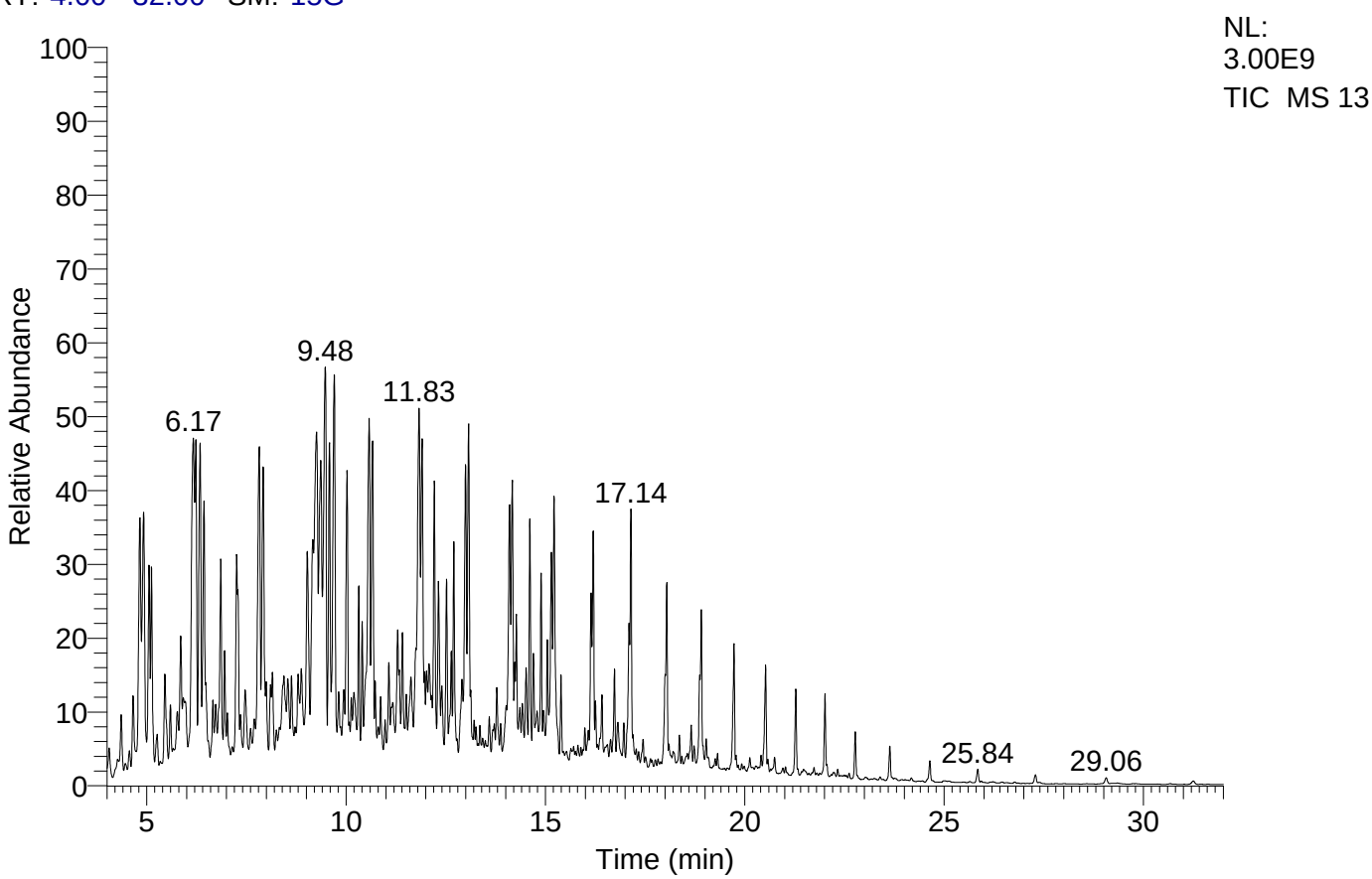
Data File:	13	Injection Volume(µl):	1.00
Sample ID:	1	Run Time(min):	28.10
Comments:		Scans:	8261
Low Mass(m/z):	50	High Mass(m/z):	500

RT: 4.00 - 32.00 SM: 15G



RT	Compound Name	Area	Area %	RSI	Cas #	Library
4.83	Decyl trifluoroacetate	3292076330	2.18	950	333-88-0	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
4.92	1-Octanol, 2-butyl-	3659660952	2.43	941	3913-02-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
5.06	Oxalic acid, 2-ethylhexyl hexyl ester	2061966047	1.37	934	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
5.12	Oxalic acid, 2-ethylhexyl hexyl ester	2068922508	1.37	932	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.17	Cyclopentane, 1-butyl-2-propyl-	5568198181	3.70	880	62199-50-2	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.23	5-Ethyl-1-nonene	3584675481	2.38	898	19780-74-6	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.34	E-11,13-Tetradecadien-1-ol	4194071753	2.78	967	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.44	Undecane	3962683466	2.63	972	1120-21-4	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.86	1-Dodecanol, 3,7,11-trimethyl-	2803781304	1.86	924	6750-34-1	mainlib

Analysed By: *Checked By:*

RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.95	1-Dodecanol, 3,7,11-trimethyl-	1095699316	0.73	940	6750-34-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.25	4-Nonene, 3-methyl-, (Z)-	3428099098	2.27	879	63830-69-3	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.82	Cyclododecane	4637415639	3.08	952	294-62-2	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.92	Dodecane	4148834202	2.75	984	112-40-3	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.02	Trichloroacetic acid, pentadecyl ester	2563756349	1.70	904	74339-53-0	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.16	10-Heneicosene (c,t)	2065147344	1.37	953	95008-11-0	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.25	1-Tridecene	4024324226	2.67	974	2437-56-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.37	10-Methylnonadecane	2800125743	1.86	936	56862-62-5	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.48	Trifluoroacetic acid, pentadecyl ester	5996302173	3.98	902	959010-23-2	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.58	1-Decanol, 2-hexyl-	3420962043	2.27	916	2425-77-6	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.71	Dichloroacetic acid, 6-ethyl-3-octyl ester	5837778482	3.87	882	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.03	3-Eicosene, (E)-	3340221279	2.22	909	74685-33-9	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.32	10-Heneicosene (c,t)	1402821131	0.93	932	95008-11-0	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.40	1,16-Hexadecanediol	920715705	0.61	866	7735-42-4	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.58	1-Tetradecene	5410424752	3.59	981	1120-36-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.66	Tetradecane	3804973538	2.53	984	629-59-4	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.29	10-Methylnonadecane	1681891823	1.12	934	56862-62-5	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.41	2-Hexyl-1-octanol	1022867847	0.68	928	19780-79-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.83	Trifluoroacetic acid, pentadecyl ester	6158870340	4.09	975	959010-23-2	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.91	Pentadecane	3994681734	2.65	968	629-62-9	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.21	1-Dodecanol, 3,7,11-trimethyl-	2695952813	1.79	925	6750-34-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.31	Trichloroacetic acid, hexadecyl ester	1831951594	1.22	923	74339-54-1	mainlib

Analysed By: *Checked By:*

RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.52	1-Dodecanol, 3,7,11-trimethyl-	1679379289	1.11	936	6750-34-1	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.70	Trichloroacetic acid, tetradecyl ester	2146033589	1.42	857	74339-52-9	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
13.00	Cyclohexadecane	3622733210	2.40	981	295-65-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
13.07	Decane, 2,4,6-trimethyl-	4317767725	2.87	937	62108-27-4	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.10	E-14-Hexadecenal	3560927978	2.36	981	330207-53-9	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.17	Heptadecane	3108859932	2.06	970	629-78-7	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.27	Nonadecyl pentafluoropropionate	1518131799	1.01	892	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.61	1-Dodecanol, 2-hexyl-	2131474151	1.41	924	110225-00-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.89	1-Dodecanol, 2-hexyl-	1517211604	1.01	933	110225-00-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.05	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	874079911	0.58	882	7225-68-5	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.15	10-Heneicosene (c,t)	2409972010	1.60	982	95008-11-0	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.22	Eicosane	3680539172	2.44	969	112-95-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
16.14	1-Heneicosanol	1539463410	1.02	984	15594-90-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
16.20	Eicosane	2626909217	1.74	983	112-95-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
17.14	2-methylhexacosane	4086590346	2.71	957	NA	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
18.04	Eicosane	2891362267	1.92	982	112-95-8	mainlib

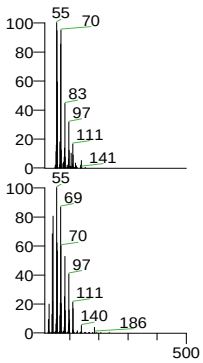
RT	Compound Name	Area	Area %	RSI	Cas #	Library
18.91	Eicosane	2465669529	1.64	977	112-95-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
19.73	Eicosane	1640671809	1.09	975	112-95-8	mainlib

RT	Compound Name	Area	Area %	RSI	Cas #	Library
20.52	Eicosane	1391924842	0.92	966	112-95-8	mainlib

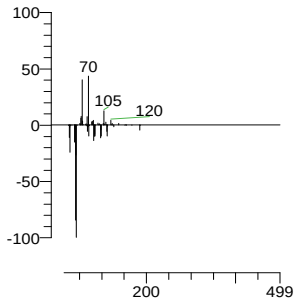
Analysed By: *Checked By:*

Hit Spectrum	Delta	Compound Structure

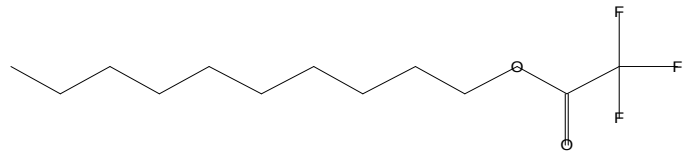


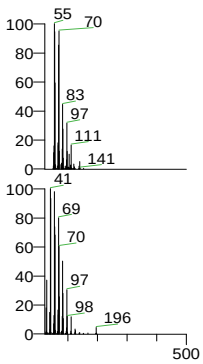
NL: 9.98E2
13245 4.83 1 11
22 220-230 260-270
1.28E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 911, RSI 950,
mainlib, Entry# 18827,
CAS# 333-88-0, Decyl
trifluoroacetate



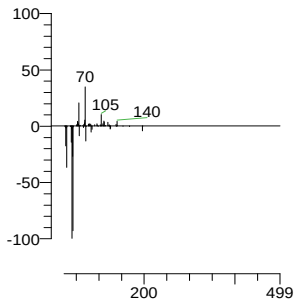
Decyl trifluoroacetate
Formula C12H21F3O2, MW 254, CAS# 333-88-0, Entry# 18827
Decyl 2,2,2-trifluoroacetate



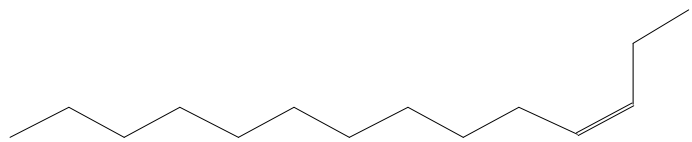


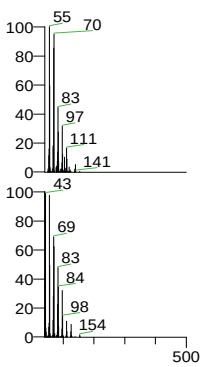
NL: 9.98E2
13245 4.83 1 11
22 220-230 260-270
1.28E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 914, RSI 948,
mainlib, Entry# 2508,
CAS# 41446-67-7,
3-Tetradecene, (Z)-



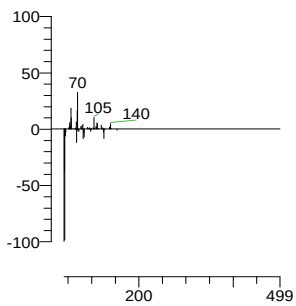
3-Tetradecene, (Z)-
Formula C14H28, MW 196, CAS# 41446-67-7, Entry# 2508
(3Z)-3-Tetradecene



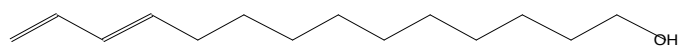


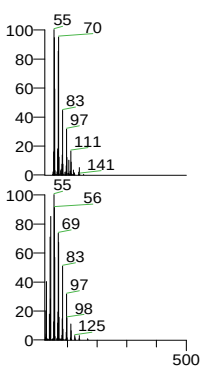
NL: 9.98E2
13245 4.83 1 11
22 220-230 260-270
1.28E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 898, RSI 948,
mainlib, Entry# 2200,
CAS# NA,
E-11,13-Tetradecadien-
1-ol



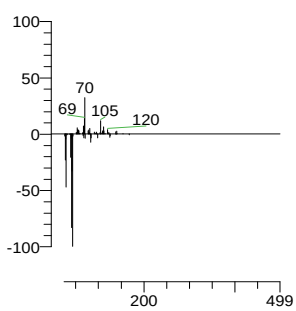
E-11,13-Tetradecadien-1-ol
Formula C14H26O, MW 210, CAS# NA, Entry# 2200
(11E)-11,13-Tetradecadien-1-ol #



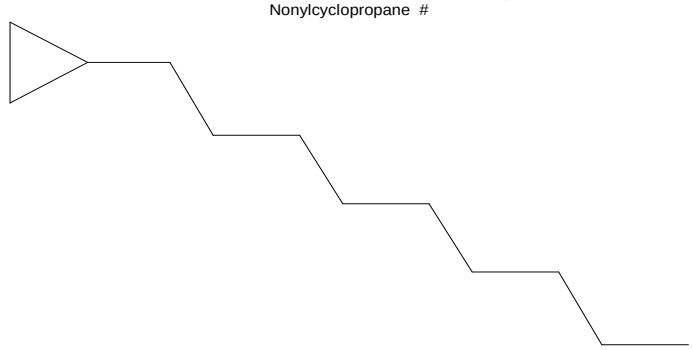


NL: 9.98E2
13245 4.83 1 11
22 220-230 260-270
1.28E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 909, RSI 946,
mainlib, Entry# 18566,
CAS# 74663-85-7,
Cyclopropane, nonyl-

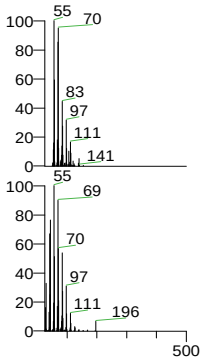


Cyclopropane, nonyl-
Formula C12H24, MW 168, CAS# 74663-85-7, Entry# 18566
Nonylcyclopropane #

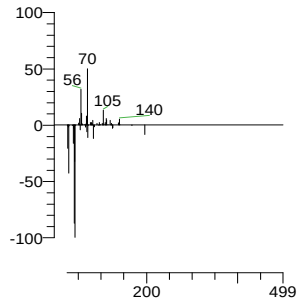


Analysed By: *Checked By:*

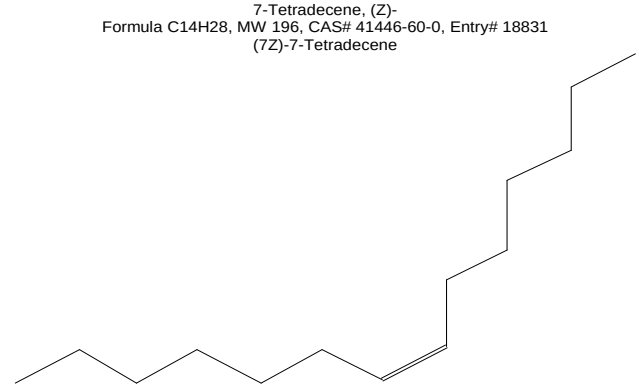
Hit Spectrum



Delta



Compound Structure

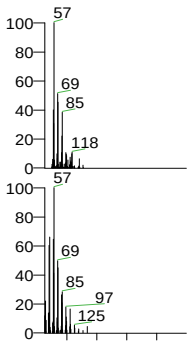


RT	Compound Name	Area	Area %	RSI	Cas #	Library
4.83	Decyl trifluoroacetate	3292076330	2.18	950	333-88-0	mainlib
4.83	E-11,13-Tetradecadien-1-ol	3292076330	2.18	948	NA	mainlib
4.83	3-Tetradecene, (Z)-	3292076330	2.18	948	41446-67-7	mainlib

Analysed By:

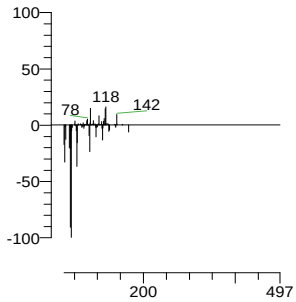
Checked By:

Hit Spectrum	Delta	Compound Structure

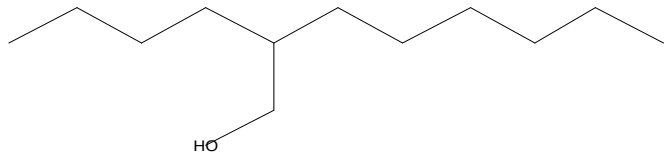


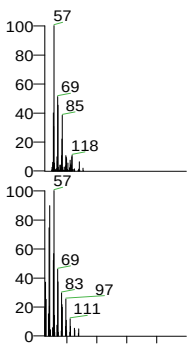
NL: 9.99E2
13271 4.92 1 11
22 246-256 286-296
1.85E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 829, RSI 941,
mainlib, Entry# 22453,
CAS# 3913-02-8,
1-Octanol, 2-butyl-



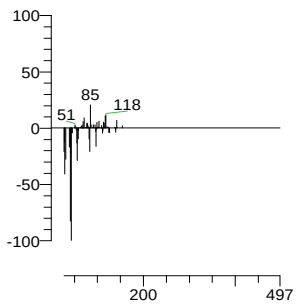
1-Octanol, 2-butyl-
Formula C12H26O, MW 186, CAS# 3913-02-8, Entry# 22453
2-Butyl-1-octanol



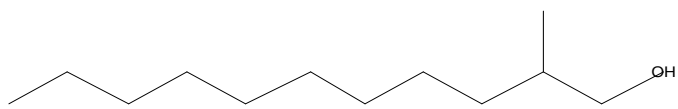


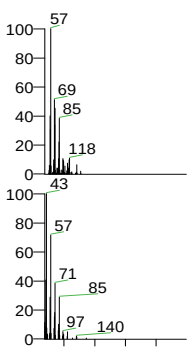
NL: 9.99E2
13271 4.92 1 11
22 246-256 286-296
1.85E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 788, RSI 935,
mainlib, Entry# 22393,
CAS# 10522-26-6,
2-Methyl-1-undecanol



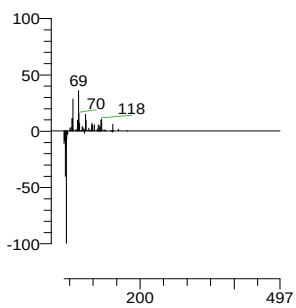
2-Methyl-1-undecanol
Formula C12H26O, MW 186, CAS# 10522-26-6, Entry# 22393
1-Undecanol, 2-methyl-



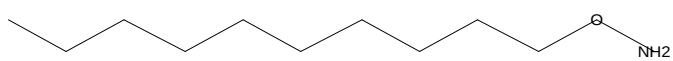


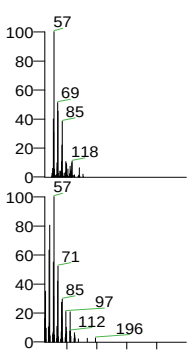
NL: 9.99E2
13271 4.92 1 11
22 246-256 286-296
1.85E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 772, RSI 932,
mainlib, Entry# 7242,
CAS# 29812-79-1,
Hydroxylamine,
O-decyl-



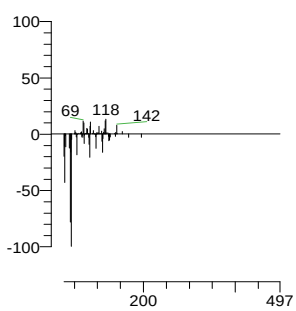
Hydroxylamine, O-decyl-
Formula C10H23NO, MW 173, CAS# 29812-79-1, Entry# 7242
O-Decylhydroxylamine



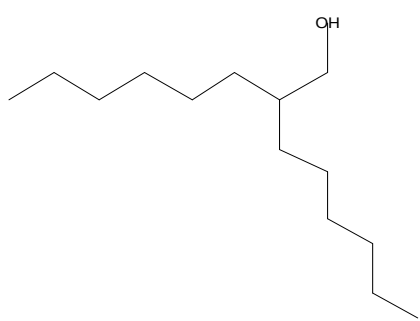


NL: 9.99E2
13271 4.92 1 11
22 246-256 286-296
1.85E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 800, RSI 930,
mainlib, Entry# 22406,
CAS# 19780-79-1,
2-Hexyl-1-octanol

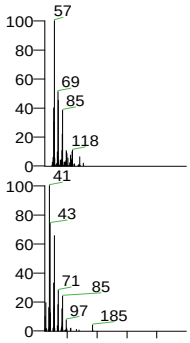


2-Hexyl-1-octanol
Formula C14H30O, MW 214, CAS# 19780-79-1, Entry# 22406



Analysed By: *Checked By:*

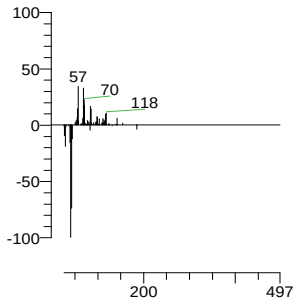
Hit Spectrum



NL: 9.99E2
13271 4.92 1 11
22 246-256 286-296
1.85E8 + c EI Full ms
[50.00-500.00]

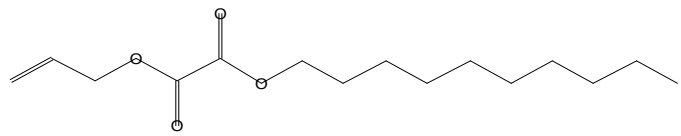
NL: 9.99E2
SI 789, RSI 930,
mainlib, Entry# 2293,
CAS# NA, Oxalic acid,
allyl decyl ester

Delta



Compound Structure

Oxalic acid, allyl decyl ester
Formula C15H26O4, MW 270, CAS# NA, Entry# 2293

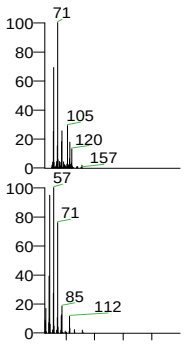


RT	Compound Name	Area	Area %	RSI	Cas #	Library
4.92	1-Octanol, 2-butyl-	3659660952	2.43	941	3913-02-8	mainlib
4.92	2-Methyl-1-undecanol	3659660952	2.43	935	10522-26-6	mainlib
4.92	Hydroxylamine, O-decyl-	3659660952	2.43	932	29812-79-1	mainlib

Analysed By:

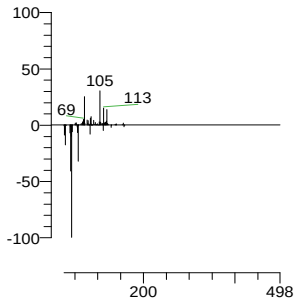
Checked By:

Hit Spectrum	Delta	Compound Structure

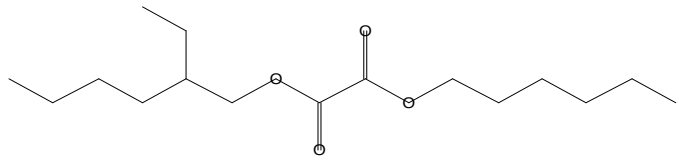


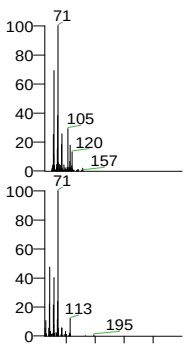
NL: 9.99E2
13312 5.06 1 11 22
287-297 327-337
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 737, RSI 934,
mainlib, Entry# 22519,
CAS# NA, Oxalic acid,
2-ethylhexyl hexyl ester



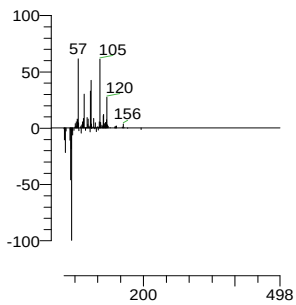
Oxalic acid, 2-ethylhexyl hexyl ester
Formula C16H30O4, MW 286, CAS# NA, Entry# 22519



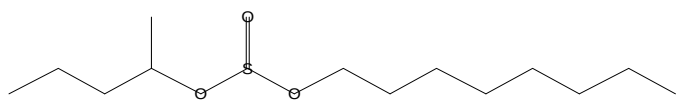


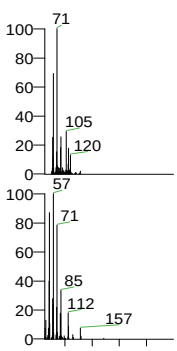
NL: 9.99E2
13312 5.06 1 11
22 287-297 327-337
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 734, RSI 928,
mainlib, Entry# 35068,
CAS# NA, Sulfurous
acid, octyl 2-pentyl ester



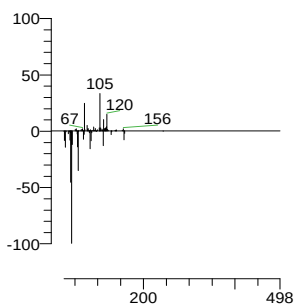
Sulfurous acid, octyl 2-pentyl ester
Formula C13H28O3S, MW 264, CAS# NA, Entry# 35068



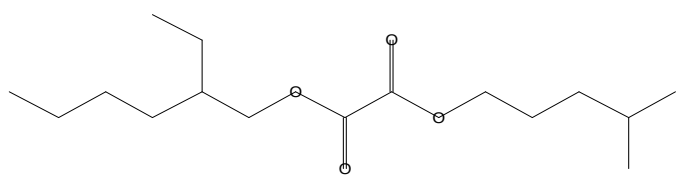


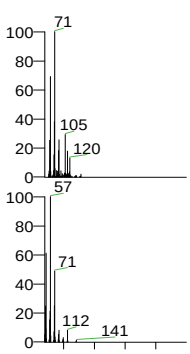
NL: 9.99E2
13312 5.06 1 11 22
287-297 327-337
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 751, RSI 916, mainlib,
Entry# 22518, CAS# NA,
Oxalic acid, 2-ethylhexyl
isohexyl ester



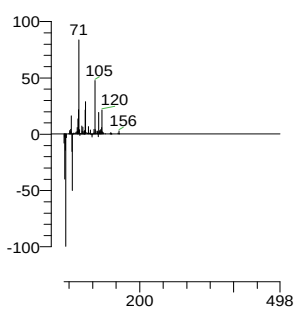
Oxalic acid, 2-ethylhexyl isohexyl ester
Formula C16H30O4, MW 286, CAS# NA, Entry# 22518



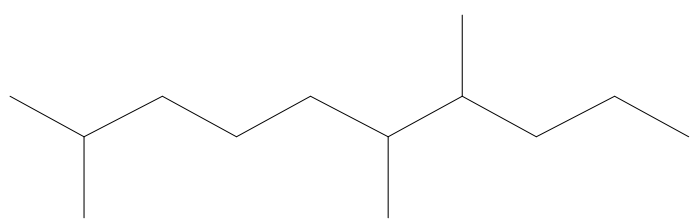


NL: 9.99E2
13312 5.06 1 11
22 287-297 327-337
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 718, RSI 909,
mainlib, Entry# 22617,
CAS# 62108-25-2,
Decane, 2,6,7-trimethyl-

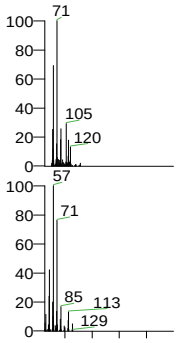


Decane, 2,6,7-trimethyl-
Formula C13H28, MW 184, CAS# 62108-25-2, Entry# 22617
2,6,7-Trimethyldecane #



Analysed By: *Checked By:*

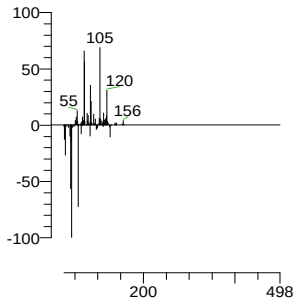
Hit Spectrum



NL: 9.99E2
13312 5.06 1 11 22
287-297 327-337
1.63E8 + c EI Full ms
[50.00-500.00]

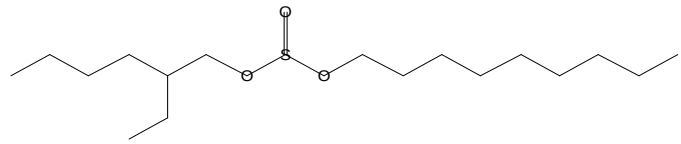
NL: 9.99E2
SI 725, RSI 908, mainlib,
Entry# 23480, CAS# NA,
Sulfurous acid,
2-ethylhexyl nonyl ester

Delta



Compound Structure

Sulfurous acid, 2-ethylhexyl nonyl ester
Formula C17H36O3S, MW 320, CAS# NA, Entry# 23480

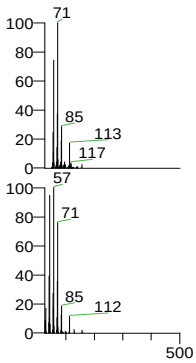


RT	Compound Name	Area	Area %	RSI	Cas #	Library
5.06	Oxalic acid, 2-ethylhexyl hexyl ester	2061966047	1.37	934	NA	mainlib
5.06	Sulfurous acid, octyl 2-pentyl ester	2061966047	1.37	928	NA	mainlib
5.06	Oxalic acid, 2-ethylhexyl isohexyl ester	2061966047	1.37	916	NA	mainlib

Analysed By:

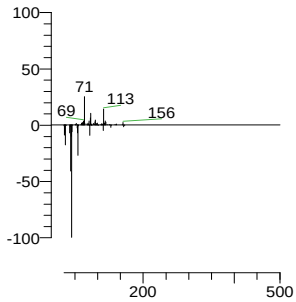
Checked By:

Hit Spectrum	Delta	Compound Structure

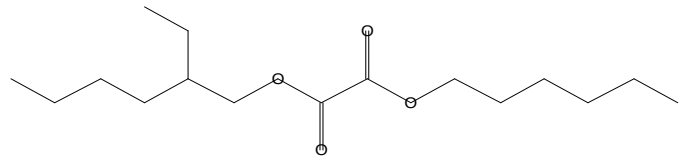


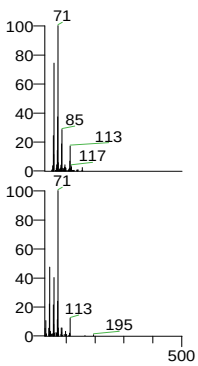
NL: 9.99E2
13330 5.12 1 11 22
305-315 345-355
1.74E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 837, RSI 932,
mainlib, Entry# 22519,
CAS# NA, Oxalic acid,
2-ethylhexyl hexyl ester



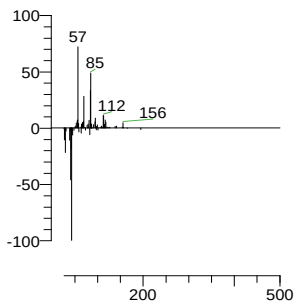
Oxalic acid, 2-ethylhexyl hexyl ester
Formula C16H30O4, MW 286, CAS# NA, Entry# 22519



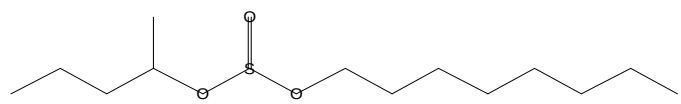


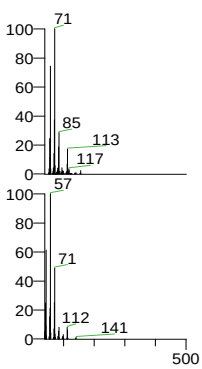
NL: 9.99E2
13330 5.12 1 11
22 305-315 345-355
1.74E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 829, RSI 916,
mainlib, Entry# 35068,
CAS# NA, Sulfurous
acid, octyl 2-pentyl ester



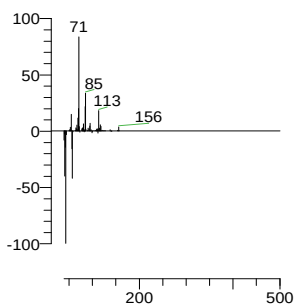
Sulfurous acid, octyl 2-pentyl ester
Formula C13H28O3S, MW 264, CAS# NA, Entry# 35068



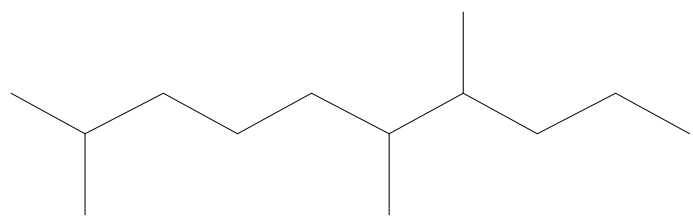


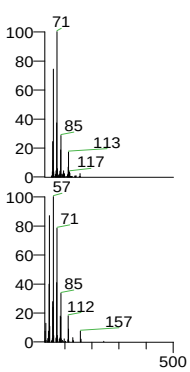
NL: 9.99E2
13330 5.12 1 11
22 305-315 345-355
1.74E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 824, RSI 916,
mainlib, Entry# 22617,
CAS# 62108-25-2,
Decane, 2,6,7-trimethyl-



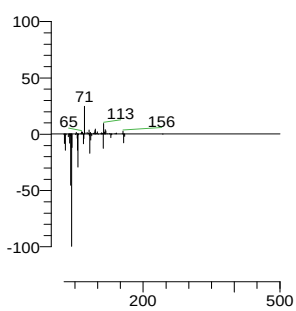
Decane, 2,6,7-trimethyl-
Formula C13H28, MW 184, CAS# 62108-25-2, Entry# 22617
2,6,7-Trimethyldecane #



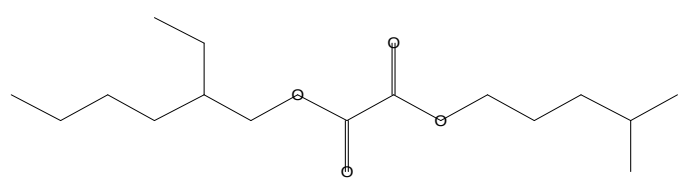


NL: 9.99E2
13330 5.12 1 11 22
305-315 345-355
1.74E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 843, RSI 915, mainlib,
Entry# 22518, CAS# NA,
Oxalic acid, 2-ethylhexyl
isohexyl ester

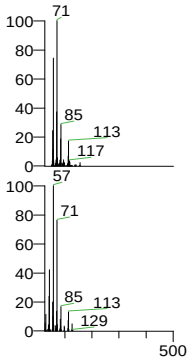


Oxalic acid, 2-ethylhexyl isohexyl ester
Formula C16H30O4, MW 286, CAS# NA, Entry# 22518



Analysed By: *Checked By:*

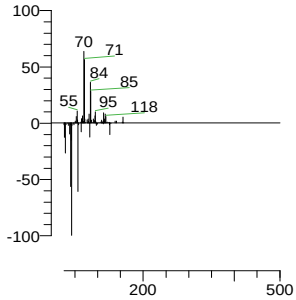
Hit Spectrum



NL: 9.99E2
13330 5.12 1 11 22
305-315 345-355
1.74E8 + c EI Full ms
[50.00-500.00]

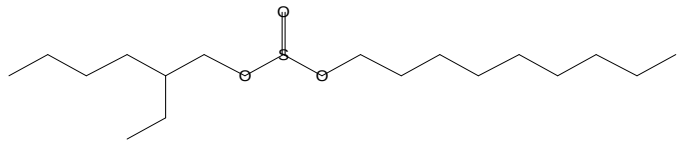
NL: 9.99E2
SI 835, RSI 914, mainlib,
Entry# 23480, CAS# NA,
Sulfurous acid,
2-ethylhexyl nonyl ester

Delta



Compound Structure

Sulfurous acid, 2-ethylhexyl nonyl ester
Formula C17H36O3S, MW 320, CAS# NA, Entry# 23480

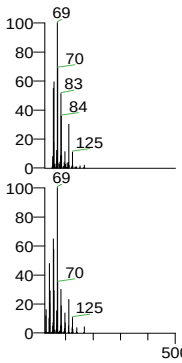


RT	Compound Name	Area	Area %	RSI	Cas #	Library
5.12	Oxalic acid, 2-ethylhexyl hexyl ester	2068922508	1.37	932	NA	mainlib
5.12	Decane, 2,6,7-trimethyl-	2068922508	1.37	916	62108-25-2	mainlib
5.12	Sulfurous acid, octyl 2-pentyl ester	2068922508	1.37	916	NA	mainlib

Analysed By:

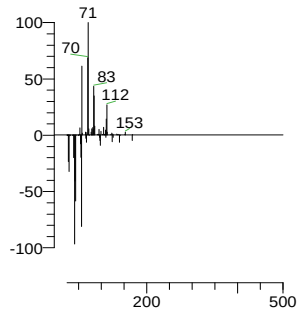
Checked By:

Hit Spectrum	Delta	Compound Structure

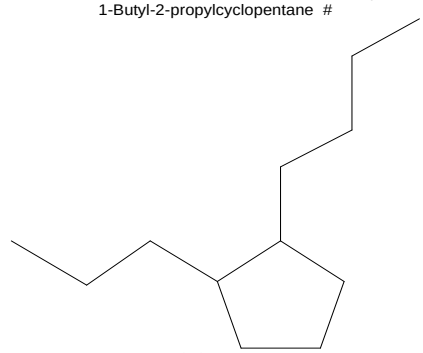


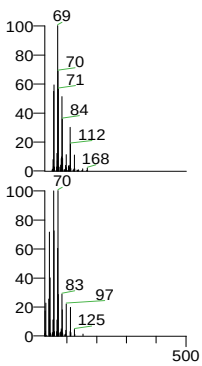
NL: 9.99E2
13639 6.17 1 11 22
614-624 654-664
1.98E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 862, RSI 880, mainlib, Entry# 32071, CAS# 62199-50-2, Cyclopentane, 1-butyl-2-propyl-



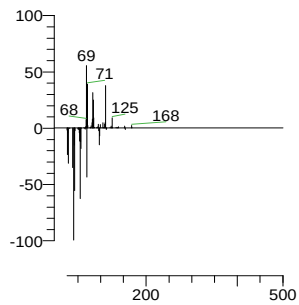
Cyclopentane, 1-butyl-2-propyl-
Formula C12H24, MW 168, CAS# 62199-50-2, Entry# 32071
1-Butyl-2-propylcyclopentane #



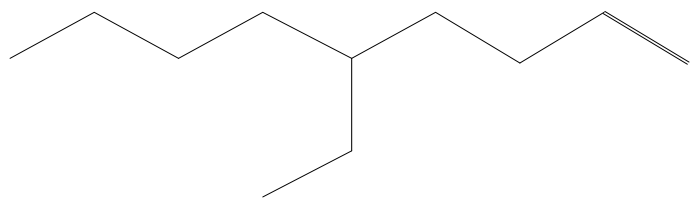


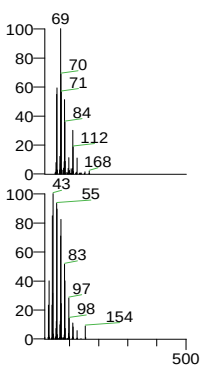
NL: 9.99E2
13639 6.17 1 11
22 614-624 654-664
1.98E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 842, RSI 880, mainlib, Entry# 34087, CAS# 19780-74-6, 5-Ethyl-1-nonene



