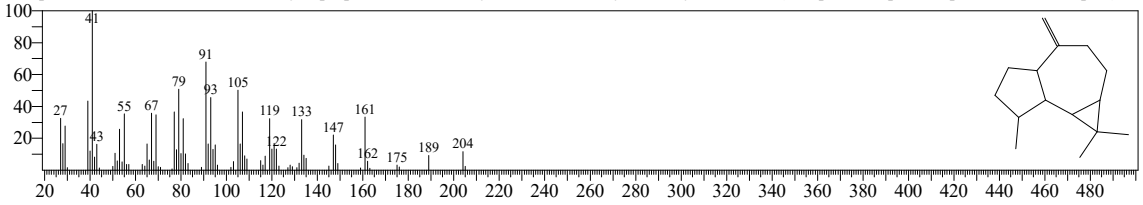
Hit#:3 Entry:52722 Library:NIST17M1.lib
SI:93 Formula:C15H24 CAS:118-65-0 MolWeight:204 RetIndex:1494
CompName:Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-,[1R-(1R*,4Z,9S*)]- $$ Isocaryophyllene $$ 4,11,11-Trimethyl-8-methylenebicyclo[



Hit#:4 Entry:22253 Library:NIST17R.lib
SI:91 Formula:C15H24 CAS:87-44-5 MolWeight:204 RetIndex:1494
CompName:Caryophyllene $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4E,9S*)]- $$ Bicyclo[7.2.0]undec-4-ene, 4,11,11-trime

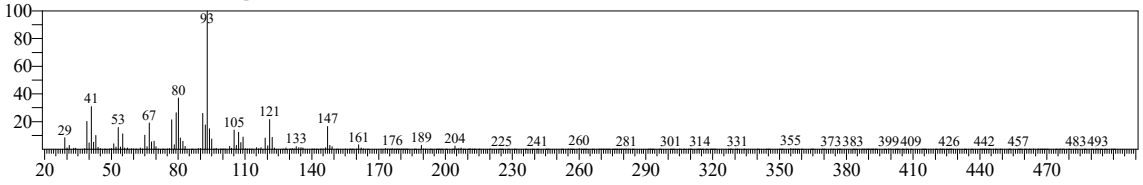


Hit#:5 Entry:22258 Library:NIST17R.lib
SI:91 Formula:C15H24 CAS:489-39-4 MolWeight:204 RetIndex:1386
CompName:Aromandendrene $$ 1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1a.alpha.,4a.alpha.,7.alpha.,7a.beta.,7b.alpha.)]- $

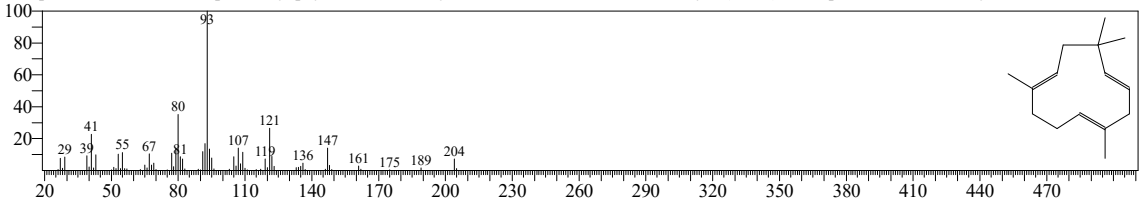


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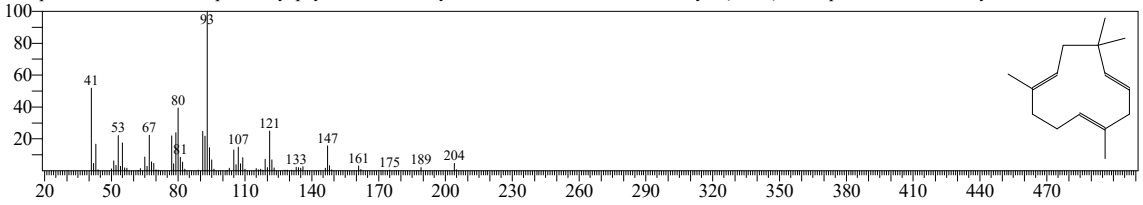
<< Target >>
Line#:11 R.Time:23.225(Scan#:4046) MassPeaks:266
RawMode:Averaged 23.220-23.230(4045-4047) BasePeak:93.05(24004)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



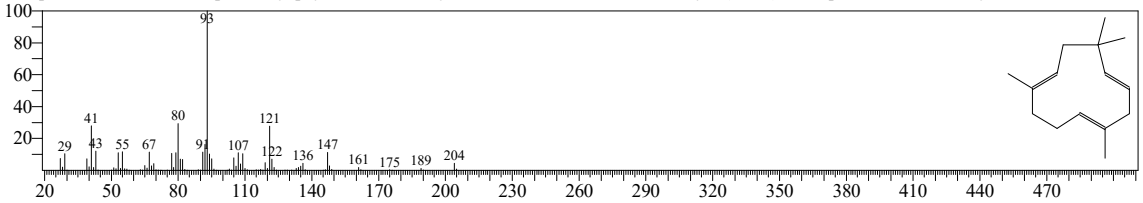
Hit#:1 Entry:22310 Library:NIST17R.lib
SI:92 Formula:C15H24 CAS:6753-98-6 MolWeight:204 RetIndex:1579
CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-trien



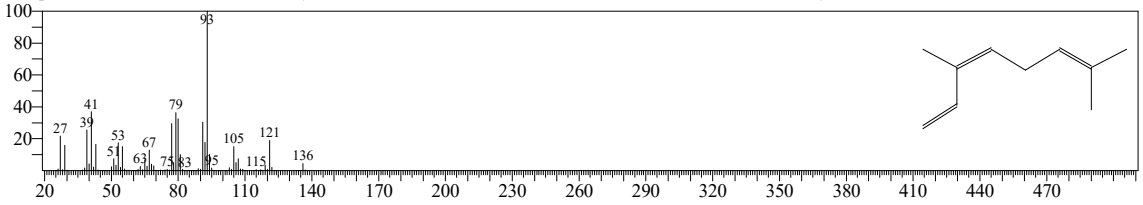
Hit#:2 Entry:22303 Library:NIST17R.lib
SI:91 Formula:C15H24 CAS:6753-98-6 MolWeight:204 RetIndex:1579
CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-trien



