Informações Suplementares

Article

Caracterização de Compostos Voláteis em Cavidades Naturais Impactadas por Mudanças Climáticas

Characterization of Volatile Composts in Natural Cavities Impacted by Climate Changes

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1. Dados Brutos para Repositório de Informação

Para garantir transparência e permitir a replicação e validação dos resultados apresentados neste estudo, disponibilizamos um conjunto de amostras representativas analisadas por diferentes técnicas experimentais. Esses dados fornecem um suporte fundamental às conclusões do artigo, permitindo que pesquisadores e profissionais da área tenham acesso direto aos valores brutos das análises realizadas.

Optamos por disponibilizar os dados, em anexo, na sua forma bruta, sem qualquer tipo de tratamento ou manipulação estatística, preservando sua integridade e permitindo que diferentes abordagens analíticas possam ser aplicadas conforme necessário. Manter esses dados acessíveis em um repositório aberto possibilita que outras pesquisas utilizem as mesmas informações para fins comparativos, desenvolvimento de novas metodologias e aprimoramento de modelos preditivos relacionados à degradação da madeira e seus produtos voláteis.

A estruturação e apresentação dos dados incluem informações detalhadas para assegurar a reprodutibilidade dos experimentos, como:

- Data da realização do experimento
- Fator de diluição.
- Número de identificação da amostra.
- Volume de injeção.
- Relatório da metodologia analítica utilizada.
- Arquivo de tunning, para avaliar a calibração e desempenho.

Com essa abordagem, garantimos que qualquer leitor ou pesquisador interessado possa acessar, analisar e utilizar os dados de maneira independente, promovendo a colaboração científica e fortalecendo a confiabilidade dos resultados apresentados. Qualquer interessado que deseje obter os dados em formato digital pode solicitá-los diretamente ao nosso grupo de pesquisa, contribuindo para um ambiente acadêmico mais aberto, verificável e replicável.

Anexos:

S1. Dados brutos das análises da fibra de microextração em fase sólida do ponto 1 de coleta na caverna do Couto.

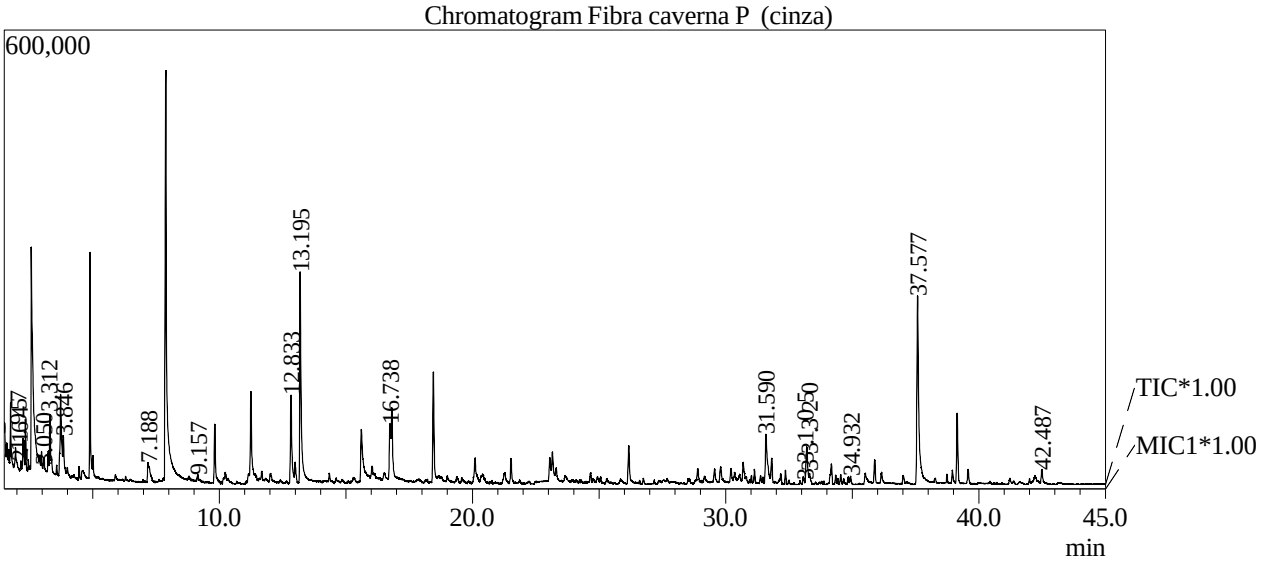
S2. Dados brutos das análises da fibra de microextração em fase sólida da madeira coletada no ponto 1 de coleta na caverna do Couto.

S3. Dados brutos das análises da *headspace* da madeira coletada no ponto 1 de coleta na caverna do Couto.

S1. Dados brutos das análises da fibra de microextração em fase sólida do ponto 1 de coleta na caverna do Couto.

Sample Information

Analyzed by	: Admin
Analyzed	: 28/01/2025 16:42:57
Sample Type	: Unknown
Level #	1
$EndIf$IS Amount	: [1] 1
Sample Amount	1
Dilution Factor	1
Vial #	1
Injection Volume	: 1.00
Data File	: C:\GCMSsolution\Data\Project1\Norberto\Voláteis Caverna\Fibra cav
Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise SPME-caverna.qg
Org Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise SPME-caverna.qg
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1\2025\23-01-2024.qgt



Peak Report TIC

Peak#	R.Time	Area	Area%	Name	Base m/z
1	1.957	82164	2.00	1-Hexanol (CAS) n-Hexanol	56.05
2	2.164	13196	0.32	Butanoic acid, 3-methylbutyl ester (CAS) Is	43.00
3	3.050	9375	0.23	3,5-DIMETHYL-4-OXO-4H-PYRAZOLE	57.05
4	3.312	209821	5.11	Disulfide, dimethyl ********	93.95
5	3.846	185529	4.52	Heptane, 3-methyl-	43.00
6	7.188	74888	1.83	2,4-Dithiapentane ********	61.00
7	9.157	22519	0.55	DIPIVALOYL SULPHIDE	57.05
8	12.833	471355	11.49	o-Cymene	119.10
9	13.195	1039510	25.34	1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol	57.05
10	16.738	251365	6.13	Nonanal (CAS) n-Nonanal	57.00
11	31.590	371171	9.05	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	151.00
12	33.105	4603	0.11	Methyl [(1R)-(1.alpha.,4.alpha.,5.beta.)-4-(b	91.00
13	33.320	59347	1.45	2-Propyl-1,3,3-trimethylcyclohexane	69.00
14	34.932	36434	0.89	7-ethyl-5-azacinnoline	159.05
15	37.577	1208866	29.46	Benzoic acid <2-[[[4-(4-hydroxy-4-methylp	149.00
16	42.487	62688	1.53	2-Octyldodecan-1-ol	57.05

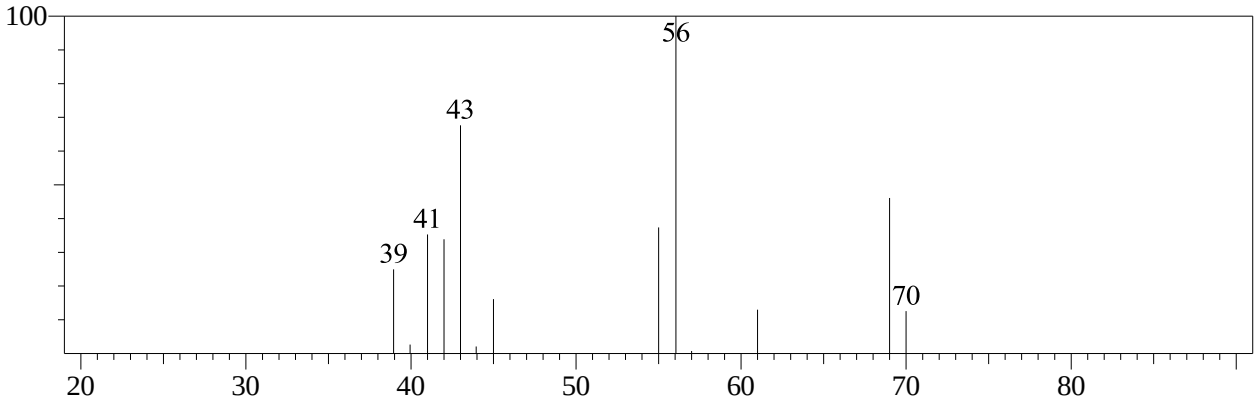
Library

<< Target >>

Line#:1 R.Time:1.955(Scan#:92) MassPeaks:13

RawMode:Averaged 1.950-1.960(91-93) BasePeak:56.05(5961)

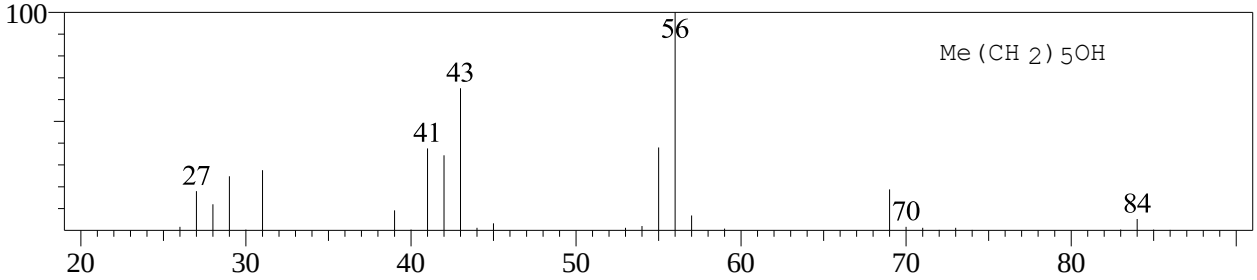
BG Mode:Calc. from Peak



Hit#:1 Entry:7937 Library:WILEY7.LIB

SI:91 Formula:C6 H14 O CAS:111-27-3 MolWeight:102 RetIndex:0

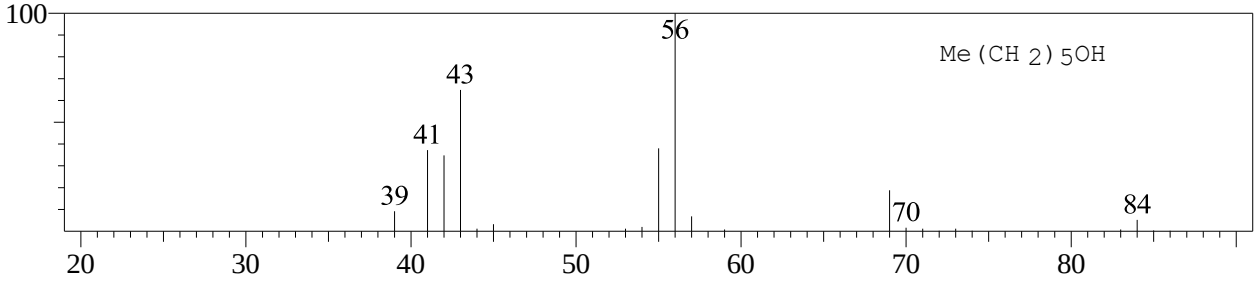
CompName:1-Hexanol (CAS) n-Hexanol $$ Amylcarbinol $$ n-Hexan-1-ol $$ Hexyl alcohol $$ Hexanol $



Hit#:2 Entry:7938 Library:WILEY7.LIB

SI:91 Formula:C6 H14 O CAS:111-27-3 MolWeight:102 RetIndex:0

CompName:1-Hexanol (CAS) n-Hexanol $$ Amylcarbinol $$ n-Hexan-1-ol $$ Hexyl alcohol $$ Hexanol $



<< Target >>
Line#:3 R.Time:3.050(Scan#:311) MassPeaks:5
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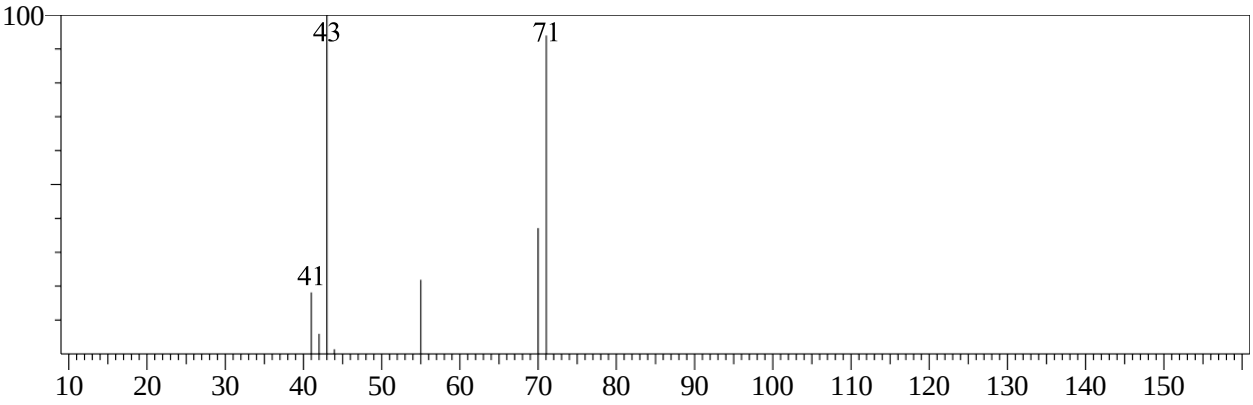
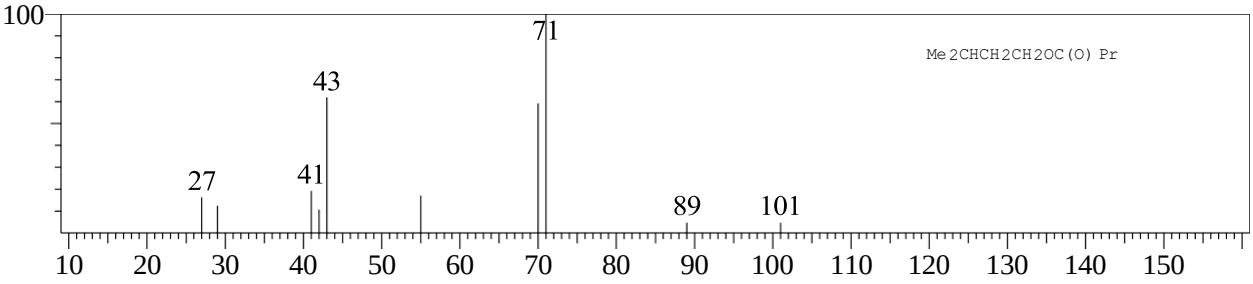
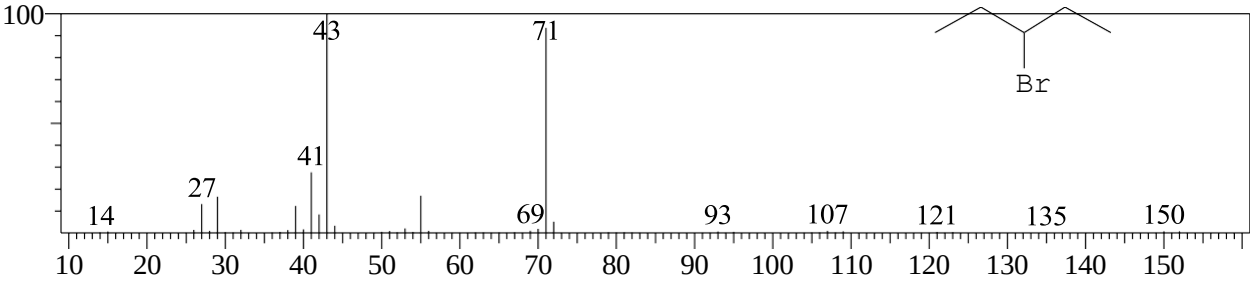
BG Mode:Calc. from Peak



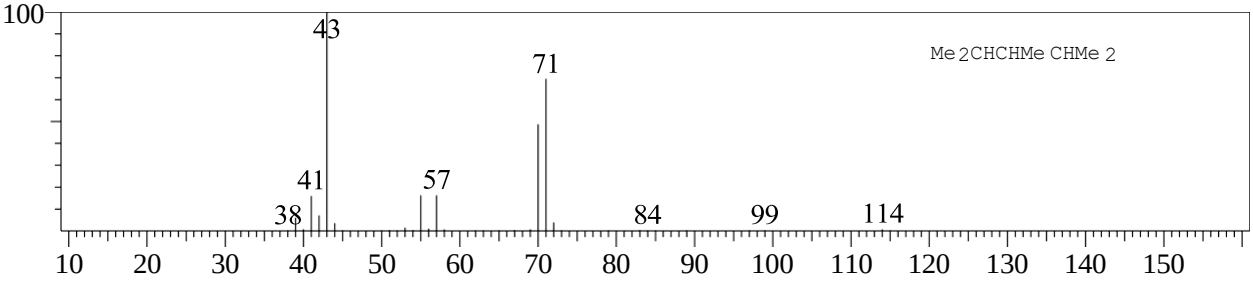
Hit#:1 Entry:47881 Library:WILEY7.LIB
SI:91 Formula:C9 H18 O2 CAS:106-27-4 MolWeight:158 RetIndex:0
CompName:Butanoic acid, 3-methylbutyl ester (CAS) Isoamyl butyrate $$ Isoamyl butylate $$ Isoamyl but



Hit#:2 Entry:8772 Library:NIST11s.lib
SI:91 Formula:C5H11Br CAS:1809-10-5 MolWeight:150 RetIndex:750
CompName:Pentane, 3-bromo- $$ 3-Bromopentane $$ 3-Pentyl bromide $$



Hit#:3 Entry:12878 Library:WILEY7.LIB
SI:91 Formula:C8 H18 CAS:565-75-3 MolWeight:114 RetIndex:0
CompName:Pentane, 2,3,4-trimethyl- (CAS) 2,3,4-Trimethylpentane $$ (CH3)2CHCH(CH3)CH(CH3)2 $$



<< Target >>
Line#:3 R.Time:3.050(Scan#:311) MassPeaks:5
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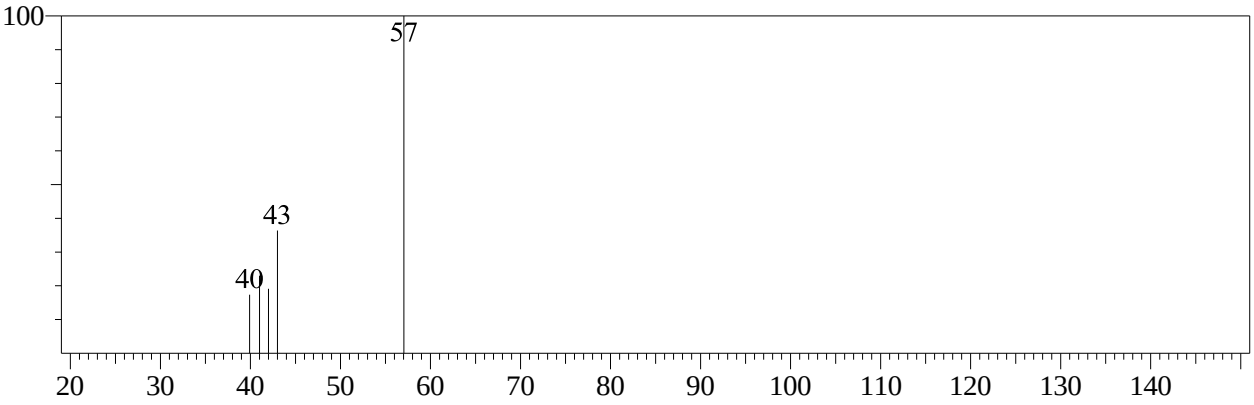
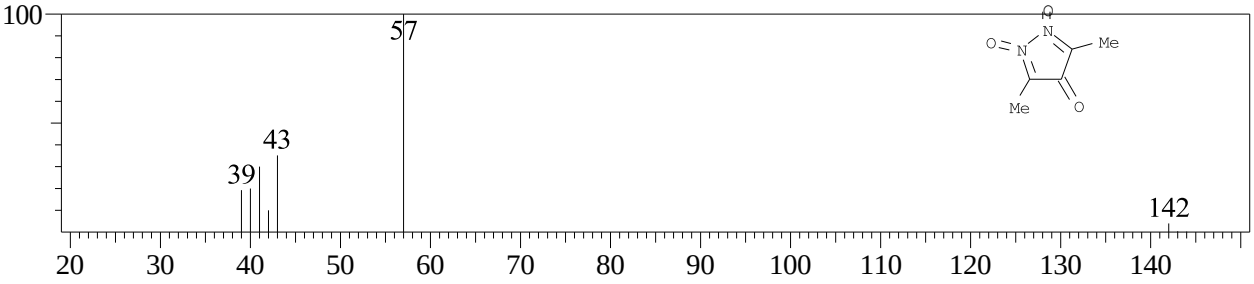
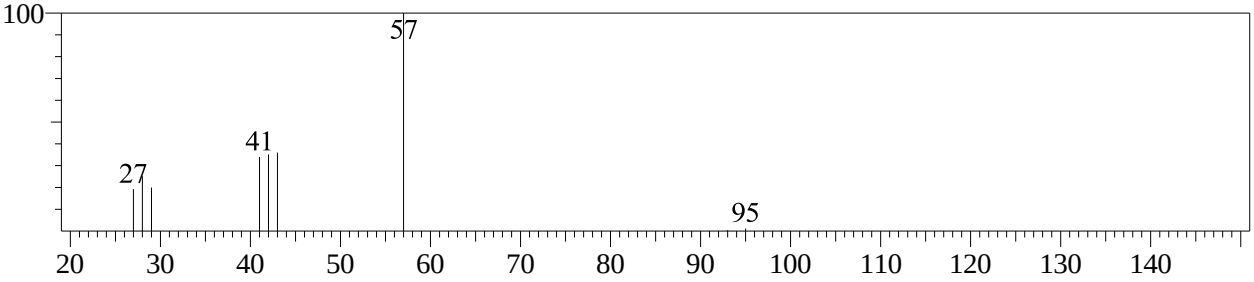
BG Mode:Calc. from Peak



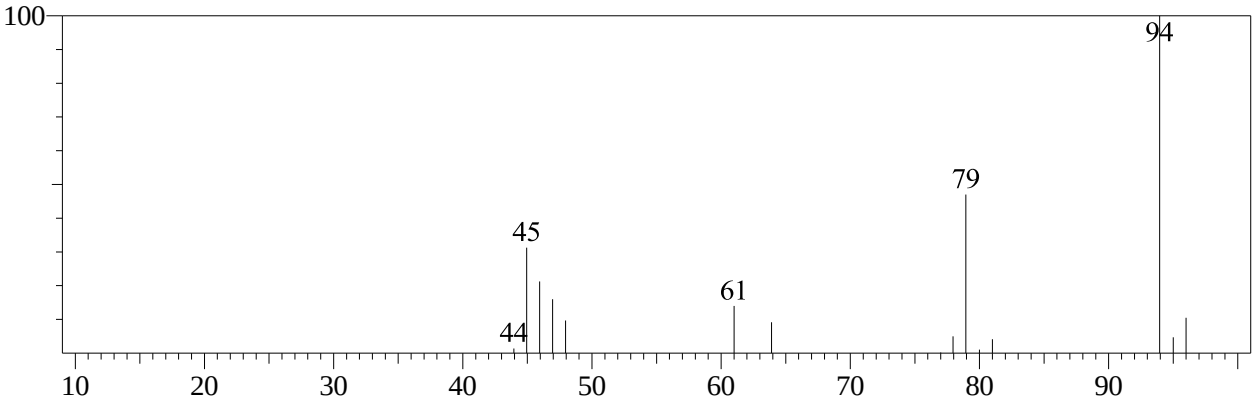
Hit#:1 Entry:30509 Library:WILEY7.LIB
SI:96 Formula:C5 H6 N2 O3 CAS:17952-97-5 MolWeight:142 RetIndex:0
CompName:3,5-DIMETHYL-4-OXO-4H-PYRAZOLE 1,2-DIOXIDE $$ 4H-Pyrazol-4-one, 3,5-dimethyl-,



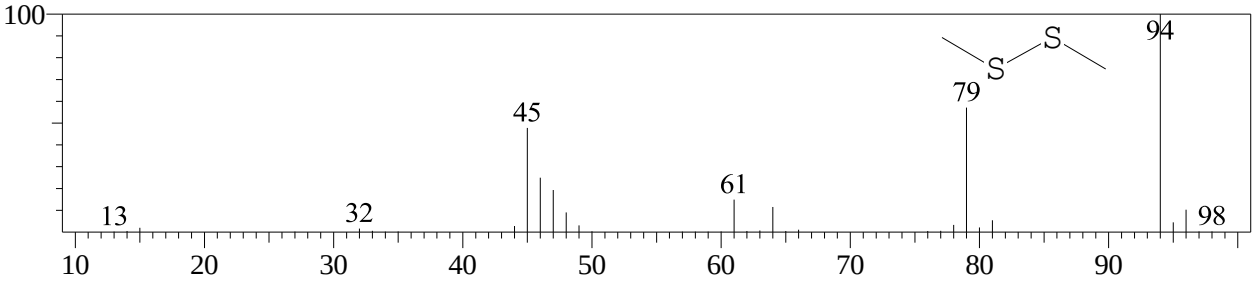
Hit#:2 Entry:4546 Library:WILEY7.LIB
SI:92 Formula:C3 13C H9 CL CAS:0-00-0 MolWeight:92 RetIndex:0
CompName:[1-13C]-Butylchloride $$



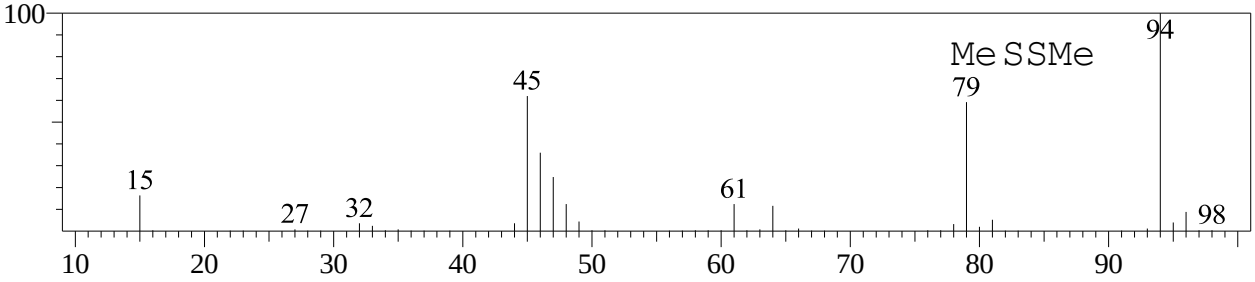
<< Target >>
Line#:5 R.Time:3.845(Scan#:470) MassPeaks:13



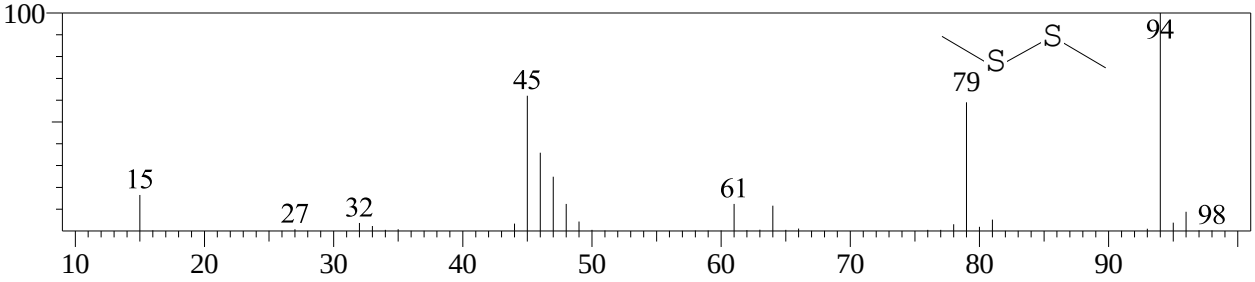
Hit#:1 Entry:1238 Library:NIST11.lib
SI:95 Formula:C2H6S2 CAS:624-92-0 MolWeight:94 RetIndex:722
CompName:Disulfide, dimethyl $$ 2,3-Dithiabutane $$ Methyl disulfide $$ (Methyldithio)methane $$ Dim



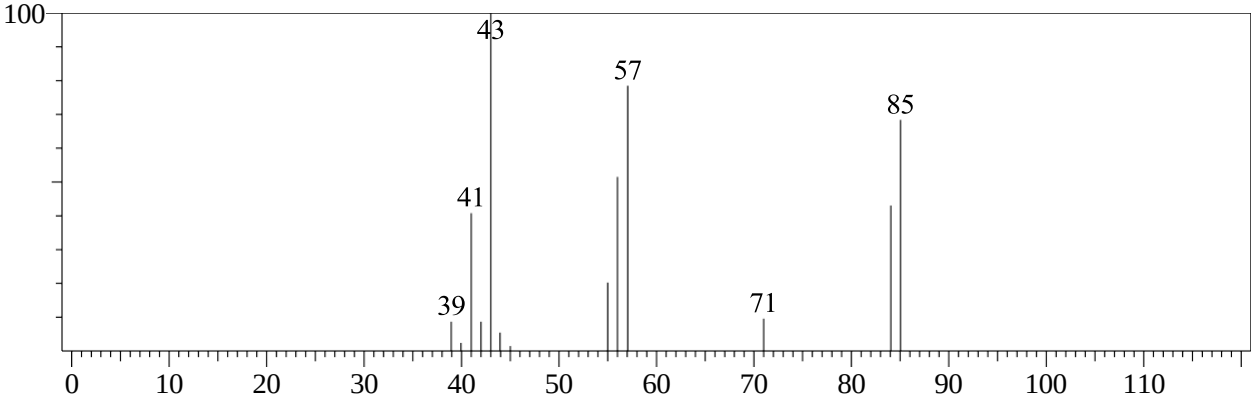
Hit#:2 Entry:4882 Library:WILEY7.LIB
SI:92 Formula:C2 H6 S2 CAS:624-92-0 MolWeight:94 RetIndex:0
CompName:Disulfide, dimethyl (CAS) 2,3-Dithiabutane $$ Dimethyl disulfide $$ Methyl disulfide $$ (Met



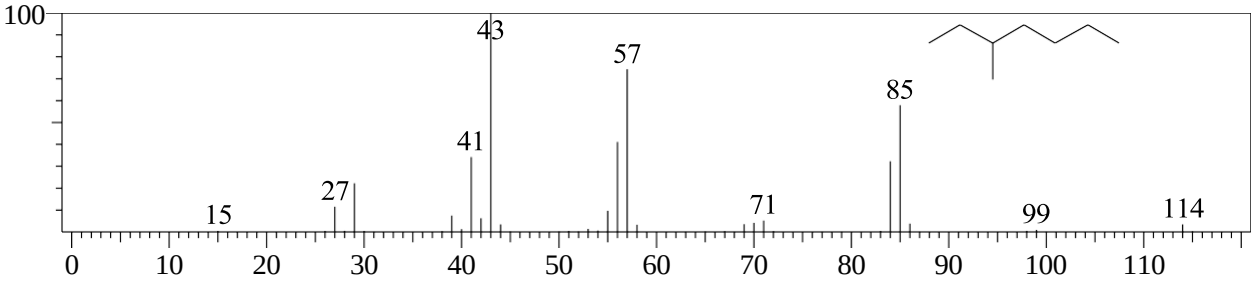
Hit#:3 Entry:1299 Library:NIST11s.lib
SI:92 Formula:C2H6S2 CAS:624-92-0 MolWeight:94 RetIndex:722
CompName:Disulfide, dimethyl $$ 2,3-Dithiabutane $$ Methyl disulfide $$ (Methyldithio)methane $$ Dim



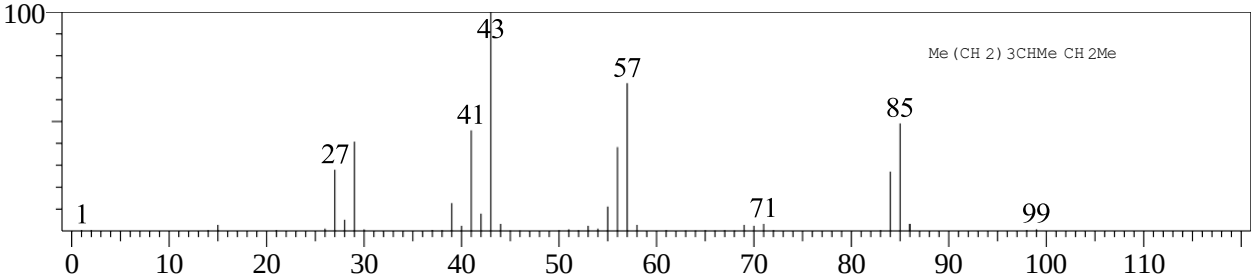
<< Target >>
Line#:5 R.Time:3.845(Scan#:470) MassPeaks:13
RawMode:Averaged 3.840-3.850(469-471) BasePeak:43.00(7674)
BG Mode:Calc. from Peak



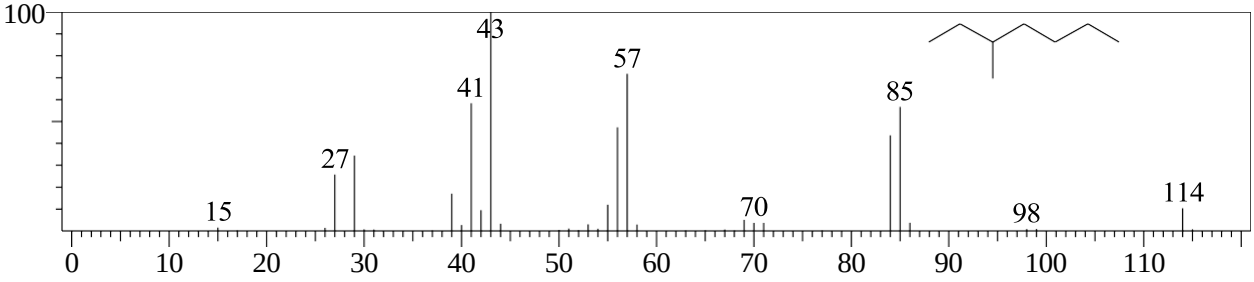
Hit#:1 Entry:3398 Library:NIST11s.lib
SI:93 Formula:C8H18 CAS:589-81-1 MolWeight:114 RetIndex:752
CompName:Heptane, 3-methyl- $$ 3-Methylheptane $$ 2-Ethylhexane $$



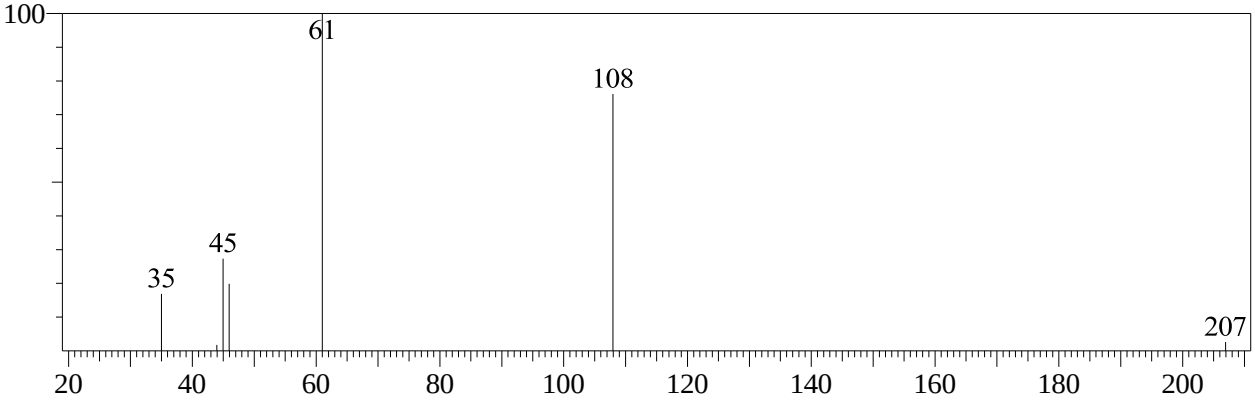
Hit#:2 Entry:12837 Library:WILEY7.LIB
SI:92 Formula:C8 H18 CAS:589-81-1 MolWeight:114 RetIndex:0
CompName:Heptane, 3-methyl- (CAS) 3-Methylheptane $$ 2-Ethylhexane $$