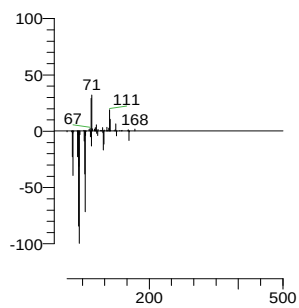
5-Ethyl-1-nonene
Formula C11H22, MW 154, CAS# 19780-74-6, Entry# 34087



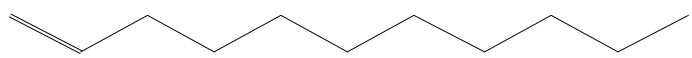


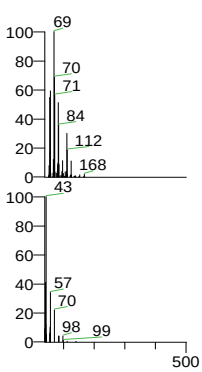
NL: 9.99E2
13639 6.17 1 11
22 614-624 654-664
1.98E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 848, RSI 865, mainlib, Entry# 6823, CAS# 821-95-4, 1-Undecene



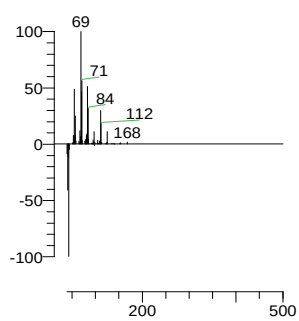
1-Undecene
Formula C11H22, MW 154, CAS# 821-95-4, Entry# 6823
n-1-Undecene



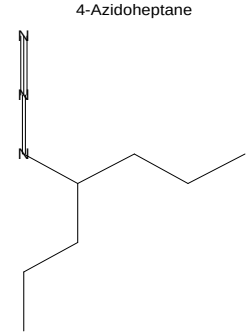


NL: 9.99E2
13639 6.17 1 11
22 614-624 654-664
1.98E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 407, RSI 865, mainlib, Entry# 5791, CAS# 27126-22-3, Heptane, 4-azido-

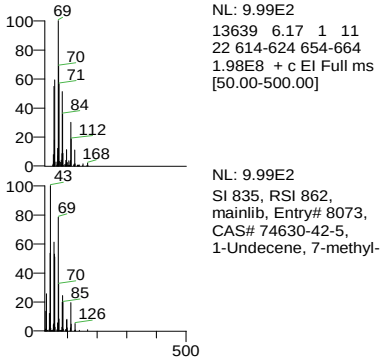


Heptane, 4-azido-
Formula C7H15N3, MW 141, CAS# 27126-22-3, Entry# 5791
4-Azidoheptane

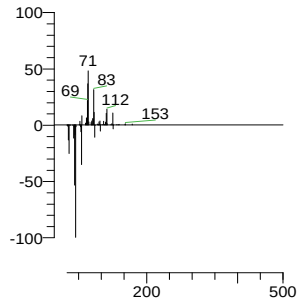


Analysed By: *Checked By:*

Hit Spectrum

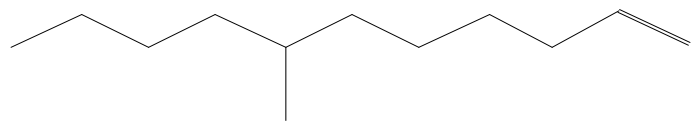


Delta



Compound Structure

1-Undecene, 7-methyl-
Formula C12H24, MW 168, CAS# 74630-42-5, Entry# 8073
7-Methyl-1-undecene #

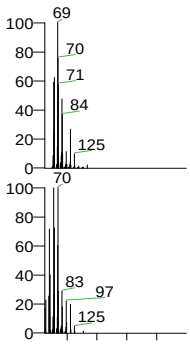


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.17	5-Ethyl-1-nonene	5568198181	3.70	880	19780-74-6	mainlib
6.17	Cyclopentane, 1-butyl-2-propyl-	5568198181	3.70	880	62199-50-2	mainlib
6.17	1-Undecene	5568198181	3.70	865	821-95-4	mainlib

Analysed By:

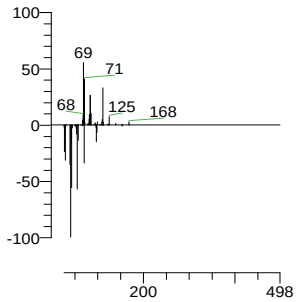
Checked By:

Hit Spectrum	Delta	Compound Structure

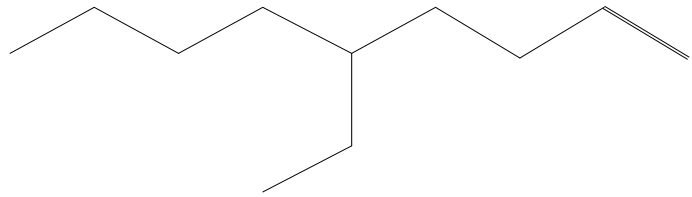


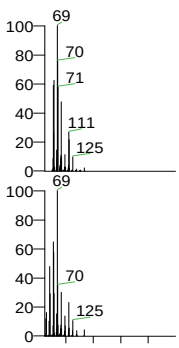
NL: 9.99E2
13659 6.23 1 11 22 634-644 674-684
1.88E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 871, RSI 898, mainlib, Entry# 34087, CAS# 19780-74-6, 5-Ethyl-1-nonene



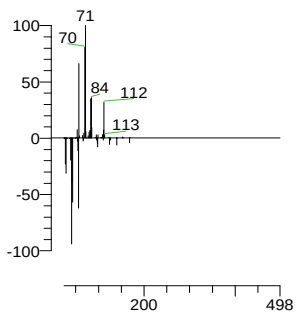
5-Ethyl-1-nonene
Formula C11H22, MW 154, CAS# 19780-74-6, Entry# 34087



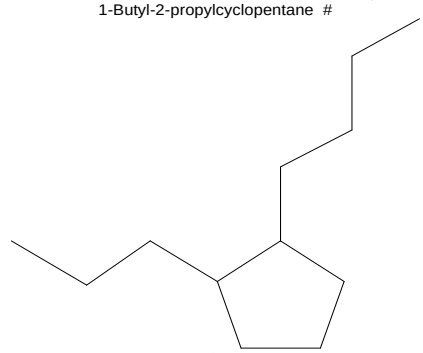


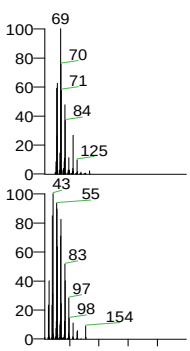
NL: 9.99E2
13659 6.23 1 11 22 634-644 674-684
1.88E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 887, RSI 893, mainlib, Entry# 32071, CAS# 62199-50-2, Cyclopentane, 1-butyl-2-propyl-



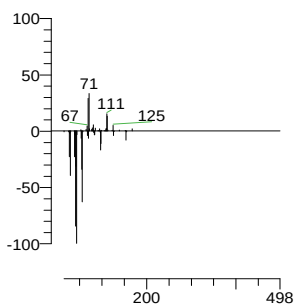
Cyclopentane, 1-butyl-2-propyl-
Formula C12H24, MW 168, CAS# 62199-50-2, Entry# 32071
1-Butyl-2-propylcyclopentane #



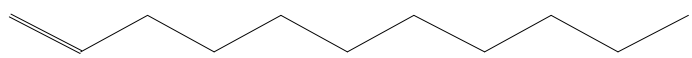


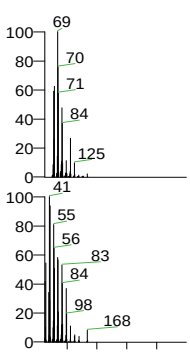
NL: 9.99E2
13659 6.23 1 11 22 634-644 674-684
1.88E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 885, RSI 893, mainlib, Entry# 6823, CAS# 821-95-4, 1-Undecene



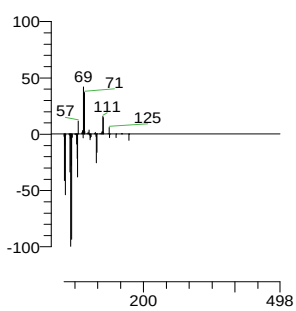
1-Undecene
Formula C11H22, MW 154, CAS# 821-95-4, Entry# 6823
n-1-Undecene



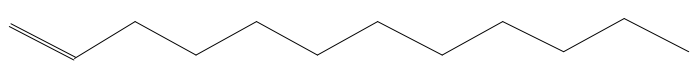


NL: 9.99E2
13659 6.23 1 11 22 634-644 674-684
1.88E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 877, RSI 882, mainlib, Entry# 2237, CAS# 112-41-4, 1-Dodecene

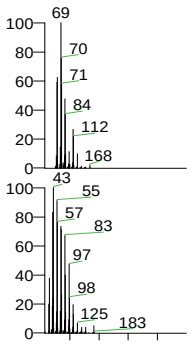


1-Dodecene
Formula C12H24, MW 168, CAS# 112-41-4, Entry# 2237
à-Dodecene

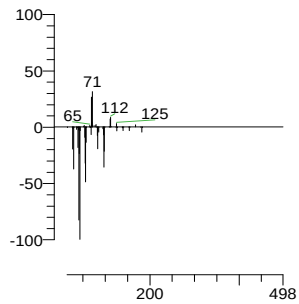


Analysed By: *Checked By:*

Hit Spectrum

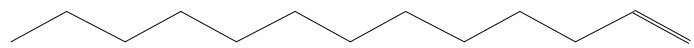


Delta



Compound Structure

1-Tridecene
Formula C13H26, MW 182, CAS# 2437-56-1, Entry# 6779
n-Tridec-1-ene

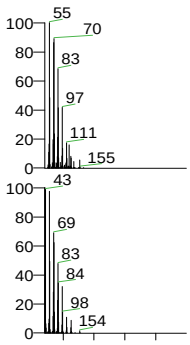


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.23	5-Ethyl-1-nonene	3584675481	2.38	898	19780-74-6	mainlib
6.23	1-Undecene	3584675481	2.38	893	821-95-4	mainlib
6.23	Cyclopentane, 1-butyl-2-propyl-	3584675481	2.38	893	62199-50-2	mainlib

Analysed By:

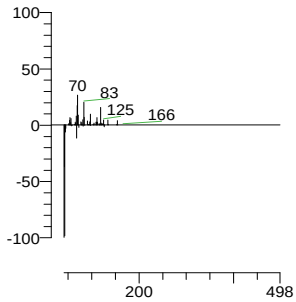
Checked By:

Hit Spectrum	Delta	Compound Structure

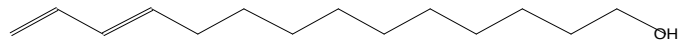


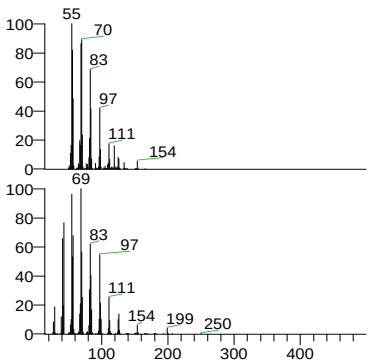
NL: 9.99E2
13691 6.34 1 11
22 666-676 706-716
1.44E8 + c EI Full ms
[50.00-500.00]

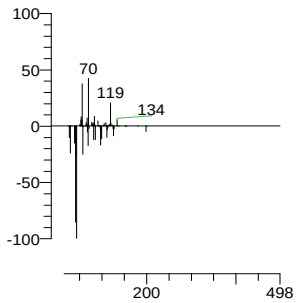
NL: 9.99E2
SI 914, RSI 967,
mainlib, Entry# 2200,
CAS# NA,
E-11,13-Tetradecadien-
1-ol



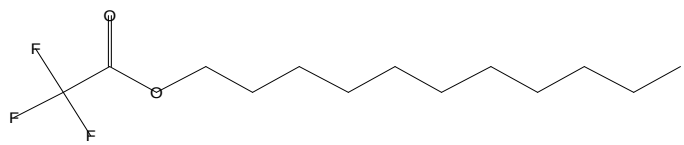
E-11,13-Tetradecadien-1-ol
Formula C14H26O, MW 210, CAS# NA, Entry# 2200
(11E)-11,13-Tetradecadien-1-ol #

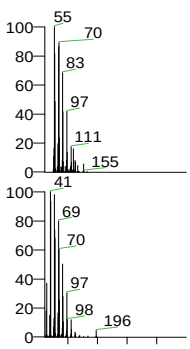






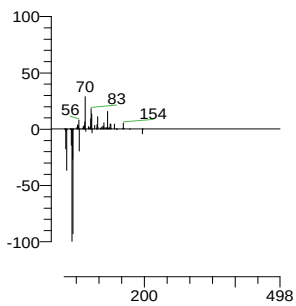
Acetic acid, trifluoro-, undecyl ester
Formula C13H23F3O2, MW 268, CAS# 53800-01-4, Entry# 32052



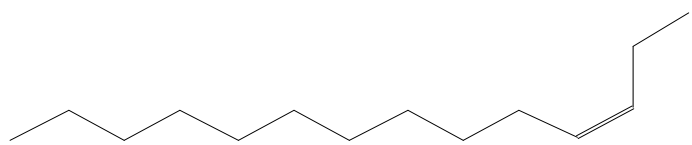


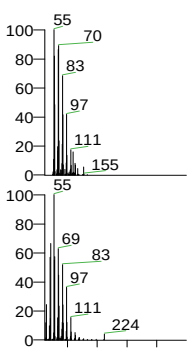
NL: 9.99E2
13691 6.34 1 11
22 666-676 706-716
1.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 906, RSI 951,
mainlib, Entry# 2508,
CAS# 41446-67-7,
3-Tetradecene, (Z)-



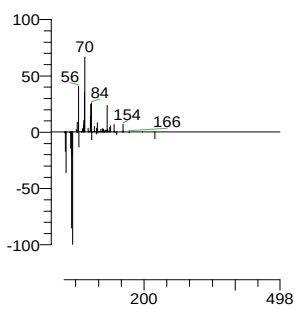
3-Tetradecene, (Z)-
Formula C14H28, MW 196, CAS# 41446-67-7, Entry# 2508
(3Z)-3-Tetradecene



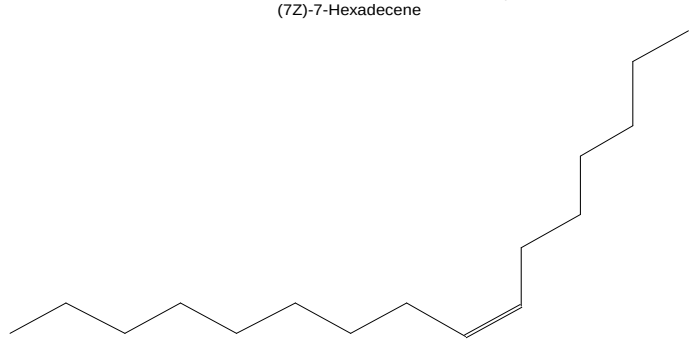


NL: 9.99E2
13691 6.34 1 11
22 666-676 706-716
1.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 907, RSI 950,
mainlib, Entry# 18425,
CAS# 35507-09-6,
7-Hexadecene, (Z)-

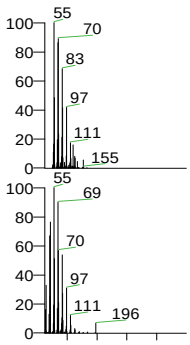


7-Hexadecene, (Z)-
Formula C16H32, MW 224, CAS# 35507-09-6, Entry# 18425
(7Z)-7-Hexadecene



Analysed By: *Checked By:*

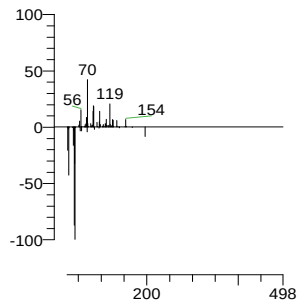
Hit Spectrum



NL: 9.99E2
13691 6.34 1 11
22 666-676 706-716
1.44E8 + c EI Full ms
[50.00-500.00]

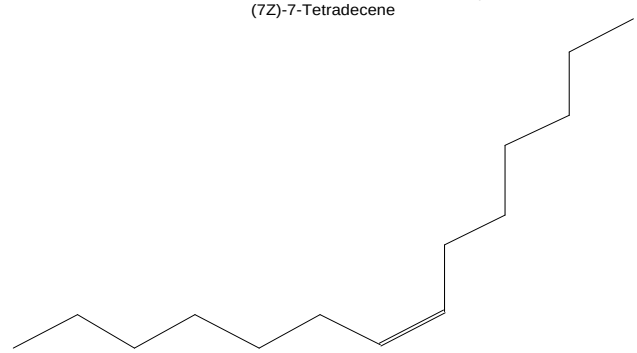
NL: 9.99E2
SI 903, RSI 949,
mainlib, Entry# 18831,
CAS# 41446-60-0,
7-Tetradecene, (Z)-

Delta



Compound Structure

7-Tetradecene, (Z)-
Formula C14H28, MW 196, CAS# 41446-60-0, Entry# 18831
(7Z)-7-Tetradecene

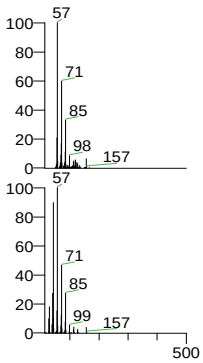


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.34	E-11,13-Tetradecadien-1-ol	4194071753	2.78	967	NA	mainlib
6.34	Acetic acid, trifluoro-, undecyl ester	4194071753	2.78	952	53800-01-4	mainlib
6.34	3-Tetradecene, (Z)-	4194071753	2.78	951	41446-67-7	mainlib

Analysed By:

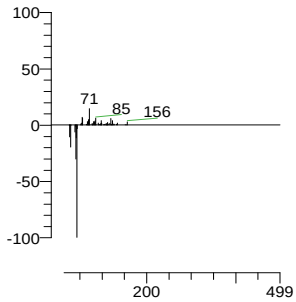
Checked By:

Hit Spectrum	Delta	Compound Structure

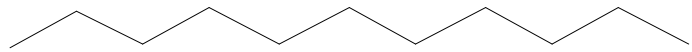


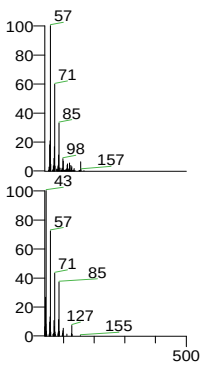
NL: 9.98E2
13719 6.44 1 11
22 694-704 734-744
2.54E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 866, RSI 972,
mainlib, Entry# 22688,
CAS# 1120-21-4,
Undecane



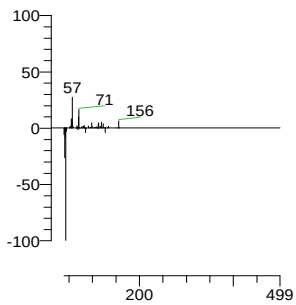
Undecane
Formula C11H24, MW 156, CAS# 1120-21-4, Entry# 22688
n-Undecane



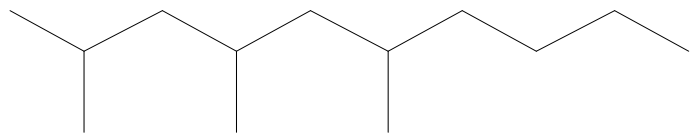


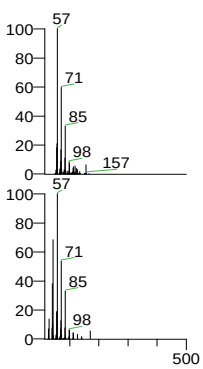
NL: 9.98E2
13719 6.44 1 11
22 694-704 734-744
2.54E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 757, RSI 956,
mainlib, Entry# 7452,
CAS# 62108-27-4,
Decane, 2,4,6-trimethyl-



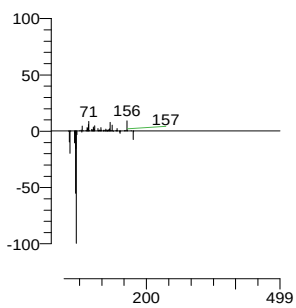
Decane, 2,4,6-trimethyl-
Formula C13H28, MW 184, CAS# 62108-27-4, Entry# 7452
2,4,6-Trimethyldecane #



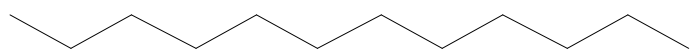


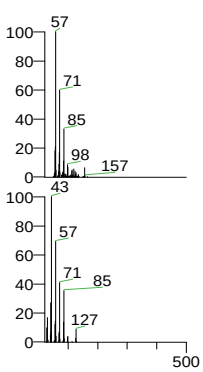
NL: 9.98E2
13719 6.44 1 11
22 694-704 734-744
2.54E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 839, RSI 954,
mainlib, Entry# 22550,
CAS# 112-40-3,
Dodecane



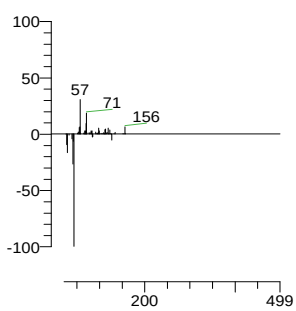
Dodecane
Formula C12H26, MW 170, CAS# 112-40-3, Entry# 22550
n-Dodecane



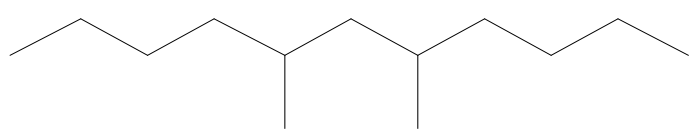


NL: 9.98E2
13719 6.44 1 11
22 694-704 734-744
2.54E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 748, RSI 944,
mainlib, Entry# 7436,
CAS# 17312-83-3,
Undecane,
5,7-dimethyl-

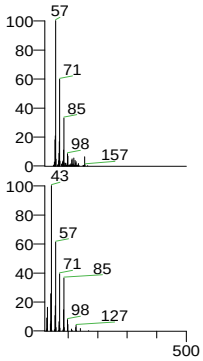


Undecane, 5,7-dimethyl-
Formula C13H28, MW 184, CAS# 17312-83-3, Entry# 7436
5,7-Dimethylundecane #

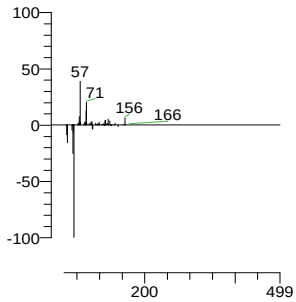


Analysed By: *Checked By:*

Hit Spectrum

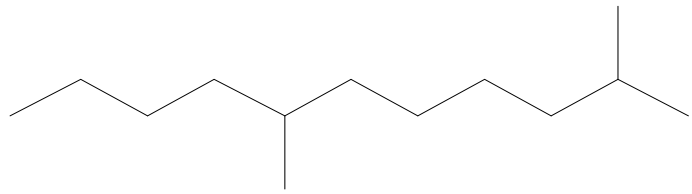


Delta



Compound Structure

Undecane, 2,7-dimethyl-
Formula C13H28, MW 184, CAS# 17301-24-5, Entry# 7484
2,7-Dimethylundecane #

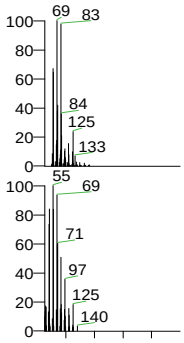


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.44	Undecane	3962683466	2.63	972	1120-21-4	mainlib
6.44	Decane, 2,4,6-trimethyl-	3962683466	2.63	956	62108-27-4	mainlib
6.44	Dodecane	3962683466	2.63	954	112-40-3	mainlib

Analysed By:

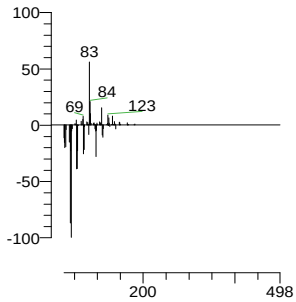
Checked By:

Hit Spectrum	Delta	Compound Structure

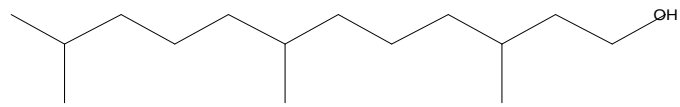


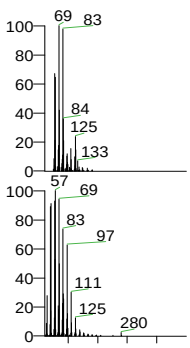
NL: 9.99E2
13841 6.86 1 11 22
816-826 856-866
8.91E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 863, RSI 924,
mainlib, Entry# 18829,
CAS# 6750-34-1,
1-Dodecanol,
3,7,11-trimethyl-



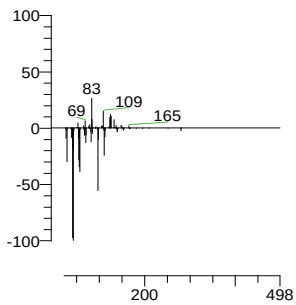
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



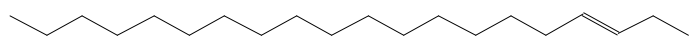


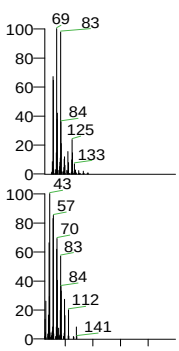
NL: 9.99E2
13841 6.86 1 11
22 816-826 856-866
8.91E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 871, RSI 894,
mainlib, Entry# 23390,
CAS# 74685-33-9,
3-Eicosene, (E)-



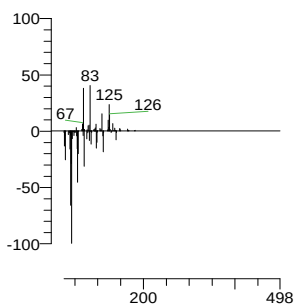
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



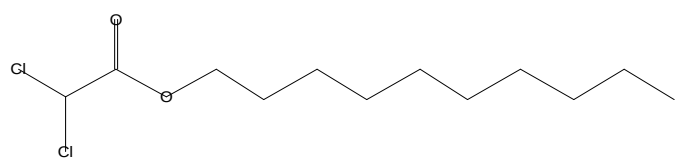


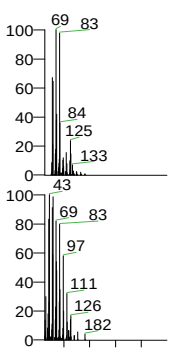
NL: 9.99E2
13841 6.86 1 11 22
816-826 856-866
8.91E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 763, RSI 894, mainlib,
Entry# 7338, CAS#
83005-00-9,
Dichloroacetic acid,
decyl ester



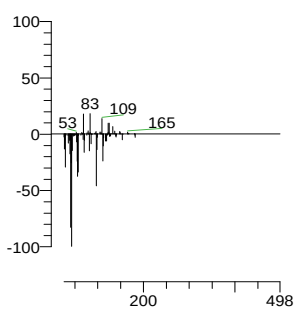
Dichloroacetic acid, decyl ester
Formula C12H22Cl2O2, MW 268, CAS# 83005-00-9, Entry# 7338
Decyl dichloroacetate #



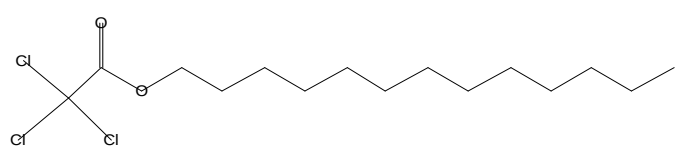


NL: 9.99E2
13841 6.86 1 11 22
816-826 856-866 8.91E7
+ c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 848, RSI 892, mainlib,
Entry# 7357, CAS#
74339-51-8,
Trichloroacetic acid,
tridecyl ester

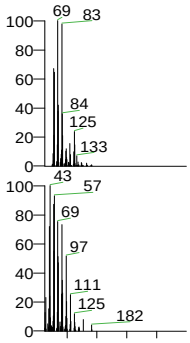


Trichloroacetic acid, tridecyl ester
Formula C15H27Cl3O2, MW 344, CAS# 74339-51-8, Entry# 7357
Tridecyl trichloroacetate #



Analysed By: *Checked By:*

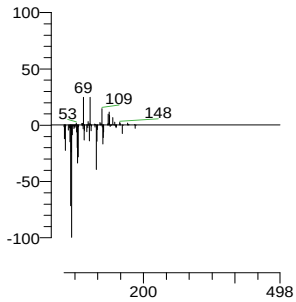
Hit Spectrum



NL: 9.99E2
13841 6.86 1 11
22 816-826 856-866
8.91E7 + c EI Full ms
[50.00-500.00]

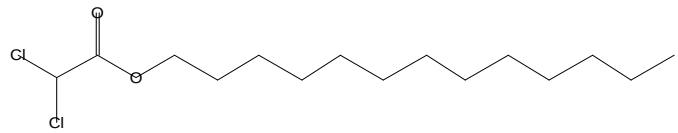
NL: 9.99E2
SI 844, RSI 891,
mainlib, Entry# 7309,
CAS# NA,
Dichloroacetic acid,
tridecyl ester

Delta



Compound Structure

Dichloroacetic acid, tridecyl ester
Formula C15H28Cl2O2, MW 310, CAS# NA, Entry# 7309
Tridecyl dichloroacetate #

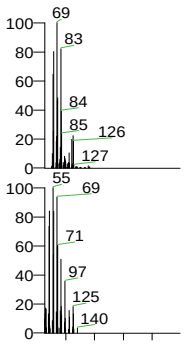


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.86	1-Dodecanol, 3,7,11-trimethyl-	2803781304	1.86	924	6750-34-1	mainlib
6.86	Dichloroacetic acid, decyl ester	2803781304	1.86	894	83005-00-9	mainlib
6.86	3-Eicosene, (E)-	2803781304	1.86	894	74685-33-9	mainlib

Analysed By:

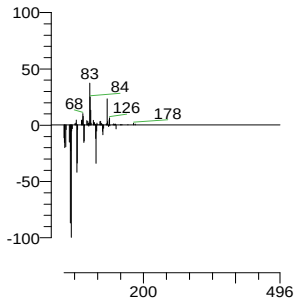
Checked By:

Hit Spectrum	Delta	Compound Structure

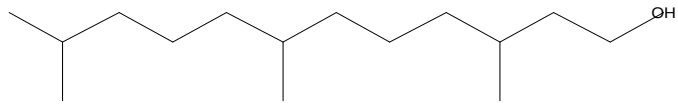


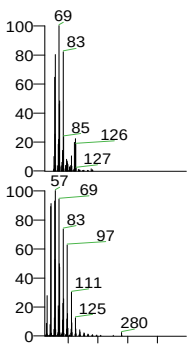
NL: 9.99E2
13868 6.95 1 11 22 843-853 883-893 4.09E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 858, RSI 940, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-



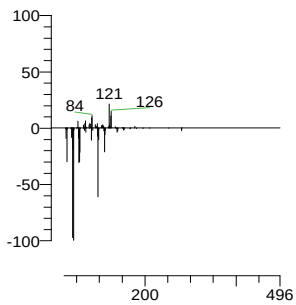
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



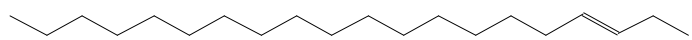


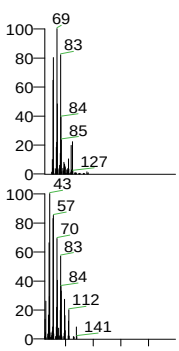
NL: 9.99E2
13868 6.95 1 11 22 843-853 883-893 4.09E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 865, RSI 901, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-



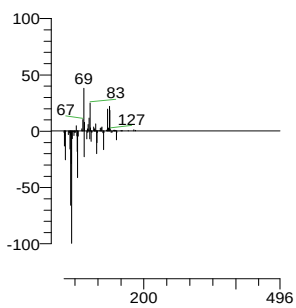
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



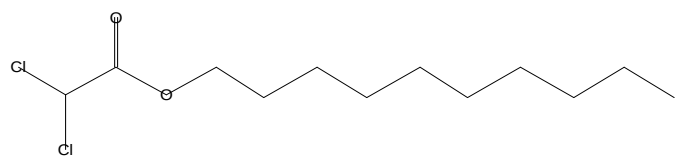


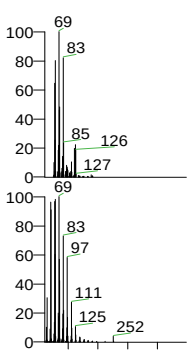
NL: 9.99E2
13868 6.95 1 11 22 843-853 883-893 4.09E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 774, RSI 900, mainlib, Entry# 7338, CAS# 83005-00-9, Dichloroacetic acid, decyl ester



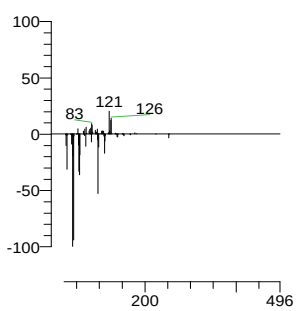
Dichloroacetic acid, decyl ester
Formula C12H22Cl2O2, MW 268, CAS# 83005-00-9, Entry# 7338
Decyl dichloroacetate #



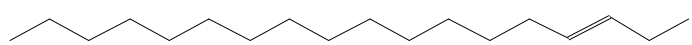


NL: 9.99E2
13868 6.95 1 11 22 843-853 883-893 4.09E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 856, RSI 899, mainlib, Entry# 32223, CAS# 7206-19-1, 3-Octadecene, (E)-

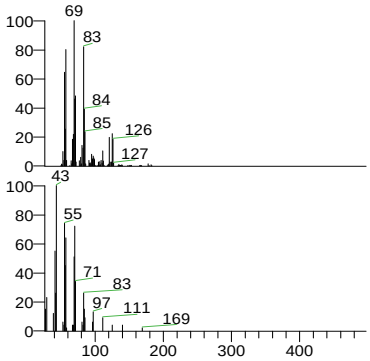


3-Octadecene, (E)-
Formula C18H36, MW 252, CAS# 7206-19-1, Entry# 32223
(3E)-3-Octadecene

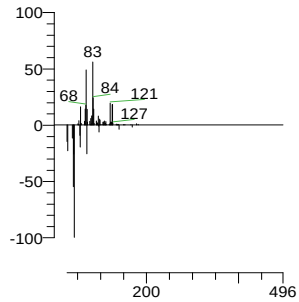


Analysed By: *Checked By:*

Hit Spectrum

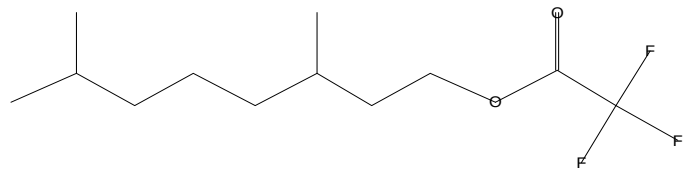


Delta



Compound Structure

Acetic acid, trifluoro-, 3,7-dimethyloctyl ester
Formula C12H21F3O2, MW 254, CAS# 28745-07-5, Entry# 6926
Trifluoroacetyl-3,7-dimethyloctanol

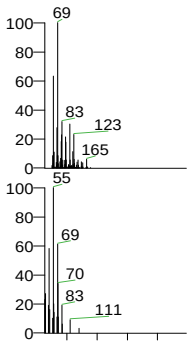


RT	Compound Name	Area	Area %	RSI	Cas #	Library
6.95	1-Dodecanol, 3,7,11-trimethyl-	1095699316	0.73	940	6750-34-1	mainlib
6.95	3-Eicosene, (E)-	1095699316	0.73	901	74685-33-9	mainlib
6.95	Dichloroacetic acid, decyl ester	1095699316	0.73	900	83005-00-9	mainlib

Analysed By:

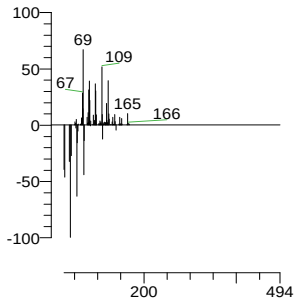
Checked By:

Hit Spectrum	Delta	Compound Structure

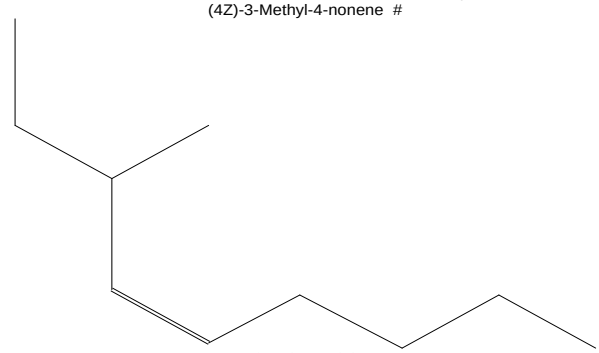


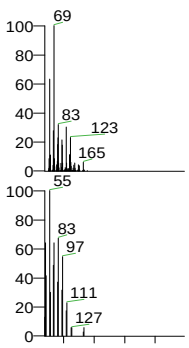
NL: 9.99E2
13958 7.25 1 11
22 933-943 973-983
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 442, RSI 879,
mainlib, Entry# 18798,
CAS# 63830-69-3,
4-Nonene, 3-methyl-,
(Z)-



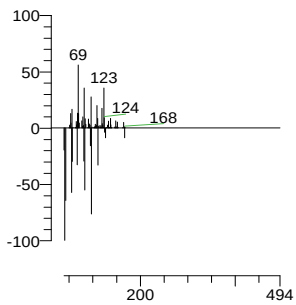
4-Nonene, 3-methyl-, (Z)-
Formula C10H20, MW 140, CAS# 63830-69-3, Entry# 18798
(4Z)-3-Methyl-4-nonene #



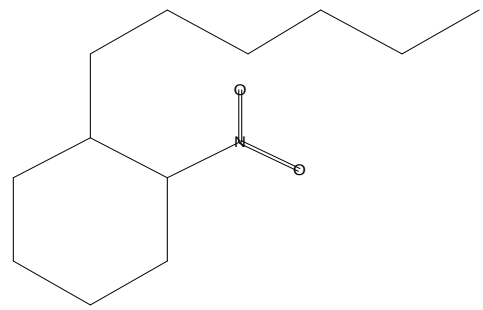


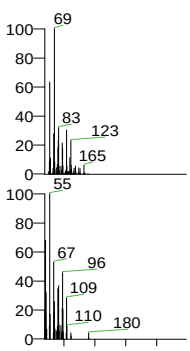
NL: 9.99E2
13958 7.25 1 11
22 933-943 973-983
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 490, RSI 855,
mainlib, Entry# 19313,
CAS# 118252-04-3,
1-Hexyl-2-
nitrocyclohexane



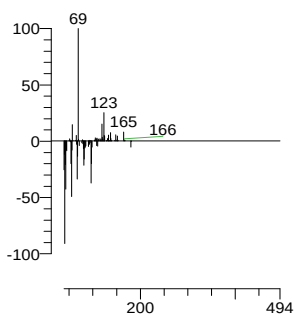
1-Hexyl-2-nitrocyclohexane
Formula C12H23NO2, MW 213, CAS# 118252-04-3, Entry# 19313