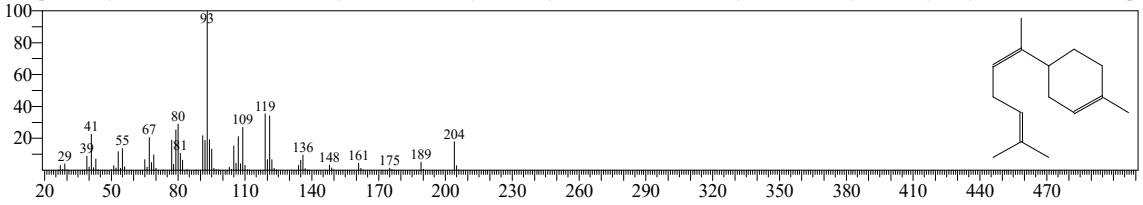
Hit#:3 Entry:52774 Library:NIST17M1.lib
SI:91 Formula:C15H24 CAS:6753-98-6 MolWeight:204 RetIndex:1579
CompName:Humulene $$ .alpha.-Caryophyllene $$ 1,4,8-Cycloundecatriene, 2,6,6,9-tetramethyl-, (E,E,E)- $$ .alpha.-Humulene $$ Cycloundeca-1,4,8-trien



Hit#:4 Entry:7927 Library:NIST17R.lib
SI:88 Formula:C10H16 CAS:3338-55-4 MolWeight:136 RetIndex:976
CompName:1,3,6-Octatriene, 3,7-dimethyl-, (Z)- $$ .beta.-cis-Ocimene $$ cis-.beta.-Ocimene $$ cis-3,7-Dimethyl-1,3,6-octatriene $$ Ocimene, cis-.beta.- $

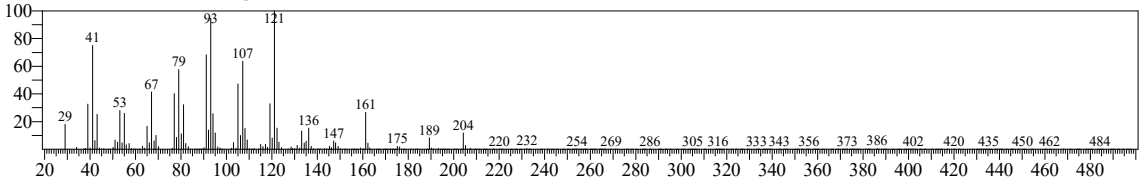


Hit#:5 Entry:52782 Library:NIST17M1.lib
SI:88 Formula:C15H24 CAS:25532-79-0 MolWeight:204 RetIndex:1518
CompName:Cyclohexene, 4-[(1E)-1,5-dimethyl-1,4-hexadien-1-yl]-1-methyl- $$ 4-[(1E)-1,5-Dimethyl-1,4-hexadienyl]-1-methyl-1-cyclohexene $$ 2,5-Hept

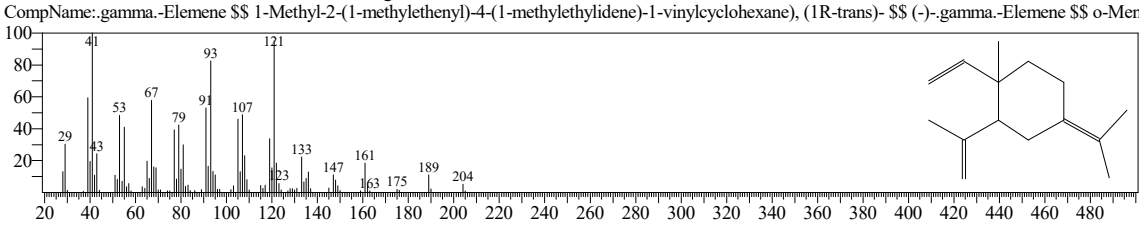


Qualitative Analysis Report

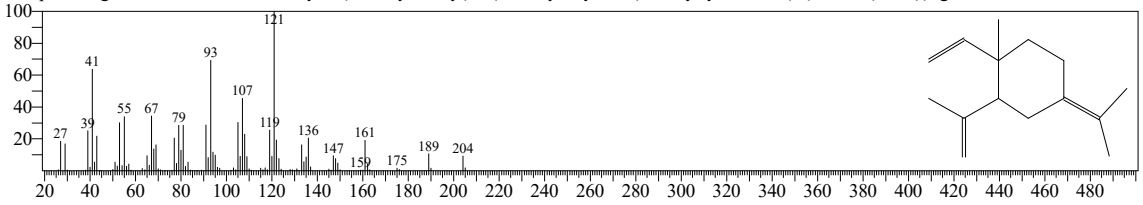
<< Target >>
Line#:12 R.Time:23.910(Scan#:4183) MassPeaks:294
RawMode:Averaged 23.905-23.915(4182-4184) BasePeak:121.10(39948)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



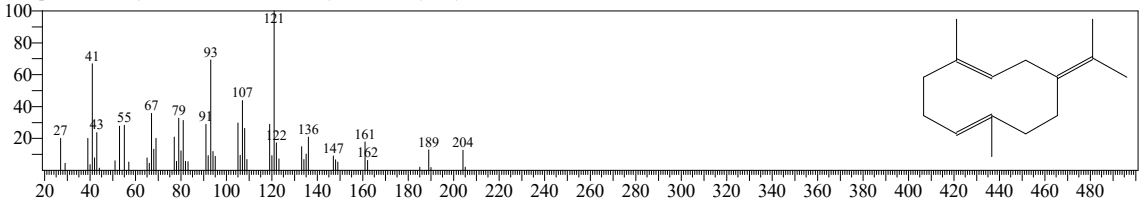
Hit#:1 Entry:22271 Library:NIST17R.lib
SI:92 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