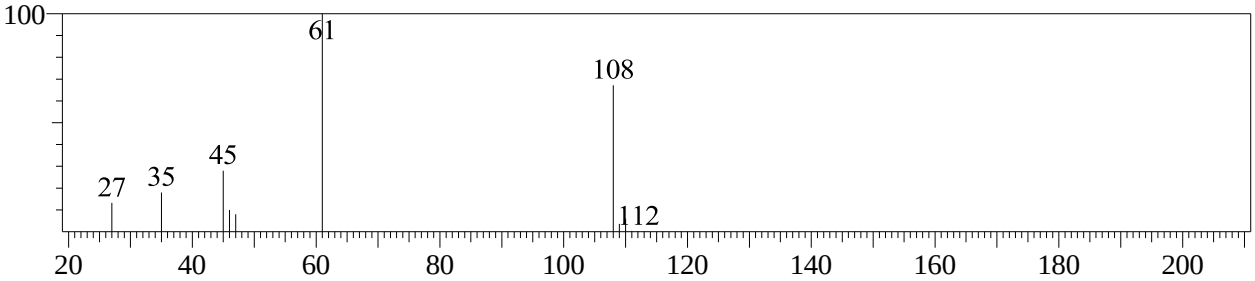
Hit#:3 Entry:4237 Library:NIST11.lib
SI:92 Formula:C8H18 CAS:589-81-1 MolWeight:114 RetIndex:752
CompName:Heptane, 3-methyl- $$ 3-Methylheptane $$ 2-Ethylhexane $$



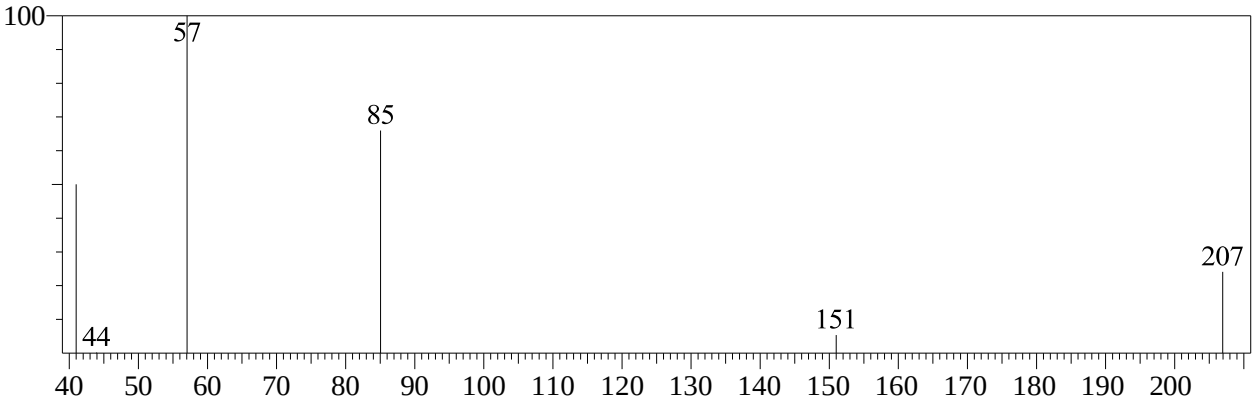
<< Target >>
Line#:7 R.Time:9.155(Scan#:1532) MassPeaks:6
RawMode:Averaged 9.150-9.160(1538-1540) BasePeak:61.00(2866)
BG Mode:Calc. from Peak



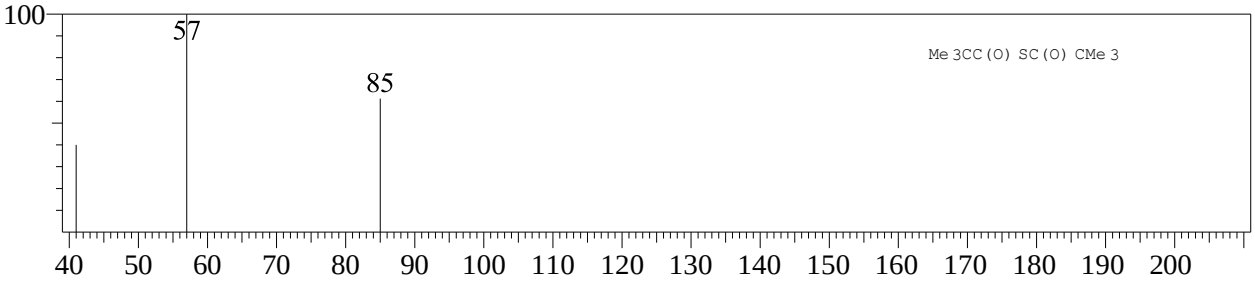
Hit#:1 Entry:9320 Library:WILEY7.LIB
SI:93 Formula:C3 H8 S2 CAS:1618-26-4 MolWeight:108 RetIndex:0
CompName:2,4-Dithiapentane $$ Bis-(methylthio)-methane $$ CH3SCH2SCH3 $$ Bis(methylthio)methan



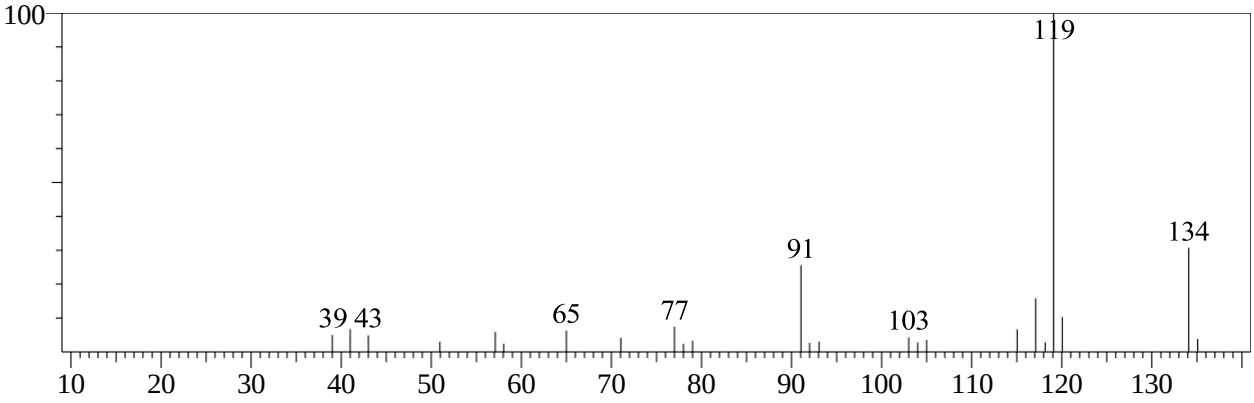
<< Target >>
Line#:7 R.Time:9.155(Scan#:1532) MassPeaks:6
RawMode:Averaged 9.150-9.160(1531-1533) BasePeak:57.05(2865)
BG Mode:Calc. from Peak



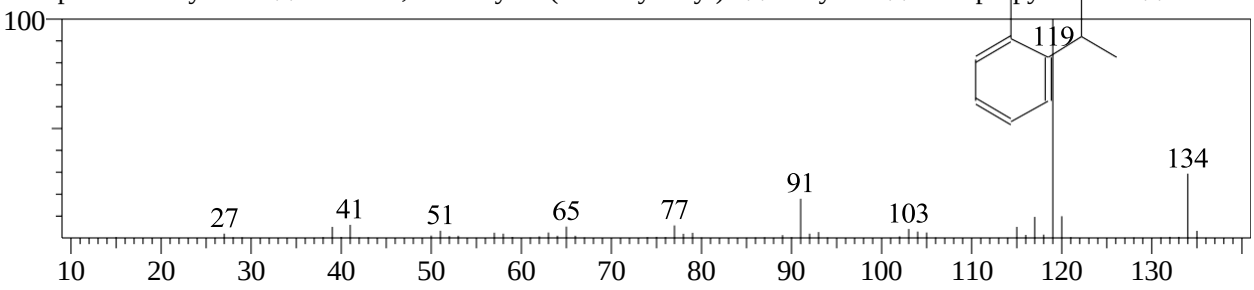
Hit#:1 Entry:97009 Library:WILEY7.LIB
SI:92 Formula:C10 H18 O2 S CAS:36911-20-3 MolWeight:202 RetIndex:0
CompName:DIPIVALOYL SULPHIDE $$ Propanethioic acid, 2,2-dimethyl-, anhydrosulfide (CAS) Dipiva



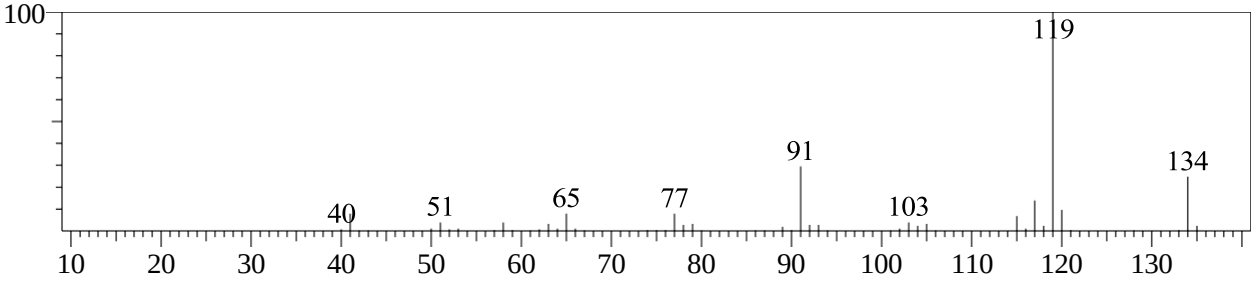
<< Target >>
Line#:9 R.Time:13.195(Scan#:2340) MassPeaks:26
RawMode:Averaged 12.830-12.840(2267-2269) BasePeak:119.10(42397)
BG Mode:Calc. from Peak



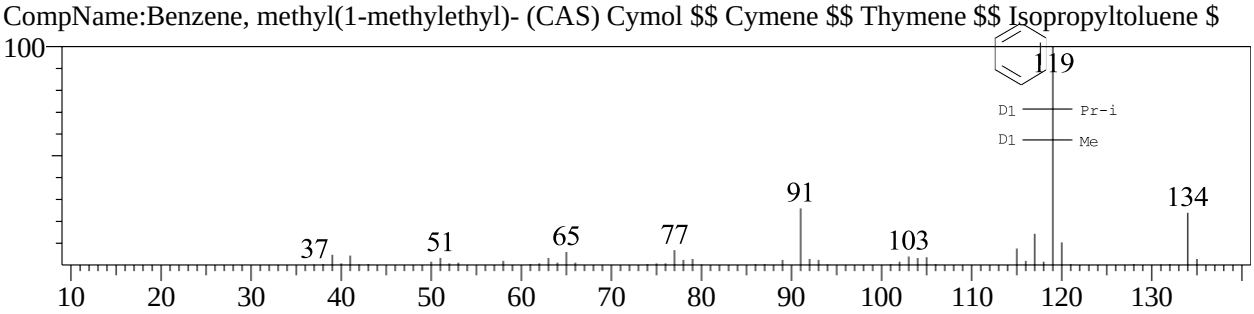
Hit#:1 Entry:6234 Library:NIST11s.lib
SI:92 Formula:C10H14 CAS:527-84-4 MolWeight:134 RetIndex:1042
CompName:o-Cymene $$ Benzene, 1-methyl-2-(1-methylethyl)- $$ o-Cymol $$ o-Isopropyltoluene $$ 1-Is



Hit#:2 Entry:317 Library:FFNSC1.3.lib
SI:92 Formula:C10 H14 CAS:99-87-6 MolWeight:134 RetIndex:1025
CompName:Cymene <para->



Hit#:3 Entry:24425 Library:WILEY7.LIB
SI:92 Formula:C10 H14 CAS:25155-15-1 MolWeight:134 RetIndex:0
CompName:Benzene, methyl(1-methylethyl)- (CAS) Cymol $$ Cymene $$ Thymene $$ Isopropyltoluene $



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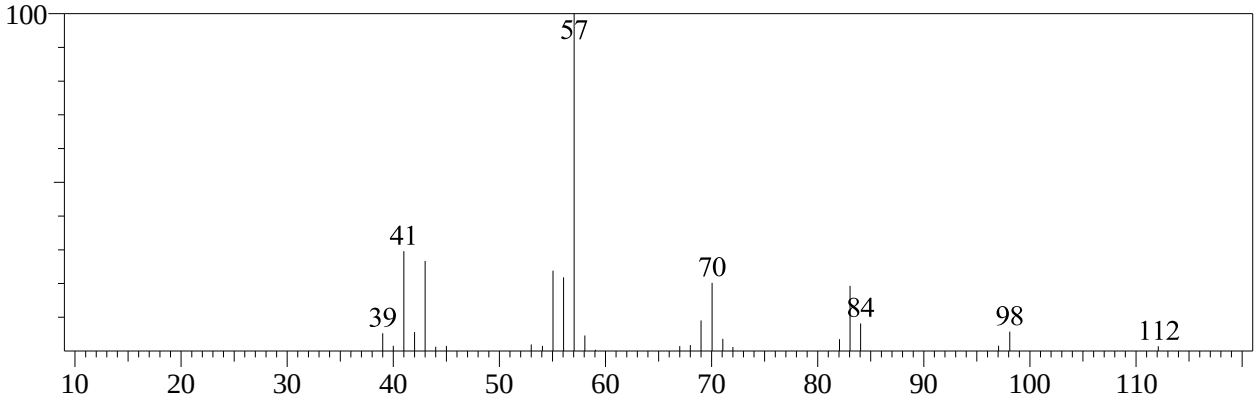
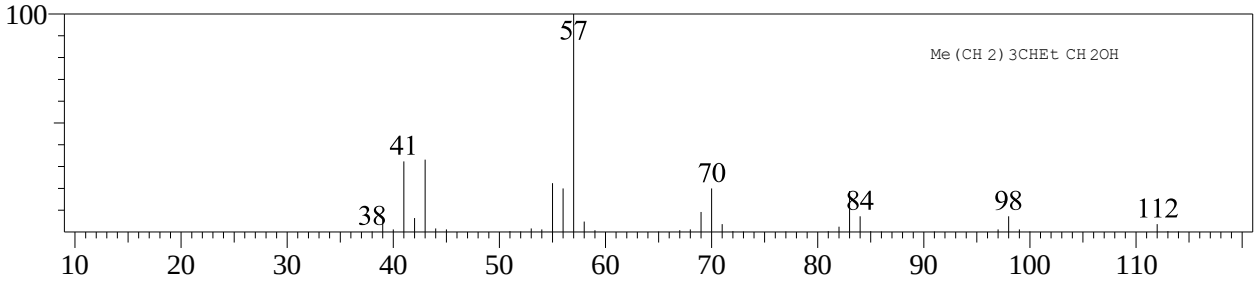
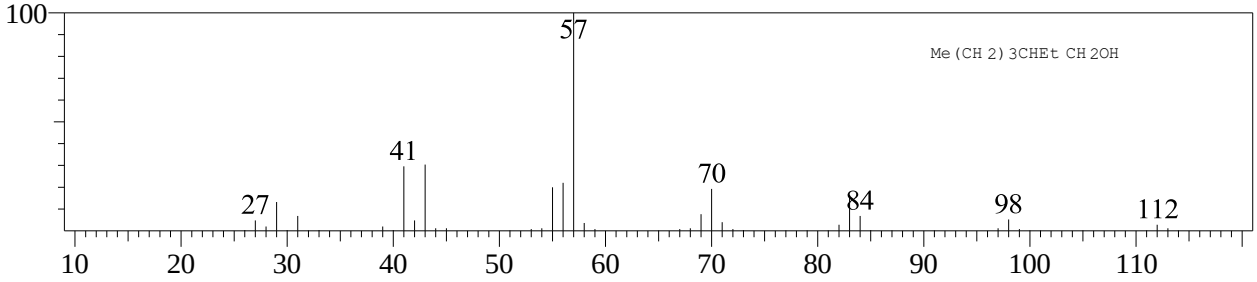
RawMode:Averaged 13.190-13.200(2339-2341) BasePeak:57.05(89306)
BG Mode:Calc. from Peak



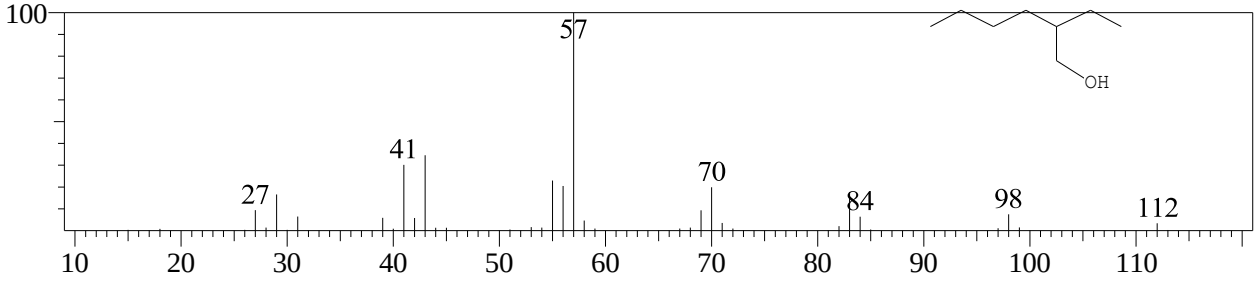
Hit#:1 Entry:22067 Library:WILEY7.LIB
SI:98 Formula:C8 H18 O CAS:104-76-7 MolWeight:130 RetIndex:0
CompName:1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol $$ 2-Ethyl-1-hexanol $$ Ethylhexanol $$ 2-Ethylhe



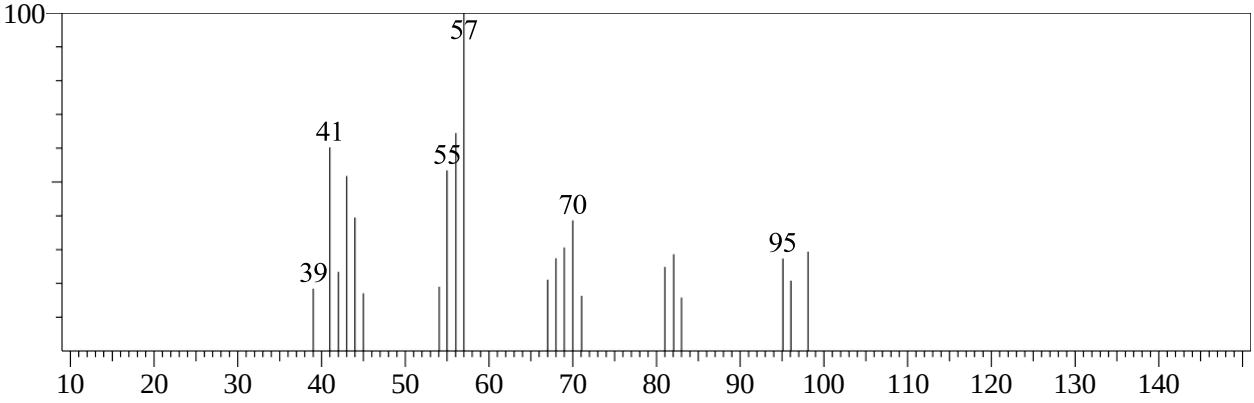
Hit#:2 Entry:22058 Library:WILEY7.LIB
SI:97 Formula:C8 H18 O CAS:104-76-7 MolWeight:130 RetIndex:0
CompName:1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol $$ 2-Ethyl-1-hexanol $$ Ethylhexanol $$ 2-Ethylhe



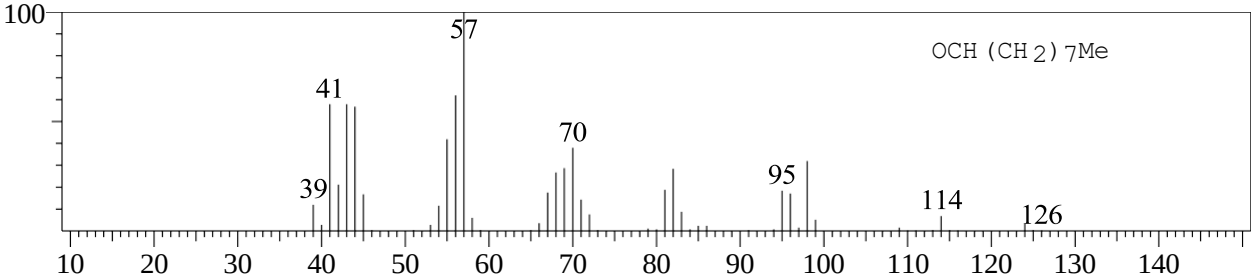
Hit#:3 Entry:5630 Library:NIST11s.lib
SI:97 Formula:C8H18O CAS:104-76-7 MolWeight:130 RetIndex:995
CompName:1-Hexanol, 2-ethyl- $$ 2-Ethyl-1-hexanol $$ 2-Ethylhexan-1-ol $$ 2-Ethylhexanol $$ Ethylhex



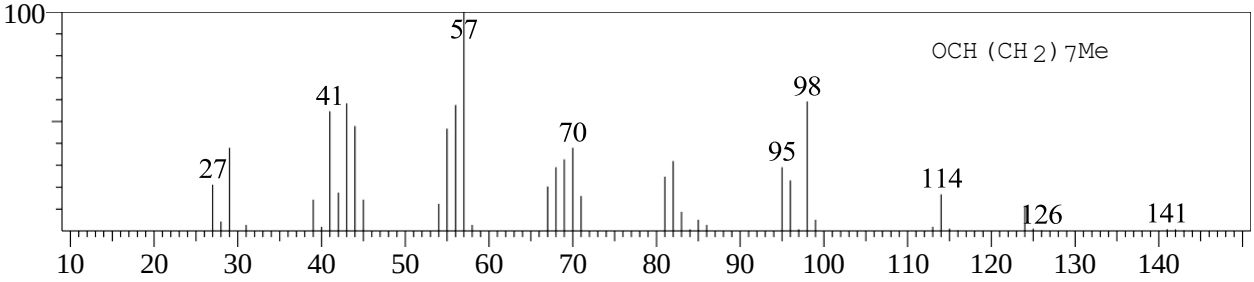
<< Target >>
Line#:9 R.Time:13.195(Scan#:2340) MassPeaks:26
RawMode:Averaged 16.730-16.740(3047-3049) BasePeak:57.00(7098)
BG Mode:Calc. from Peak



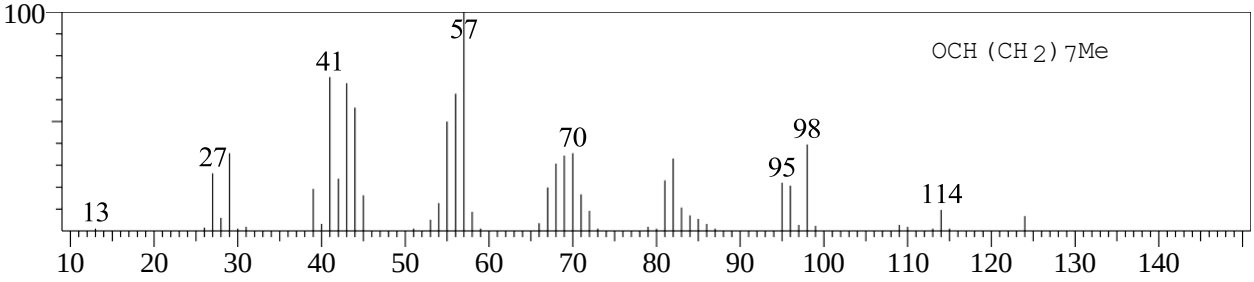
Hit#:1 Entry:31645 Library:WILEY7.LIB
SI:93 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



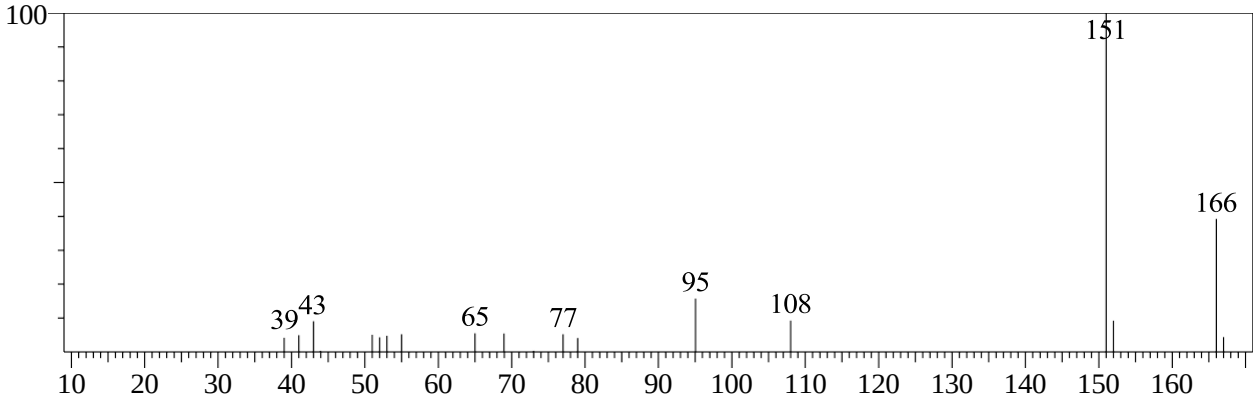
Hit#:2 Entry:31649 Library:WILEY7.LIB
SI:93 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



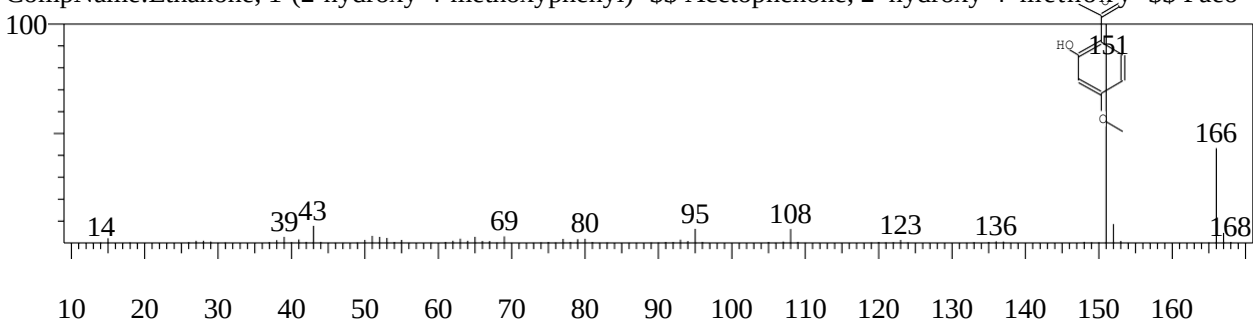
Hit#:3 Entry:31655 Library:WILEY7.LIB
SI:92 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



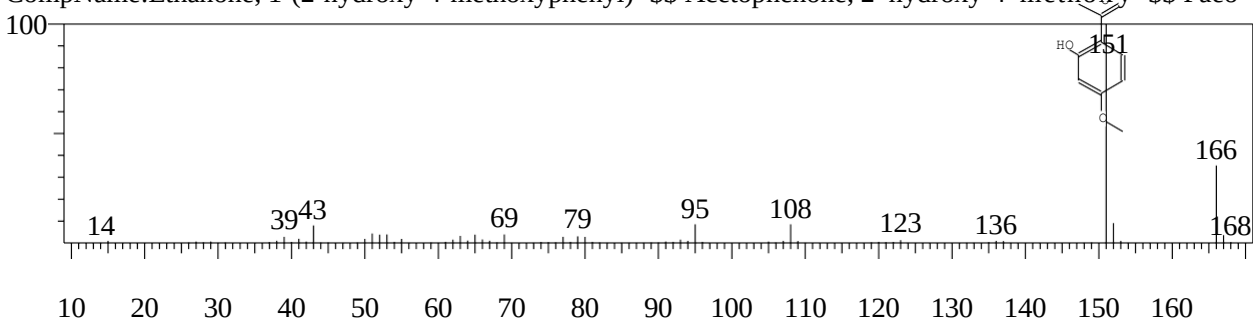
<< Target >>
Line#:11 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 31.585-31.595(6018-6020) BasePeak:151.00(26364)
BG Mode:Calc. from Peak



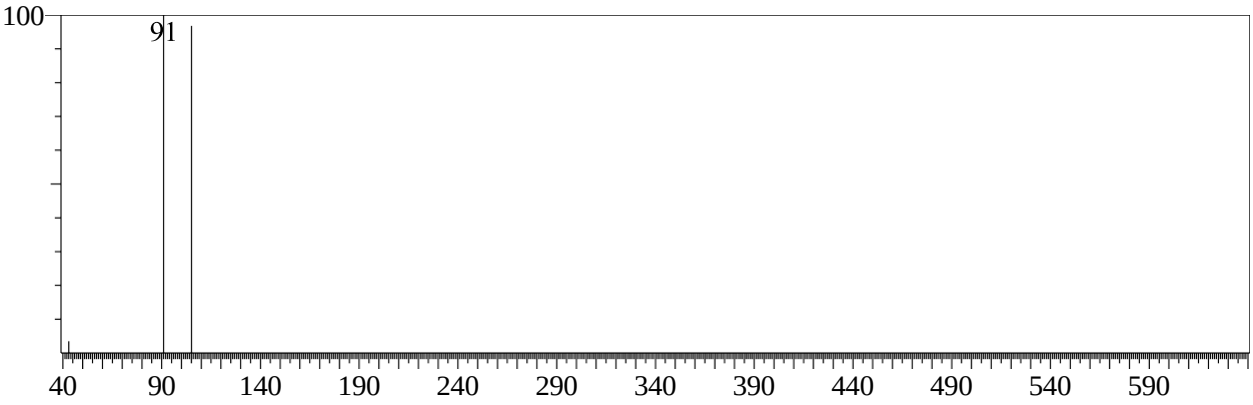
Hit#:1 Entry:12015 Library:NIST11s.lib
SI:90 Formula:C9H10O3 CAS:552-41-0 MolWeight:166 RetIndex:1439
CompName:Ethanone, 1-(2-hydroxy-4-methoxyphenyl)- $$ Acetophenone, 2'-hydroxy-4'-methoxy- $$ Paeo



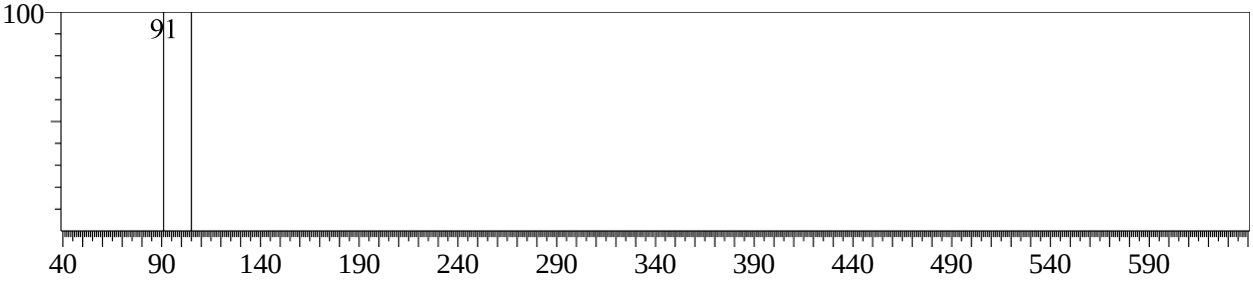
Hit#:2 Entry:23324 Library:NIST11.lib
SI:90 Formula:C9H10O3 CAS:552-41-0 MolWeight:166 RetIndex:1439
CompName:Ethanone, 1-(2-hydroxy-4-methoxyphenyl)- $$ Acetophenone, 2'-hydroxy-4'-methoxy- $$ Paeo



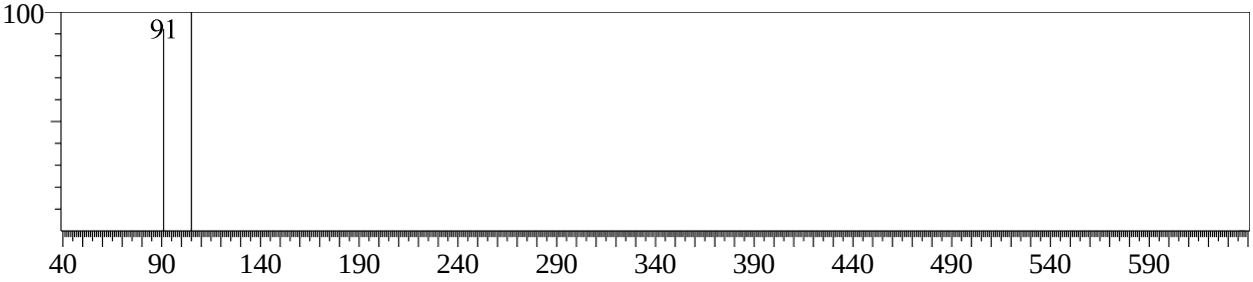
<< Target >>
Line#:12 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 33.100-33.110(6321-6323) BasePeak:91.00(256)
BG Mode:Calc. from Peak



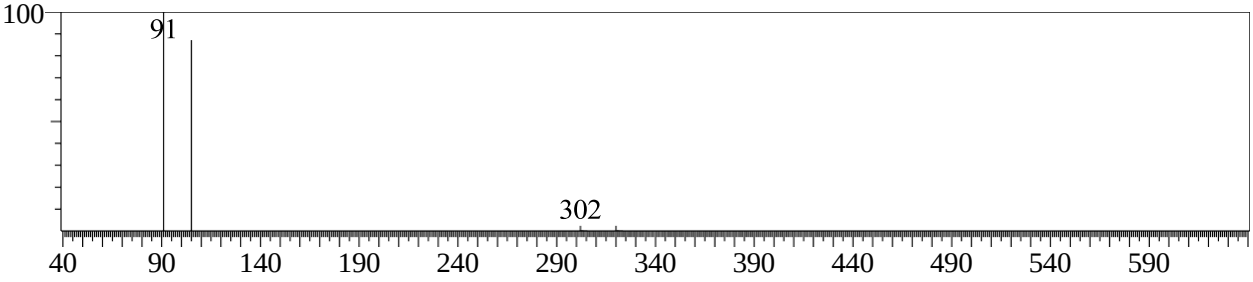
Hit#:1 Entry:320967 Library:WILEY7.LIB
SI:99 Formula:C29 H38 O7 SI CAS:0-00-0 MolWeight:526 RetIndex:0
CompName:Methyl [(1R)-(1.alpha.,4.alpha.,5.beta.)-4-(benzoyloxy)-5-[[(benzyloxy)methyl]oxy]-1-[[(1,1-di



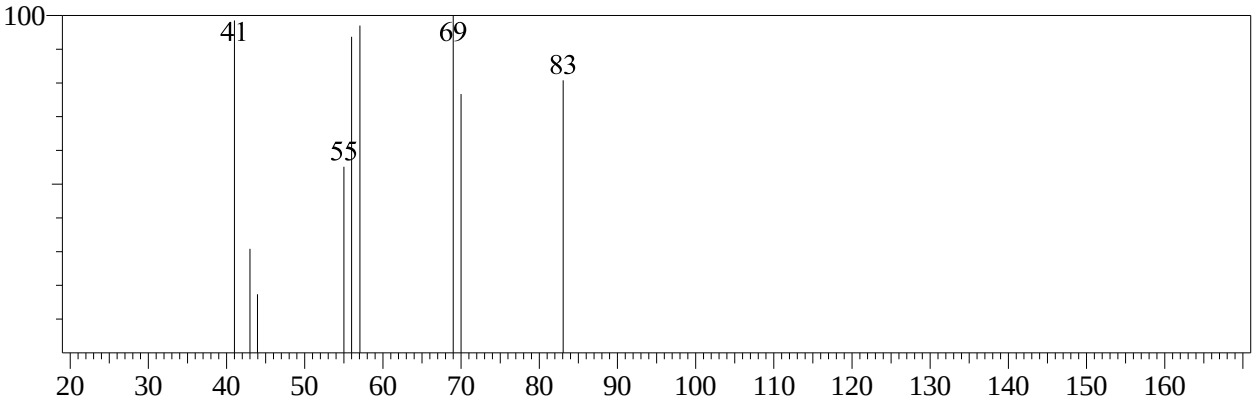
Hit#:2 Entry:331371 Library:WILEY7.LIB
SI:98 Formula:C33 H28 N6 O8 CAS:131682-13-8 MolWeight:636 RetIndex:0
CompName:7'-[2-phenyoxy-3-formyoxyl-4-(benzyoxy-methyl)-5-nitro-cyclopentene]-4'-benzyamino-purino



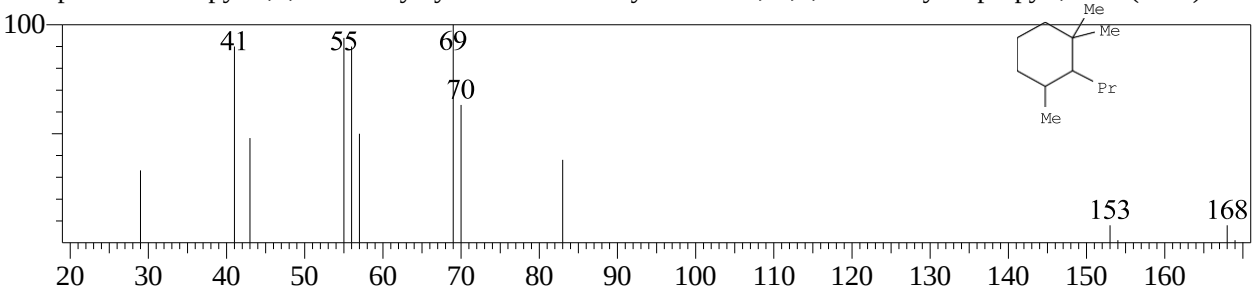
Hit#:3 Entry:230601 Library:WILEY7.LIB
SI:97 Formula:C23 H28 O CAS:113519-73-6 MolWeight:320 RetIndex:0
CompName:(4E)-7-ethyl-3,5-diphenylnona-4,6-dien-3-ol $$ Benzenemethanol, .alpha.-ethyl-.alpha.-(4-ethy



