10.1071/CH15476_AC

Australian Journal of Chemistry 2016, 69(2), 169-173

SUPPLEMENTARY MATERIAL

Identification of the Cat Attractants Isodihydronepetalactone and Isoiridomyrmecin from *Acalypha indica**

Adrian Scaffidi,[A] Dave Algar,[B] Björn Bohman,[A,C] Emilio L. Ghisalberti,[A,D] and Gavin Flematti[A,E]

[A]School of Chemistry and Biochemistry, University of Western Australia, Perth, WA 6009, Australia.

[B]Department of Parks and Wildlife's Science and Conservation Division, Wanneroo, WA 6946, Australia.

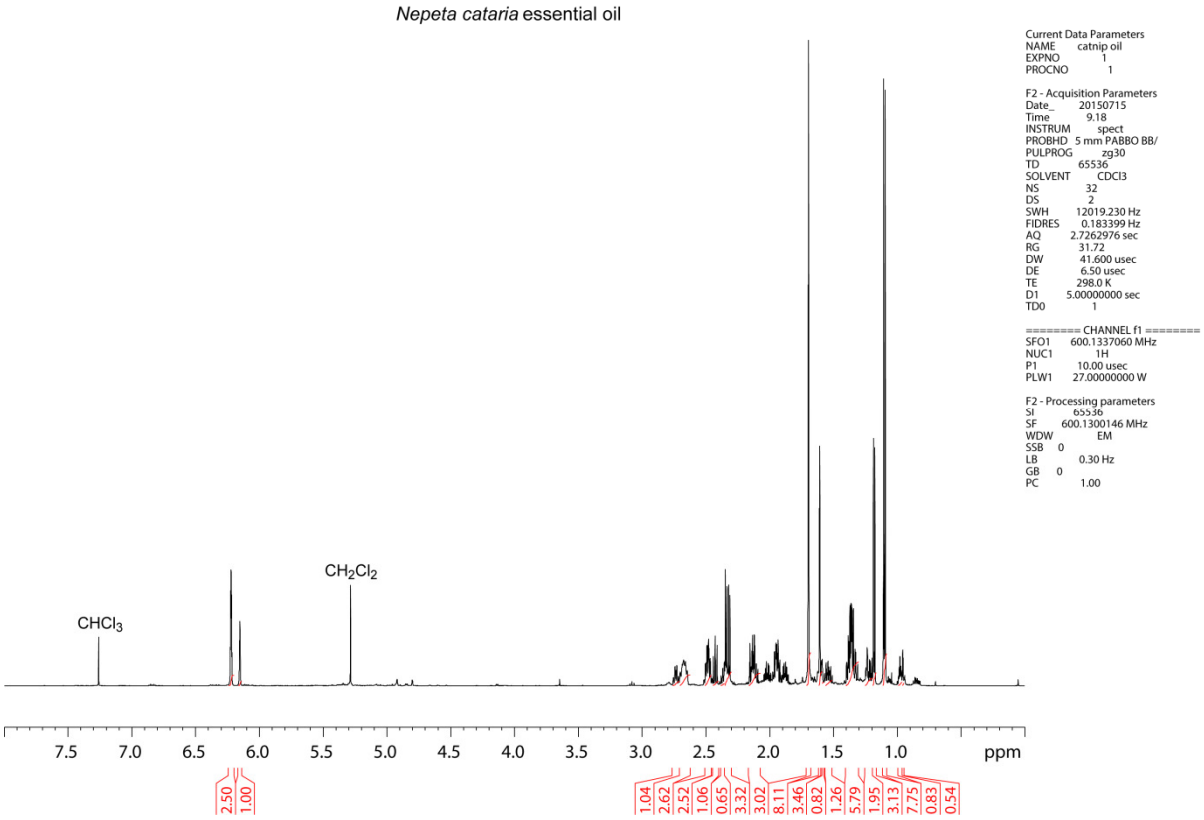
[C]Research School of Biology, The Australian National University, Canberra, ACT 0200, Australia.

[D]Deceased.

[E]Corresponding author. Email: gavin.flematti@uwa.edu.au

*In honour of the late Professor Emilio Ghisalberti.

Fig. S1. ^{1}H NMR spectrum of essential oil derived from *Nepeta cataria* in this study showing the 2:5 ratio of *cis*:*trans*-fused nepetalactones respectively.[1]



For NMR comparison see:

[1] E. J. Eisenbraun, C. E. Browne, R. L. Irvinwillis, D. J. Mcgurk, E. L. Eliel, D. L. Harris. Structure and stereochemistry of 4a*β*,7*α*,7a*β* -Nepetalactone from *Nepeta mussini* and its relationship to the 4a*α*,7*α*,7a*α* and 4a*α*,7*α*,7a*β*-nepetalactones from *N. Cataria*. *J Org Chem*. **1980**, *45*, 3811.

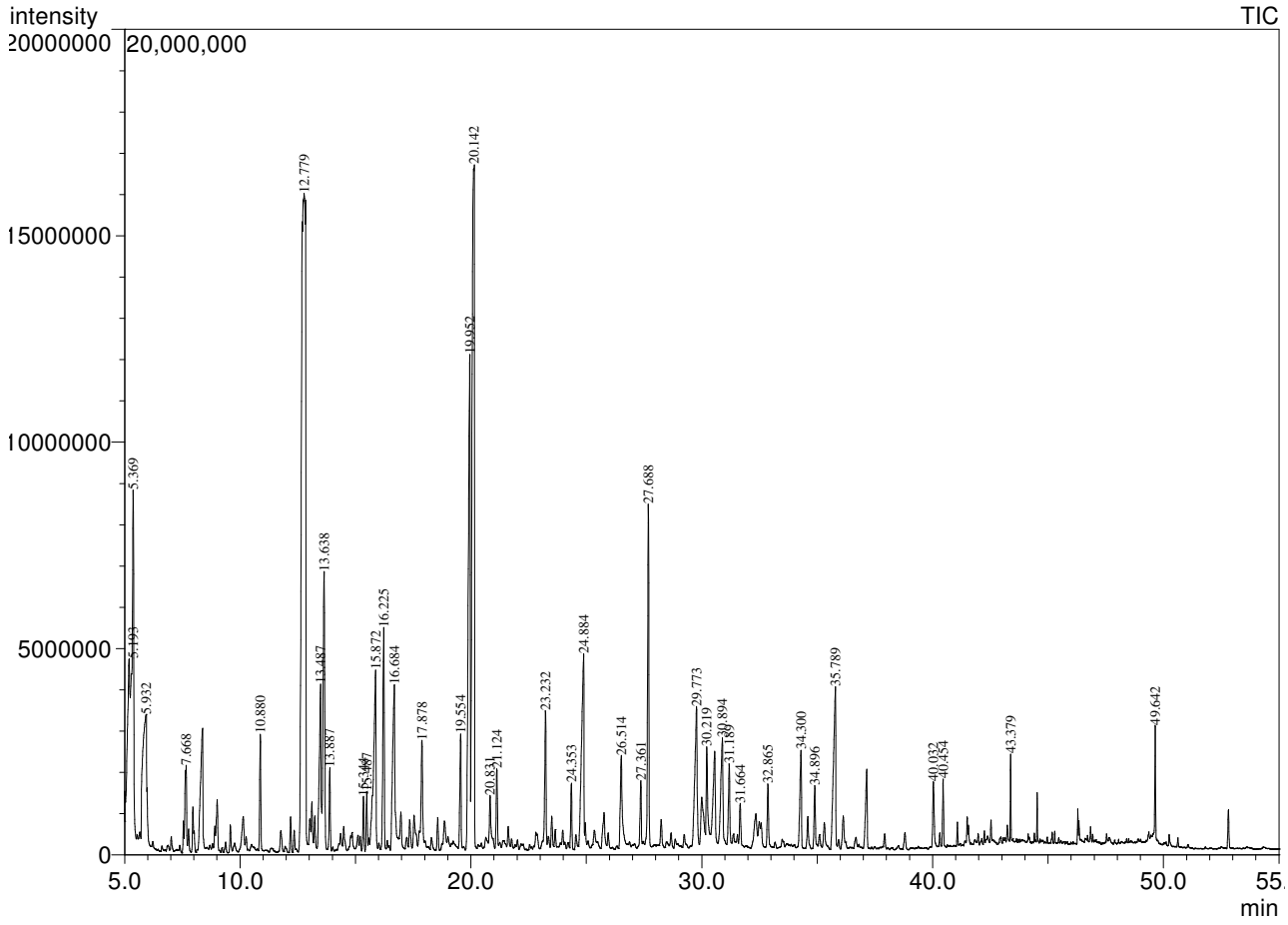
GC-MS supplementary information

The following is the GC-MS library report for the thermal desorption chromatogram shown in Fig. 2. The report shows the experimental mass spectra for the main peaks detected and the closest matching library mass spectrum directly below it. A percentage indication of the library match to the experimental spectrum is given by the similarity index (SI) value. These are tentative library matches only and have not been confirmed with authentic standards.

Sample Information

Analyzed by	: grf	Analyzed	: 24/08/2011 6:16:00 AM
Sample Type	:	Level #	: 0
Sample Name	: Acalypha indica thermal desorption	Sample Amount	: 1
Dilution Factor	: 1 Vial # : 0	Injection Volume	: 0.00

Data File : E:\GC-MS\Christmas Island\thermal desorp\24081104_CDF.QGD
Org Data File :
Method File :
Org Method File :
Report File :
Tuning File :
[Comment]
Thermal desorption from Tenax trap
Modified by : Admin
Modified : 10/12/2015 12:42:33 PM



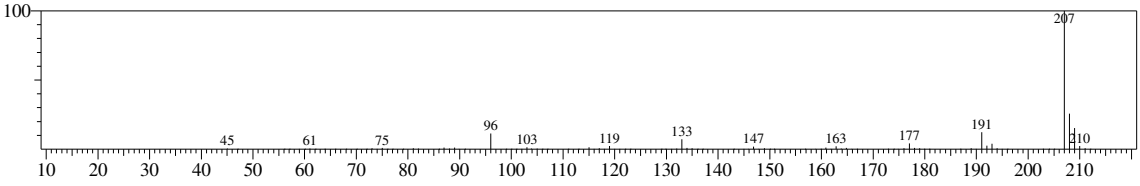
Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	5.193	24809707	2.87	Cyclotrisiloxane, hexamethyl-
2	5.369	45422305	5.25	Cyclotrisiloxane, hexamethyl-
3	5.932	37237398	4.30	Formamide, N,N-dimethyl-
4	7.668	9360989	1.08	4-Hexen-1-ol, (Z)-
5	10.880	9143836	1.06	Methyl ethyl cyclopentene
6	12.779	195993648	22.65	Cyclotetrasiloxane, octamethyl-
7	13.487	20198347	2.33	1-Octen-3-ol
8	13.638	32057345	3.70	1,7-Octadien-3-ol, 2,6-dimethyl-
9	13.887	6692714	0.77	Benzene, 1,2,3-trimethyl-
10	15.344	4134341	0.48	Benzene, 1-methyl-2-(1-methylethyl)-
11	15.487	4153563	0.48	Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate
12	15.872	17765370	2.05	1-Hexanol, 2-ethyl-
13	16.225	22236723	2.57	Benzene, iodo-
14	16.684	25285183	2.92	Benzyl Alcohol
15	17.878	9201867	1.06	Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)-
16	19.554	9874768	1.14	Nonanal
17	19.952	66782592	7.72	3-Isopropylidene-5-methyl-hex-4-en-2-one
18	20.142	119750189	13.84	Cyclopentasiloxane, decamethyl-
19	20.831	3304634	0.38	3-Isopropylidene-5-methyl-hex-4-en-2-one
20	21.124	6558957	0.76	Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)-
21	23.232	11715169	1.35	Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)-
22	24.353	5294293	0.61	Decanal
23	24.884	29239099	3.38	1-Cyclopentene-1-methanol, 2-methyl-5-(1-methylethyl)-
24	26.514	10119742	1.17	2,6-Octadien-1-ol, 3,7-dimethyl-, (E)-
25	27.361	5288964	0.61	2,6-Octadienal, 3,7-dimethyl-, (E)-
26	27.688	30038014	3.47	Cyclohexasiloxane, dodecamethyl-
27	29.773	11233026	1.30	Oxacycloheptadec-8-en-2-one
28	30.219	7920855	0.92	Quinoline, 1,2,3,4-tetrahydro-2-methyl-
29	30.894	11098948	1.28	2-Methylbicyclo[3.2.1]octane
30	31.189	6985707	0.81	Cyclohexene, 1-methyl-4-(1-methylethyl)-, (R)-
31	31.664	3253176	0.38	Copaene