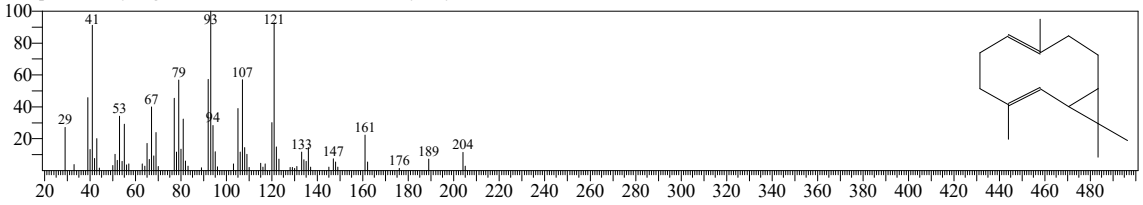
Hit#:2 Entry:52870 Library:NIST17M1.lib
SI:91 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer



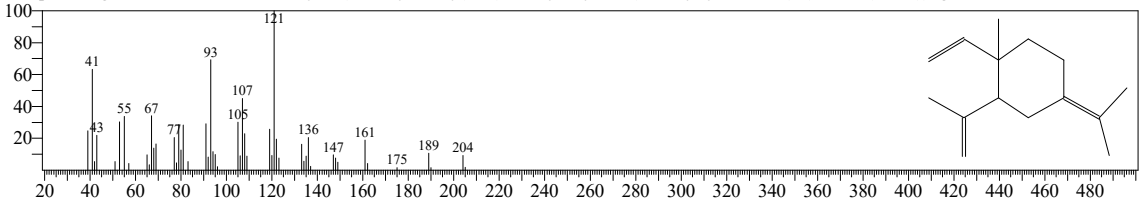
Hit#:3 Entry:22390 Library:NIST17R.lib
SI:91 Formula:C15H24 CAS:15423-57-1 MolWeight:204 RetIndex:1603
CompName:1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethylidene)-, (E,E)- $$ Germacrene B $$ Germacra-1(10),4,7(11)-triene $$ Germacra-1(10),4,7(1



Hit#:4 Entry:52783 Library:NIST17M1.lib
SI:90 Formula:C15H24 CAS:67650-90-2 MolWeight:204 RetIndex:1499
CompName:Bicyclogermacrene $$ 3,7,11,11-Tetramethylbicyclo[8.1.0]undeca-2,6-diene #

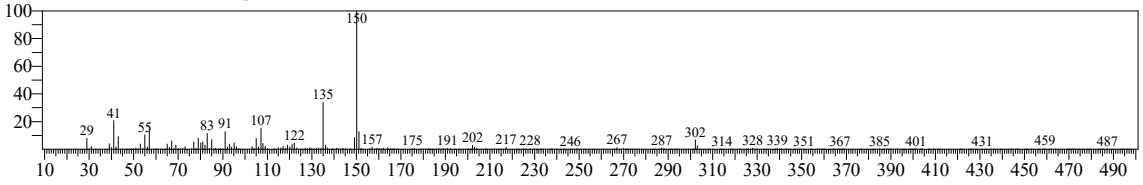


Hit#:5 Entry:22389 Library:NIST17R.lib
SI:89 Formula:C15H24 CAS:29873-99-2 MolWeight:204 RetIndex:1431
CompName:.gamma.-Elemene $$ 1-Methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-1-vinylcyclohexane), (1R-trans)- $$ (-)-.gamma.-Elemene $$ o-Mer

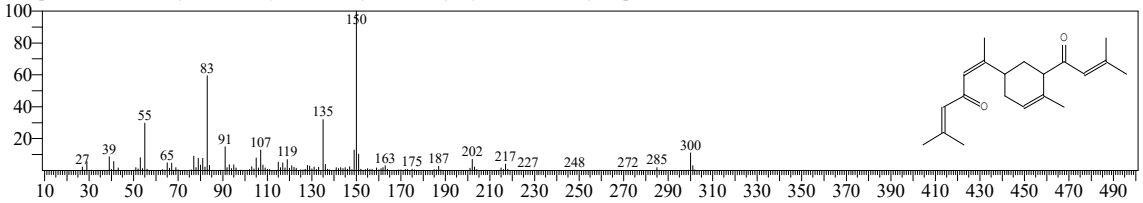


Qualitative Analysis Report

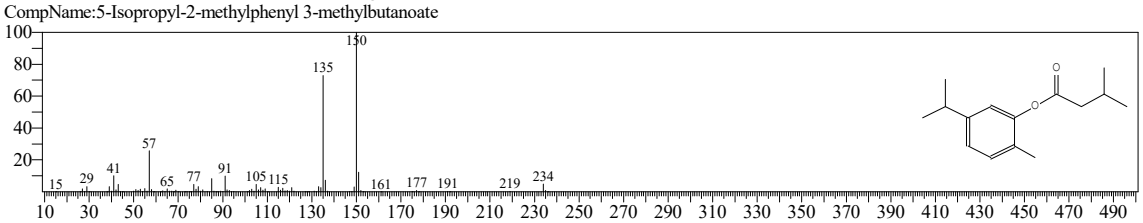
<< Target >>
Line#:13 R.Time:27.160(Scan#:4833) MassPeaks:275
RawMode:Averaged 27.155-27.165(4832-4834) BasePeak:150.10(53959)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



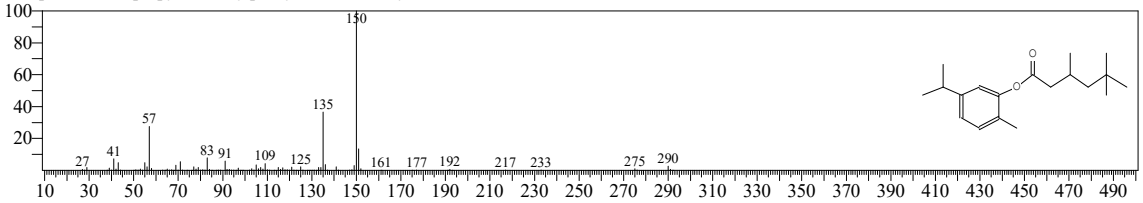
Hit#:1 Entry:144154 Library:NIST17M1.lib
SI:79 Formula:C20H28O2 CAS:0-00-0 MolWeight:300 RetIndex:2234
CompName:(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)hepta-2,5-dien-4-one