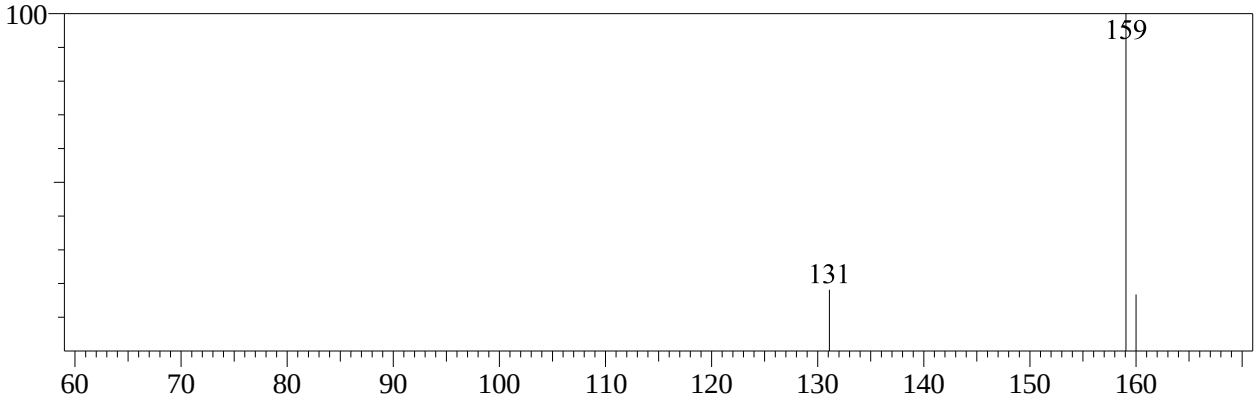
<< Target >>
Line#:13 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 33.315-33.325(6364-6366) BasePeak:69.00(1407)
BG Mode:Calc. from Peak



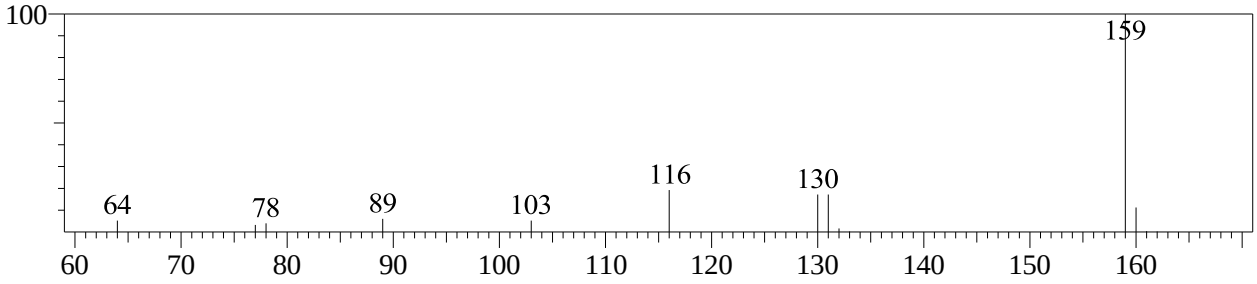
Hit#:1 Entry:58352 Library:WILEY7.LIB
SI:90 Formula:C12 H24 CAS:81983-69-9 MolWeight:168 RetIndex:0
CompName:2-Propyl-1,3,3-trimethylcyclohexane $$ Cyclohexane, 1,1,3-trimethyl-2-propyl-, cis- (CAS)



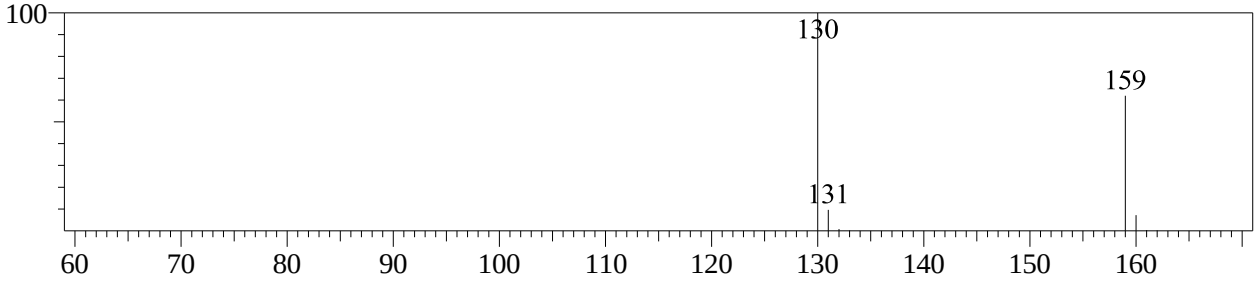
<< Target >>
Line#:14 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 34.925-34.935(6686-6688) BasePeak:159.05(7063)
BG Mode:Calc. from Peak



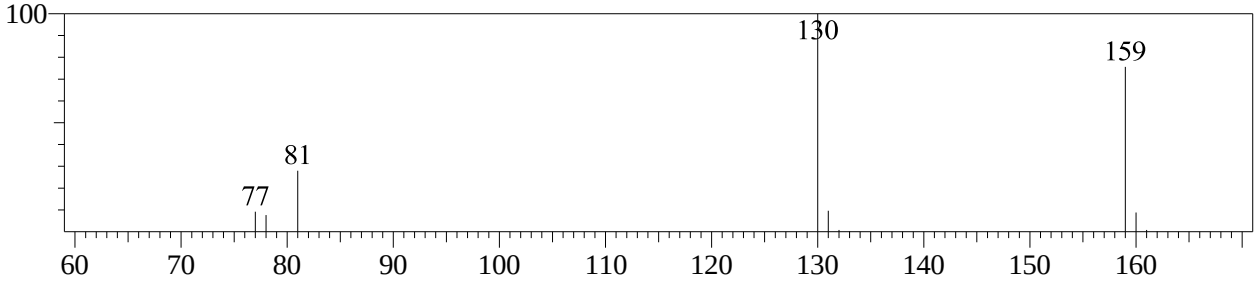
Hit#:1 Entry:48298 Library:WILEY7.LIB
SI:98 Formula:C9 H9 N3 CAS:0-00-0 MolWeight:159 RetIndex:0
CompName:7-ethyl-5-azacinnoline $$



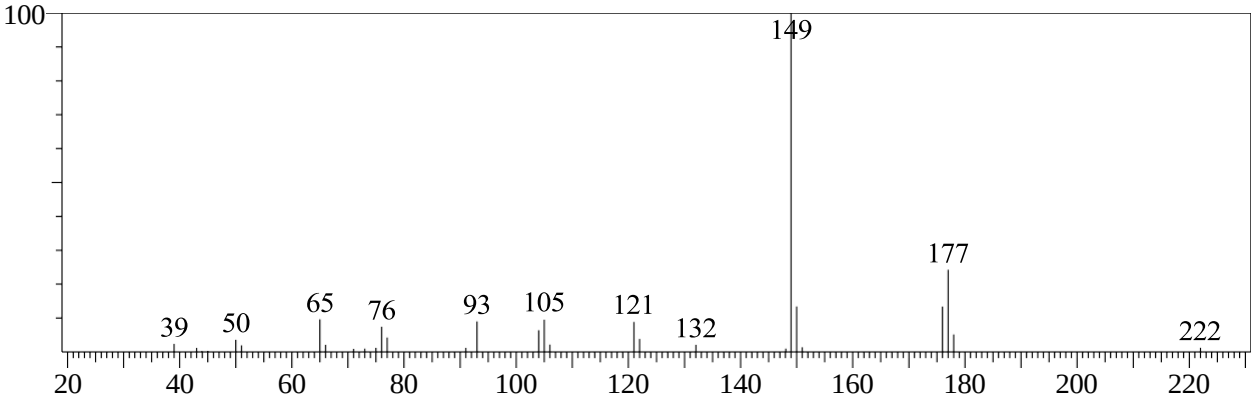
Hit#:2 Entry:48346 Library:WILEY7.LIB
SI:98 Formula:C10 H9 N O CAS:120696-99-3 MolWeight:159 RetIndex:0
CompName:(E)-4-hydroxy-2-phenylbut-2-enenitrile $$ Benzeneacetonitrile, .alpha.-(2-hydroxyethylidene)-,



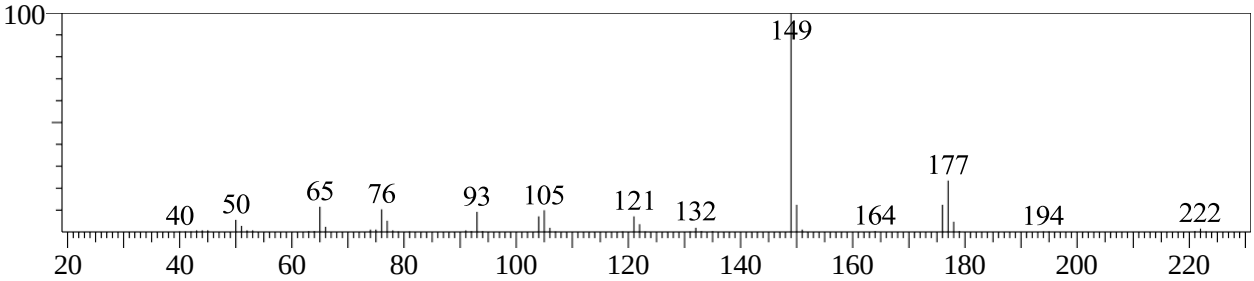
Hit#:3 Entry:48349 Library:WILEY7.LIB
SI:97 Formula:C10 H9 N O CAS:0-00-0 MolWeight:159 RetIndex:0
CompName:2-(2-Furylmethyl)pyridine $$



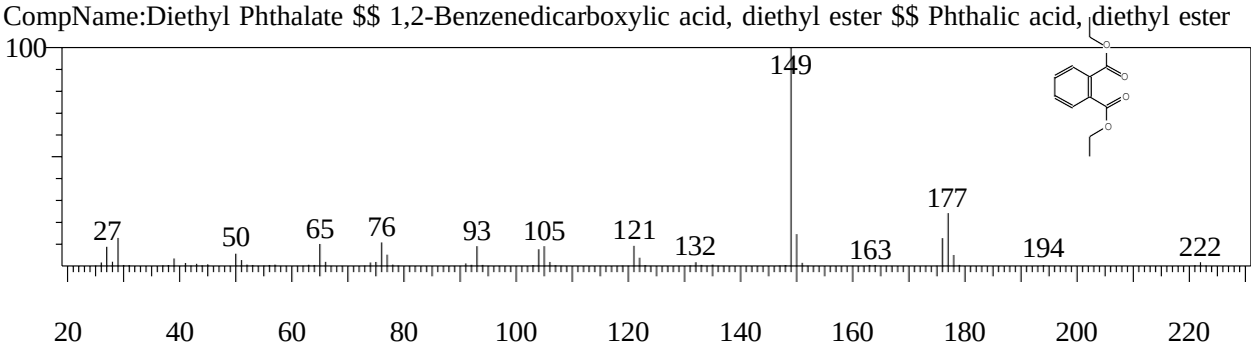
<< Target >>
Line#:15 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 37.570-37.580(7215-7217) BasePeak:149.00(100590)
BG Mode:Calc. from Peak



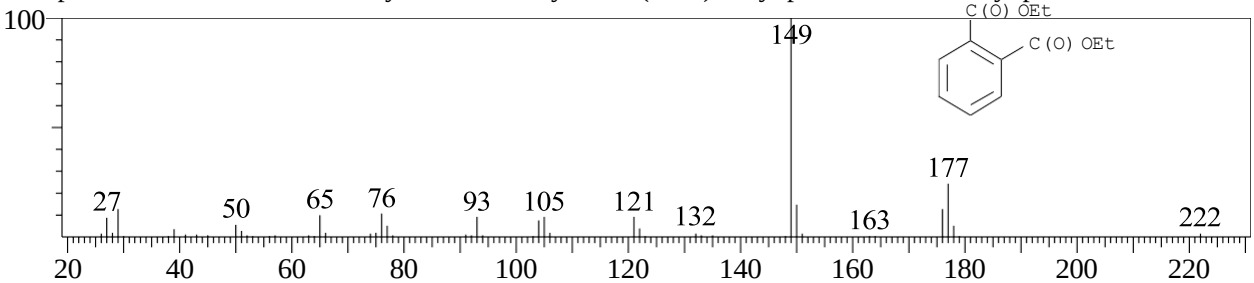
Hit#:1 Entry:1318 Library:FFNSC1.3.lib
SI:96 Formula:C21 H29 N O3 CAS:67634-12-2 MolWeight:343 RetIndex:1589
CompName:Benzoic acid <2-[[[4-(4-hydroxy-4-methylpentyl)-, 3-cyclohexen-1-yl]methylene]amino]-, met



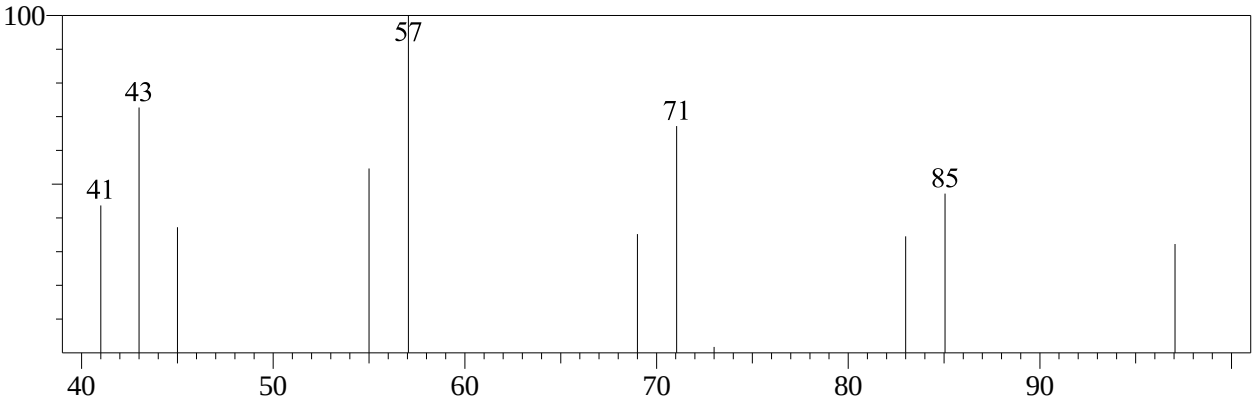
Hit#:2 Entry:20183 Library:NIST11s.lib
SI:96 Formula:C12H14O4 CAS:84-66-2 MolWeight:222 RetIndex:1639
CompName:Diethyl Phthalate $$ 1,2-Benzenedicarboxylic acid, diethyl ester $$ Phthalic acid, diethyl ester



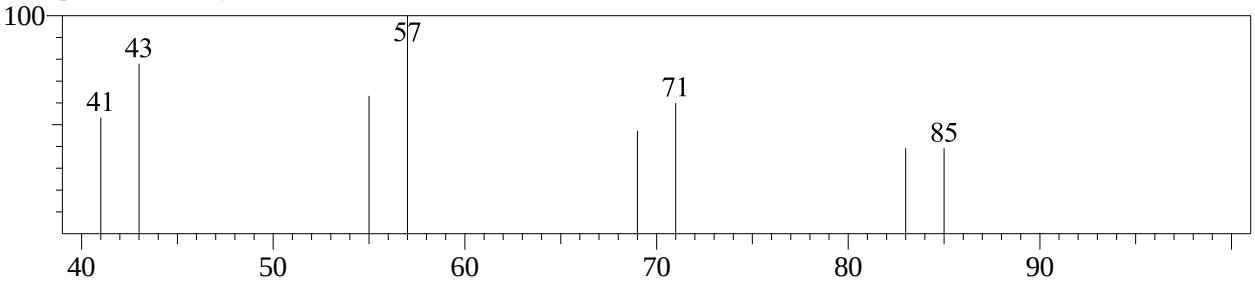
Hit#:3 Entry:123701 Library:WILEY7.LIB
SI:96 Formula:C12 H14 O4 CAS:84-66-2 MolWeight:222 RetIndex:0
CompName:1,2-Benzenedicarboxylic acid, diethyl ester (CAS) Ethyl phthalate $$ Diethyl phthalate $$ Ano



<< Target >>
Line#:16 R.Time:31.590(Scan#:6019) MassPeaks:19
RawMode:Averaged 42.480-42.490(8197-8199) BasePeak:57.05(3306)
BG Mode:Calc. from Peak



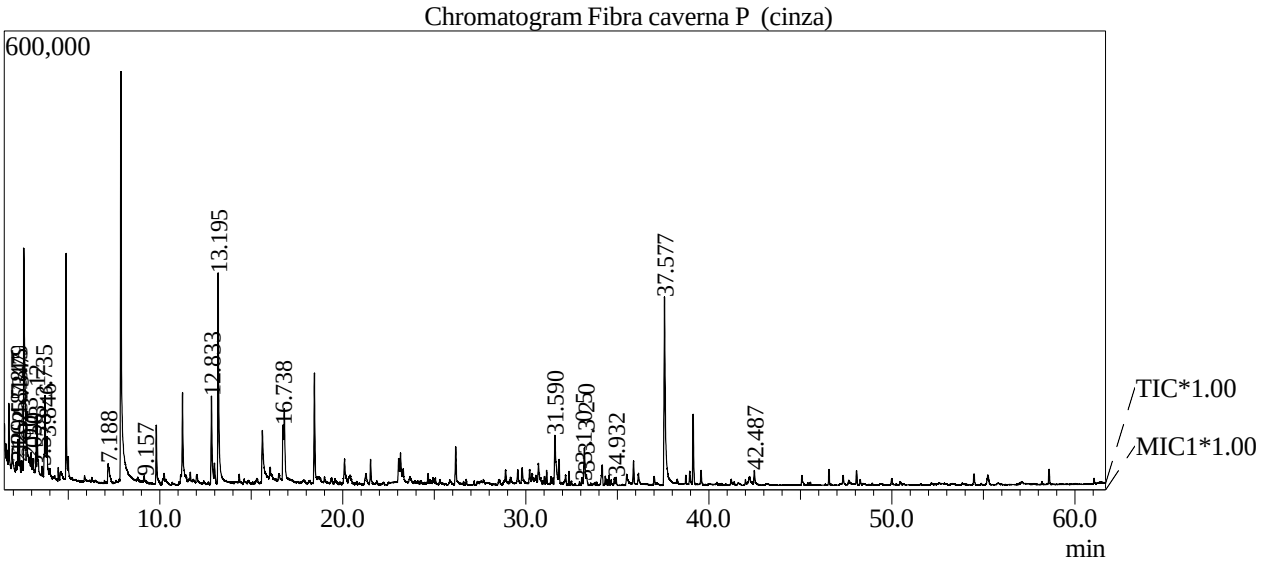
Hit#:1 Entry:209613 Library:WILEY7.LIB
SI:90 Formula:C20 H42 O CAS:0-00-0 MolWeight:298 RetIndex:0
CompName:2-Octyldodecan-1-ol $$



S2. Dados brutos das análises da fibra de microextração em fase sólida da madeira coletada no ponto 1 de coleta na caverna do Couto.

Sample Information

Analyzed by	: Admin
Analyzed	: 28/01/2025 16:42:57
Sample Type	: Unknown
Level #	1
$EndIf$IS Amount	: [1]=1
Sample Amount	1
Dilution Factor	1
Vial #	1
Injection Volume	: 1.00
Data File	: C:\GCMSsolution\Data\Project1\Norberto\Voláteis Caverna\Fibra cav
Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise SPME-caverna.qg
Org Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise SPME-caverna.qg
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1\2025\23-01-2024.qgt



Peak Report TIC

Peak#	R.Time	Area	Area%	Name	Base m/z
1	1.759	171086	3.40	Hexane (CAS) n-Hexane	57.05
2	1.957	82164	1.63	1-Hexanol (CAS) n-Hexanol	56.05
3	2.164	13196	0.26	Butanoic acid, 3-methylbutyl ester (CAS) Is	43.00
4	2.254	78520	1.56	Hexane <2-methyl->	43.00
5	2.288	62145	1.24	Pentane, 2,3-dimethyl- (CAS) 2,3-Dimethyl	56.05
6	2.347	123923	2.46	Hexane, 3-methyl-	43.00
7	2.903	14681	0.29	Pentane, 2,2,4,4-tetramethyl- (CAS) 2,2,4,4-	57.05
8	3.050	9375	0.19	3,5-DIMETHYL-4-OXO-4H-PYRAZOLE	57.05
9	3.312	209821	4.17	Disulfide, dimethyl **********	93.95
10	3.578	26780	0.53	Pentane, 2,3,4-trimethyl-	43.00
11	3.735	450523	8.96	Toluene	91.05
12	3.846	185529	3.69	Heptane, 3-methyl-	43.00
13	7.188	74888	1.49	2,4-Dithiapentane **********	61.00
14	9.157	22519	0.45	DIPIVALOYL SULPHIDE	57.05

Peak#	R.Time	Area	Area%	Name	Base m/z
15	12.833	471355	9.37	o-Cymene	119.10
16	13.195	1039510	20.66	1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol	57.05
17	16.738	251365	5.00	Nonanal (CAS) n-Nonanal	57.00
18	31.590	371171	7.38	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	151.00
19	33.105	4603	0.09	Methyl [(1R)-(1.alpha.,4.alpha.,5.beta.)-4-(b	91.00
20	33.320	59347	1.18	2-Propyl-1,3,3-trimethylcyclohexane	69.00
21	34.932	36434	0.72	7-ethyl-5-azacinnoline	159.05
22	37.577	1208866	24.03	Benzoic acid <2-[[[4-(4-hydroxy-4-methylp	149.00
23	42.487	62688	1.25	2-Octyldodecan-1-ol	57.05
		5030489	100.00		

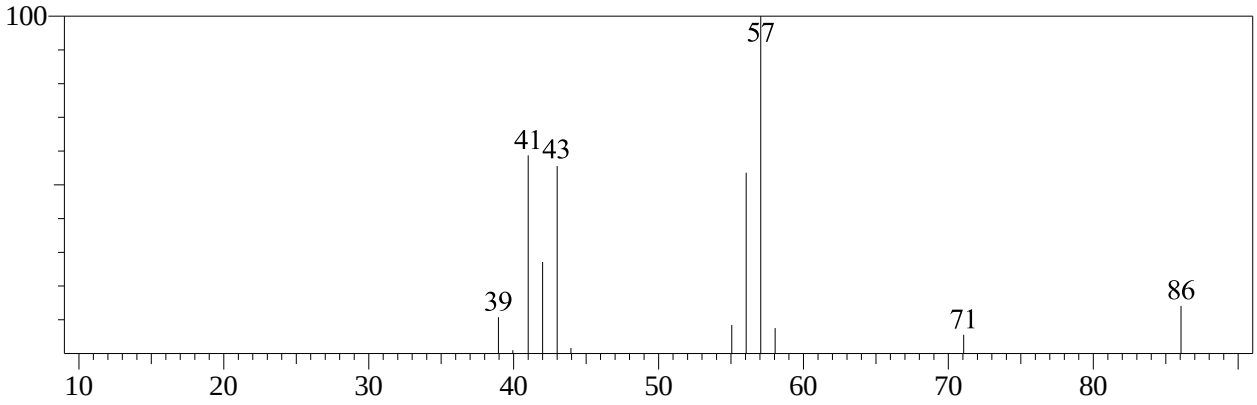
Library

<< Target >>

Line#:1 R.Time:1.760(Scan#:53) MassPeaks:12

RawMode:Averaged 1.755-1.765(52-54) BasePeak:57.05(22064)

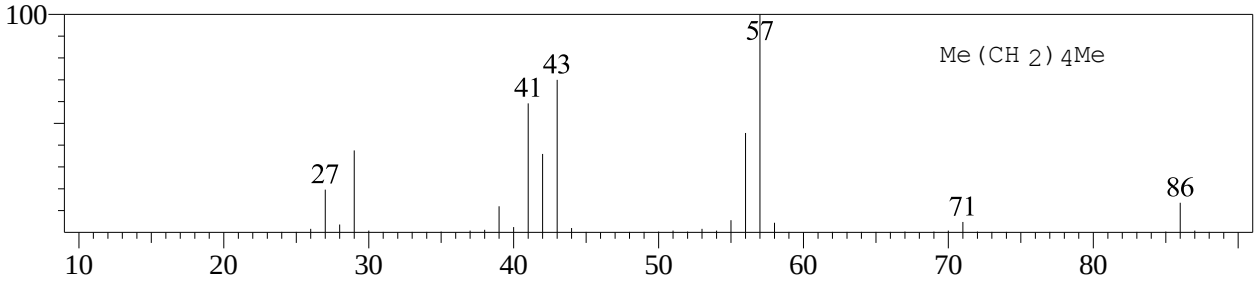
BG Mode:Calc. from Peak



Hit#:1 Entry:3573 Library:WILEY7.LIB

SI:96 Formula:C6 H14 CAS:110-54-3 MolWeight:86 RetIndex:0

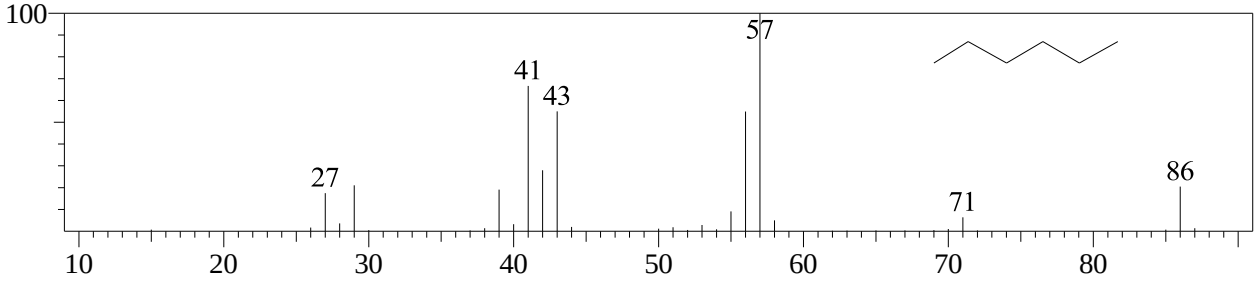
CompName:Hexane (CAS) n-Hexane $$ Skellysolve B $$



Hit#:2 Entry:936 Library:NIST11s.lib

SI:96 Formula:C6H14 CAS:110-54-3 MolWeight:86 RetIndex:618

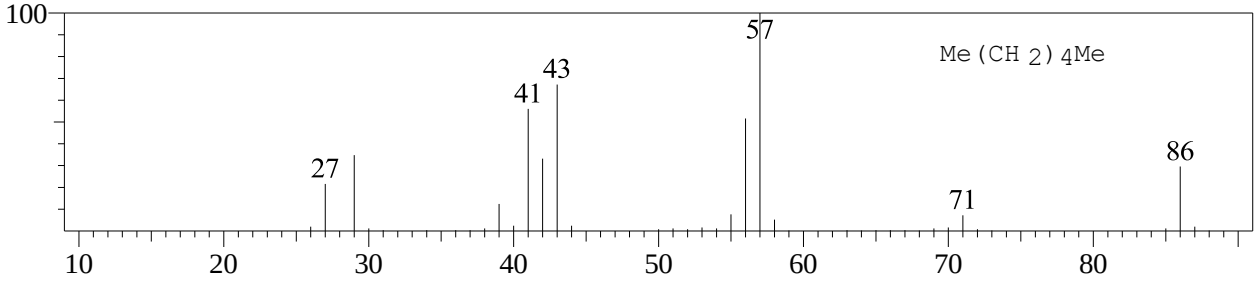
CompName:n-Hexane $$ Hexane $$ Skellysolve B $$ n-C6H14 $$ Esani $$ Heksan $$ Hexanen $$ Hexyl



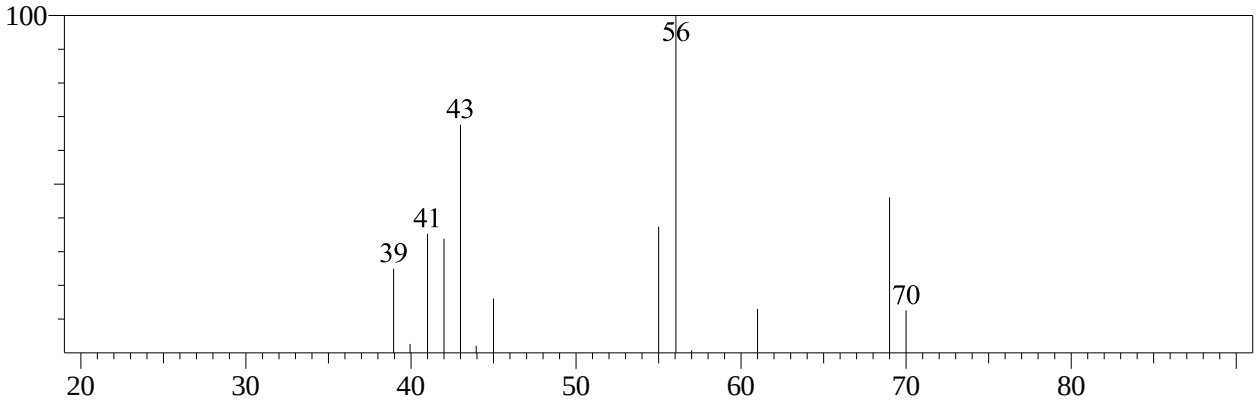
Hit#:3 Entry:3574 Library:WILEY7.LIB

SI:95 Formula:C6 H14 CAS:110-54-3 MolWeight:86 RetIndex:0

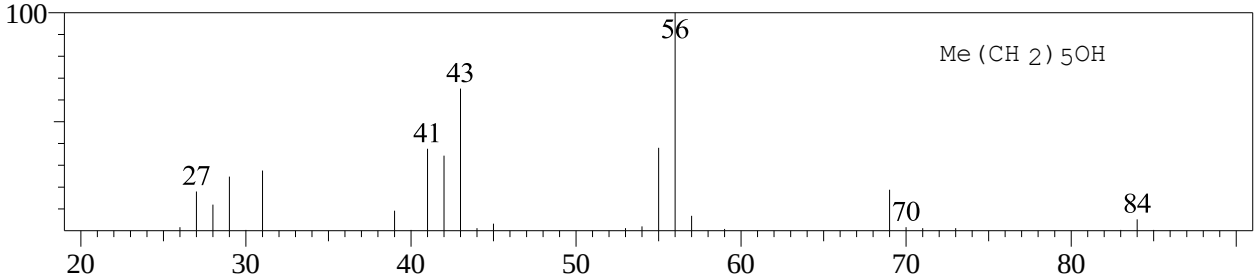
CompName:Hexane (CAS) n-Hexane $$ Skellysolve B $$ n-C6H14 $$ Esani $$ Heksan $$ Hexanen $$ He



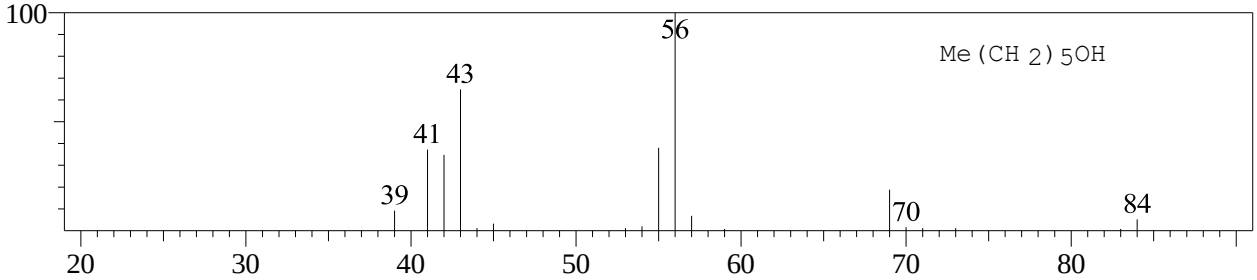
<< Target >>
Line#:3 R.Time:2.165(Scan#:134) MassPeaks:7
RawMode:Averaged 1.950-1.960(91-93) BasePeak:56.05(5961)
BG Mode:Calc. from Peak



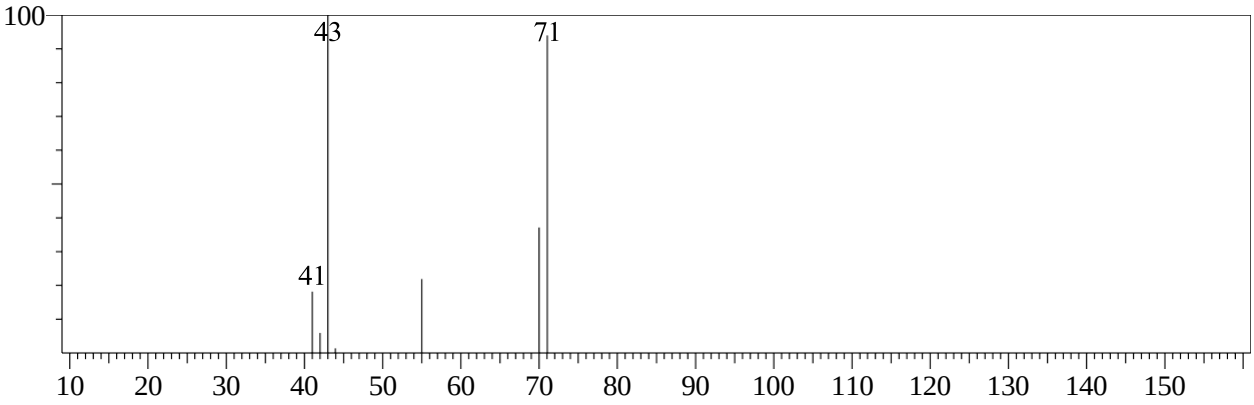
Hit#:1 Entry:7937 Library:WILEY7.LIB
SI:91 Formula:C6 H14 O CAS:111-27-3 MolWeight:102 RetIndex:0
CompName:1-Hexanol (CAS) n-Hexanol $$ Amylcarbinol $$ n-Hexan-1-ol $$ Hexyl alcohol $$ Hexanol $



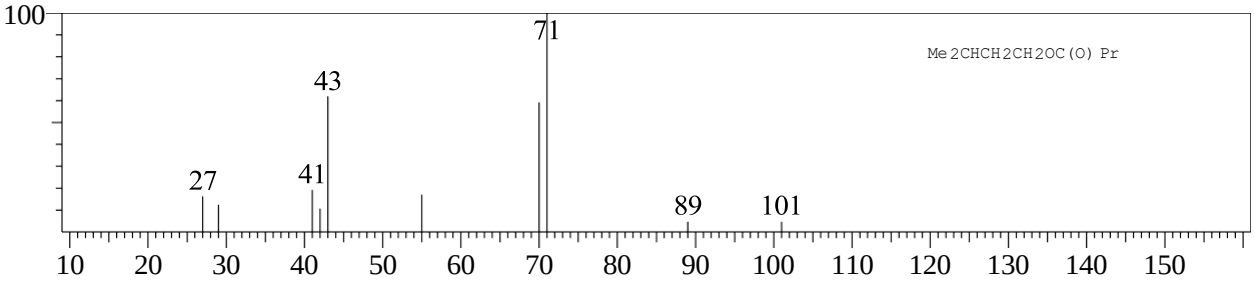
Hit#:2 Entry:7938 Library:WILEY7.LIB
SI:91 Formula:C6 H14 O CAS:111-27-3 MolWeight:102 RetIndex:0
CompName:1-Hexanol (CAS) n-Hexanol $$ Amylcarbinol $$ n-Hexan-1-ol $$ Hexyl alcohol $$ Hexanol $