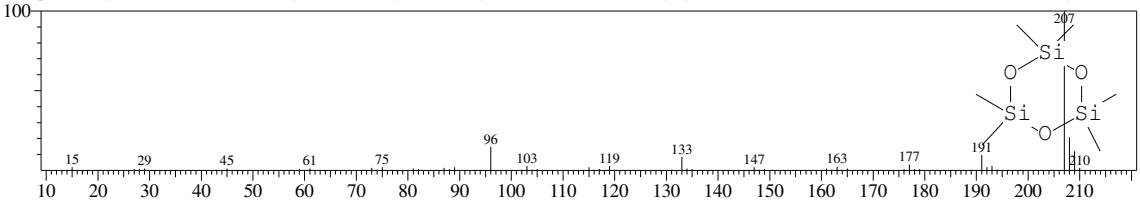
Peak#	R.Time	Area	Area%	Name
32	32.865	5423654	0.63	3H-3a,7-Methanoazulene, 2,4,5,6,7,8-hexahydro-1,4,9,9-tetramethyl-, [3aR-(3a.alpha.,4.beta.,7.alpha.)]-
33	34.300	9464621	1.09	Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4.alpha.,4a.alpha.,7.alpha.,7a.alpha.)-
34	34.896	4970527	0.57	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-
35	35.789	22940528	2.65	Iridomyrmecin
36	40.032	5934754	0.69	Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester
37	40.454	4705126	0.54	Cyclooctasiloxane, hexadecamethyl-
38	43.379	3965183	0.46	Cyclononasiloxane, octadecamethyl-
39	49.642	5744161	0.66	4-Amino-4'-(N,N-dimethylamino)stilbene
		865300023	100.00	

Library

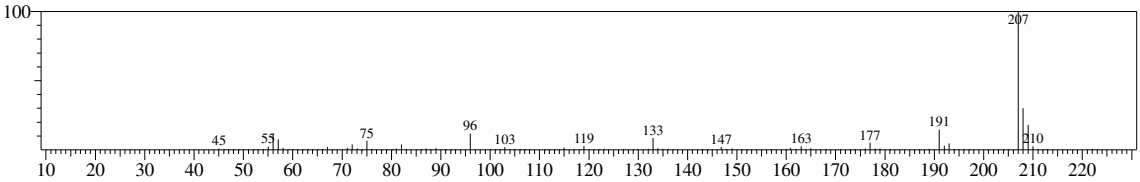
<< Target >>
Line#:1 R.Time:5.196(Scan#:613) MassPeaks:102
RawMode:Averaged 5.188-5.205(612-614) BasePeak:207.00(711693)
BG Mode:Calc. from Peak



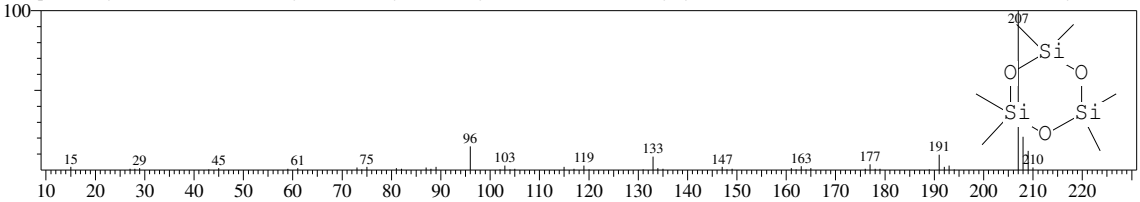
Hit#:1 Entry:53689 Library:NIST05.LIB
SI:96 Formula:C6H18O3Si3 CAS:541-05-9 MolWeight:222 RetIndex:620
CompName:Cyclotrisiloxane, hexamethyl- $$ Dimethylsiloxane cyclic trimer $$ Hexamethylcyclotrisiloxane $$ CH7260 $$ 2,2,4,4,6,6-Hexamethyl-1,3,5,2



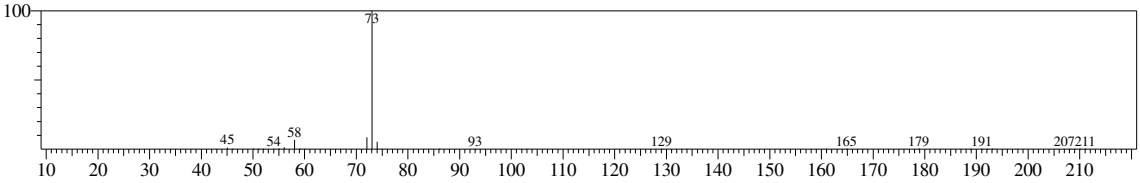
<< Target >>
Line#:2 R.Time:5.371(Scan#:634) MassPeaks:134
RawMode:Averaged 5.363-5.380(633-635) BasePeak:207.00(2347210)
BG Mode:Calc. from Peak



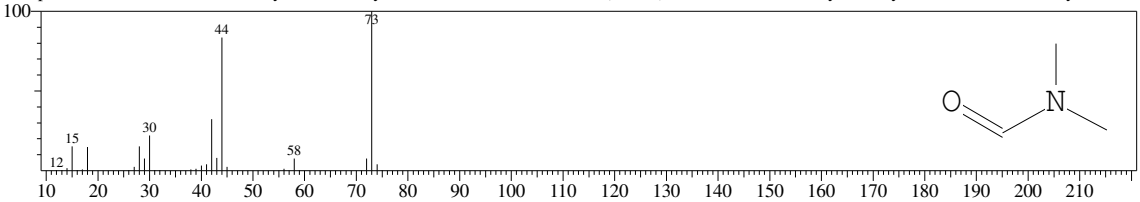
Hit#:1 Entry:53689 Library:NIST05.LIB
SI:89 Formula:C6H18O3Si3 CAS:541-05-9 MolWeight:222 RetIndex:620
CompName:Cyclotrisiloxane, hexamethyl- $$ Dimethylsiloxane cyclic trimer $$ Hexamethylcyclotrisiloxane $$ CH7260 $$ 2,2,4,4,6,6-Hexamethyl-1,3,5,2



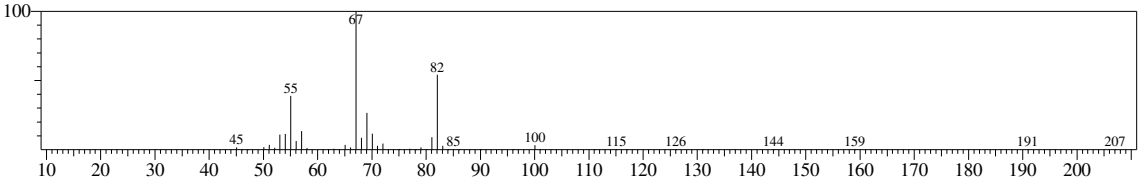
<< Target >>
Line#:3 R.Time:5.930(Scan#:701) MassPeaks:30
RawMode:Averaged 5.921-5.938(700-702) BasePeak:73.05(2510117)
BG Mode:Calc. from Peak



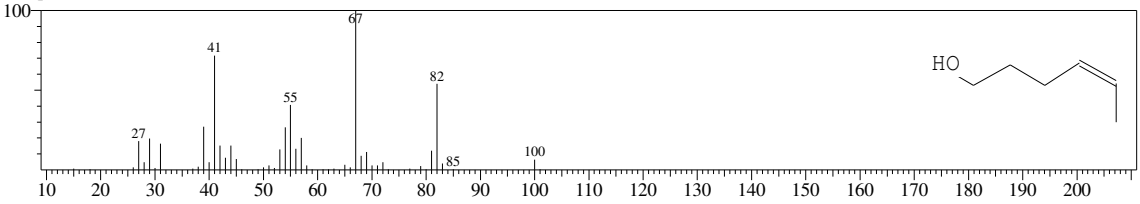
Hit#:1 Entry:384 Library:NIST05s.LIB
SI:98 Formula:C3H7NO CAS:68-12-2 MolWeight:73 RetIndex:557
CompName:Formamide, N,N-dimethyl- $$ Dimethylformamide $$ DMF $$ DMF (Amide) $$ DMFA $$ N-Formyldimethylamine $$ N,N-Dimethylformam



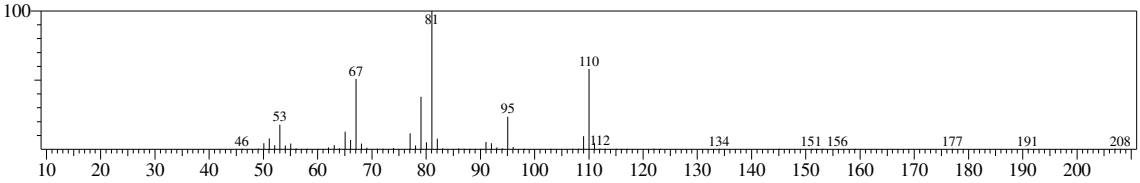
<< Target >>
Line#:4 R.Time:7.671(Scan#:910) MassPeaks:52
RawMode:Averaged 7.663-7.680(909-911) BasePeak:67.05(541859)
BG Mode:Calc. from Peak



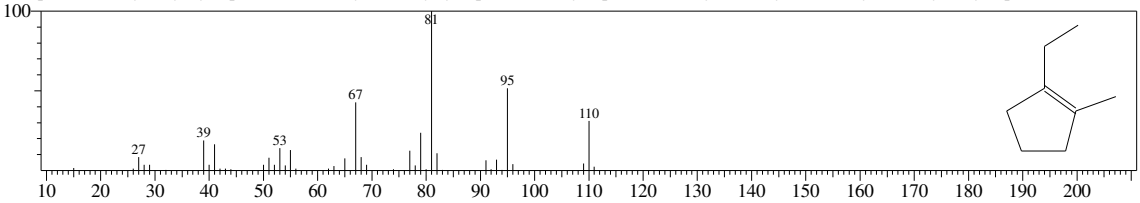
Hit#:1 Entry:2017 Library:NIST05.LIB
SI:94 Formula:C6H12O CAS:928-91-6 MolWeight:100 RetIndex:868
CompName:4-Hexen-1-ol, (Z)- $$ cis-4-Hexen-1-Ol $$ (4Z)-4-Hexen-1-ol # $$



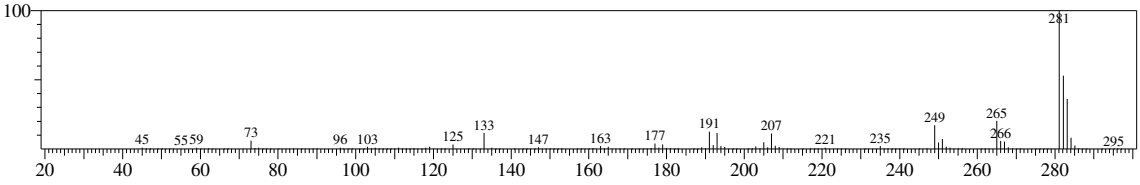
<< Target >>
Line#:5 R.Time:10.880(Scan#:1295) MassPeaks:77
RawMode:Averaged 10.871-10.888(1294-1296) BasePeak:81.05(661886)
BG Mode:Calc. from Peak