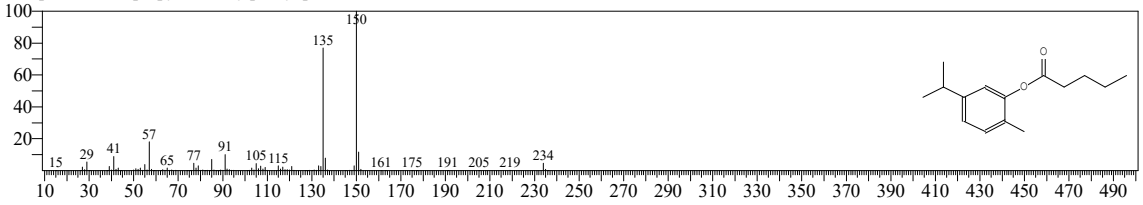
Hit#:2 Entry:79288 Library:NIST17M1.lib
SI:79 Formula:C15H22O2 CAS:0-00-0 MolWeight:234 RetIndex:1656
CompName:5-Isopropyl-2-methylphenyl 3-methylbutanoate



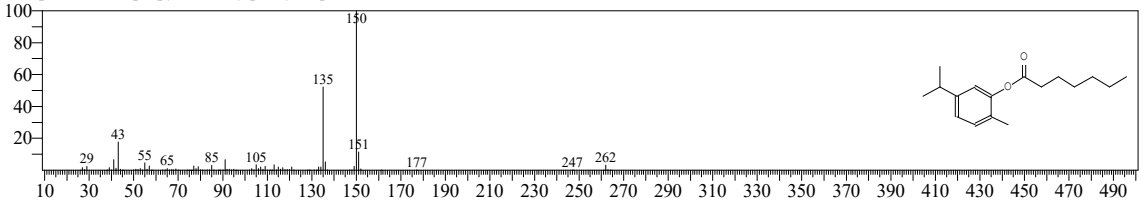
Hit#:3 Entry:133691 Library:NIST17M1.lib
SI:79 Formula:C19H30O2 CAS:0-00-0 MolWeight:290 RetIndex:1969
CompName:5-Isopropyl-2-methylphenyl 3,5,5-trimethylhexanoate



Hit#:4 Entry:79289 Library:NIST17M1.lib
SI:78 Formula:C15H22O2 CAS:0-00-0 MolWeight:234 RetIndex:1720
CompName:5-Isopropyl-2-methylphenyl pentanoate

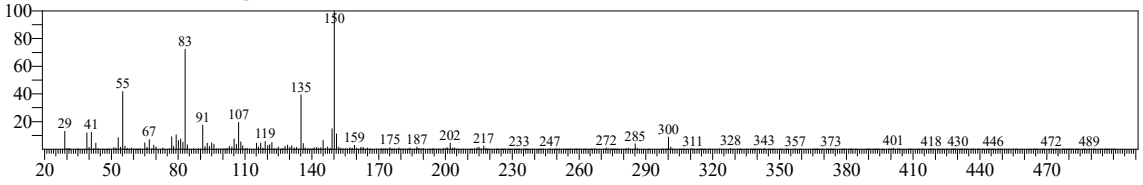


Hit#:5 Entry:105725 Library:NIST17M1.lib
SI:78 Formula:C17H26O2 CAS:0-00-0 MolWeight:262 RetIndex:1918
CompName:5-Isopropyl-2-methylphenyl heptanoate

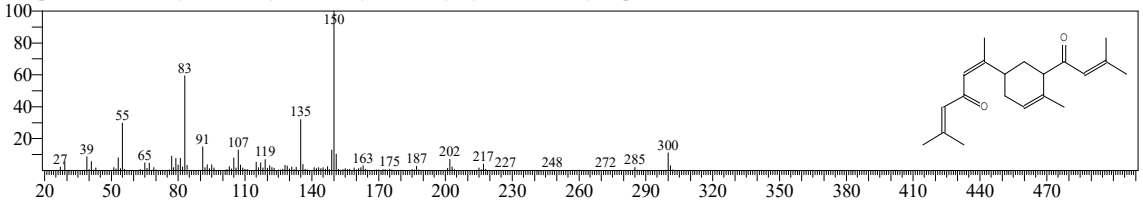


Qualitative Analysis Report

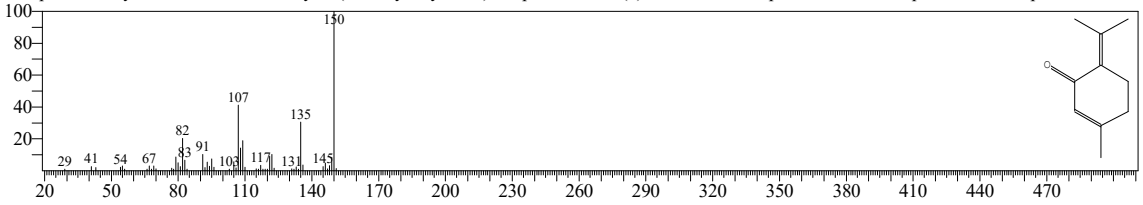
<< Target >>
Line#:14 R.Time:27.300(Scan#:4861) MassPeaks:314
RawMode:Averaged 27.295-27.305(4860-4862) BasePeak:150.10(78793)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