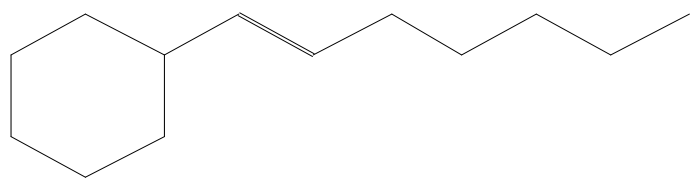


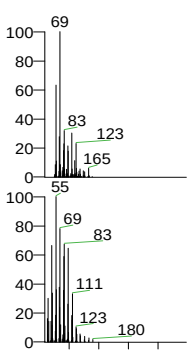
NL: 9.99E2
13958 7.25 1 11
22 933-943 973-983
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 685, RSI 853,
mainlib, Entry# 17941,
CAS# 114614-83-4,
1-Cyclohexylheptene



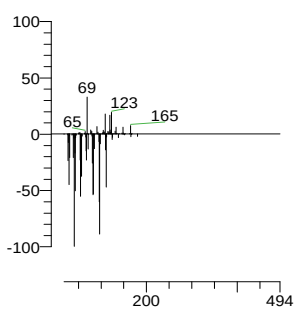
1-Cyclohexylheptene
Formula C13H24, MW 180, CAS# 114614-83-4, Entry# 17941
(1E)-1-Heptenylcyclohexane #



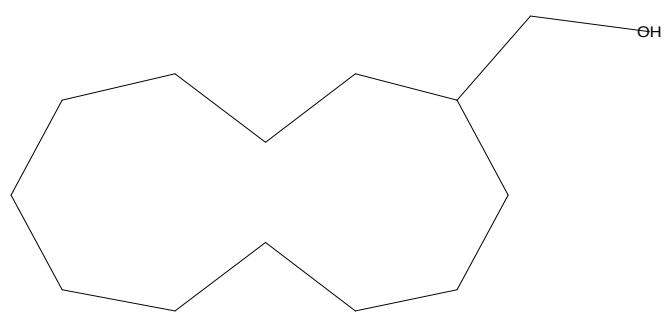


NL: 9.99E2
13958 7.25 1 11
22 933-943 973-983
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 755, RSI 847,
mainlib, Entry# 18944,
CAS# 1892-12-2,
Cyclododecanemethano
l

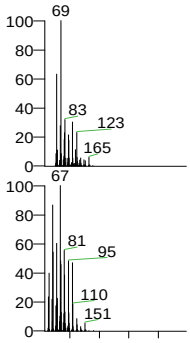


Cyclododecanemethanol
Formula C13H26O, MW 198, CAS# 1892-12-2, Entry# 18944
Cyclododecylmethanol #



Analysed By: *Checked By:*

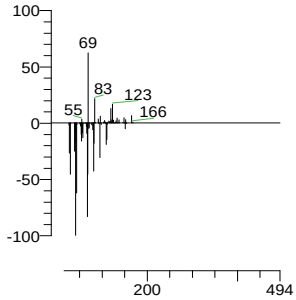
Hit Spectrum



NL: 9.99E2
13958 7.25 1 11
22 933-943 973-983
1.26E8 + c EI Full ms
[50.00-500.00]

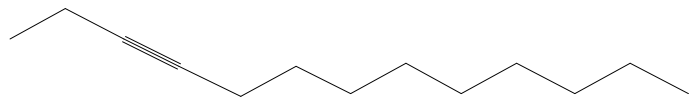
NL: 9.99E2
SI 772, RSI 840,
mainlib, Entry# 29745,
CAS# 60186-78-9,
3-Tridecene

Delta



Compound Structure

3-Tridecene
Formula C13H24, MW 180, CAS# 60186-78-9, Entry# 29745
3-C13H24

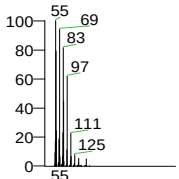


RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.25	4-Nonene, 3-methyl-, (Z)-	3428099098	2.27	879	63830-69-3	mainlib
7.25	1-Hexyl-2-nitrocyclohexane	3428099098	2.27	855	118252-04-3	mainlib
7.25	1-Cyclohexylheptene	3428099098	2.27	853	114614-83-4	mainlib

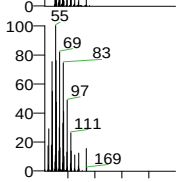
Analysed By:

Checked By:

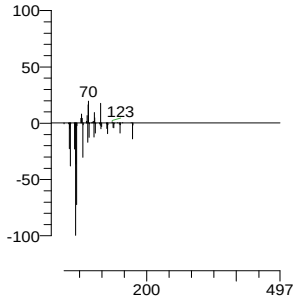
Hit Spectrum	Delta	Compound Structure



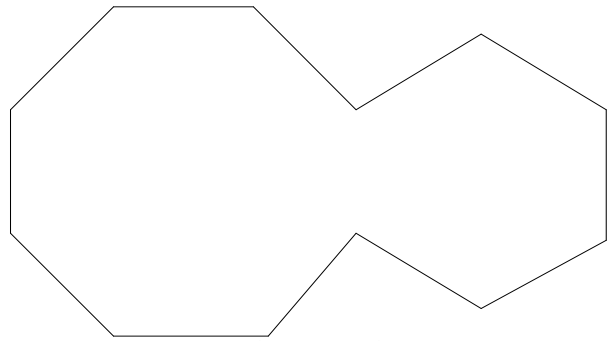
NL: 9.99E2
131126 7.82 1 11
22 1101-1111
1141-1151 1.24E8 + c
EI Full ms [50.00-500.00]

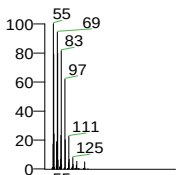


NL: 9.99E2
SI 948, RSI 952, mainlib, Entry# 18863, CAS# 294-62-2, Cyclododecane

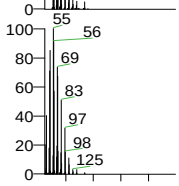


Cyclododecane
Formula C12H24, MW 168, CAS# 294-62-2, Entry# 18863

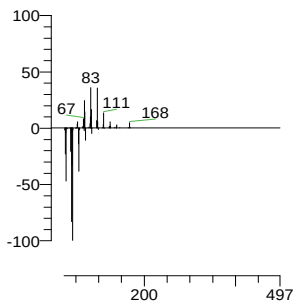




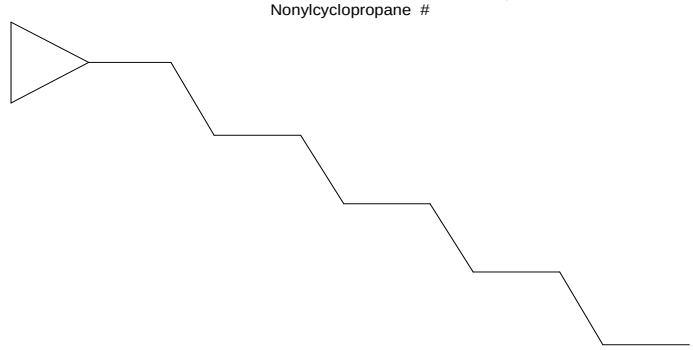
NL: 9.99E2
131126 7.82 1 11
22 1101-1111
1141-1151 1.24E8 + c
EI Full ms [50.00-500.00]

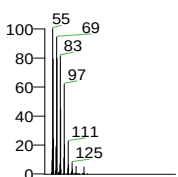


NL: 9.99E2
SI 939, RSI 948, mainlib, Entry# 18566, CAS# 74663-85-7, Cyclopropane, nonyl-

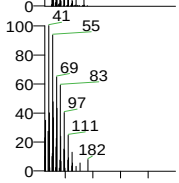


Cyclopropane, nonyl-
Formula C12H24, MW 168, CAS# 74663-85-7, Entry# 18566
Nonylcyclopropane #

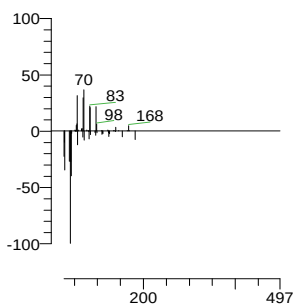




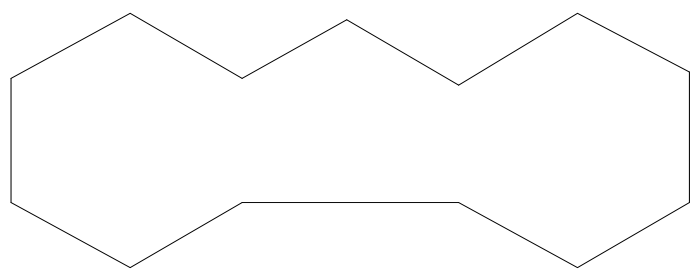
NL: 9.99E2
131126 7.82 1 11
22 1101-1111
1141-1151 1.24E8 + c
EI Full ms [50.00-500.00]

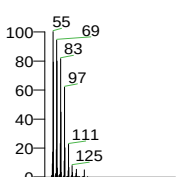


NL: 9.99E2
SI 917, RSI 944, mainlib, Entry# 2642, CAS# 295-02-3, Cyclotridecane

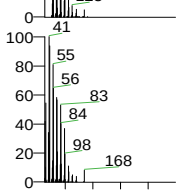


Cyclotridecane
Formula C13H26, MW 182, CAS# 295-02-3, Entry# 2642

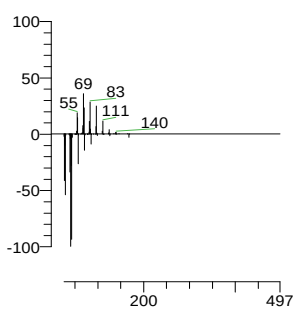




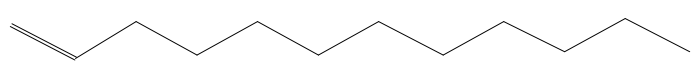
NL: 9.99E2
131126 7.82 1 11
22 1101-1111
1141-1151 1.24E8 + c
EI Full ms [50.00-500.00]



NL: 9.99E2
SI 939, RSI 943, mainlib, Entry# 2237, CAS# 112-41-4, 1-Dodecene

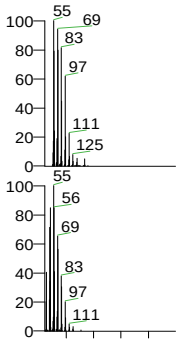


1-Dodecene
Formula C12H24, MW 168, CAS# 112-41-4, Entry# 2237
à-Dodecene

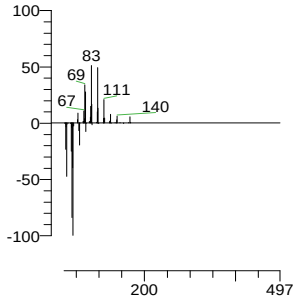


Analysed By: *Checked By:*

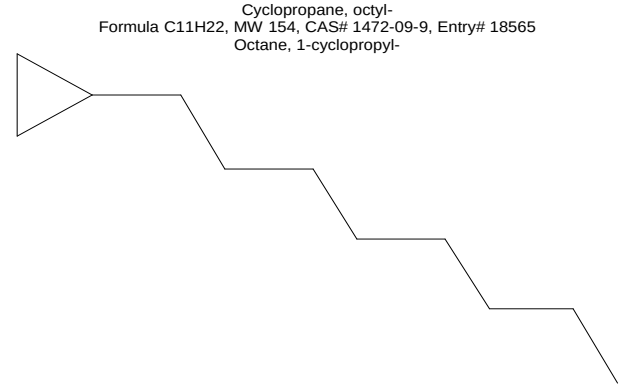
Hit Spectrum



Delta



Compound Structure

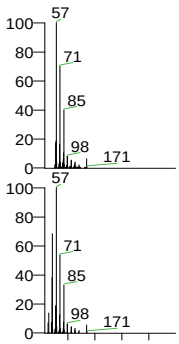


RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.82	Cyclododecane	4637415639	3.08	952	294-62-2	mainlib
7.82	Cyclopropane, nonyl-	4637415639	3.08	948	74663-85-7	mainlib
7.82	Cyclotridecane	4637415639	3.08	944	295-02-3	mainlib

Analysed By:

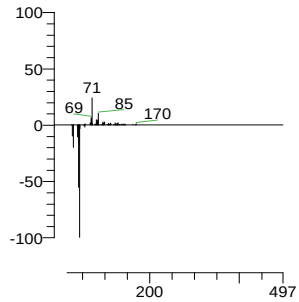
Checked By:

Hit Spectrum	Delta	Compound Structure

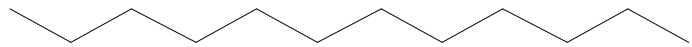


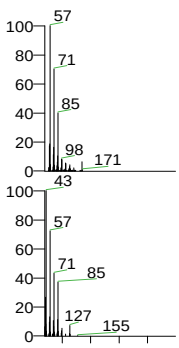
NL: 9.99E2
131156 7.92 1 11
22 1131-1141
1171-1181 2.64E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 929, RSI 984, mainlib, Entry# 22550, CAS# 112-40-3, Dodecane



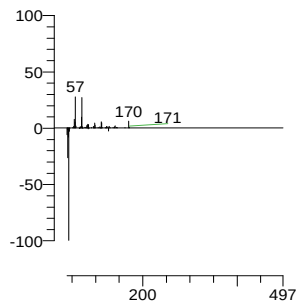
Dodecane
Formula C12H26, MW 170, CAS# 112-40-3, Entry# 22550
n-Dodecane



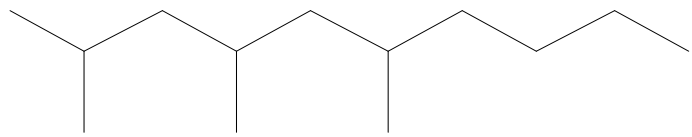


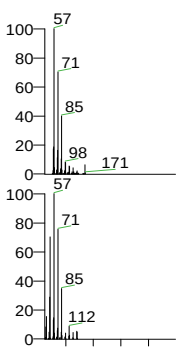
NL: 9.99E2
131156 7.92 1 11
22 1131-1141
1171-1181 2.64E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 816, RSI 970, mainlib, Entry# 7452, CAS# 62108-27-4, Decane, 2,4,6-trimethyl-



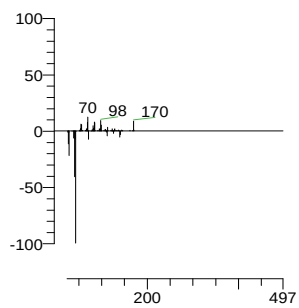
Decane, 2,4,6-trimethyl-
Formula C13H28, MW 184, CAS# 62108-27-4, Entry# 7452
2,4,6-Trimethyldecane #



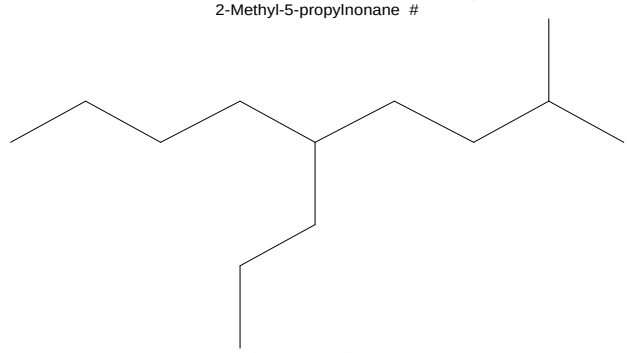


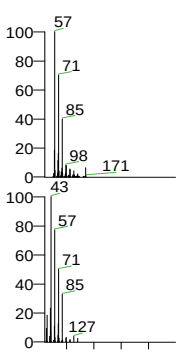
NL: 9.99E2
131156 7.92 1 11
22 1131-1141
1171-1181 2.64E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 857, RSI 959, mainlib, Entry# 23616, CAS# 31081-17-1, Nonane, 2-methyl-5-propyl-



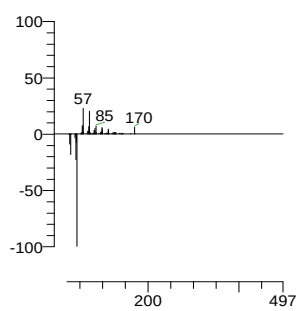
Nonane, 2-methyl-5-propyl-
Formula C13H28, MW 184, CAS# 31081-17-1, Entry# 23616
2-Methyl-5-propylnonane #



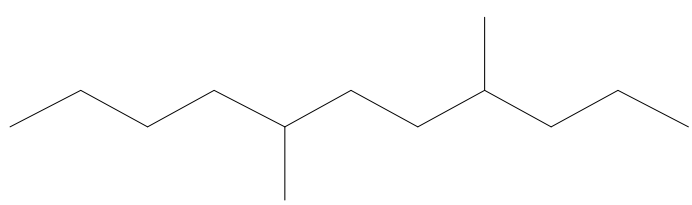


NL: 9.99E2
131156 7.92 1 11
22 1131-1141
1171-1181 2.64E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 832, RSI 959, mainlib, Entry# 7443, CAS# 17301-32-5, Undecane, 4,7-dimethyl-

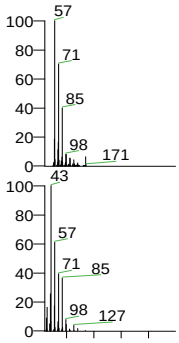


Undecane, 4,7-dimethyl-
Formula C13H28, MW 184, CAS# 17301-32-5, Entry# 7443
4,7-Dimethylundecane #

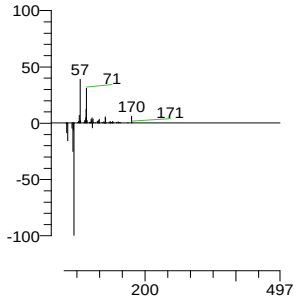


Analysed By: *Checked By:*

Hit Spectrum

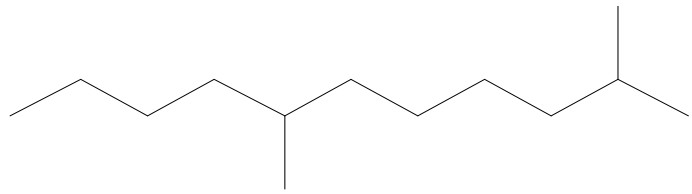


Delta



Compound Structure

Undecane, 2,7-dimethyl-
Formula C13H28, MW 184, CAS# 17301-24-5, Entry# 7484
2,7-Dimethylundecane #

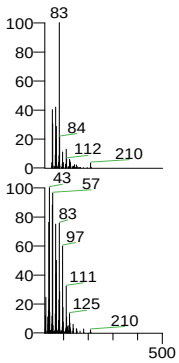


RT	Compound Name	Area	Area %	RSI	Cas #	Library
7.92	Dodecane	4148834202	2.75	984	112-40-3	mainlib
7.92	Decane, 2,4,6-trimethyl-	4148834202	2.75	970	62108-27-4	mainlib
7.92	Nonane, 2-methyl-5-propyl-	4148834202	2.75	959	31081-17-1	mainlib

Analysed By:

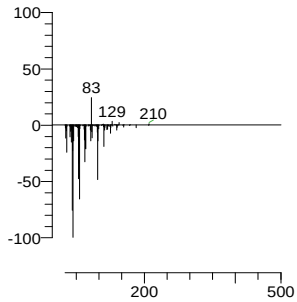
Checked By:

Hit Spectrum	Delta	Compound Structure

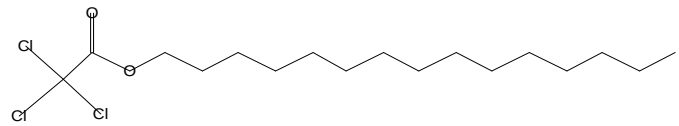


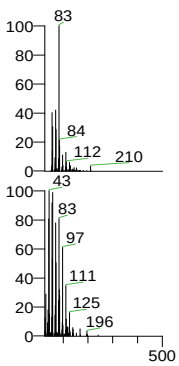
NL: 9.99E2
131478 9.02 1 11 22 1453-1463 1493-1503 1.48E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 876, RSI 904, mainlib, Entry# 7360, CAS# 74339-53-0, Trichloroacetic acid, pentadecyl ester



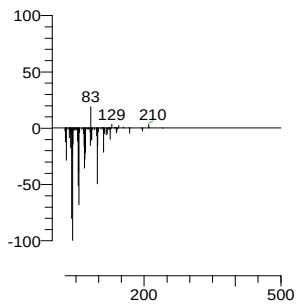
Trichloroacetic acid, pentadecyl ester
Formula C17H31Cl3O2, MW 372, CAS# 74339-53-0, Entry# 7360
Pentadecyl trichloroacetate #



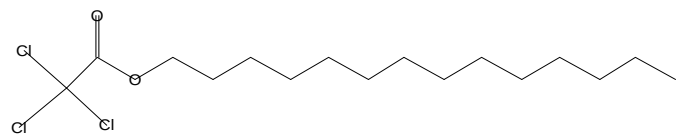


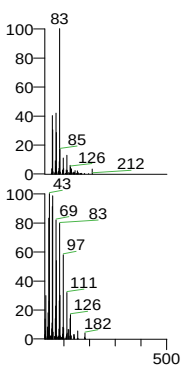
NL: 9.99E2
131478 9.02 1 11 22 1453-1463 1493-1503 1.48E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 861, RSI 901, mainlib, Entry# 7359, CAS# 74339-52-9, Trichloroacetic acid, tetradecyl ester



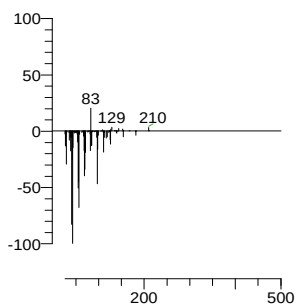
Trichloroacetic acid, tetradecyl ester
Formula C16H29Cl3O2, MW 358, CAS# 74339-52-9, Entry# 7359
Tetradecyl trichloroacetate #



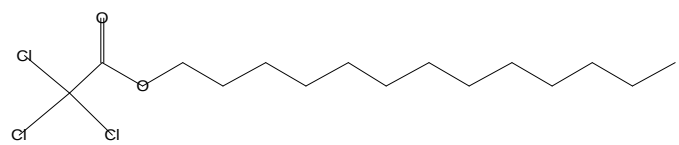


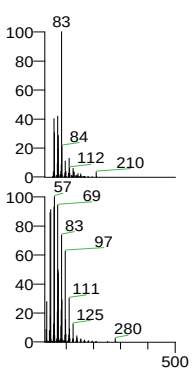
NL: 9.99E2
131478 9.02 1 11 22 1453-1463 1493-1503 1.48E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 860, RSI 899, mainlib, Entry# 7357, CAS# 74339-51-8, Trichloroacetic acid, tridecyl ester



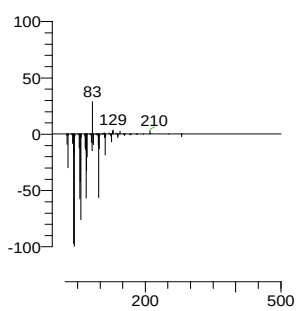
Trichloroacetic acid, tridecyl ester
Formula C15H27Cl3O2, MW 344, CAS# 74339-51-8, Entry# 7357
Tridecyl trichloroacetate #



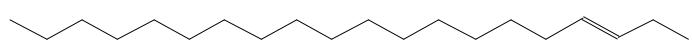


NL: 9.99E2
131478 9.02 1 11 22 1453-1463 1493-1503 1.48E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 865, RSI 898, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-

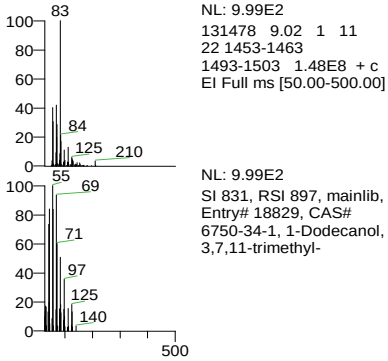


3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



Analysed By: *Checked By:*

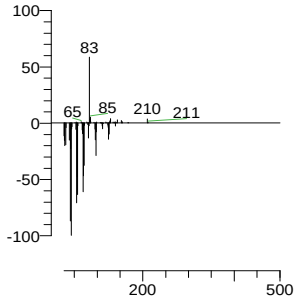
Hit Spectrum



NL: 9.99E2
131478 9.02 1 11
22 1453-1463
1493-1503 1.48E8 + c
EI Full ms [50.00-500.00]

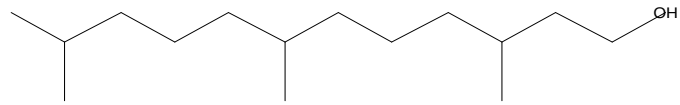
NL: 9.99E2
SI 831, RSI 897, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-

Delta



Compound Structure

1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol

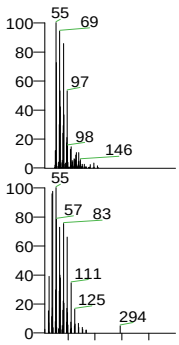


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.02	Trichloroacetic acid, pentadecyl ester	2563756349	1.70	904	74339-53-0	mainlib
9.02	Trichloroacetic acid, tetradecyl ester	2563756349	1.70	901	74339-52-9	mainlib
9.02	Trichloroacetic acid, tridecyl ester	2563756349	1.70	899	74339-51-8	mainlib

Analysed By:

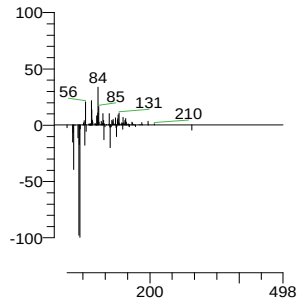
Checked By:

Hit Spectrum	Delta	Compound Structure

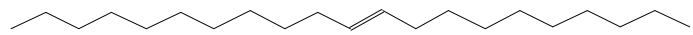


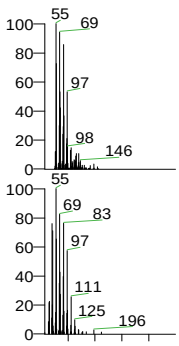
NL: 9.99E2
131519 9.16 1 11
22 1494-1504
1534-1544 6.69E7 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 849, RSI 953, mainlib, Entry# 18363, CAS# 95008-11-0, 10-Heneicosene (c,t)



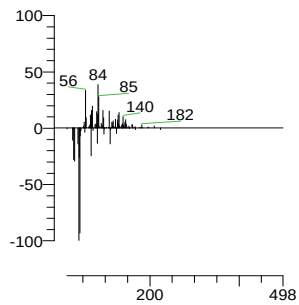
10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



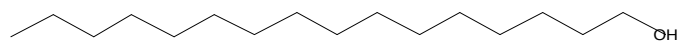


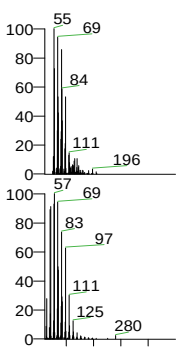
NL: 9.99E2
131519 9.16 1 11
22 1494-1504
1534-1544 6.69E7 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 860, RSI 947, mainlib, Entry# 18939, CAS# 36653-82-4, 1-Hexadecanol



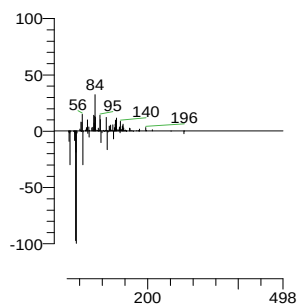
1-Hexadecanol
Formula C16H34O, MW 242, CAS# 36653-82-4, Entry# 18939
n-Cetyl alcohol



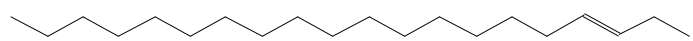


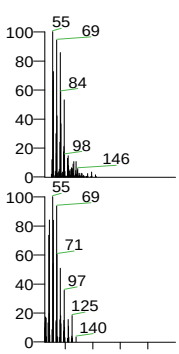
NL: 9.99E2
131519 9.16 1 11
22 1494-1504
1534-1544 6.69E7 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 878, RSI 946, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-



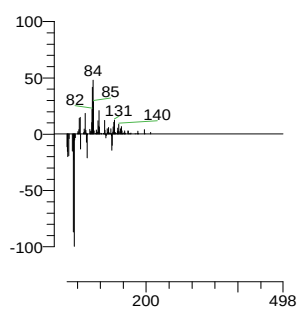
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



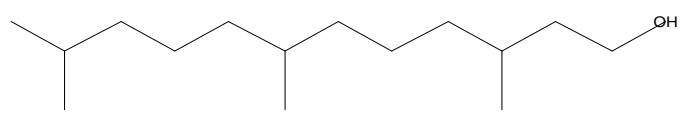


NL: 9.99E2
131519 9.16 1 11
22 1494-1504
1534-1544 6.69E7 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 821, RSI 946, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-

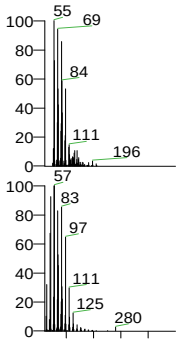


1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



Analysed By: *Checked By:*

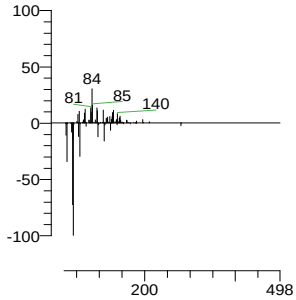
Hit Spectrum



NL: 9.99E2
131519 9.16 1 11
22 1494-1504
1534-1544 6.69E7 + c
EI Full ms [50.00-500.00]

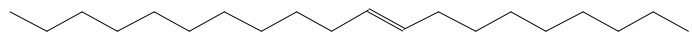
NL: 9.99E2
SI 875, RSI 944, mainlib, Entry# 23002, CAS# 74685-29-3, 9-Eicosene, (E)-

Delta



Compound Structure

9-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-29-3, Entry# 23002
(9E)-9-Icosene #

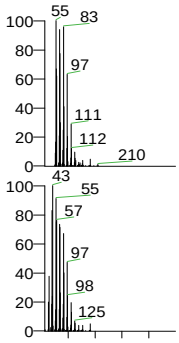


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.16	10-Heneicosene (c,t)	2065147344	1.37	953	95008-11-0	mainlib
9.16	1-Hexadecanol	2065147344	1.37	947	36653-82-4	mainlib
9.16	3-Eicosene, (E)-	2065147344	1.37	946	74685-33-9	mainlib

Analysed By:

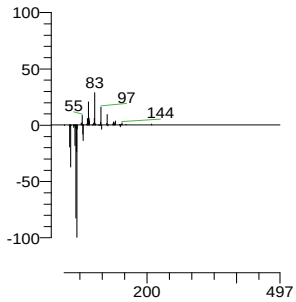
Checked By:

Hit Spectrum	Delta	Compound Structure

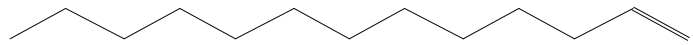


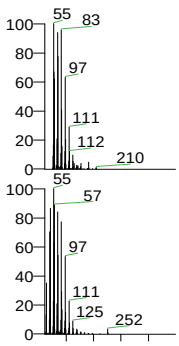
NL: 9.99E2
131550 9.25 1 11
22 1525-1535
1565-1575 1.30E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 962, RSI 974, mainlib,
Entry# 6779, CAS#
2437-56-1, 1-Tridecene



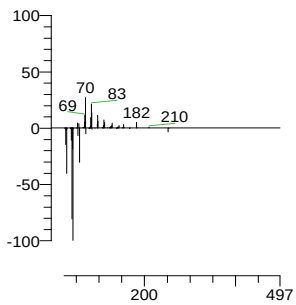
1-Tridecene
Formula C13H26, MW 182, CAS# 2437-56-1, Entry# 6779
n-Tridec-1-ene



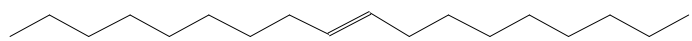


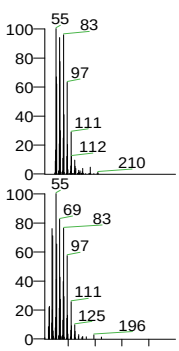
NL: 9.99E2
131550 9.25 1 11
22 1525-1535
1565-1575 1.30E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 951, RSI 968, mainlib,
Entry# 18644, CAS#
7206-25-9,
9-Octadecene, (E)-



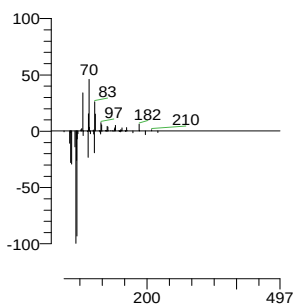
9-Octadecene, (E)-
Formula C18H36, MW 252, CAS# 7206-25-9, Entry# 18644
(9E)-9-Octadecene



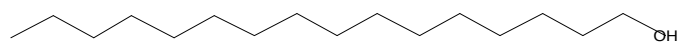


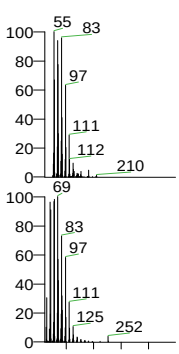
NL: 9.99E2
131550 9.25 1 11
22 1525-1535
1565-1575 1.30E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 931, RSI 968, mainlib,
Entry# 18939, CAS#
36653-82-4,
1-Hexadecanol



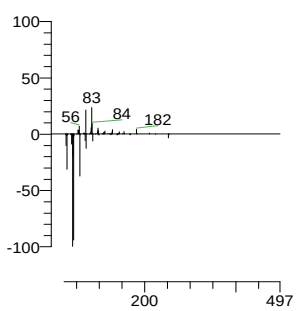
1-Hexadecanol
Formula C16H34O, MW 242, CAS# 36653-82-4, Entry# 18939
n-Cetyl alcohol



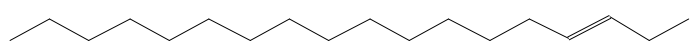


NL: 9.99E2
131550 9.25 1 11
22 1525-1535
1565-1575 1.30E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 951, RSI 967, mainlib,
Entry# 32223, CAS#
7206-19-1,
3-Octadecene, (E)-

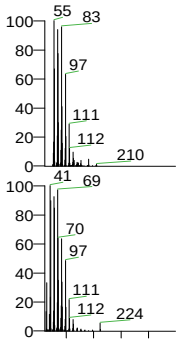


3-Octadecene, (E)-
Formula C18H36, MW 252, CAS# 7206-19-1, Entry# 32223
(3E)-3-Octadecene



Analysed By: *Checked By:*

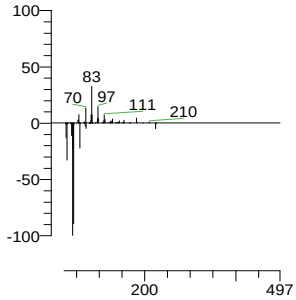
Hit Spectrum



NL: 9.99E2
131550 9.25 1 11
22 1525-1535
1565-1575 1.30E8 + c
EI Full ms [50.00-500.00]

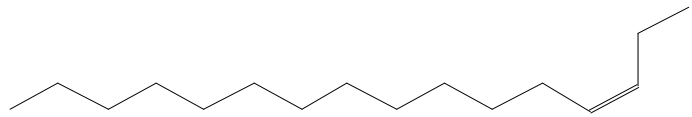
NL: 9.99E2
SI 949, RSI 966, mainlib,
Entry# 3165, CAS#
34303-81-6,
3-Hexadecene, (Z)-

Delta



Compound Structure

3-Hexadecene, (Z)-
Formula C16H32, MW 224, CAS# 34303-81-6, Entry# 3165
(3Z)-3-Hexadecene

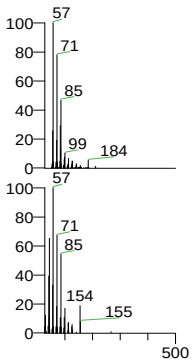


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.25	1-Tridecene	4024324226	2.67	974	2437-56-1	mainlib
9.25	1-Hexadecanol	4024324226	2.67	968	36653-82-4	mainlib
9.25	9-Octadecene, (E)-	4024324226	2.67	968	7206-25-9	mainlib

Analysed By:

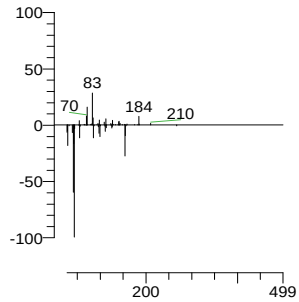
Checked By:

Hit Spectrum	Delta	Compound Structure

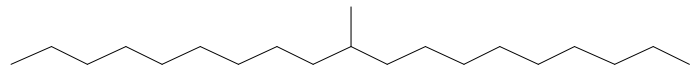


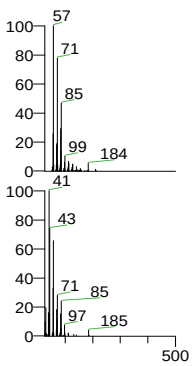
NL: 9.99E2
131579 9.37 1 11
22 1554-1564
1594-1604 2.20E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 895, RSI 936, mainlib, Entry# 23599, CAS# 56862-62-5, 10-Methylnonadecane



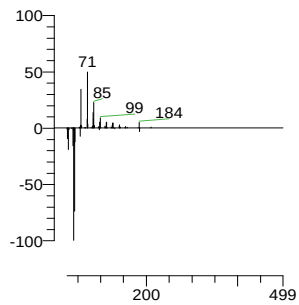
10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



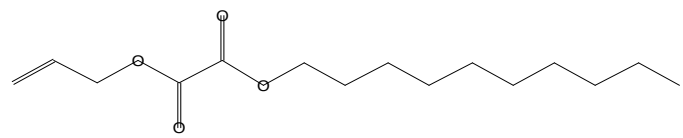


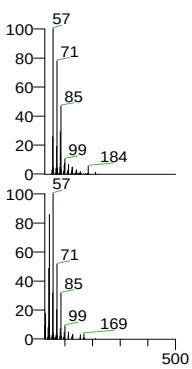
NL: 9.99E2
131579 9.37 1 11
22 1554-1564
1594-1604 2.20E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 855, RSI 935, mainlib, Entry# 2293, CAS# NA, Oxalic acid, allyl decyl ester



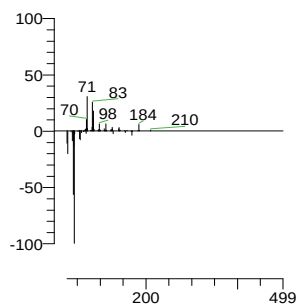
Oxalic acid, allyl decyl ester
Formula C15H26O4, MW 270, CAS# NA, Entry# 2293



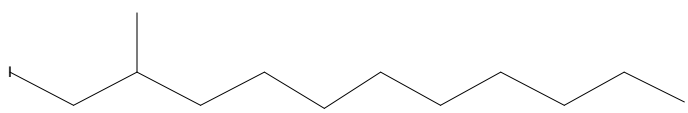


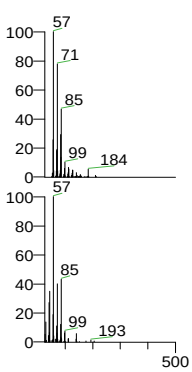
NL: 9.99E2
131579 9.37 1 11
22 1554-1564
1594-1604 2.20E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 888, RSI 933, mainlib, Entry# 22546, CAS# 73105-67-6, 1-Iodo-2-methylundecane



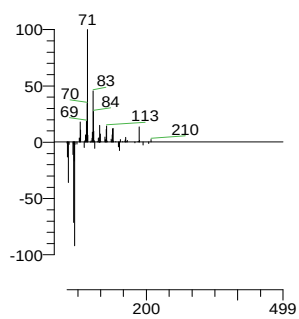
1-Iodo-2-methylundecane
Formula C12H25I, MW 296, CAS# 73105-67-6, Entry# 22546