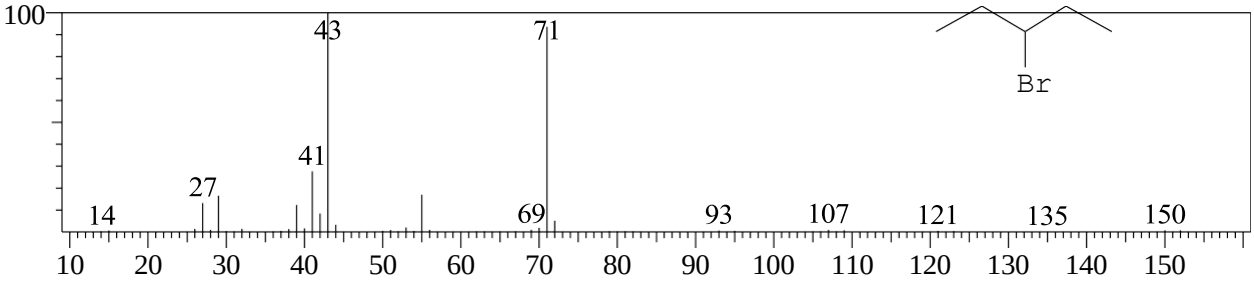
<< Target >>
Line#:3 R.Time:2.165(Scan#:134) MassPeaks:7
RawMode:Averaged 2.160-2.170(133-135) BasePeak:43.00(3325)
BG Mode:Calc. from Peak



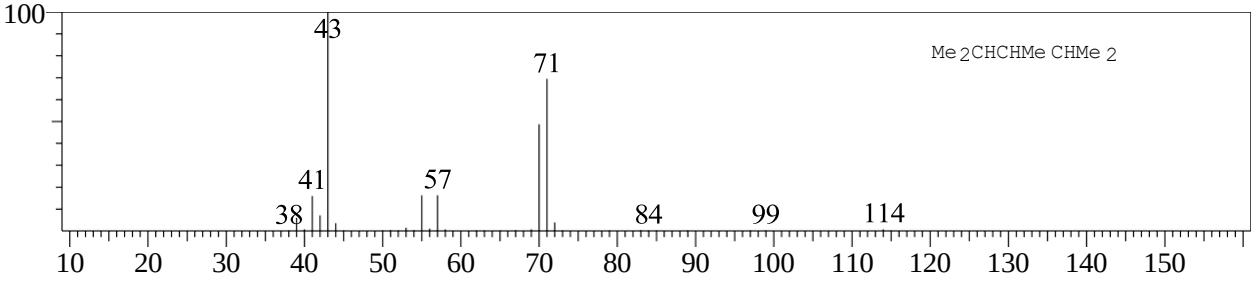
Hit#:1 Entry:47881 Library:WILEY7.LIB
SI:91 Formula:C9 H18 O2 CAS:106-27-4 MolWeight:158 RetIndex:0
CompName:Butanoic acid, 3-methylbutyl ester (CAS) Isoamyl butyrate $$ Isoamyl butylate $$ Isoamyl but



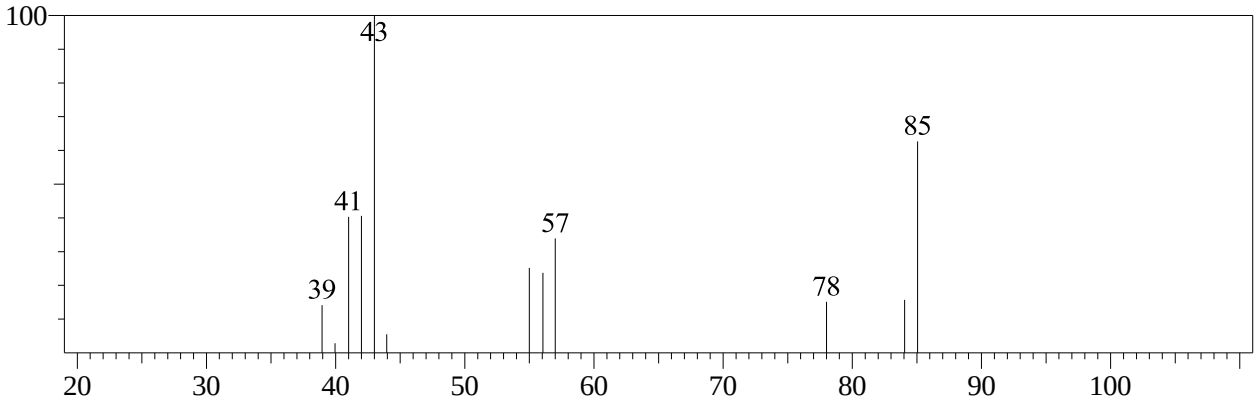
Hit#:2 Entry:8772 Library:NIST11s.lib
SI:91 Formula:C5H11Br CAS:1809-10-5 MolWeight:150 RetIndex:750
CompName:Pentane, 3-bromo- $$ 3-Bromopentane $$ 3-Pentyl bromide $$



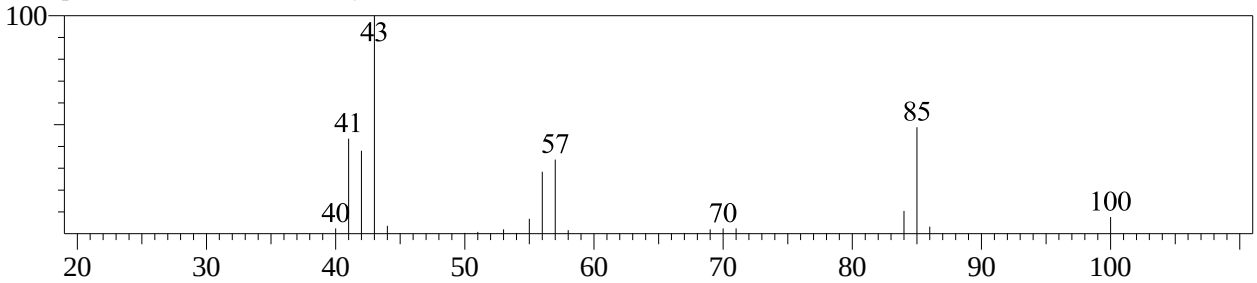
Hit#:3 Entry:12878 Library:WILEY7.LIB
SI:91 Formula:C8 H18 CAS:565-75-3 MolWeight:114 RetIndex:0
CompName:Pentane, 2,3,4-trimethyl- (CAS) 2,3,4-Trimethylpentane $$ (CH3)2CHCH(CH3)CH(CH3)2 $$



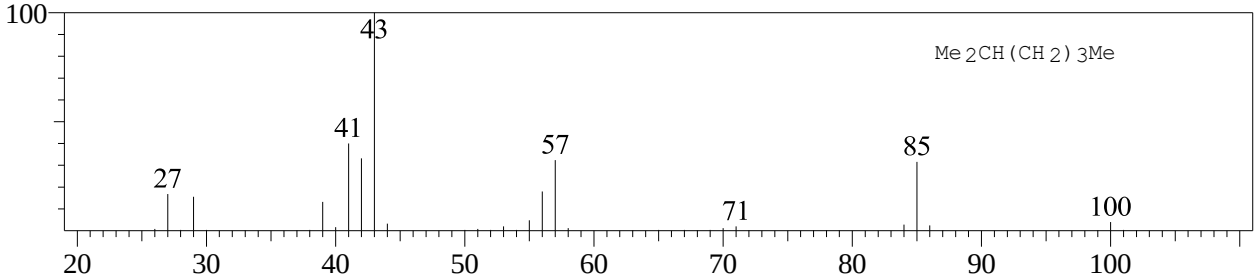
<< Target >>
Line#:4 R.Time:3.4(Scan#:4) MassPeaks:4
RawMode:Averaged 2.250-2.260(151-153) BasePeak:43.00(5649)
BG Mode:Calc. from Peak



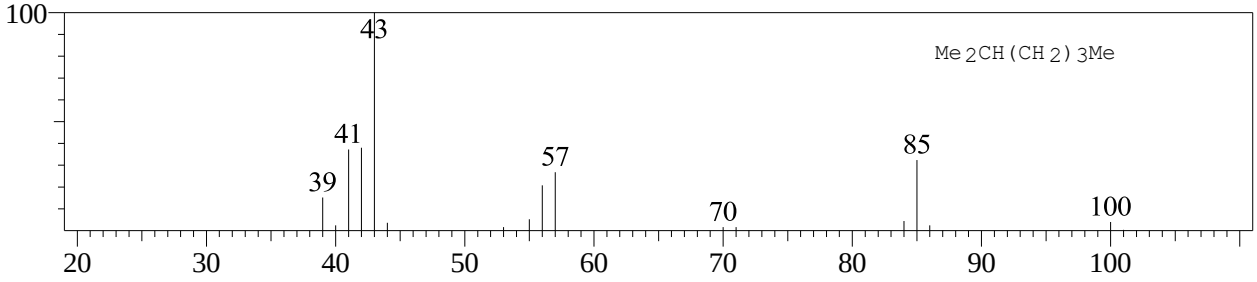
Hit#:1 Entry:1487 Library:FFNSC1.3.lib
SI:90 Formula:C7 H16 CAS:591-76-4 MolWeight:100 RetIndex:680
CompName:Hexane <2-methyl->



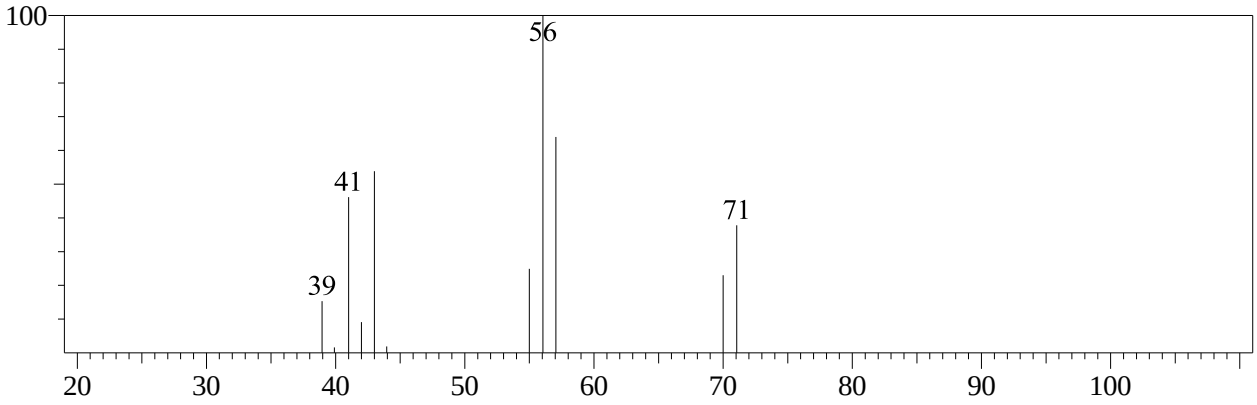
Hit#:2 Entry:7210 Library:WILEY7.LIB
SI:90 Formula:C7 H16 CAS:591-76-4 MolWeight:100 RetIndex:0
CompName:Hexane, 2-methyl- (CAS) 2-Methylhexane $$ Isoheptane $$



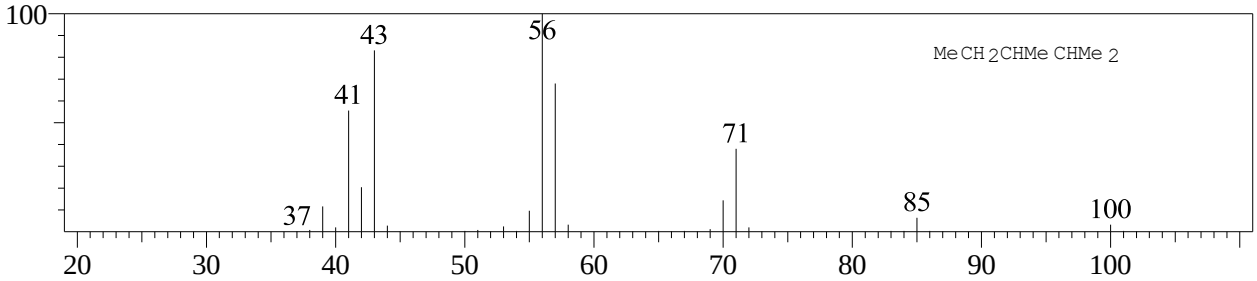
Hit#:3 Entry:7212 Library:WILEY7.LIB
SI:90 Formula:C7 H16 CAS:591-76-4 MolWeight:100 RetIndex:0
CompName:Hexane, 2-methyl- (CAS) 2-Methylhexane $$ Isoheptane $$



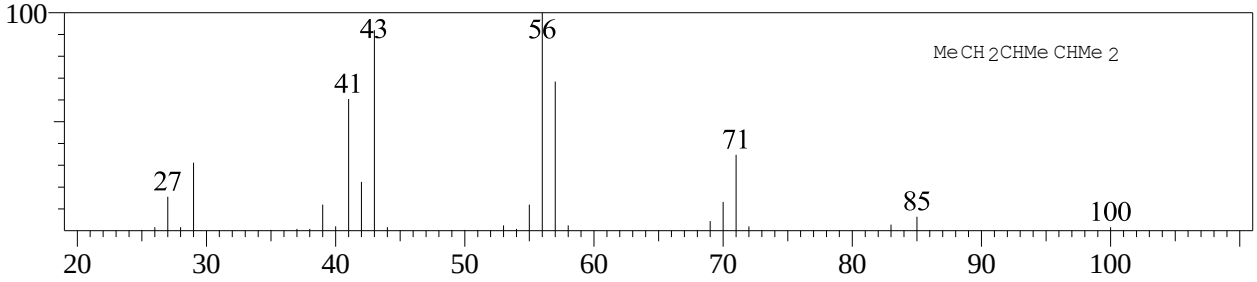
<< Target >>
Line#:5 R.Time:3.5(Scan#:5) MassPeaks:5
RawMode:Averaged 2.285-2.295(158-160) BasePeak:56.05(5565)
BG Mode:Calc. from Peak



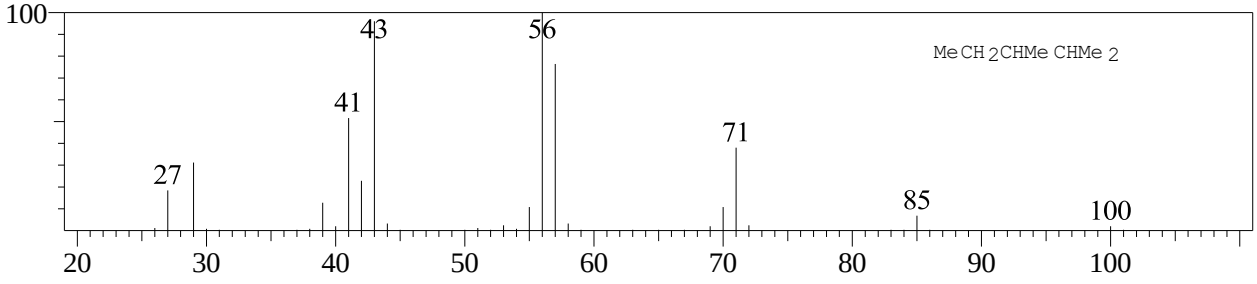
Hit#:1 Entry:7228 Library:WILEY7.LIB
SI:92 Formula:C7 H16 CAS:565-59-3 MolWeight:100 RetIndex:0
CompName:Pentane, 2,3-dimethyl- (CAS) 2,3-Dimethylpentane $$ 3,4-Dimethylpentane $$



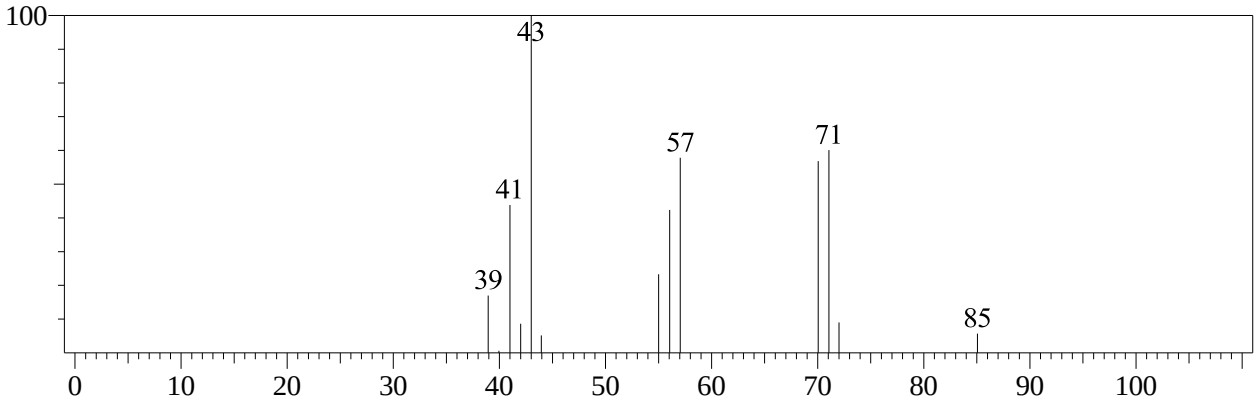
Hit#:2 Entry:7226 Library:WILEY7.LIB
SI:91 Formula:C7 H16 CAS:565-59-3 MolWeight:100 RetIndex:0
CompName:Pentane, 2,3-dimethyl- (CAS) 2,3-Dimethylpentane $$ 3,4-Dimethylpentane $$



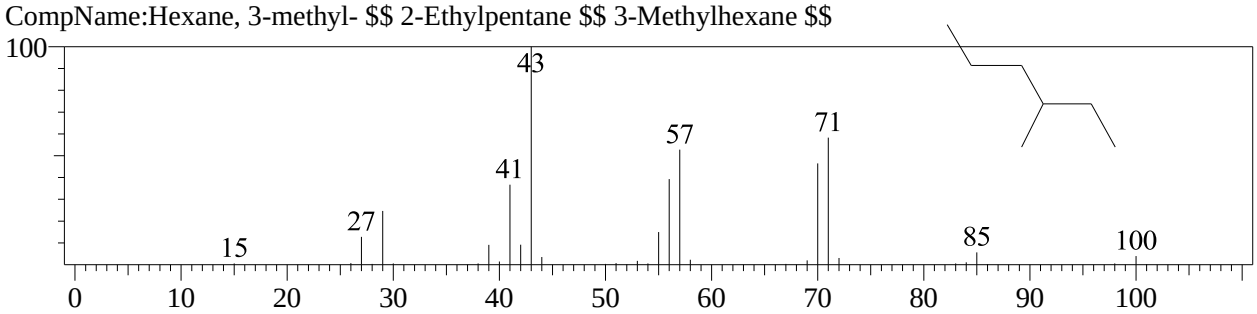
Hit#:3 Entry:7224 Library:WILEY7.LIB
SI:91 Formula:C7 H16 CAS:565-59-3 MolWeight:100 RetIndex:0
CompName:Pentane, 2,3-dimethyl- (CAS) 2,3-Dimethylpentane $$ 3,4-Dimethylpentane $$



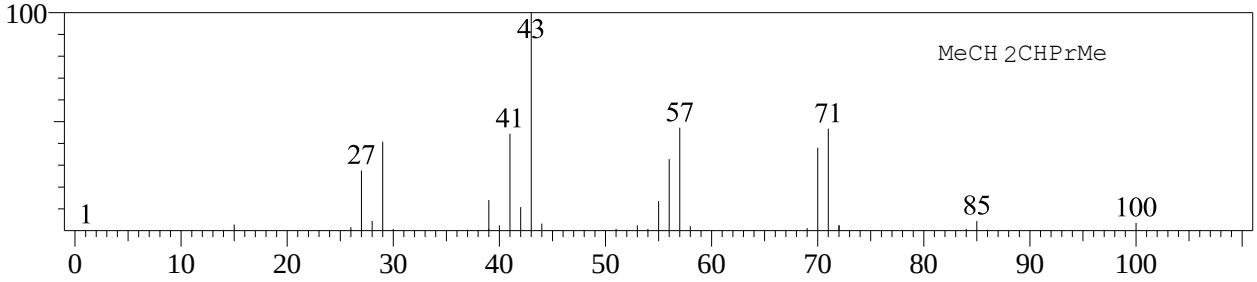
<< Target >>
Line#:6 R.Time:3.6(Scan#:6) MassPeaks:6
RawMode:Averaged 2.340-2.350(169-171) BasePeak:43.00(13338)
BG Mode:Calc. from Peak



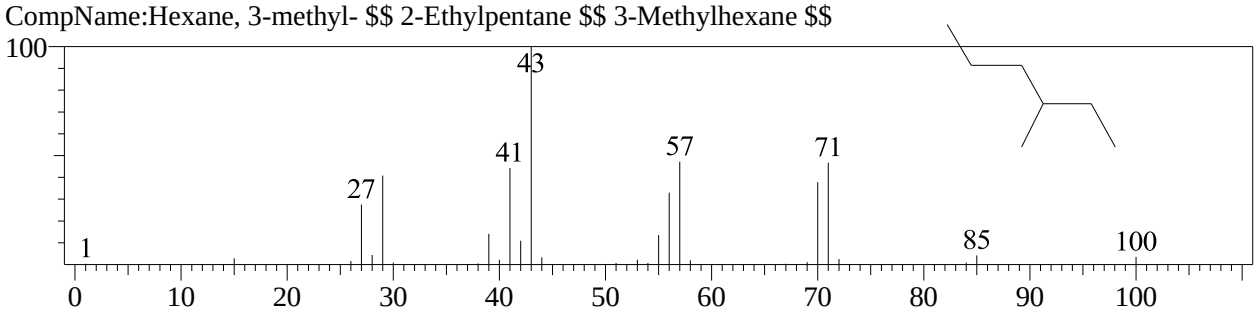
Hit#:1 Entry:2087 Library:NIST11.lib
SI:95 Formula:C7H16 CAS:589-34-4 MolWeight:100 RetIndex:653
CompName:Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane $$



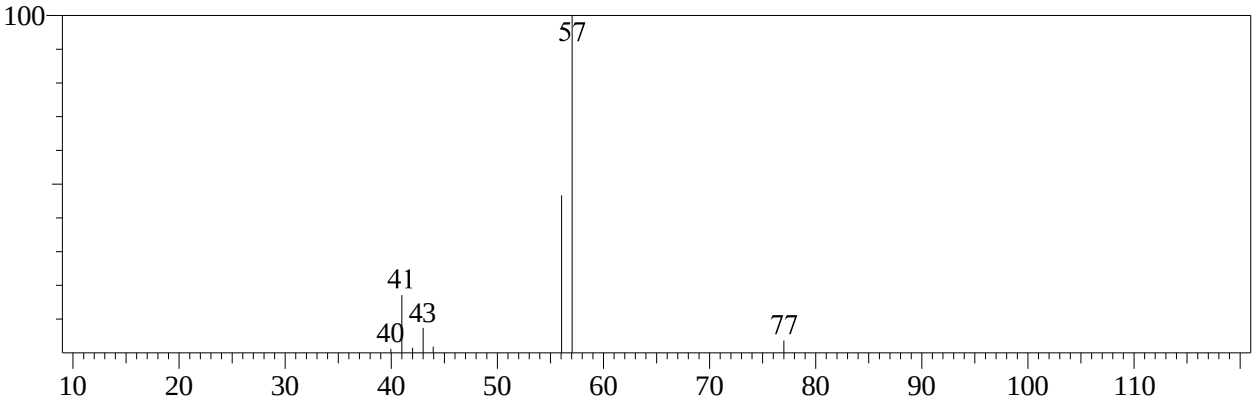
Hit#:2 Entry:7213 Library:WILEY7.LIB
SI:94 Formula:C7 H16 CAS:589-34-4 MolWeight:100 RetIndex:0
CompName:Hexane, 3-methyl- (CAS) 3-Methylhexane $$ 2-Ethylpentane $$



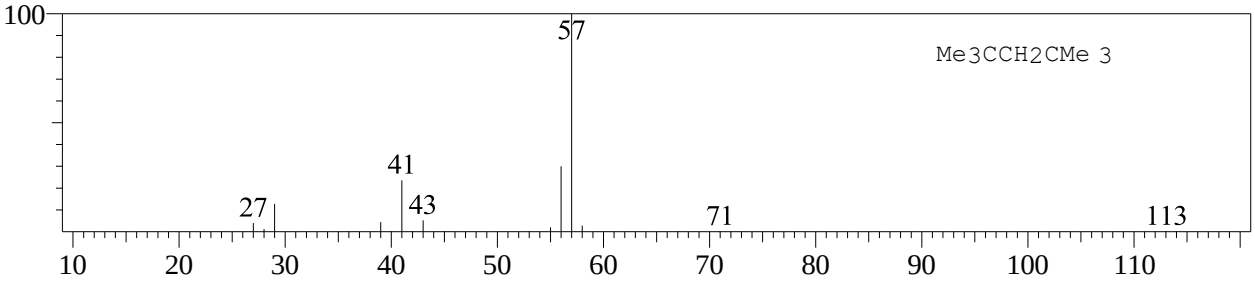
Hit#:3 Entry:1899 Library:NIST11s.lib
SI:93 Formula:C7H16 CAS:589-34-4 MolWeight:100 RetIndex:653
CompName:Hexane, 3-methyl- $$ 2-Ethylpentane $$ 3-Methylhexane $$



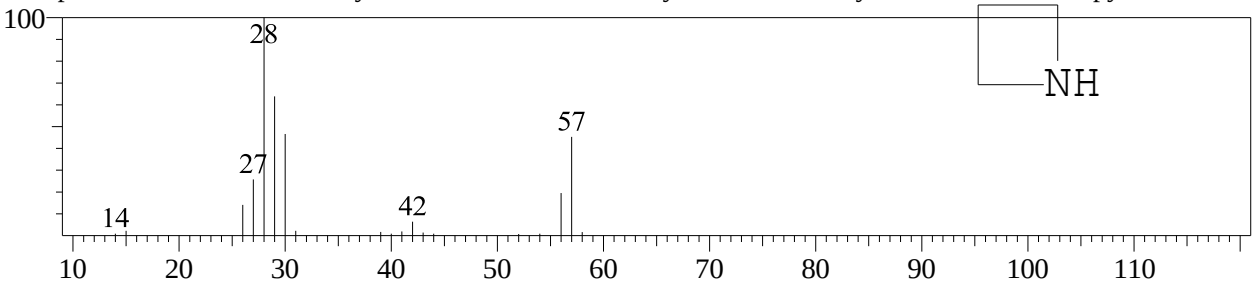
<< Target >>
Line#:7 R.Time:3.7(Scan#:7) MassPeaks:7
RawMode:Averaged 2.900-2.910(281-283) BasePeak:57.05(4627)
BG Mode:Calc. from Peak



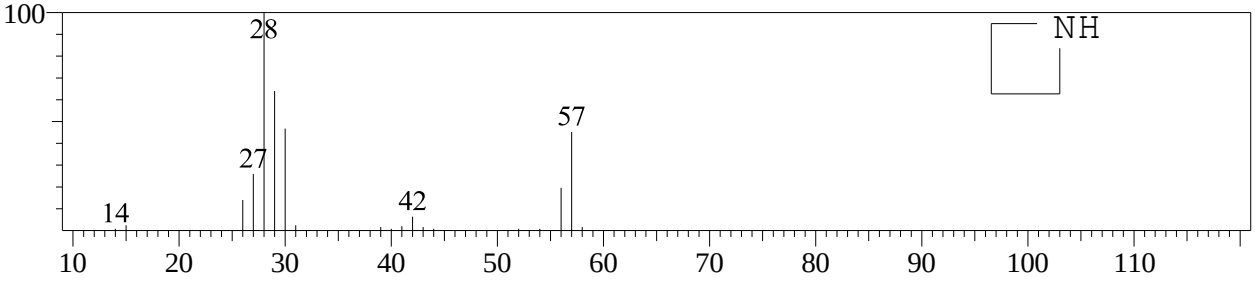
Hit#:1 Entry:20685 Library:WILEY7.LIB
SI:93 Formula:C9 H20 CAS:1070-87-7 MolWeight:128 RetIndex:0
CompName:Pentane, 2,2,4,4-tetramethyl- (CAS) 2,2,4,4-Tetramethylpentane $$ Di-tert-Butylmethane $$



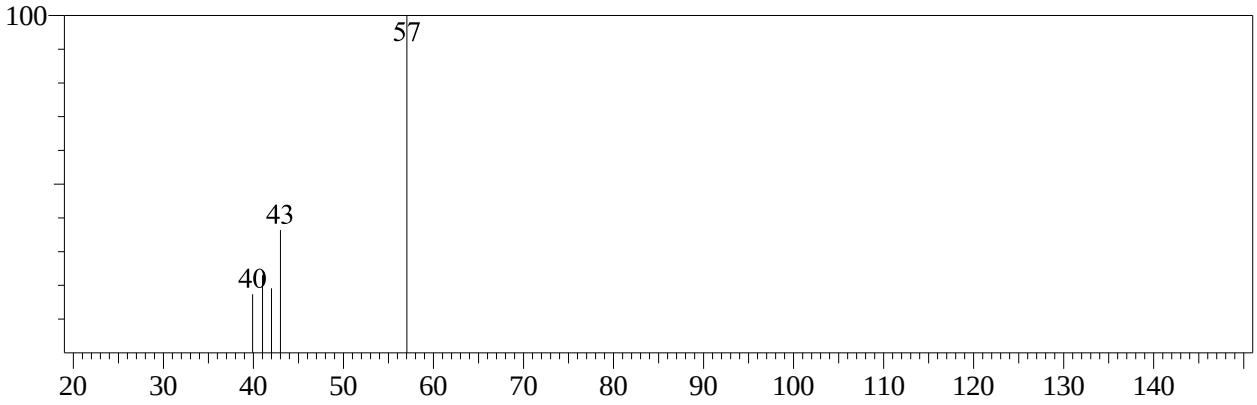
Hit#:2 Entry:101 Library:NIST11.lib
SI:92 Formula:C3H7N CAS:503-29-7 MolWeight:57 RetIndex:625
CompName:Azetidine $$ Azacyclobutane $$ Azete, tetrahydro- $$ Trimethylenimine $$ 1,3-Propylenimine



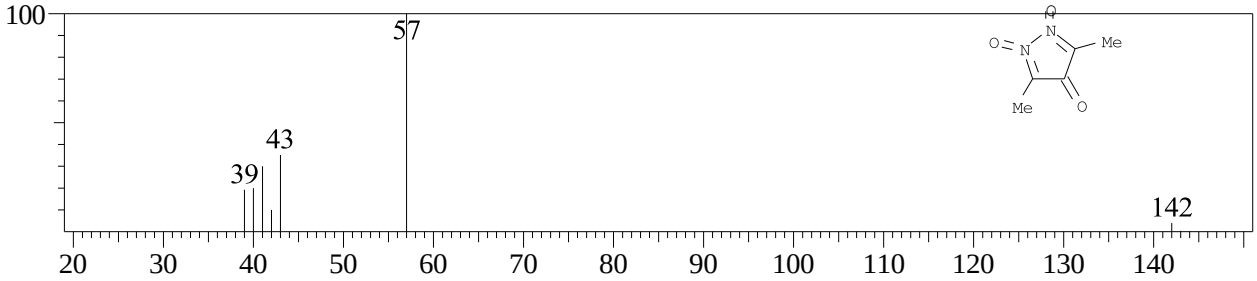
Hit#:3 Entry:448 Library:WILEY7.LIB
SI:92 Formula:C3 H7 N CAS:503-29-7 MolWeight:57 RetIndex:0
CompName:Azetidine (CAS) Azacyclobutane $$ Trimethylenimine $$ 1,3-Propylenimine $$ Azete, tetrahyd



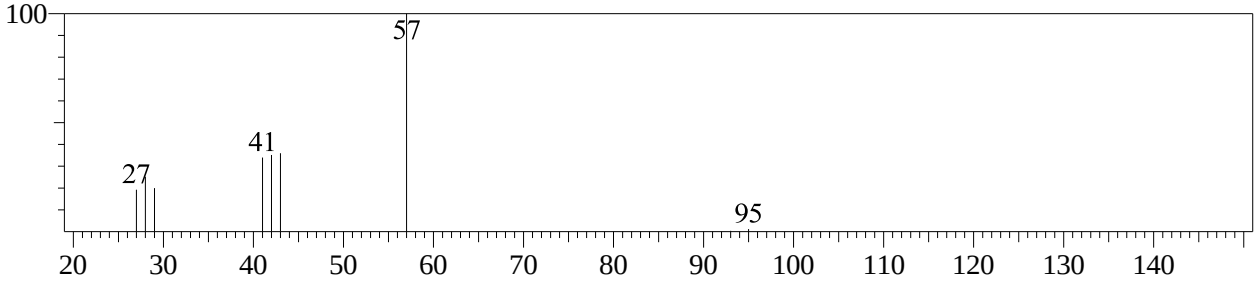
<< Target >>
Line#:8 R.Time:3.8(Scan#:8) MassPeaks:8
RawMode:Averaged 3.045-3.055(310-312) BasePeak:57.05(800)
BG Mode:Calc. from Peak



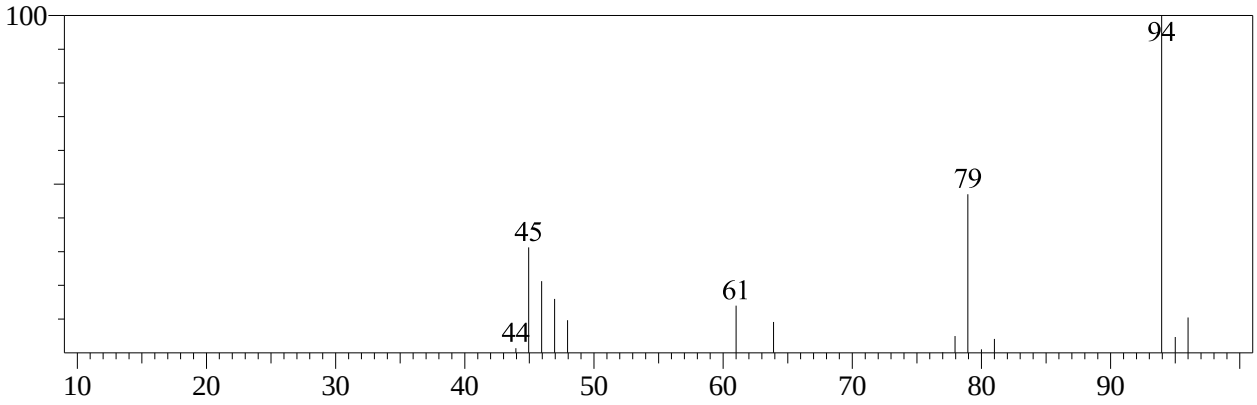
Hit#:1 Entry:30509 Library:WILEY7.LIB
SI:96 Formula:C5 H6 N2 O3 CAS:17952-97-5 MolWeight:142 RetIndex:0
CompName:3,5-DIMETHYL-4-OXO-4H-PYRAZOLE 1,2-DIOXIDE $$ 4H-Pyrazol-4-one, 3,5-dimethyl-,



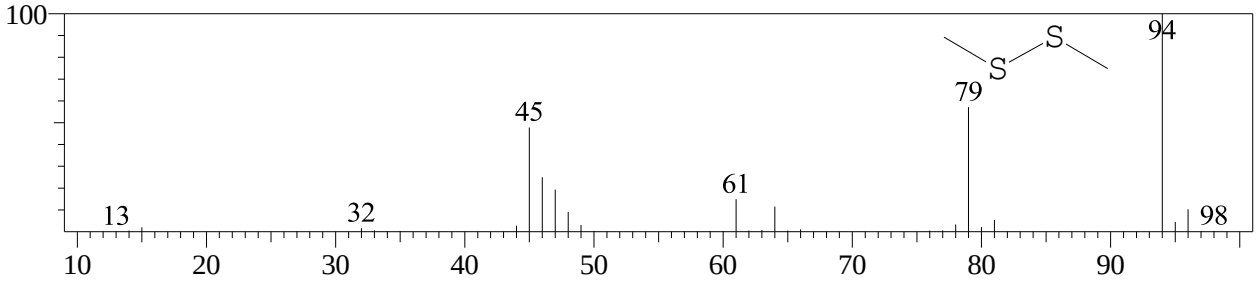
Hit#:2 Entry:4546 Library:WILEY7.LIB
SI:92 Formula:C3 13C H9 CL CAS:0-00-0 MolWeight:92 RetIndex:0
CompName:[1-13C]-Butylchloride $$



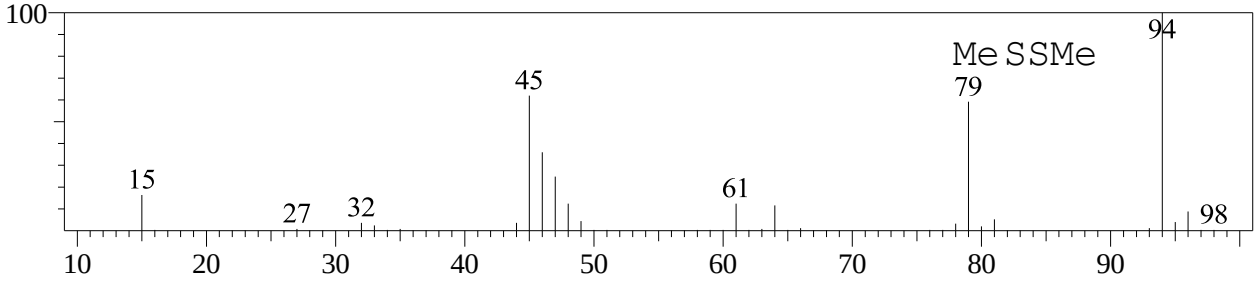
<< Target >>
Line#:9 R.Time:3.9(Scan#:9) MassPeaks:9
RawMode:Averaged 3.305-3.315(362-364) BasePeak:93.95(24304)
BG Mode:Calc. from Peak