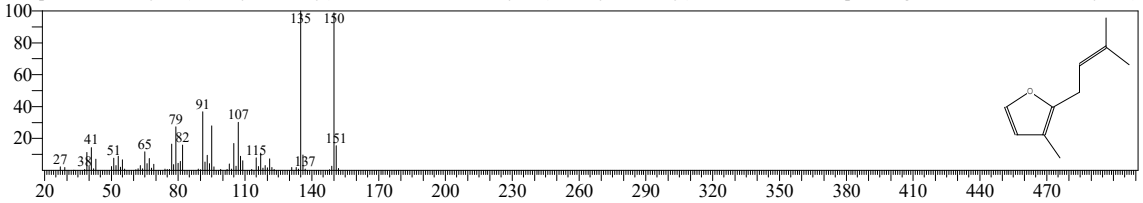
Hit#:1 Entry:144154 Library:NIST17M1.lib
SI:90 Formula:C20H28O2 CAS:0-00-0 MolWeight:300 RetIndex:2234
CompName:(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)hepta-2,5-dien-4-one



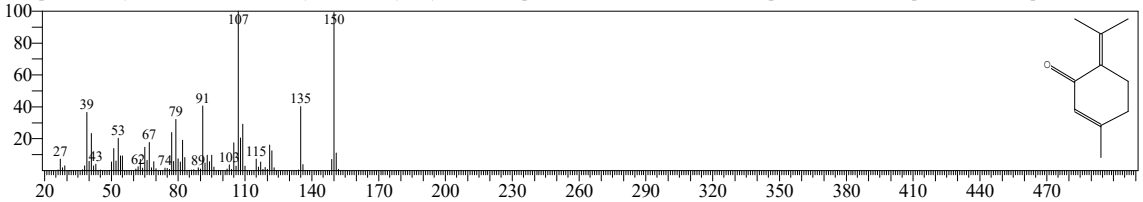
Hit#:2 Entry:10887 Library:NIST17R.lib
SI:75 Formula:C10H14O CAS:491-09-8 MolWeight:150 RetIndex:1223
CompName:2-Cyclohexen-1-one, 3-methyl-6-(1-methylethylidene)- $$ p-Mentha-1,4(8)-dien-3-one $$ Piperitenone $$ Pulespenone $$ 3-Terpinolenone $$



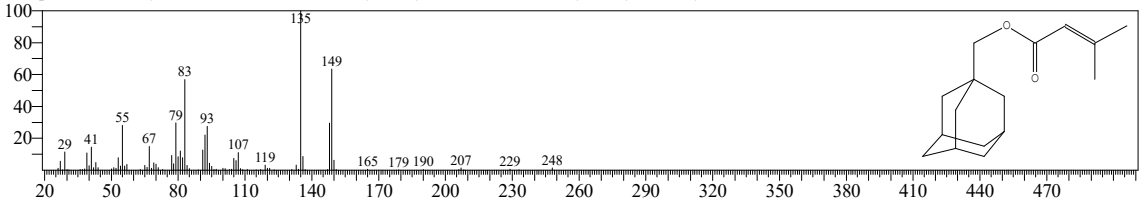
Hit#:3 Entry:16509 Library:NIST17M1.lib
SI:75 Formula:C10H14O CAS:15186-51-3 MolWeight:150 RetIndex:1115
CompName:3-Methyl-2-(2-methyl-2-butenyl)-furan $$ Furan, 3-methyl-2-(3-methyl-2-butenyl)- $$ Rosefuran $$ .alpha.-Naginatene $$ Furan, 3-methyl-2-(3



Hit#:4 Entry:16457 Library:NIST17M1.lib
SI:74 Formula:C10H14O CAS:491-09-8 MolWeight:150 RetIndex:1223
CompName:2-Cyclohexen-1-one, 3-methyl-6-(1-methylethylidene)- $$ p-Mentha-1,4(8)-dien-3-one $$ Piperitenone $$ Pulespenone $$ 3-Terpinolenone $$

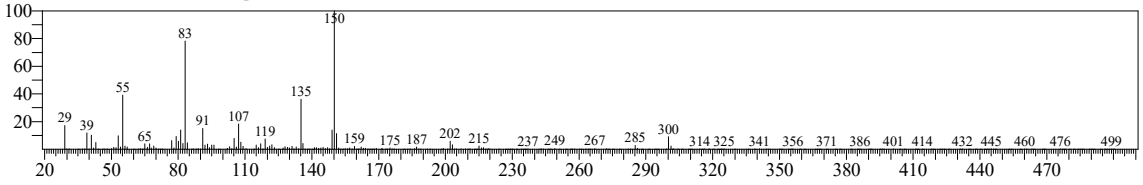


Hit#:5 Entry:92275 Library:NIST17M1.lib
SI:72 Formula:C16H24O2 CAS:0-00-0 MolWeight:248 RetIndex:1603
CompName:3-Methyl-2-butenoic acid, 1-adamantylmethyl ester $$ 1-Adamantylmethyl 3-methyl-2-butenoate #

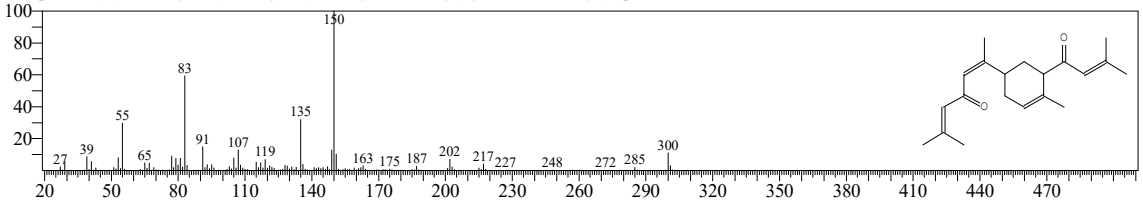


Qualitative Analysis Report

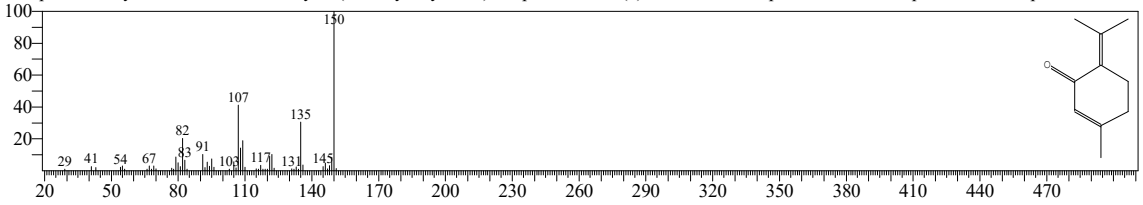
<< Target >>
Line#:15 R.Time:27.490(Scan#:4899) MassPeaks:285
RawMode:Averaged 27.485-27.495(4898-4900) BasePeak:150.10(90663)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