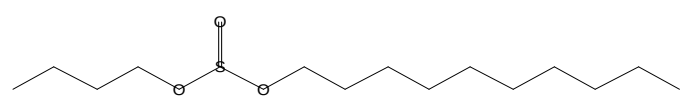


NL: 9.99E2
131579 9.37 1 11
22 1554-1564
1594-1604 2.20E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 858, RSI 932, mainlib, Entry# 23989, CAS# NA, Sulfurous acid, butyl decyl ester

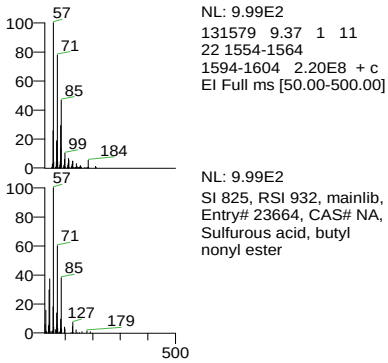


Sulfurous acid, butyl decyl ester
Formula C14H30O3S, MW 278, CAS# NA, Entry# 23989

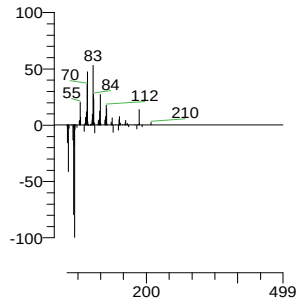


Analysed By: *Checked By:*

Hit Spectrum

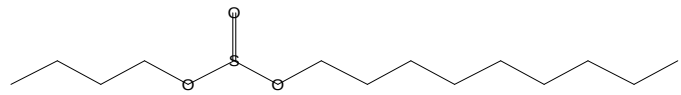


Delta



Compound Structure

Sulfurous acid, butyl nonyl ester
Formula C13H28O3S, MW 264, CAS# NA, Entry# 23664

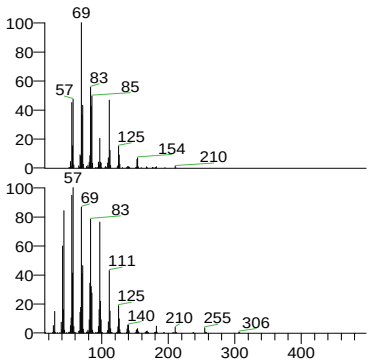


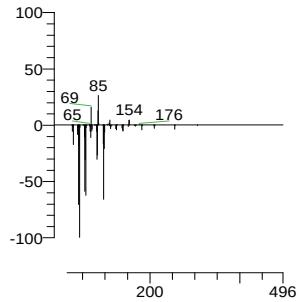
RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.37	10-Methylnonadecane	2800125743	1.86	936	56862-62-5	mainlib
9.37	Oxalic acid, allyl decyl ester	2800125743	1.86	935	NA	mainlib
9.37	1-Iodo-2-methylundecane	2800125743	1.86	933	73105-67-6	mainlib

Analysed By:

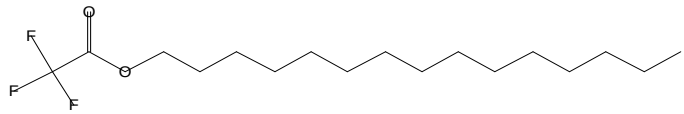
Checked By:

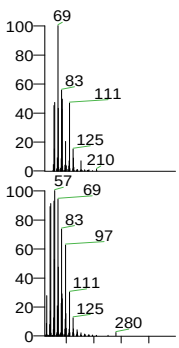
Hit Spectrum	Delta	Compound Structure





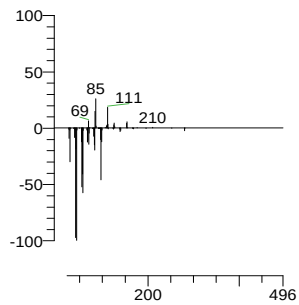
Trifluoroacetic acid, pentadecyl ester
Formula C17H31F3O2, MW 324, CAS# 959010-23-2, Entry# 23039



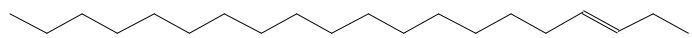


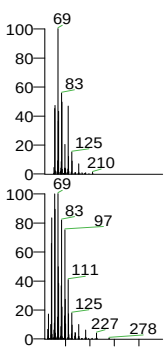
NL: 9.99E2
131609 9.48 1 11 22 1584-1594 1624-1634 2.20E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 895, RSI 900, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-



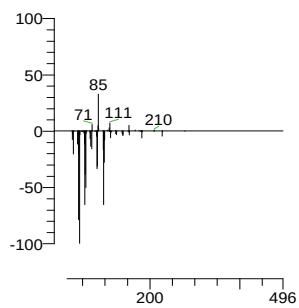
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



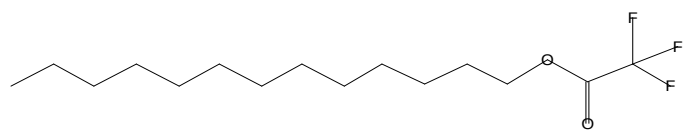


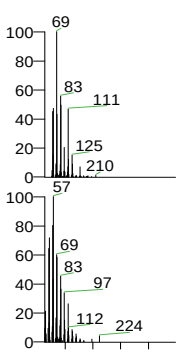
NL: 9.99E2
131609 9.48 1 11 22 1584-1594 1624-1634 2.20E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 892, RSI 899, mainlib, Entry# 32079, CAS# 53800-02-5, Trifluoroacetic acid,n-tridecyl ester



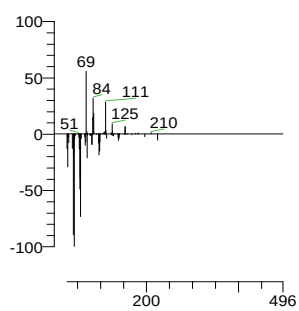
Trifluoroacetic acid,n-tridecyl ester
Formula C15H27F3O2, MW 296, CAS# 53800-02-5, Entry# 32079
Tridecyl trifluoroacetate #



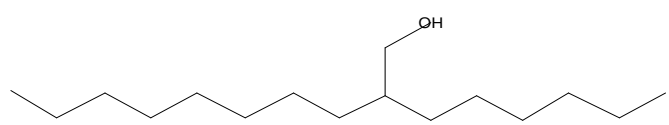


NL: 9.99E2
131609 9.48 1 11 22 1584-1594 1624-1634 2.20E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 887, RSI 897, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-

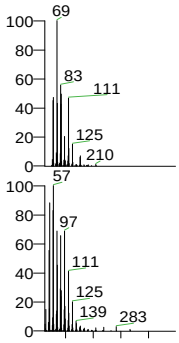


1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol



Analysed By: *Checked By:*

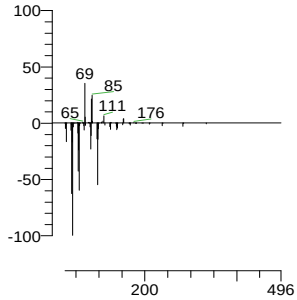
Hit Spectrum



NL: 9.99E2
131609 9.48 1 11
22 1584-1594
1624-1634 2.20E8 + c
EI Full ms [50.00-500.00]

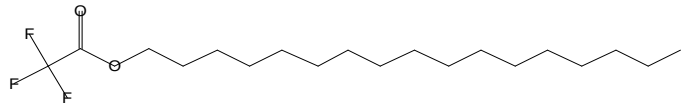
NL: 9.99E2
SI 887, RSI 893, mainlib, Entry# 22444, CAS# NA, Heptadecyl trifluoroacetate

Delta



Compound Structure

Heptadecyl trifluoroacetate
Formula C19H35F3O2, MW 352, CAS# NA, Entry# 22444
Heptadecyl 2,2,2-trifluoroacetate

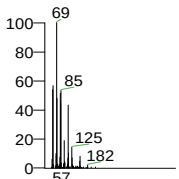


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.48	Trifluoroacetic acid, pentadecyl ester	5996302173	3.98	902	959010-23-2	mainlib
9.48	3-Eicosene, (E)-	5996302173	3.98	900	74685-33-9	mainlib
9.48	Trifluoroacetic acid,n-tridecyl ester	5996302173	3.98	899	53800-02-5	mainlib

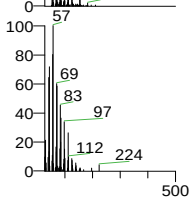
Analysed By:

Checked By:

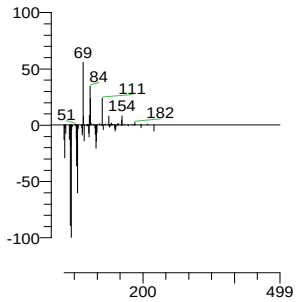
Hit Spectrum	Delta	Compound Structure



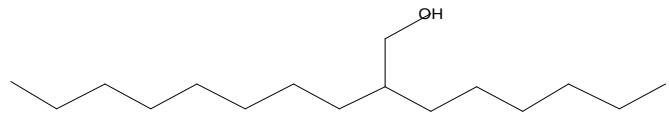
NL: 9.99E2
131644 9.58 1 11
22 1619-1629
1659-1669 1.66E8 + c
EI Full ms [50.00-500.00]

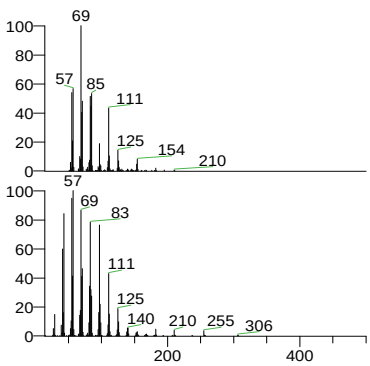


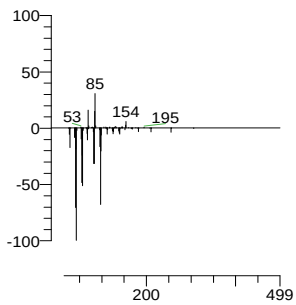
NL: 9.99E2
SI 896, RSI 916, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-



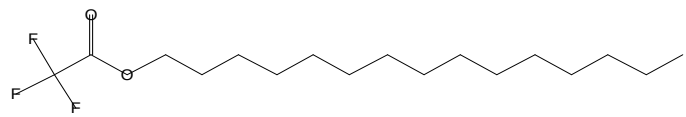
1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol

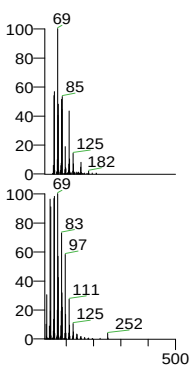






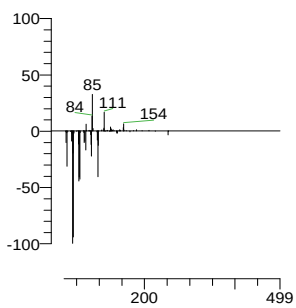
Trifluoroacetic acid, pentadecyl ester
Formula C17H31F3O2, MW 324, CAS# 959010-23-2, Entry# 23039



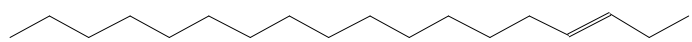


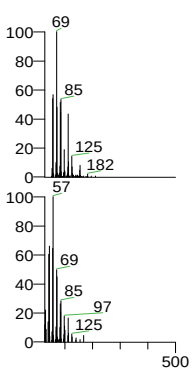
NL: 9.99E2
131644 9.58 1 11
22 1619-1629
1659-1669 1.66E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 887, RSI 905, mainlib, Entry# 32223, CAS# 7206-19-1, 3-Octadecene, (E)-



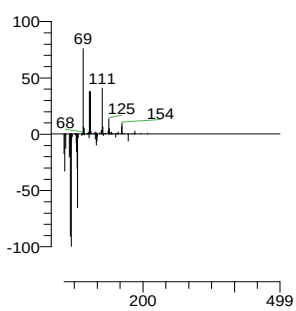
3-Octadecene, (E)-
Formula C18H36, MW 252, CAS# 7206-19-1, Entry# 32223
(3E)-3-Octadecene



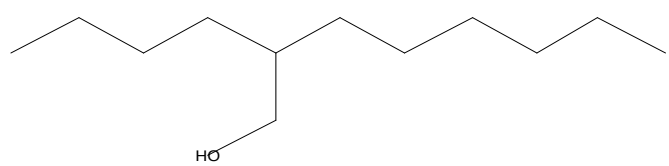


NL: 9.99E2
131644 9.58 1 11
22 1619-1629
1659-1669 1.66E8 + c
EI Full ms [50.00-500.00]

NL: 9.99E2
SI 863, RSI 901, mainlib, Entry# 22453, CAS# 3913-02-8, 1-Octanol, 2-butyl-

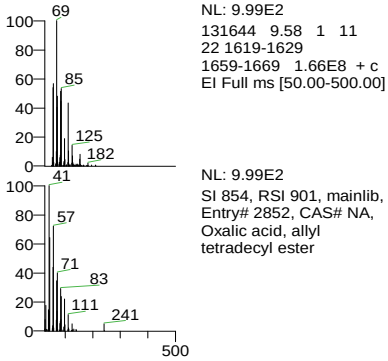


1-Octanol, 2-butyl-
Formula C12H26O, MW 186, CAS# 3913-02-8, Entry# 22453
2-Butyl-1-octanol

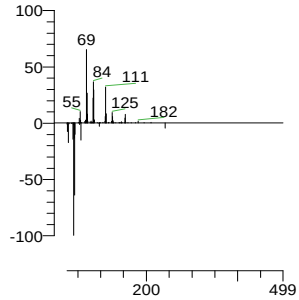


Analysed By: *Checked By:*

Hit Spectrum

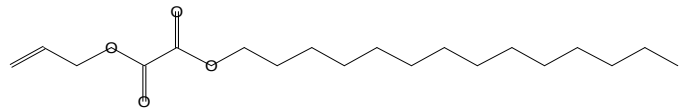


Delta



Compound Structure

Oxalic acid, allyl tetradecyl ester
Formula C19H34O4, MW 326, CAS# NA, Entry# 2852

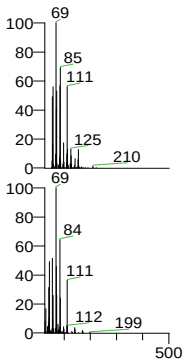


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.58	1-Decanol, 2-hexyl-	3420962043	2.27	916	2425-77-6	mainlib
9.58	Trifluoroacetic acid, pentadecyl ester	3420962043	2.27	908	959010-23-2	mainlib
9.58	3-Octadecene, (E)-	3420962043	2.27	905	7206-19-1	mainlib

Analysed By:

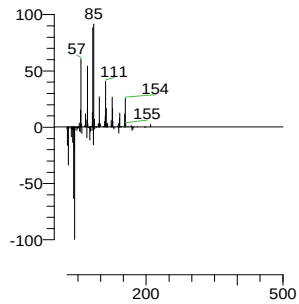
Checked By:

Hit Spectrum	Delta	Compound Structure

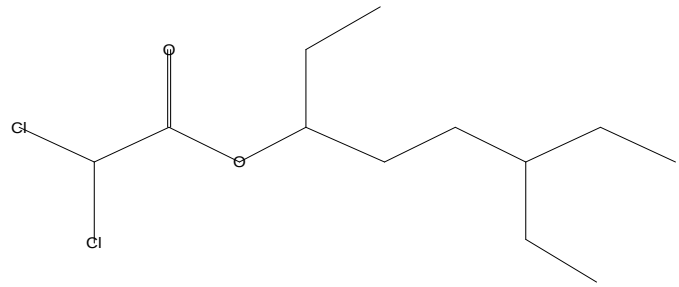


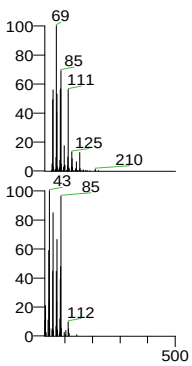
NL: 9.99E2
131678 9.71 1 11 22 1653-1663 1693-1703 1.56E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 818, RSI 882, mainlib, Entry# 32562, CAS# NA, Dichloroacetic acid, 6-ethyl-3-octyl ester



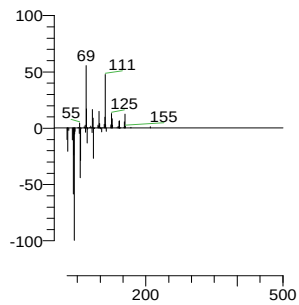
Dichloroacetic acid, 6-ethyl-3-octyl ester
Formula C12H22Cl2O2, MW 268, CAS# NA, Entry# 32562
1,4-Diethylhexyl dichloroacetate #



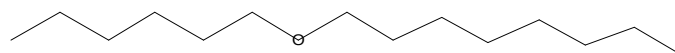


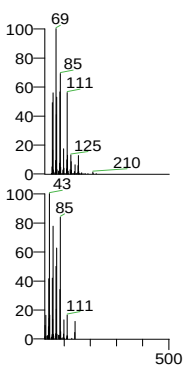
NL: 9.99E2
131678 9.71 1 11 22 1653-1663 1693-1703 1.56E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 758, RSI 878, mainlib, Entry# 9315, CAS# 17071-54-4, Hexyl octyl ether



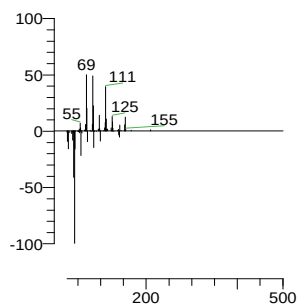
Hexyl octyl ether
Formula C14H30O, MW 214, CAS# 17071-54-4, Entry# 9315
1-(Hexyloxy)octane #



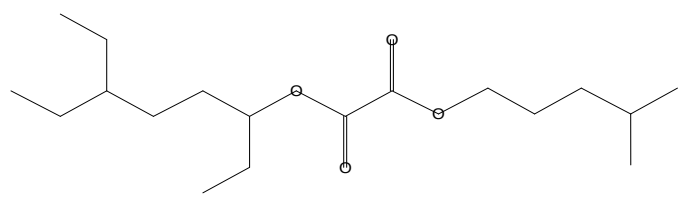


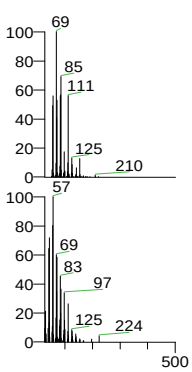
NL: 9.99E2
131678 9.71 1 11 22 1653-1663 1693-1703 1.56E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 798, RSI 873, mainlib, Entry# 9293, CAS# NA, Oxalic acid, 6-ethyloct-3-yl isohexyl ester



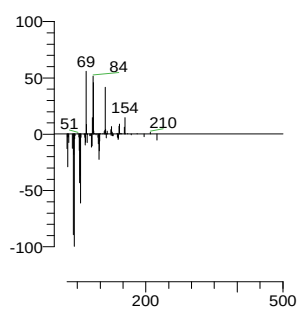
Oxalic acid, 6-ethyloct-3-yl isohexyl ester
Formula C18H34O4, MW 314, CAS# NA, Entry# 9293



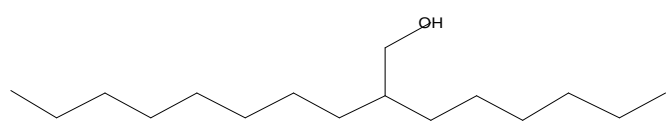


NL: 9.99E2
131678 9.71 1 11 22 1653-1663 1693-1703 1.56E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 850, RSI 870, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-

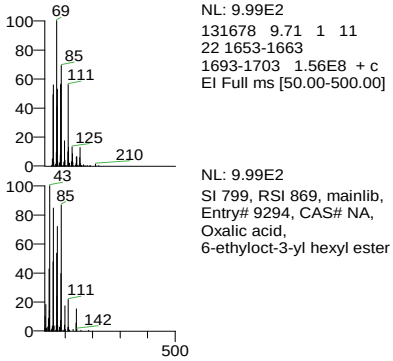


1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol

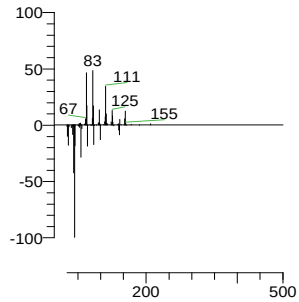


Analysed By: *Checked By:*

Hit Spectrum

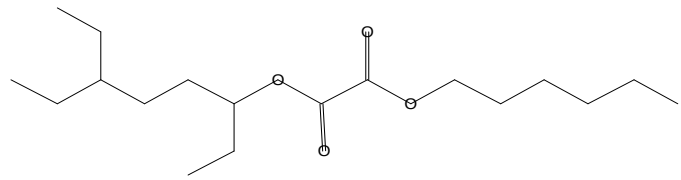


Delta



Compound Structure

Oxalic acid, 6-ethyloct-3-yl hexyl ester
Formula C18H34O4, MW 314, CAS# NA, Entry# 9294

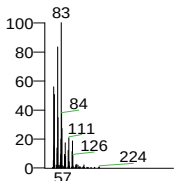


RT	Compound Name	Area	Area %	RSI	Cas #	Library
9.71	Dichloroacetic acid, 6-ethyl-3-octyl ester	5837778482	3.87	882	NA	mainlib
9.71	Hexyl octyl ether	5837778482	3.87	878	17071-54-4	mainlib
9.71	Oxalic acid, 6-ethyloct-3-yl isohexyl ester	5837778482	3.87	873	NA	mainlib

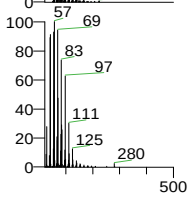
Analysed By:

Checked By:

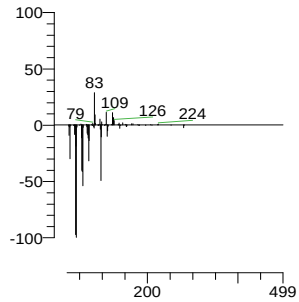
Hit Spectrum	Delta	Compound Structure



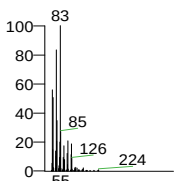
NL: 9.99E2
131774 10.03 1 11
22 1749-1759 1789-1799
1.50E8 + c EI Full ms
[50.00-500.00]



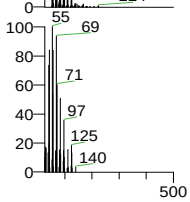
NL: 9.99E2
SI 889, RSI 909, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-



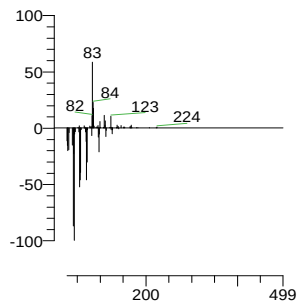
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



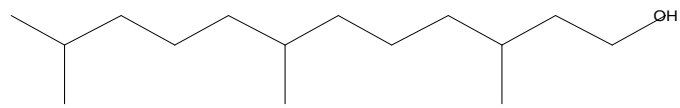
NL: 9.99E2
131774 10.03 1 11
22 1749-1759 1789-1799
1.50E8 + c EI Full ms
[50.00-500.00]

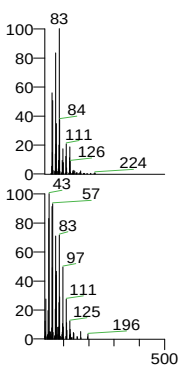


NL: 9.99E2
SI 853, RSI 906, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-



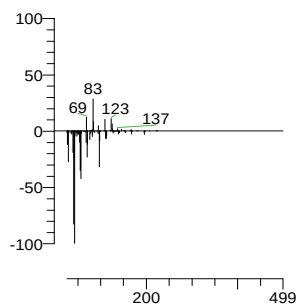
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



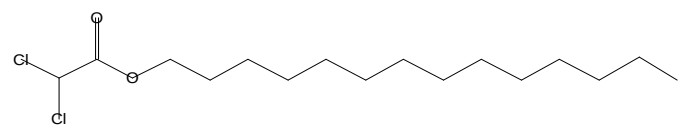


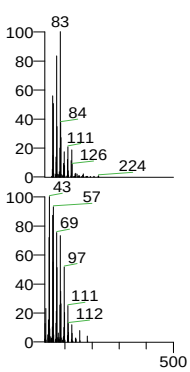
NL: 9.99E2
131774 10.03 1 11
22 1749-1759 1789-1799
1.50E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 856, RSI 900, mainlib, Entry# 7343, CAS# 83005-02-1, Dichloroacetic acid, tetradecyl ester



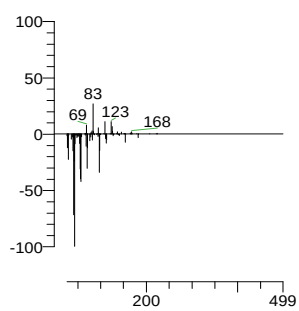
Dichloroacetic acid, tetradecyl ester
Formula C16H30Cl2O2, MW 324, CAS# 83005-02-1, Entry# 7343
Tetradecyl dichloroacetate #



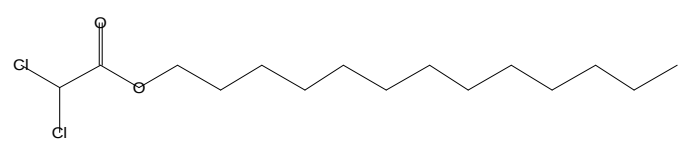


NL: 9.99E2
131774 10.03 1 11
22 1749-1759 1789-1799
1.50E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 852, RSI 900, mainlib, Entry# 7309, CAS# NA, Dichloroacetic acid, tridecyl ester

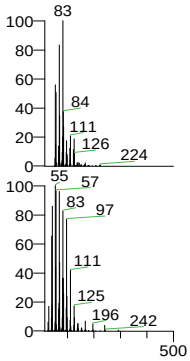


Dichloroacetic acid, tridecyl ester
Formula C15H28Cl2O2, MW 310, CAS# NA, Entry# 7309
Tridecyl dichloroacetate #



Analysed By: *Checked By:*

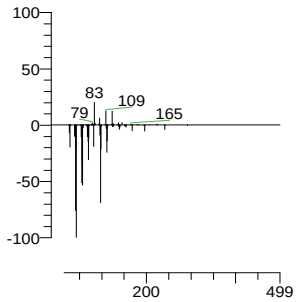
Hit Spectrum



NL: 9.99E2
131774 10.03 1 11 22 1749-1759 1789-1799 1.50E8 + c EI Full ms [50.00-500.00]

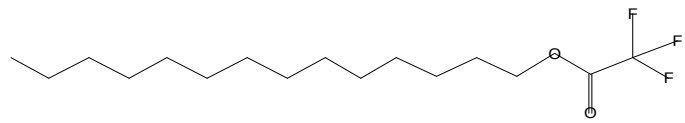
NL: 9.99E2
SI 882, RSI 899, mainlib, Entry# 18657, CAS# 6222-02-2, Tetradecyl trifluoroacetate

Delta



Compound Structure

Tetradecyl trifluoroacetate
Formula C16H29F3O2, MW 310, CAS# 6222-02-2, Entry# 18657
Tetradecyl 2,2,2-trifluoroacetate

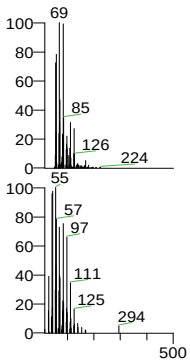


RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.03	3-Eicosene, (E)-	3340221279	2.22	909	74685-33-9	mainlib
10.03	1-Dodecanol, 3,7,11-trimethyl-	3340221279	2.22	906	6750-34-1	mainlib
10.03	Dichloroacetic acid, tetradecyl ester	3340221279	2.22	900	83005-02-1	mainlib

Analysed By:

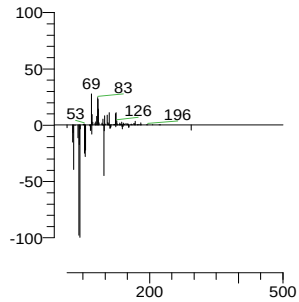
Checked By:

Hit Spectrum	Delta	Compound Structure

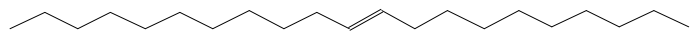


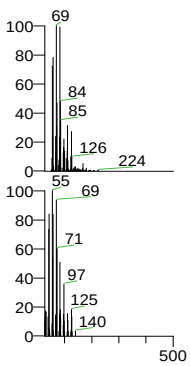
NL: 9.99E2
131858 10.32 1 11
22 1833-1843 1873-1883
5.82E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 868, RSI 932, mainlib,
Entry# 18363, CAS#
95008-11-0,
10-Heneicosene (c,t)



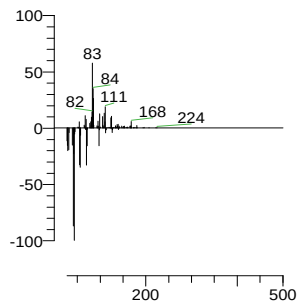
10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



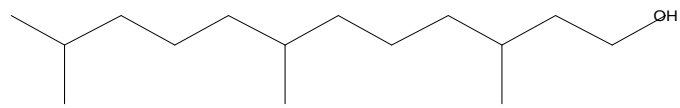


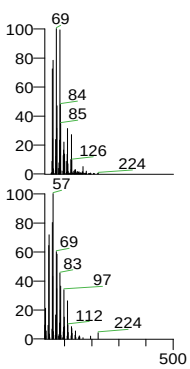
NL: 9.99E2
131858 10.32 1 11
22 1833-1843 1873-1883
5.82E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 849, RSI 927, mainlib,
Entry# 18829, CAS#
6750-34-1, 1-Dodecanol,
3,7,11-trimethyl-



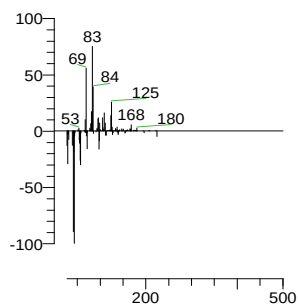
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



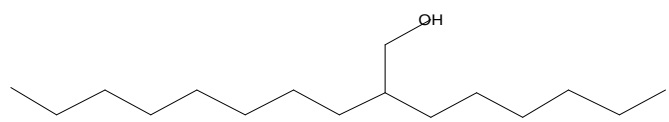


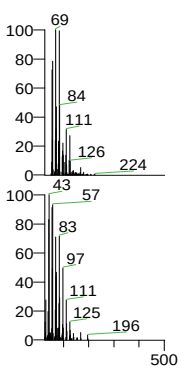
NL: 9.99E2
131858 10.32 1 11
22 1833-1843 1873-1883
5.82E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 869, RSI 923, mainlib,
Entry# 23004, CAS#
2425-77-6, 1-Decanol,
2-hexyl-



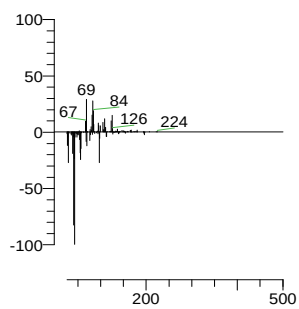
1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol



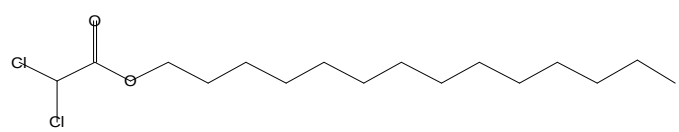


NL: 9.99E2
131858 10.32 1 11
22 1833-1843 1873-1883
5.82E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 873, RSI 922, mainlib,
Entry# 7343, CAS#
83005-02-1,
Dichloroacetic acid,
tetradecyl ester

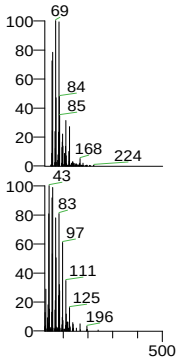


Dichloroacetic acid, tetradecyl ester
Formula C16H30Cl2O2, MW 324, CAS# 83005-02-1, Entry# 7343
Tetradecyl dichloroacetate #

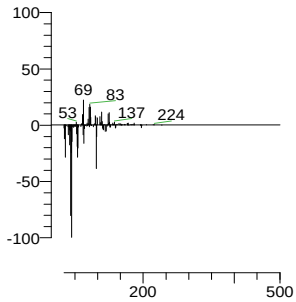


Analysed By: *Checked By:*

Hit Spectrum

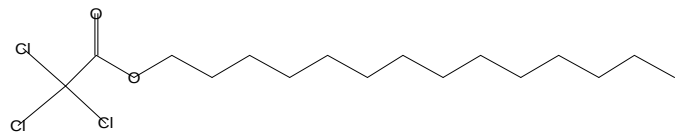


Delta



Compound Structure

Trichloroacetic acid, tetradecyl ester
Formula C16H29Cl3O2, MW 358, CAS# 74339-52-9, Entry# 7359
Tetradecyl trichloroacetate #

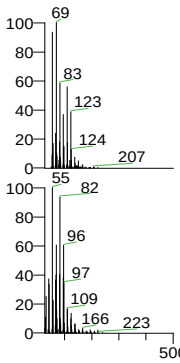


RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.32	10-Heneicosene (c,t)	1402821131	0.93	932	95008-11-0	mainlib
10.32	1-Dodecanol, 3,7,11-trimethyl-	1402821131	0.93	927	6750-34-1	mainlib
10.32	1-Decanol, 2-hexyl-	1402821131	0.93	923	2425-77-6	mainlib

Analysed By:

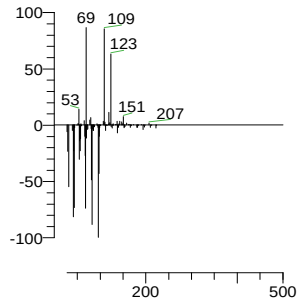
Checked By:

Hit Spectrum	Delta	Compound Structure

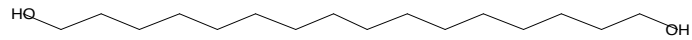


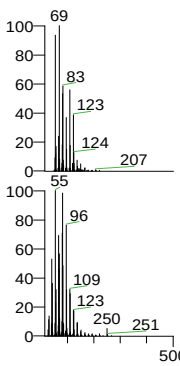
NL: 9.99E2
131884 10.40 1 11
22 1859-1869 1899-1909
5.60E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 838, RSI 866, mainlib, Entry# 19250, CAS# 7735-42-4, 1,16-Hexadecanediol



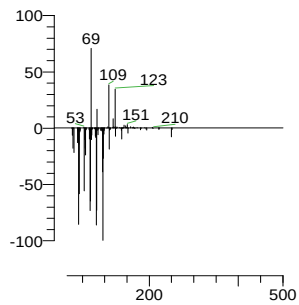
1,16-Hexadecanediol
Formula C16H34O2, MW 258, CAS# 7735-42-4, Entry# 19250



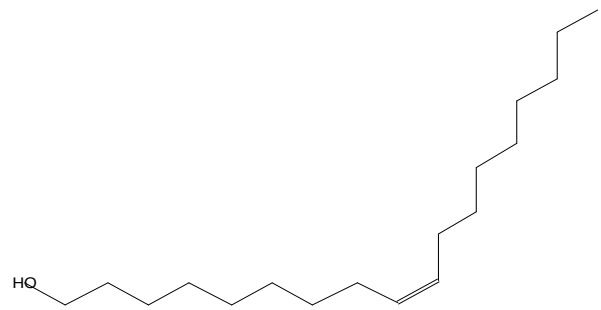


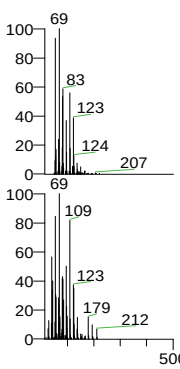
NL: 9.99E2
131884 10.40 1 11
22 1859-1869 1899-1909
5.60E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 832, RSI 855, mainlib, Entry# 19267, CAS# 143-28-2, 9-Octadecen-1-ol, (Z)-



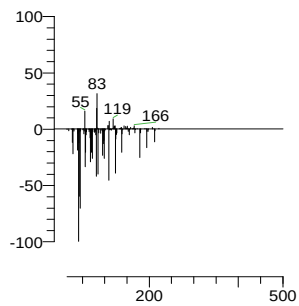
9-Octadecen-1-ol, (Z)-
Formula C18H36O, MW 268, CAS# 143-28-2, Entry# 19267
cis-9-Octadecen-1-ol



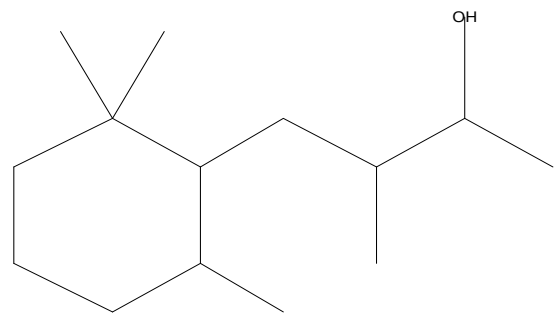


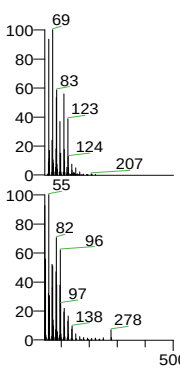
NL: 9.99E2
131884 10.40 1 11
22 1859-1869 1899-1909
5.60E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 821, RSI 847, mainlib, Entry# 32148, CAS# 60241-53-4, Methyl tetrahydroionol



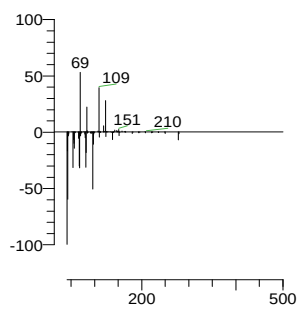
Methyl tetrahydroionol
Formula C14H28O, MW 212, CAS# 60241-53-4, Entry# 32148
Cyclohexanepropanol, à,á,2,2,6-pentamethyl-



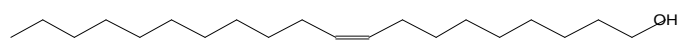


NL: 9.99E2
131884 10.40 1 11
22 1859-1869 1899-1909
5.60E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 820, RSI 847, mainlib, Entry# 18153, CAS# 112248-30-3, Eicosen-1-ol, cis-9-

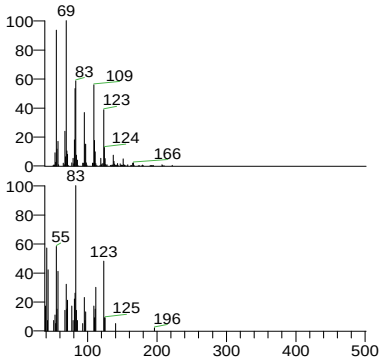


Eicosen-1-ol, cis-9-
Formula C20H40O, MW 296, CAS# 112248-30-3, Entry# 18153
(9Z)-9-Icosen-1-ol #