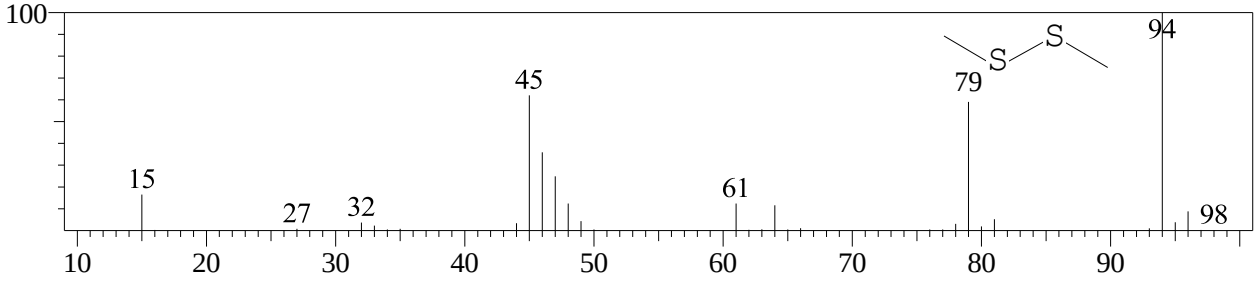
Hit#:1 Entry:1238 Library:NIST11.lib
SI:95 Formula:C2H6S2 CAS:624-92-0 MolWeight:94 RetIndex:722
CompName:Disulfide, dimethyl $$ 2,3-Dithiabutane $$ Methyl disulfide $$ (Methyldithio)methane $$ Dim



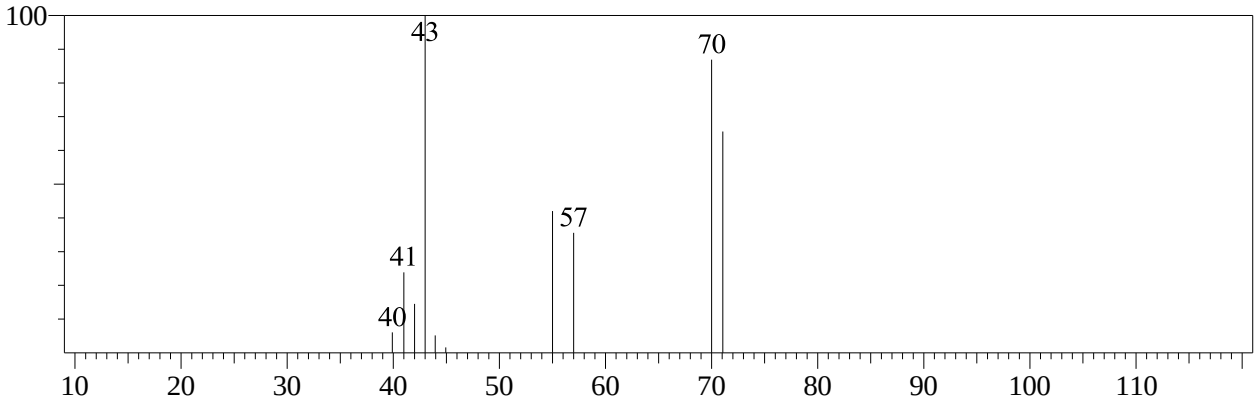
Hit#:2 Entry:4882 Library:WILEY7.LIB
SI:92 Formula:C2 H6 S2 CAS:624-92-0 MolWeight:94 RetIndex:0
CompName:Disulfide, dimethyl (CAS) 2,3-Dithiabutane $$ Dimethyl disulfide $$ Methyl disulfide $$ (Met



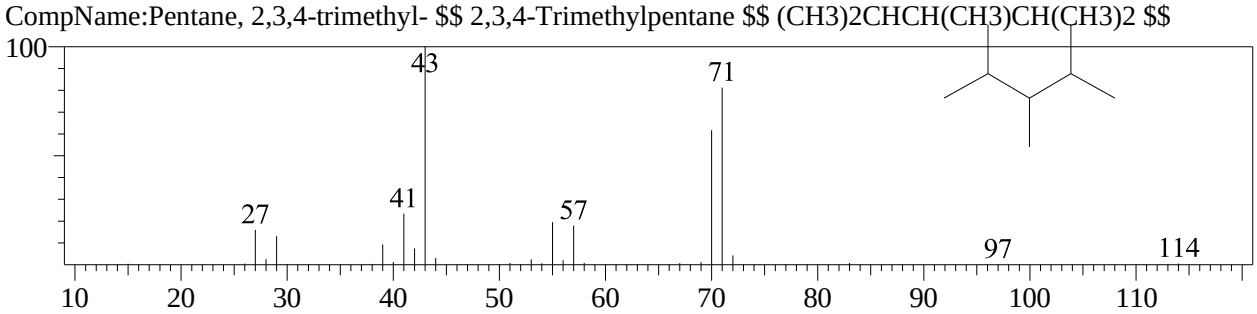
Hit#:3 Entry:1299 Library:NIST11s.lib
SI:92 Formula:C2H6S2 CAS:624-92-0 MolWeight:94 RetIndex:722
CompName:Disulfide, dimethyl $$ 2,3-Dithiabutane $$ Methyl disulfide $$ (Methyldithio)methane $$ Dim



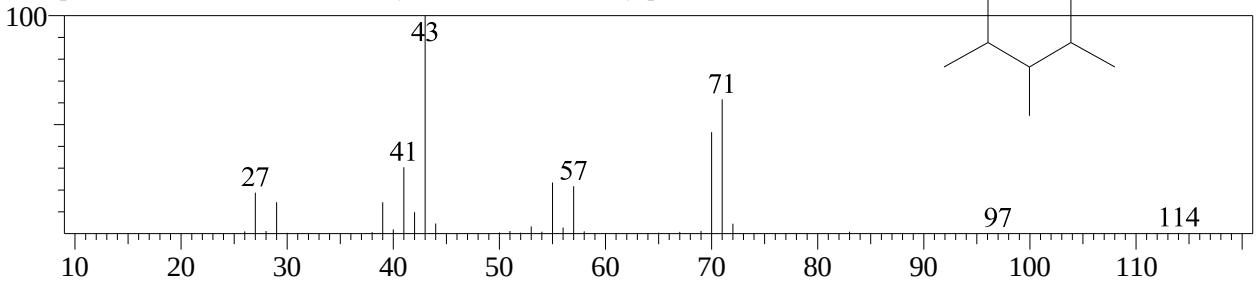
<< Target >>
Line#:10 R.Time:3.10(Scan#:10) MassPeaks:10
RawMode:Averaged 3.575-3.585(416-418) BasePeak:43.00(3318)
BG Mode:Calc. from Peak



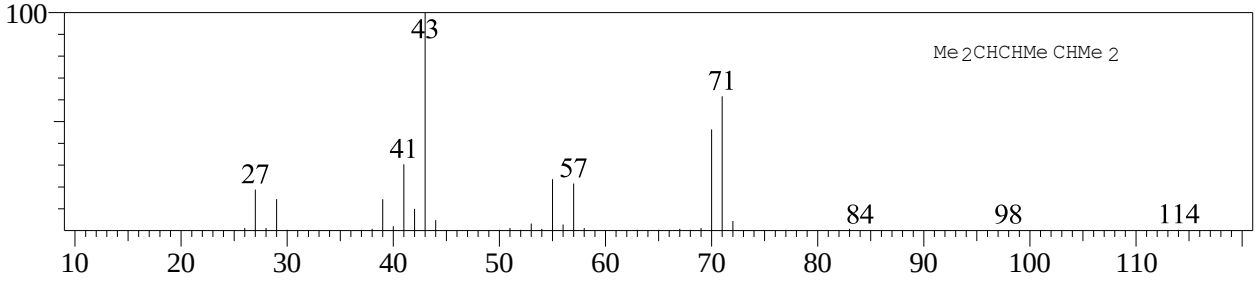
Hit#:1 Entry:3409 Library:NIST11s.lib
SI:91 Formula:C8H18 CAS:565-75-3 MolWeight:114 RetIndex:624
CompName:Pentane, 2,3,4-trimethyl- $$ 2,3,4-Trimethylpentane $$ (CH3)2CHCH(CH3)CH(CH3)2 $$



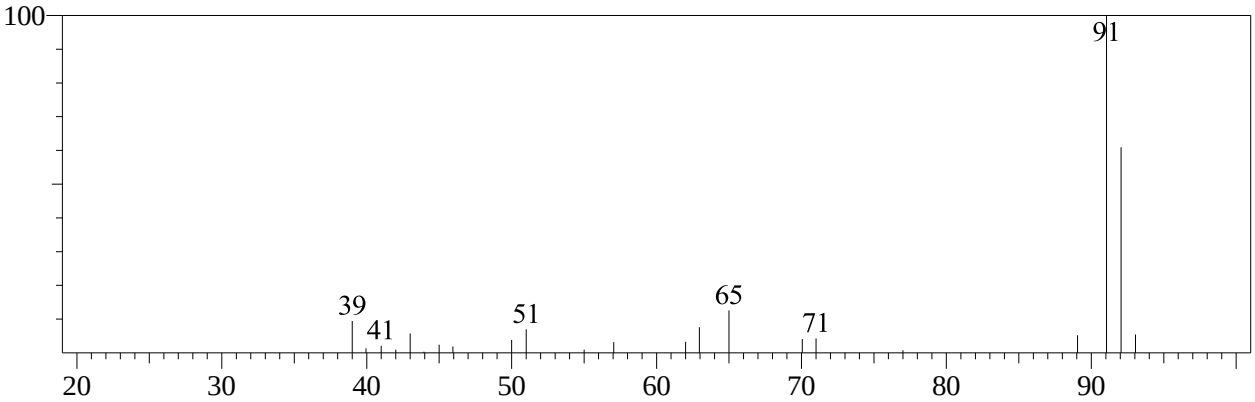
Hit#:2 Entry:3410 Library:NIST11s.lib
SI:91 Formula:C8H18 CAS:565-75-3 MolWeight:114 RetIndex:624
CompName:Pentane, 2,3,4-trimethyl- $$ 2,3,4-Trimethylpentane $$ (CH3)2CHCH(CH3)CH(CH3)2 $$



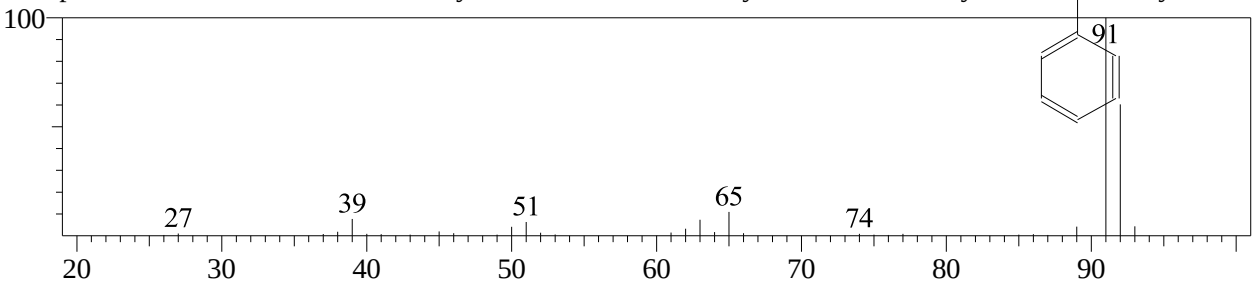
Hit#:3 Entry:12875 Library:WILEY7.LIB
SI:91 Formula:C8 H18 CAS:565-75-3 MolWeight:114 RetIndex:0
CompName:Pentane, 2,3,4-trimethyl- (CAS) 2,3,4-Trimethylpentane $$



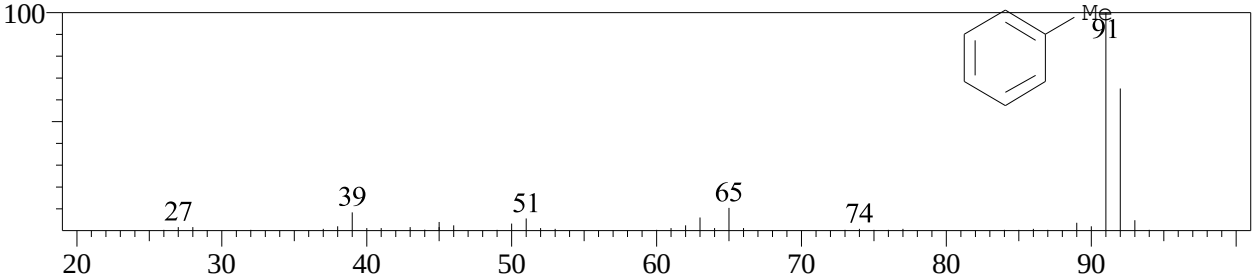
<< Target >>
Line#:11 R.Time:3.11(Scan#:11) MassPeaks:11
RawMode:Averaged 3.730-3.740(447-449) BasePeak:91.05(36916)
BG Mode:Calc. from Peak



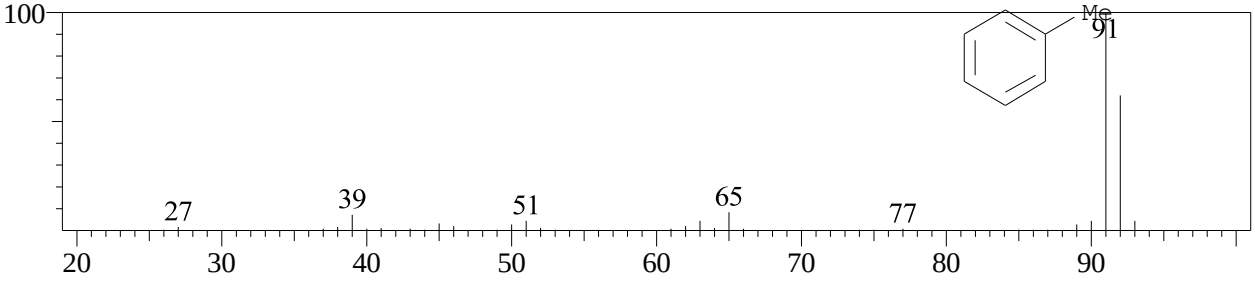
Hit#:1 Entry:1261 Library:NIST11s.lib
SI:93 Formula:C7H8 CAS:108-88-3 MolWeight:92 RetIndex:794
CompName:Toluene $$ Benzene, methyl $$ Methacide $$ Methylbenzene $$ Methylbenzol $$ Phenylmeth



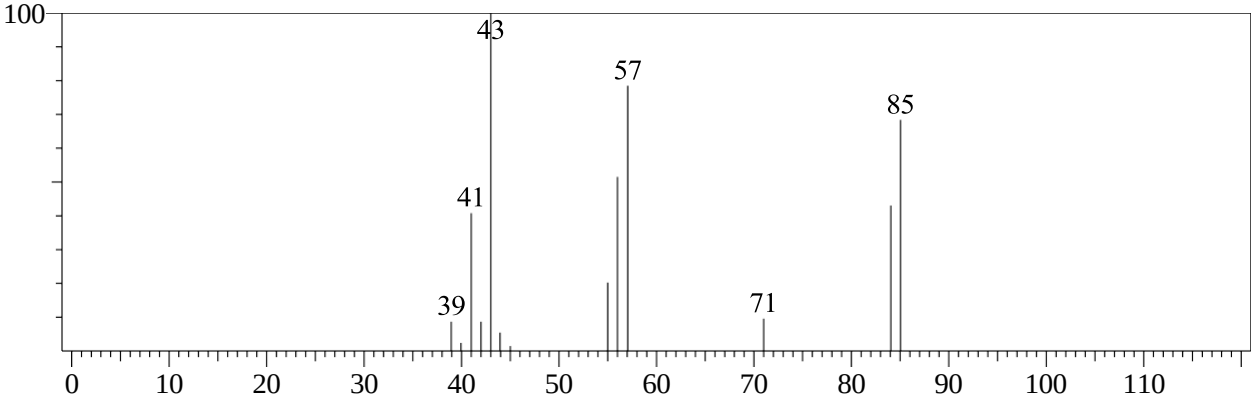
Hit#:2 Entry:4672 Library:WILEY7.LIB
SI:93 Formula:C7 H8 CAS:108-88-3 MolWeight:92 RetIndex:0
CompName:Benzene, methyl- (CAS) Toluene $$ CP 25 $$ Methylbenzene $$ Toluol $$ Methacide $$ Antis



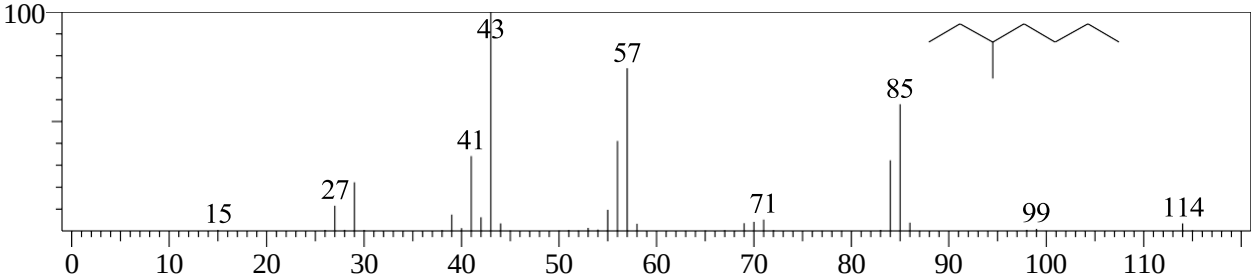
Hit#:3 Entry:4668 Library:WILEY7.LIB
SI:92 Formula:C7 H8 CAS:108-88-3 MolWeight:92 RetIndex:0
CompName:Benzene, methyl- (CAS) Toluene $$ CP 25 $$ Methylbenzene $$ Toluol $$ Methacide $$ Antis



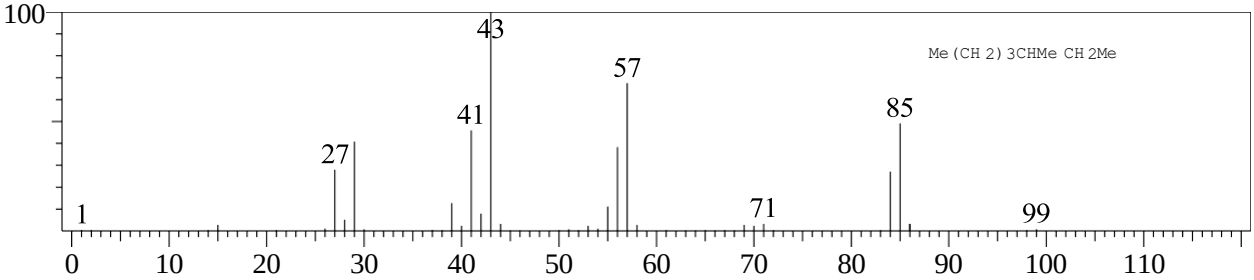
<< Target >>
Line#:12 R.Time:3.12(Scan#:12) MassPeaks:12
RawMode:Averaged 3.840-3.850(469-471) BasePeak:43.00(7674)
BG Mode:Calc. from Peak



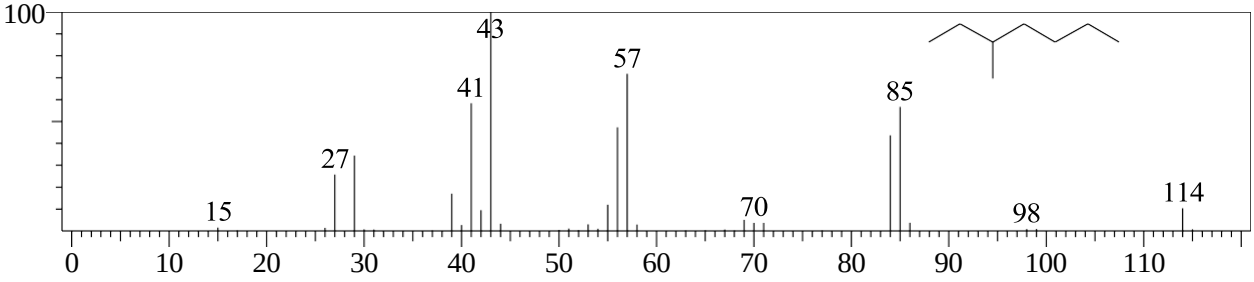
Hit#:1 Entry:3398 Library:NIST11s.lib
SI:93 Formula:C8H18 CAS:589-81-1 MolWeight:114 RetIndex:752
CompName:Heptane, 3-methyl- $$ 3-Methylheptane $$ 2-Ethylhexane $$



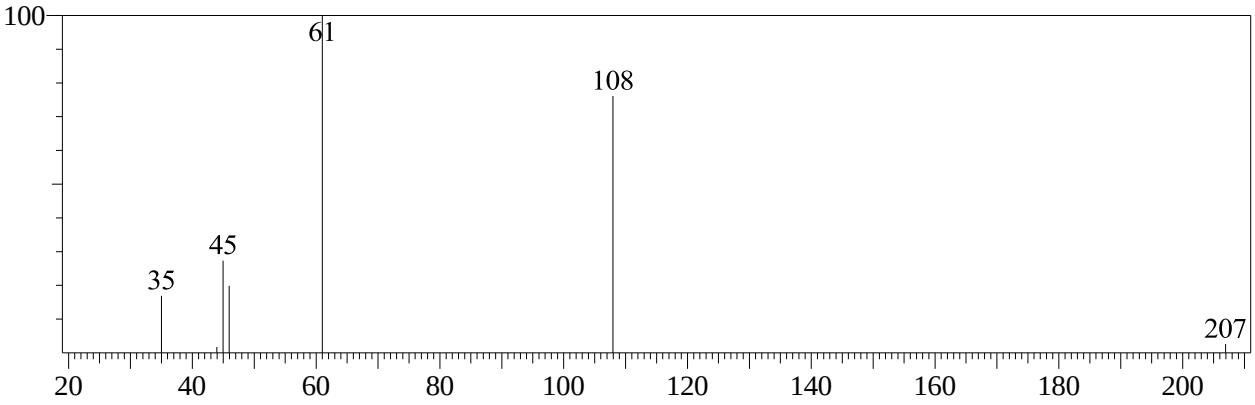
Hit#:2 Entry:12837 Library:WILEY7.LIB
SI:92 Formula:C8 H18 CAS:589-81-1 MolWeight:114 RetIndex:0
CompName:Heptane, 3-methyl- (CAS) 3-Methylheptane $$ 2-Ethylhexane $$



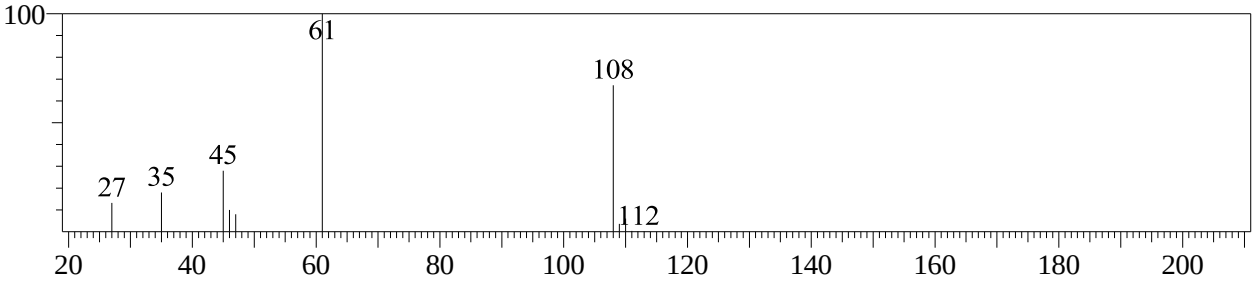
Hit#:3 Entry:4237 Library:NIST11.lib
SI:92 Formula:C8H18 CAS:589-81-1 MolWeight:114 RetIndex:752
CompName:Heptane, 3-methyl- $$ 3-Methylheptane $$ 2-Ethylhexane $$



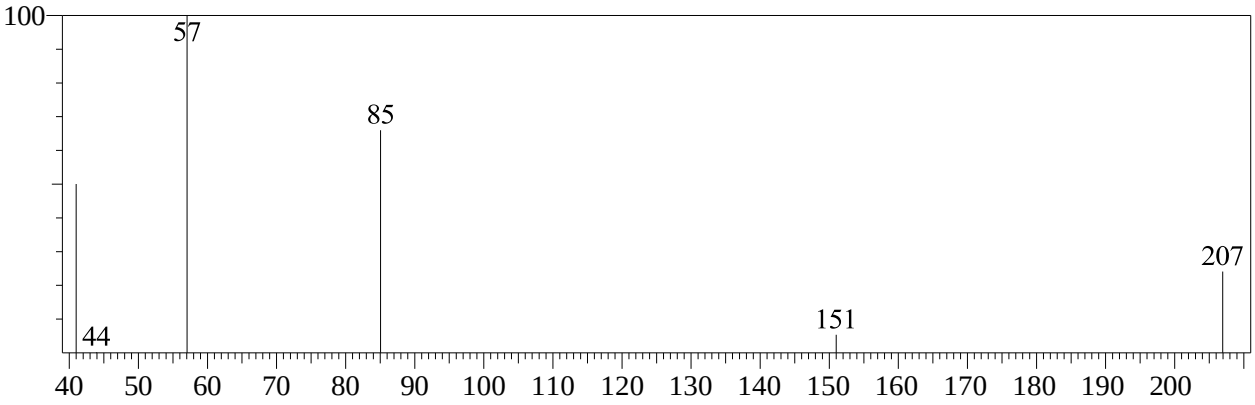
<< Target >>
Line#:13 R.Time:3.13(Scan#:13) MassPeaks:13
RawMode:Averaged 7.185-7.195(1138-1140) BasePeak:61.00(6316)
BG Mode:Calc. from Peak



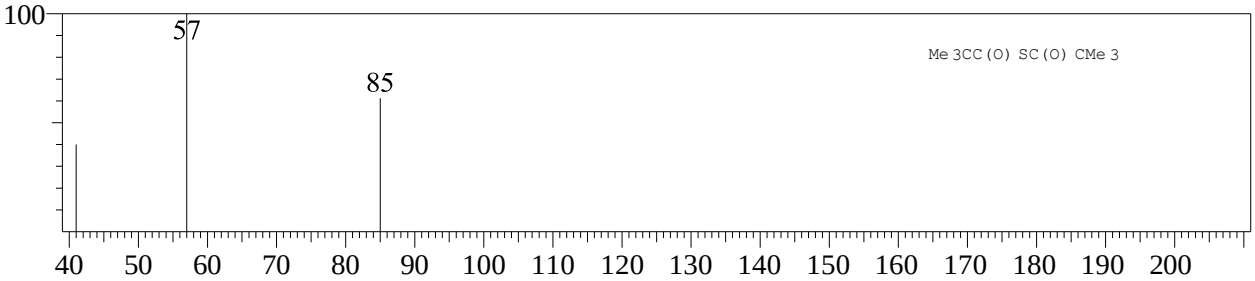
Hit#:1 Entry:9320 Library:WILEY7.LIB
SI:93 Formula:C3 H8 S2 CAS:1618-26-4 MolWeight:108 RetIndex:0
CompName:2,4-Dithiapentane $$ Bis-(methylthio)-methane $$ CH3SCH2SCH3 $$ Bis(methylthio)methan



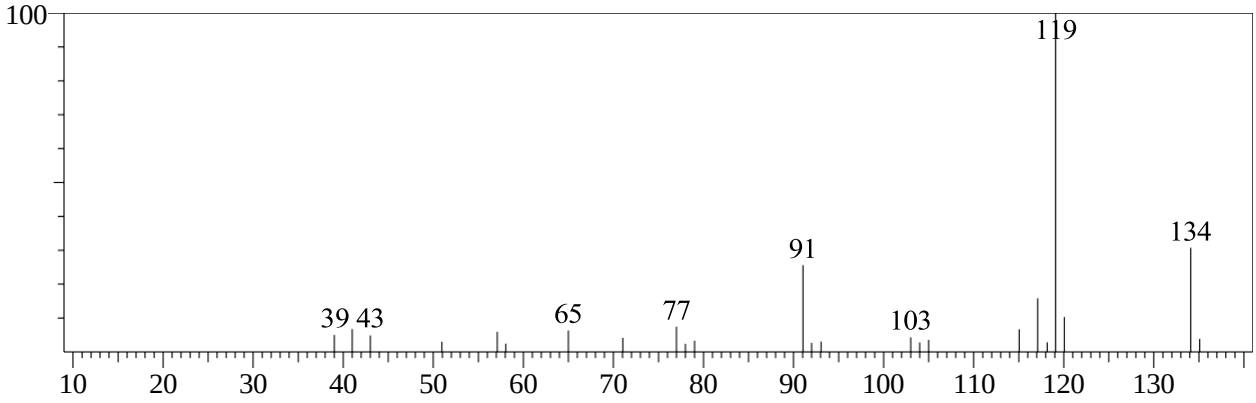
<< Target >>
Line#:14 R.Time:3.14(Scan#:14) MassPeaks:14
RawMode:Averaged 9.150-9.160(1531-1533) BasePeak:57.05(2865)
BG Mode:Calc. from Peak



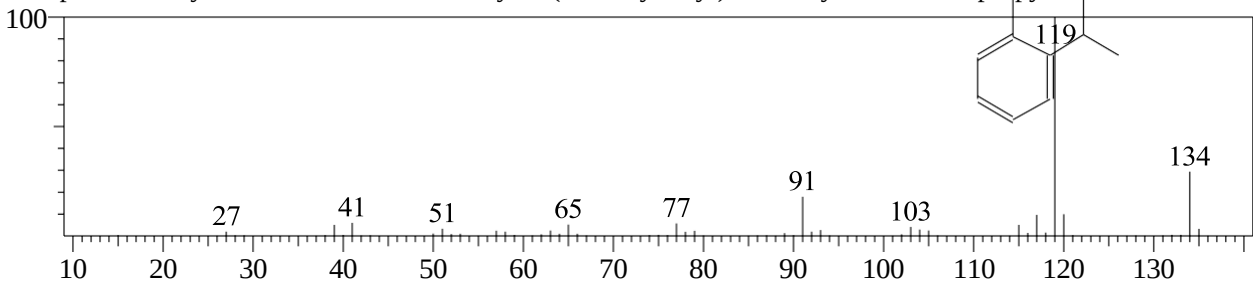
Hit#:1 Entry:97009 Library:WILEY7.LIB
SI:92 Formula:C10 H18 O2 S CAS:36911-20-3 MolWeight:202 RetIndex:0
CompName:DIPIVALOYL SULPHIDE $$ Propanethioic acid, 2,2-dimethyl-, anhydrosulfide (CAS) Dipiva



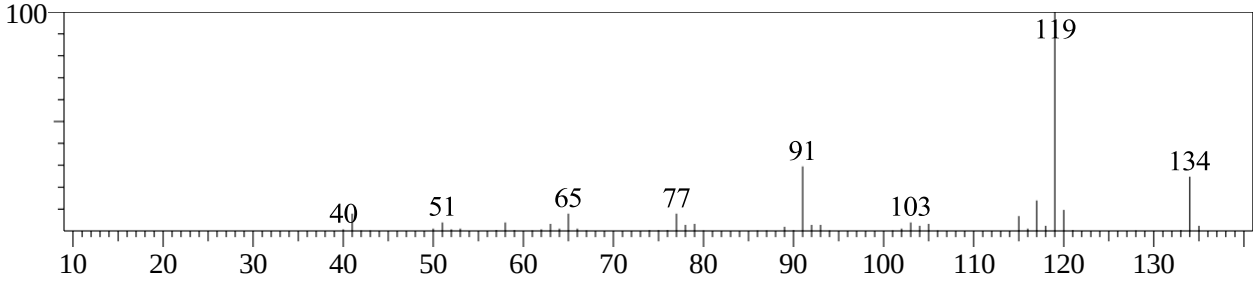
<< Target >>
Line#:15 R.Time:3.15(Scan#:15) MassPeaks:15
RawMode:Averaged 12.830-12.840(2267-2269) BasePeak:119.10(42397)
BG Mode:Calc. from Peak



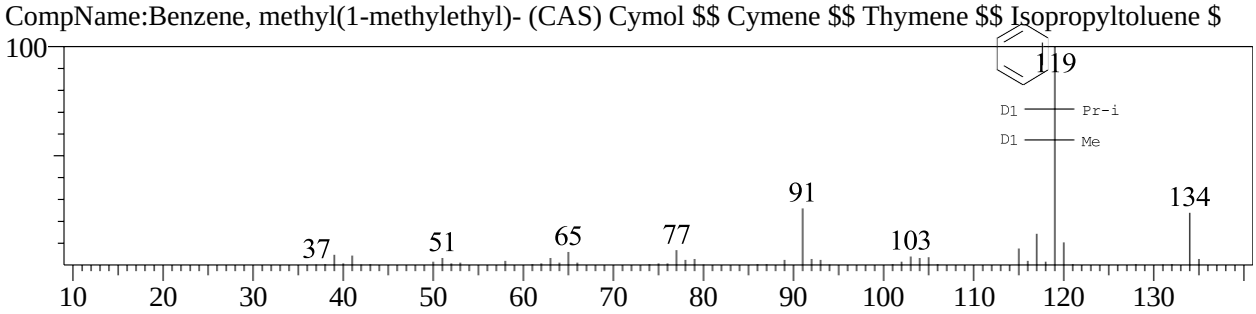
Hit#:1 Entry:6234 Library:NIST11s.lib
SI:92 Formula:C10H14 CAS:527-84-4 MolWeight:134 RetIndex:1042
CompName:o-Cymene $$ Benzene, 1-methyl-2-(1-methylethyl)- $$ o-Cymol $$ o-Isopropyltoluene $$ 1-Is



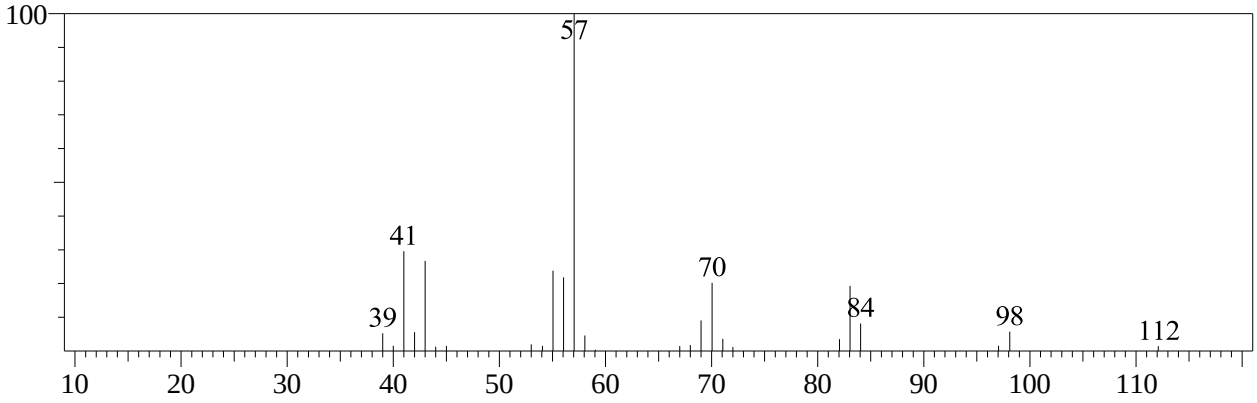
Hit#:2 Entry:317 Library:FFNSC1.3.lib
SI:92 Formula:C10 H14 CAS:99-87-6 MolWeight:134 RetIndex:1025
CompName:Cymene <para->



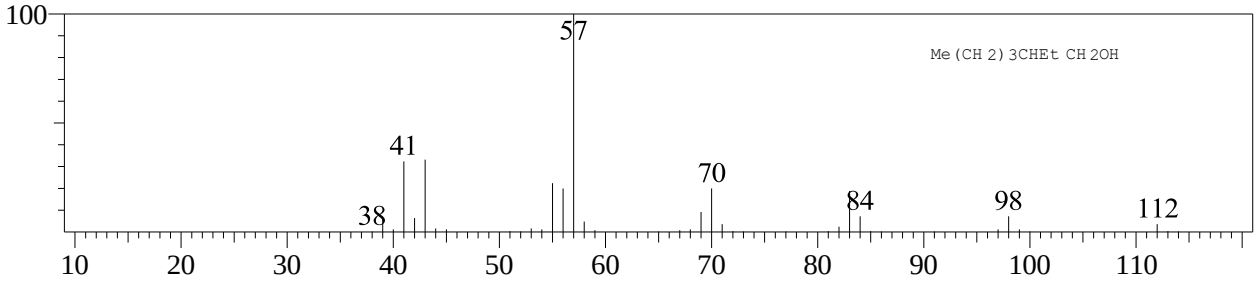
Hit#:3 Entry:24425 Library:WILEY7.LIB
SI:92 Formula:C10 H14 CAS:25155-15-1 MolWeight:134 RetIndex:0
CompName:Benzene, methyl(1-methylethyl)- (CAS) Cymol $$ Cymene $$ Thymene $$ Isopropyltoluene $