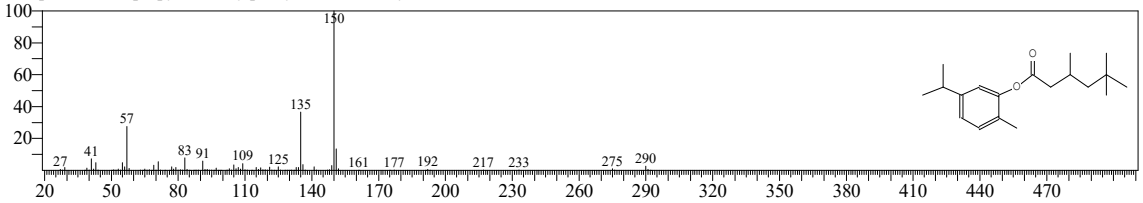
Hit#:1 Entry:144154 Library:NIST17M1.lib
SI:91 Formula:C20H28O2 CAS:0-00-0 MolWeight:300 RetIndex:2234
CompName:(Z)-2-Methyl-6-(4-methyl-5-(3-methylbut-2-enoyl)cyclohex-3-en-1-yl)hepta-2,5-dien-4-one



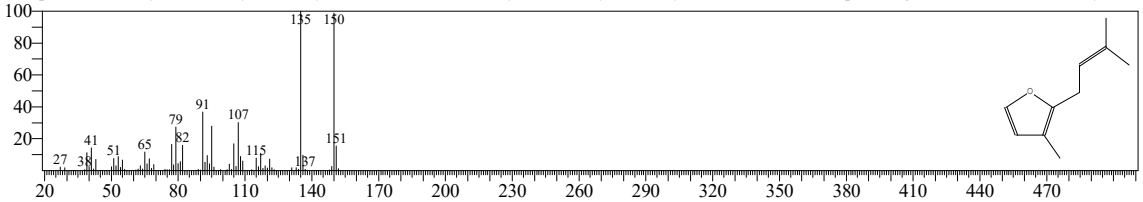
Hit#:2 Entry:10887 Library:NIST17R.lib
SI:73 Formula:C10H14O CAS:491-09-8 MolWeight:150 RetIndex:1223
CompName:2-Cyclohexen-1-one, 3-methyl-6-(1-methylethylidene)- $$ p-Mentha-1,4(8)-dien-3-one $$ Piperitenone $$ Pulespenone $$ 3-Terpinolenone $$



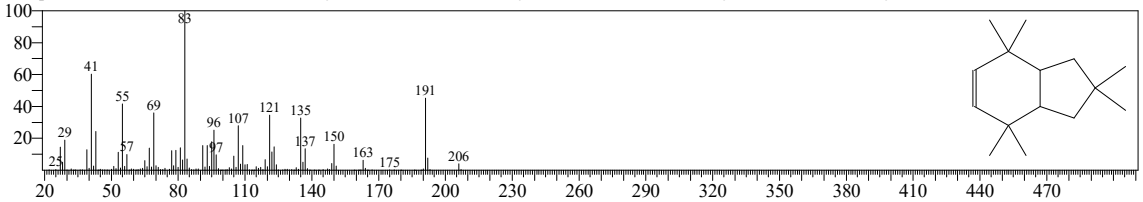
Hit#:3 Entry:133691 Library:NIST17M1.lib
SI:72 Formula:C19H30O2 CAS:0-00-0 MolWeight:290 RetIndex:1969
CompName:5-Isopropyl-2-methylphenyl 3,5,5-trimethylhexanoate



Hit#:4 Entry:16509 Library:NIST17M1.lib
SI:71 Formula:C10H14O CAS:15186-51-3 MolWeight:150 RetIndex:1115
CompName:3-Methyl-2-(2-methyl-2-butenyl)-furan $$ Furan, 3-methyl-2-(3-methyl-2-butenyl)- $$ Rosefuran $$ .alpha.-Naginatene $$ Furan, 3-methyl-2-(3

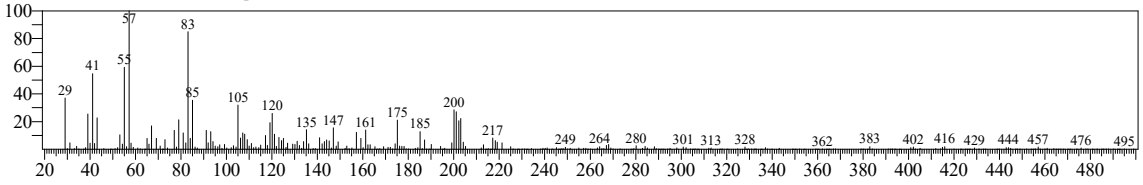


Hit#:5 Entry:54622 Library:NIST17M1.lib
SI:71 Formula:C15H26 CAS:61142-60-7 MolWeight:206 RetIndex:1367
CompName:1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7-hexamethyl- $$ 2,2,4,4,7,7-Hexamethyl-2,3,3a,4,7,7a-hexahydro-1H-indene #