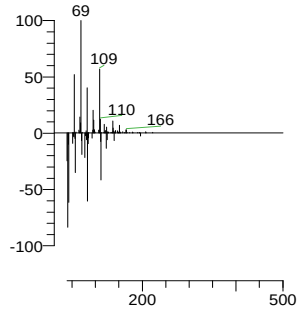


Analysed By: *Checked By:*

Hit Spectrum

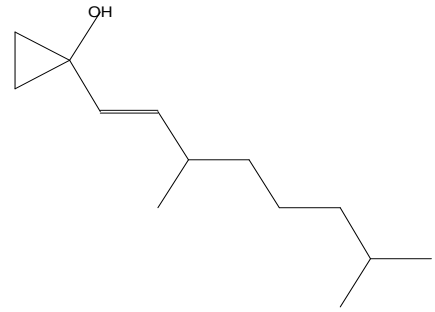


Delta



Compound Structure

Cyclopropanol, 1-(3,7-dimethyl-1-octenyl)-
Formula C13H24O, MW 196, CAS# 65147-72-0, Entry# 47465
1-[(1E)-3,7-Dimethyl-1-octenyl]cyclopropanol #

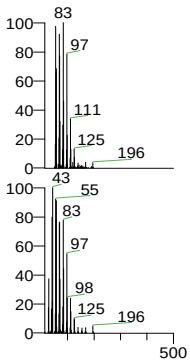


RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.40	1,16-Hexadecanediol	920715705	0.61	866	7735-42-4	mainlib
10.40	9-Octadecen-1-ol, (Z)-	920715705	0.61	855	143-28-2	mainlib
10.40	Methyl tetrahydroionol	920715705	0.61	847	60241-53-4	mainlib

Analysed By:

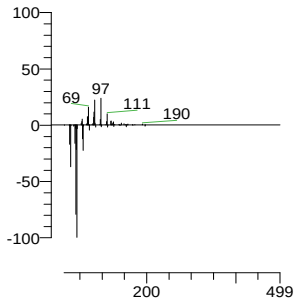
Checked By:

Hit Spectrum	Delta	Compound Structure

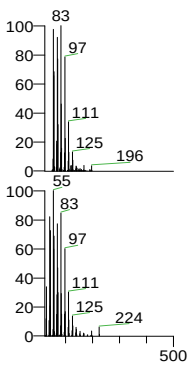


NL: 9.98E2
131938 10.58 1 11
22 1913-1923 1953-1963
1.19E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 958, RSI 981, mainlib,
Entry# 6847, CAS#
1120-36-1,
1-Tetradecene

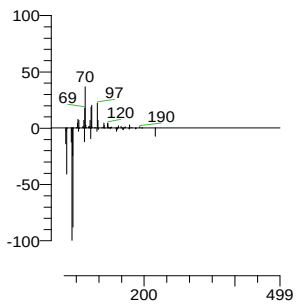


1-Tetradecene
Formula C14H28, MW 196, CAS# 1120-36-1, Entry# 6847
n-Tetradec-1-ene

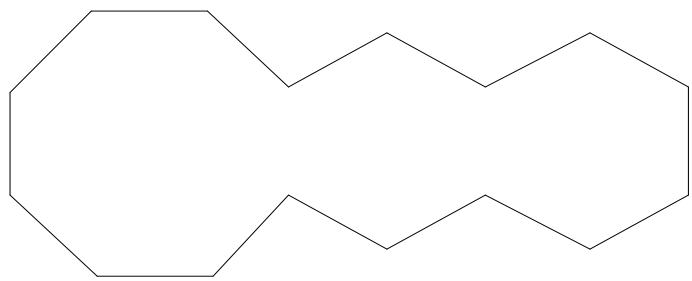


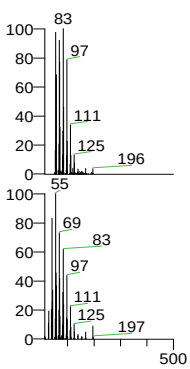
NL: 9.98E2
131938 10.58 1 11
22 1913-1923 1953-1963
1.19E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 947, RSI 972, mainlib,
Entry# 19398, CAS#
295-65-8,
Cyclohexadecane



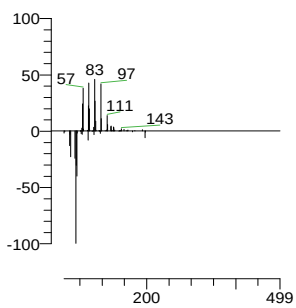
Cyclohexadecane
Formula C16H32, MW 224, CAS# 295-65-8, Entry# 19398



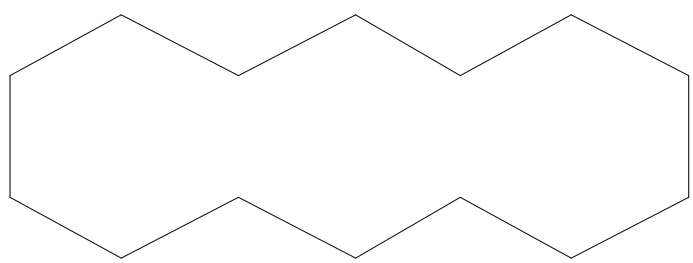


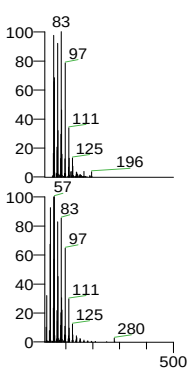
NL: 9.98E2
131938 10.58 1 11
22 1913-1923 1953-1963
1.19E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 946, RSI 972, mainlib,
Entry# 17995, CAS#
295-17-0,
Cyclotetradecane



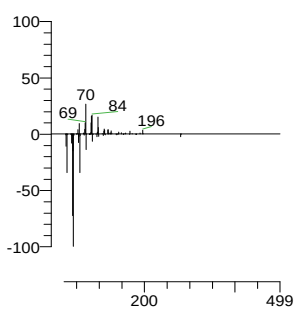
Cyclotetradecane
Formula C14H28, MW 196, CAS# 295-17-0, Entry# 17995



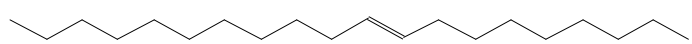


NL: 9.98E2
131938 10.58 1 11
22 1913-1923 1953-1963
1.19E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 934, RSI 971, mainlib,
Entry# 23002, CAS#
74685-29-3, 9-Eicosene,
(E)-

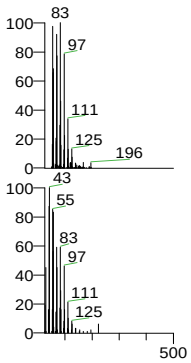


9-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-29-3, Entry# 23002
(9E)-9-Icosene #



Analysed By: *Checked By:*

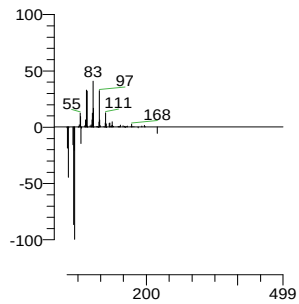
Hit Spectrum



NL: 9.98E2
131938 10.58 1 11
22 1913-1923 1953-1963
1.19E8 + c EI Full ms
[50.00-500.00]

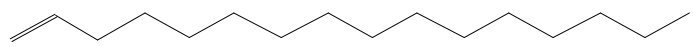
NL: 9.99E2
SI 929, RSI 971, mainlib,
Entry# 5717, CAS#
629-73-2, Cetene

Delta



Compound Structure

Cetene
Formula C16H32, MW 224, CAS# 629-73-2, Entry# 5717
1-Hexadecene

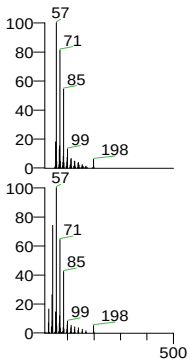


RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.58	1-Tetradecene	5410424752	3.59	981	1120-36-1	mainlib
10.58	Cyclotetradecane	5410424752	3.59	972	295-17-0	mainlib
10.58	Cyclohexadecane	5410424752	3.59	972	295-65-8	mainlib

Analysed By:

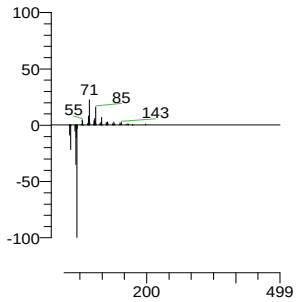
Checked By:

Hit Spectrum	Delta	Compound Structure

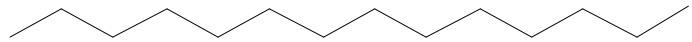


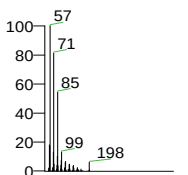
NL: 9.98E2
131962 10.66 1 11
22 1937-1947 1977-1987
2.59E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 958, RSI 984, mainlib, Entry# 22616, CAS# 629-59-4, Tetradecane

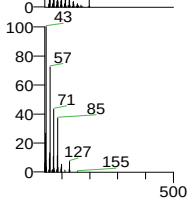


Tetradecane
Formula C14H30, MW 198, CAS# 629-59-4, Entry# 22616
n-Tetradecane

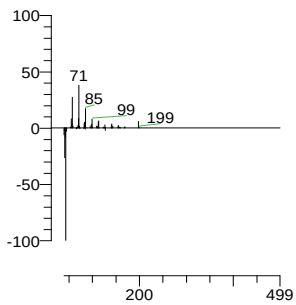




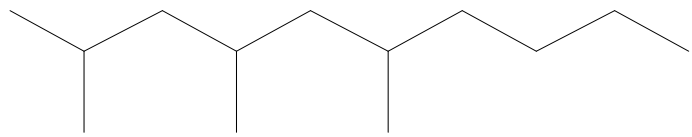
NL: 9.98E2
131962 10.66 1 11
22 1937-1947 1977-1987
2.59E8 + c EI Full ms
[50.00-500.00]

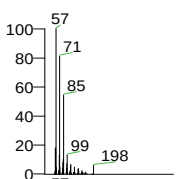


NL: 9.99E2
SI 836, RSI 968, mainlib, Entry# 7452, CAS# 62108-27-4, Decane, 2,4,6-trimethyl-

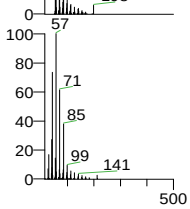


Decane, 2,4,6-trimethyl-
Formula C13H28, MW 184, CAS# 62108-27-4, Entry# 7452
2,4,6-Trimethyldecane #

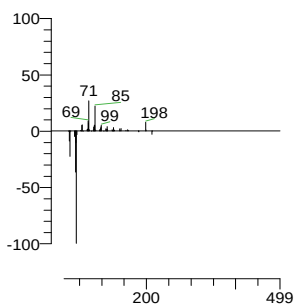




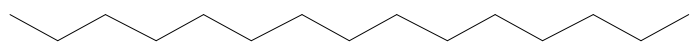
NL: 9.98E2
131962 10.66 1 11
22 1937-1947 1977-1987
2.59E8 + c EI Full ms
[50.00-500.00]

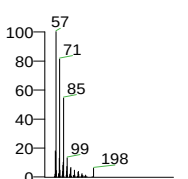


NL: 9.99E2
SI 931, RSI 964, mainlib, Entry# 22638, CAS# 629-62-9, Pentadecane

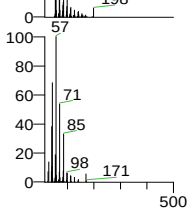


Pentadecane
Formula C15H32, MW 212, CAS# 629-62-9, Entry# 22638
n-Pentadecane

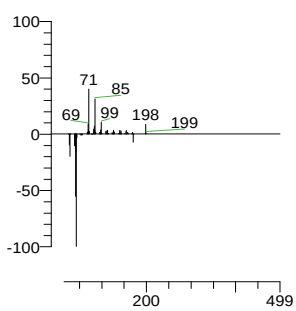




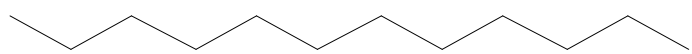
NL: 9.98E2
131962 10.66 1 11
22 1937-1947 1977-1987
2.59E8 + c EI Full ms
[50.00-500.00]



NL: 9.99E2
SI 899, RSI 957, mainlib, Entry# 22550, CAS# 112-40-3, Dodecane

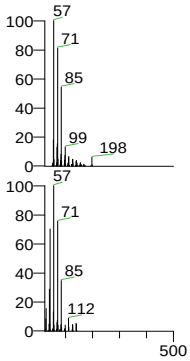


Dodecane
Formula C12H26, MW 170, CAS# 112-40-3, Entry# 22550
n-Dodecane

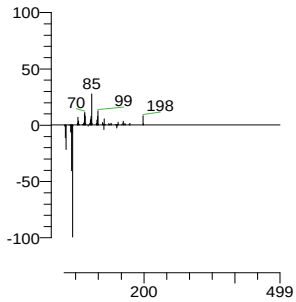


Analysed By: *Checked By:*

Hit Spectrum

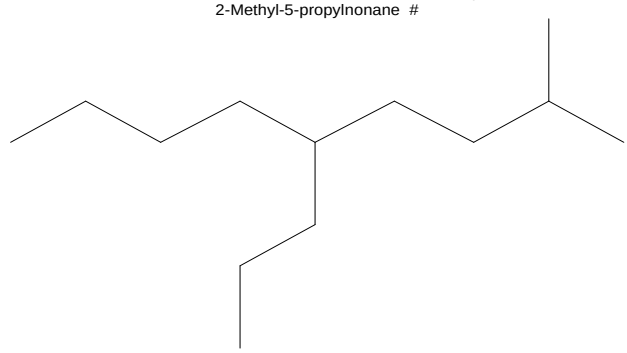


Delta



Compound Structure

Nonane, 2-methyl-5-propyl-
Formula C13H28, MW 184, CAS# 31081-17-1, Entry# 23616
2-Methyl-5-propylnonane #

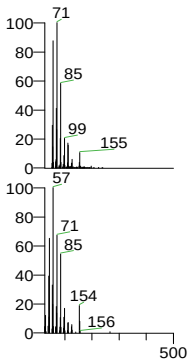


RT	Compound Name	Area	Area %	RSI	Cas #	Library
10.66	Tetradecane	3804973538	2.53	984	629-59-4	mainlib
10.66	Decane, 2,4,6-trimethyl-	3804973538	2.53	968	62108-27-4	mainlib
10.66	Pentadecane	3804973538	2.53	964	629-62-9	mainlib

Analysed By:

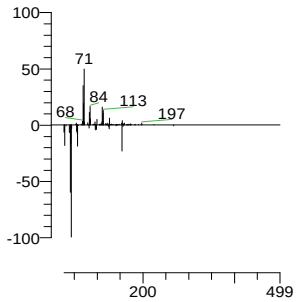
Checked By:

Hit Spectrum	Delta	Compound Structure

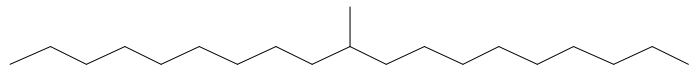


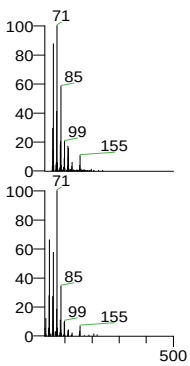
NL: 9.98E2
132145 11.29 1 11
22 2120-2130 2160-2170
6.14E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 889, RSI 934, mainlib, Entry# 23599, CAS# 56862-62-5, 10-Methylnonadecane



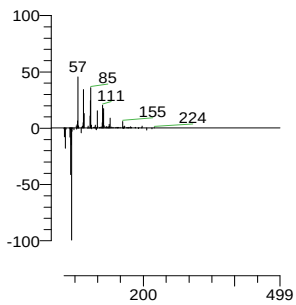
10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



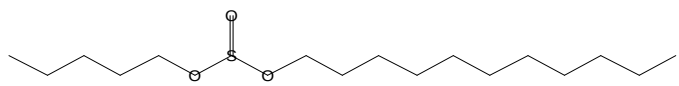


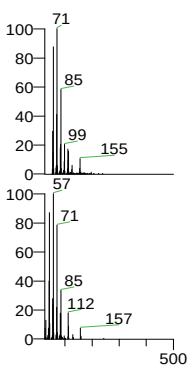
NL: 9.98E2
132145 11.29 1 11
22 2120-2130 2160-2170
6.14E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 879, RSI 928, mainlib, Entry# 35060, CAS# NA, Sulfurous acid, pentyl undecyl ester



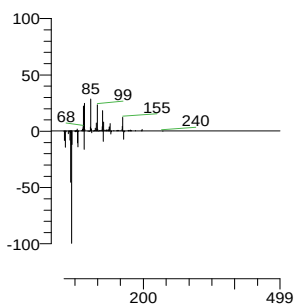
Sulfurous acid, pentyl undecyl ester
Formula C16H34O3S, MW 306, CAS# NA, Entry# 35060



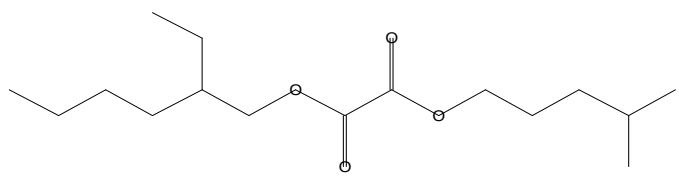


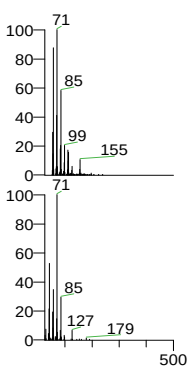
NL: 9.98E2
132145 11.29 1 11
22 2120-2130 2160-2170
6.14E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 808, RSI 926, mainlib, Entry# 22518, CAS# NA, Oxalic acid, 2-ethylhexyl isohexyl ester



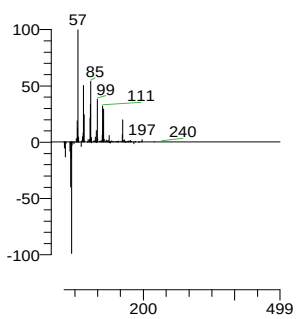
Oxalic acid, 2-ethylhexyl isohexyl ester
Formula C16H30O4, MW 286, CAS# NA, Entry# 22518



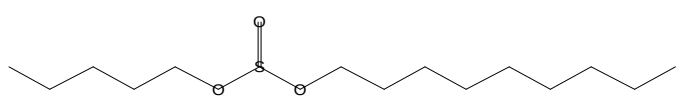


NL: 9.98E2
132145 11.29 1 11
22 2120-2130 2160-2170
6.14E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 740, RSI 926, mainlib, Entry# 35058, CAS# NA, Sulfurous acid, nonyl pentyl ester

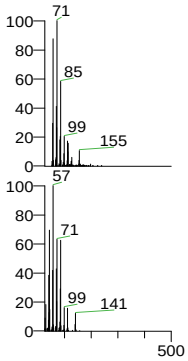


Sulfurous acid, nonyl pentyl ester
Formula C14H30O3S, MW 278, CAS# NA, Entry# 35058

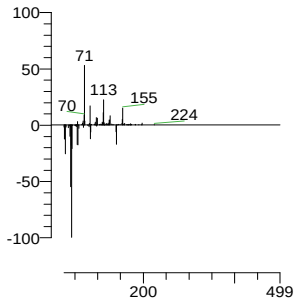


Analysed By: *Checked By:*

Hit Spectrum

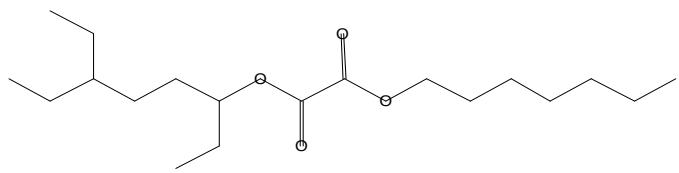


Delta



Compound Structure

Oxalic acid, 6-ethyloct-3-yl heptyl ester
Formula C19H36O4, MW 328, CAS# NA, Entry# 22517

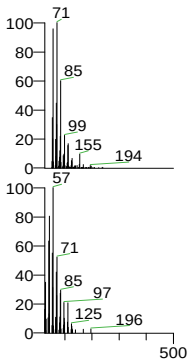


RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.29	10-Methylnonadecane	1681891823	1.12	934	56862-62-5	mainlib
11.29	Sulfurous acid, pentyl undecyl ester	1681891823	1.12	928	NA	mainlib
11.29	Oxalic acid, 2-ethylhexyl isohexyl ester	1681891823	1.12	926	NA	mainlib

Analysed By:

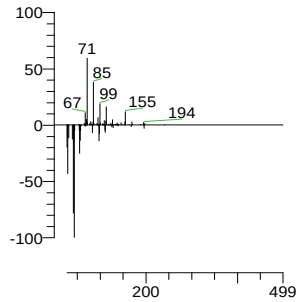
Checked By:

Hit Spectrum	Delta	Compound Structure

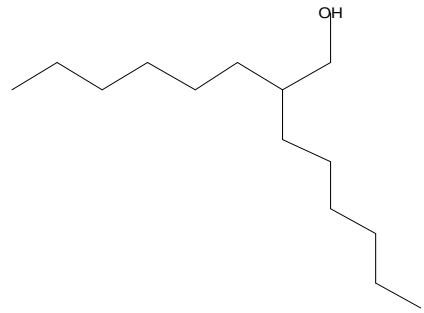


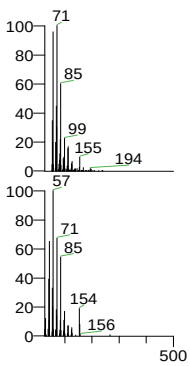
NL: 9.99E2
132180 11.41 1 11
22 2155-2165 2195-2205
5.25E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 862, RSI 928, mainlib,
Entry# 22406, CAS#
19780-79-1,
2-Hexyl-1-octanol



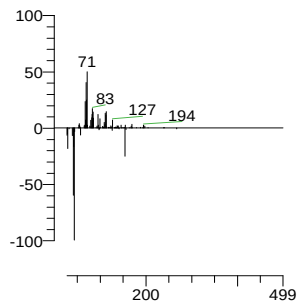
2-Hexyl-1-octanol
Formula C14H30O, MW 214, CAS# 19780-79-1, Entry# 22406



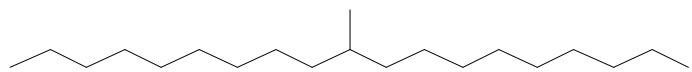


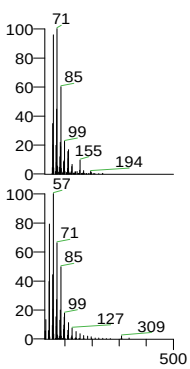
NL: 9.99E2
132180 11.41 1 11
22 2155-2165 2195-2205
5.25E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 864, RSI 927, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane



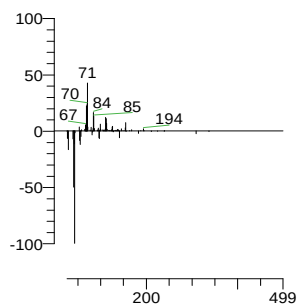
10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



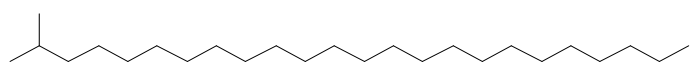


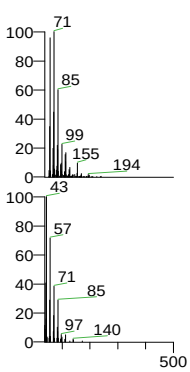
NL: 9.99E2
132180 11.41 1 11
22 2155-2165 2195-2205
5.25E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 901, RSI 924, mainlib,
Entry# 22537, CAS# NA,
2-methyltetracosane



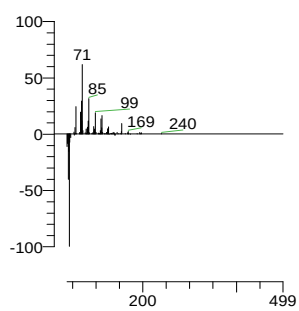
2-methyltetracosane
Formula C25H52, MW 352, CAS# NA, Entry# 22537



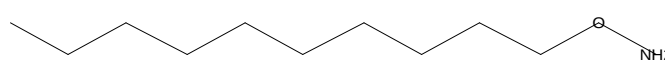


NL: 9.99E2
132180 11.41 1 11
22 2155-2165 2195-2205
5.25E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 766, RSI 917, mainlib,
Entry# 7242, CAS#
29812-79-1,
Hydroxylamine, O-decyl-

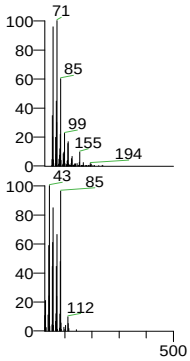


Hydroxylamine, O-decyl-
Formula C10H23NO, MW 173, CAS# 29812-79-1, Entry# 7242
O-Decylhydroxylamine



Analysed By: *Checked By:*

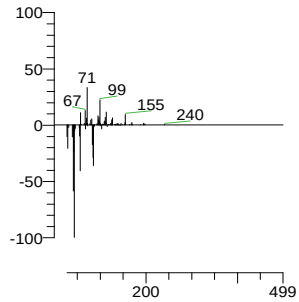
Hit Spectrum



NL: 9.99E2
132180 11.41 1 11
22 2155-2165 2195-2205
5.25E7 + c EI Full ms
[50.00-500.00]

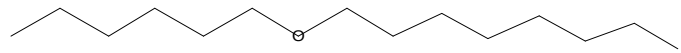
NL: 9.99E2
SI 752, RSI 915, mainlib,
Entry# 9315, CAS#
17071-54-4, Hexyl octyl
ether

Delta



Compound Structure

Hexyl octyl ether
Formula C14H30O, MW 214, CAS# 17071-54-4, Entry# 9315
1-(Hexyloxy)octane #

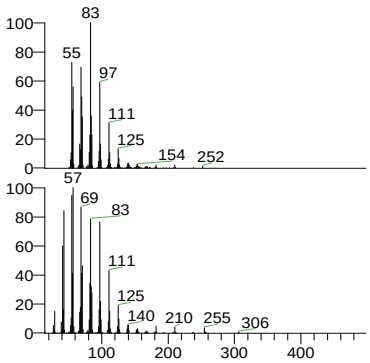


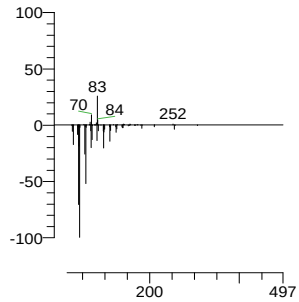
RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.41	2-Hexyl-1-octanol	1022867847	0.68	928	19780-79-1	mainlib
11.41	10-Methylnonadecane	1022867847	0.68	927	56862-62-5	mainlib
11.41	2-methyltetracosane	1022867847	0.68	924	NA	mainlib

Analysed By:

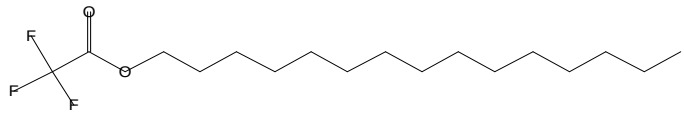
Checked By:

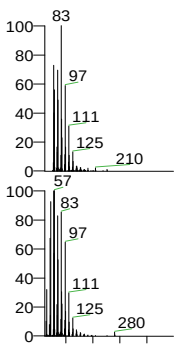
Hit Spectrum	Delta	Compound Structure





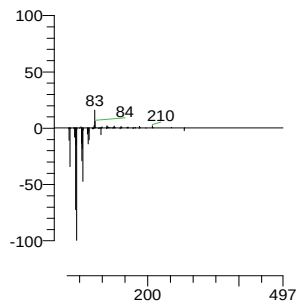
Trifluoroacetic acid, pentadecyl ester
Formula C17H31F3O2, MW 324, CAS# 959010-23-2, Entry# 23039



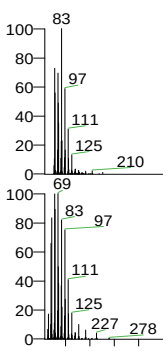


NL: 9.99E2
132305 11.83 1 11 22 2280-2290 2320-2330 1.62E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 962, RSI 974, mainlib, Entry# 23002, CAS# 74685-29-3, 9-Eicosene, (E)-

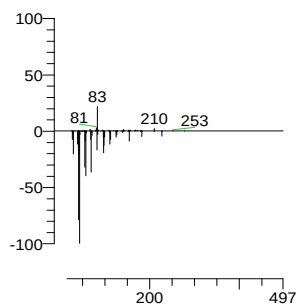


9-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-29-3, Entry# 23002
(9E)-9-Icosene #

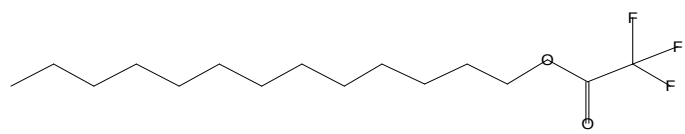


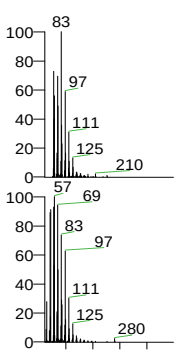
NL: 9.99E2
132305 11.83 1 11 22 2280-2290 2320-2330 1.62E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 959, RSI 974, mainlib, Entry# 32079, CAS# 53800-02-5, Trifluoroacetic acid,n-tridecyl ester



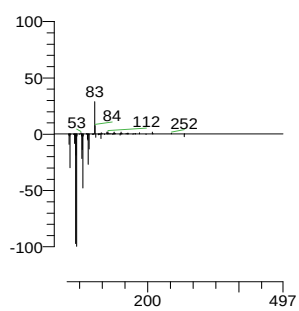
Trifluoroacetic acid,n-tridecyl ester
Formula C15H27F3O2, MW 296, CAS# 53800-02-5, Entry# 32079
Tridecyl trifluoroacetate #



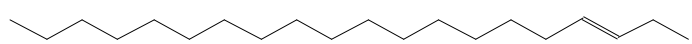


NL: 9.99E2
132305 11.83 1 11 22 2280-2290 2320-2330 1.62E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 962, RSI 973, mainlib, Entry# 23390, CAS# 74685-33-9, 3-Eicosene, (E)-

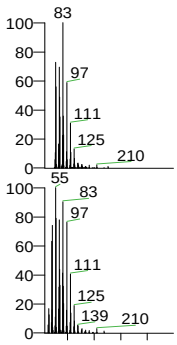


3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #



Analysed By: *Checked By:*

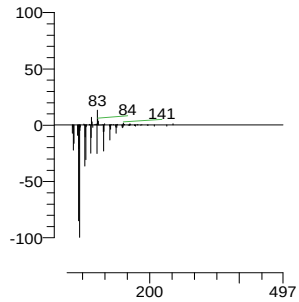
Hit Spectrum



NL: 9.99E2
132305 11.83 1 11
22 2280-2290 2320-2330
1.62E8 + c EI Full ms
[50.00-500.00]

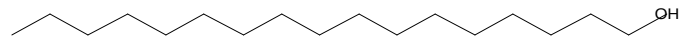
NL: 9.99E2
SI 962, RSI 973, mainlib,
Entry# 19432, CAS#
1454-85-9,
n-Heptadecanol-1

Delta



Compound Structure

n-Heptadecanol-1
Formula C17H36O, MW 256, CAS# 1454-85-9, Entry# 19432
1-Hydroxyheptadecane

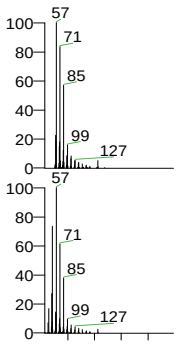


RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.83	Trifluoroacetic acid, pentadecyl ester	6158870340	4.09	975	959010-23-2	mainlib
11.83	Trifluoroacetic acid,n-tridecyl ester	6158870340	4.09	974	53800-02-5	mainlib
11.83	9-Eicosene, (E)-	6158870340	4.09	974	74685-29-3	mainlib

Analysed By:

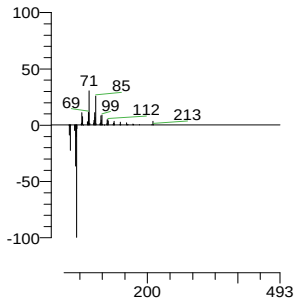
Checked By:

Hit Spectrum	Delta	Compound Structure

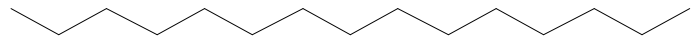


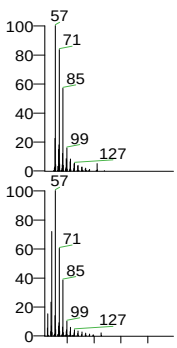
NL: 9.98E2
132327 11.91 1 11
22 2302-2312 2342-2352
2.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 962, RSI 968, mainlib,
Entry# 22638, CAS#
629-62-9, Pentadecane



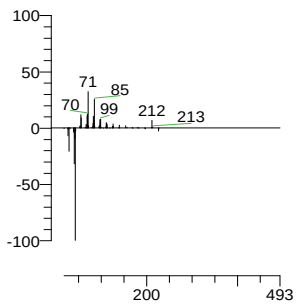
Pentadecane
Formula C15H32, MW 212, CAS# 629-62-9, Entry# 22638
n-Pentadecane



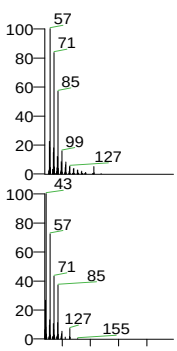


NL: 9.98E2
132327 11.91 1 11
22 2302-2312 2342-2352
2.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 945, RSI 962, mainlib,
Entry# 22719, CAS#
544-76-3, Hexadecane

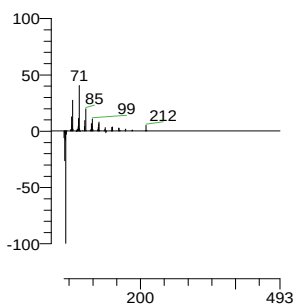


Hexadecane
Formula C16H34, MW 226, CAS# 544-76-3, Entry# 22719
n-Cetane

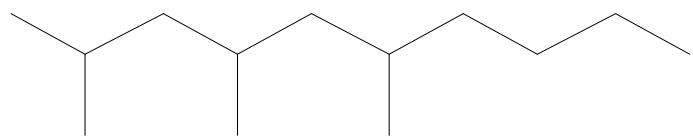


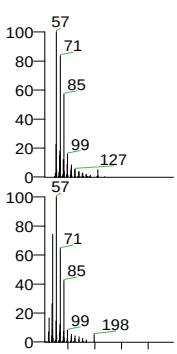
NL: 9.98E2
132327 11.91 1 11
22 2302-2312 2342-2352
2.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 839, RSI 955, mainlib,
Entry# 7452, CAS#
62108-27-4, Decane,
2,4,6-trimethyl-



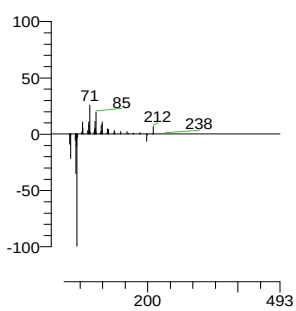
Decane, 2,4,6-trimethyl-
Formula C13H28, MW 184, CAS# 62108-27-4, Entry# 7452
2,4,6-Trimethyldecane #



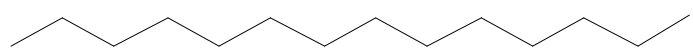


NL: 9.98E2
132327 11.91 1 11
22 2302-2312 2342-2352
2.44E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 931, RSI 953, mainlib,
Entry# 22616, CAS#
629-59-4, Tetradecane

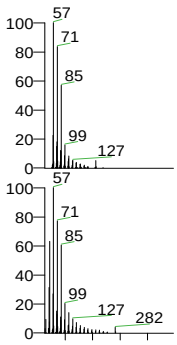


Tetradecane
Formula C14H30, MW 198, CAS# 629-59-4, Entry# 22616
n-Tetradecane

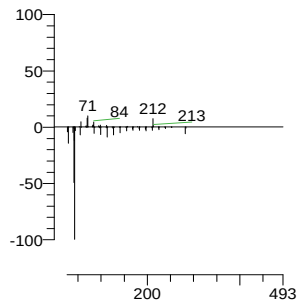


Analysed By: *Checked By:*

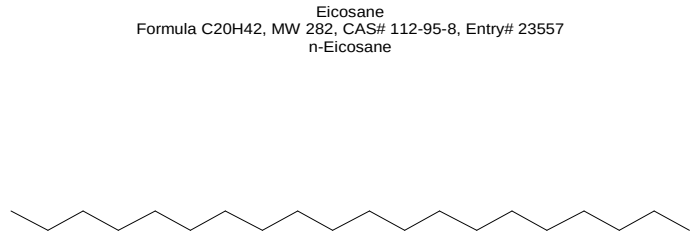
Hit Spectrum



Delta



Compound Structure

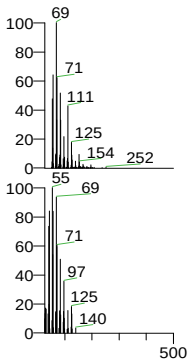


RT	Compound Name	Area	Area %	RSI	Cas #	Library
11.91	Pentadecane	3994681734	2.65	968	629-62-9	mainlib
11.91	Hexadecane	3994681734	2.65	962	544-76-3	mainlib
11.91	Decane, 2,4,6-trimethyl-	3994681734	2.65	955	62108-27-4	mainlib

Analysed By:

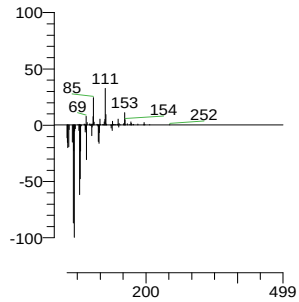
Checked By:

Hit Spectrum	Delta	Compound Structure

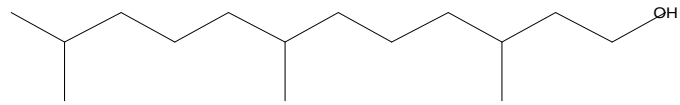


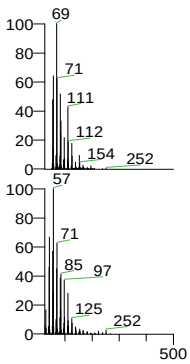
NL: 9.99E2
132416 12.21 1 11
22 2391-2401 2431-2441
1.35E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 862, RSI 925, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-



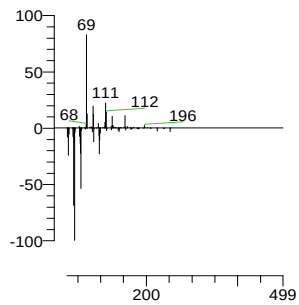
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



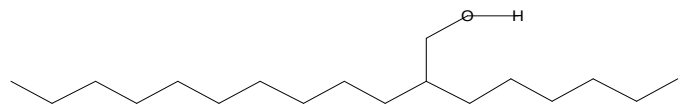


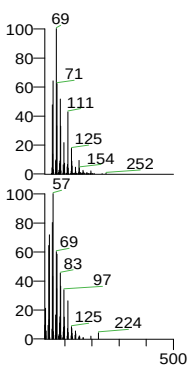
NL: 9.99E2
132416 12.21 1 11
22 2391-2401 2431-2441
1.35E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 914, RSI 920, mainlib, Entry# 22630, CAS# 110225-00-8, 1-Dodecanol, 2-hexyl-



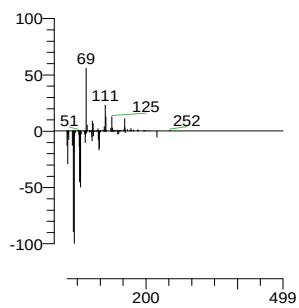
1-Dodecanol, 2-hexyl-
Formula C18H38O, MW 270, CAS# 110225-00-8, Entry# 22630
2-Hexyldodecan-1-ol