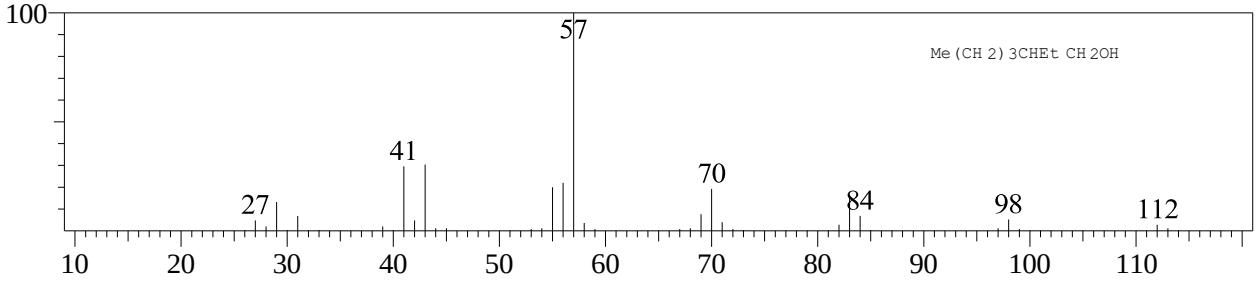
<< Target >>
Line#:16 R.Time:3.16(Scan#:16) MassPeaks:16
RawMode:Averaged 13.190-13.200(2339-2341) BasePeak:57.05(89306)
BG Mode:Calc. from Peak



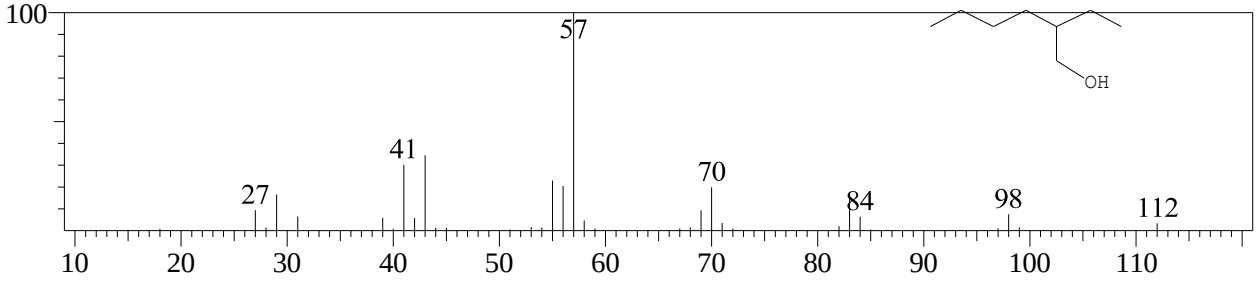
Hit#:1 Entry:22067 Library:WILEY7.LIB
SI:98 Formula:C8 H18 O CAS:104-76-7 MolWeight:130 RetIndex:0
CompName:1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol $$ 2-Ethyl-1-hexanol $$ Ethylhexanol $$ 2-Ethylhe



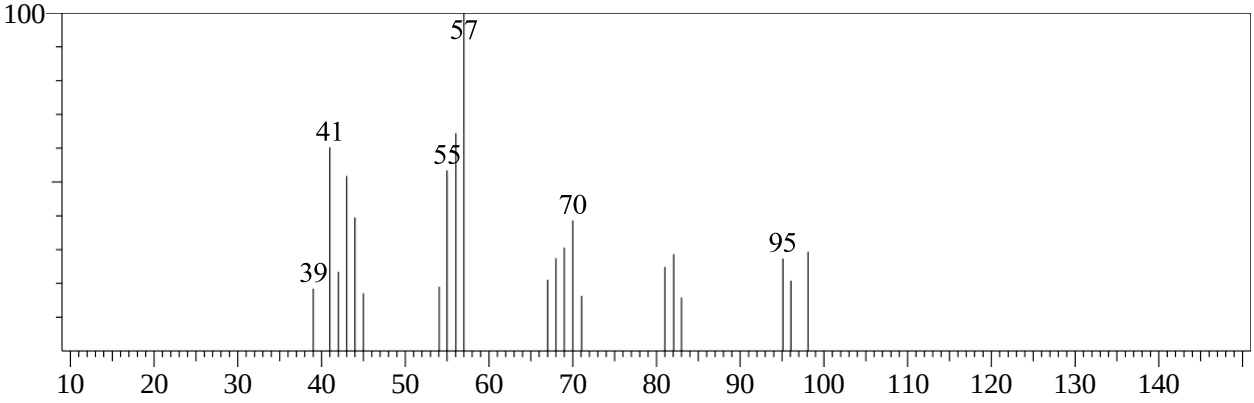
Hit#:2 Entry:22058 Library:WILEY7.LIB
SI:97 Formula:C8 H18 O CAS:104-76-7 MolWeight:130 RetIndex:0
CompName:1-Hexanol, 2-ethyl- (CAS) 2-Ethylhexanol $$ 2-Ethyl-1-hexanol $$ Ethylhexanol $$ 2-Ethylhe



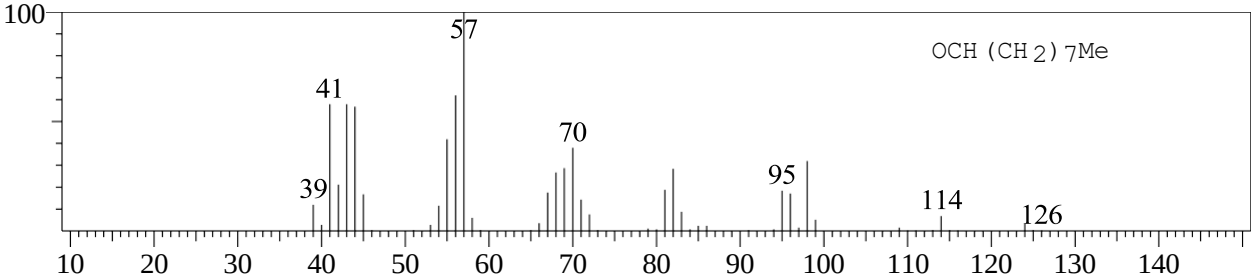
Hit#:3 Entry:5630 Library:NIST11s.lib
SI:97 Formula:C8H18O CAS:104-76-7 MolWeight:130 RetIndex:995
CompName:1-Hexanol, 2-ethyl- $$ 2-Ethyl-1-hexanol $$ 2-Ethylhexan-1-ol $$ 2-Ethylhexanol $$ Ethylhex



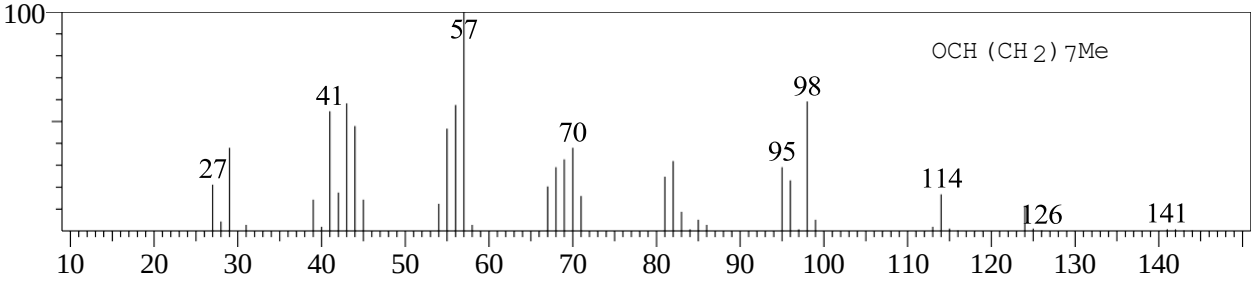
<< Target >>
Line#:17 R.Time:3.17(Scan#:17) MassPeaks:17
RawMode:Averaged 16.730-16.740(3047-3049) BasePeak:57.00(7098)
BG Mode:Calc. from Peak



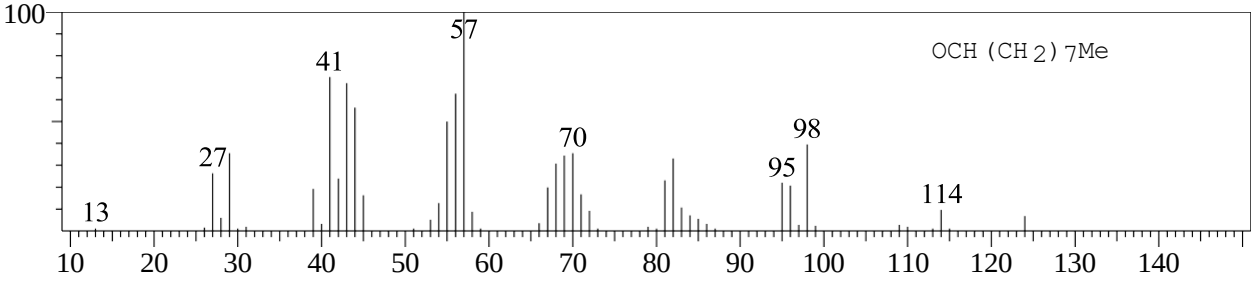
Hit#:1 Entry:31645 Library:WILEY7.LIB
SI:93 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



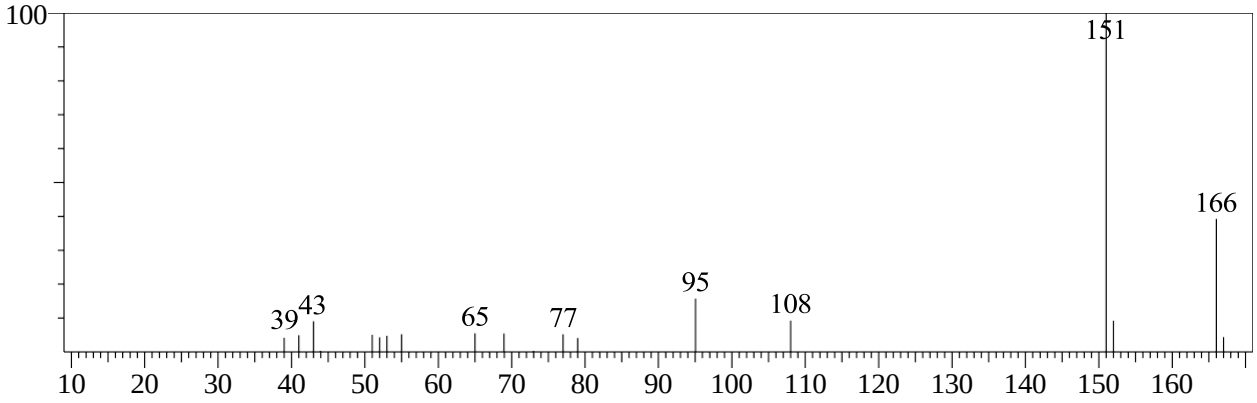
Hit#:2 Entry:31649 Library:WILEY7.LIB
SI:93 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



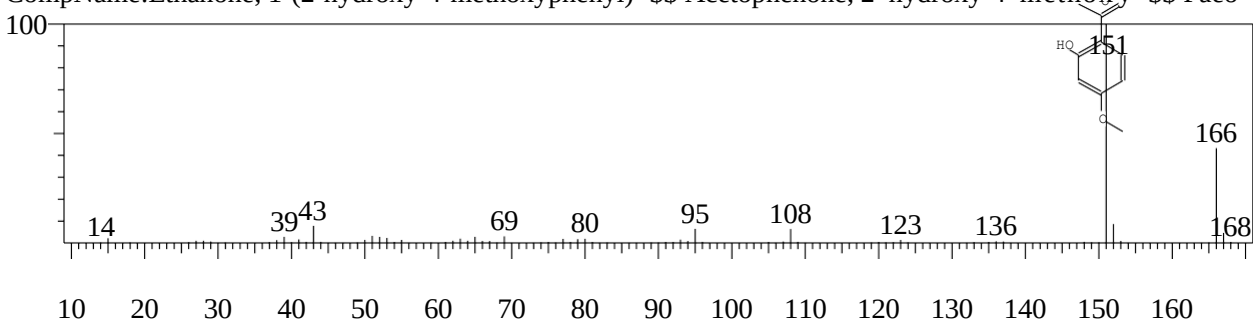
Hit#:3 Entry:31655 Library:WILEY7.LIB
SI:92 Formula:C9 H18 O CAS:124-19-6 MolWeight:142 RetIndex:0
CompName:Nonanal (CAS) n-Nonanal $$ n-Nonylaldehyde $$ Nonaldehyde $$ n-Nonaldehyde $$ Nonana



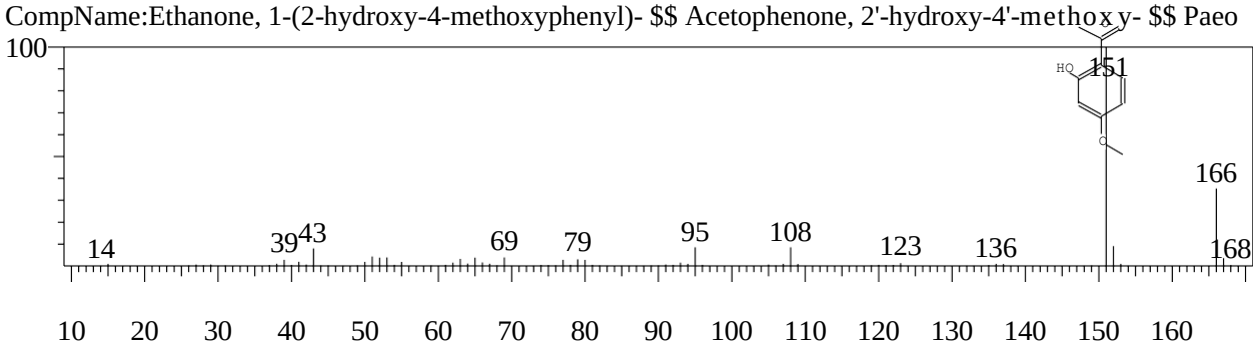
<< Target >>
Line#:18 R.Time:3.18(Scan#:18) MassPeaks:18
RawMode:Averaged 31.585-31.595(6018-6020) BasePeak:151.00(26364)
BG Mode:Calc. from Peak



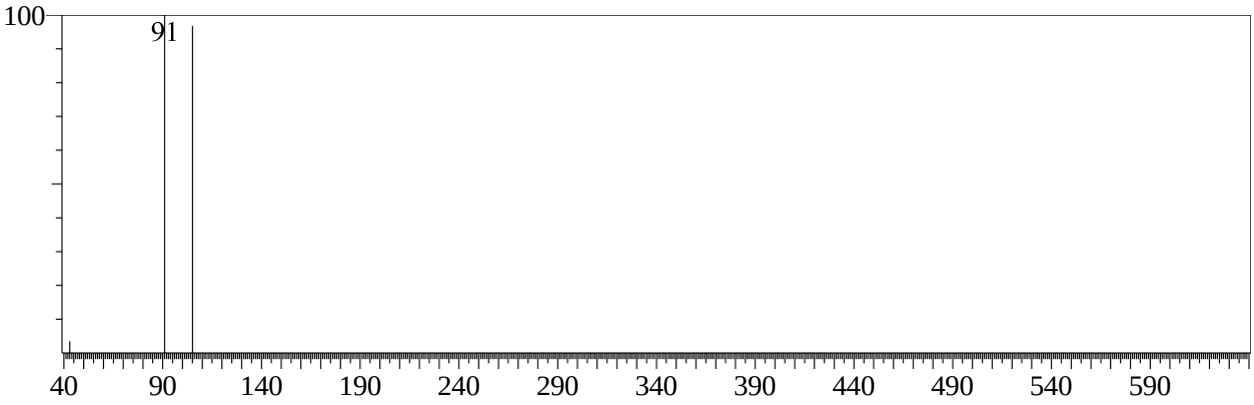
Hit#:1 Entry:12015 Library:NIST11s.lib
SI:90 Formula:C9H10O3 CAS:552-41-0 MolWeight:166 RetIndex:1439
CompName:Ethanone, 1-(2-hydroxy-4-methoxyphenyl)- $$ Acetophenone, 2'-hydroxy-4'-methoxy- $$ Paeo



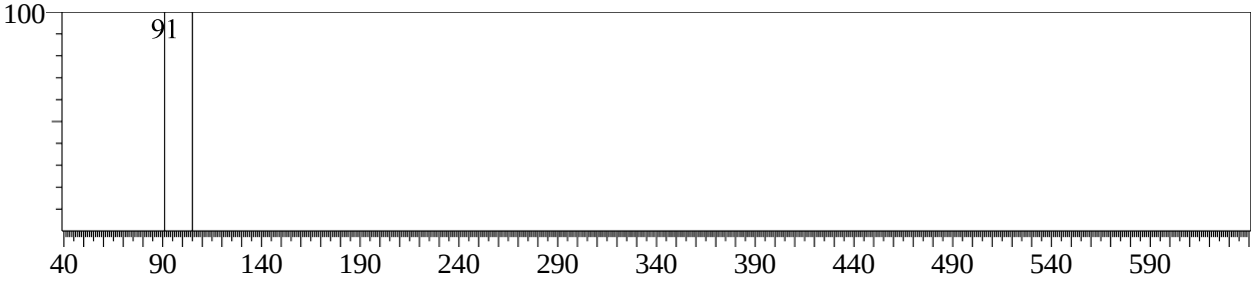
Hit#:2 Entry:23324 Library:NIST11.lib
SI:90 Formula:C9H10O3 CAS:552-41-0 MolWeight:166 RetIndex:1439
CompName:Ethanone, 1-(2-hydroxy-4-methoxyphenyl)- $$ Acetophenone, 2'-hydroxy-4'-methoxy- $$ Paeo



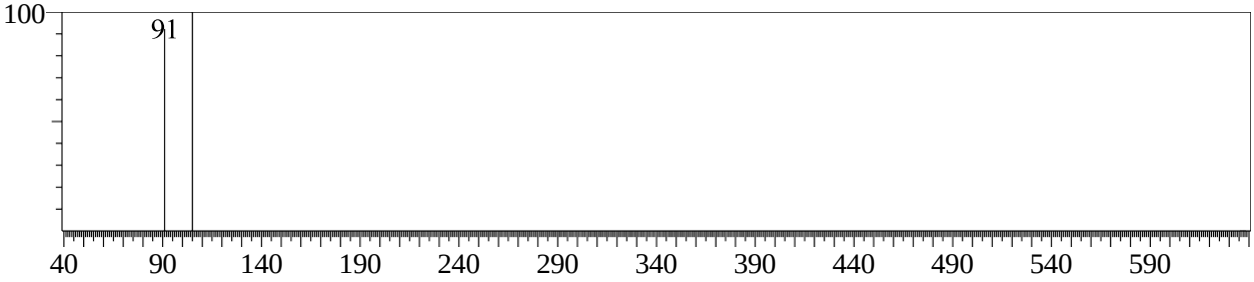
<< Target >>
Line#:19 R.Time:3.19(Scan#:19) MassPeaks:19
RawMode:Averaged 33.100-33.110(6321-6323) BasePeak:91.00(256)
BG Mode:Calc. from Peak



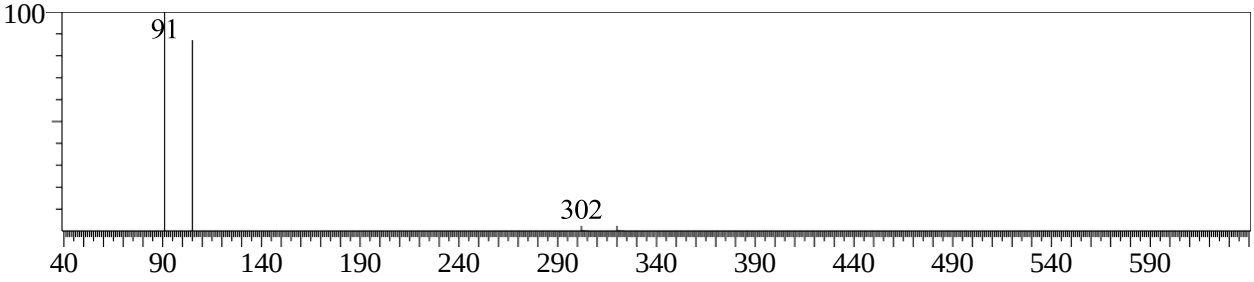
Hit#:1 Entry:320967 Library:WILEY7.LIB
SI:99 Formula:C29 H38 O7 SI CAS:0-00-0 MolWeight:526 RetIndex:0
CompName:Methyl [(1R)-(1.alpha.,4.alpha.,5.beta.)-4-(benzoyloxy)-5-[[(benzyloxy)methyl]oxy]-1-[[(1,1-di



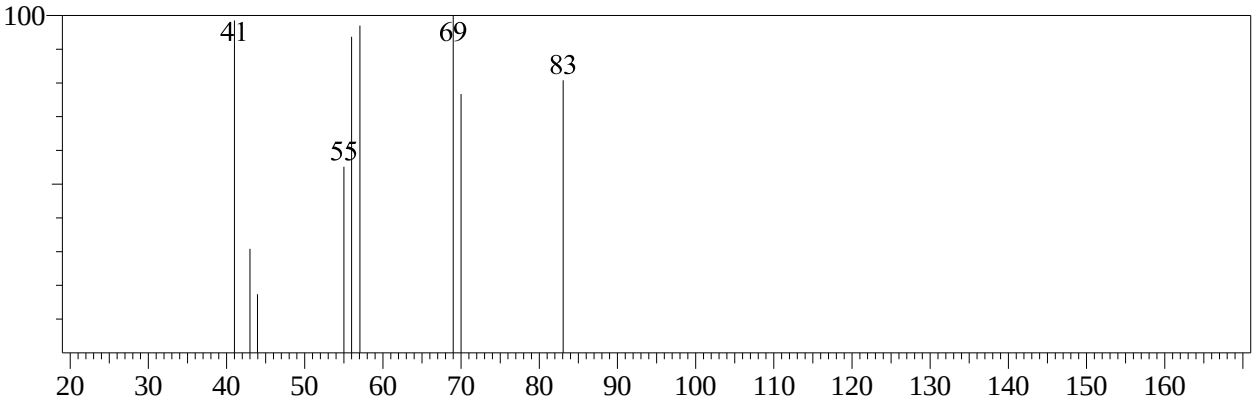
Hit#:2 Entry:331371 Library:WILEY7.LIB
SI:98 Formula:C33 H28 N6 O8 CAS:131682-13-8 MolWeight:636 RetIndex:0
CompName:7'-[2-phenyoxy-3-formyoxyl-4-(benzyoxy-methyl)-5-nitro-cyclopentene]-4'-benzyamino-purino



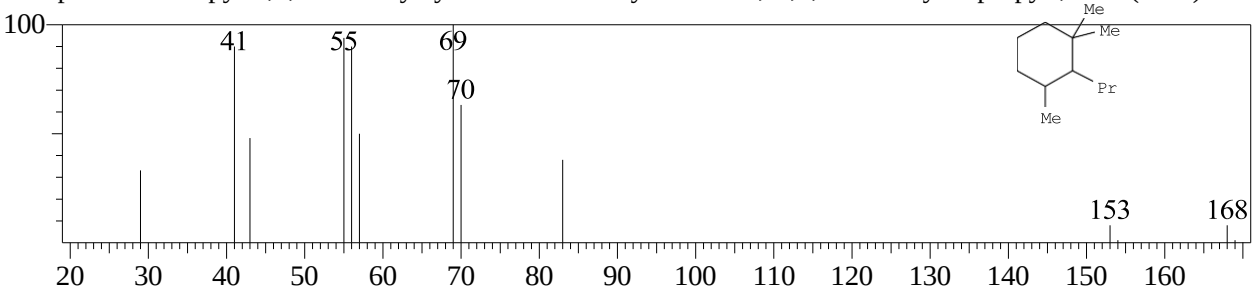
Hit#:3 Entry:230601 Library:WILEY7.LIB
SI:97 Formula:C23 H28 O CAS:113519-73-6 MolWeight:320 RetIndex:0
CompName:(4E)-7-ethyl-3,5-diphenylnona-4,6-dien-3-ol $$ Benzenemethanol, .alpha.-ethyl-.alpha.-(4-ethy



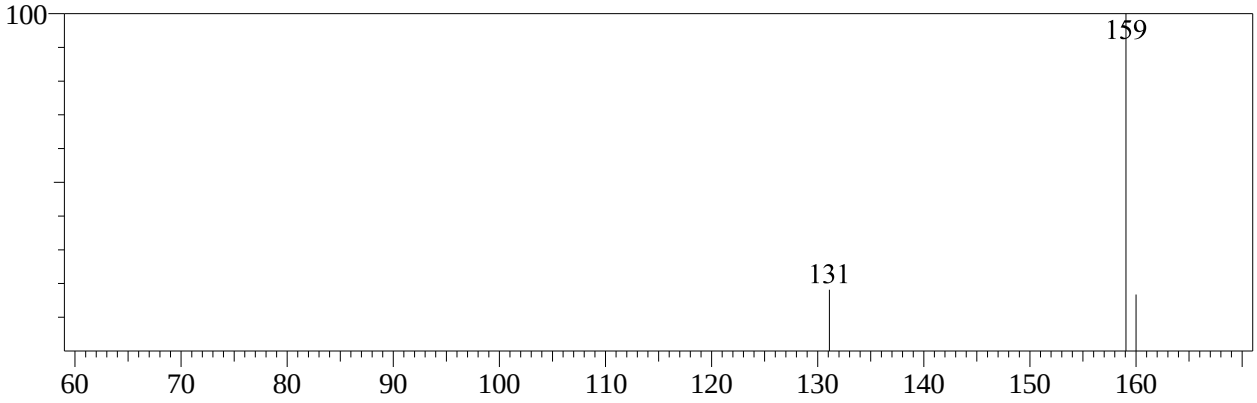
<< Target >>
Line#:20 R.Time:3.20(Scan#:20) MassPeaks:20
RawMode:Averaged 33.315-33.325(6364-6366) BasePeak:69.00(1407)
BG Mode:Calc. from Peak



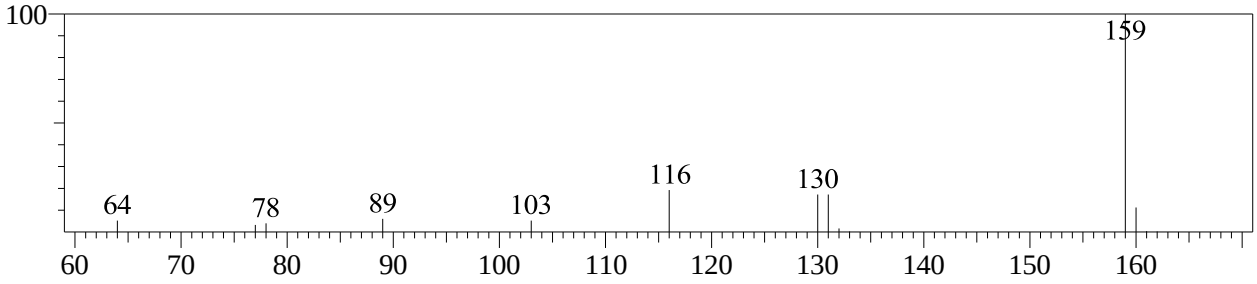
Hit#:1 Entry:58352 Library:WILEY7.LIB
SI:90 Formula:C12 H24 CAS:81983-69-9 MolWeight:168 RetIndex:0
CompName:2-Propyl-1,3,3-trimethylcyclohexane $$ Cyclohexane, 1,1,3-trimethyl-2-propyl-, cis- (CAS)



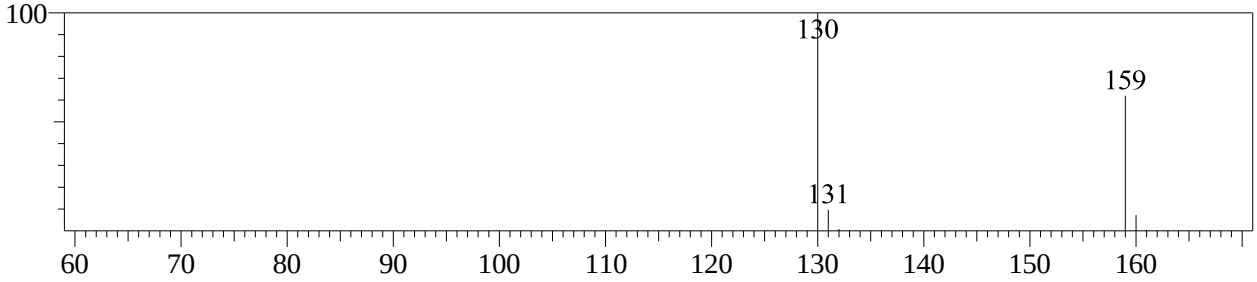
<< Target >>
Line#:21 R.Time:3.21(Scan#:21) MassPeaks:21
RawMode:Averaged 34.925-34.935(6686-6688) BasePeak:159.05(7063)
BG Mode:Calc. from Peak



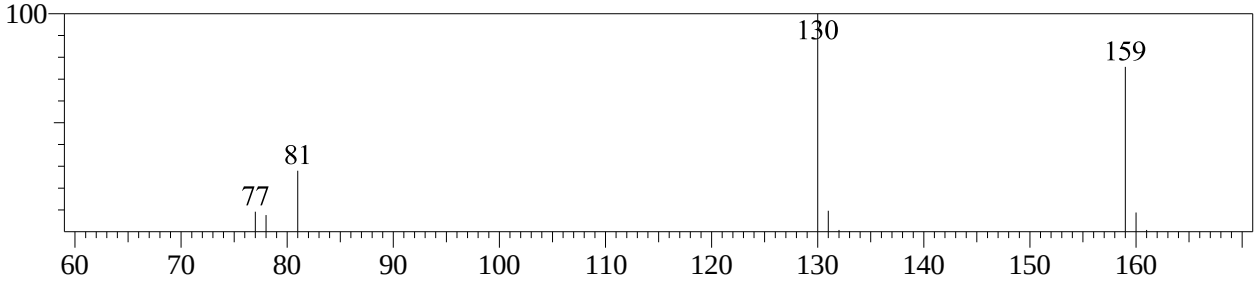
Hit#:1 Entry:48298 Library:WILEY7.LIB
SI:98 Formula:C9 H9 N3 CAS:0-00-0 MolWeight:159 RetIndex:0
CompName:7-ethyl-5-azacinnoline $$



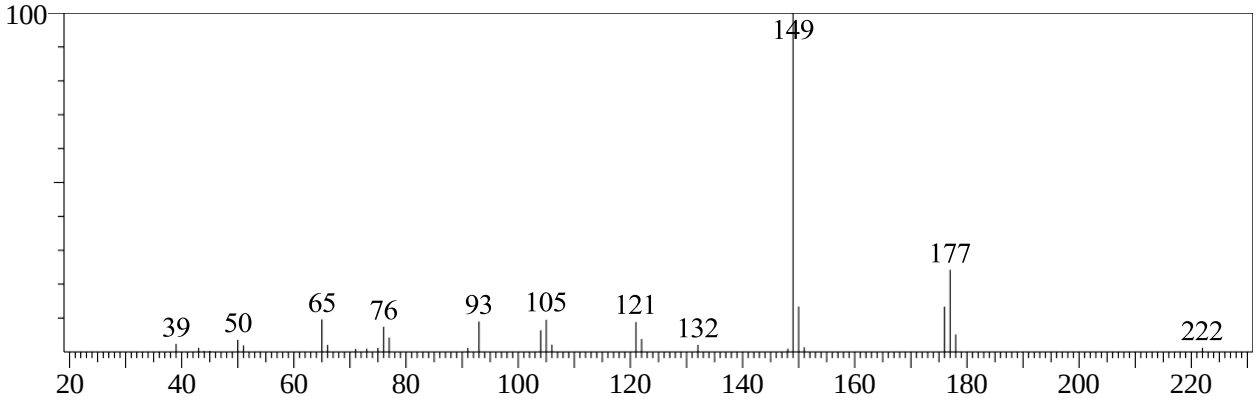
Hit#:2 Entry:48346 Library:WILEY7.LIB
SI:98 Formula:C10 H9 N O CAS:120696-99-3 MolWeight:159 RetIndex:0
CompName:(E)-4-hydroxy-2-phenylbut-2-enenitrile $$ Benzeneacetonitrile, .alpha.-(2-hydroxyethylidene)-,



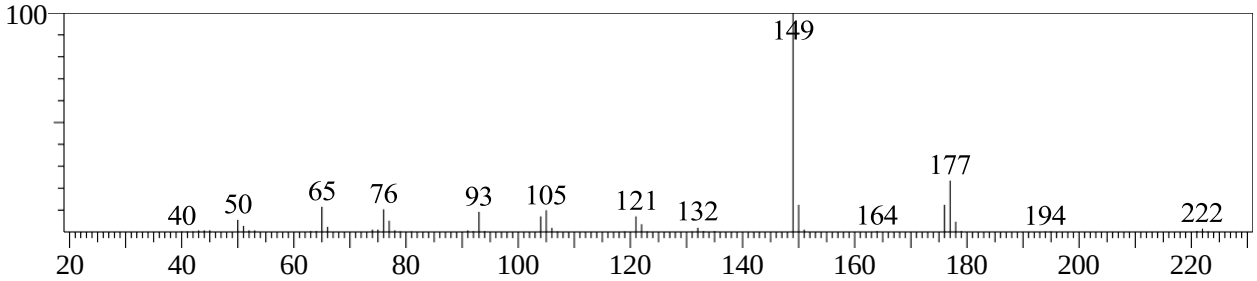
Hit#:3 Entry:48349 Library:WILEY7.LIB
SI:97 Formula:C10 H9 N O CAS:0-00-0 MolWeight:159 RetIndex:0
CompName:2-(2-Furylmethyl)pyridine $$



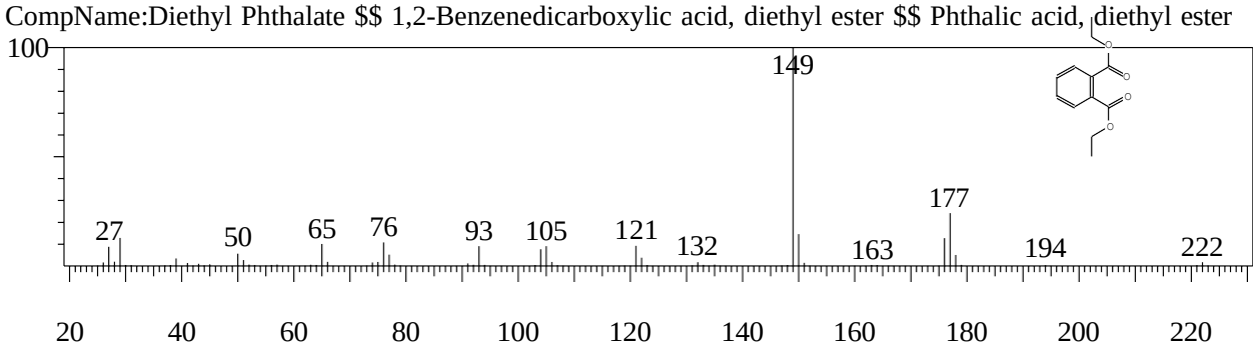
<< Target >>
Line#:22 R.Time:3.22(Scan#:22) MassPeaks:22
RawMode:Averaged 37.570-37.580(7215-7217) BasePeak:149.00(100590)
BG Mode:Calc. from Peak