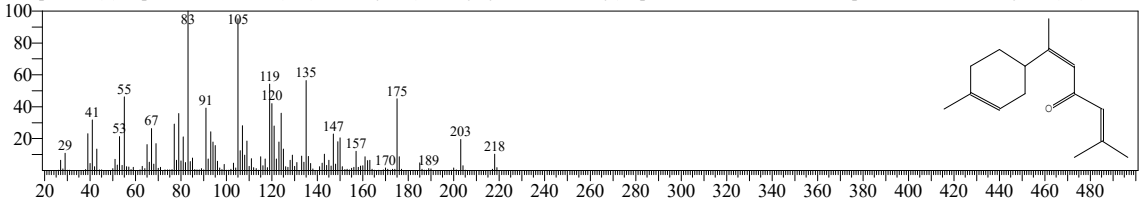


Qualitative Analysis Report

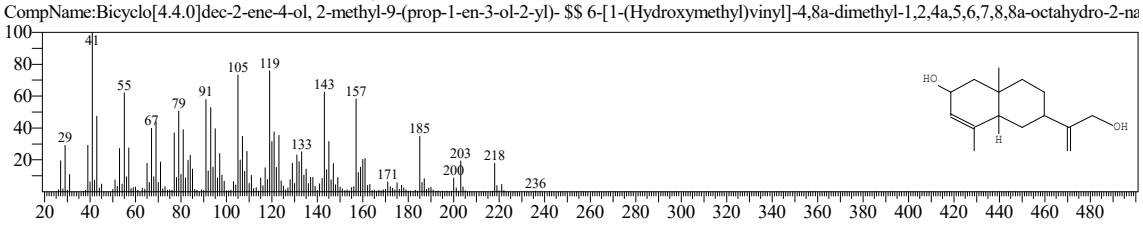
<< Target >>
Line#:16 R.Time:27.665(Scan#:4934) MassPeaks:296
RawMode:Averaged 27.660-27.670(4933-4935) BasePeak:57.10(14042)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



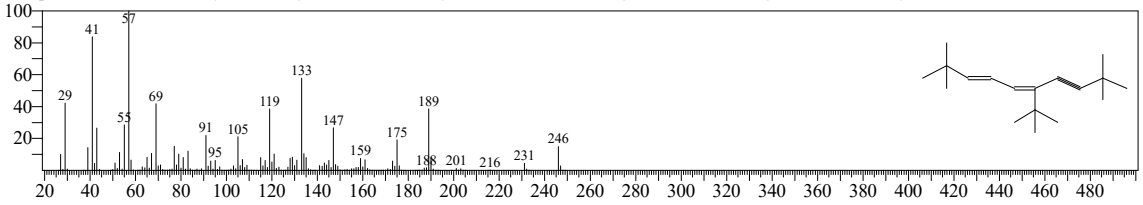
Hit#:1 Entry:64771 Library:NIST17M1.lib
SI:68 Formula:C15H22O CAS:56192-70-2 MolWeight:218 RetIndex:1654
CompName:(Z)-.alpha.-Atlantone $$ (R,Z)-2-Methyl-6-(4-methylcyclohex-3-en-1-yl)hepta-2,5-dien-4-one $$ 2,5-Heptadien-4-one, 2-methyl-6-[(1R)-4-meth



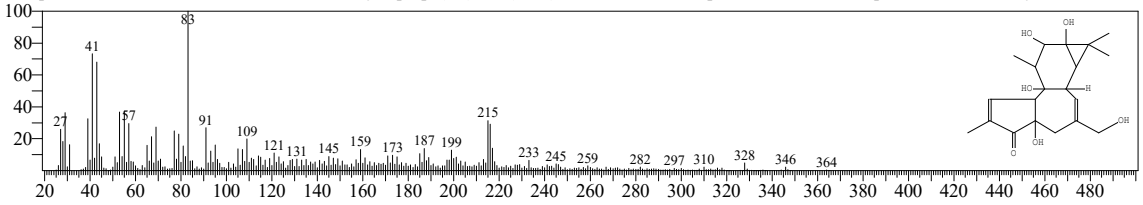
Hit#:2 Entry:81046 Library:NIST17M1.lib
SI:68 Formula:C15H24O2 CAS:0-00-0 MolWeight:236 RetIndex:1904
CompName:Bicyclo[4.4.0]dec-2-ene-4-ol, 2-methyl-9-(prop-1-en-3-ol-2-yl)- $$ 6-[1-(Hydroxymethyl)vinyl]-4,8a-dimethyl-1,2,4a,5,6,7,8,8a-octahydro-2-na



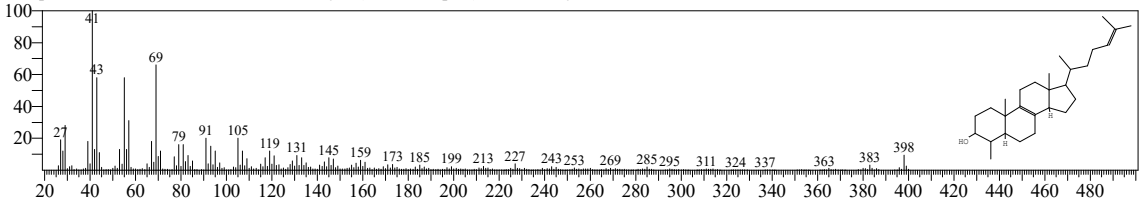
Hit#:3 Entry:90505 Library:NIST17M1.lib
SI:66 Formula:C18H30 CAS:0-00-0 MolWeight:246 RetIndex:1567
CompName:3,5-Decadien-7-yne, 6-t-butyl-2,2,9,9-tetramethyl- $$ (3E,5Z)-6-tert-Butyl-2,2,9,9-tetramethyl-3,5-decadien-7-yne #



Hit#:4 Entry:203867 Library:NIST17M1.lib
SI:66 Formula:C20H28O6 CAS:17673-25-5 MolWeight:364 RetIndex:2774
CompName:Phorbol $$ 4-.beta.-Phorbol $$ 5H-Cyclopropa(3,4)benz(1,2-e)azulen-5-one, 1,1a.alpha.,1b.beta.,4,4a,7a.alpha.,7b,8,9,9a-decahydro-4a.beta.,7b