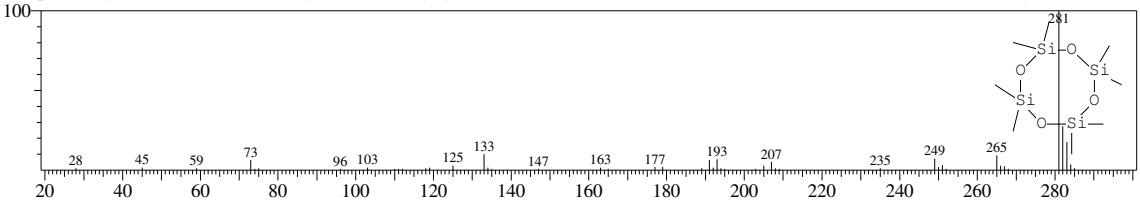
Hit#:1 Entry:3169 Library:NIST05.LIB
SI:90 Formula:C8H14 CAS:19780-56-4 MolWeight:110 RetIndex:860
CompName:Methyl ethyl cyclopentene $$ 1-Ethyl-2-methylcyclopentene $$ Cyclopentene, 1-ethyl-2-methyl- $$ 1-Ethyl-2-methyl-1-cyclopentene # $$



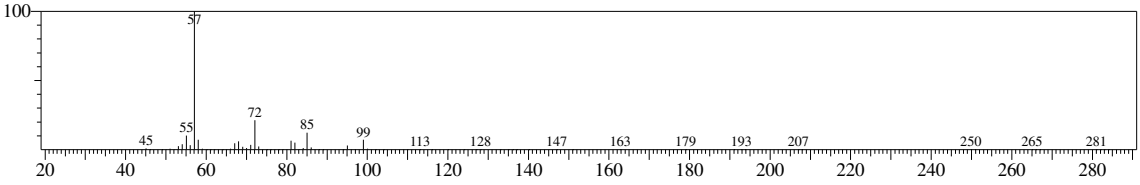
<< Target >>
Line#:6 R.Time:12.780(Scan#:1523) MassPeaks:192
RawMode:Averaged 12.771-12.788(1522-1524) BasePeak:281.10(4081615)
BG Mode:Calc. from Peak



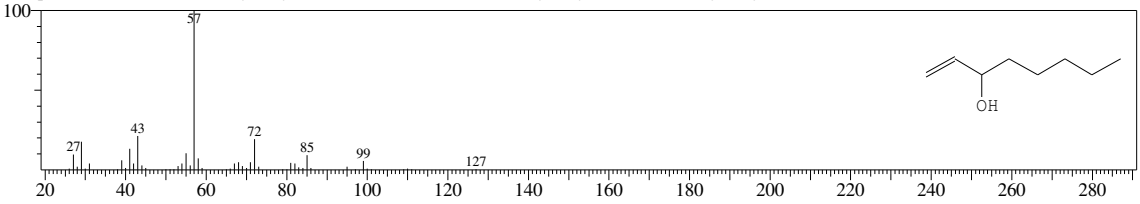
Hit#:1 Entry:23532 Library:NIST05s.LIB
SI:89 Formula:C8H24O4Si4 CAS:556-67-2 MolWeight:296 RetIndex:827
CompName:Cyclotetrasiloxane, octamethyl- $$ Oktamethylcyklotetrasiloxan $$ NUC Silicone VS 7207 $$ CO9810 $$ O9810 $$ Octamethyltetrasiloxane $



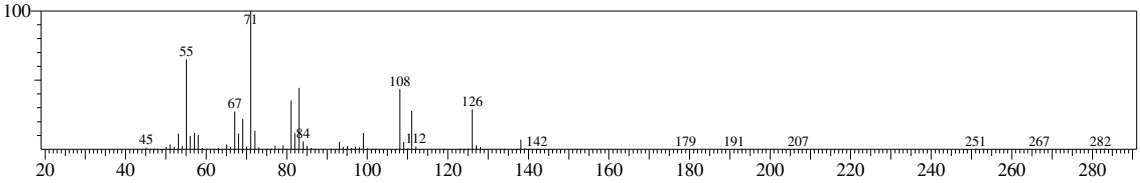
<< Target >>
Line#:7 R.Time:13.488(Scan#:1608) MassPeaks:83
RawMode:Averaged 13.480-13.496(1607-1609) BasePeak:57.05(1510568)
BG Mode:Calc. from Peak



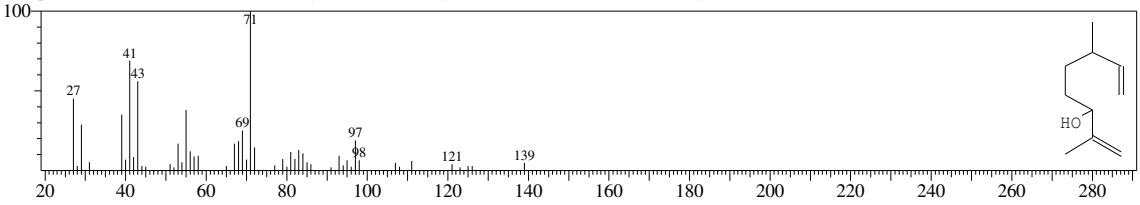
Hit#:1 Entry:7193 Library:NIST05.LIB
SI:97 Formula:C8H16O CAS:3391-86-4 MolWeight:128 RetIndex:969
CompName:1-Octen-3-ol $$ Amyl vinyl carbinol $$ Oct-1-en-3-ol $$ Vinyl amyl carbinol $$ 3-Hydroxy-1-octene $$ Matsutake alcohol $$ 1-Okten-3-ol $$



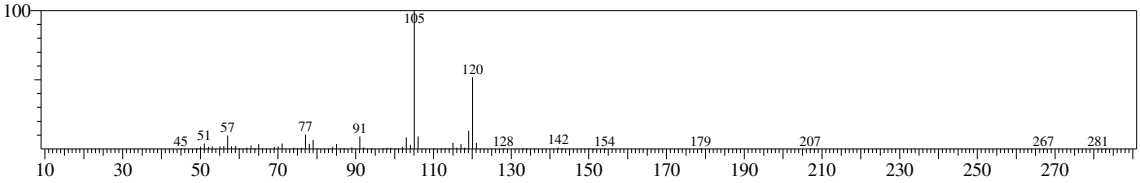
<< Target >>
Line#:8 R.Time:13.638(Scan#:1626) MassPeaks:92
RawMode:Averaged 13.630-13.646(1625-1627) BasePeak:71.05(1088936)
BG Mode:Calc. from Peak



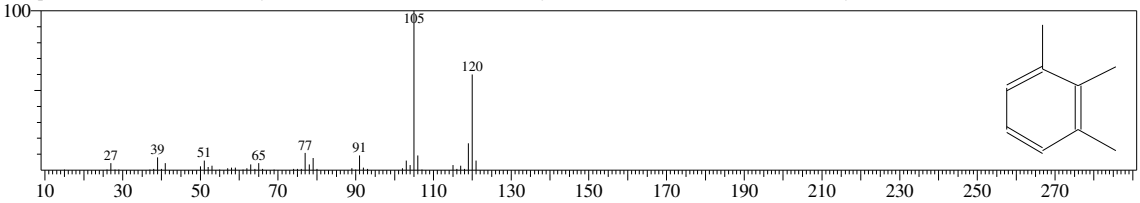
Hit#:1 Entry:16975 Library:NIST05.LIB
SI:81 Formula:C10H18O CAS:22460-59-9 MolWeight:154 RetIndex:1071
CompName:1,7-Octadien-3-ol, 2,6-dimethyl- $$ 3,7-Dimethyl-1, 7-octadien-6-ol $$ 2,6-Dimethyl-1,7-octadien-3-ol # $$



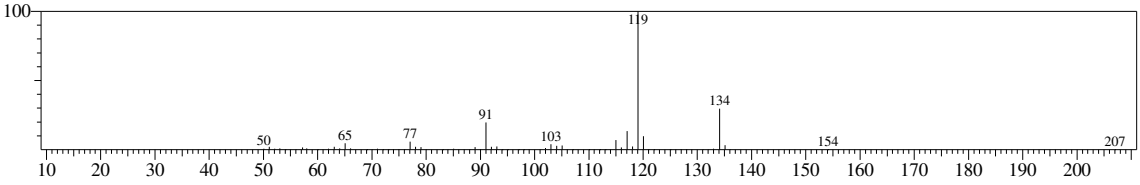
<< Target >>
Line#:9 R.Time:13.888(Scan#:1656) MassPeaks:84
RawMode:Averaged 13.880-13.896(1655-1657) BasePeak:105.05(655097)
BG Mode:Calc. from Peak



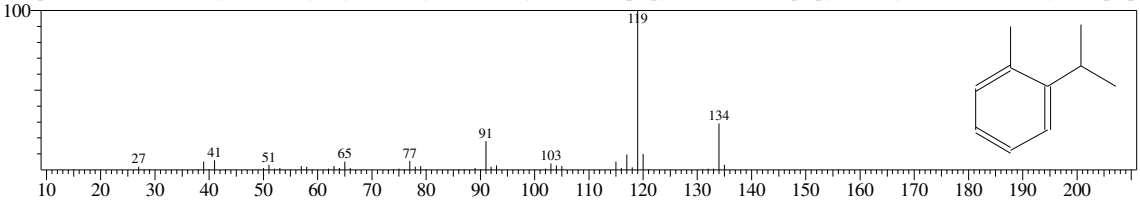
Hit#:1 Entry:3934 Library:NIST05s.LIB
SI:93 Formula:C9H12 CAS:526-73-8 MolWeight:120 RetIndex:1020
CompName:Benzene, 1,2,3-trimethyl- $$ Hemimellitene $$ 1,2,3-Trimethylbenzene $$ Hemellitol $$ 1,2,3-Trimethyl benzene $$



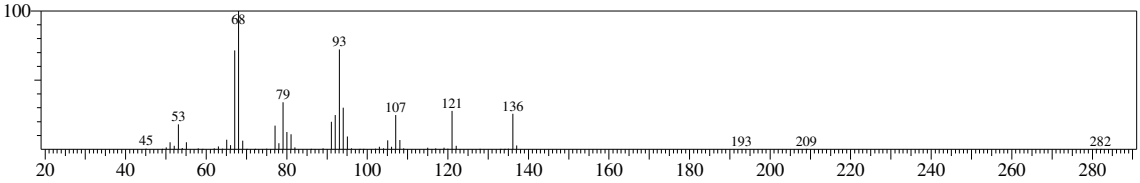
<< Target >>
Line#:10 R.Time:15.346(Scan#:1831) MassPeaks:77
RawMode:Averaged 15.338-15.355(1830-1832) BasePeak:119.05(517542)
BG Mode:Calc. from Peak



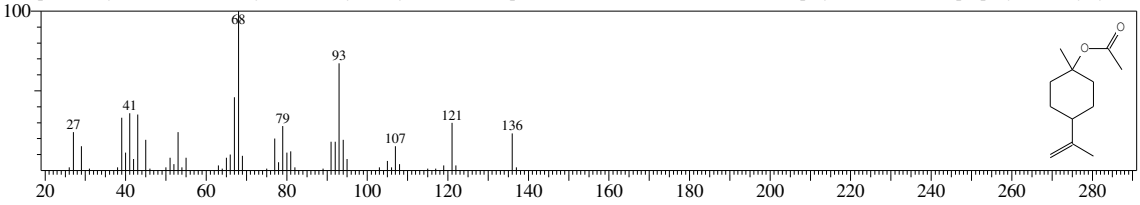
Hit#:1 Entry:5934 Library:NIST05s.LIB
SI:97 Formula:C10H14 CAS:527-84-4 MolWeight:134 RetIndex:1042
CompName:Benzene, 1-methyl-2-(1-methylethyl)- $$ o-Cymene $$ o-Cymol $$ o-Isopropyltoluene $$ 1-Isopropyl-2-methylbenzene $$ 1-Methyl-2-isoprop