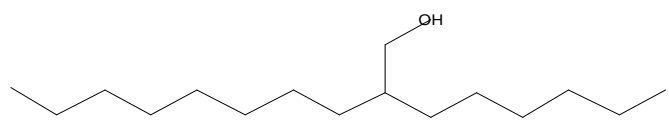


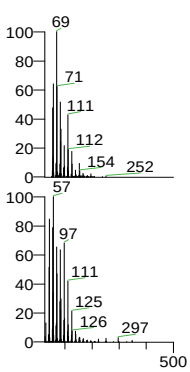
NL: 9.99E2
132416 12.21 1 11
22 2391-2401 2431-2441
1.35E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 898, RSI 918, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-



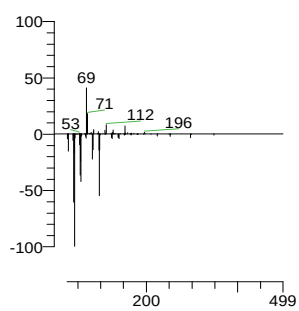
1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol



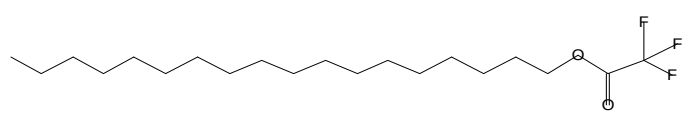


NL: 9.99E2
132416 12.21 1 11
22 2391-2401 2431-2441
1.35E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 907, RSI 913, mainlib, Entry# 22467, CAS# 79392-43-1, Octadecyl trifluoroacetate

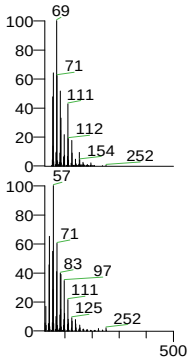


Octadecyl trifluoroacetate
Formula C20H37F3O2, MW 366, CAS# 79392-43-1, Entry# 22467
Octadecyl 2,2,2-trifluoroacetate



Analysed By: *Checked By:*

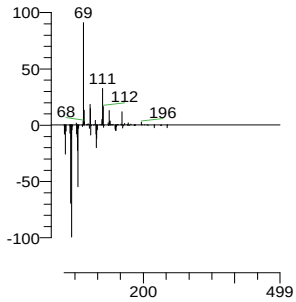
Hit Spectrum



NL: 9.99E2
132416 12.21 1 11
22 2391-2401 2431-2441
1.35E8 + c EI Full ms
[50.00-500.00]

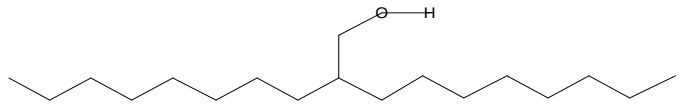
NL: 9.99E2
SI 905, RSI 911, mainlib,
Entry# 22554, CAS#
45235-48-1, 1-Decanol,
2-octyl-

Delta



Compound Structure

1-Decanol, 2-octyl-
Formula C18H38O, MW 270, CAS# 45235-48-1, Entry# 22554
2-Octyldecan-1-ol

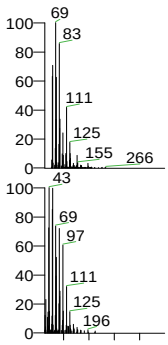


RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.21	1-Dodecanol, 3,7,11-trimethyl-	2695952813	1.79	925	6750-34-1	mainlib
12.21	1-Dodecanol, 2-hexyl-	2695952813	1.79	920	110225-00-8	mainlib
12.21	1-Decanol, 2-hexyl-	2695952813	1.79	918	2425-77-6	mainlib

Analysed By:

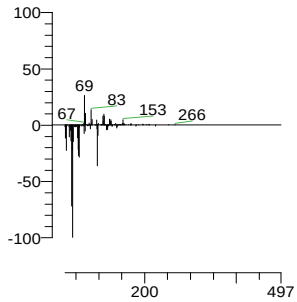
Checked By:

Hit Spectrum	Delta	Compound Structure

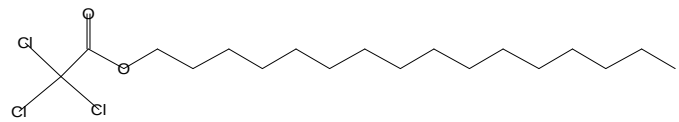


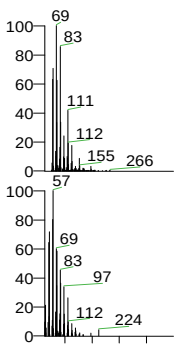
NL: 9.99E2
132446 12.31 1 11 22 2421-2431 2461-2471 6.08E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 884, RSI 923, mainlib, Entry# 7365, CAS# 74339-54-1, Trichloroacetic acid, hexadecyl ester



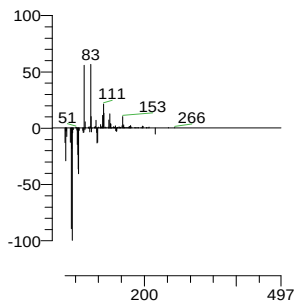
Trichloroacetic acid, hexadecyl ester
Formula C18H33Cl3O2, MW 386, CAS# 74339-54-1, Entry# 7365
Hexadecyl trichloroacetate #



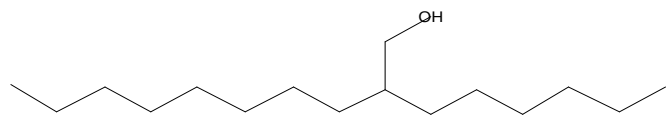


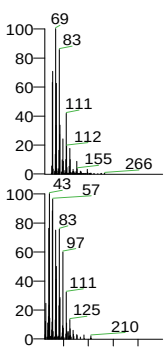
NL: 9.99E2
132446 12.31 1 11 22 2421-2431 2461-2471 6.08E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 873, RSI 921, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-



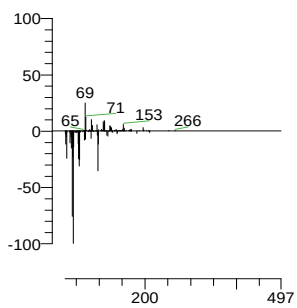
1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol



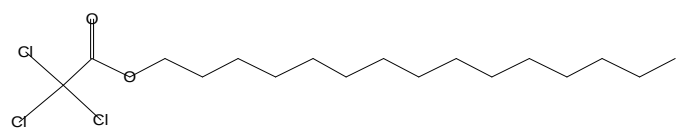


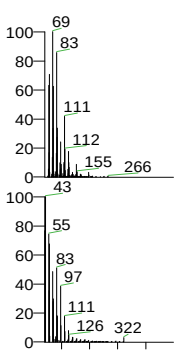
NL: 9.99E2
132446 12.31 1 11 22 2421-2431 2461-2471 6.08E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 878, RSI 917, mainlib, Entry# 7360, CAS# 74339-53-0, Trichloroacetic acid, pentadecyl ester



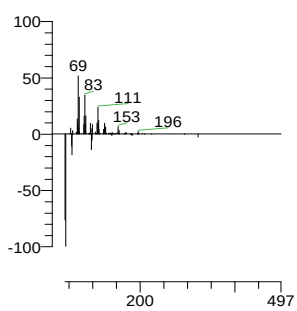
Trichloroacetic acid, pentadecyl ester
Formula C17H31Cl3O2, MW 372, CAS# 74339-53-0, Entry# 7360
Pentadecyl trichloroacetate #



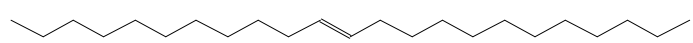


NL: 9.99E2
132446 12.31 1 11 22 2421-2431 2461-2471 6.08E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 769, RSI 915, mainlib, Entry# 5718, CAS# 52078-56-5, 11-Tricosene

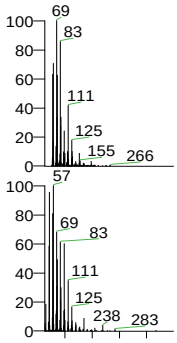


11-Tricosene
Formula C23H46, MW 322, CAS# 52078-56-5, Entry# 5718
(11E)-11-Tricosene #

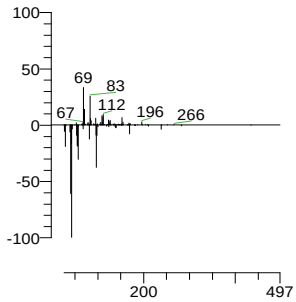


Analysed By: *Checked By:*

Hit Spectrum

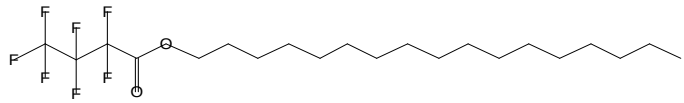


Delta



Compound Structure

Heptadecyl heptafluorobutyrate
Formula C21H35F7O2, MW 452, CAS# 959085-66-6, Entry# 22456
Heptadecyl 2,2,3,3,4,4,4-heptafluorobutanoate

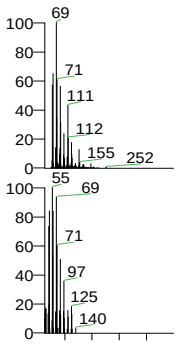


RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.31	Trichloroacetic acid, hexadecyl ester	1831951594	1.22	923	74339-54-1	mainlib
12.31	1-Decanol, 2-hexyl-	1831951594	1.22	921	2425-77-6	mainlib
12.31	Trichloroacetic acid, pentadecyl ester	1831951594	1.22	917	74339-53-0	mainlib

Analysed By:

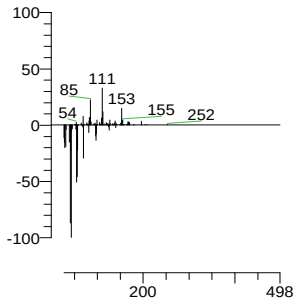
Checked By:

Hit Spectrum	Delta	Compound Structure

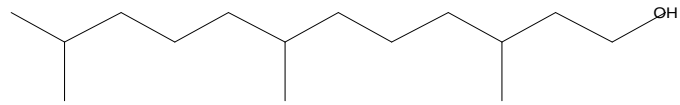


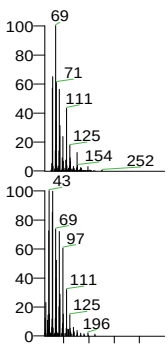
NL: 9.99E2
132505 12.52 1 11 22 2480-2490 2520-2530 7.67E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 836, RSI 936, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-



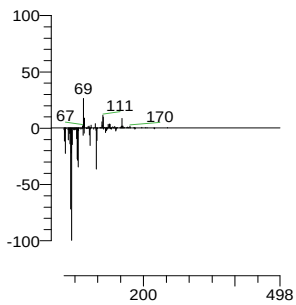
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



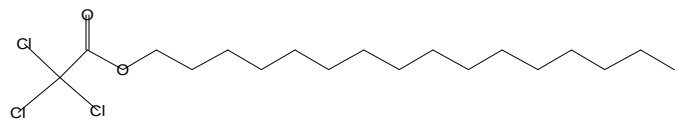


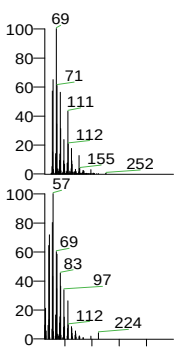
NL: 9.99E2
132505 12.52 1 11 22 2480-2490 2520-2530 7.67E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 896, RSI 930, mainlib, Entry# 7365, CAS# 74339-54-1, Trichloroacetic acid, hexadecyl ester



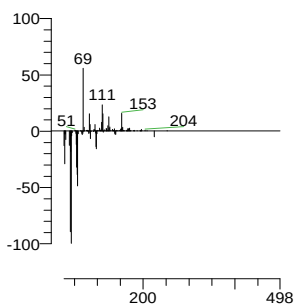
Trichloroacetic acid, hexadecyl ester
Formula C18H33Cl3O2, MW 386, CAS# 74339-54-1, Entry# 7365
Hexadecyl trichloroacetate #



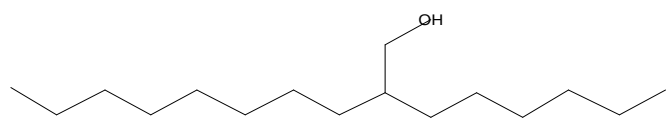


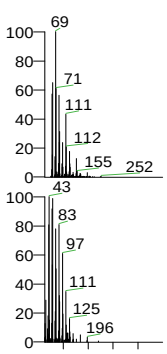
NL: 9.99E2
132505 12.52 1 11 22 2480-2490 2520-2530 7.67E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 879, RSI 926, mainlib, Entry# 23004, CAS# 2425-77-6, 1-Decanol, 2-hexyl-



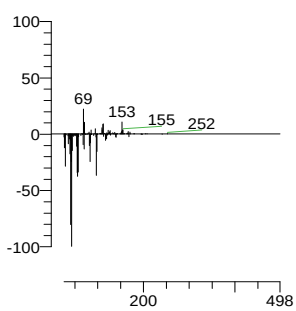
1-Decanol, 2-hexyl-
Formula C16H34O, MW 242, CAS# 2425-77-6, Entry# 23004
2-Hexyl-1-decanol



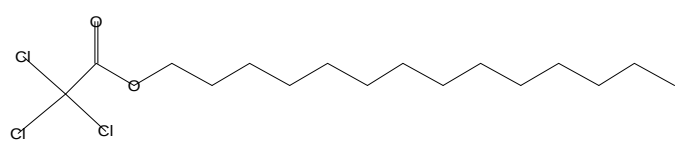


NL: 9.99E2
132505 12.52 1 11 22 2480-2490 2520-2530 7.67E7 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 876, RSI 924, mainlib, Entry# 7359, CAS# 74339-52-9, Trichloroacetic acid, tetradecyl ester

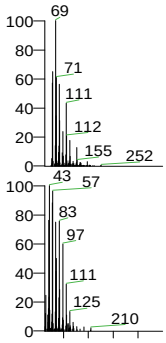


Trichloroacetic acid, tetradecyl ester
Formula C16H29Cl3O2, MW 358, CAS# 74339-52-9, Entry# 7359
Tetradecyl trichloroacetate #



Analysed By: *Checked By:*

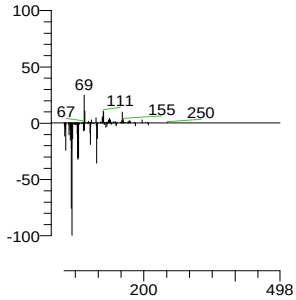
Hit Spectrum



NL: 9.99E2
132505 12.52 1 11 22
2480-2490 2520-2530
7.67E7 + c EI Full ms
[50.00-500.00]

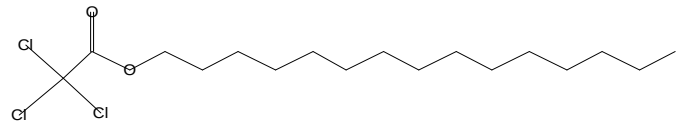
NL: 9.99E2
SI 881, RSI 920, mainlib, Entry# 7360, CAS# 74339-53-0, Trichloroacetic acid, pentadecyl ester

Delta



Compound Structure

Trichloroacetic acid, pentadecyl ester
Formula C17H31Cl3O2, MW 372, CAS# 74339-53-0, Entry# 7360
Pentadecyl trichloroacetate #

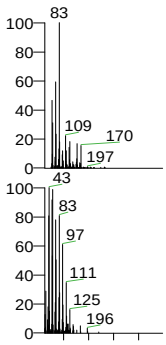


RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.52	1-Dodecanol, 3,7,11-trimethyl-	1679379289	1.11	936	6750-34-1	mainlib
12.52	Trichloroacetic acid, hexadecyl ester	1679379289	1.11	930	74339-54-1	mainlib
12.52	1-Decanol, 2-hexyl-	1679379289	1.11	926	2425-77-6	mainlib

Analysed By:

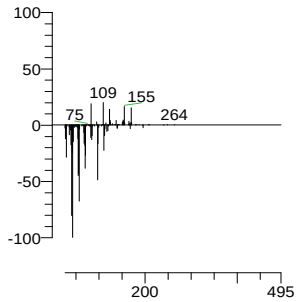
Checked By:

Hit Spectrum	Delta	Compound Structure

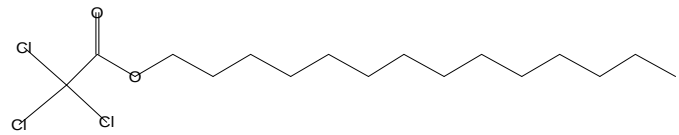


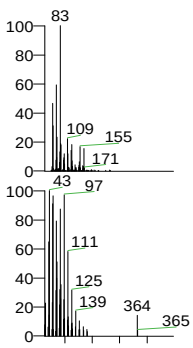
NL: 9.98E2
132559 12.70 1 11 22 2534-2544 2574-2584 1.04E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 732, RSI 857, mainlib, Entry# 7359, CAS# 74339-52-9, Trichloroacetic acid, tetradecyl ester



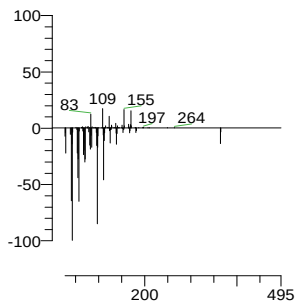
Trichloroacetic acid, tetradecyl ester
Formula C16H29Cl3O2, MW 358, CAS# 74339-52-9, Entry# 7359
Tetradecyl trichloroacetate #



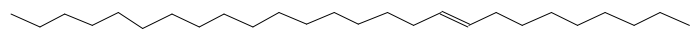


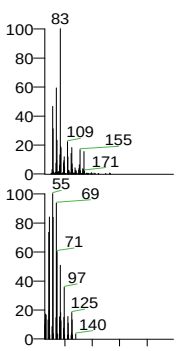
NL: 9.98E2
132559 12.70 1 11 22 2534-2544 2574-2584 1.04E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 730, RSI 850, mainlib, Entry# 9856, CAS# 71502-22-2, 9-Hexacosene



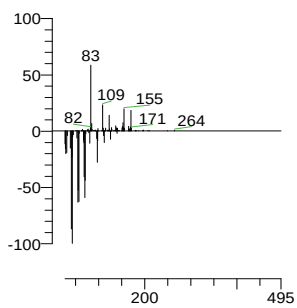
9-Hexacosene
Formula C26H52, MW 364, CAS# 71502-22-2, Entry# 9856
(9E)-9-Hexacosene #



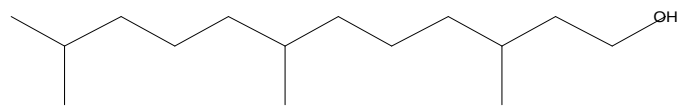


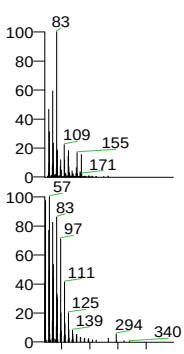
NL: 9.98E2
132559 12.70 1 11 22 2534-2544 2574-2584 1.04E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 700, RSI 850, mainlib, Entry# 18829, CAS# 6750-34-1, 1-Dodecanol, 3,7,11-trimethyl-



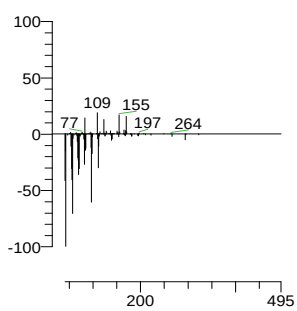
1-Dodecanol, 3,7,11-trimethyl-
Formula C15H32O, MW 228, CAS# 6750-34-1, Entry# 18829
Hexa-hydro-farnesol



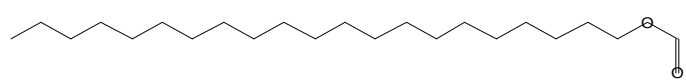


NL: 9.98E2
132559 12.70 1 11 22 2534-2544 2574-2584 1.04E8 + c EI Full ms [50.00-500.00]

NL: 9.99E2
SI 745, RSI 848, mainlib, Entry# 22753, CAS# 77899-03-7, 1-Heneicosyl formate

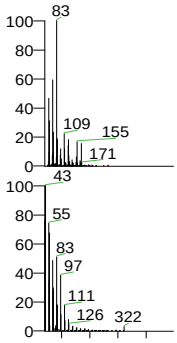


1-Heneicosyl formate
Formula C22H44O2, MW 340, CAS# 77899-03-7, Entry# 22753
Henicosyl formate #



Analysed By: *Checked By:*

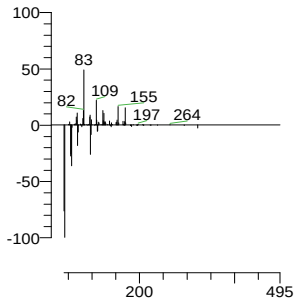
Hit Spectrum



NL: 9.98E2
132559 12.70 1 11
22 2534-2544 2574-2584
1.04E8 + c EI Full ms
[50.00-500.00]

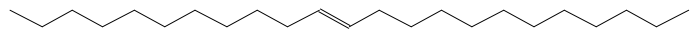
NL: 9.99E2
SI 633, RSI 844, mainlib,
Entry# 5718, CAS#
52078-56-5, 11-Tricosene

Delta



Compound Structure

11-Tricosene
Formula C23H46, MW 322, CAS# 52078-56-5, Entry# 5718
(11E)-11-Tricosene #

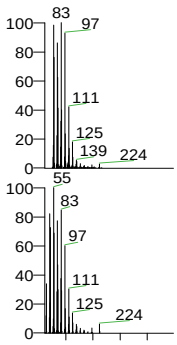


RT	Compound Name	Area	Area %	RSI	Cas #	Library
12.70	Trichloroacetic acid, tetradecyl ester	2146033589	1.42	857	74339-52-9	mainlib
12.70	1-Dodecanol, 3,7,11-trimethyl-	2146033589	1.42	850	6750-34-1	mainlib
12.70	9-Hexacosene	2146033589	1.42	850	71502-22-2	mainlib

Analysed By:

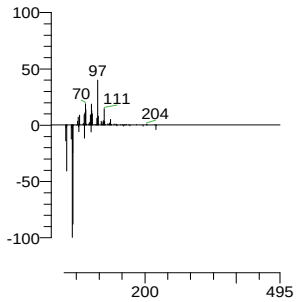
Checked By:

Hit Spectrum	Delta	Compound Structure

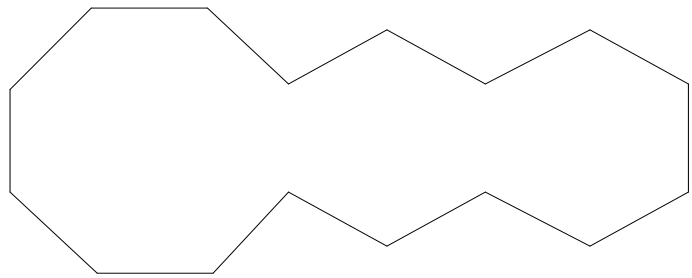


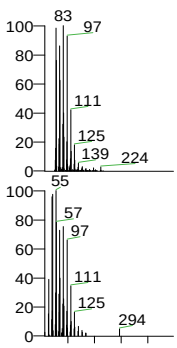
NL: 9.99E2
132647 13.00 1 11
22 2622-2632 2662-2672
1.00E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 964, RSI 981, mainlib,
Entry# 19398, CAS#
295-65-8,
Cyclohexadecane



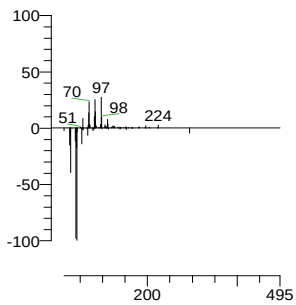
Cyclohexadecane
Formula C16H32, MW 224, CAS# 295-65-8, Entry# 19398



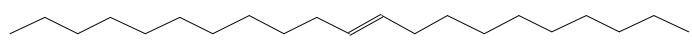


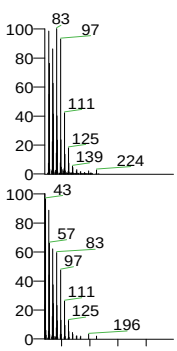
NL: 9.99E2
132647 13.00 1 11
22 2622-2632 2662-2672
1.00E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 947, RSI 980, mainlib,
Entry# 18363, CAS#
95008-11-0,
10-Heneicosene (c,t)



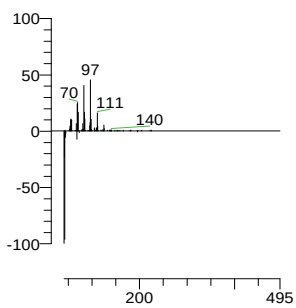
10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



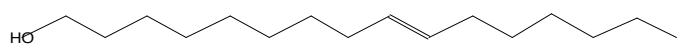


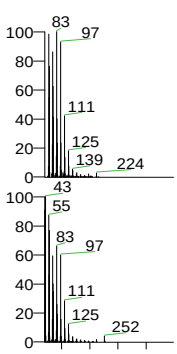
NL: 9.99E2
132647 13.00 1 11
22 2622-2632 2662-2672
1.00E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 946, RSI 980, mainlib,
Entry# 2269, CAS#
64437-47-4,
Hexadecen-1-ol, trans-9-



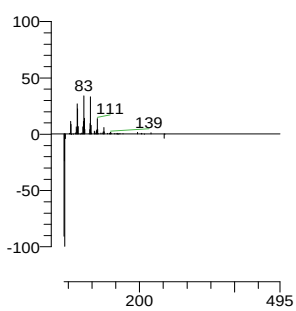
Hexadecen-1-ol, trans-9-
Formula C16H32O, MW 240, CAS# 64437-47-4, Entry# 2269
(9E)-9-Hexadecen-1-ol



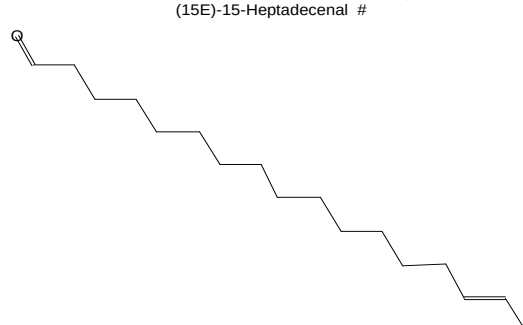


NL: 9.99E2
132647 13.00 1 11
22 2622-2632 2662-2672
1.00E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 970, RSI 979, mainlib,
Entry# 5592, CAS# NA,
E-15-Heptadecenal

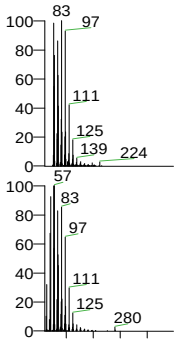


E-15-Heptadecenal
Formula C17H32O, MW 252, CAS# NA, Entry# 5592
(15E)-15-Heptadecenal #



Analysed By: *Checked By:*

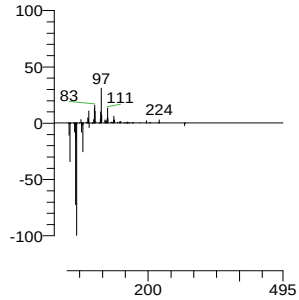
Hit Spectrum



NL: 9.99E2
132647 13.00 1 11
22 2622-2632 2662-2672
1.00E8 + c EI Full ms
[50.00-500.00]

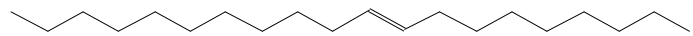
NL: 9.99E2
SI 956, RSI 978, mainlib,
Entry# 23002, CAS#
74685-29-3, 9-Eicosene,
(E)-

Delta



Compound Structure

9-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-29-3, Entry# 23002
(9E)-9-Icosene #

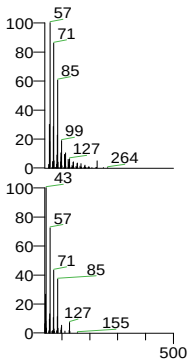


RT	Compound Name	Area	Area %	RSI	Cas #	Library
13.00	Cyclohexadecane	3622733210	2.40	981	295-65-8	mainlib
13.00	Hexadecen-1-ol, trans-9-	3622733210	2.40	980	64437-47-4	mainlib
13.00	10-Heneicosene (c,t)	3622733210	2.40	980	95008-11-0	mainlib

Analysed By:

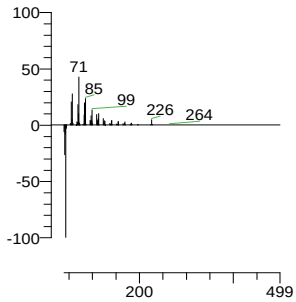
Checked By:

Hit Spectrum	Delta	Compound Structure

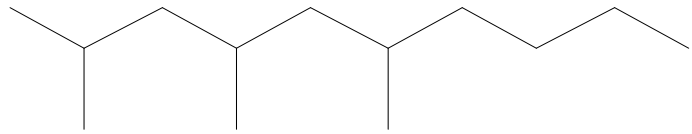


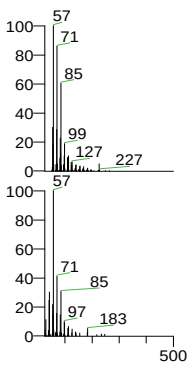
NL: 9.99E2
132671 13.07 1 11
22 2646-2656 2686-2696
2.13E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 768, RSI 937, mainlib, Entry# 7452, CAS# 62108-27-4, Decane, 2,4,6-trimethyl-



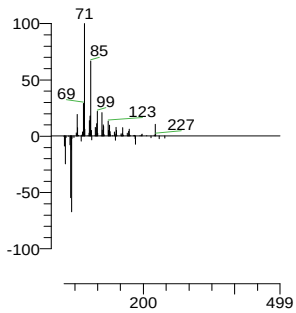
Decane, 2,4,6-trimethyl-
Formula C13H28, MW 184, CAS# 62108-27-4, Entry# 7452
2,4,6-Trimethyldecane #



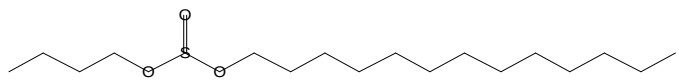


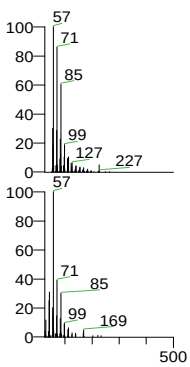
NL: 9.99E2
132671 13.07 1 11
22 2646-2656 2686-2696
2.13E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 835, RSI 934, mainlib, Entry# 23666, CAS# NA, Sulfurous acid, butyl tridecyl ester



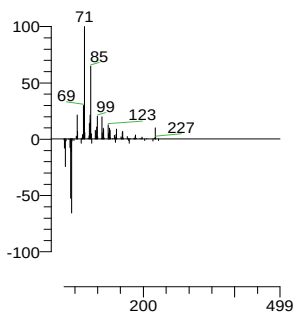
Sulfurous acid, butyl tridecyl ester
Formula C17H36O3S, MW 320, CAS# NA, Entry# 23666



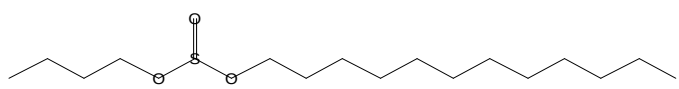


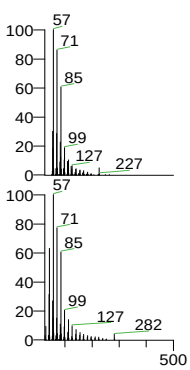
NL: 9.99E2
132671 13.07 1 11
22 2646-2656 2686-2696
2.13E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 826, RSI 934, mainlib, Entry# 23475, CAS# NA, Sulfurous acid, butyl dodecyl ester



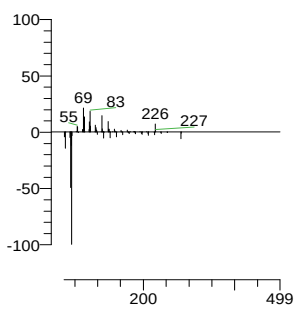
Sulfurous acid, butyl dodecyl ester
Formula C16H34O3S, MW 306, CAS# NA, Entry# 23475



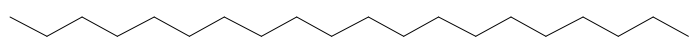


NL: 9.99E2
132671 13.07 1 11
22 2646-2656 2686-2696
2.13E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 908, RSI 933, mainlib, Entry# 23557, CAS# 112-95-8, Eicosane

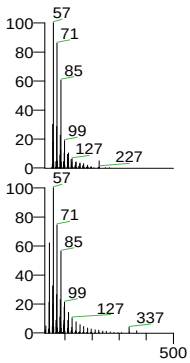


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

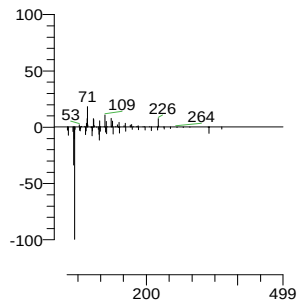


Analysed By: *Checked By:*

Hit Spectrum

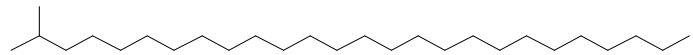


Delta



Compound Structure

2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535

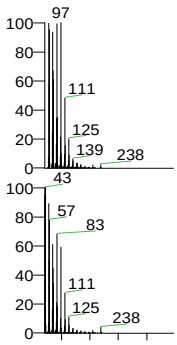


RT	Compound Name	Area	Area %	RSI	Cas #	Library
13.07	Decane, 2,4,6-trimethyl-	4317767725	2.87	937	62108-27-4	mainlib
13.07	Sulfurous acid, butyl dodecyl ester	4317767725	2.87	934	NA	mainlib
13.07	Sulfurous acid, butyl tridecyl ester	4317767725	2.87	934	NA	mainlib

Analysed By:

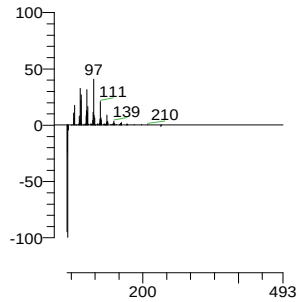
Checked By:

Hit Spectrum	Delta	Compound Structure

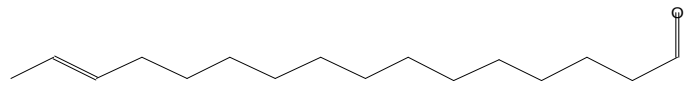


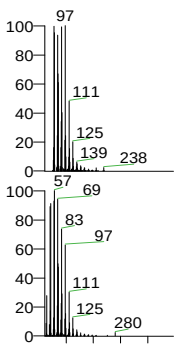
NL: 9.99E2
132971 14.10 1 11
22 2946-2956 2986-2996
7.79E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 977, RSI 981, mainlib,
Entry# 5664, CAS#
330207-53-9,
E-14-Hexadecenal



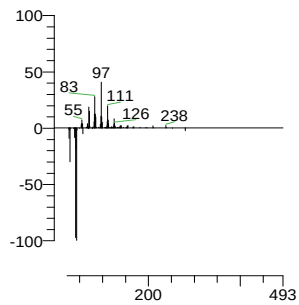
E-14-Hexadecenal
Formula C16H30O, MW 238, CAS# 330207-53-9, Entry# 5664
(14E)-14-Hexadecenal



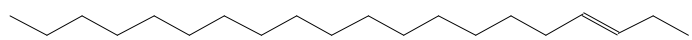


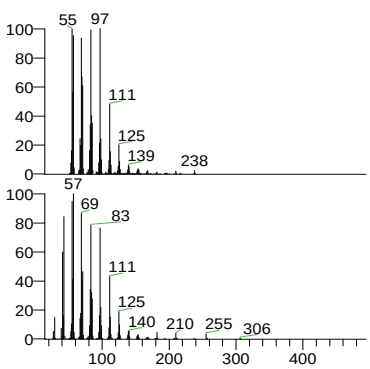
NL: 9.99E2
132971 14.10 1 11
22 2946-2956 2986-2996
7.79E7 + c EI Full ms
[50.00-500.00]

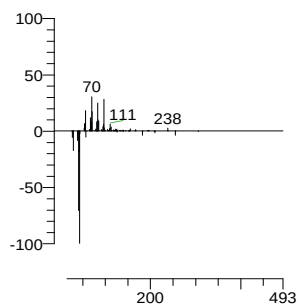
NL: 9.99E2
SI 966, RSI 981, mainlib,
Entry# 23390, CAS#
74685-33-9, 3-Eicosene,
(E)-



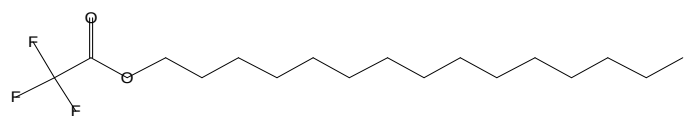
3-Eicosene, (E)-
Formula C20H40, MW 280, CAS# 74685-33-9, Entry# 23390
(3E)-3-Icosene #

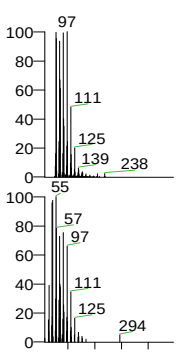






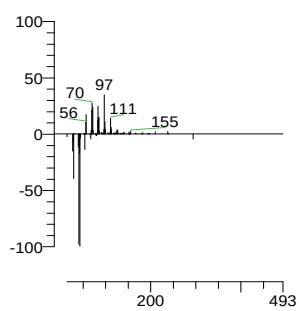
Trifluoroacetic acid, pentadecyl ester
Formula C17H31F3O2, MW 324, CAS# 959010-23-2, Entry# 23039



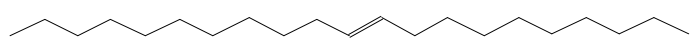


NL: 9.99E2
132971 14.10 1 11
22 2946-2956 2986-2996
7.79E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 941, RSI 980, mainlib,
Entry# 18363, CAS#
95008-11-0,
10-Heneicosene (c,t)

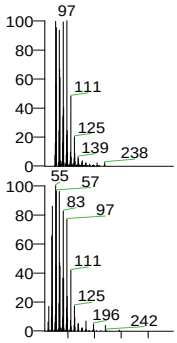


10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



Analysed By: *Checked By:*

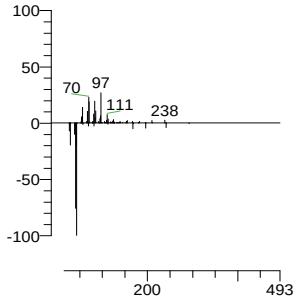
Hit Spectrum



NL: 9.99E2
132971 14.10 1 11
22 2946-2956 2986-2996
7.79E7 + c EI Full ms
[50.00-500.00]

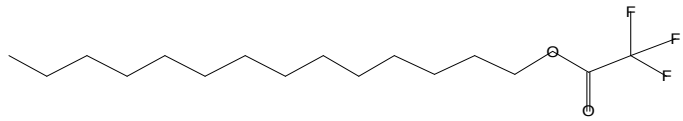
NL: 9.99E2
SI 956, RSI 979, mainlib,
Entry# 18657, CAS#
6222-02-2, Tetradecyl
trifluoroacetate

Delta



Compound Structure

Tetradecyl trifluoroacetate
Formula C16H29F3O2, MW 310, CAS# 6222-02-2, Entry# 18657
Tetradecyl 2,2,2-trifluoroacetate