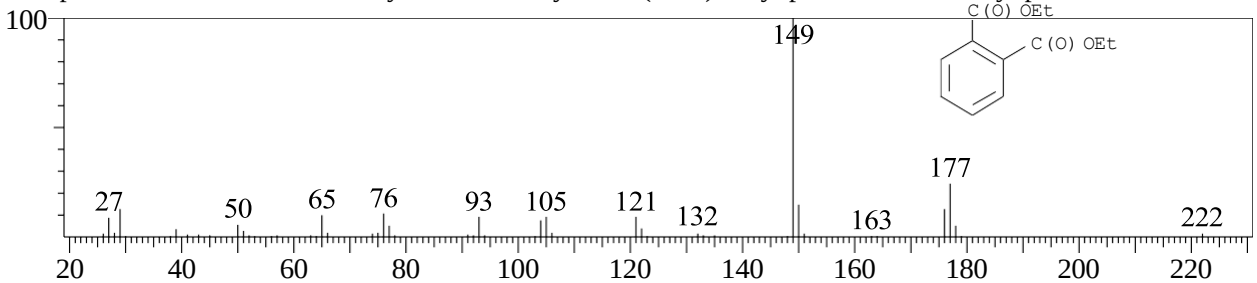
Hit#:1 Entry:1318 Library:FFNSC1.3.lib
SI:96 Formula:C21 H29 N O3 CAS:67634-12-2 MolWeight:343 RetIndex:1589
CompName:Benzoic acid <2-[[[4-(4-hydroxy-4-methylpentyl)-, 3-cyclohexen-1-yl]methylene]amino]-, met



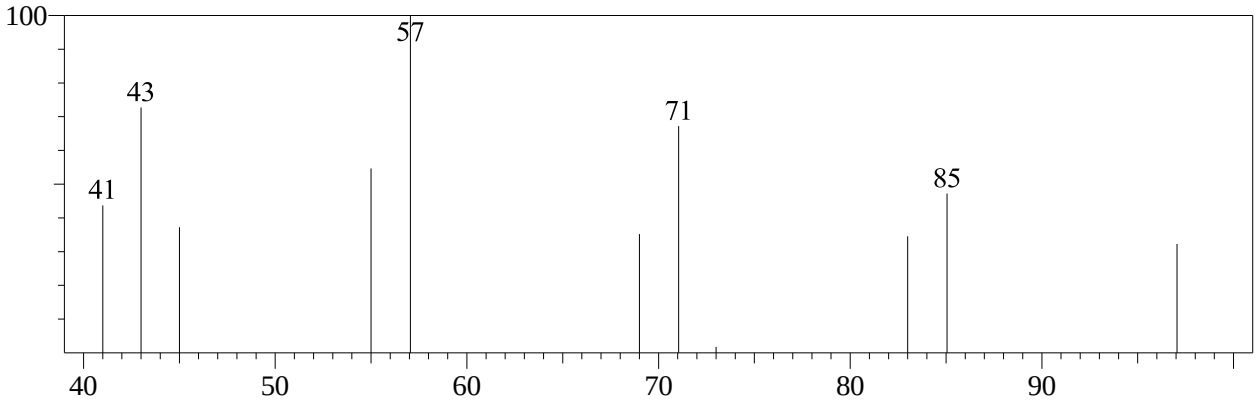
Hit#:2 Entry:20183 Library:NIST11s.lib
SI:96 Formula:C12H14O4 CAS:84-66-2 MolWeight:222 RetIndex:1639
CompName:Diethyl Phthalate $$ 1,2-Benzenedicarboxylic acid, diethyl ester $$ Phthalic acid, diethyl ester



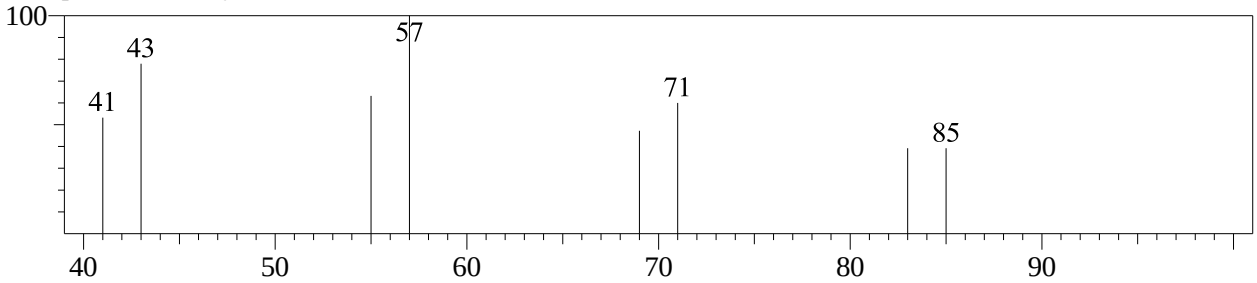
Hit#:3 Entry:123701 Library:WILEY7.LIB
SI:96 Formula:C12 H14 O4 CAS:84-66-2 MolWeight:222 RetIndex:0
CompName:1,2-Benzenedicarboxylic acid, diethyl ester (CAS) Ethyl phthalate $$ Diethyl phthalate $$ Ano



<< Target >>
Line#:23 R.Time:3.23(Scan#:23) MassPeaks:23
RawMode:Averaged 42.480-42.490(8197-8199) BasePeak:57.05(3306)
BG Mode:Calc. from Peak



Hit#:1 Entry:209613 Library:WILEY7.LIB
SI:90 Formula:C20 H42 O CAS:0-00-0 MolWeight:298 RetIndex:0
CompName:2-Octyldodecan-1-ol $$



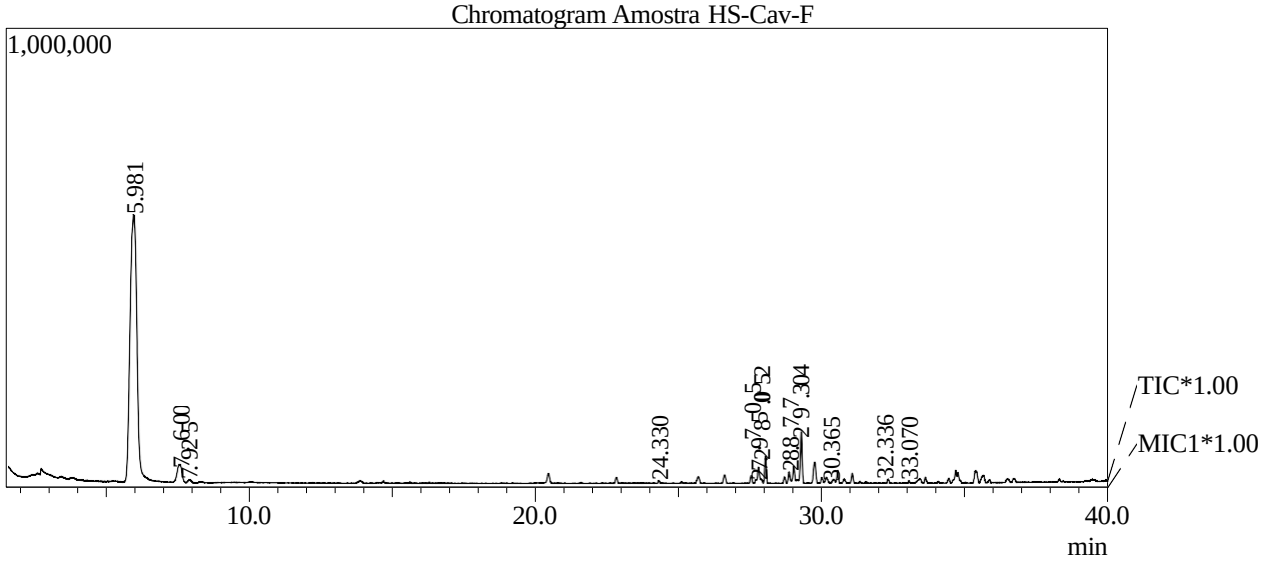
S3. Dados brutos das análises da headspace da madeira coletada no ponto 1 de coleta na caverna do Couto.

<< Target >>
Line#:24 R.Time:3.24(Scan#:24) MassPeaks:24

Sample Information

Analyzed by	: Admin
Analyzed	: 28/01/2025 09:22:38
Sample Type	: Unknown
Level #	1
$EndIf$IS Amount	: [1]=1.58
Sample Amount	1
Dilution Factor	1
Vial #	2
Injection Volume	: 1.00
Data File	: C:\GCMSsolution\Data\Project1\Norberto\Voláteis Caverna\Amostra
Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise HS-caverna.qgm
Org Method File	: C:\GCMSsolution\Data\Project1\Norberto\Análise HS-caverna.qgm
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1\2025\23-01-2024.qgt

Chromatogram Amostra HS-Cav-F



Peak Report TIC

Peak#	R.Time	Area	Area%	Name	Base m/z
1	5.981	9598364	86.73	Silanol, trimethyl- (CAS) Trimethylsilanol	75.00
2	7.600	434274	3.92	Disiloxane, hexamethyl- (CAS) Hexamethyl	147.05
3	7.925	51925	0.47		41.00
4	24.330	21088	0.19	Undecane, 5-methyl- (CAS) 5-Methylundec	43.05
5	27.705	30019	0.27	1-(2-Tetrahydrofuryl)-1-methyl-pent-4-ene-	85.10
6	27.950	31552	0.29	Octane (CAS) n-Octane	43.00
7	28.052	235698	2.13	Dodecane, 4-methyl-	43.00
8	28.877	97198	0.88	Pentadecane (CAS) n-Pentadecane	57.05
9	29.304	465047	4.20	Decane, 3-ethyl-3-methyl-	43.00
10	30.365	53605	0.48	Di-n-octyl disulfide	43.05
11	32.336	35833	0.32	Hexadecane (CAS) n-Hexadecane	57.05
12	33.070	12141	0.11	Di-n-octyl disulfide	57.05
		11066744	100.00		

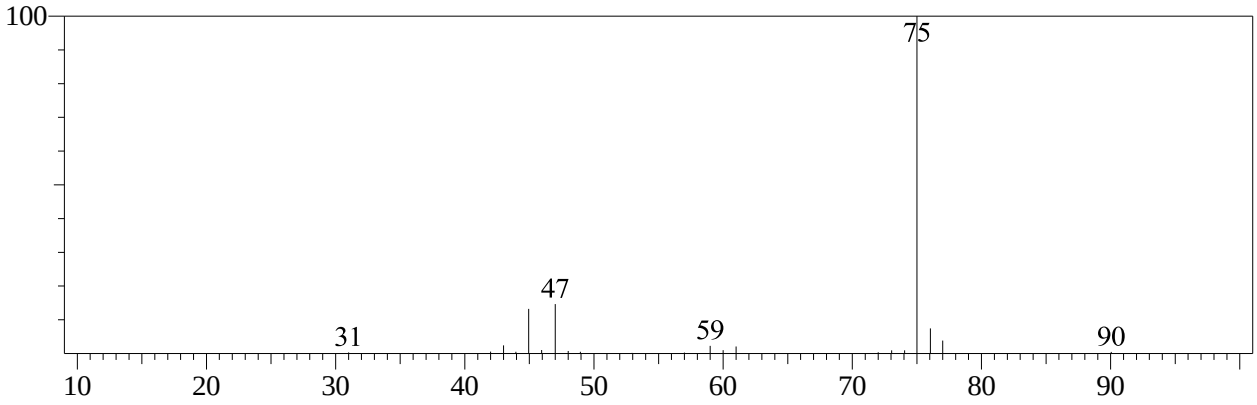
Library

<< Target >>

Line#:1 R.Time:5.980(Scan#:877) MassPeaks:23

RawMode:Averaged 5.975-5.985(876-878) BasePeak:75.00(379079)

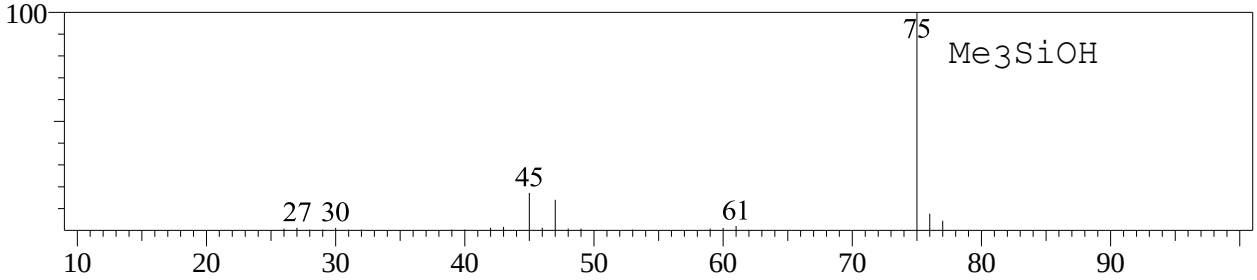
BG Mode:Calc. from Peak



Hit#:1 Entry:4389 Library:WILEY7.LIB

SI:97 Formula:C3 H10 O SI CAS:1066-40-6 MolWeight:90 RetIndex:0

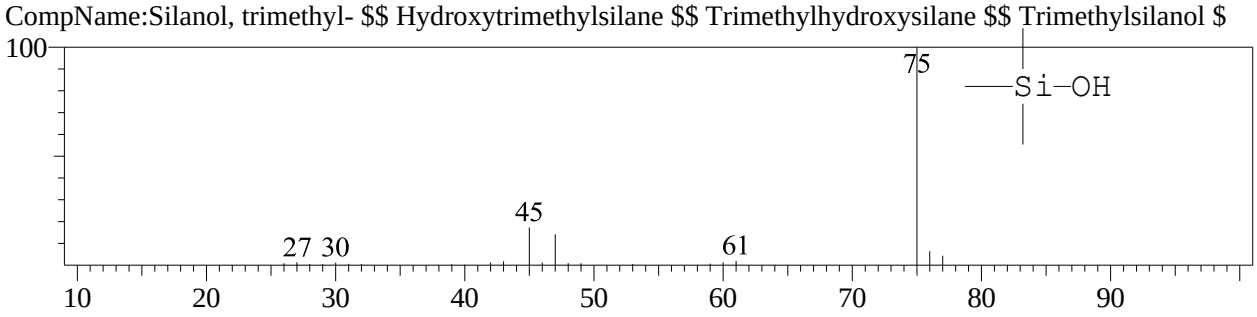
CompName:Silanol, trimethyl- (CAS) Trimethylsilanol $$ Hydroxytrimethylsilane $$ Trimethylhydroxysila



Hit#:2 Entry:1161 Library:NIST11s.lib

SI:97 Formula:C3H10OSi CAS:1066-40-6 MolWeight:90 RetIndex:369

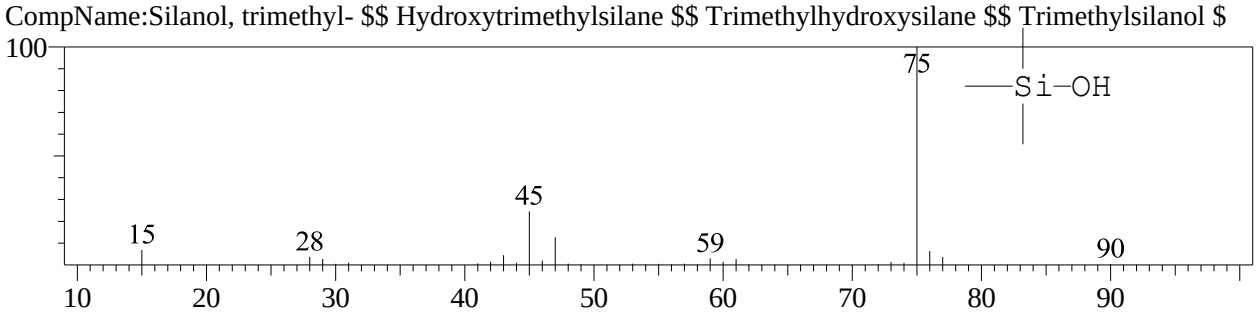
CompName:Silanol, trimethyl- $$ Hydroxytrimethylsilane $$ Trimethylhydroxysilane $$ Trimethylsilanol $



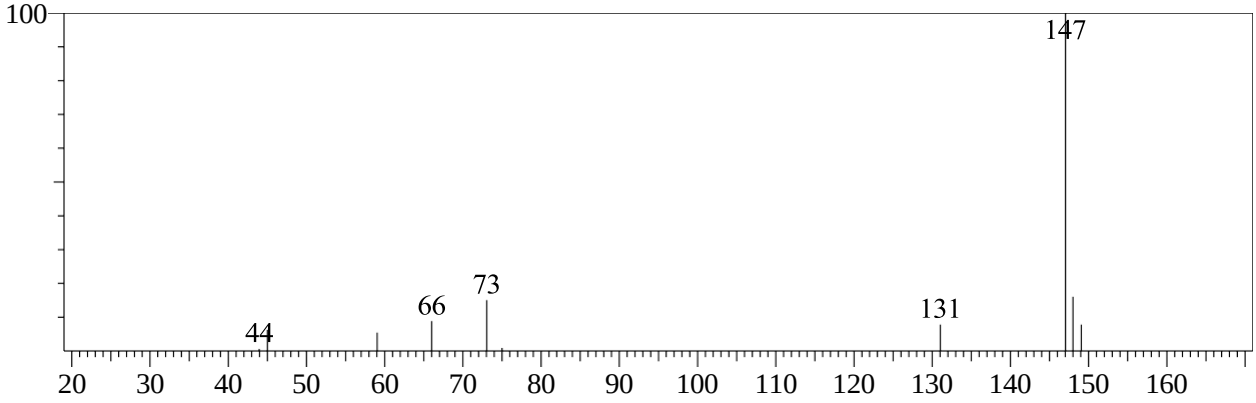
Hit#:3 Entry:1125 Library:NIST11.lib

SI:96 Formula:C3H10OSi CAS:1066-40-6 MolWeight:90 RetIndex:369

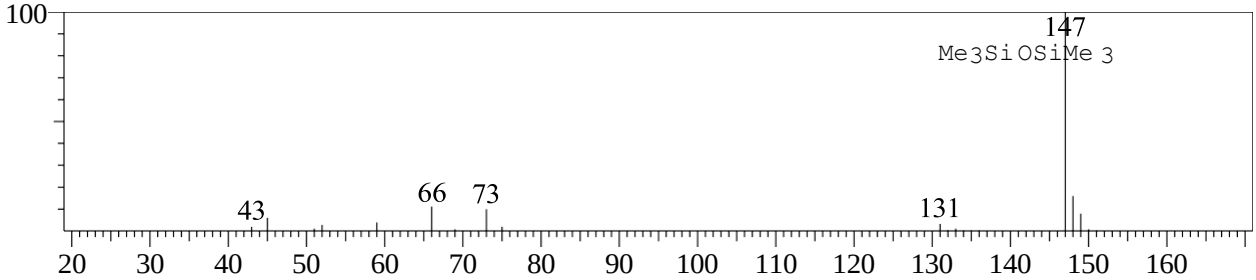
CompName:Silanol, trimethyl- $$ Hydroxytrimethylsilane $$ Trimethylhydroxysilane $$ Trimethylsilanol $



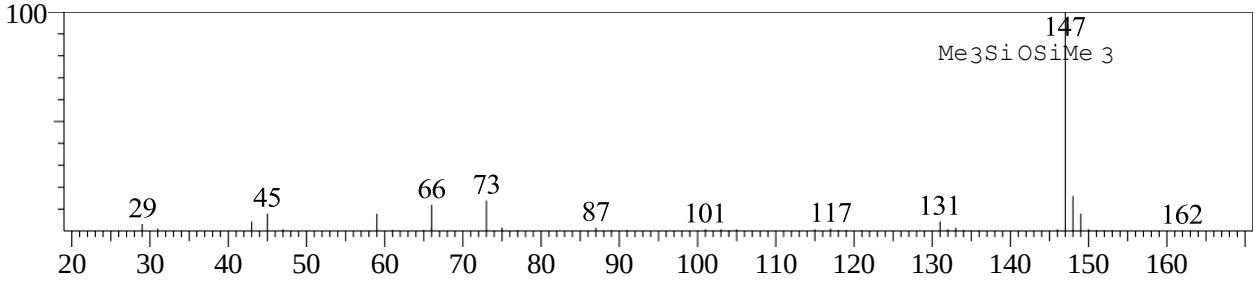
<< Target >>
Line#:3 R.Time:7.925(Scan#:1266) MassPeaks:6
RawMode:Averaged 7.595-7.605(1200-1202) BasePeak:147.05(22976)
BG Mode:Calc. from Peak



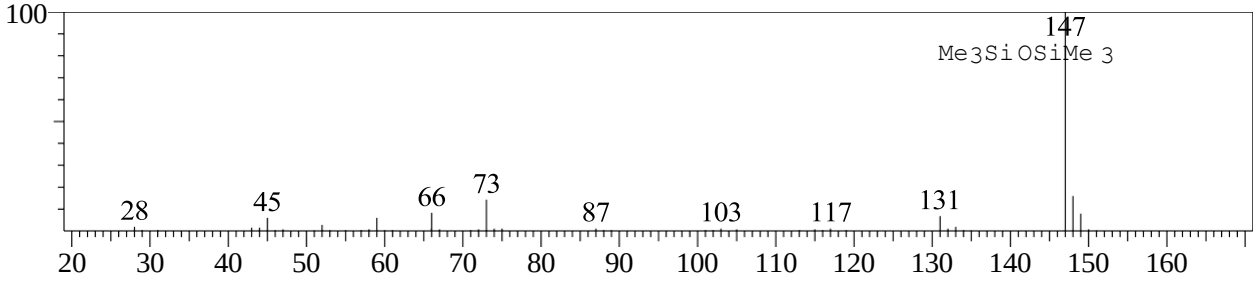
Hit#:1 Entry:51356 Library:WILEY7.LIB
SI:96 Formula:C6 H18 O SI2 CAS:107-46-0 MolWeight:162 RetIndex:0
CompName:Disiloxane, hexamethyl- (CAS) Hexamethyldisiloxane $$ BIS-(TRIMETHYLSILYL)ETHER $



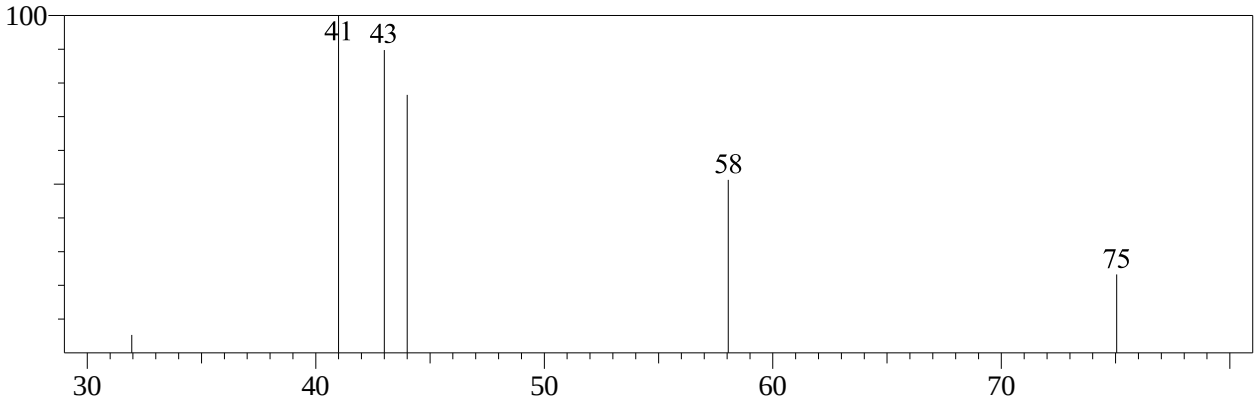
Hit#:2 Entry:51354 Library:WILEY7.LIB
SI:94 Formula:C6 H18 O SI2 CAS:107-46-0 MolWeight:162 RetIndex:0
CompName:Disiloxane, hexamethyl- (CAS) Hexamethyldisiloxane $$ BIS-(TRIMETHYLSILYL)ETHER $



Hit#:3 Entry:51350 Library:WILEY7.LIB
SI:93 Formula:C6 H18 O SI2 CAS:107-46-0 MolWeight:162 RetIndex:0
CompName:Disiloxane, hexamethyl- (CAS) Hexamethyldisiloxane $$ BIS-(TRIMETHYLSILYL)ETHER $

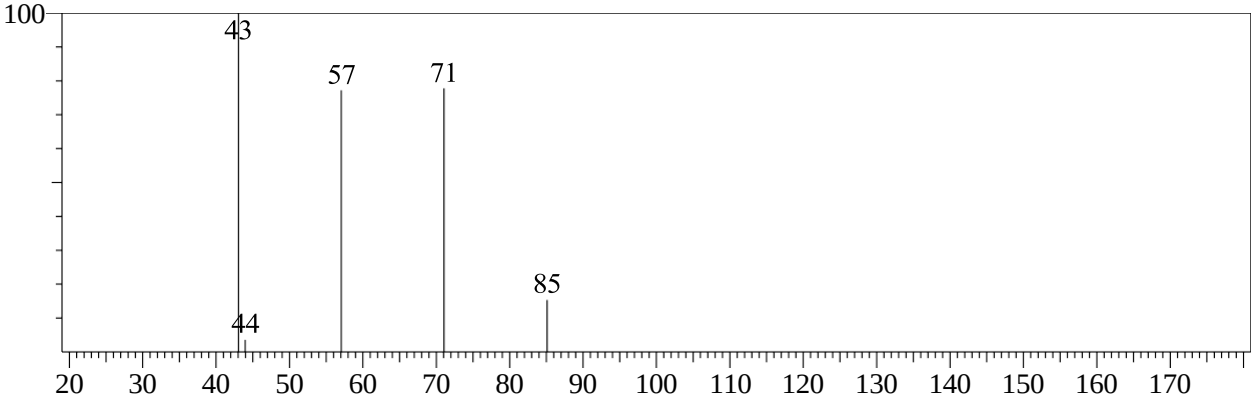


<< Target >>
Line#:3 R.Time:7.925(Scan#:1266) MassPeaks:6
RawMode:Averaged 7.920-7.930(1265-1267) BasePeak:41.00(2030)
BG Mode:Calc. from Peak

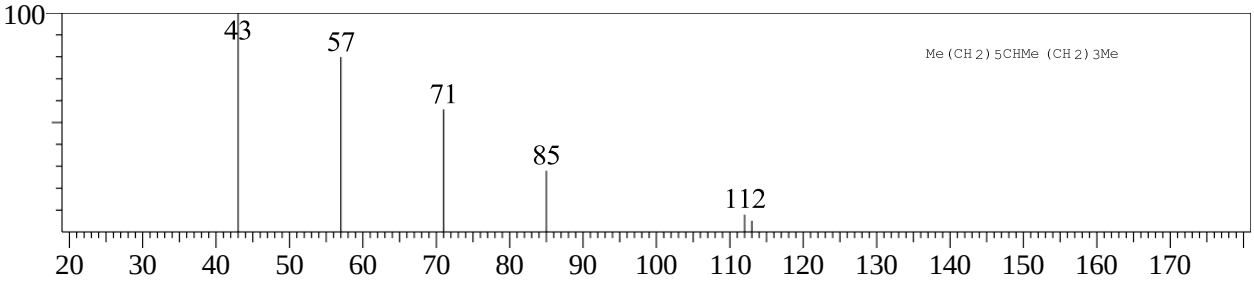


No hit compound

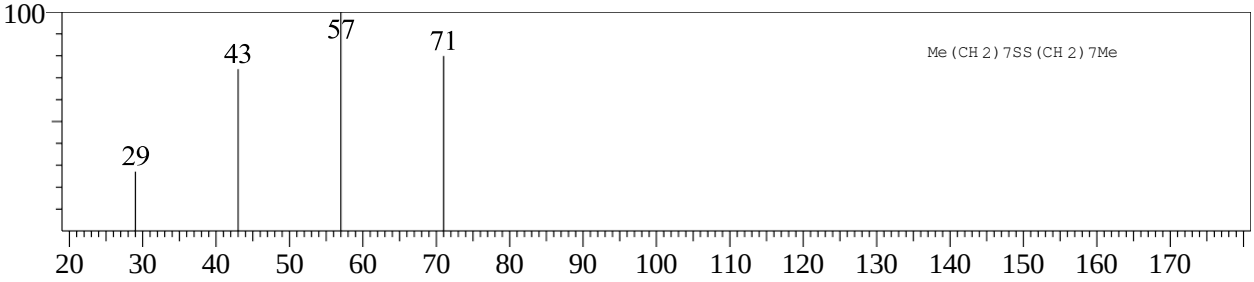
<< Target >>
Line#:4 R.Time:4.45(Scan#:4) MassPeaks:4
RawMode:Averaged 24.325-24.335(4546-4548) BasePeak:43.05(2178)
BG Mode:Calc. from Peak



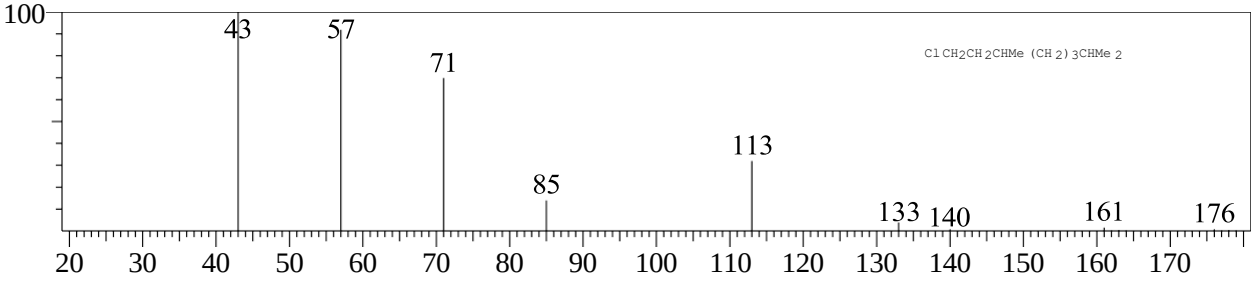
Hit#:1 Entry:61359 Library:WILEY7.LIB
SI:94 Formula:C12 H26 CAS:1632-70-8 MolWeight:170 RetIndex:0
CompName:Undecane, 5-methyl- (CAS) 5-Methylundecane $$ Methylundecane $$



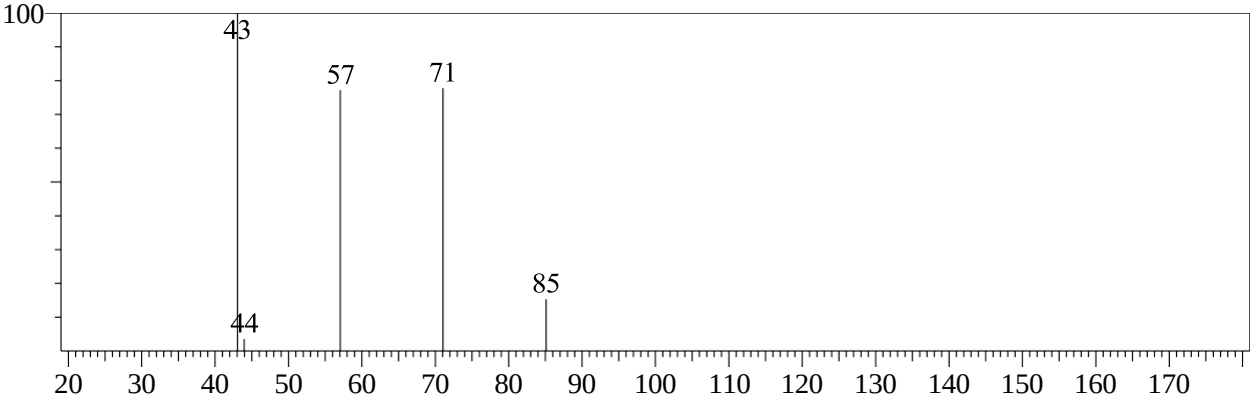
Hit#:2 Entry:201724 Library:WILEY7.LIB
SI:92 Formula:C16 H34 S2 CAS:822-27-5 MolWeight:290 RetIndex:0
CompName:Di-n-octyl disulfide $$ Disulfide, dioctyl (CAS) Dioctyl disulfide $$ Octyl disulfide $$ n-Octyl



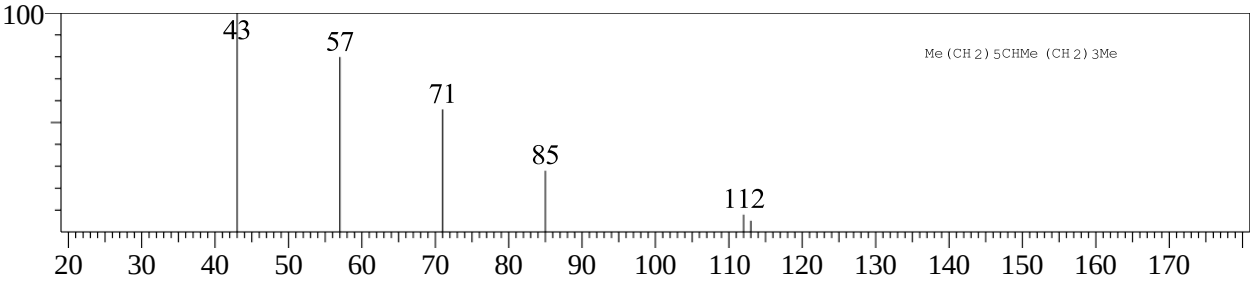
Hit#:3 Entry:66414 Library:WILEY7.LIB
SI:91 Formula:C10 H21 CL CAS:66261-41-4 MolWeight:176 RetIndex:0
CompName:(-)-(R)-1-CHLORO-3,7-DIMETHYLOCTANE $$ Octane, 1-chloro-3,7-dimethyl-, (R)- (CAS)



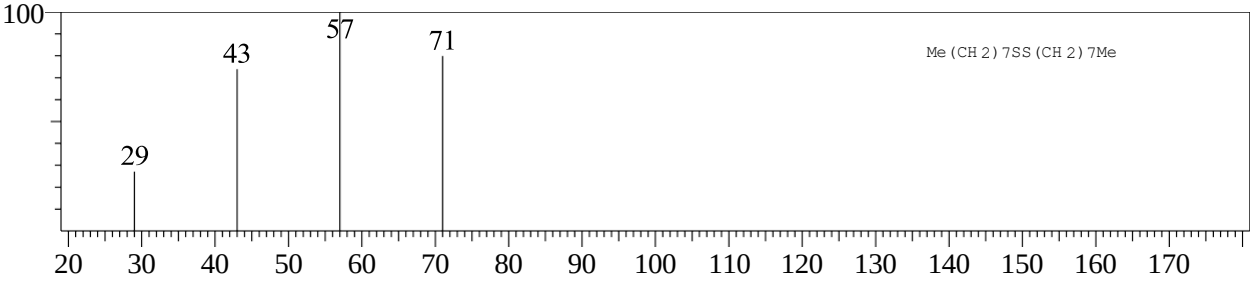
<< Target >>
Line#:5 R.Time:5.55(Scan#:5) MassPeaks:5
RawMode:Averaged 24.325-24.335(4546-4548) BasePeak:43.05(2178)
BG Mode:Calc. from Peak



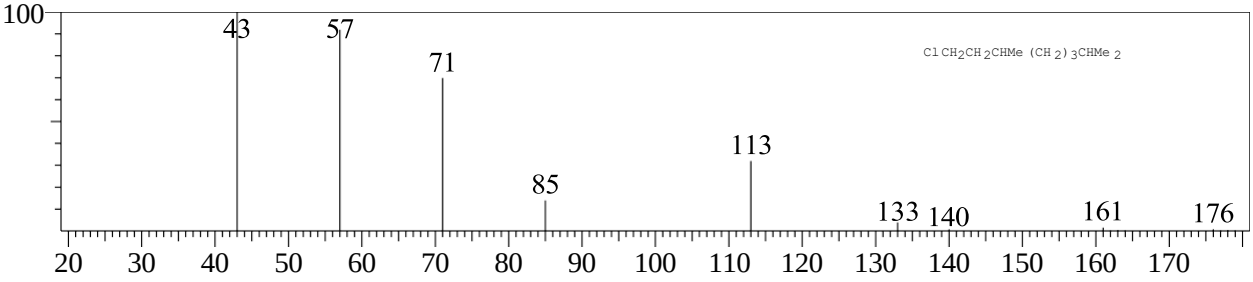
Hit#:1 Entry:61359 Library:WILEY7.LIB
SI:94 Formula:C12 H26 CAS:1632-70-8 MolWeight:170 RetIndex:0
CompName:Undecane, 5-methyl- (CAS) 5-Methylundecane $$ Methylundecane $$



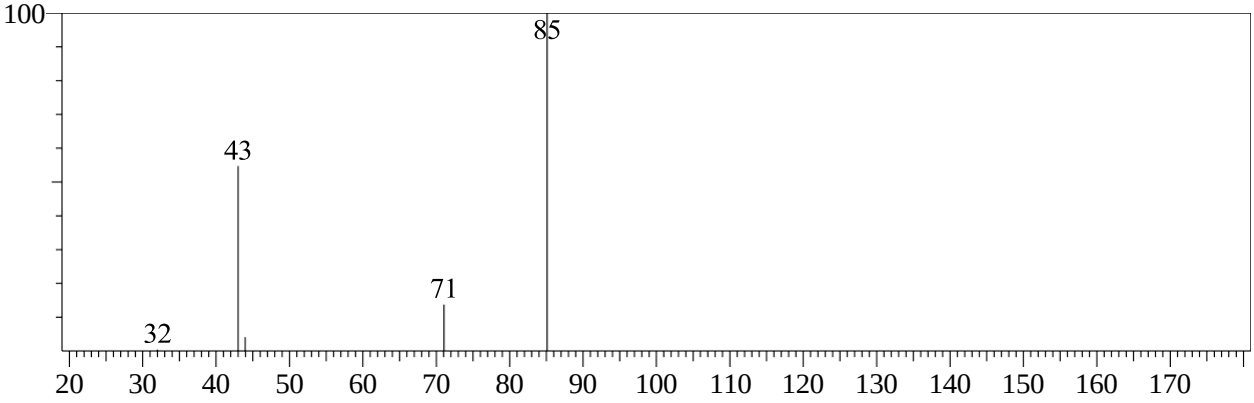
Hit#:2 Entry:201724 Library:WILEY7.LIB
SI:92 Formula:C16 H34 S2 CAS:822-27-5 MolWeight:290 RetIndex:0
CompName:Di-n-octyl disulfide $$ Disulfide, dioctyl (CAS) Dioctyl disulfide $$ Octyl disulfide $$ n-Octyl



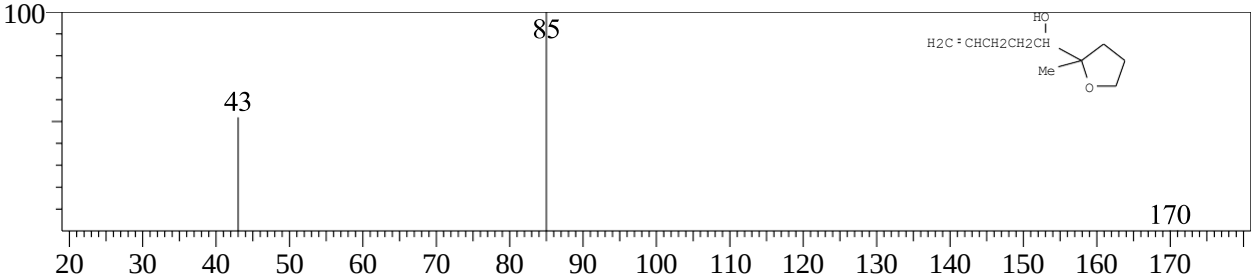
Hit#:3 Entry:66414 Library:WILEY7.LIB
SI:91 Formula:C10 H21 CL CAS:66261-41-4 MolWeight:176 RetIndex:0
CompName:(-)-(R)-1-CHLORO-3,7-DIMETHYLOCTANE $$ Octane, 1-chloro-3,7-dimethyl-, (R)- (CAS)



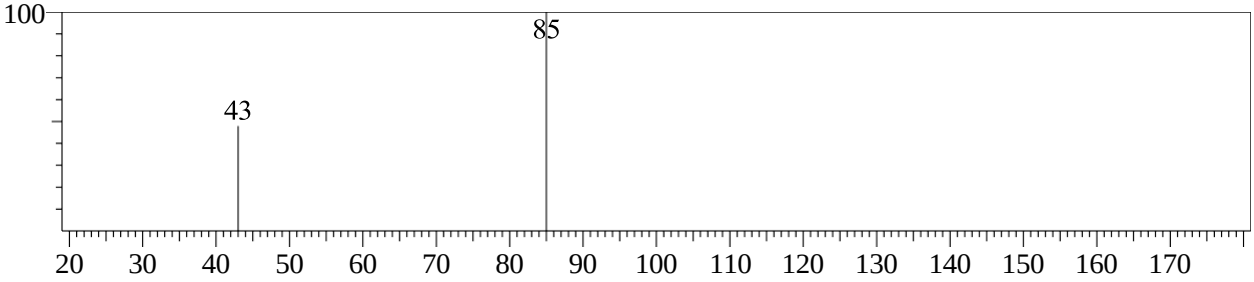
<< Target >>
Line#:6 R.Time:6.65(Scan#:6) MassPeaks:6
RawMode:Averaged 27.700-27.710(5221-5223) BasePeak:85.10(1751)
BG Mode:Calc. from Peak



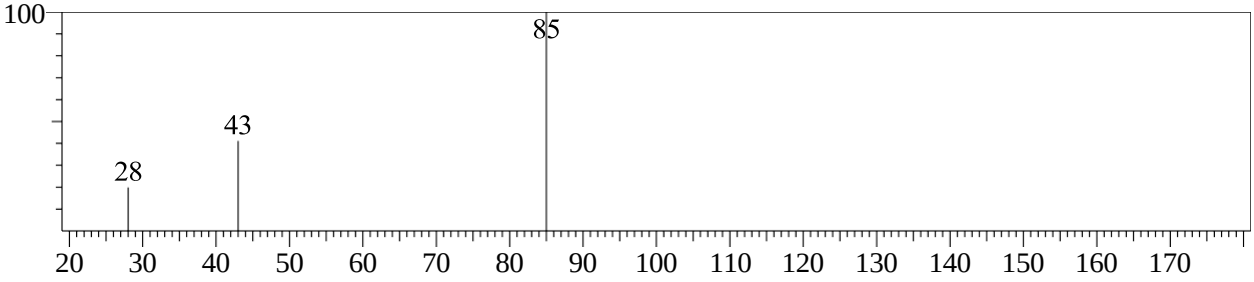
Hit#:1 Entry:60230 Library:WILEY7.LIB
SI:94 Formula:C10 H18 O2 CAS:80275-38-3 MolWeight:170 RetIndex:0
CompName:1-(2-Tetrahydrofuryl)-1-methyl-pent-4-ene-1-ol $$ 2-Furanmethanol, .alpha.-3-butenyltetrahyd



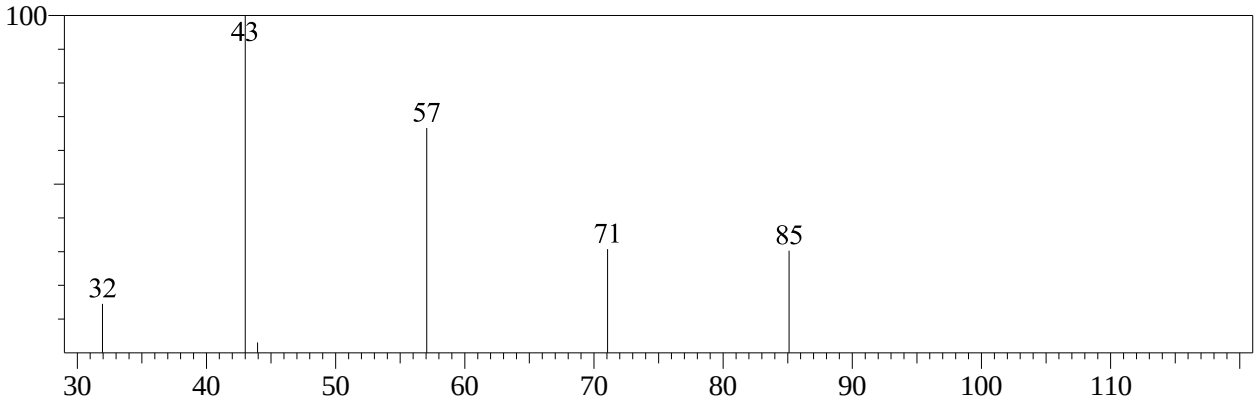
Hit#:2 Entry:78245 Library:WILEY7.LIB
SI:93 Formula:C10 H18 O3 CAS:112041-38-0 MolWeight:186 RetIndex:0
CompName:methyl (3-(2'methyl)tetrahydrofuran-2'-yl)-2-methylpropanoate $$ 2-Furanpropanoic acid, tetra



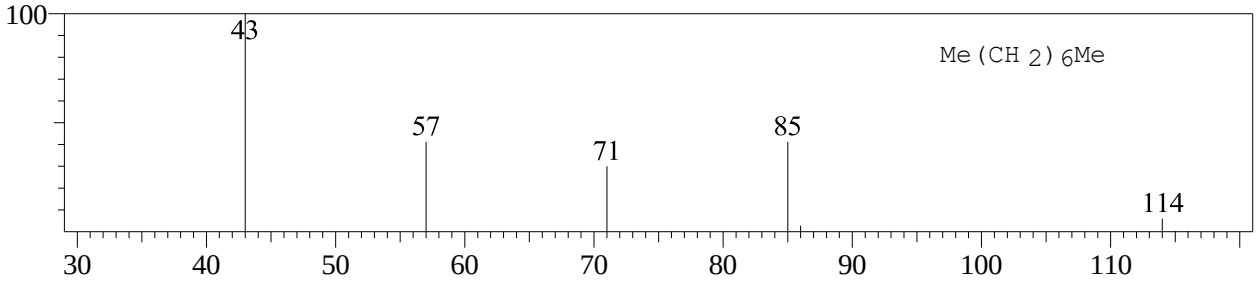
Hit#:3 Entry:62404 Library:WILEY7.LIB
SI:92 Formula:C9 H16 O3 CAS:112039-55-1 MolWeight:172 RetIndex:0
CompName:3-(2'-methyltetrahydrofuran-2'-yl)-2-methylpropanoic acid $$ 2-Furanpropanoic acid, tetrahydr



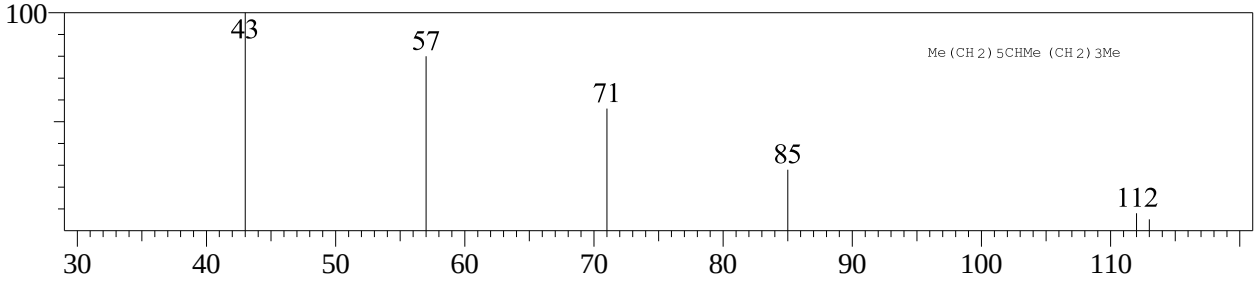
<< Target >>
Line#:7 R.Time:7.75(Scan#:7) MassPeaks:7
RawMode:Averaged 27.945-27.955(5270-5272) BasePeak:43.00(1103)
BG Mode:Calc. from Peak



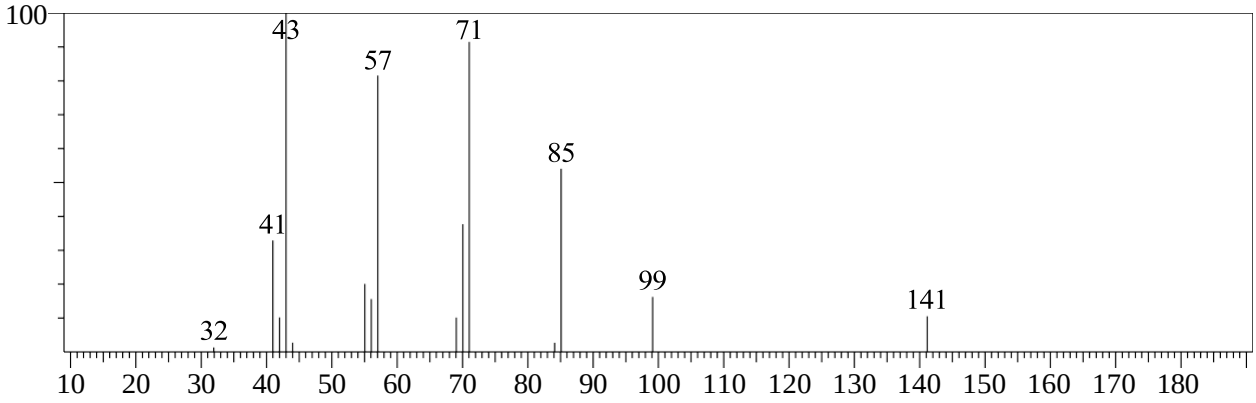
Hit#:1 Entry:12832 Library:WILEY7.LIB
SI:90 Formula:C8 H18 CAS:111-65-9 MolWeight:114 RetIndex:0
CompName:Octane (CAS) n-Octane $$ Octane (DOT) $$ Isooctane $$ n-C8H18 $$ Oktan $$ Oktanen $$ O



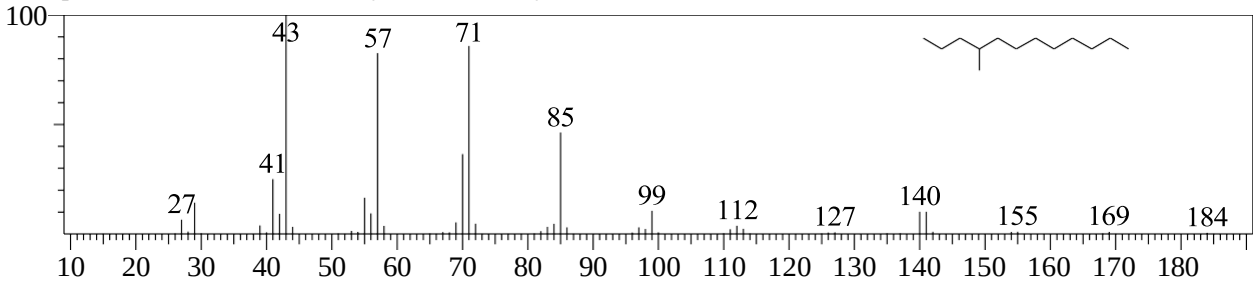
Hit#:2 Entry:61359 Library:WILEY7.LIB
SI:90 Formula:C12 H26 CAS:1632-70-8 MolWeight:170 RetIndex:0
CompName:Undecane, 5-methyl- (CAS) 5-Methylundecane $$ Methylundecane $$



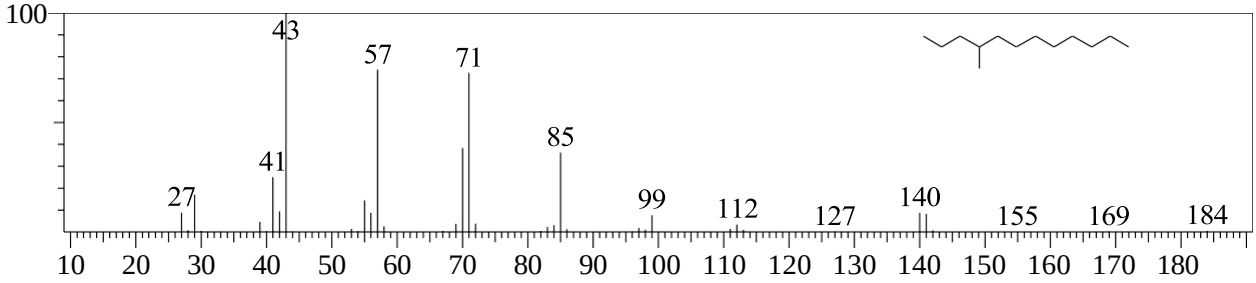
<< Target >>
Line#:8 R.Time:8.85(Scan#:8) MassPeaks:8
RawMode:Averaged 28.045-28.055(5290-5292) BasePeak:43.00(12041)
BG Mode:Calc. from Peak



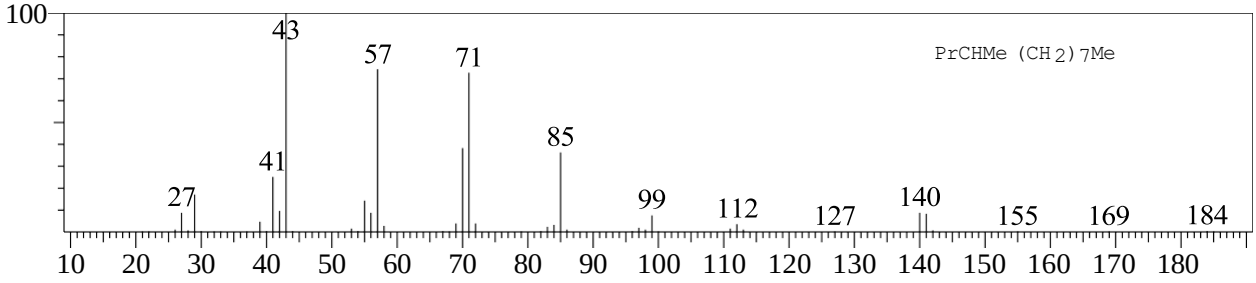
Hit#:1 Entry:34144 Library:NIST11.lib
SI:92 Formula:C13H28 CAS:6117-97-1 MolWeight:184 RetIndex:1249
CompName:Dodecane, 4-methyl- $$ 4-Methyldodecane $$



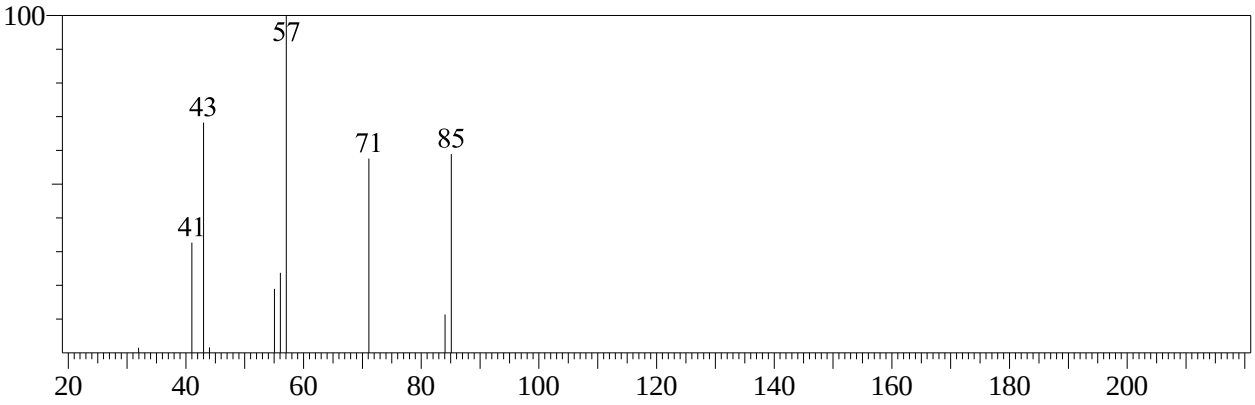
Hit#:2 Entry:15154 Library:NIST11s.lib
SI:91 Formula:C13H28 CAS:6117-97-1 MolWeight:184 RetIndex:1249
CompName:Dodecane, 4-methyl- $$ 4-Methyldodecane $$



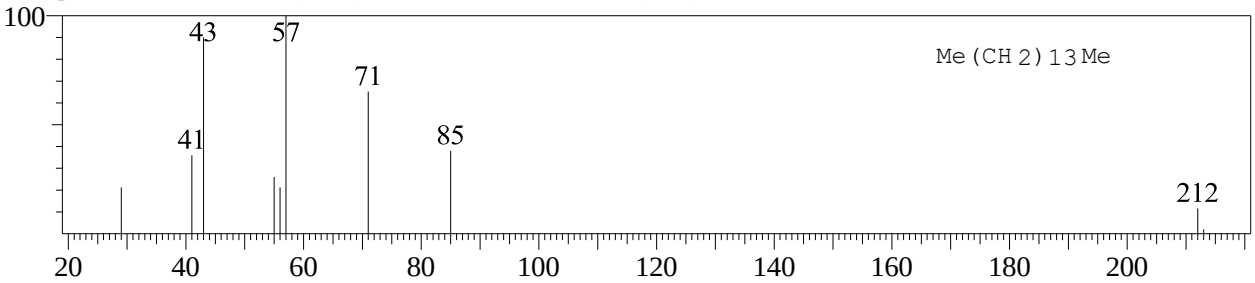
Hit#:3 Entry:76398 Library:WILEY7.LIB
SI:91 Formula:C13 H28 CAS:6117-97-1 MolWeight:184 RetIndex:0
CompName:Dodecane, 4-methyl- (CAS) 4-Methyldodecane $$



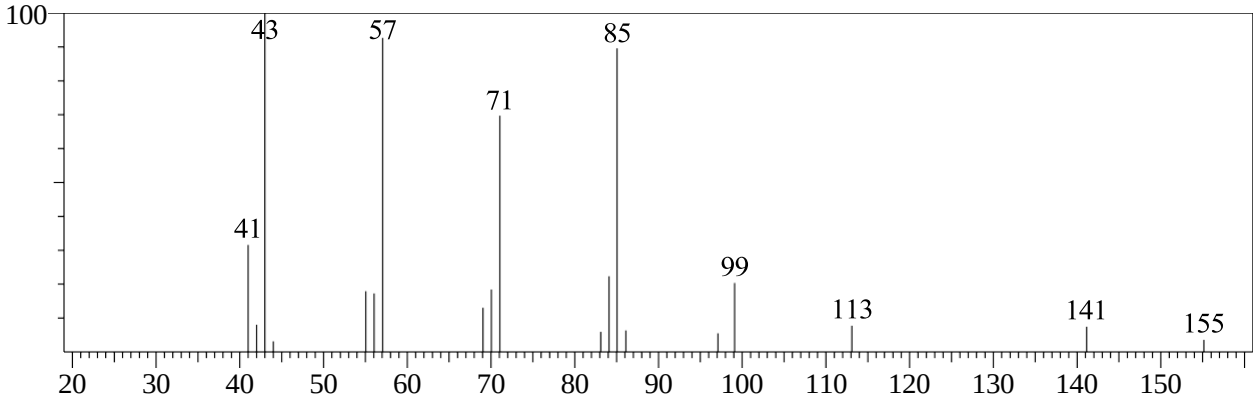
<< Target >>
Line#:9 R.Time:9.95(Scan#:9) MassPeaks:9
RawMode:Averaged 28.870-28.880(5455-5457) BasePeak:57.05(5868)
BG Mode:Calc. from Peak



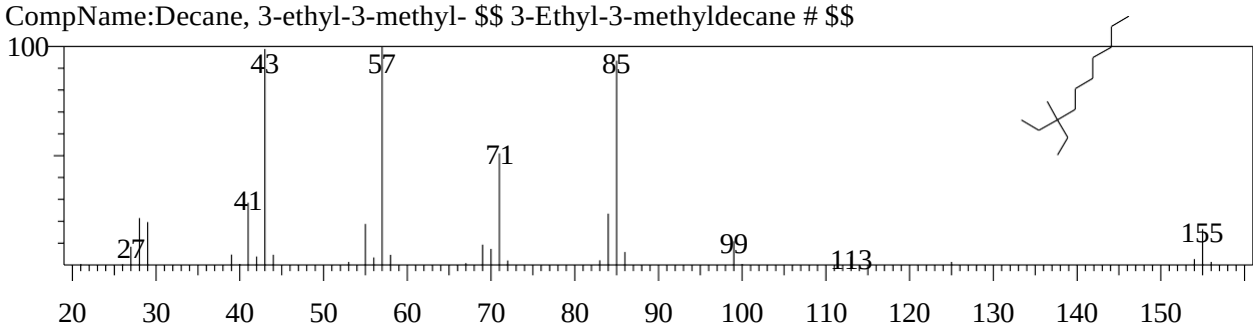
Hit#:1 Entry:111406 Library:WILEY7.LIB
SI:92 Formula:C15 H32 CAS:629-62-9 MolWeight:212 RetIndex:0
CompName:Pentadecane (CAS) n-Pentadecane $$ CH3(CH2)13CH3 $$



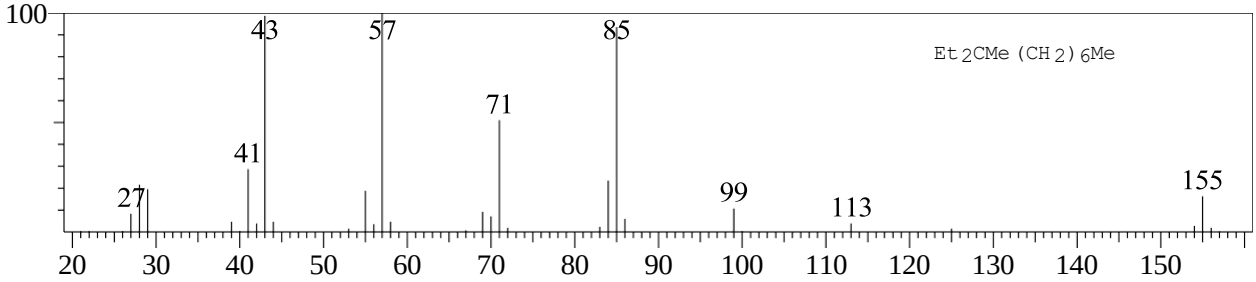
<< Target >>
Line#:10 R.Time:10.105(Scan#:10) MassPeaks:10
RawMode:Averaged 29.300-29.310(5541-5543) BasePeak:43.00(20023)
BG Mode:Calc. from Peak



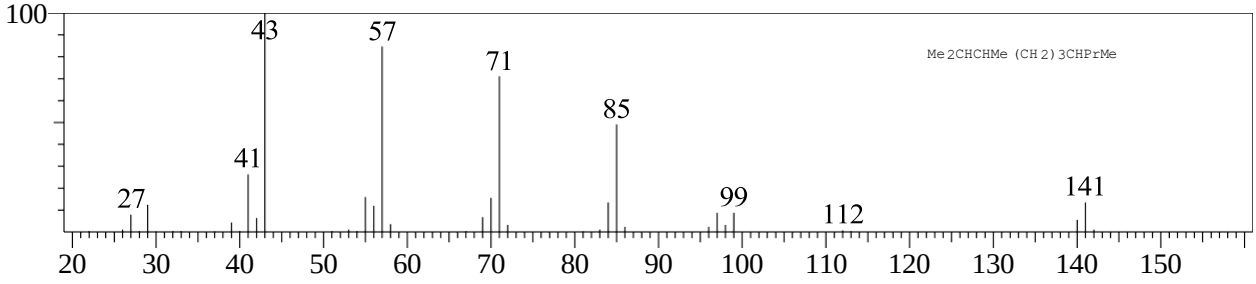
Hit#:1 Entry:34171 Library:NIST11.lib
SI:93 Formula:C13H28 CAS:17312-66-2 MolWeight:184 RetIndex:1229
CompName:Decane, 3-ethyl-3-methyl- $$ 3-Ethyl-3-methyldecane # $$



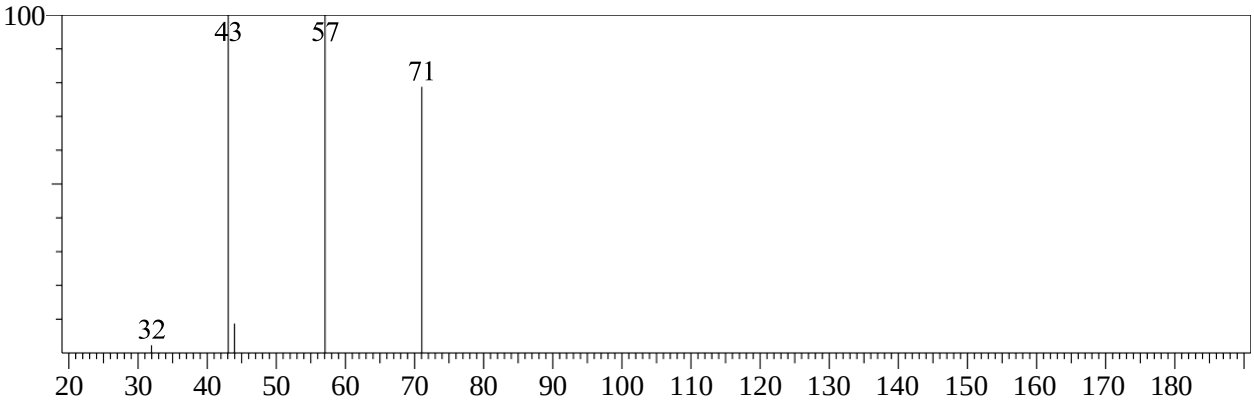
Hit#:2 Entry:76426 Library:WILEY7.LIB
SI:92 Formula:C13 H28 CAS:17312-66-2 MolWeight:184 RetIndex:0
CompName:Decane, 3-ethyl-3-methyl- (CAS)



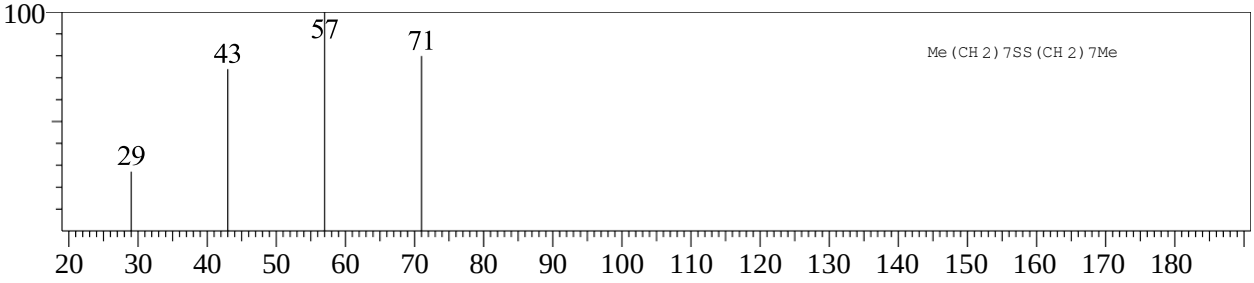
Hit#:3 Entry:76439 Library:WILEY7.LIB
SI:91 Formula:C13 H28 CAS:62238-13-5 MolWeight:184 RetIndex:0
CompName:Decane, 2,3,7-trimethyl- (CAS)



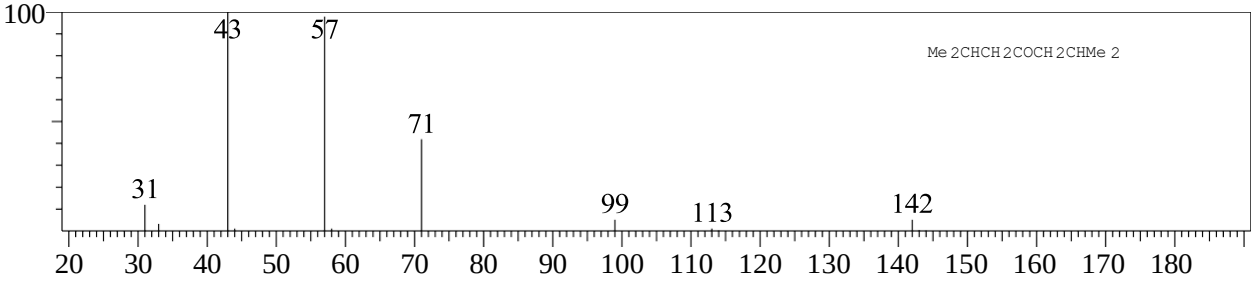
<< Target >>
Line#:11 R.Time:11.115(Scan#:11) MassPeaks:11
RawMode:Averaged 30.360-30.370(5753-5755) BasePeak:43.05(955)
BG Mode:Calc. from Peak



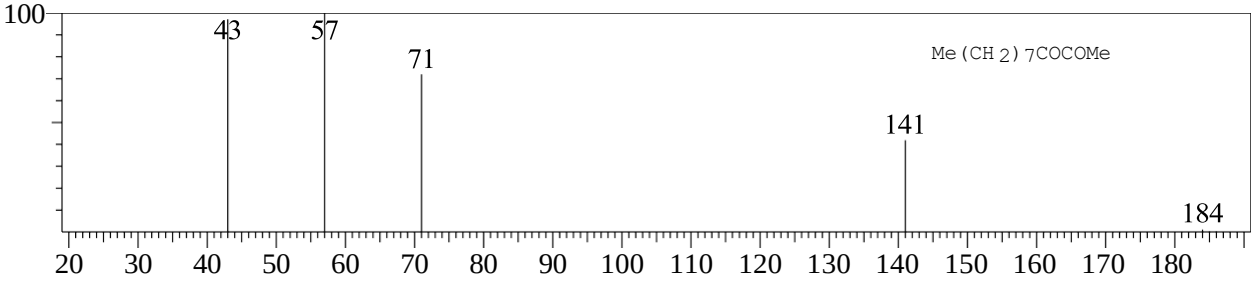
Hit#:1 Entry:201724 Library:WILEY7.LIB
SI:96 Formula:C16 H34 S2 CAS:822-27-5 MolWeight:290 RetIndex:0
CompName:Di-n-octyl disulfide $$ Disulfide, dioctyl (CAS) Dioctyl disulfide $$ Octyl disulfide $$ n-Octyl



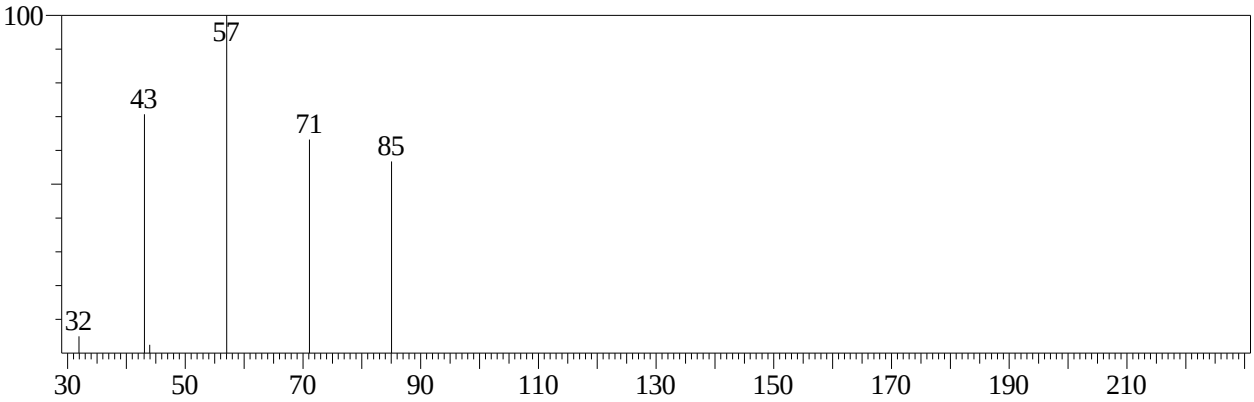
Hit#:2 Entry:31727 Library:WILEY7.LIB
SI:92 Formula:C9 H18 O CAS:108-83-8 MolWeight:142 RetIndex:0
CompName:4-Heptanone, 2,6-dimethyl- (CAS) 2,6-Dimethyl-4-heptanone $$ DIBK $$ DIBC $$ Isovaleron



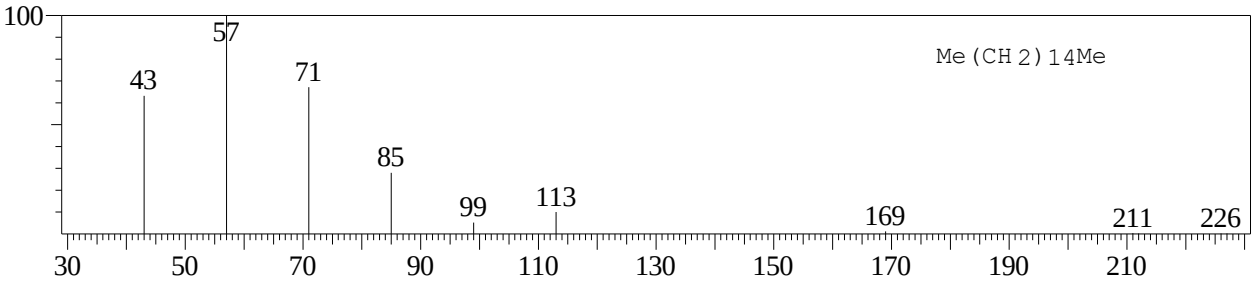
Hit#:3 Entry:76022 Library:WILEY7.LIB
SI:90 Formula:C11 H20 O2 CAS:7493-59-6 MolWeight:184 RetIndex:0
CompName:2,3-Undecandione $$ 2,3-Undecanedione (CAS)



<< Target >>
Line#:12 R.Time:12.125(Scan#:12) MassPeaks:12
RawMode:Averaged 32.330-32.340(6147-6149) BasePeak:57.05(2858)
BG Mode:Calc. from Peak



Hit#:1 Entry:129213 Library:WILEY7.LIB
SI:92 Formula:C16 H34 CAS:544-76-3 MolWeight:226 RetIndex:0
CompName:Hexadecane (CAS) n-Hexadecane $$ Cetane $$ n-Cetane $$ Isohexadecane $$ HEXADECAN



Hit#:2 Entry:46256 Library:WILEY7.LIB
SI:91 Formula:C11 H24 CAS:1120-21-4 MolWeight:156 RetIndex:0
CompName:Undecane (CAS) n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330 $$