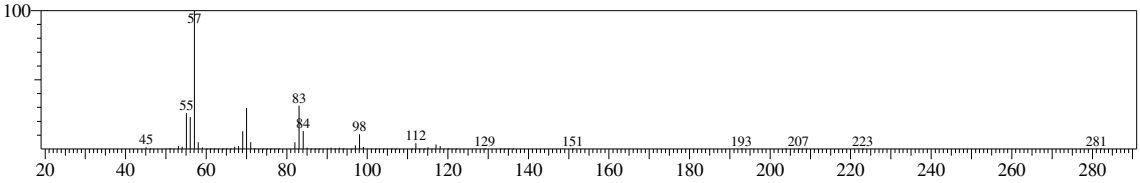
<< Target >>
Line#:11 R.Time:15.488(Scan#:1848) MassPeaks:71
RawMode:Averaged 15.480-15.496(1847-1849) BasePeak:68.05(226263)
BG Mode:Calc. from Peak



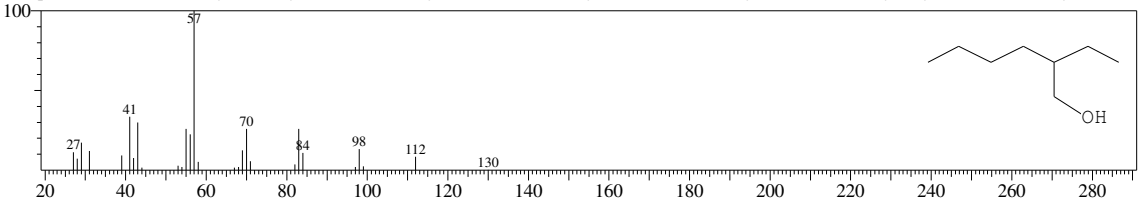
Hit#:1 Entry:15684 Library:NIST05s.LIB
SI:94 Formula:C12H20O2 CAS:10198-23-9 MolWeight:196 RetIndex:1348
CompName:Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, acetate $$ p-Menth-8-en-1-ol, acetate $$ .beta.-Terpinyl acetate $$ 4-Isopropenyl-1-methylcycloh



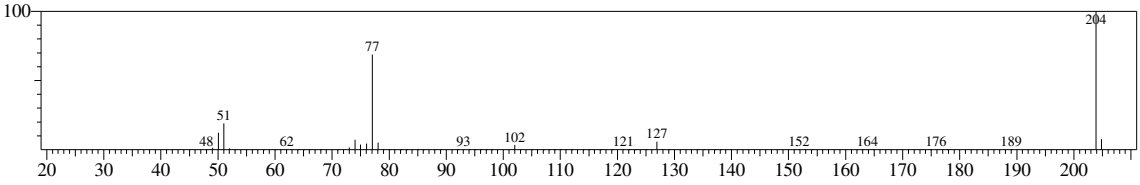
<< Target >>
Line#:12 R.Time:15.871(Scan#:1894) MassPeaks:82
RawMode:Averaged 15.863-15.880(1893-1895) BasePeak:57.05(1299833)
BG Mode:Calc. from Peak



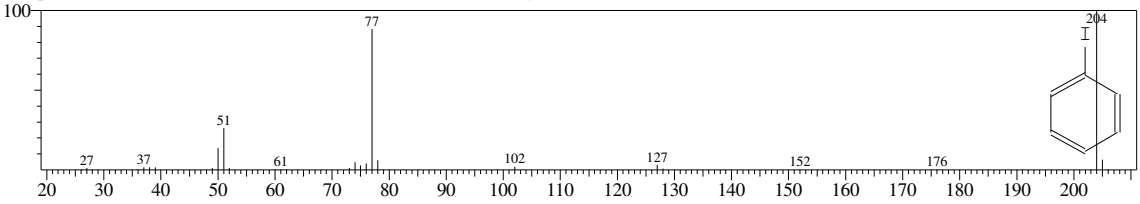
Hit#:1 Entry:5356 Library:NIST05s.LIB
SI:95 Formula:C8H18O CAS:104-76-7 MolWeight:130 RetIndex:995
CompName:1-Hexanol, 2-ethyl- $$ Ethylhexanol $$ 2-Ethyl-1-hexanol $$ 2-Ethylhexan-1-ol $$ 2-Ethylhexanol $$ 2-Ethylhexyl alcohol $$ 2-Ethyl-hexanol



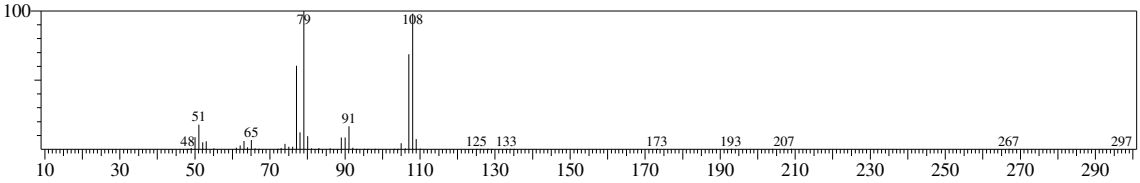
<< Target >>
Line#:13 R.Time:16.221(Scan#:1936) MassPeaks:85
RawMode:Averaged 16.213-16.230(1935-1937) BasePeak:203.85(2116314)
BG Mode:Calc. from Peak



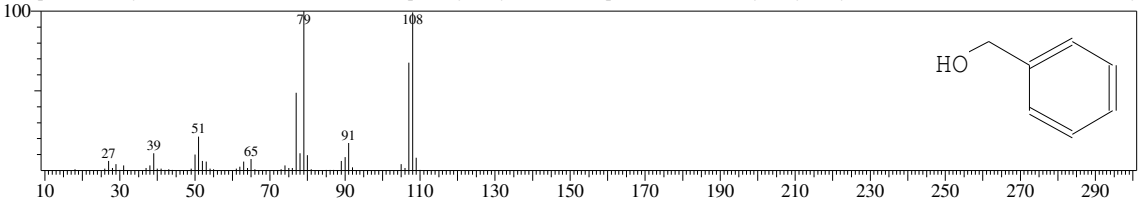
Hit#:1 Entry:16558 Library:NIST05s.LIB
SI:95 Formula:C6H5I CAS:591-50-4 MolWeight:204 RetIndex:1085
CompName:Benzene, iodo- $$ Benzene iodide $$ Iodobenzene $$ Phenyl iodide $$



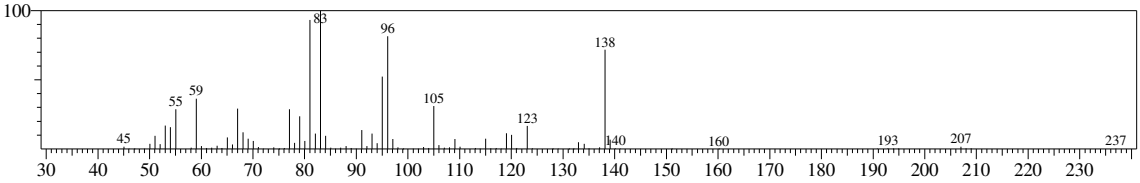
<< Target >>
Line#:14 R.Time:16.688(Scan#:1992) MassPeaks:63
RawMode:Averaged 16.680-16.696(1991-1993) BasePeak:79.05(774983)
BG Mode:Calc. from Peak



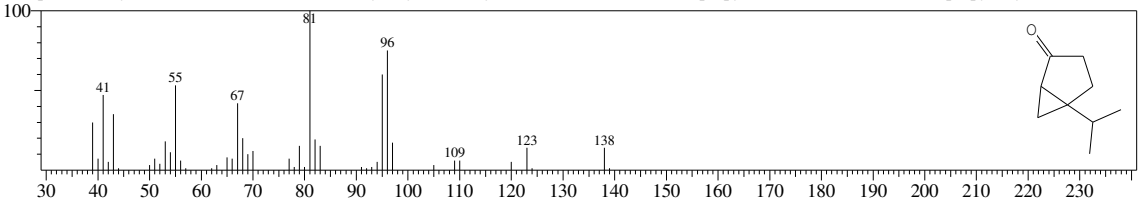
Hit#:1 Entry:2454 Library:NIST05s.LIB
SI:98 Formula:C7H8O CAS:100-51-6 MolWeight:108 RetIndex:1036
CompName:Benzyl Alcohol $$ Benzenemethanol $$ .alpha.-Hydroxytoluene $$ .alpha.-Toluenol $$ (Hydroxymethyl)benzene $$ Benzenecarbinol $$ Pheny



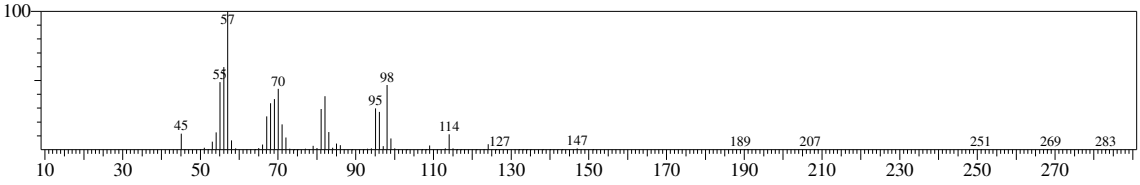
<< Target >>
Line#:15 R.Time:17.880(Scan#:2135) MassPeaks:94
RawMode:Averaged 17.871-17.888(2134-2136) BasePeak:83.05(269825)
BG Mode:Calc. from Peak



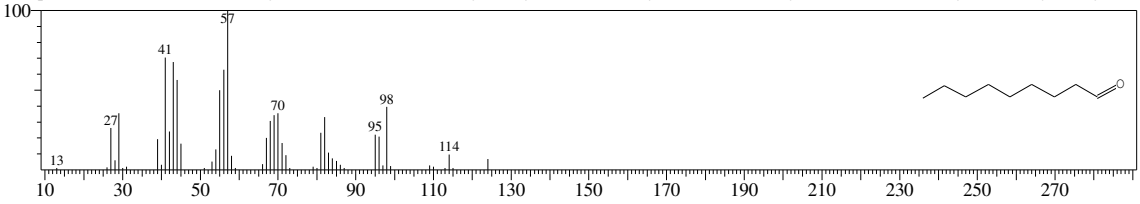
Hit#:1 Entry:10187 Library:NIST05.LIB
SI:80 Formula:C9H14O CAS:513-20-2 MolWeight:138 RetIndex:1001
CompName:Bicyclo[3.1.0]hexan-2-one, 5-(1-methylethyl)- $$ Bicyclo[3.1.0]hexan-2-one, 5-isopropyl- $$ Sabina ketone $$ 5-Isopropylbicyclo[3.1.0]hexan



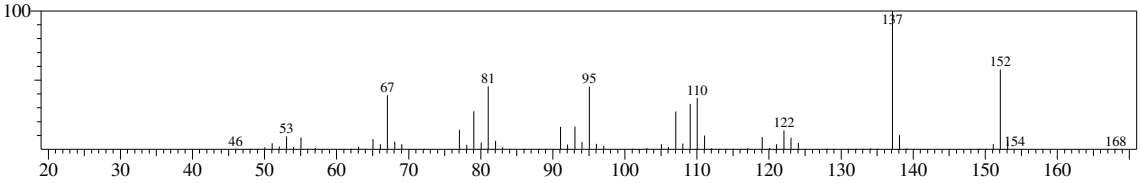
<< Target >>
Line#:16 R.Time:19.555(Scan#:2336) MassPeaks:93
RawMode:Averaged 19.546-19.563(2335-2337) BasePeak:57.05(397973)
BG Mode:Calc. from Peak



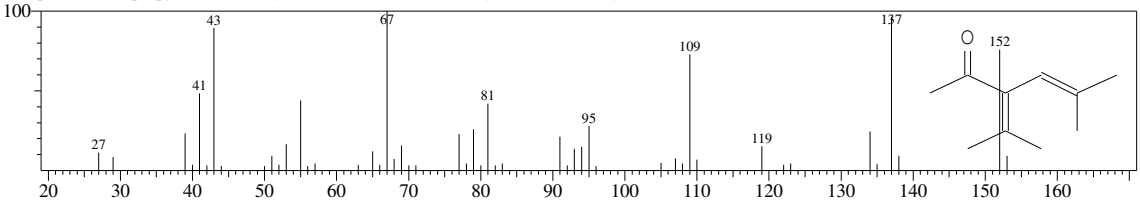
Hit#:1 Entry:7237 Library:NIST05s.LIB
SI:96 Formula:C9H18O CAS:124-19-6 MolWeight:142 RetIndex:1104
CompName:Nonanal $$ n-Nonaldehyde $$ n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ Nonanaldehyde $$ Nonanoic aldehyde $$ Nonylaldehyde $$



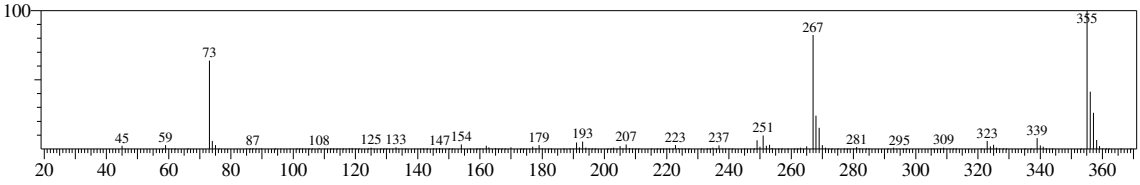
<< Target >>
Line#:17 R.Time:19.955(Scan#:2384) MassPeaks:90
RawMode:Averaged 19.946-19.963(2383-2385) BasePeak:137.10(1771952)
BG Mode:Calc. from Peak



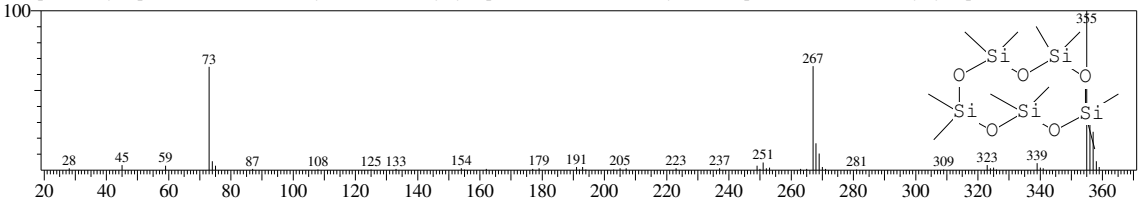
Hit#:1 Entry:15816 Library:NIST05.LIB
SI:84 Formula:C10H16O CAS:64149-32-2 MolWeight:152 RetIndex:1099
CompName:3-Isopropylidene-5-methyl-hex-4-en-2-one $$ 5-Methyl-3-(1-methylethylidene)-4-hexen-2-one # $$



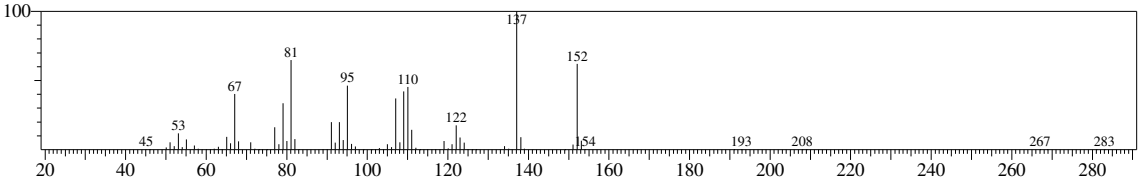
<< Target >>
Line#:18 R.Time:20.146(Scan#:2407) MassPeaks:209
RawMode:Averaged 20.138-20.155(2406-2408) BasePeak:355.10(3134207)
BG Mode:Calc. from Peak



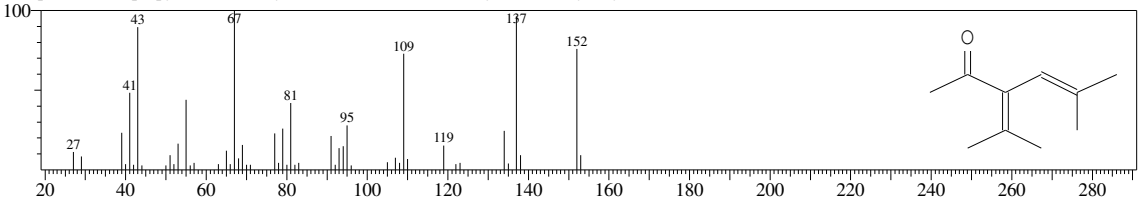
Hit#:1 Entry:135081 Library:NIST05.LIB
SI:95 Formula:C10H30O5Si5 CAS:541-02-6 MolWeight:370 RetIndex:1034
CompName:Cyclopentasiloxane, decamethyl- $$ Decamethylcyclopentasiloxane $$ Dimethylsiloxane pentamer $$ Dekamethylcyklopentasiloxan $$ CD377



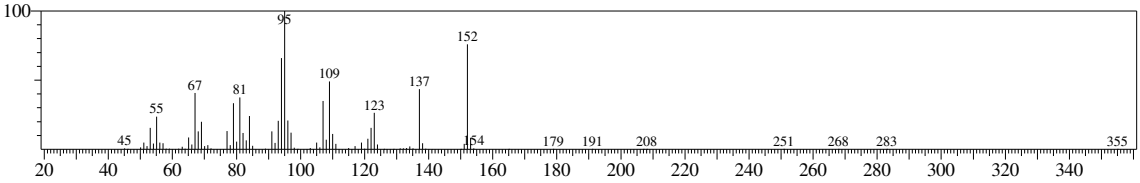
<< Target >>
Line#:19 R.Time:20.830(Scan#:2489) MassPeaks:91
RawMode:Averaged 20.821-20.838(2488-2490) BasePeak:137.10(135392)
BG Mode:Calc. from Peak



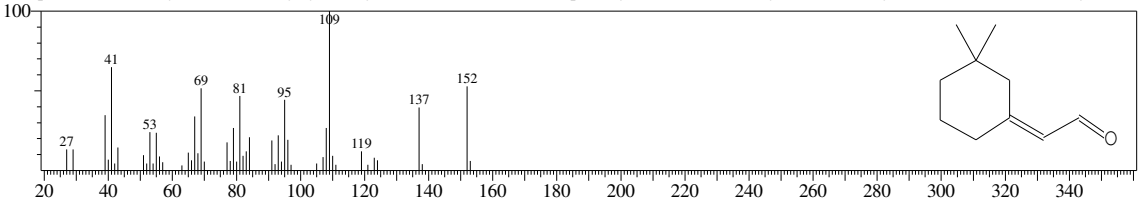
Hit#:1 Entry:15816 Library:NIST05.LIB
SI:83 Formula:C10H16O CAS:64149-32-2 MolWeight:152 RetIndex:1099
CompName:3-Isopropylidene-5-methyl-hex-4-en-2-one $$ 5-Methyl-3-(1-methylethylidene)-4-hexen-2-one # $$



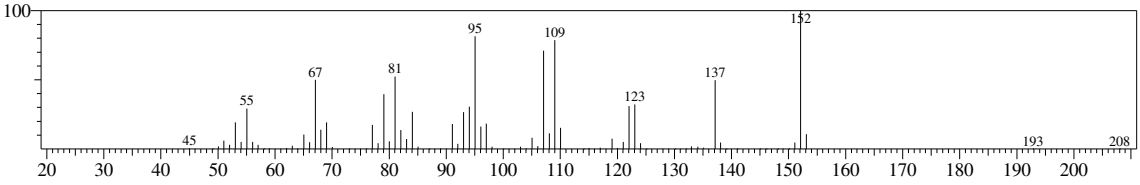
<< Target >>
Line#:20 R.Time:21.121(Scan#:2524) MassPeaks:98
RawMode:Averaged 21.113-21.130(2523-2525) BasePeak:95.05(210915)
BG Mode:Calc. from Peak



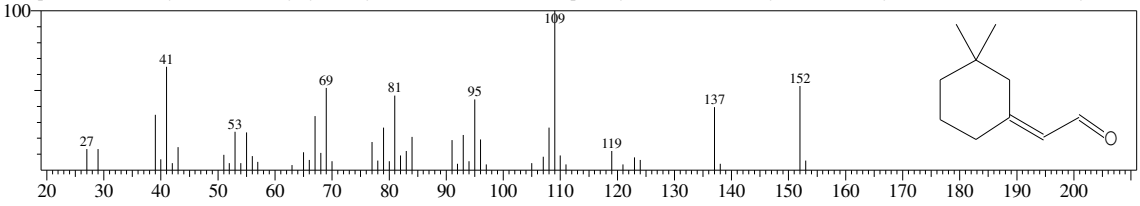
Hit#:1 Entry:15942 Library:NIST05.LIB
SI:86 Formula:C10H16O CAS:26532-25-2 MolWeight:152 RetIndex:1226
CompName:Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)- $$ .delta.1,.alpha.-Cyclohexaneacetaldehyde, 3,3-dimethyl-, (E)- $$ (E)-3,3-Dimethyl-.delta



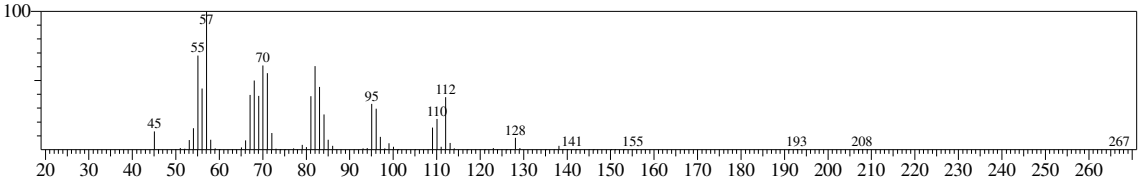
<< Target >>
Line#:21 R.Time:23.230(Scan#:2777) MassPeaks:94
RawMode:Averaged 23.221-23.238(2776-2778) BasePeak:152.10(309964)
BG Mode:Calc. from Peak



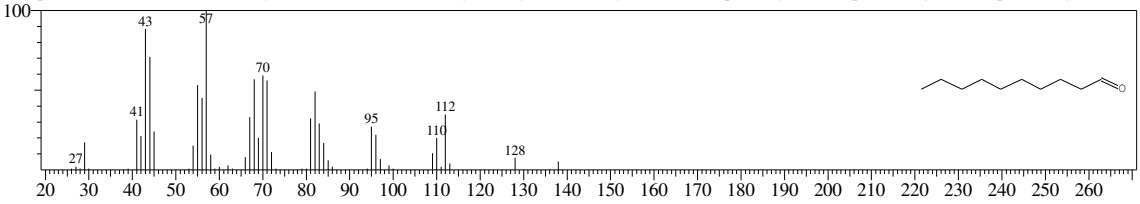
Hit#:1 Entry:15942 Library:NIST05.LIB
SI:85 Formula:C10H16O CAS:26532-25-2 MolWeight:152 RetIndex:1226
CompName:Acetaldehyde, (3,3-dimethylcyclohexylidene)-, (E)- $$ .delta.1,.alpha.-Cyclohexaneacetaldehyde, 3,3-dimethyl-, (E)- $$ (E)-3,3-Dimethyl-.delta



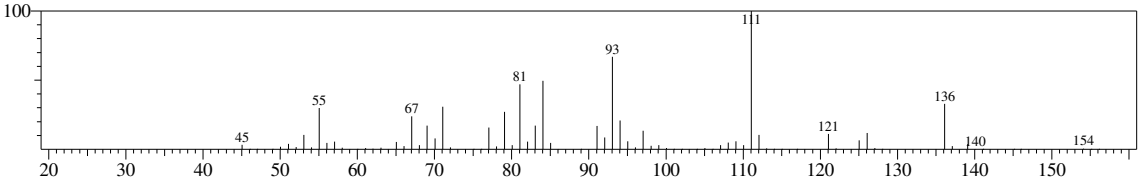
<< Target >>
Line#:22 R.Time:24.355(Scan#:2912) MassPeaks:87
RawMode:Averaged 24.346-24.363(2911-2913) BasePeak:57.05(168637)
BG Mode:Calc. from Peak



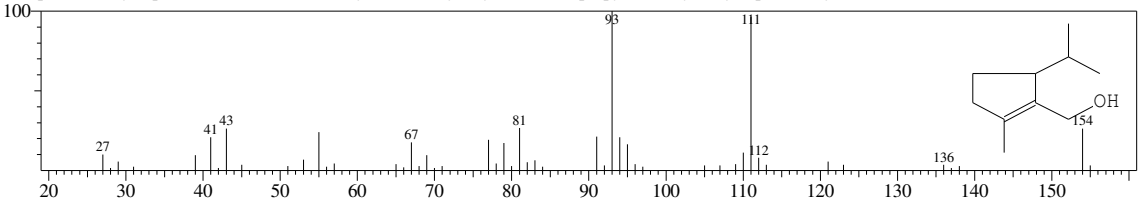
Hit#:1 Entry:9741 Library:NIST05s.LIB
SI:94 Formula:C10H20O CAS:112-31-2 MolWeight:156 RetIndex:1204
CompName:Decanal $$ n-Decaldehyde $$ n-Decanal $$ n-Decyl aldehyde $$ Aldehyde C10 $$ Capraldehyde $$ Capric aldehyde $$ Caprinaldehyde $$ Ca



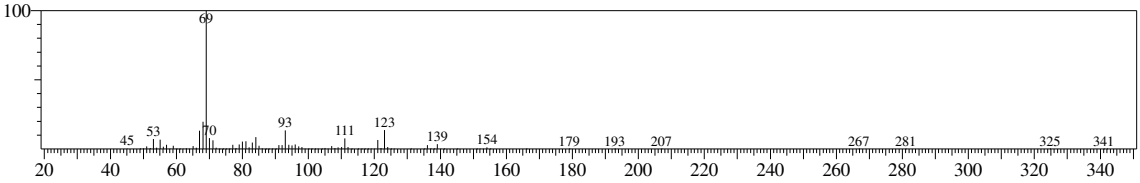
<< Target >>
Line#:23 R.Time:24.888(Scan#:2976) MassPeaks:86
RawMode:Averaged 24.880-24.896(2975-2977) BasePeak:111.05(633254)
BG Mode:Calc. from Peak



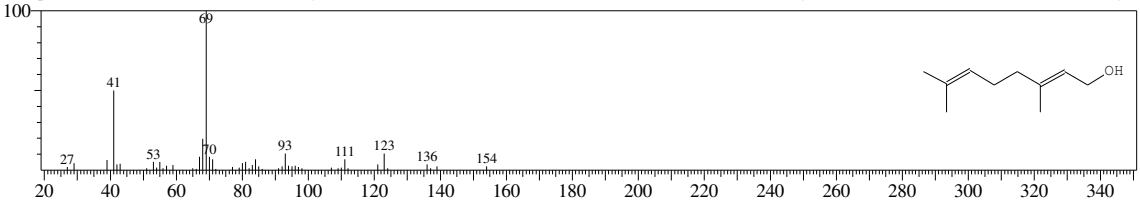
Hit#:1 Entry:17025 Library:NIST05.LIB
SI:81 Formula:C10H18O CAS:80113-82-2 MolWeight:154 RetIndex:1199
CompName:1-Cyclopentene-1-methanol, 2-methyl-5-(1-methylethyl)- $$ (5-Isopropyl-2-methyl-1-cyclopenten-1-yl)methanol # $$



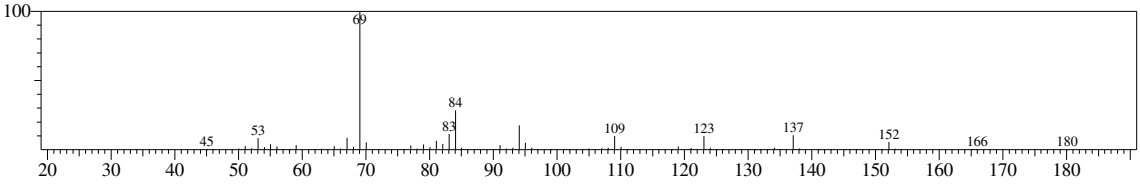
<< Target >>
Line#:24 R.Time:26.513(Scan#:3171) MassPeaks:101
RawMode:Averaged 26.505-26.521(3170-3172) BasePeak:69.05(681491)
BG Mode:Calc. from Peak



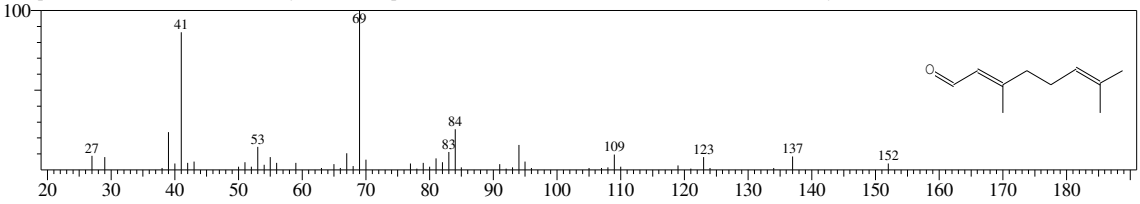
Hit#:1 Entry:9387 Library:NIST05s.LIB
SI:96 Formula:C10H18O CAS:106-24-1 MolWeight:154 RetIndex:1228
CompName:2,6-Octadien-1-ol, 3,7-dimethyl-, (E)- $$ trans-Geraniol $$ Guaniol $$ Lemonol $$ Nerol $$ Neryl Alcohol $$ Geraniol $$ trans-3,7-Dimethyl-



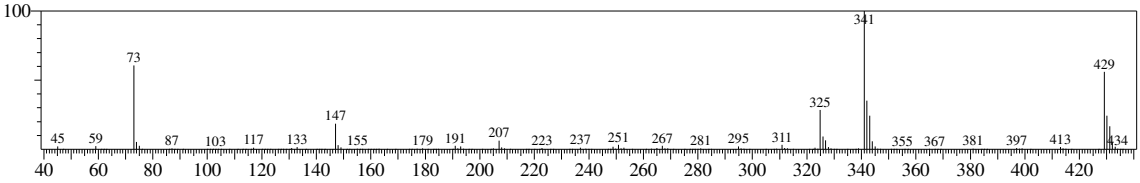
<< Target >>
Line#:25 R.Time:27.363(Scan#:3273) MassPeaks:93
RawMode:Averaged 27.355-27.371(3272-3274) BasePeak:69.05(504766)
BG Mode:Calc. from Peak



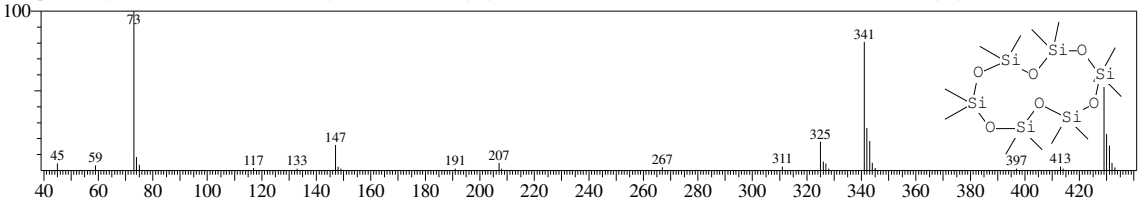
Hit#:1 Entry:8947 Library:NIST05s.LIB
SI:96 Formula:C10H16O CAS:141-27-5 MolWeight:152 RetIndex:1174
CompName:2,6-Octadienal, 3,7-dimethyl-, (E)- $$ .alpha.-Citral $$ (E)-Citral $$ trans-Citral $$ trans-3,7-Dimethyl-2,6-octadienal $$ Citral a $$ Geranaldeł



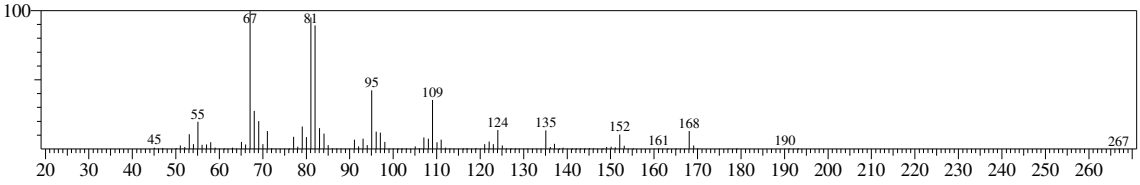
<< Target >>
Line#:26 R.Time:27.688(Scan#:3312) MassPeaks:230
RawMode:Averaged 27.680-27.696(3311-3313) BasePeak:341.00(1654503)
BG Mode:Calc. from Peak



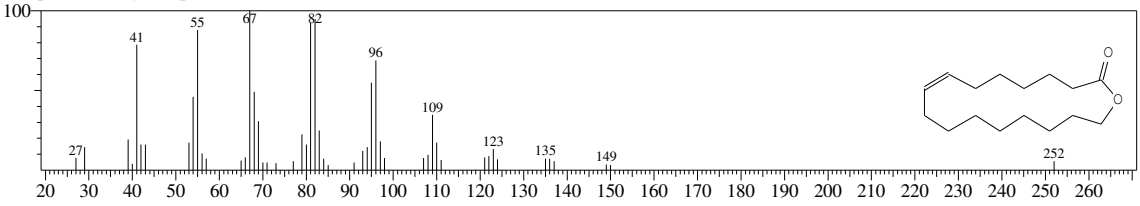
Hit#:1 Entry:27001 Library:NIST05s.LIB
SI:91 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:1240
CompName:Cyclohexasiloxane, dodecamethyl- $$ Dodecamethylcyclohexasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12-Dodecamethylcyclohexasiloxane # $$



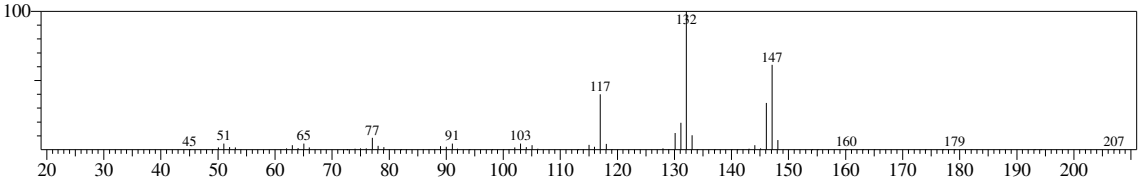
<< Target >>
Line#:27 R.Time:29.771(Scan#:3562) MassPeaks:127
RawMode:Averaged 29.763-29.780(3561-3563) BasePeak:67.05(344949)
BG Mode:Calc. from Peak



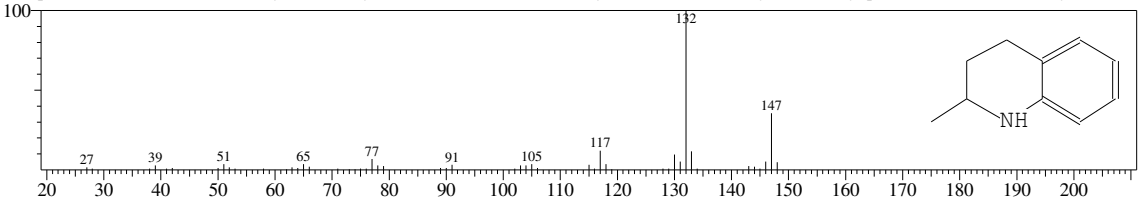
Hit#:1 Entry:72510 Library:NIST05.LIB
SI:86 Formula:C16H28O2 CAS:123-69-3 MolWeight:252 RetIndex:2246
CompName:Oxacycloheptadec-8-en-2-one $$ Ambrettolid $$ Ambrettolide $$ Musk ambrette $$ Musk ambrette, natural $$ Musk natural $$ 7-Hexadeceno



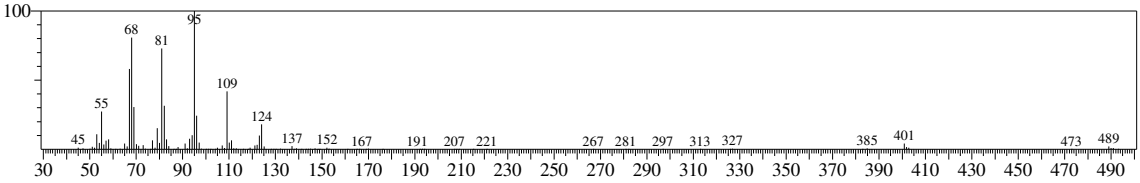
<< Target >>
Line#:28 R.Time:30.221(Scan#:3616) MassPeaks:79
RawMode:Averaged 30.213-30.230(3615-3617) BasePeak:132.10(573711)
BG Mode:Calc. from Peak



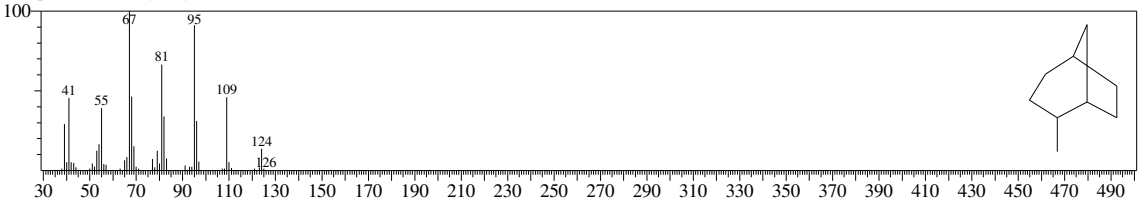
Hit#:1 Entry:13748 Library:NIST05.LIB
SI:89 Formula:C10H13N CAS:1780-19-4 MolWeight:147 RetIndex:1373
CompName:Quinoline, 1,2,3,4-tetrahydro-2-methyl- $$ Quinaldine, 1,2,3,4-tetrahydro- $$ 1,2,3,4-Tetahydro-2-methylquinoline $$ 1,2,3,4-Tetrahydro-2-me



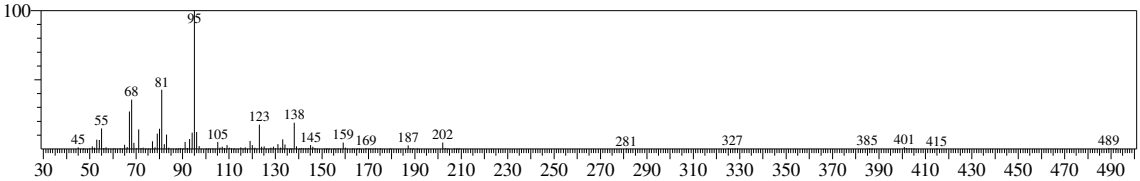
<< Target >>
Line#:29 R.Time:30.896(Scan#:3697) MassPeaks:143
RawMode:Averaged 30.888-30.905(3696-3698) BasePeak:95.05(322459)
BG Mode:Calc. from Peak



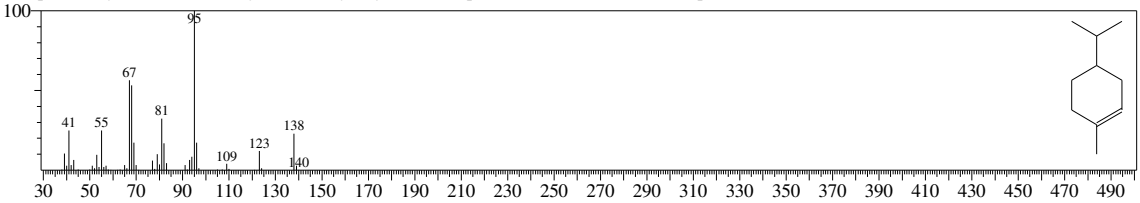
Hit#:1 Entry:5945 Library:NIST05.LIB
SI:89 Formula:C9H16 CAS:0-00-0 MolWeight:124 RetIndex:923
CompName:2-Methylbicyclo[3.2.1]octane



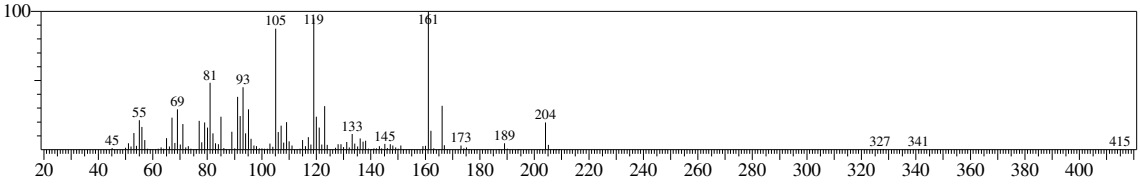
<< Target >>
Line#:30 R.Time:31.188(Scan#:3732) MassPeaks:150
RawMode:Averaged 31.180-31.196(3731-3733) BasePeak:95.05(376282)
BG Mode:Calc. from Peak



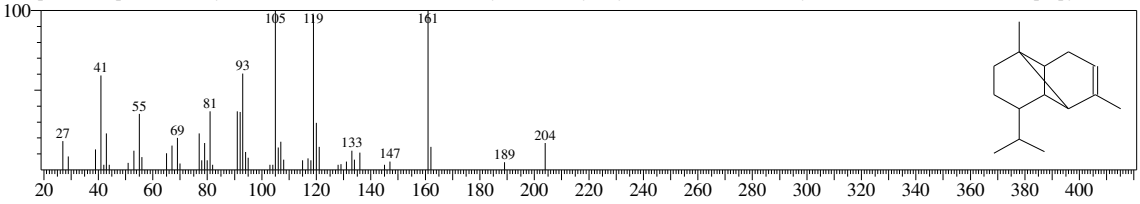
Hit#:1 Entry:6667 Library:NIST05s.LIB
SI:84 Formula:C10H18 CAS:1195-31-9 MolWeight:138 RetIndex:987
CompName:Cyclohexene, 1-methyl-4-(1-methylethyl)-, (R)- $$ p-Menth-1-ene, (R)-(+)- $$ (+)-p-Menth-1-ene $$ (+)-Carvomenthene $$ (+)-1-Menthene $$



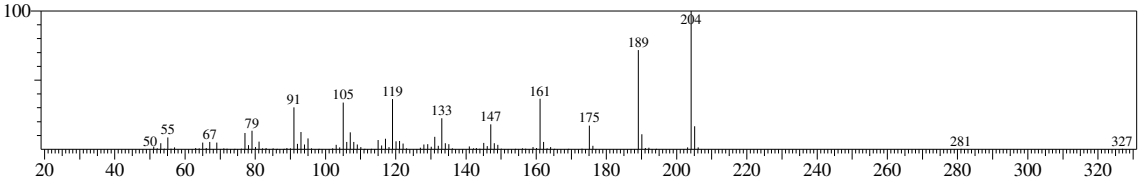
<< Target >>
Line#:31 R.Time:31.663(Scan#:3789) MassPeaks:135
RawMode:Averaged 31.655-31.671(3788-3790) BasePeak:161.10(79553)
BG Mode:Calc. from Peak



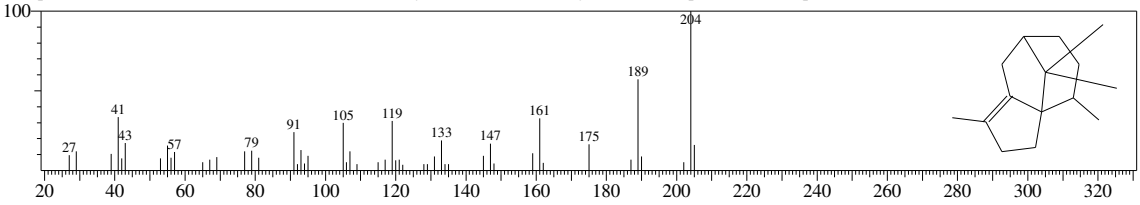
Hit#:1 Entry:16777 Library:NIST05s.LIB
SI:84 Formula:C15H24 CAS:3856-25-5 MolWeight:204 RetIndex:1221
CompName:Copaene $$ Tricyclo[4.4.0.02,7]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, stereoisomer $$ Tricyclo[4.4.0.02,7]dec-3-ene, 8-isopropyl-1,3-din



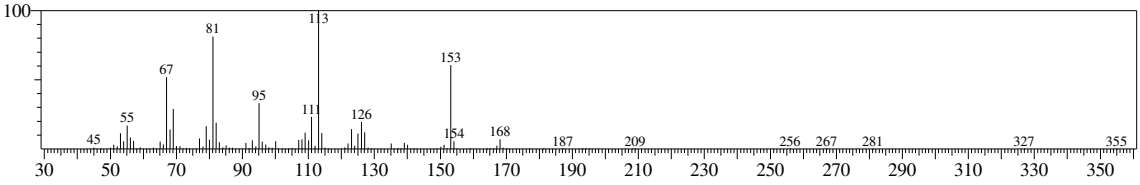
<< Target >>
Line#:32 R.Time:32.863(Scan#:3933) MassPeaks:125
RawMode:Averaged 32.855-32.871(3932-3934) BasePeak:204.10(222889)
BG Mode:Calc. from Peak



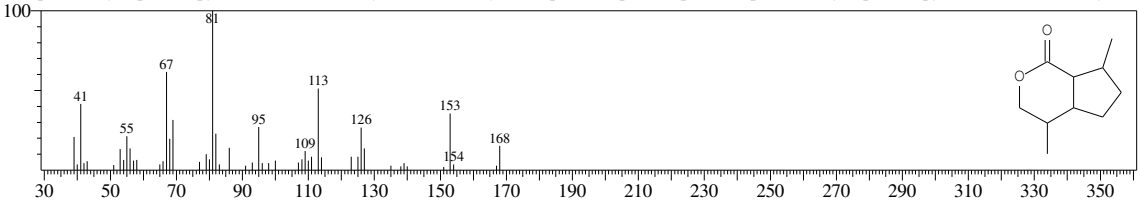
Hit#:1 Entry:43588 Library:NIST05.LIB
SI:91 Formula:C15H24 CAS:2387-78-2 MolWeight:204 RetIndex:1432
CompName:3H-3a,7-Methanoazulene, 2,4,5,6,7,8-hexahydro-1,4,9,9-tetramethyl-, [3aR-(3a.alpha.,4.beta.,7.alpha.)]- $$ 3H-3a.beta.,7-Methanoazulene, 2,4.



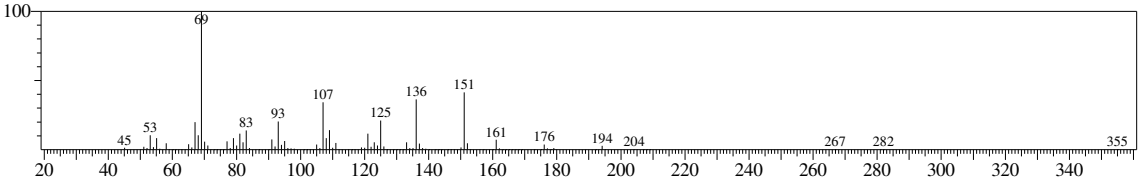
<< Target >>
Line#:33 R.Time:34.296(Scan#:4105) MassPeaks:120
RawMode:Averaged 34.288-34.305(4104-4106) BasePeak:113.05(310282)
BG Mode:Calc. from Peak



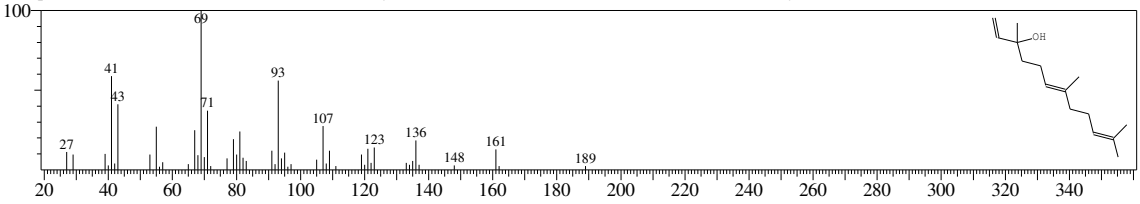
Hit#:1 Entry:23555 Library:NIST05.LIB
SI:89 Formula:C10H16O2 CAS:17672-96-7 MolWeight:168 RetIndex:1329
CompName:Cyclopenta[c]pyran-1(3H)-one, hexahydro-4,7-dimethyl-, (4.alpha.,4a.alpha.,7.alpha.,7a.alpha.)- $$ Cyclopenta[c]pyran-1(3H)-one, hexahydro-



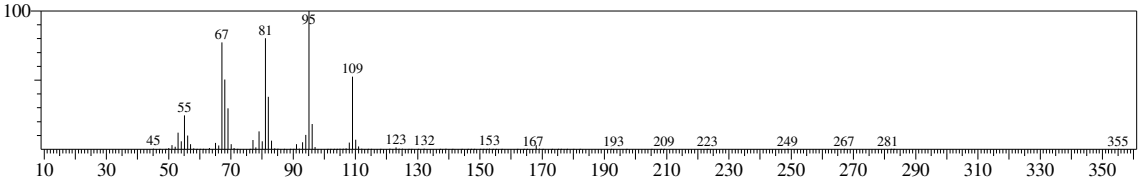
<< Target >>
Line#:34 R.Time:34.896(Scan#:4177) MassPeaks:131
RawMode:Averaged 34.888-34.905(4176-4178) BasePeak:69.05(269575)
BG Mode:Calc. from Peak



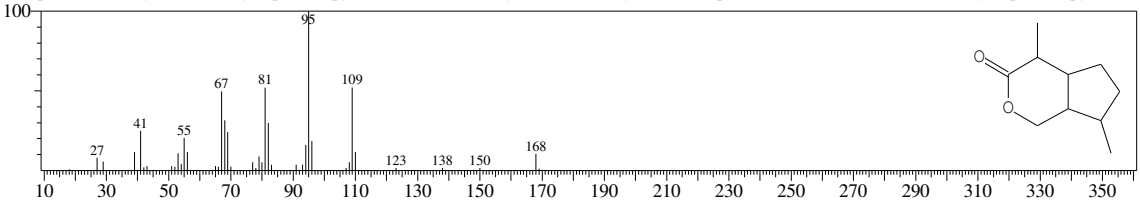
Hit#:1 Entry:54490 Library:NIST05.LIB
SI:78 Formula:C15H26O CAS:40716-66-3 MolWeight:222 RetIndex:1564
CompName:1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)- $$.+/-.-trans-Nerolidol $$ (6E)-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol # $$



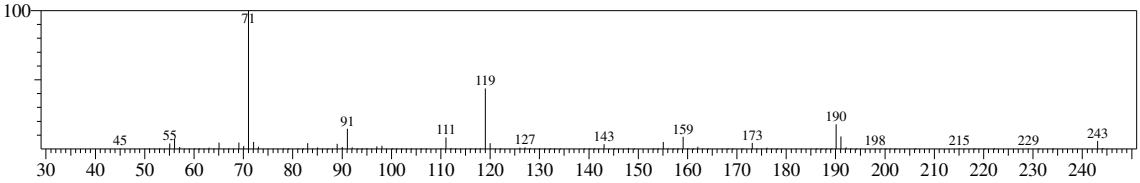
<< Target >>
Line#:35 R.Time:35.788(Scan#:4284) MassPeaks:126
RawMode:Averaged 35.780-35.796(4283-4285) BasePeak:95.05(604393)
BG Mode:Calc. from Peak



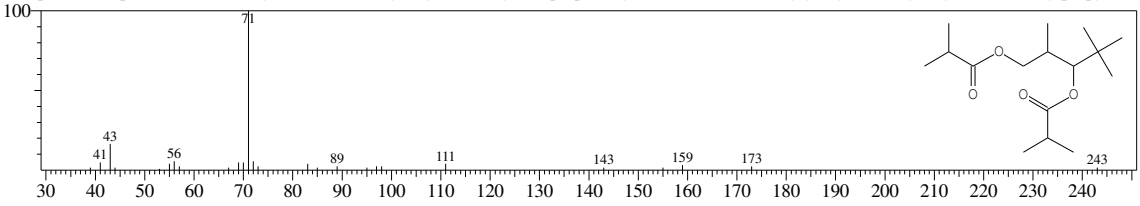
Hit#:1 Entry:11640 Library:NIST05s.LIB
SI:92 Formula:C10H16O2 CAS:485-43-8 MolWeight:168 RetIndex:1329
CompName:Iridomyrmecin $$ Cyclopenta[c]pyran-3(1H)-one, hexahydro-4,7-dimethyl-, [4S-(4.alpha.,4a.beta.,7.beta.,7a.beta.)]- $$ Cyclopenta[c]pyran-3(1



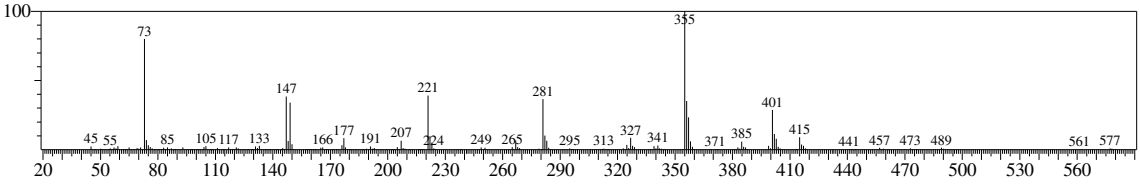
<< Target >>
Line#:36 R.Time:40.030(Scan#:4793) MassPeaks:144
RawMode:Averaged 40.021-40.038(4792-4794) BasePeak:71.05(486468)
BG Mode:Calc. from Peak



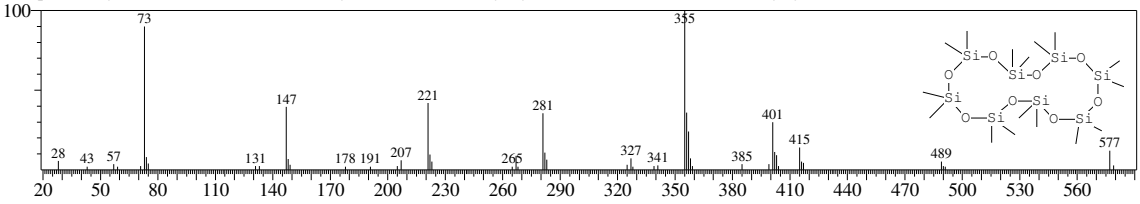
Hit#:1 Entry:92898 Library:NIST05.LIB
SI:72 Formula:C16H30O4 CAS:74381-40-1 MolWeight:286 RetIndex:1605
CompName:Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl ester $$ 1-[2-(Isobutyryloxy)-1-methylethyl]-2,2-dimethylpropyl 2-n



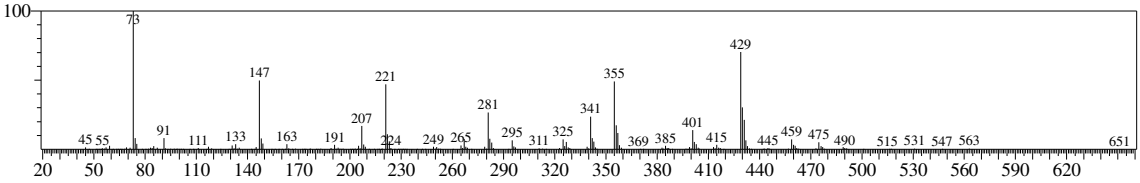
<< Target >>
Line#:37 R.Time:40.455(Scan#:4844) MassPeaks:259
RawMode:Averaged 40.446-40.463(4843-4845) BasePeak:355.00(219869)
BG Mode:Calc. from Peak



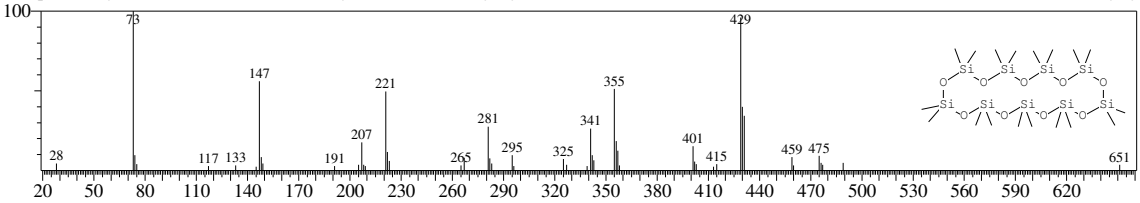
Hit#:1 Entry:160758 Library:NIST05.LIB
SI:92 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



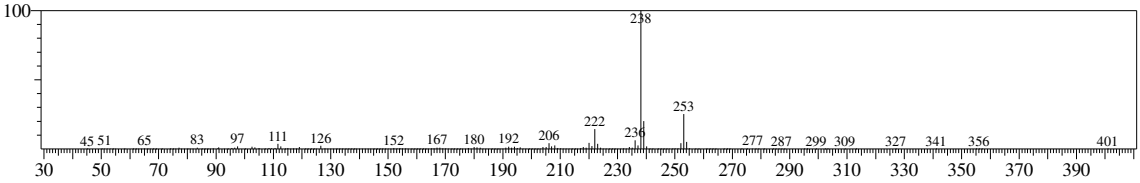
<< Target >>
Line#:38 R.Time:43.380(Scan#:5195) MassPeaks:312
RawMode:Averaged 43.371-43.388(5194-5196) BasePeak:73.05(236258)
BG Mode:Calc. from Peak



Hit#:1 Entry:162013 Library:NIST05.LIB
SI:92 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



<< Target >>
Line#:39 R.Time:49.638(Scan#:5946) MassPeaks:222
RawMode:Averaged 49.630-49.646(5945-5947) BasePeak:238.10(910975)
BG Mode:Calc. from Peak



Hit#:1 Entry:64116 Library:NIST05.LIB
SI:76 Formula:C16H18N2 CAS:22525-43-5 MolWeight:238 RetIndex:2148
CompName:4-Amino-4'-(N,N-dimethylamino)stilbene $$ Benzenamine, 4-[2-(4-aminophenyl)ethenyl]-N,N-dimethyl- $$ N-(4-[(E)-2-(4-Aminophenyl)ethen