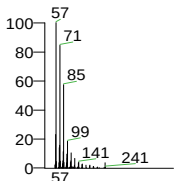


RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.10	3-Eicosene, (E)-	3560927978	2.36	981	74685-33-9	mainlib
14.10	E-14-Hexadecenal	3560927978	2.36	981	330207-53-9	mainlib
14.10	Trifluoroacetic acid, pentadecyl ester	3560927978	2.36	980	959010-23-2	mainlib

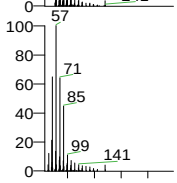
Analysed By:

Checked By:

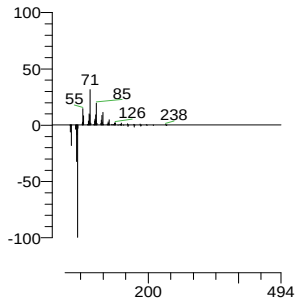
Hit Spectrum	Delta	Compound Structure



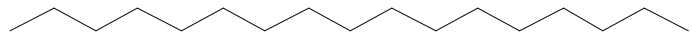
NL: 9.99E2
132993 14.17 1 11
22 2968-2978 3008-3018
1.98E8 + c EI Full ms
[50.00-500.00]

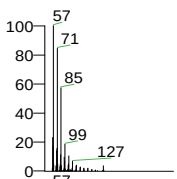


NL: 9.99E2
SI 968, RSI 970, mainlib,
Entry# 22556, CAS#
629-78-7, Heptadecane

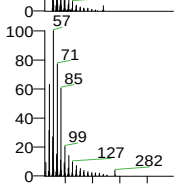


Heptadecane
Formula C17H36, MW 240, CAS# 629-78-7, Entry# 22556
n-Heptadecane

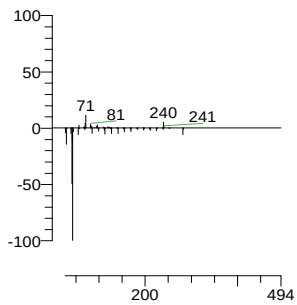




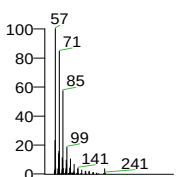
NL: 9.99E2
132993 14.17 1 11
22 2968-2978 3008-3018
1.98E8 + c EI Full ms
[50.00-500.00]



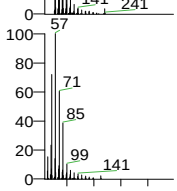
NL: 9.99E2
SI 956, RSI 962, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane



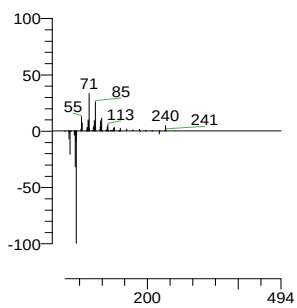
Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane



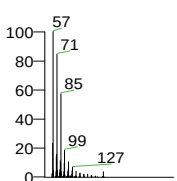
NL: 9.99E2
132993 14.17 1 11
22 2968-2978 3008-3018
1.98E8 + c EI Full ms
[50.00-500.00]



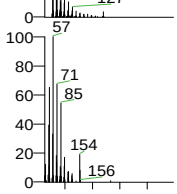
NL: 9.99E2
SI 949, RSI 962, mainlib,
Entry# 22719, CAS#
544-76-3, Hexadecane



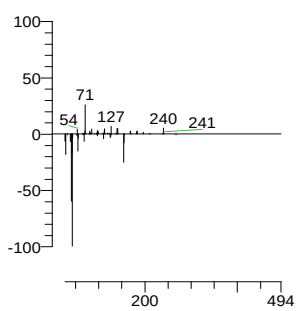
Hexadecane
Formula C16H34, MW 226, CAS# 544-76-3, Entry# 22719
n-Cetane



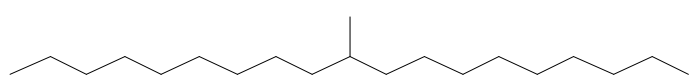
NL: 9.99E2
132993 14.17 1 11
22 2968-2978 3008-3018
1.98E8 + c EI Full ms
[50.00-500.00]



NL: 9.99E2
SI 887, RSI 958, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane

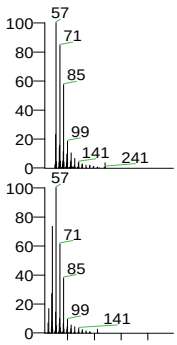


10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



Analysed By: *Checked By:*

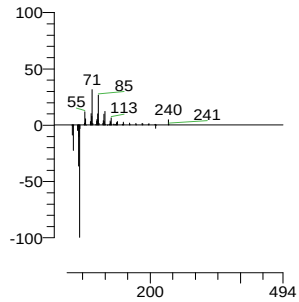
Hit Spectrum



NL: 9.99E2
132993 14.17 1 11
22 2968-2978 3008-3018
1.98E8 + c EI Full ms
[50.00-500.00]

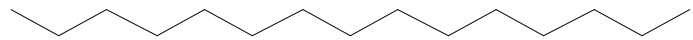
NL: 9.99E2
SI 935, RSI 954, mainlib,
Entry# 22638, CAS#
629-62-9, Pentadecane

Delta



Compound Structure

Pentadecane
Formula C15H32, MW 212, CAS# 629-62-9, Entry# 22638
n-Pentadecane

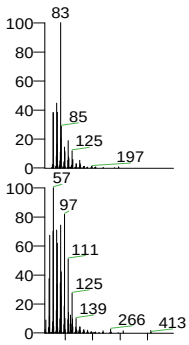


RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.17	Heptadecane	3108859932	2.06	970	629-78-7	mainlib
14.17	Hexadecane	3108859932	2.06	962	544-76-3	mainlib
14.17	Eicosane	3108859932	2.06	962	112-95-8	mainlib

Analysed By:

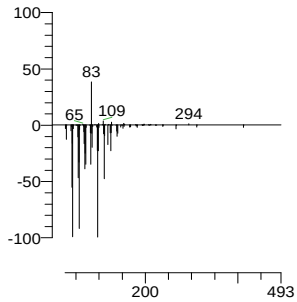
Checked By:

Hit Spectrum	Delta	Compound Structure

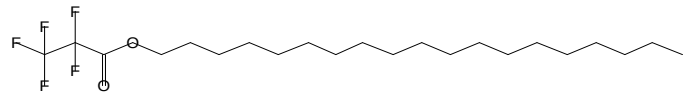


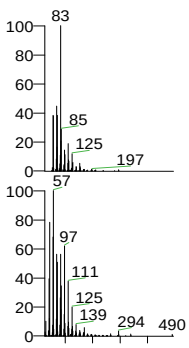
NL: 9.99E2
133020 14.27 1 11
22 2995-3005 3035-3045
7.71E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 888, RSI 892, mainlib, Entry# 24210, CAS# NA, Nonadecyl pentafluoropropionate



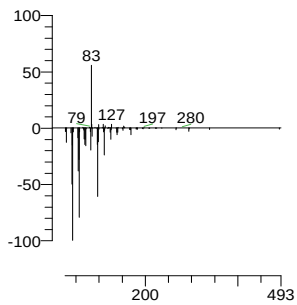
Nonadecyl pentafluoropropionate
Formula C22H39F5O2, MW 430, CAS# NA, Entry# 24210
Nonadecyl 2,2,3,3,3-pentafluoropropanoate



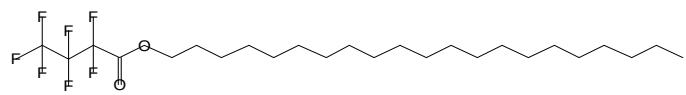


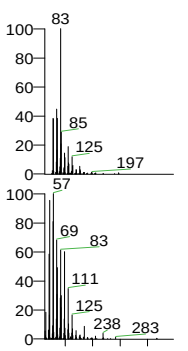
NL: 9.99E2
133020 14.27 1 11
22 2995-3005 3035-3045
7.71E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 887, RSI 891, mainlib, Entry# 22443, CAS# NA, Heneicosyl heptafluorobutyrate



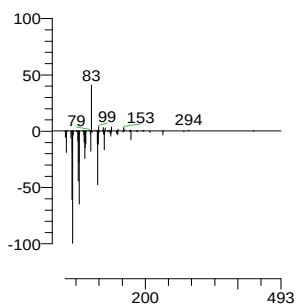
Heneicosyl heptafluorobutyrate
Formula C25H43F7O2, MW 508, CAS# NA, Entry# 22443
Heneicosyl 2,2,3,3,4,4,4-heptafluorobutanoate



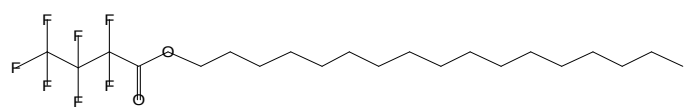


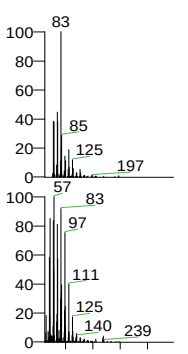
NL: 9.99E2
133020 14.27 1 11
22 2995-3005 3035-3045
7.71E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 883, RSI 891, mainlib, Entry# 22456, CAS# 959085-66-6, Heptadecyl heptafluorobutyrate



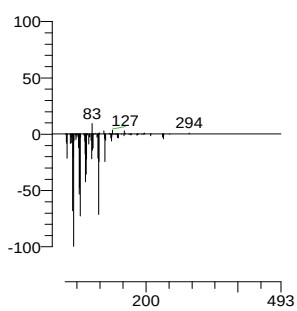
Heptadecyl heptafluorobutyrate
Formula C21H35F7O2, MW 452, CAS# 959085-66-6, Entry# 22456
Heptadecyl 2,2,3,3,4,4,4-heptafluorobutanoate



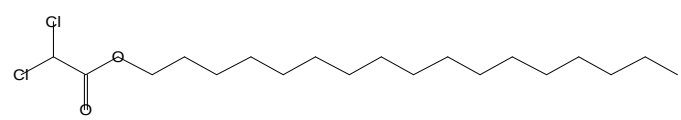


NL: 9.99E2
133020 14.27 1 11
22 2995-3005 3035-3045
7.71E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 884, RSI 889, mainlib, Entry# 23863, CAS# NA, Dichloroacetic acid, heptadecyl ester

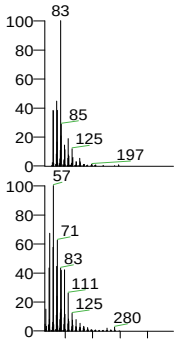


Dichloroacetic acid, heptadecyl ester
Formula C19H36Cl2O2, MW 366, CAS# NA, Entry# 23863
Heptadecyl dichloroacetate #



Analysed By: *Checked By:*

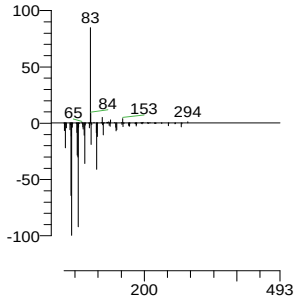
Hit Spectrum



NL: 9.99E2
133020 14.27 1 11
22 2995-3005 3035-3045
7.71E7 + c EI Full ms
[50.00-500.00]

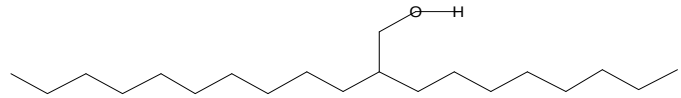
NL: 9.99E2
SI 882, RSI 888, mainlib,
Entry# 22667, CAS#
5333-42-6, 1-Dodecanol,
2-octyl-

Delta



Compound Structure

1-Dodecanol, 2-octyl-
Formula C20H42O, MW 298, CAS# 5333-42-6, Entry# 22667
Eutanol G

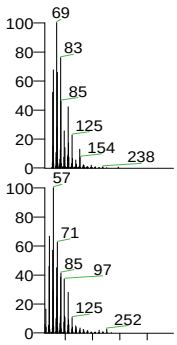


RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.27	Nonadecyl pentafluoropropionate	1518131799	1.01	892	NA	mainlib
14.27	Heptadecyl heptafluorobutyrate	1518131799	1.01	891	959085-66-6	mainlib
14.27	Heneicosyl heptafluorobutyrate	1518131799	1.01	891	NA	mainlib

Analysed By:

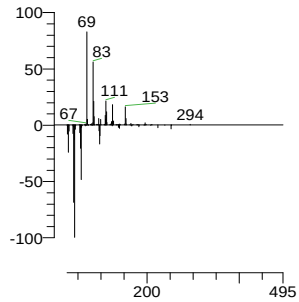
Checked By:

Hit Spectrum	Delta	Compound Structure

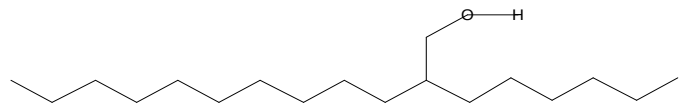


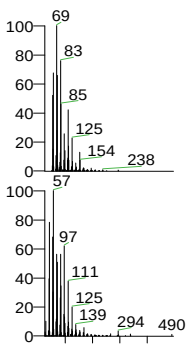
NL: 9.99E2
133120 14.61 1 11
22 3095-3105 3135-3145
1.10E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 920, RSI 924, mainlib, Entry# 22630, CAS# 110225-00-8, 1-Dodecanol, 2-hexyl-



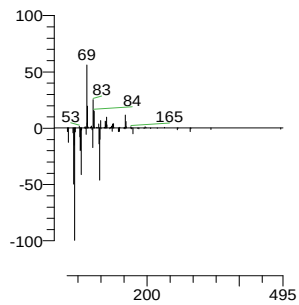
1-Dodecanol, 2-hexyl-
Formula C18H38O, MW 270, CAS# 110225-00-8, Entry# 22630
2-Hexyldodecan-1-ol



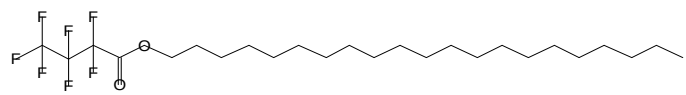


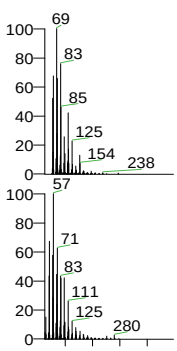
NL: 9.99E2
133120 14.61 1 11
22 3095-3105 3135-3145
1.10E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 917, RSI 920, mainlib, Entry# 22443, CAS# NA, Heneicosyl heptafluorobutyrate



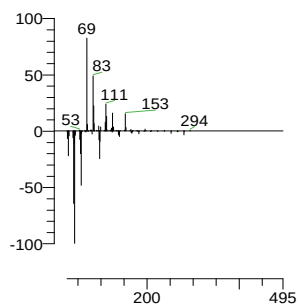
Heneicosyl heptafluorobutyrate
Formula C25H43F7O2, MW 508, CAS# NA, Entry# 22443
Heneicosyl 2,2,3,3,4,4,4-heptafluorobutanoate



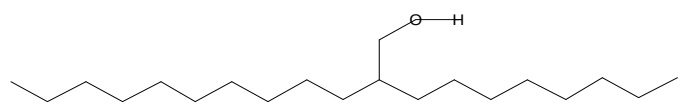


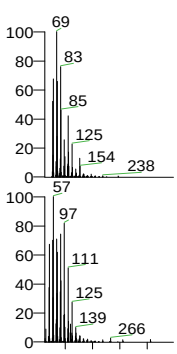
NL: 9.99E2
133120 14.61 1 11
22 3095-3105 3135-3145
1.10E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 916, RSI 919, mainlib, Entry# 22667, CAS# 5333-42-6, 1-Dodecanol, 2-octyl-



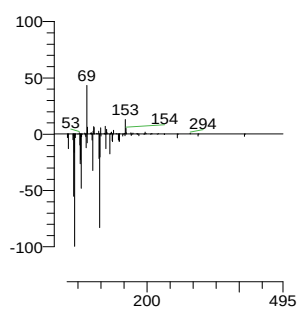
1-Dodecanol, 2-octyl-
Formula C20H42O, MW 298, CAS# 5333-42-6, Entry# 22667
Eutanol G



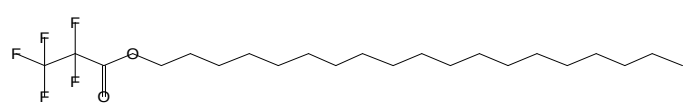


NL: 9.99E2
133120 14.61 1 11
22 3095-3105 3135-3145
1.10E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 915, RSI 919, mainlib, Entry# 24210, CAS# NA, Nonadecyl pentafluoropropionate

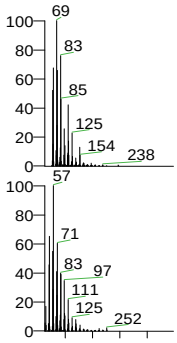


Nonadecyl pentafluoropropionate
Formula C22H39F5O2, MW 430, CAS# NA, Entry# 24210
Nonadecyl 2,2,3,3,3-pentafluoropropanoate



Analysed By: *Checked By:*

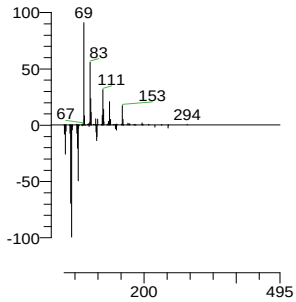
Hit Spectrum



NL: 9.99E2
133120 14.61 1 11
22 3095-3105 3135-3145
1.10E8 + c EI Full ms
[50.00-500.00]

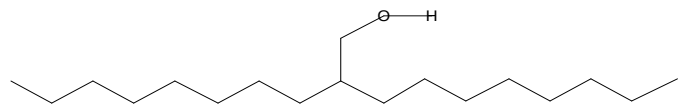
NL: 9.99E2
SI 914, RSI 918, mainlib,
Entry# 22554, CAS#
45235-48-1, 1-Decanol,
2-octyl-

Delta



Compound Structure

1-Decanol, 2-octyl-
Formula C18H38O, MW 270, CAS# 45235-48-1, Entry# 22554
2-Octyldecan-1-ol

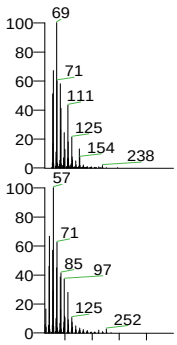


RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.61	1-Dodecanol, 2-hexyl-	2131474151	1.41	924	110225-00-8	mainlib
14.61	Heneicosyl heptafluorobutyrate	2131474151	1.41	920	NA	mainlib
14.61	1-Dodecanol, 2-octyl-	2131474151	1.41	919	5333-42-6	mainlib

Analysed By:

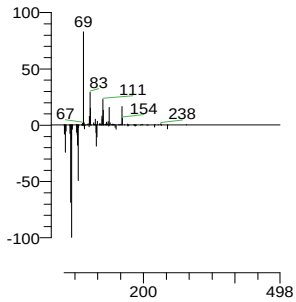
Checked By:

Hit Spectrum	Delta	Compound Structure

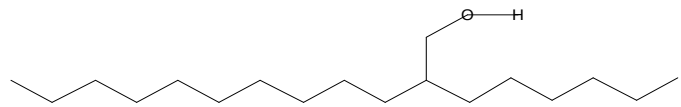


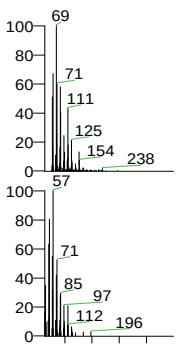
NL: 9.99E2
133203 14.89 1 11
22 3178-3188 3218-3228
8.33E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 919, RSI 933, mainlib,
Entry# 22630, CAS#
110225-00-8,
1-Dodecanol, 2-hexyl-



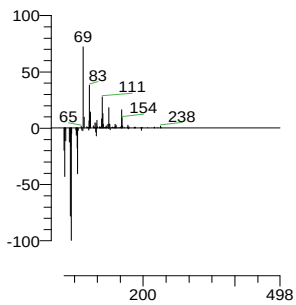
1-Dodecanol, 2-hexyl-
Formula C18H38O, MW 270, CAS# 110225-00-8, Entry# 22630
2-Hexyldodecan-1-ol



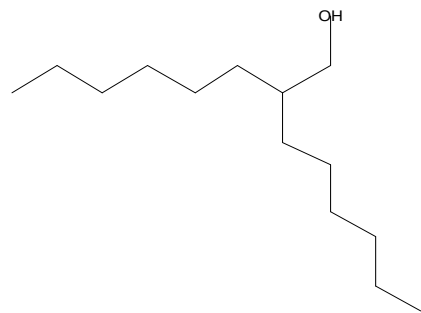


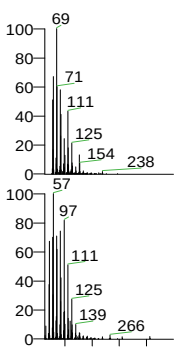
NL: 9.99E2
133203 14.89 1 11
22 3178-3188 3218-3228
8.33E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 840, RSI 931, mainlib,
Entry# 22406, CAS#
19780-79-1,
2-Hexyl-1-octanol



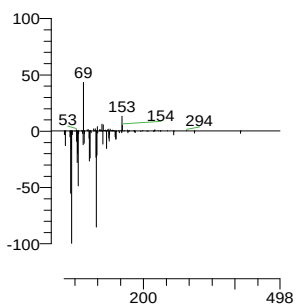
2-Hexyl-1-octanol
Formula C14H30O, MW 214, CAS# 19780-79-1, Entry# 22406



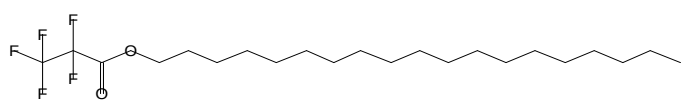


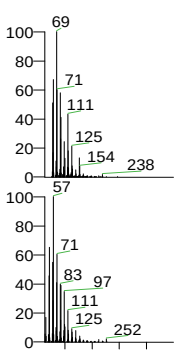
NL: 9.99E2
133203 14.89 1 11
22 3178-3188 3218-3228
8.33E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 910, RSI 925, mainlib,
Entry# 24210, CAS# NA,
Nonadecyl
pentafluoropropionate



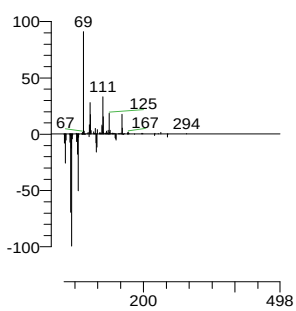
Nonadecyl pentafluoropropionate
Formula C22H39F5O2, MW 430, CAS# NA, Entry# 24210
Nonadecyl 2,2,3,3,3-pentafluoropropanoate



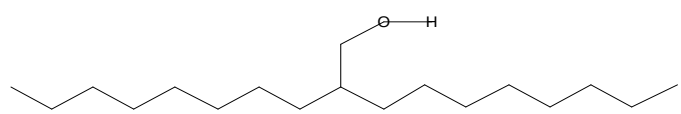


NL: 9.99E2
133203 14.89 1 11
22 3178-3188 3218-3228
8.33E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 910, RSI 924, mainlib,
Entry# 22554, CAS#
45235-48-1, 1-Decanol,
2-octyl-

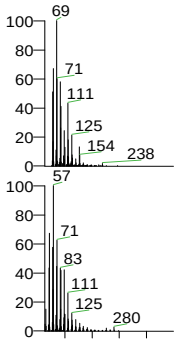


1-Decanol, 2-octyl-
Formula C18H38O, MW 270, CAS# 45235-48-1, Entry# 22554
2-Octyldecan-1-ol

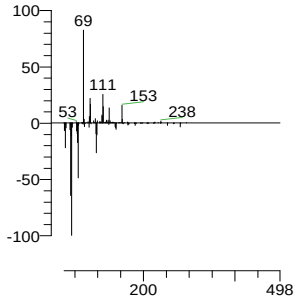


Analysed By: *Checked By:*

Hit Spectrum

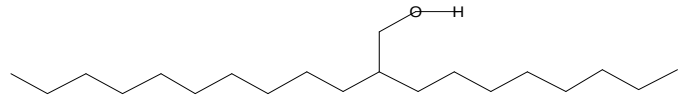


Delta



Compound Structure

1-Dodecanol, 2-octyl-
Formula C20H42O, MW 298, CAS# 5333-42-6, Entry# 22667
Eutanol G

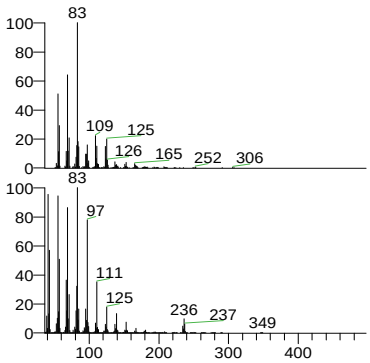


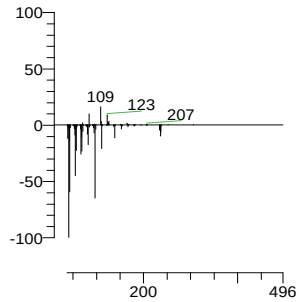
RT	Compound Name	Area	Area %	RSI	Cas #	Library
14.89	1-Dodecanol, 2-hexyl-	1517211604	1.01	933	110225-00-8	mainlib
14.89	2-Hexyl-1-octanol	1517211604	1.01	931	19780-79-1	mainlib
14.89	Nonadecyl pentafluoropropionate	1517211604	1.01	925	NA	mainlib

Analysed By:

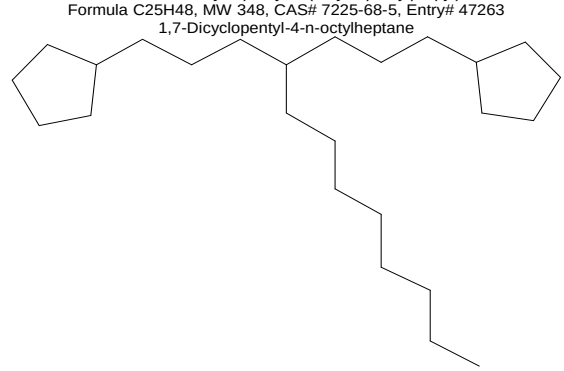
Checked By:

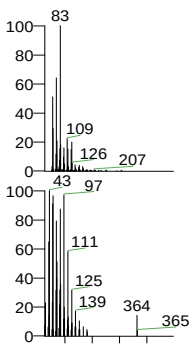
Hit Spectrum	Delta	Compound Structure





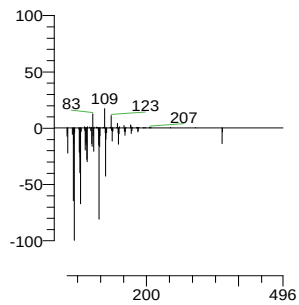
Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-
Formula C25H48, MW 348, CAS# 7225-68-5, Entry# 47263
1,7-Dicyclopentyl-4-n-octylheptane



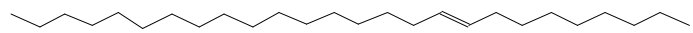


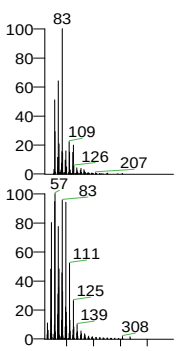
NL: 9.99E2
133249 15.05 1 11
22 3224-3234 3264-3274
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 817, RSI 869, mainlib,
Entry# 9856, CAS#
71502-22-2,
9-Hexacosene



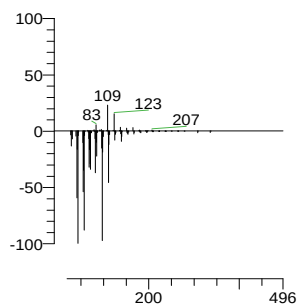
9-Hexacosene
Formula C26H52, MW 364, CAS# 71502-22-2, Entry# 9856
(9E)-9-Hexacosene #



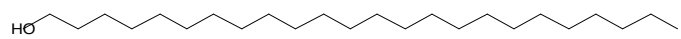


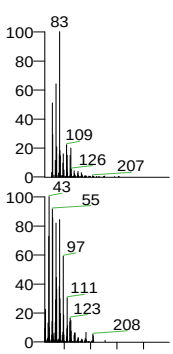
NL: 9.99E2
133249 15.05 1 11
22 3224-3234 3264-3274
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 863, RSI 867, mainlib,
Entry# 23874, CAS#
506-51-4,
n-Tetracosanol-1



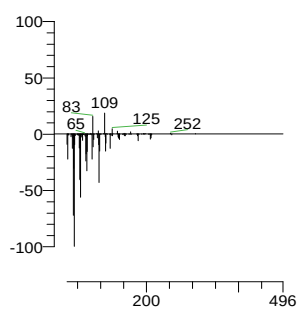
n-Tetracosanol-1
Formula C24H50O, MW 354, CAS# 506-51-4, Entry# 23874
Lignoceric alcohol



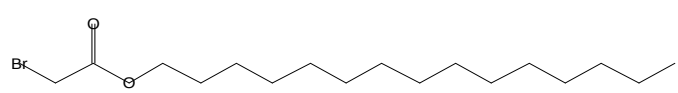


NL: 9.99E2
133249 15.05 1 11
22 3224-3234 3264-3274
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 860, RSI 865, mainlib,
Entry# 6846, CAS#
131143-01-6,
Bromoacetic acid,
pentadecyl ester

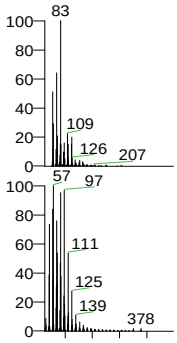


Bromoacetic acid, pentadecyl ester
Formula C17H33BrO2, MW 348, CAS# 131143-01-6, Entry# 6846
Pentadecyl bromoacetate #



Analysed By: *Checked By:*

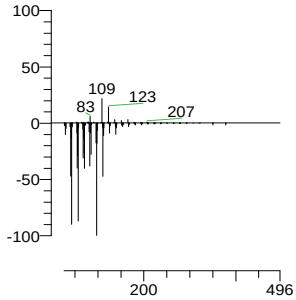
Hit Spectrum



NL: 9.99E2
133249 15.05 1 11
22 3224-3234 3264-3274
7.02E7 + c EI Full ms
[50.00-500.00]

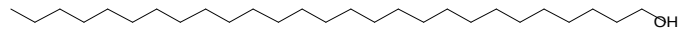
NL: 9.99E2
SI 859, RSI 865, mainlib,
Entry# 24212, CAS#
2004-39-9,
1-Heptacosanol

Delta



Compound Structure

1-Heptacosanol
Formula C27H56O, MW 396, CAS# 2004-39-9, Entry# 24212
Heptacosan-1-ol

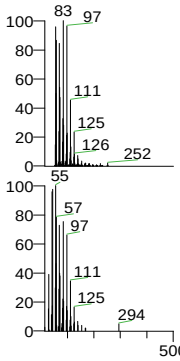


RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.05	Dodecane, 1-cyclopentyl-4-(3-cyclopentylpropyl)-	874079911	0.58	882	7225-68-5	mainlib
15.05	9-Hexacosene	874079911	0.58	869	71502-22-2	mainlib
15.05	n-Tetracosanol-1	874079911	0.58	867	506-51-4	mainlib

Analysed By:

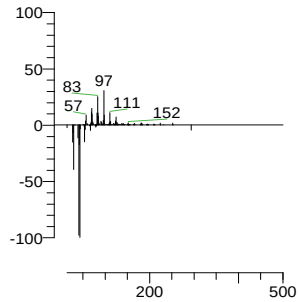
Checked By:

Hit Spectrum	Delta	Compound Structure

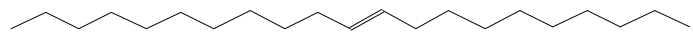


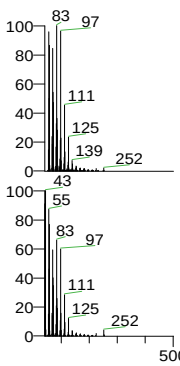
NL: 9.99E2
133280 15.15 1 11
22 3255-3265 3295-3305
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 926, RSI 982, mainlib,
Entry# 18363, CAS#
95008-11-0,
10-Heneicosene (c,t)



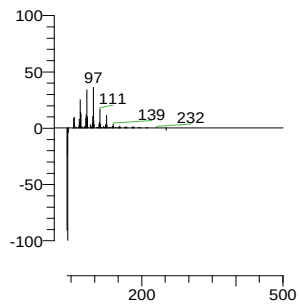
10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



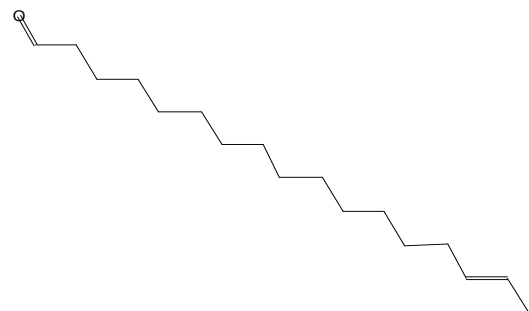


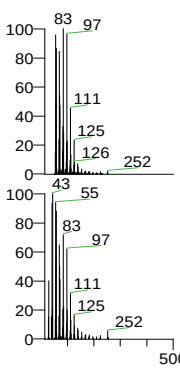
NL: 9.99E2
133280 15.15 1 11
22 3255-3265 3295-3305
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 968, RSI 980, mainlib,
Entry# 5592, CAS# NA,
E-15-Heptadecenal



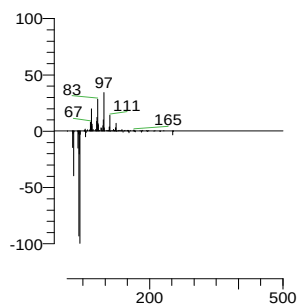
E-15-Heptadecenal
Formula C17H32O, MW 252, CAS# NA, Entry# 5592
(15E)-15-Heptadecenal #



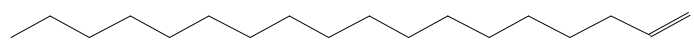


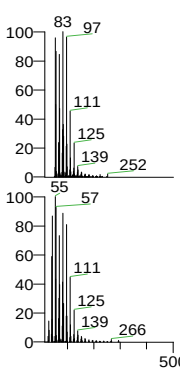
NL: 9.99E2
133280 15.15 1 11
22 3255-3265 3295-3305
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 956, RSI 978, mainlib,
Entry# 6808, CAS#
112-88-9, 1-Octadecene



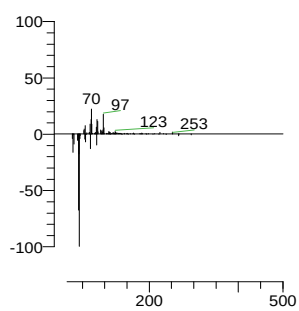
1-Octadecene
Formula C18H36, MW 252, CAS# 112-88-9, Entry# 6808
à-Octadecene



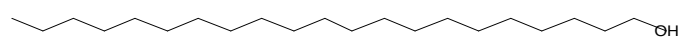


NL: 9.99E2
133280 15.15 1 11
22 3255-3265 3295-3305
7.02E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 954, RSI 977, mainlib,
Entry# 18669, CAS#
15594-90-8,
1-Heneicosanol

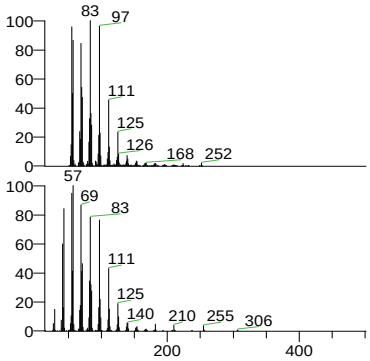


1-Heneicosanol
Formula C21H44O, MW 312, CAS# 15594-90-8, Entry# 18669
Henicosan-1-ol

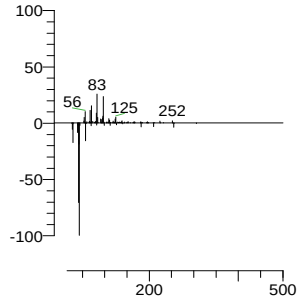


Analysed By: *Checked By:*

Hit Spectrum

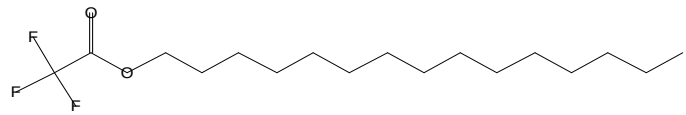


Delta



Compound Structure

Trifluoroacetic acid, pentadecyl ester
Formula C17H31F3O2, MW 324, CAS# 959010-23-2, Entry# 23039

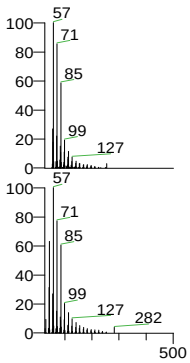


RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.15	10-Heneicosene (c,t)	2409972010	1.60	982	95008-11-0	mainlib
15.15	E-15-Heptadecenal	2409972010	1.60	980	NA	mainlib
15.15	1-Octadecene	2409972010	1.60	978	112-88-9	mainlib

Analysed By:

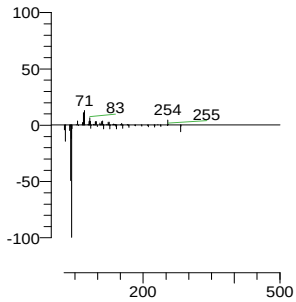
Checked By:

Hit Spectrum	Delta	Compound Structure

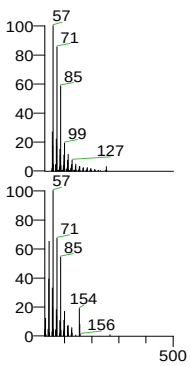


NL: 9.99E2
133300 15.22 1 11
22 3275-3285 3315-3325
1.77E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 949, RSI 969, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

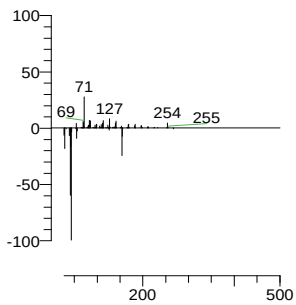


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

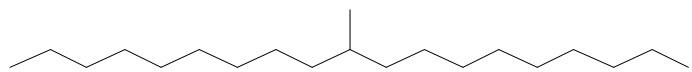


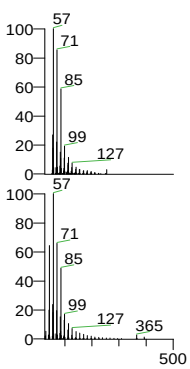
NL: 9.99E2
133300 15.22 1 11
22 3275-3285 3315-3325
1.77E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 875, RSI 962, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane



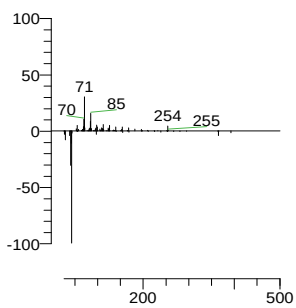
10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



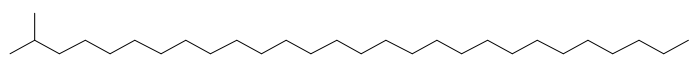


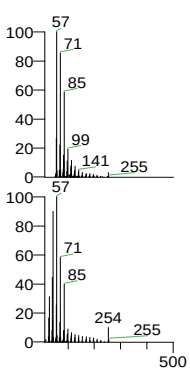
NL: 9.99E2
133300 15.22 1 11
22 3275-3285 3315-3325
1.77E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 920, RSI 955, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane