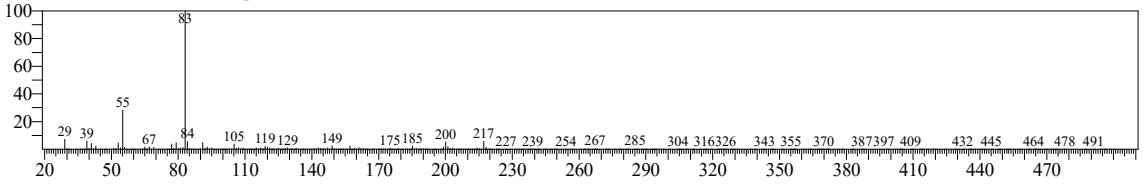


Hit#:5 Entry:226859 Library:NIST17M1.lib
SI:66 Formula:C28H46O CAS:7199-92-0 MolWeight:398 RetIndex:2735
CompName:Cholesta-8,24-dien-3-ol, 4-methyl-, (3.beta.,4.alpha.)- $$ 4-Methylcholesta-8,24-dien-3-ol #

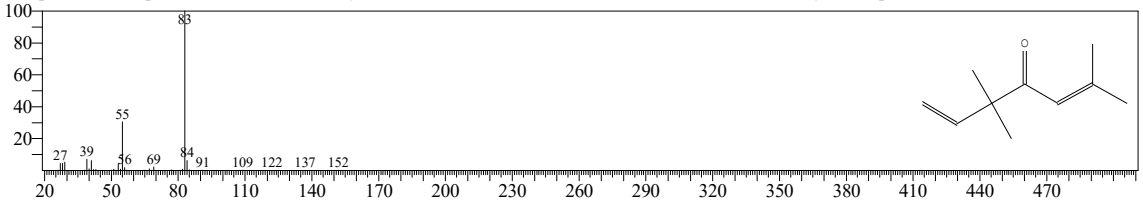


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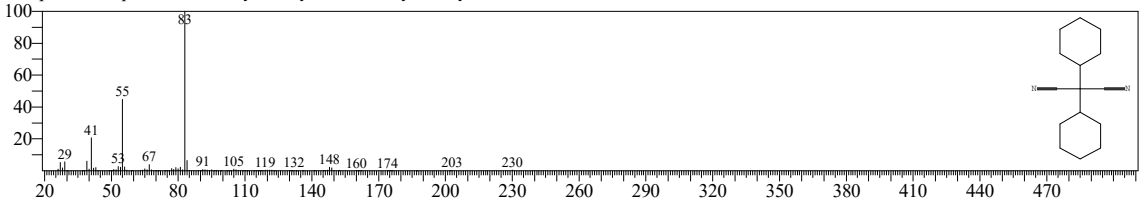
<< Target >>
Line#:17 R.Time:27.800(Scan#:4961) MassPeaks:309
RawMode:Averaged 27.795-27.805(4960-4962) BasePeak:83.05(386436)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



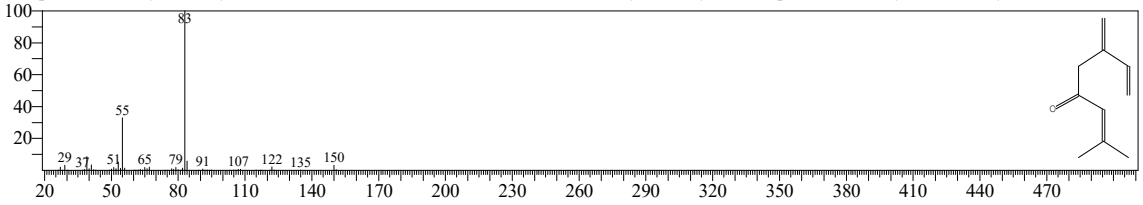
Hit#:1 Entry:17535 Library:NIST17M1.lib
SI:85 Formula:C10H16O CAS:546-49-6 MolWeight:152 RetIndex:1042
CompName:1,5-Heptadien-4-one, 3,3,6-trimethyl- $$ Artemisia ketone $$ Isoartemisia ketone $$ 2,5,5-Trimethyl-2,6-heptadien-4-one $$ Artemesia $$ 3,3,(



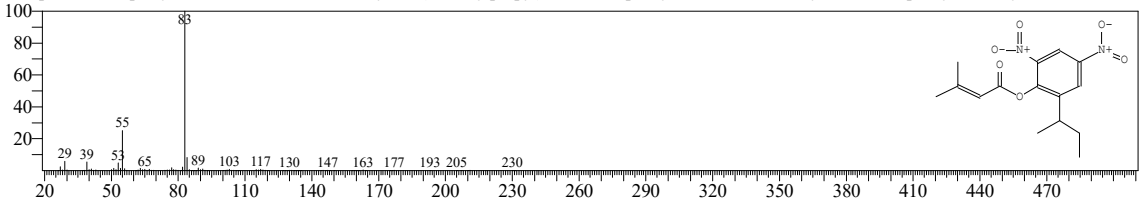
Hit#:2 Entry:75912 Library:NIST17M1.lib
SI:83 Formula:C15H22N2 CAS:74764-28-6 MolWeight:230 RetIndex:2045
CompName:Propanedinitrile, dicyclohexyl- $$ 2,2-Dicyclohexylmalononitrile #



Hit#:3 Entry:16401 Library:NIST17M1.lib
SI:83 Formula:C10H14O CAS:539-70-8 MolWeight:150 RetIndex:1094
CompName:2-Methyl-6-methyleneocta-2,7-dien-4-one $$ 2,7-Octadien-4-one, 2-methyl-6-methylene- $$ Ipsdienone $$ Myrcenon $$ Myrcenone



Hit#:4 Entry:165527 Library:NIST17M1.lib
SI:83 Formula:C15H18N2O6 CAS:485-31-4 MolWeight:322 RetIndex:2482
CompName:Binapacryl $$ 2-Butenoic acid, 3-methyl-, 2-(1-methylpropyl)-4,6-dinitrophenyl ester $$ 2-sec-Butyl-4,6-dinitrophenyl 3-methylcrotonate $$ Cr



Hit#:5 Entry:146005 Library:NIST17M1.lib
SI:82 Formula:C20H30O2 CAS:108546-82-3 MolWeight:302 RetIndex:2089
CompName:Cyclopropanecarboxylic acid, 2-methyl-, 2,6-di-t-butyl-4-methylphenyl ester $$ 2,6-Ditert-butyl-4-methylphenyl 2-methylcyclopropanecarboxyl