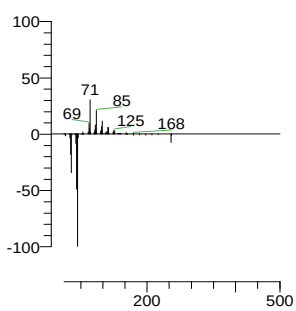
2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536



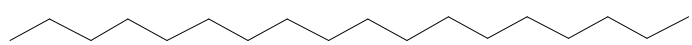


NL: 9.99E2
133300 15.22 1 11
22 3275-3285 3315-3325
1.77E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 938, RSI 950, mainlib,
Entry# 22577, CAS#
593-45-3, Octadecane

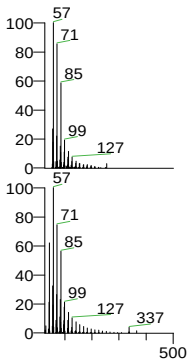


Octadecane
Formula C18H38, MW 254, CAS# 593-45-3, Entry# 22577
n-Octadecane

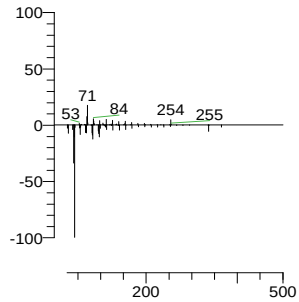


Analysed By: *Checked By:*

Hit Spectrum

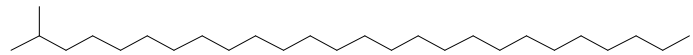


Delta



Compound Structure

2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535

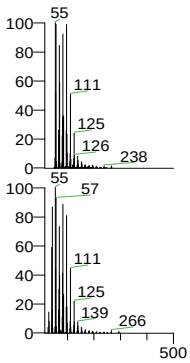


RT	Compound Name	Area	Area %	RSI	Cas #	Library
15.22	Eicosane	3680539172	2.44	969	112-95-8	mainlib
15.22	10-Methylnonadecane	3680539172	2.44	962	56862-62-5	mainlib
15.22	2-methyloctacosane	3680539172	2.44	955	NA	mainlib

Analysed By:

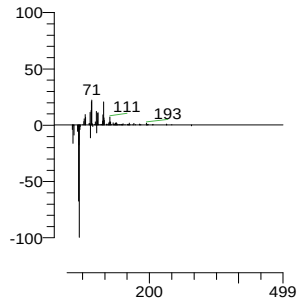
Checked By:

Hit Spectrum	Delta	Compound Structure

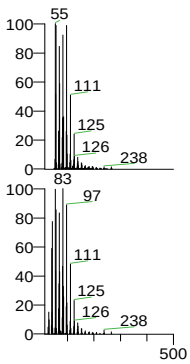


NL: 9.98E2
133571 16.14 1 11
22 3546-3556 3586-3596
4.96E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 972, RSI 984, mainlib,
Entry# 18669, CAS#
15594-90-8,
1-Heneicosanol

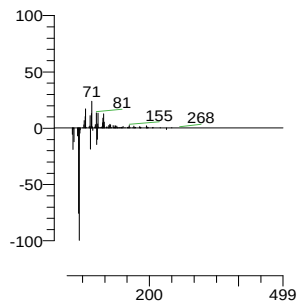


1-Heneicosanol
Formula C21H44O, MW 312, CAS# 15594-90-8, Entry# 18669
Henicosan-1-ol

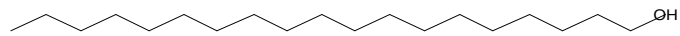


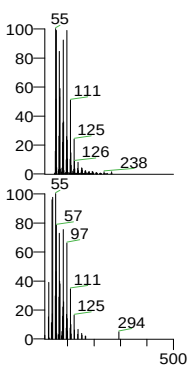
NL: 9.98E2
133571 16.14 1 11
22 3546-3556 3586-3596
4.96E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 970, RSI 983, mainlib,
Entry# 47640, CAS#
1454-84-8,
n-Nonadecanol-1



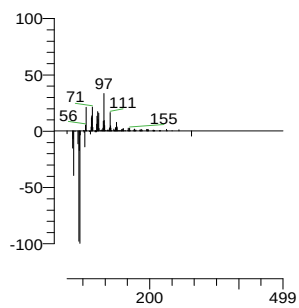
n-Nonadecanol-1
Formula C19H40O, MW 284, CAS# 1454-84-8, Entry# 47640
1-Nonadecanol



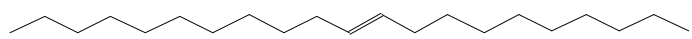


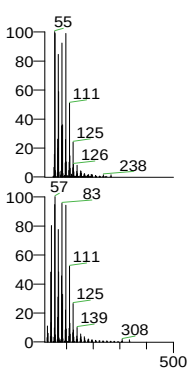
NL: 9.98E2
133571 16.14 1 11
22 3546-3556 3586-3596
4.96E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 927, RSI 982, mainlib,
Entry# 18363, CAS#
95008-11-0,
10-Heneicosene (c,t)



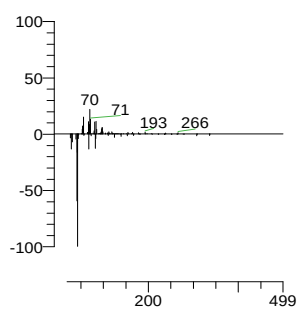
10-Heneicosene (c,t)
Formula C21H42, MW 294, CAS# 95008-11-0, Entry# 18363
(10E)-10-Henicosene #



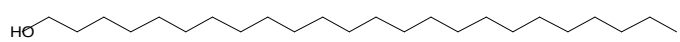


NL: 9.98E2
133571 16.14 1 11
22 3546-3556 3586-3596
4.96E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 971, RSI 979, mainlib,
Entry# 23874, CAS#
506-51-4,
n-Tetracosanol-1

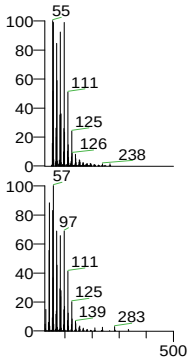


n-Tetracosanol-1
Formula C24H50O, MW 354, CAS# 506-51-4, Entry# 23874
Lignoceric alcohol



Analysed By: *Checked By:*

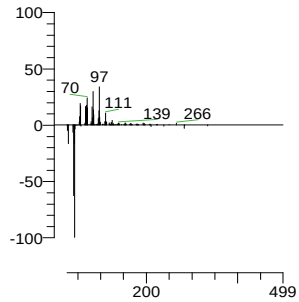
Hit Spectrum



NL: 9.98E2
133571 16.14 1 11
22 3546-3556 3586-3596
4.96E7 + c EI Full ms
[50.00-500.00]

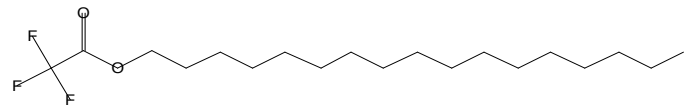
NL: 9.99E2
SI 961, RSI 978, mainlib,
Entry# 22444, CAS# NA,
Heptadecyl
trifluoroacetate

Delta



Compound Structure

Heptadecyl trifluoroacetate
Formula C19H35F3O2, MW 352, CAS# NA, Entry# 22444
Heptadecyl 2,2,2-trifluoroacetate

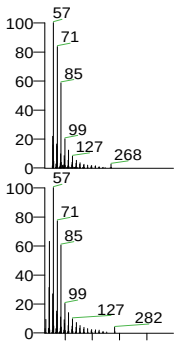


RT	Compound Name	Area	Area %	RSI	Cas #	Library
16.14	1-Heneicosanol	1539463410	1.02	984	15594-90-8	mainlib
16.14	n-Nonadecanol-1	1539463410	1.02	983	1454-84-8	mainlib
16.14	10-Heneicosene (c,t)	1539463410	1.02	982	95008-11-0	mainlib

Analysed By:

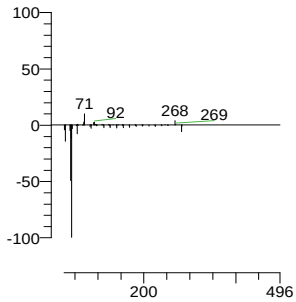
Checked By:

Hit Spectrum	Delta	Compound Structure

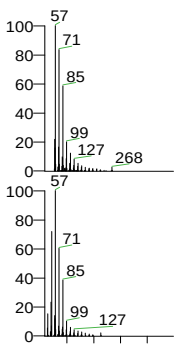


NL: 9.99E2
133589 16.20 1 11
22 3564-3574 3604-3614
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 968, RSI 983, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

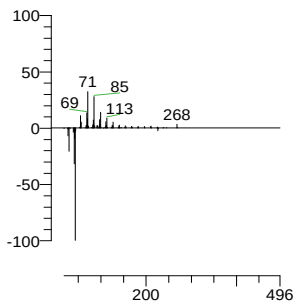


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

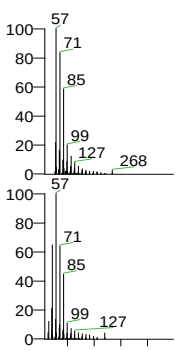


NL: 9.99E2
133589 16.20 1 11
22 3564-3574 3604-3614
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 945, RSI 966, mainlib,
Entry# 22719, CAS#
544-76-3, Hexadecane

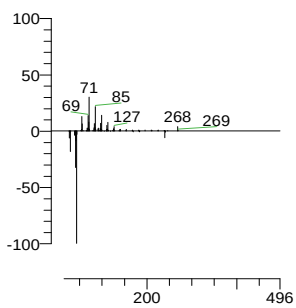


Hexadecane
Formula C16H34, MW 226, CAS# 544-76-3, Entry# 22719
n-Cetane

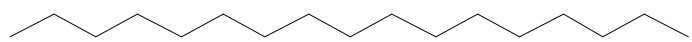


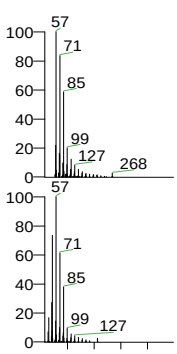
NL: 9.99E2
133589 16.20 1 11
22 3564-3574 3604-3614
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 947, RSI 962, mainlib,
Entry# 22556, CAS#
629-78-7, Heptadecane



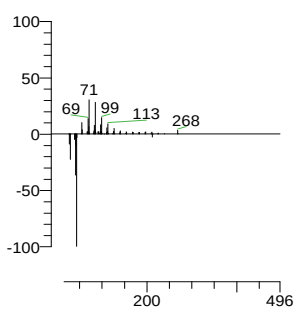
Heptadecane
Formula C17H36, MW 240, CAS# 629-78-7, Entry# 22556
n-Heptadecane



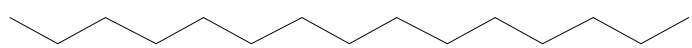


NL: 9.99E2
133589 16.20 1 11
22 3564-3574 3604-3614
1.63E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 929, RSI 960, mainlib,
Entry# 22638, CAS#
629-62-9, Pentadecane

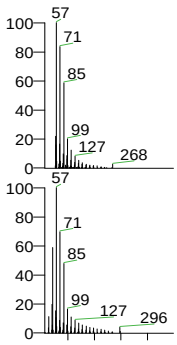


Pentadecane
Formula C15H32, MW 212, CAS# 629-62-9, Entry# 22638
n-Pentadecane



Analysed By: *Checked By:*

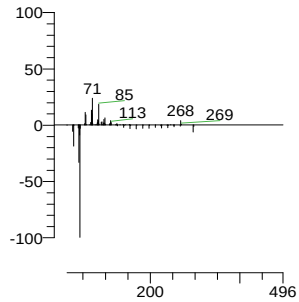
Hit Spectrum



NL: 9.99E2
133589 16.20 1 11
22 3564-3574 3604-3614
1.63E8 + c EI Full ms
[50.00-500.00]

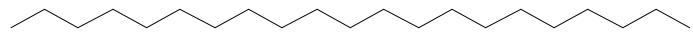
NL: 9.99E2
SI 946, RSI 957, mainlib,
Entry# 23607, CAS#
629-94-7, Heneicosane

Delta



Compound Structure

Heneicosane
Formula C21H44, MW 296, CAS# 629-94-7, Entry# 23607
n-Heneicosane

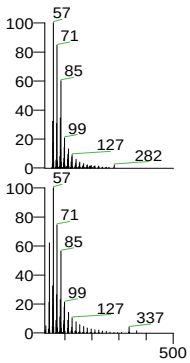


RT	Compound Name	Area	Area %	RSI	Cas #	Library
16.20	Eicosane	2626909217	1.74	983	112-95-8	mainlib
16.20	Hexadecane	2626909217	1.74	966	544-76-3	mainlib
16.20	Heptadecane	2626909217	1.74	962	629-78-7	mainlib

Analysed By:

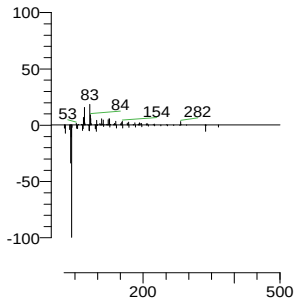
Checked By:

Hit Spectrum	Delta	Compound Structure

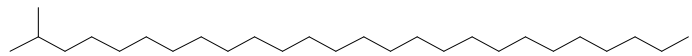


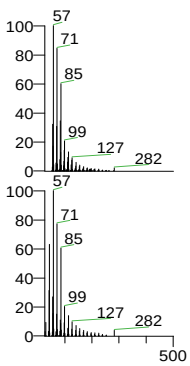
NL: 9.99E2
133866 17.14 1 11
22 3841-3851 3881-3891
1.51E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 929, RSI 957, mainlib,
Entry# 23535, CAS# NA,
2-methylhexacosane



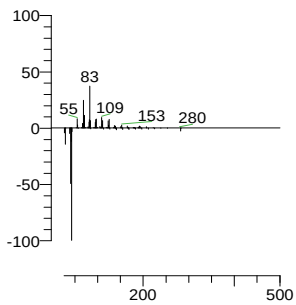
2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535



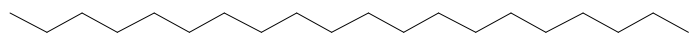


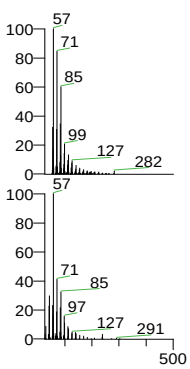
NL: 9.99E2
133866 17.14 1 11
22 3841-3851 3881-3891
1.51E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 928, RSI 956, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane



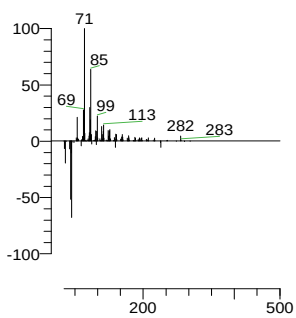
Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane



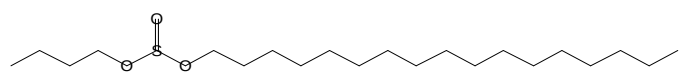


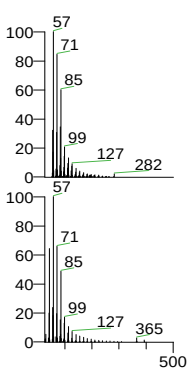
NL: 9.99E2
133866 17.14 1 11
22 3841-3851 3881-3891
1.51E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 879, RSI 944, mainlib,
Entry# 23670, CAS# NA,
Sulfurous acid, butyl
heptadecyl ester



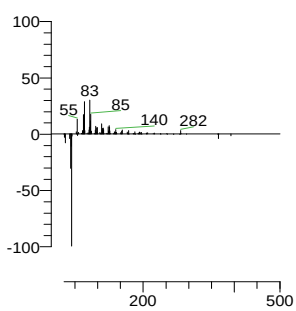
Sulfurous acid, butyl heptadecyl ester
Formula C21H44O3S, MW 376, CAS# NA, Entry# 23670



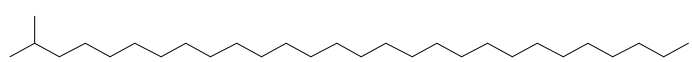


NL: 9.99E2
133866 17.14 1 11
22 3841-3851 3881-3891
1.51E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 900, RSI 943, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane

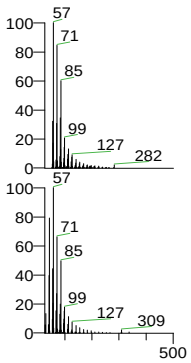


2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536

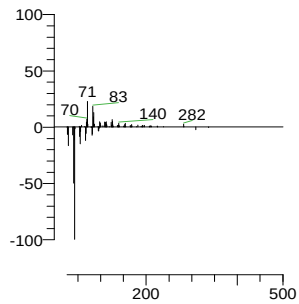


Analysed By: *Checked By:*

Hit Spectrum

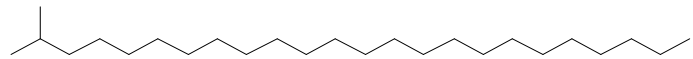


Delta



Compound Structure

2-methyltetracosane
Formula C25H52, MW 352, CAS# NA, Entry# 22537

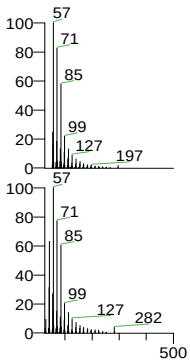


RT	Compound Name	Area	Area %	RSI	Cas #	Library
17.14	2-methylhexacosane	4086590346	2.71	957	NA	mainlib
17.14	Eicosane	4086590346	2.71	956	112-95-8	mainlib
17.14	Sulfurous acid, butyl heptadecyl ester	4086590346	2.71	944	NA	mainlib

Analysed By:

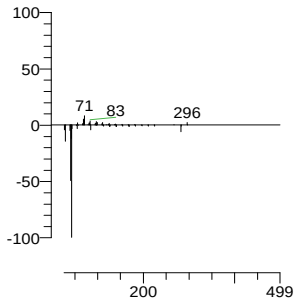
Checked By:

Hit Spectrum	Delta	Compound Structure

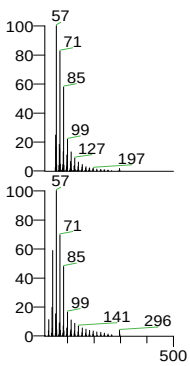


NL: 9.99E2
134131 18.04 1 11
22 4106-4116 4146-4156
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 975, RSI 982, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

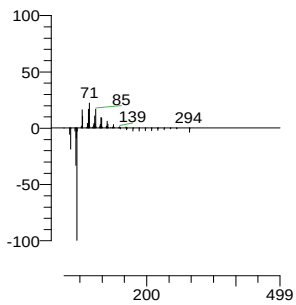


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

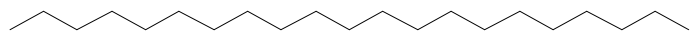


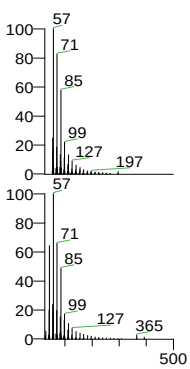
NL: 9.99E2
134131 18.04 1 11
22 4106-4116 4146-4156
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 962, RSI 966, mainlib,
Entry# 23607, CAS#
629-94-7, Heneicosane



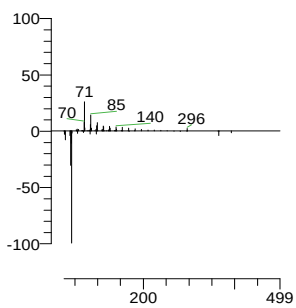
Heneicosane
Formula C21H44, MW 296, CAS# 629-94-7, Entry# 23607
n-Heneicosane



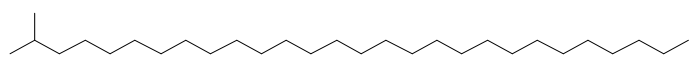


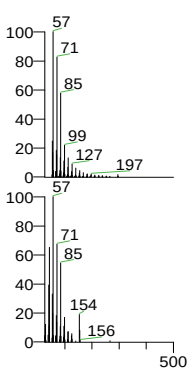
NL: 9.99E2
134131 18.04 1 11
22 4106-4116 4146-4156
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 947, RSI 964, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane



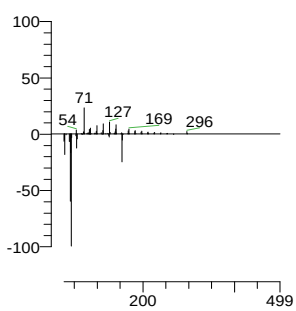
2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536



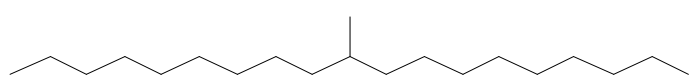


NL: 9.99E2
134131 18.04 1 11
22 4106-4116 4146-4156
1.26E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 889, RSI 960, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane

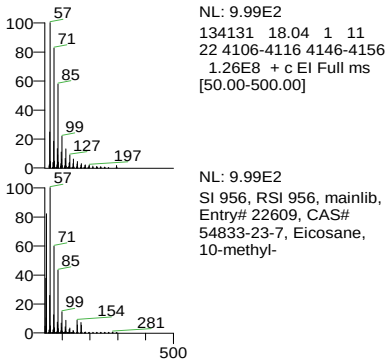


10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl

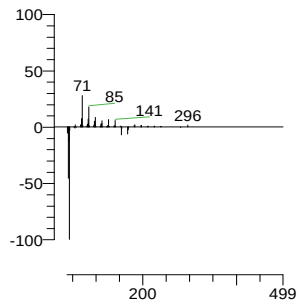


Analysed By: *Checked By:*

Hit Spectrum

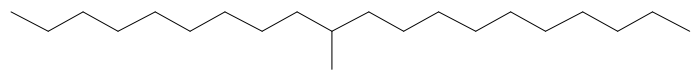


Delta



Compound Structure

Eicosane, 10-methyl-
Formula C21H44, MW 296, CAS# 54833-23-7, Entry# 22609
10-Methylicosane #

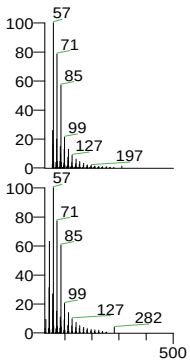


RT	Compound Name	Area	Area %	RSI	Cas #	Library
18.04	Eicosane	2891362267	1.92	982	112-95-8	mainlib
18.04	Heneicosane	2891362267	1.92	966	629-94-7	mainlib
18.04	2-methyloctacosane	2891362267	1.92	964	NA	mainlib

Analysed By:

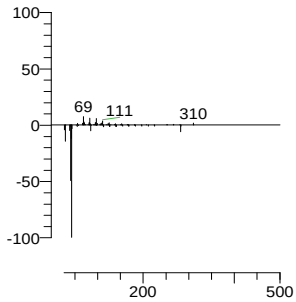
Checked By:

Hit Spectrum	Delta	Compound Structure

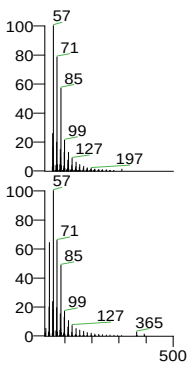


NL: 9.99E2
134385 18.91 1 11
22 4360-4370 4400-4410
1.06E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 963, RSI 977, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

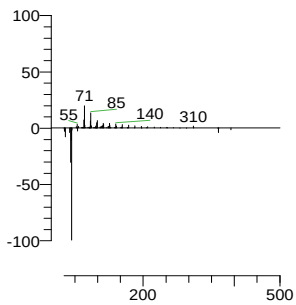


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

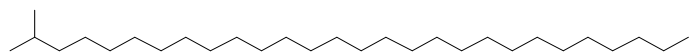


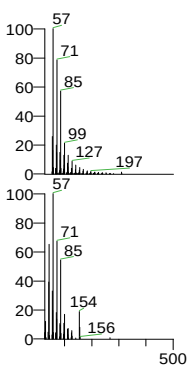
NL: 9.99E2
134385 18.91 1 11
22 4360-4370 4400-4410
1.06E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 943, RSI 964, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane



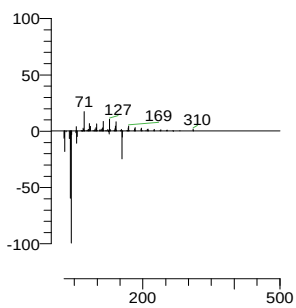
2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536



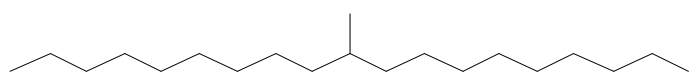


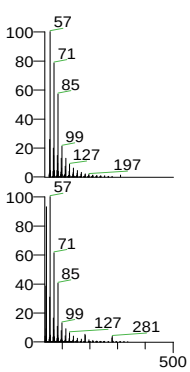
NL: 9.99E2
134385 18.91 1 11
22 4360-4370 4400-4410
1.06E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 881, RSI 960, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane



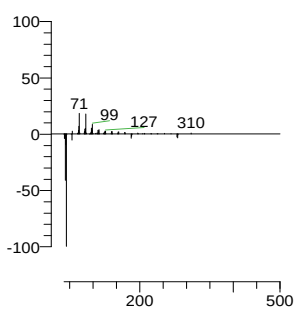
10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



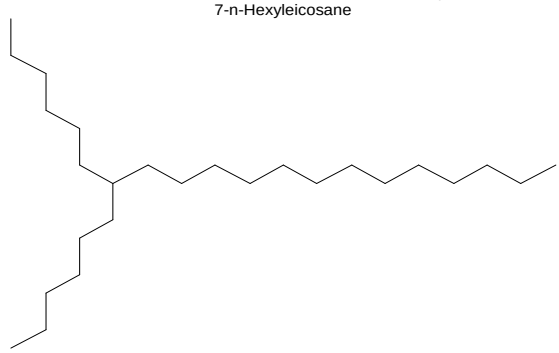


NL: 9.99E2
134385 18.91 1 11
22 4360-4370 4400-4410
1.06E8 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 956, RSI 959, mainlib,
Entry# 22628, CAS#
55333-99-8, Eicosane,
7-hexyl-

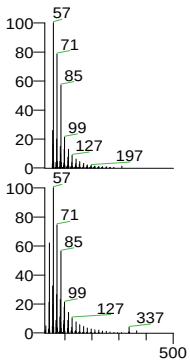


Eicosane, 7-hexyl-
Formula C26H54, MW 366, CAS# 55333-99-8, Entry# 22628
7-n-Hexyleicosane

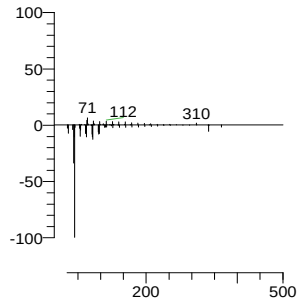


Analysed By: *Checked By:*

Hit Spectrum

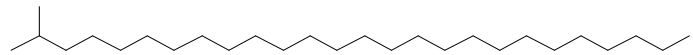


Delta



Compound Structure

2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535

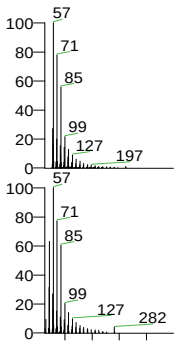


RT	Compound Name	Area	Area %	RSI	Cas #	Library
18.91	Eicosane	2465669529	1.64	977	112-95-8	mainlib
18.91	2-methyloctacosane	2465669529	1.64	964	NA	mainlib
18.91	10-Methylnonadecane	2465669529	1.64	960	56862-62-5	mainlib

Analysed By:

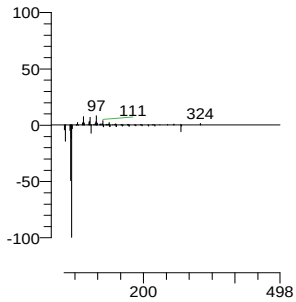
Checked By:

Hit Spectrum	Delta	Compound Structure

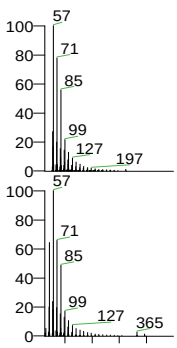


NL: 9.99E2
134626 19.73 1 11
22 4601-4611 4641-4651
8.26E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 959, RSI 975, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

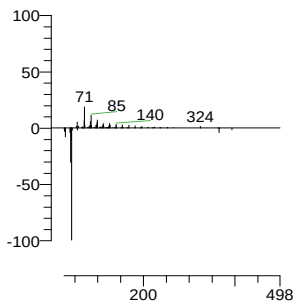


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

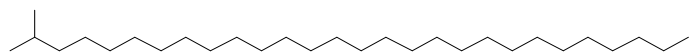


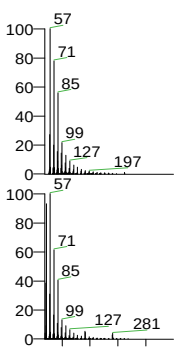
NL: 9.99E2
134626 19.73 1 11
22 4601-4611 4641-4651
8.26E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 943, RSI 966, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane



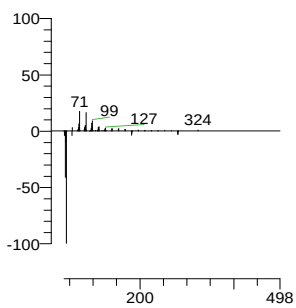
2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536



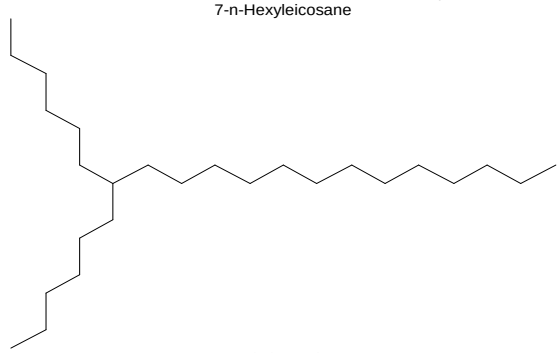


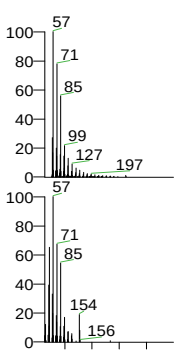
NL: 9.99E2
134626 19.73 1 11
22 4601-4611 4641-4651
8.26E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 957, RSI 962, mainlib,
Entry# 22628, CAS#
55333-99-8, Eicosane,
7-hexyl-



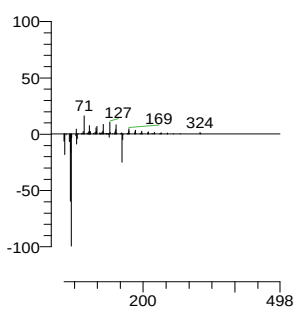
Eicosane, 7-hexyl-
Formula C26H54, MW 366, CAS# 55333-99-8, Entry# 22628
7-n-Hexyleicosane



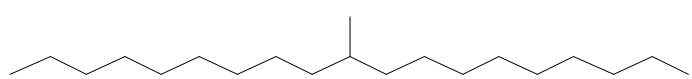


NL: 9.99E2
134626 19.73 1 11
22 4601-4611 4641-4651
8.26E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 881, RSI 960, mainlib,
Entry# 23599, CAS#
56862-62-5,
10-Methylnonadecane

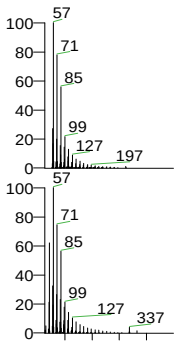


10-Methylnonadecane
Formula C20H42, MW 282, CAS# 56862-62-5, Entry# 23599
Nonadecane, 10-methyl



Analysed By: *Checked By:*

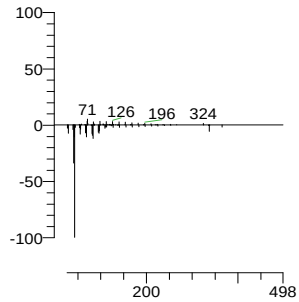
Hit Spectrum



NL: 9.99E2
134626 19.73 1 11
22 4601-4611 4641-4651
8.26E7 + c EI Full ms
[50.00-500.00]

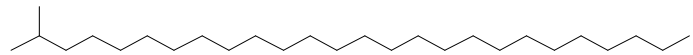
NL: 9.99E2
SI 943, RSI 958, mainlib,
Entry# 23535, CAS# NA,
2-methylhexacosane

Delta



Compound Structure

2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535

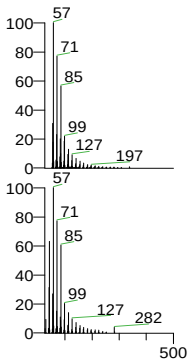


RT	Compound Name	Area	Area %	RSI	Cas #	Library
19.73	Eicosane	1640671809	1.09	975	112-95-8	mainlib
19.73	2-methyloctacosane	1640671809	1.09	966	NA	mainlib
19.73	Eicosane, 7-hexyl-	1640671809	1.09	962	55333-99-8	mainlib

Analysed By:

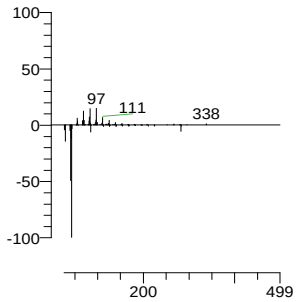
Checked By:

Hit Spectrum	Delta	Compound Structure

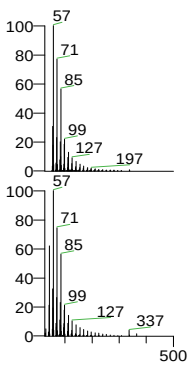


NL: 9.99E2
134859 20.52 1 11
22 4834-4844 4874-4884
6.78E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 951, RSI 966, mainlib,
Entry# 23557, CAS#
112-95-8, Eicosane

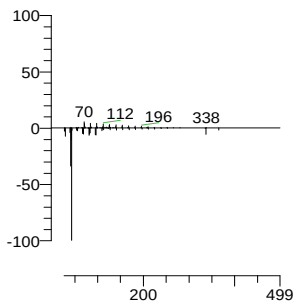


Eicosane
Formula C20H42, MW 282, CAS# 112-95-8, Entry# 23557
n-Eicosane

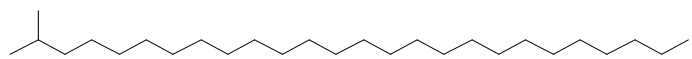


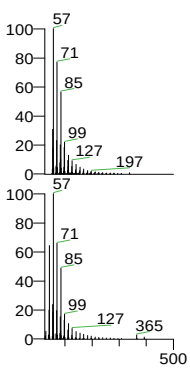
NL: 9.99E2
134859 20.52 1 11
22 4834-4844 4874-4884
6.78E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 955, RSI 964, mainlib,
Entry# 23535, CAS# NA,
2-methylhexacosane



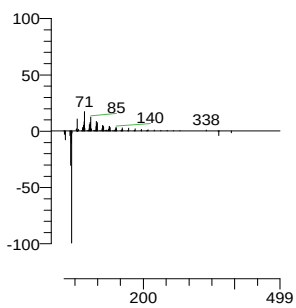
2-methylhexacosane
Formula C27H56, MW 380, CAS# NA, Entry# 23535



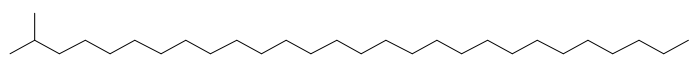


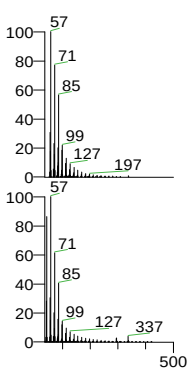
NL: 9.99E2
134859 20.52 1 11
22 4834-4844 4874-4884
6.78E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 942, RSI 961, mainlib,
Entry# 23536, CAS# NA,
2-methyloctacosane



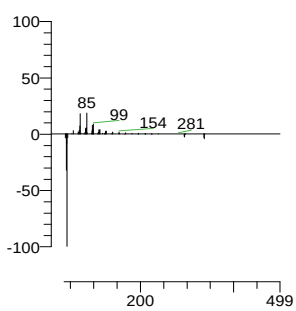
2-methyloctacosane
Formula C29H60, MW 408, CAS# NA, Entry# 23536



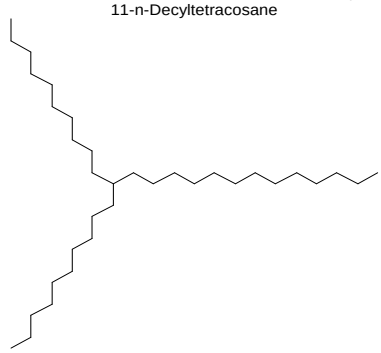


NL: 9.99E2
134859 20.52 1 11
22 4834-4844 4874-4884
6.78E7 + c EI Full ms
[50.00-500.00]

NL: 9.99E2
SI 959, RSI 960, mainlib,
Entry# 22683, CAS#
55429-84-0,
Tetracosane, 11-decyl-

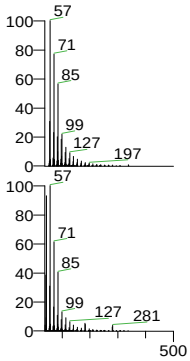


Tetracosane, 11-decyl-
Formula C34H70, MW 478, CAS# 55429-84-0, Entry# 22683
11-n-Decyltetracosane



Analysed By: *Checked By:*

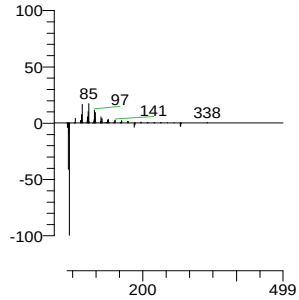
Hit Spectrum



NL: 9.99E2
134859 20.52 1 11
22 4834-4844 4874-4884
6.78E7 + c EI Full ms
[50.00-500.00]

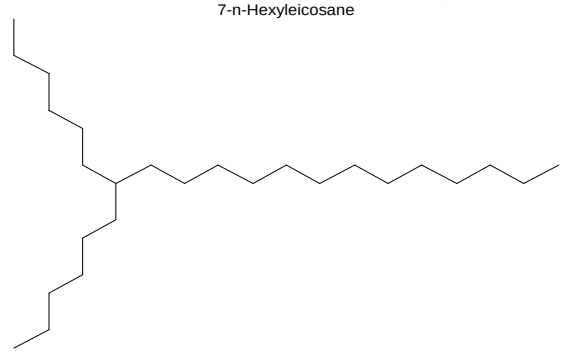
NL: 9.99E2
SI 957, RSI 959, mainlib,
Entry# 22628, CAS#
55333-99-8, Eicosane,
7-hexyl-

Delta



Compound Structure

Eicosane, 7-hexyl-
Formula C26H54, MW 366, CAS# 55333-99-8, Entry# 22628
7-n-Hexyleicosane



RT	Compound Name	Area	Area %	RSI	Cas #	Library
20.52	Eicosane	1391924842	0.92	966	112-95-8	mainlib
20.52	2-methylhexacosane	1391924842	0.92	964	NA	mainlib
20.52	2-methyloctacosane	1391924842	0.92	961	NA	mainlib

Analysed By:

Checked By: