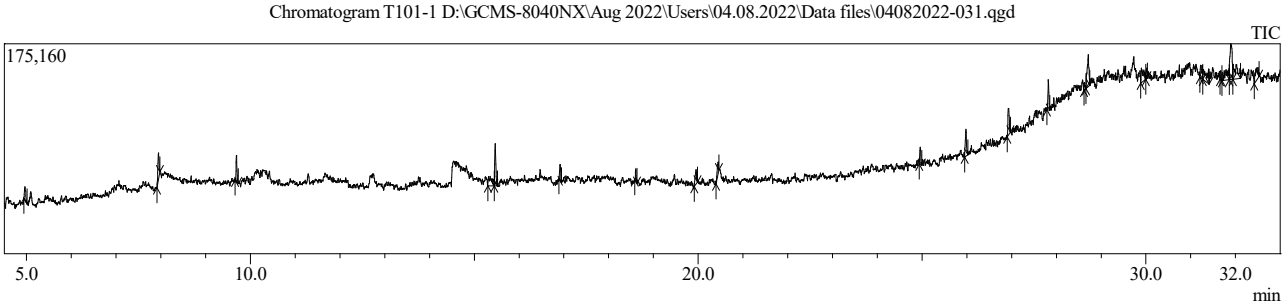
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 12:23:28 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T101-1
Sample ID	: T101-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 30
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-031.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-031.qgd
Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Org Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Report File	:
Tuning File	: D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 04082022.qgt
[Comment]	
Jerry samples	
Modified by	: Admin
Modified	: 05-Aug-22 4:47:01 PM

Chromatogram T101-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-031.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.962	21033	2.29	10864	2.95	1.94	58	Methyl butanoate
2	7.945	41917	4.56	22425	6.09	1.87	89	Undecane
3	9.687	31894	3.47	21692	5.89	1.47	89	Undecane
4	15.315	43247	4.71	7800	2.12	5.54	32	Methyl cis-10-heptadecenoate
5	15.467	59268	6.45	35279	9.58	1.68	89	2,4-Di-tert-butylphenol
6	16.915	20369	2.22	13237	3.59	1.54	78	Cyclooctasiloxane, hexadecamethyl-
7	18.606	11425	1.24	10340	2.81	1.10	50	3,4-Dihydroxymandelic acid-4TMS
8	19.947	27711	3.01	12182	3.31	2.27	61	Dimethylglycine-TMS
9	20.445	24101	2.62	9846	2.67	2.45	45	Batyl alcohol-2TMS
10	24.957	23426	2.55	14542	3.95	1.61	54	3,4-Dihydroxymandelic acid-4TMS
11	25.980	42196	4.59	22428	6.09	1.88	78	Tetracosamethyl-cyclododecasiloxane
12	26.930	46348	5.04	22127	6.01	2.09	76	Cyclodecasiloxane, eicosamethyl-
13	27.821	35483	3.86	25432	6.90	1.40	75	Cyclodecasiloxane, eicosamethyl-
14	28.625	7942	0.86	6010	1.63	1.32	33	Epinephrine-3TMS
15	28.712	73005	7.94	26584	7.22	2.75	73	Tetracosamethyl-cyclododecasiloxane
16	29.900	42450	4.62	12085	3.28	3.51	30	3-Hydroxybenzoic acid-2TMS
17	30.014	11114	1.21	8901	2.42	1.25	38	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
18	31.222	27956	3.04	10567	2.87	2.65	29	Tyrosine-3TMS
19	31.395	49660	5.40	11810	3.21	4.20	41	4-Aminobenzoic acid-2TMS
20	31.670	9001	0.98	7530	2.04	1.20	36	2-Hydroxyisobutyric acid-2TMS
21	31.745	52137	5.67	6330	1.72	8.24	33	Glycerol-3TMS
22	31.893	103136	11.22	29626	8.04	3.48	34	Docosapentaenoic acid-TMS

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Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
23	32.015	72292	7.87	11858	3.22	6.10	37	3,4-Dihydroxymandelic acid-4TMS
24	32.503	42020	4.57	8877	2.41	4.73	35	Pyridoxine-3TMS
		919131	100.00	368372	100.00			

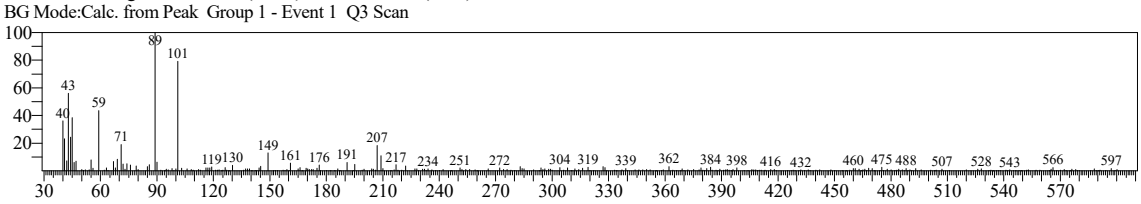
Library

<< Target >>

Line#:1 R.Time:4.960(Scan#:93) MassPeaks:296

RawMode:Averaged 4.955-4.965(92-94) BasePeak:89.00(1797)

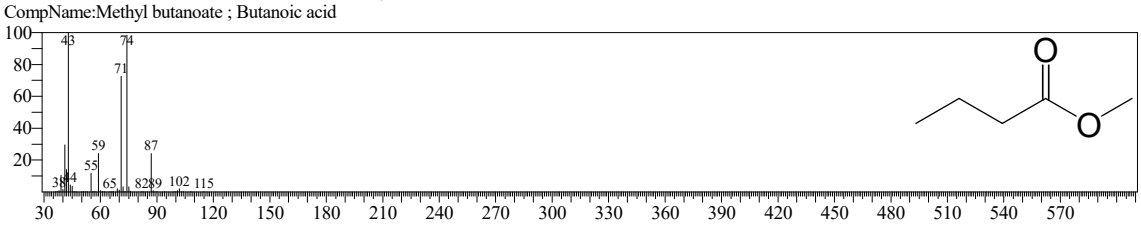
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib

SI:58 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113

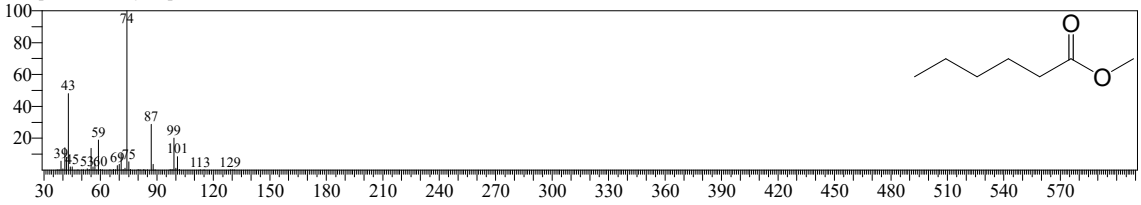
CompName:Methyl butanoate ; Butanoic acid



Hit#:2 Entry:2 Library:FA_ME_SP2560_EI_V3.lib

SI:52 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332

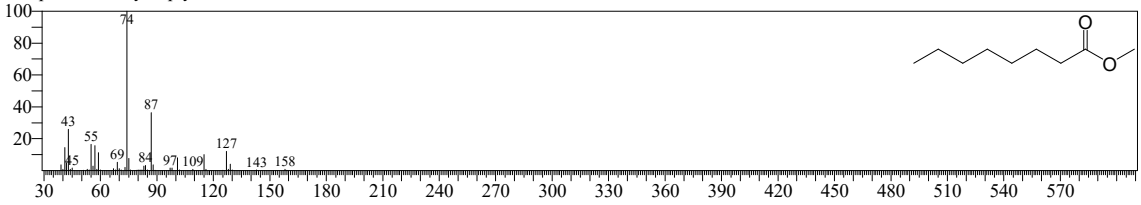
CompName:Methyl caproate ; Hexanoic acid



Hit#:3 Entry:3 Library:FA_ME_SP2560_EI_V3.lib

SI:46 Formula:C9H18O2 CAS:124-07-2 MolWeight:158 RetIndex:1550

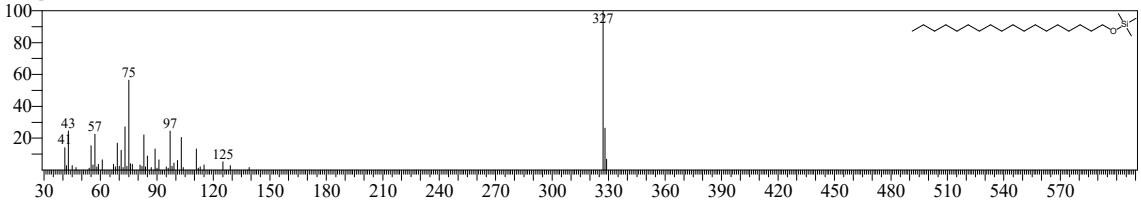
CompName:Methyl caprylate ; Octanoic acid



Hit#:4 Entry:477 Library:OA_TMS_DB5_67min_V3.lib

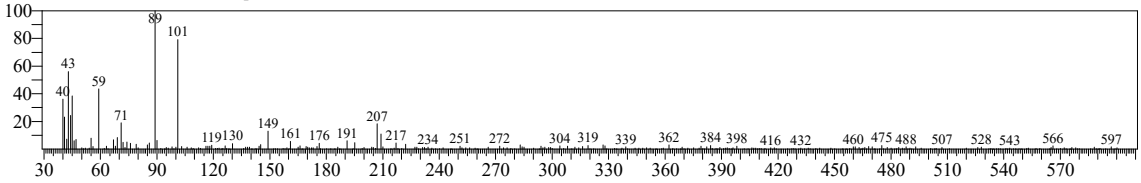
SI:41 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156

CompName:Octadecanol-TMS ; octadecan-1-ol

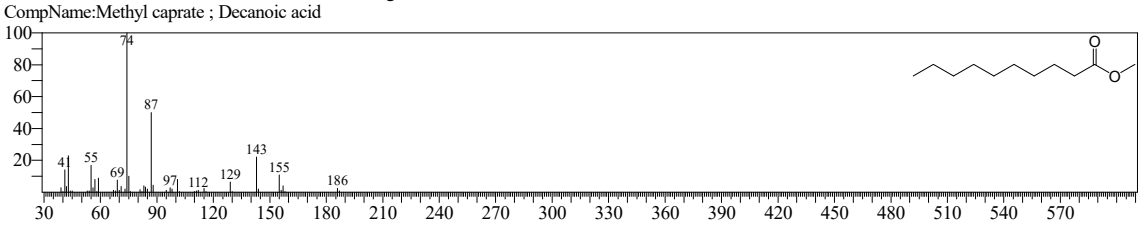


TNAU

<< Target >>
Line#:1 R.Time:4.960(Scan#:93) MassPeaks:296
RawMode:Averaged 4.955-4.965(92-94) BasePeak:89.00(1797)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

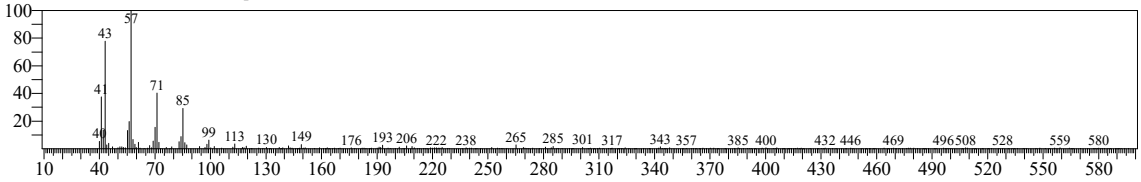


Hit#:5 Entry:4 Library:FA_ME_SP2560_EI_V3.lib
SI:38 Formula:C11H22O2 CAS:334-48-5 MolWeight:186 RetIndex:1767
CompName:Methyl caprate ; Decanoic acid

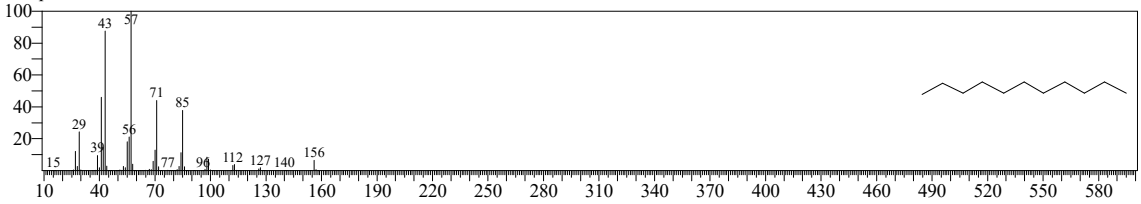


TNAU

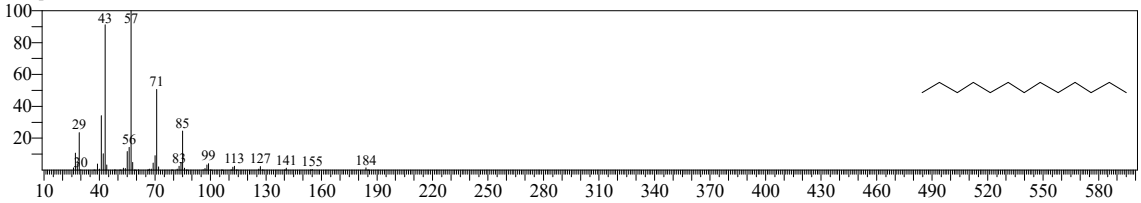
<< Target >>
Line#:2 R.Time:7.945(Scan#:690) MassPeaks:284
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5162)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



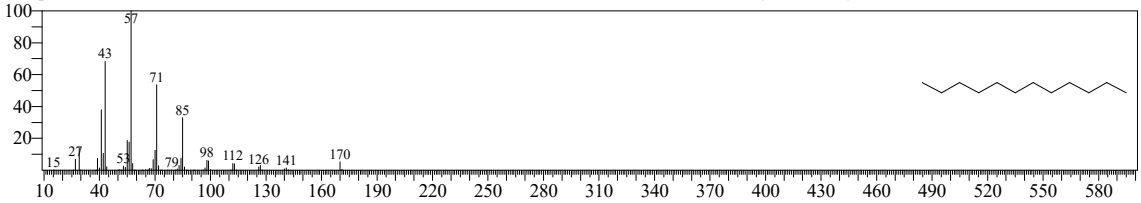
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



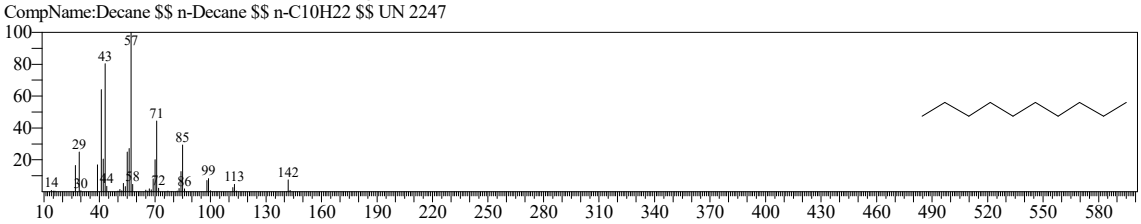
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



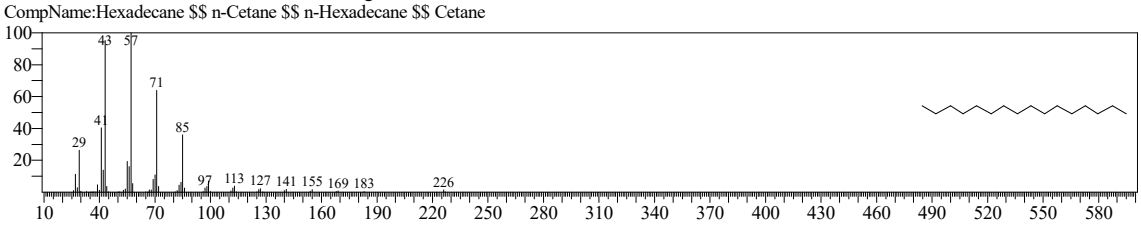
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:89 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:13604 Library:NIST20M1.lib
SI:89 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

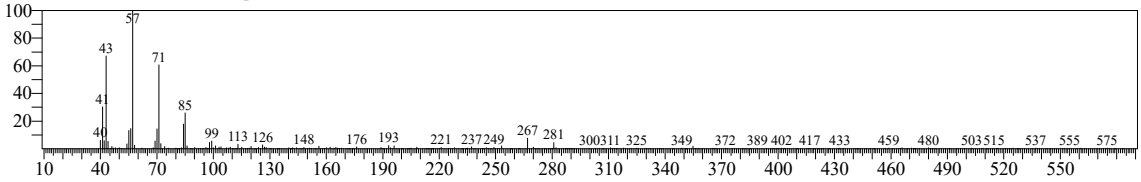


Hit#:5 Entry:27736 Library:NIST20R.lib
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

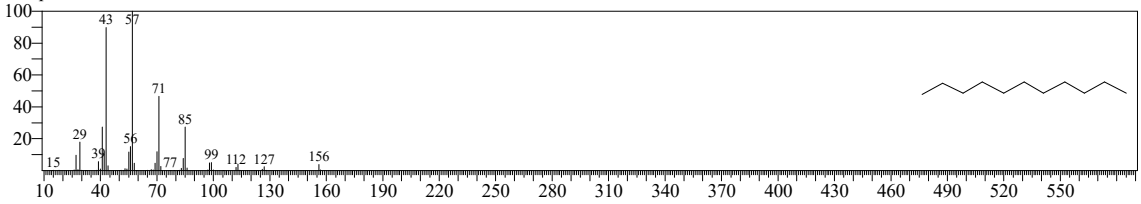


TNAU

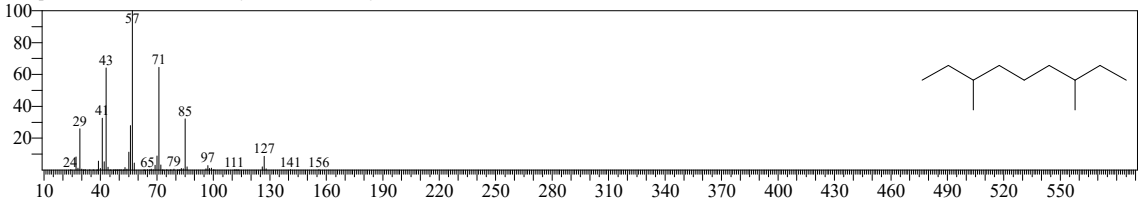
<< Target >>
Line#:3 R.Time:9.685(Scan#:1038) MassPeaks:244
RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.10(5506)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



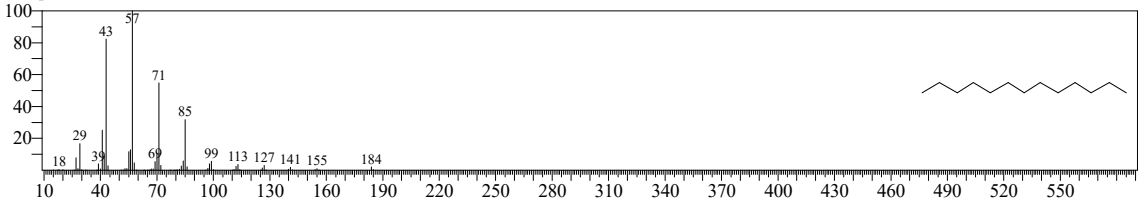
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



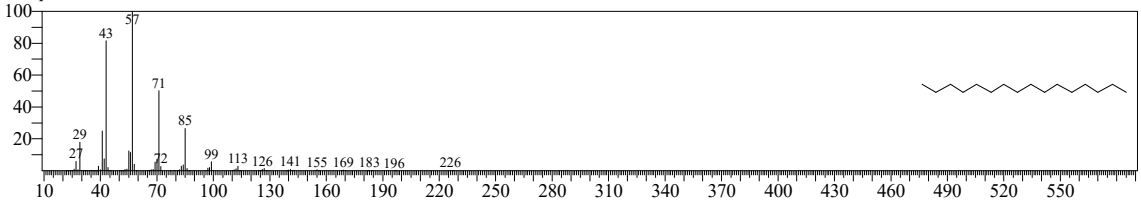
Hit#:2 Entry:21047 Library:NIST20M1.lib
SI:88 Formula:C11H24 CAS:17302-32-8 MolWeight:156 RetIndex:986
CompName:Nonane, 3,7-dimethyl- $$ 3,7-Dimethylnonane



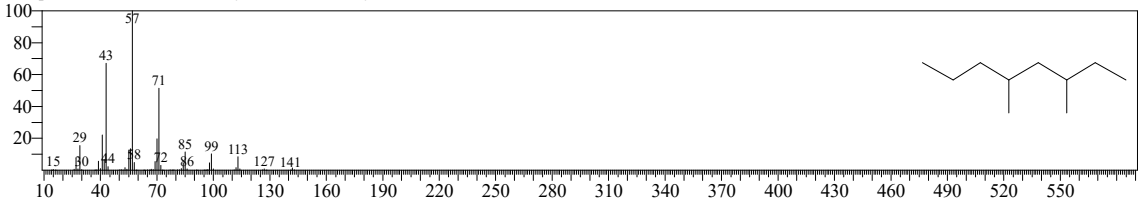
Hit#:3 Entry:19412 Library:NIST20R.lib
SI:88 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:27737 Library:NIST20R.lib
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

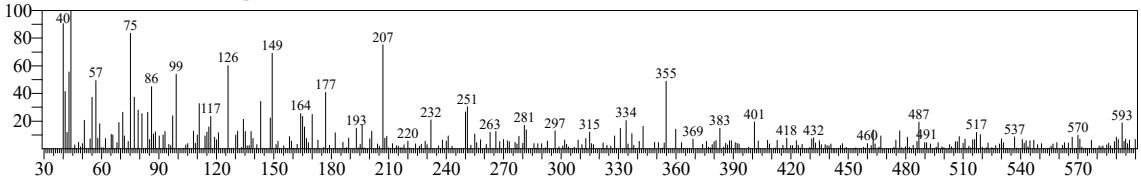


Hit#:5 Entry:13631 Library:NIST20M1.lib
SI:88 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

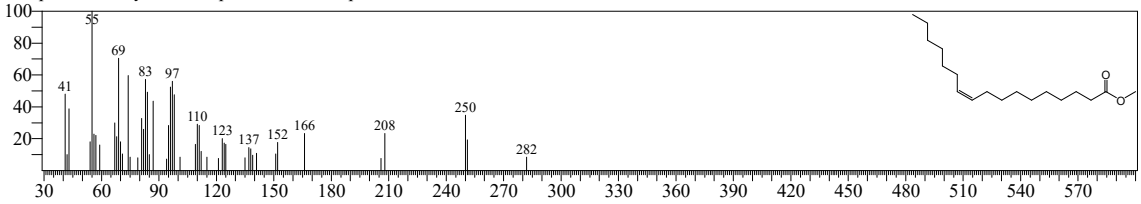


TNAU

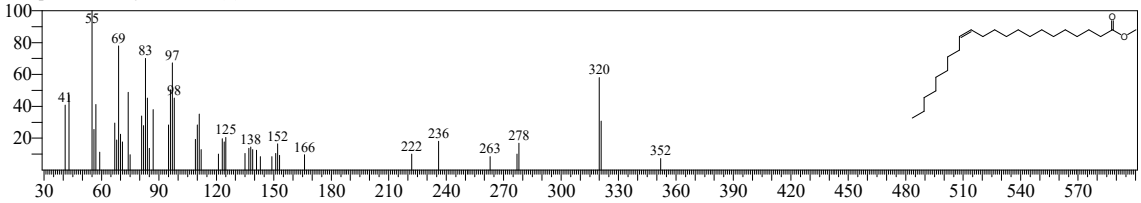
<< Target >>
Line#:4 R.Time:15.315(Scan#:2164) MassPeaks:320
RawMode:Averaged 15.310-15.320(2163-2165) BasePeak:44.00(401)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



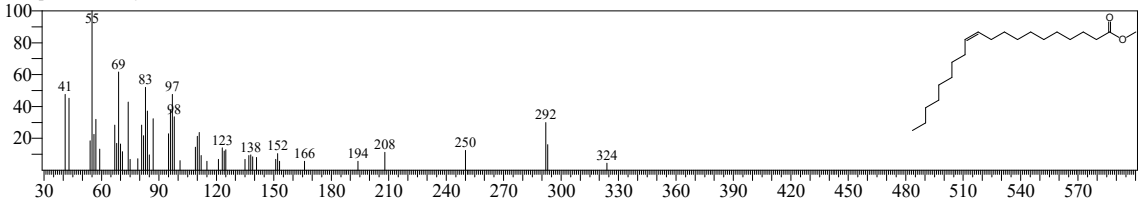
Hit#:1 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid



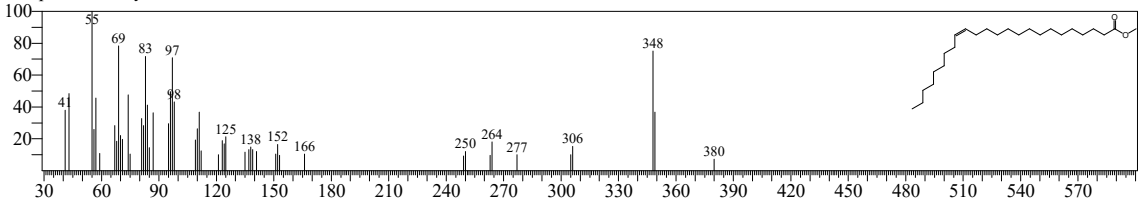
Hit#:2 Entry:30 Library:FA_ME_SP2560_EI_V3.lib
SI:31 Formula:C23H44O2 CAS:112-86-7 MolWeight:352 RetIndex:3070
CompName:Methyl erucate ; (Z)-docos-13-enoic acid



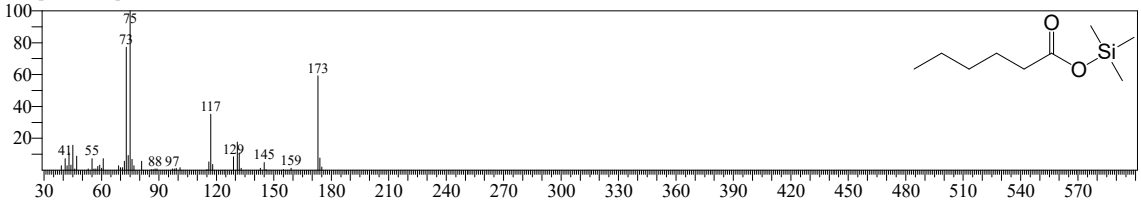
Hit#:3 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:31 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid



Hit#:4 Entry:37 Library:FA_ME_SP2560_EI_V3.lib
SI:29 Formula:C25H48O2 CAS:506-37-6 MolWeight:380 RetIndex:3263
CompName:Methyl nervonate ; Tetracos-15-enoic acid

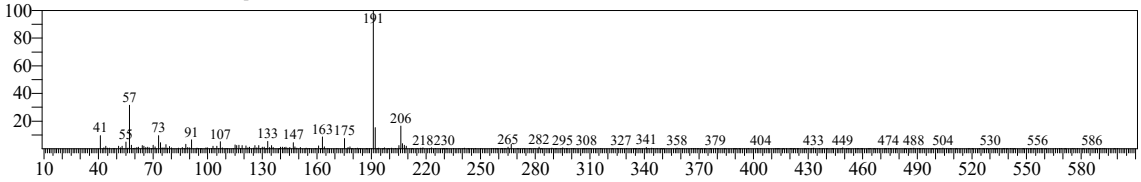


Hit#:5 Entry:11 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid

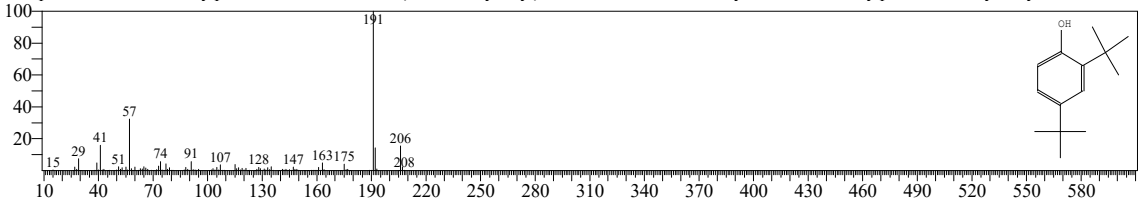


TNAU

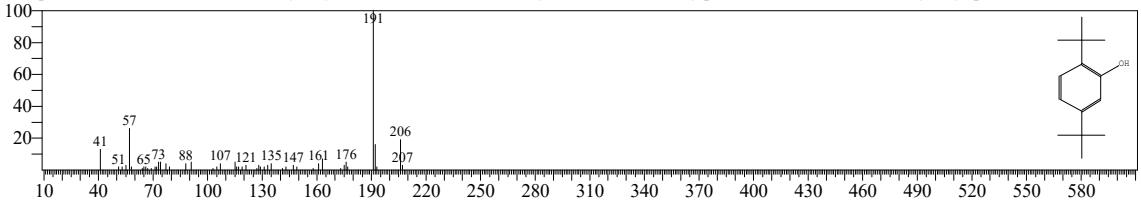
<< Target >>
Line#:5 R.Time:15.465(Scan#:2194) MassPeaks:291
RawMode:Averaged 15.460-15.470(2193-2195) BasePeak:191.10(9704)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



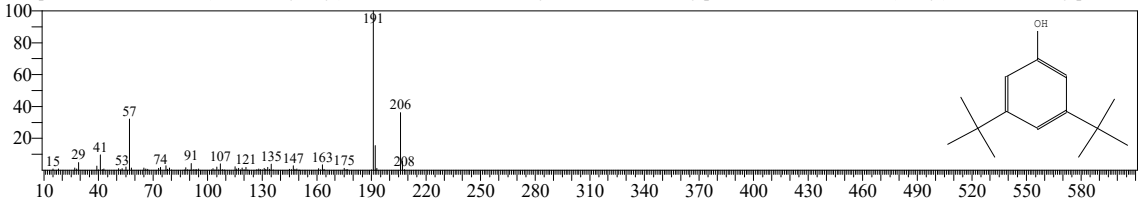
Hit#:1 Entry:59048 Library:NIST20M1.lib
SI:89 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



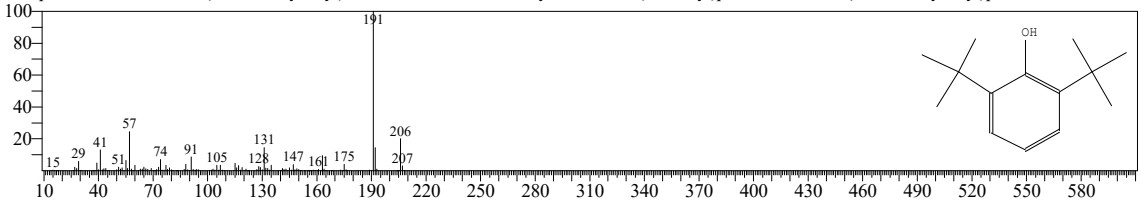
Hit#:2 Entry:24098 Library:NIST20R.lib
SI:88 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



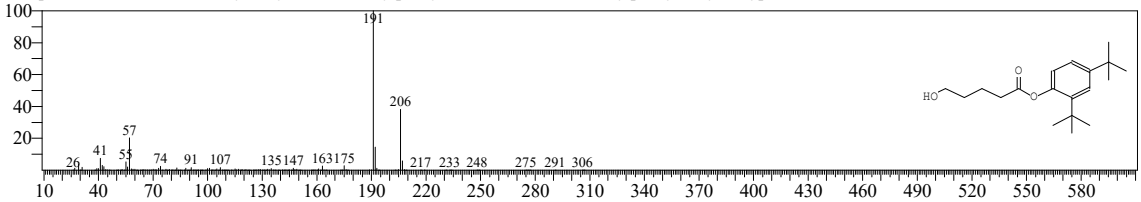
Hit#:3 Entry:24110 Library:NIST20R.lib
SI:88 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



Hit#:4 Entry:59031 Library:NIST20M1.lib
SI:86 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

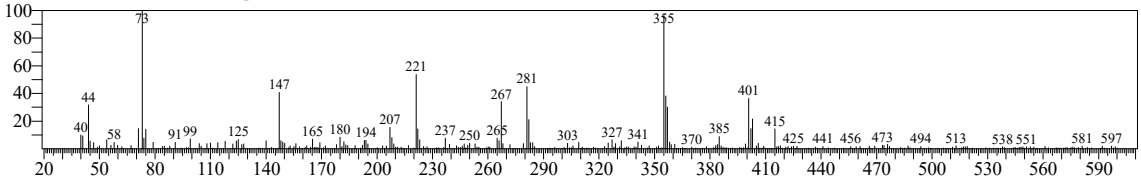


Hit#:5 Entry:170993 Library:NIST20M1.lib
SI:82 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #

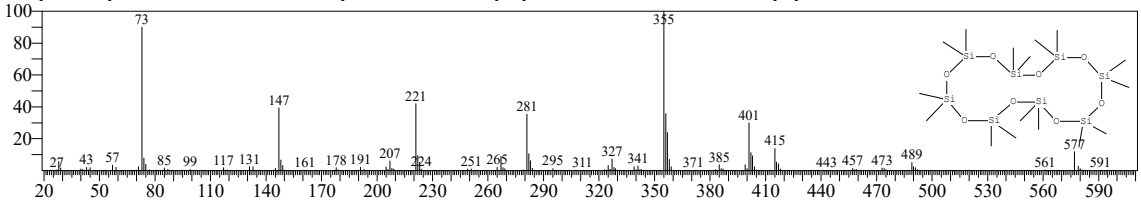


TNAU

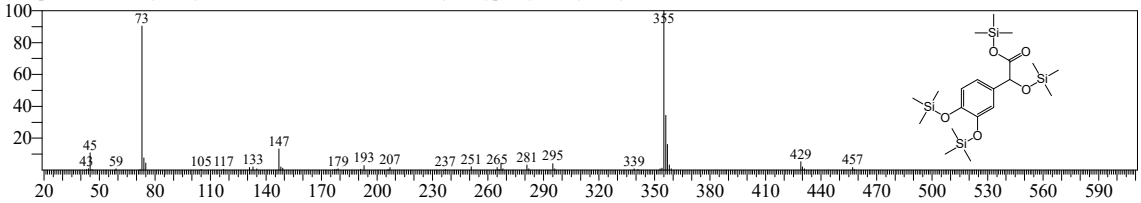
<< Target >>
Line#:6 R.Time:16.915(Scan#:2484) MassPeaks:315
RawMode:Averaged 16.910-16.920(2483-2485) BasePeak:73.05(1550)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



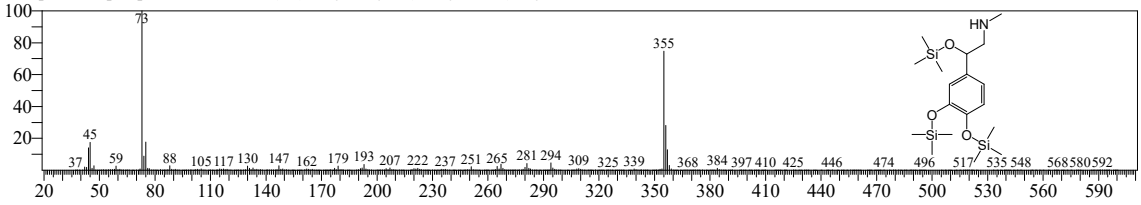
Hit#:1 Entry:42384 Library:NIST20M2.lib
SI:78 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



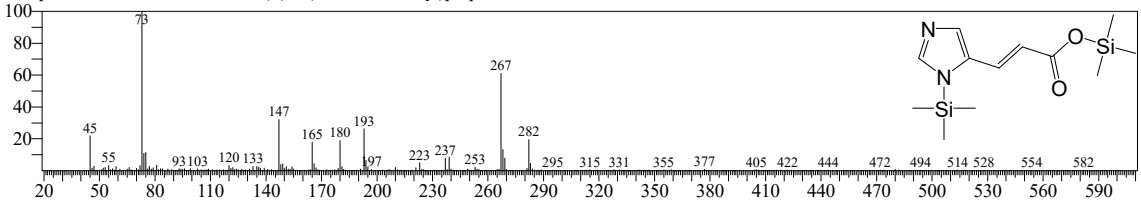
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:60 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



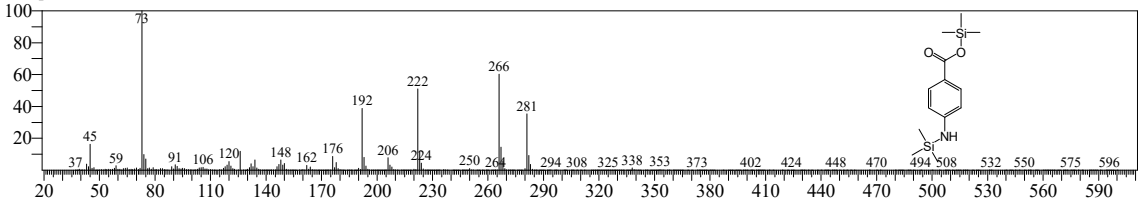
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:59 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

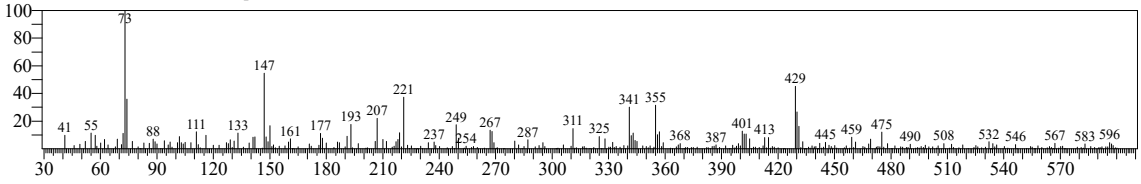


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

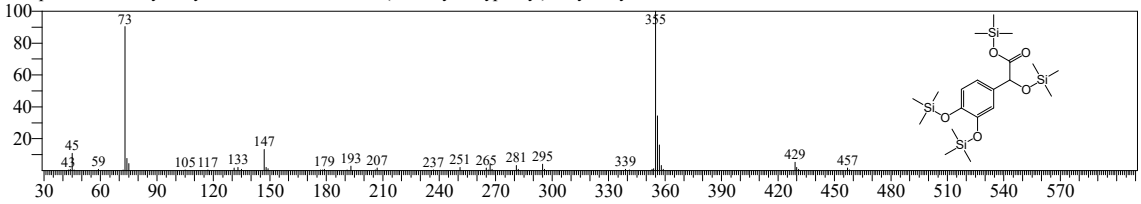


TNAU

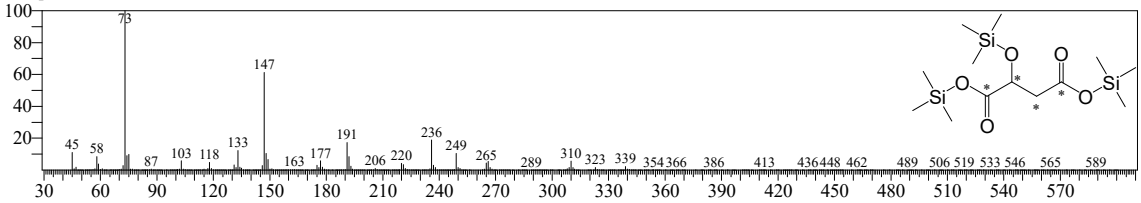
<< Target >>
Line#:7 R.Time:18.605(Scan#:2822) MassPeaks:318
RawMode:Averaged 18.600-18.610(2821-2823) BasePeak:73.05(1050)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



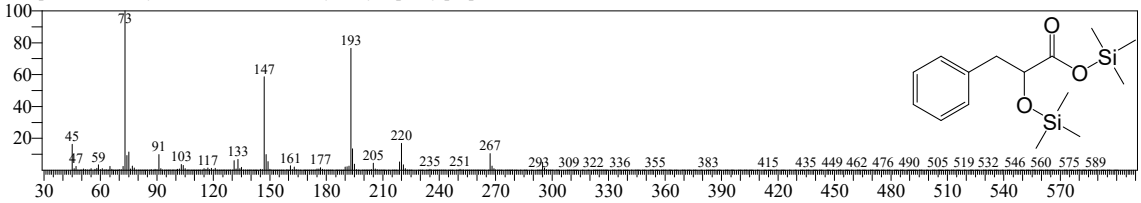
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



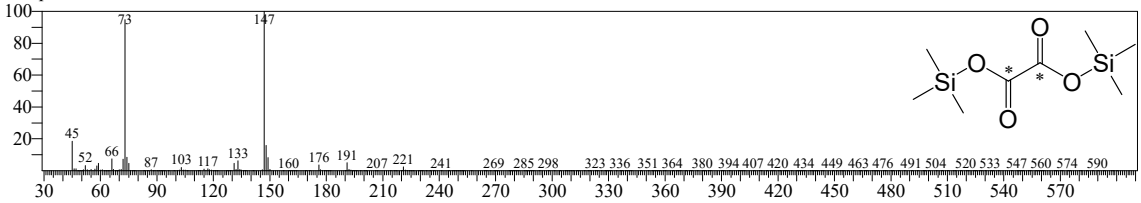
Hit#:2 Entry:143 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula: CAS:0-00-0 MolWeight:354 RetIndex:1495
CompName:Malic acid-13C4-3TMS ;



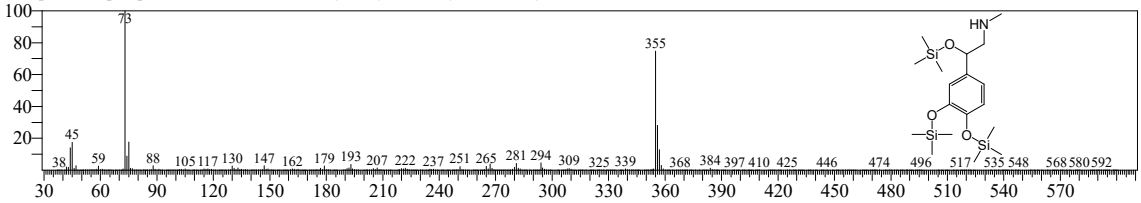
Hit#:3 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:4 Entry:24 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula: CAS:0-00-0 MolWeight:236 RetIndex:1130
CompName:Oxalic acid-13C2-2TMS ;

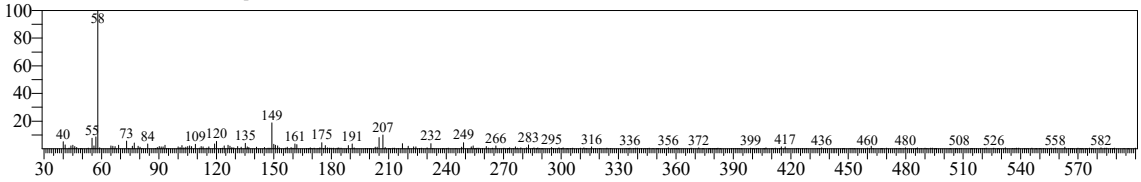


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

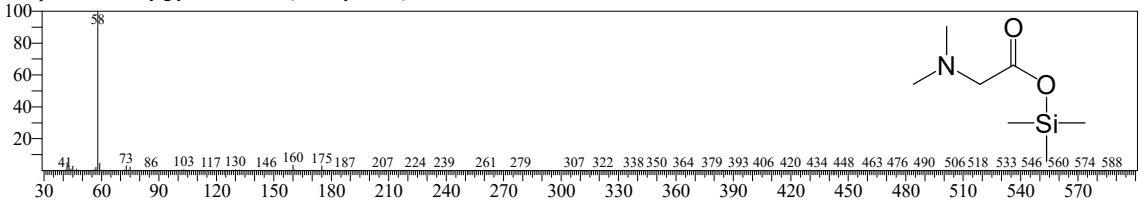


TNAU

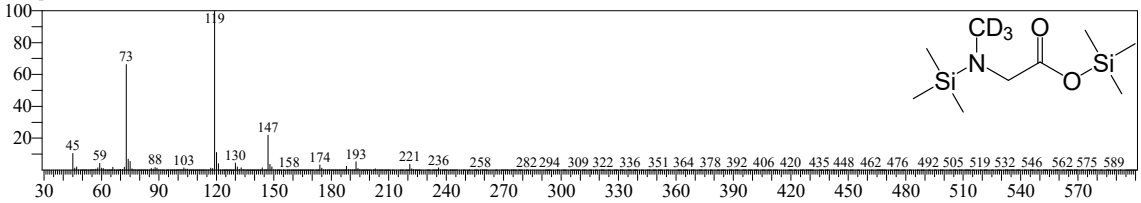
<< Target >>
Line#:8 R.Time:19.945(Scan#:3090) MassPeaks:288
RawMode:Averaged 19.940-19.950(3089-3091) BasePeak:58.10(4556)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



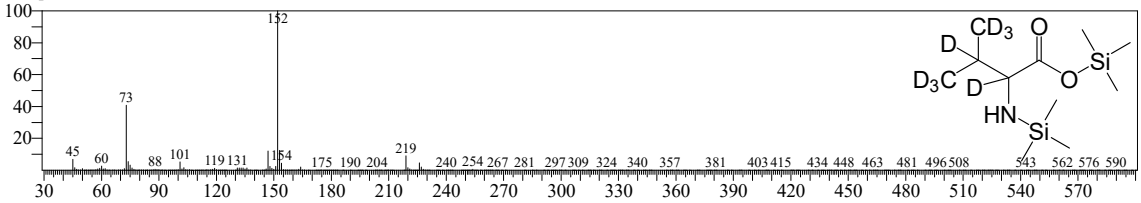
Hit#:1 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:61 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



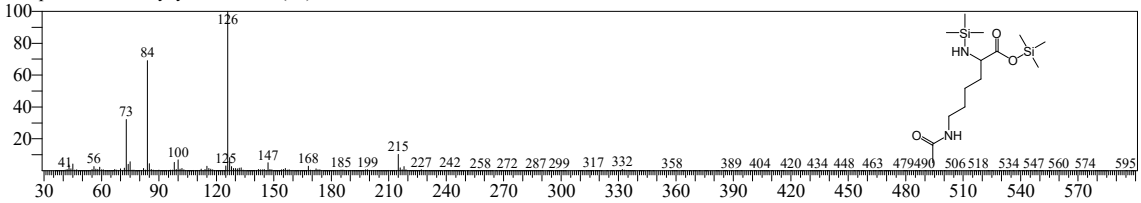
Hit#:2 Entry:28 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula: CAS:347840-04-4 MolWeight:236 RetIndex:1140
CompName:Sarcosine-d3-2TMS ;



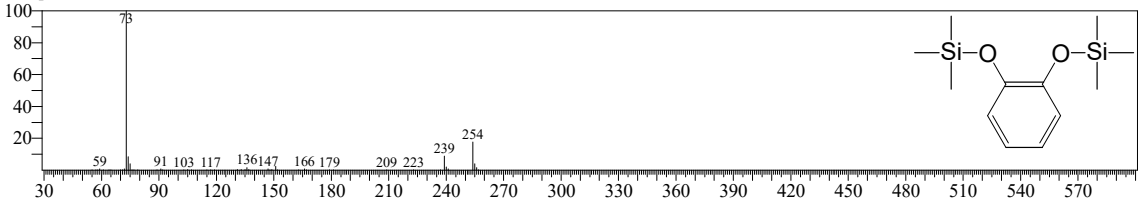
Hit#:3 Entry:53 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula: CAS:35045-72-8 MolWeight:269 RetIndex:1218
CompName:Valine-d8-2TMS ;



Hit#:4 Entry:409 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H32N2O3Si2 CAS:692-04-6 MolWeight:332 RetIndex:1951
CompName:N6-Acetyllysine-2TMS ; (2S)-6-acetamido-2-aminohexanoic acid

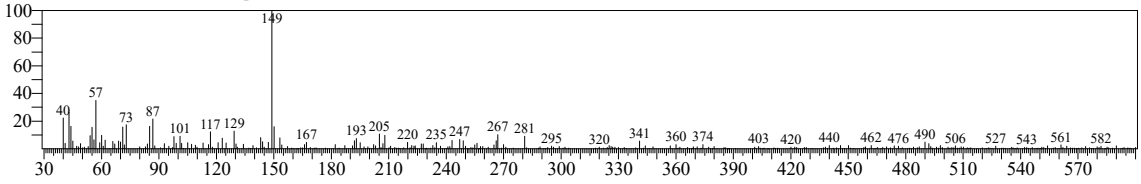


Hit#:5 Entry:94 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C12H22O2Si2 CAS:120-80-9 MolWeight:254 RetIndex:1327
CompName:Catechol-2TMS ; benzene-1,2-diol

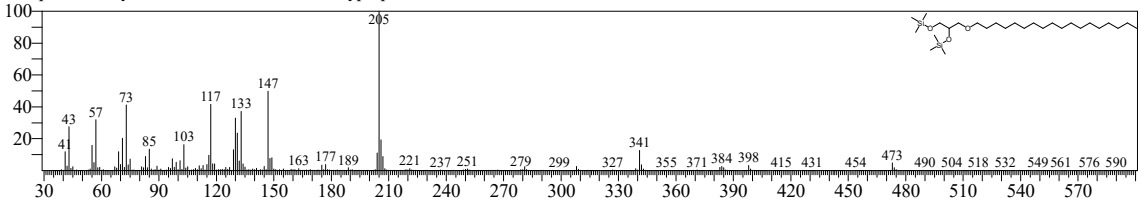


TNAU

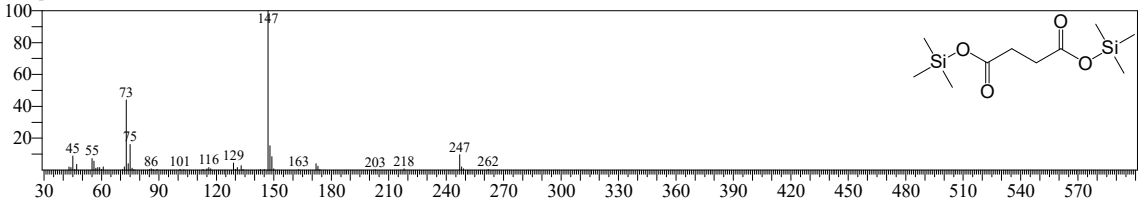
<< Target >>
Line#:9 R.Time:20.445(Scan#:3190) MassPeaks:308
RawMode:Averaged 20.440-20.450(3189-3191) BasePeak:149.05(1701)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



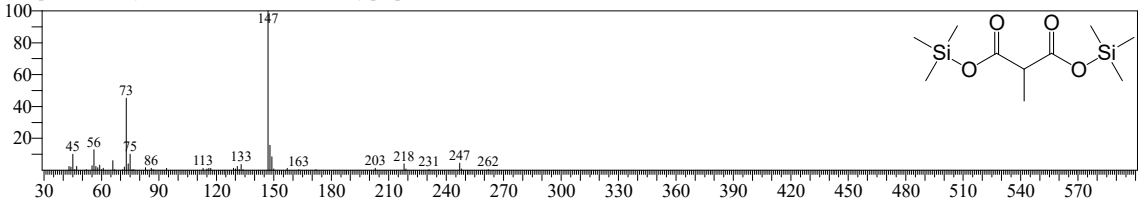
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



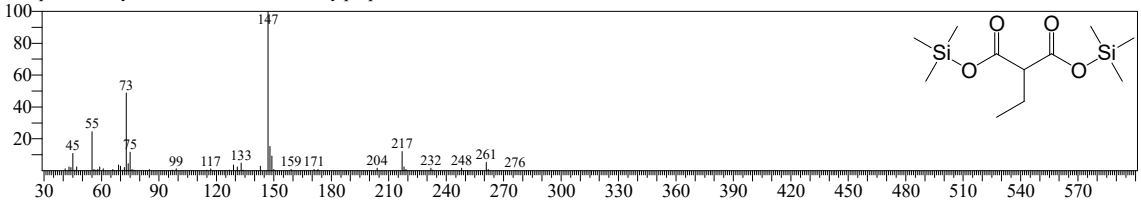
Hit#:2 Entry:92 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C10H22O4Si2 CAS:110-15-6 MolWeight:262 RetIndex:1313
CompName:Succinic acid-2TMS ; butanedioic acid



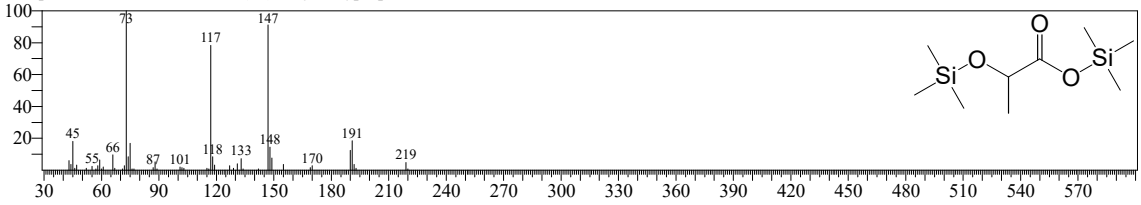
Hit#:3 Entry:52 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C10H22O4Si2 CAS:516-05-2 MolWeight:262 RetIndex:1218
CompName:Methylmalonic acid-2TMS ; 2-methylpropanedioic acid



Hit#:4 Entry:80 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C11H24O4Si2 CAS:601-75-2 MolWeight:276 RetIndex:1284
CompName:Ethylmalonic acid-2TMS ; 2-ethylpropanedioic acid

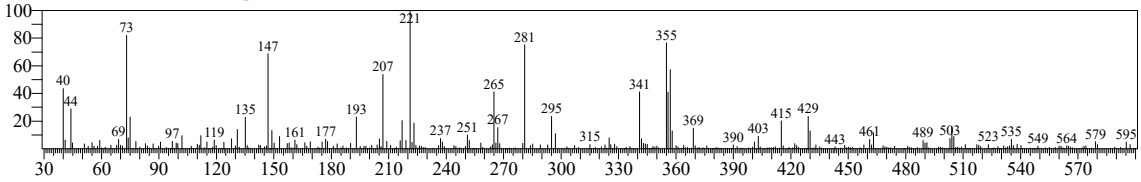


Hit#:5 Entry:8 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C9H22O3Si2 CAS:79-33-4 MolWeight:234 RetIndex:1061
CompName:Lactic acid-2TMS ; (2S)-2-hydroxypropanoic acid

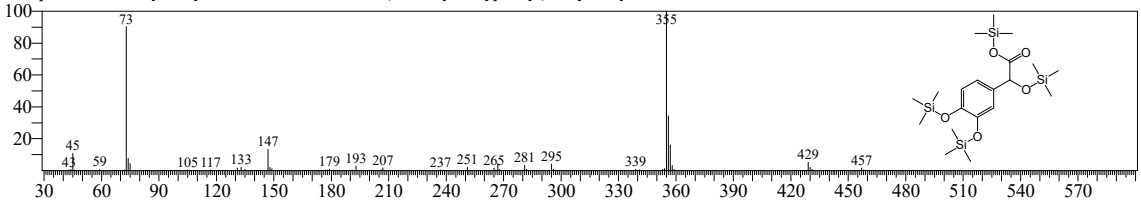


TNAU

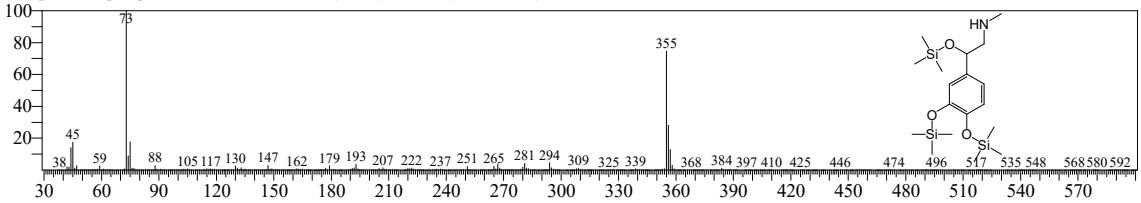
<< Target >>
Line#:10 R.Time:24.955(Scan#:4092) MassPeaks:316
RawMode:Averaged 24.950-24.960(4091-4093) BasePeak:221.10(1198)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



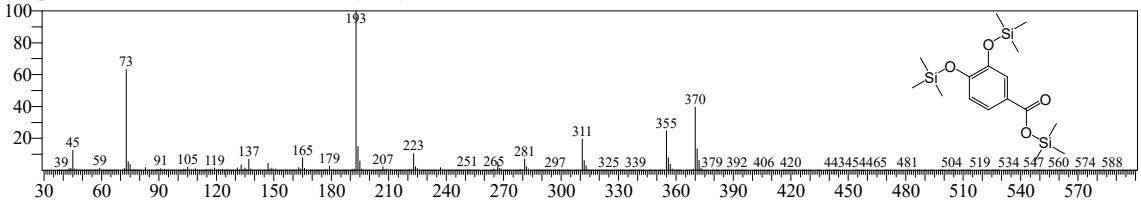
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:54 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



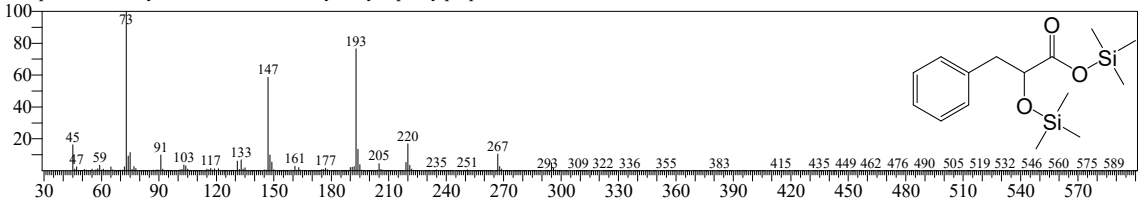
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



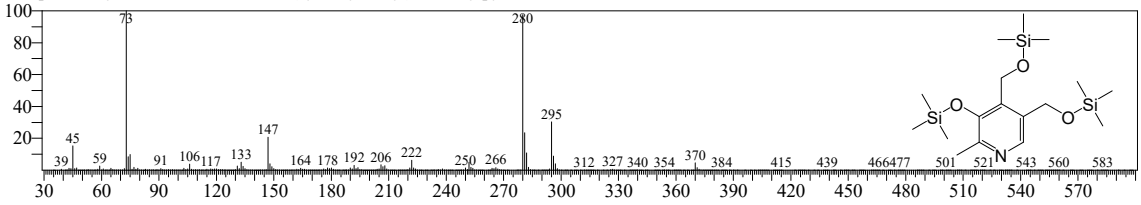
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

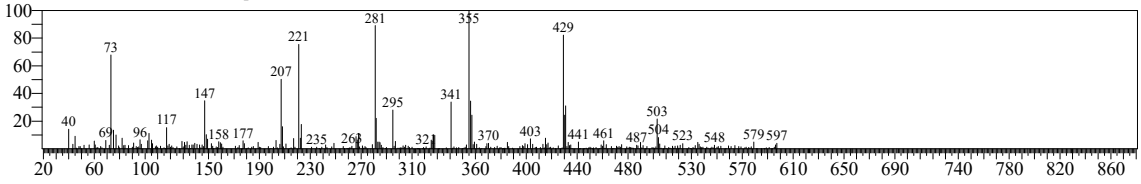


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

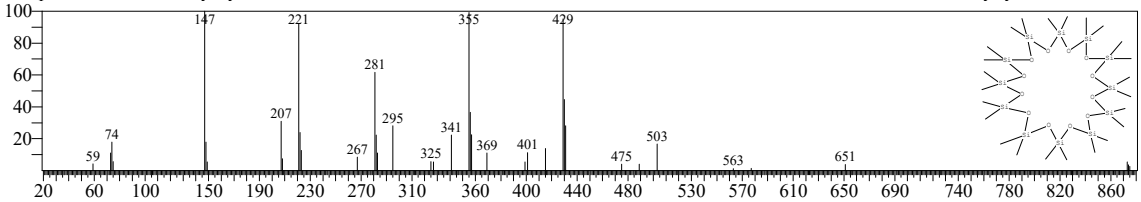


TNAU

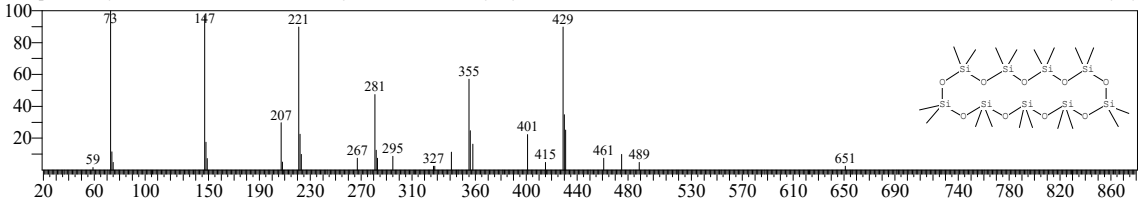
<< Target >>
Line#:11 R.Time:25.980(Scan#:4297) MassPeaks:330
RawMode:Averaged 25.975-25.985(4296-4298) BasePeak:355.00(1871)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



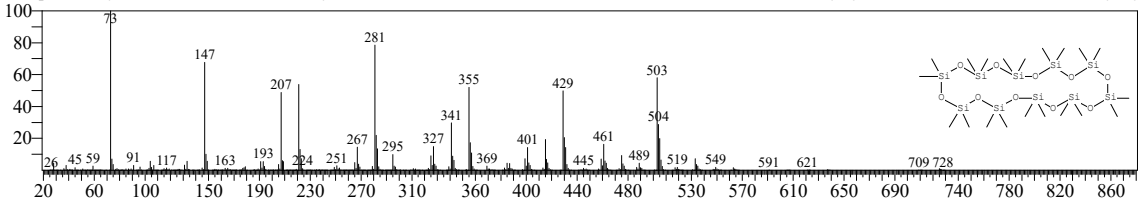
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:78 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



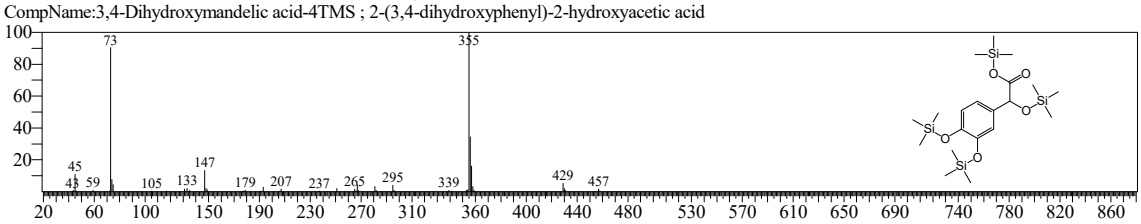
Hit#:2 Entry:43658 Library:NIST20R.lib
SI:73 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



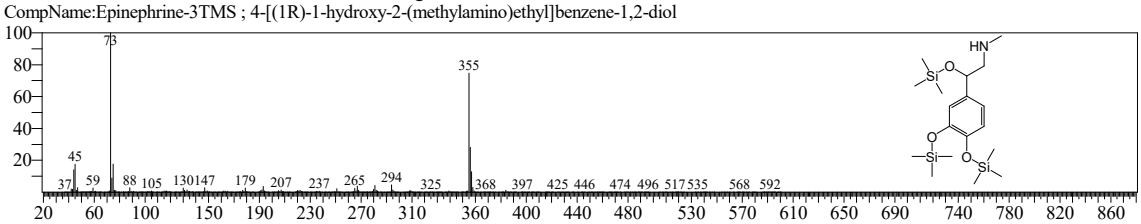
Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:72 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:58 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

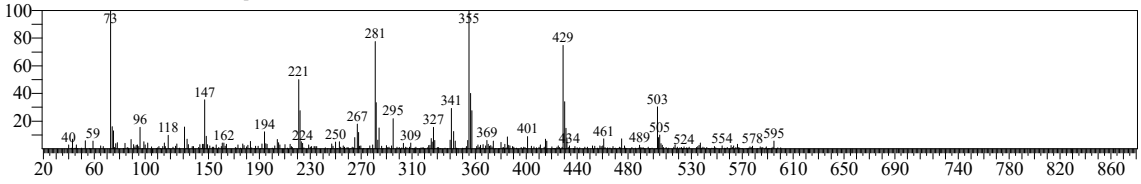


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

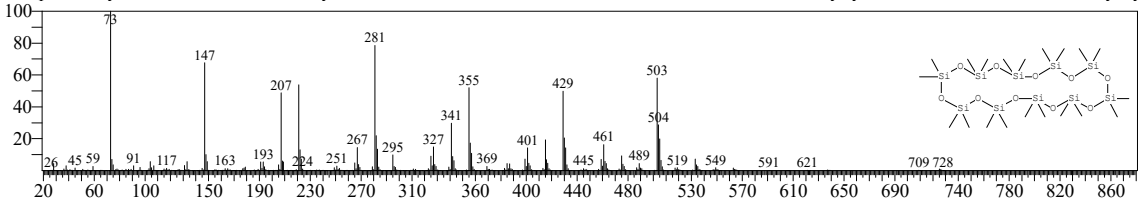


TNAU

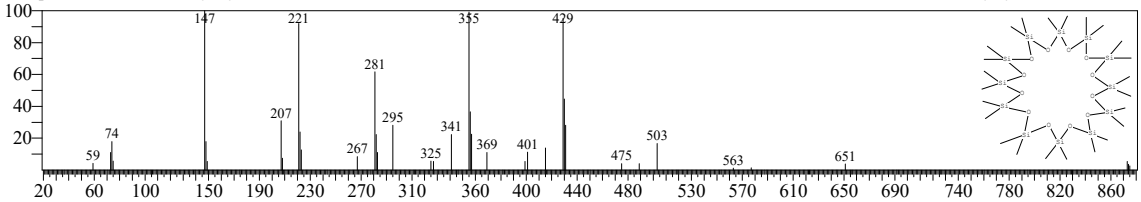
<< Target >>
Line#:12 R.Time:26.930(Scan#:4487) MassPeaks:350
RawMode:Averaged 26.925-26.935(4486-4488) BasePeak:73.00(1968)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



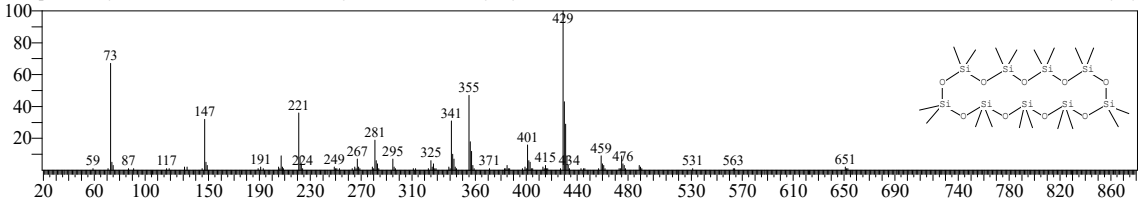
Hit#:1 Entry:45685 Library:NIST20M2.lib
SI:76 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



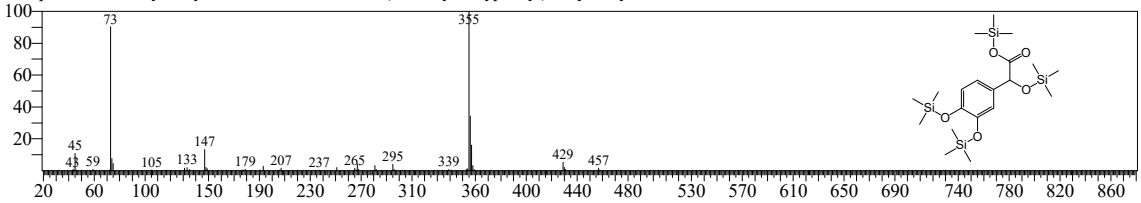
Hit#:2 Entry:46368 Library:NIST20M2.lib
SI:75 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



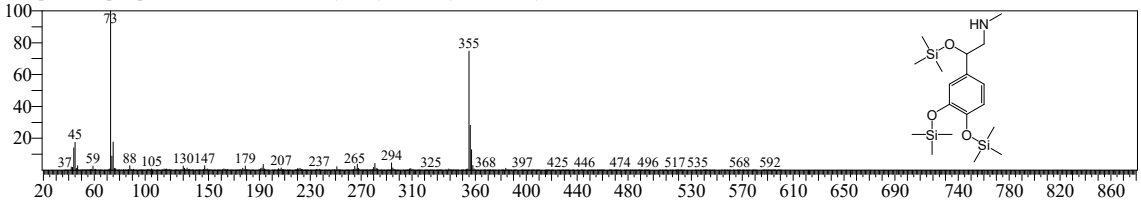
Hit#:3 Entry:43659 Library:NIST20R.lib
SI:73 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:59 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

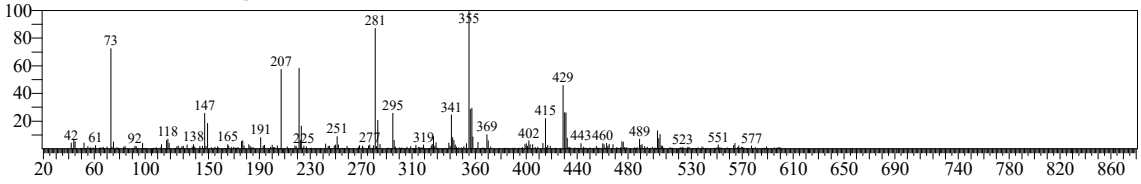


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

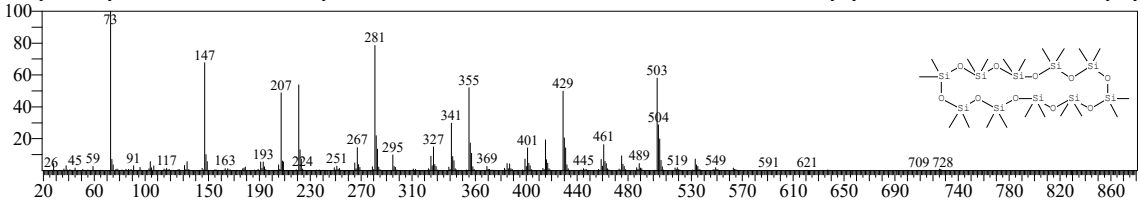


TNAU

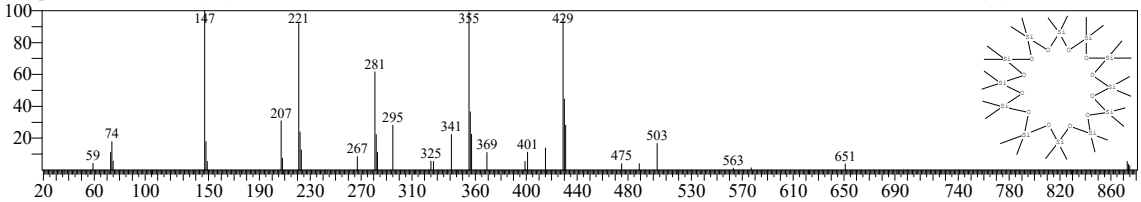
<< Target >>
Line#:13 R.Time:27.820(Scan#:4665) MassPeaks:306
RawMode:Averaged 27.815-27.825(4664-4666) BasePeak:355.05(2625)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



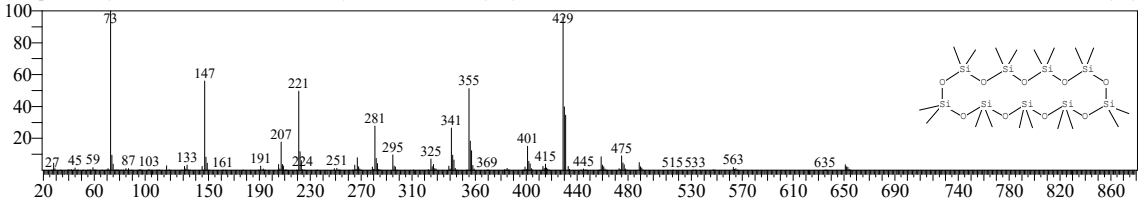
Hit#:1 Entry:45685 Library:NIST20M2.lib
SI:75 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



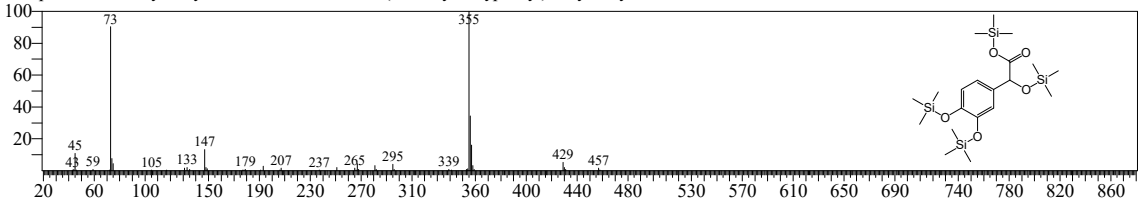
Hit#:2 Entry:46368 Library:NIST20M2.lib
SI:74 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



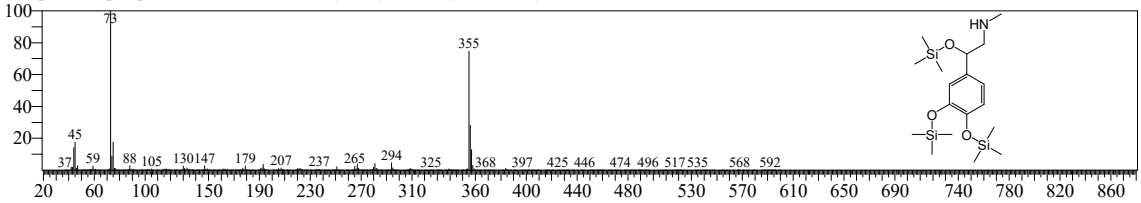
Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:73 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:60 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

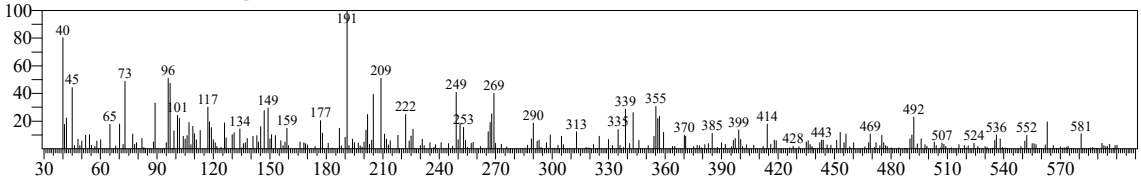


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:51 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

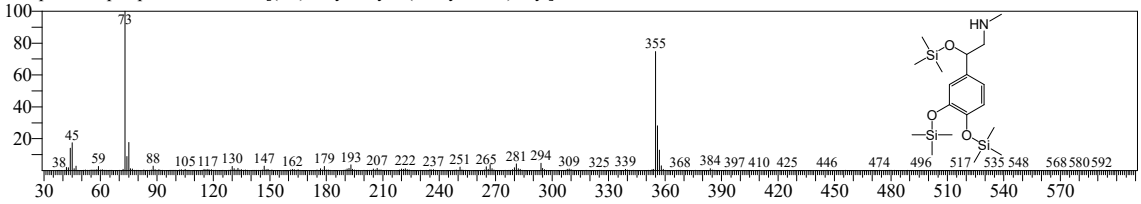


TNAU

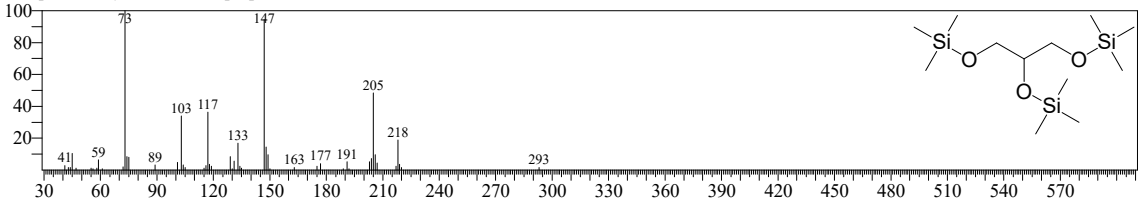
<< Target >>
Line#:14 R.Time:28.625(Scan#:4826) MassPeaks:304
RawMode:Averaged 28.620-28.630(4825-4827) BasePeak:191.00(583)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



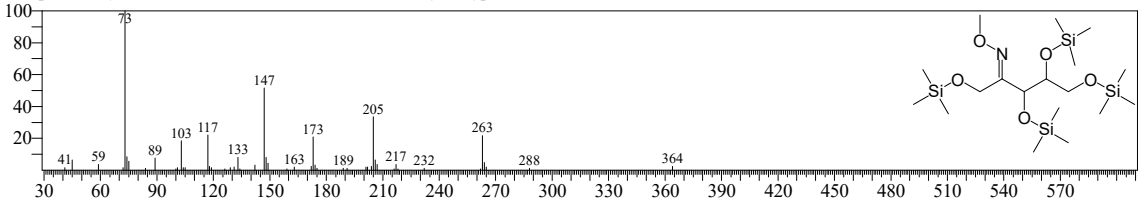
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



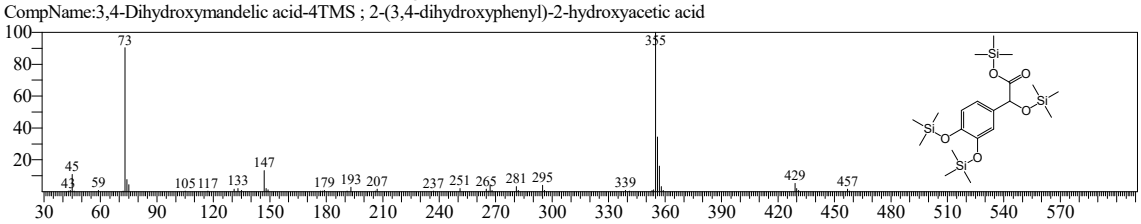
Hit#:2 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



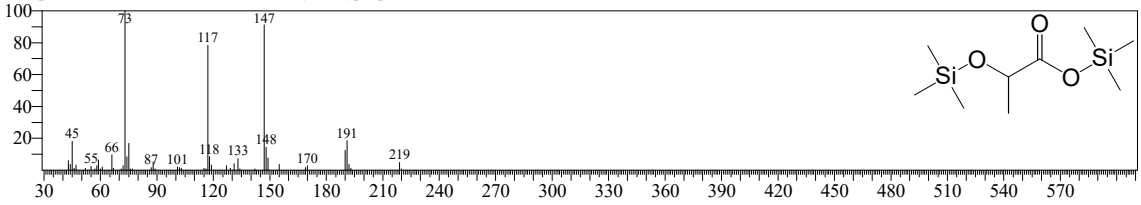
Hit#:3 Entry:255 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H45NO5Si4 CAS:551-84-8 MolWeight:467 RetIndex:1698
CompName:Xylulose-meto-4TMS ; (3S,4R)-1,3,4,5-tetrahydroxypentan-2-one



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

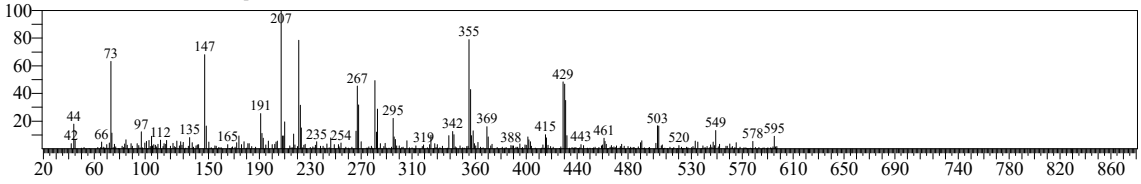


Hit#:5 Entry:8 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C9H22O3Si2 CAS:79-33-4 MolWeight:234 RetIndex:1061
CompName:Lactic acid-2TMS ; (2S)-2-hydroxypropanoic acid

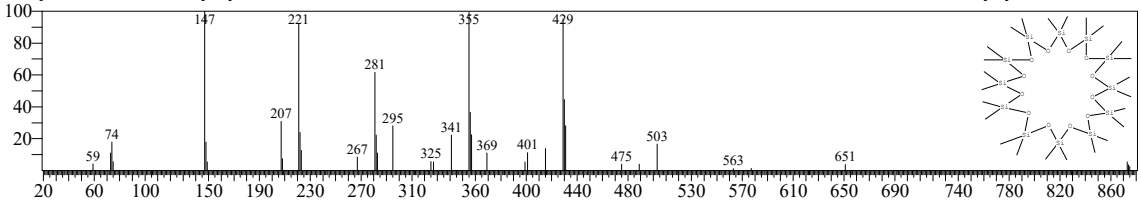


TNAU

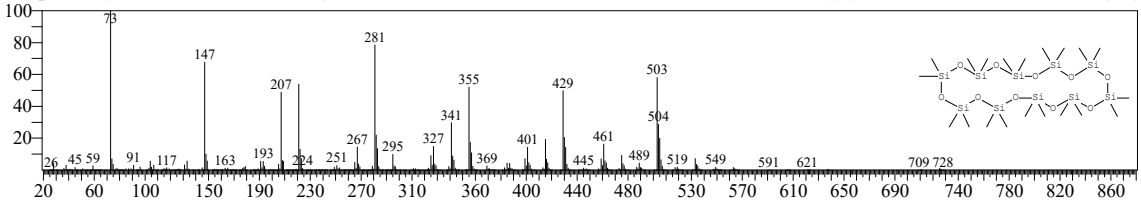
<< Target >>
Line#:15 R.Time:28.710(Scan#:4843) MassPeaks:350
RawMode:Averaged 28.705-28.715(4842-4844) BasePeak:207.00(1912)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



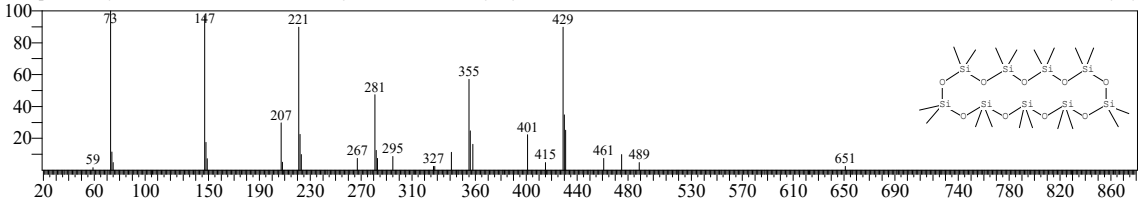
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:73 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



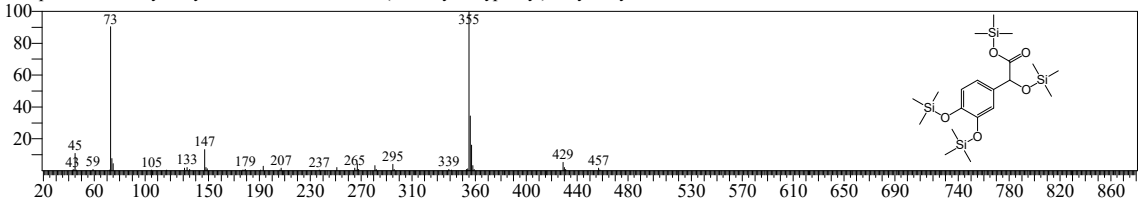
Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:71 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



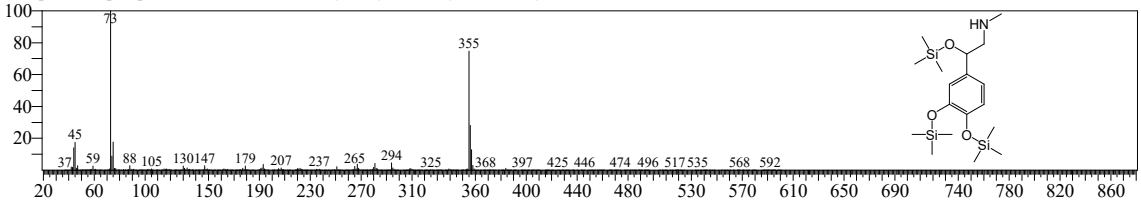
Hit#:3 Entry:43658 Library:NIST20R.lib
SI:70 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:52 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

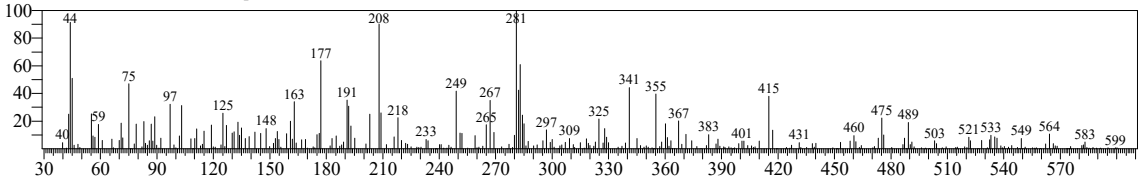


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

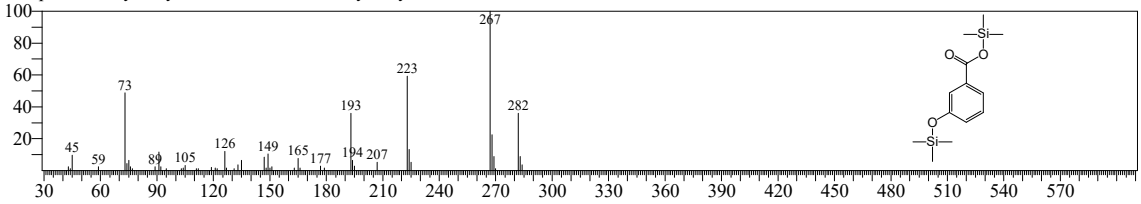


TNAU

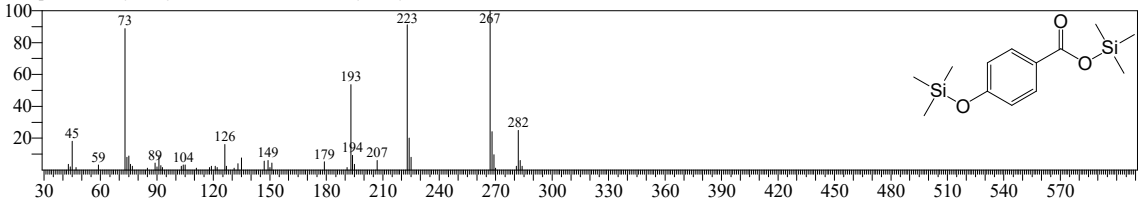
<< Target >>
Line#:16 R.Time:29.900(Scan#:5081) MassPeaks:297
RawMode:Averaged 29.895-29.905(5080-5082) BasePeak:281.00(868)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



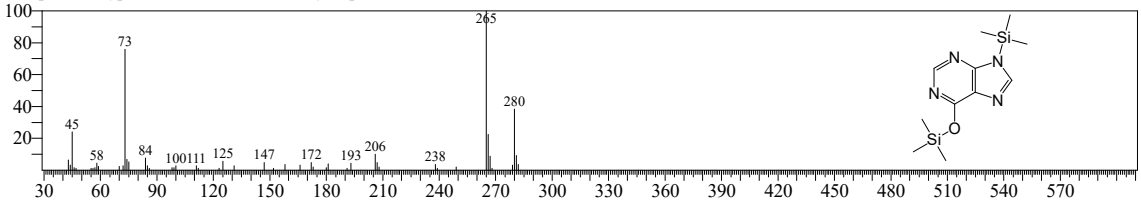
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



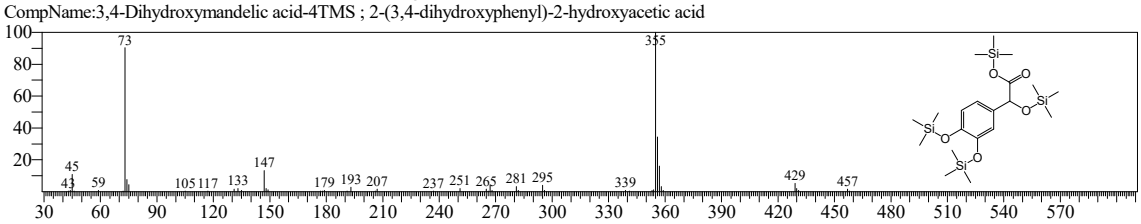
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



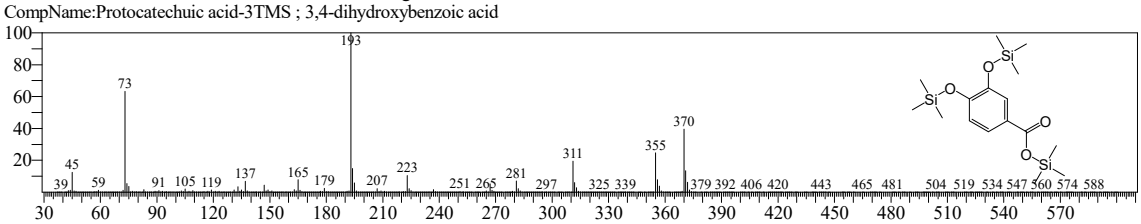
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

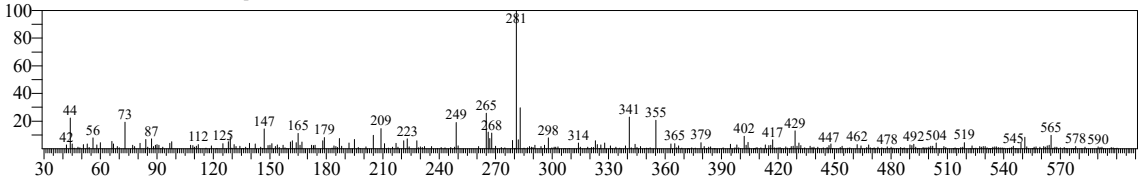


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

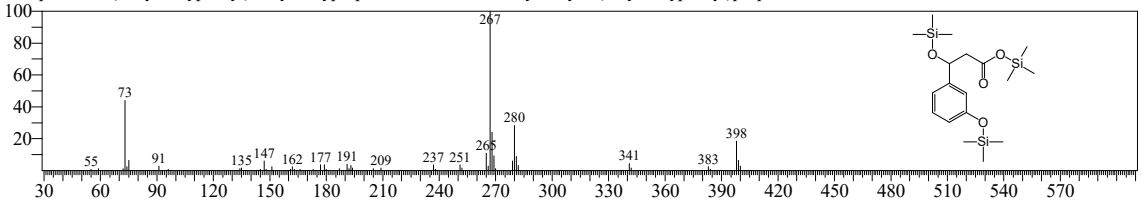


TNAU

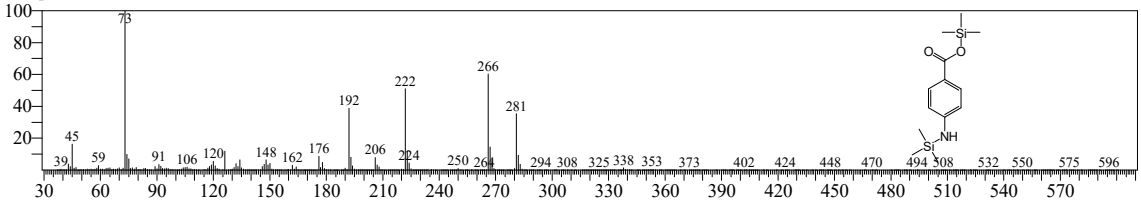
<< Target >>
Line#:17 R.Time:30.015(Scan#:5104) MassPeaks:318
RawMode:Averaged 30.010-30.020(5103-5105) BasePeak:281.05(2054)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



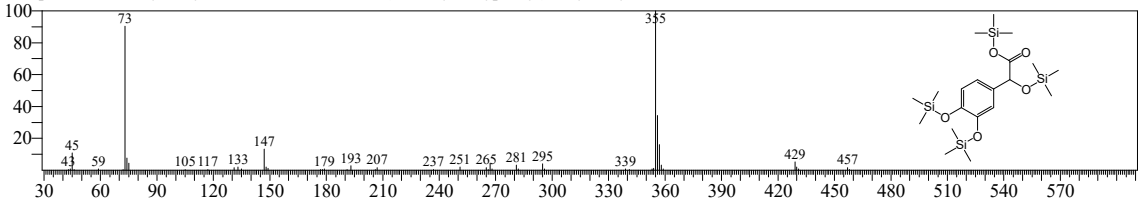
Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



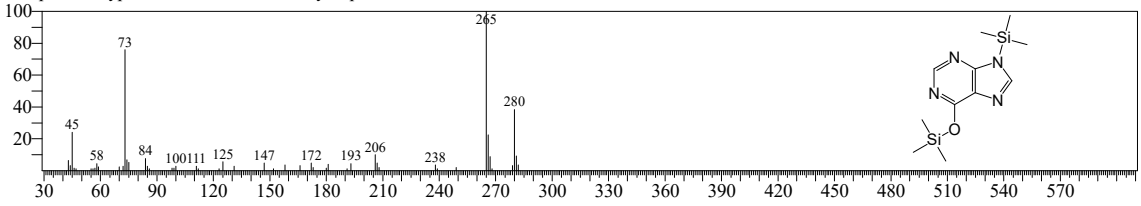
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



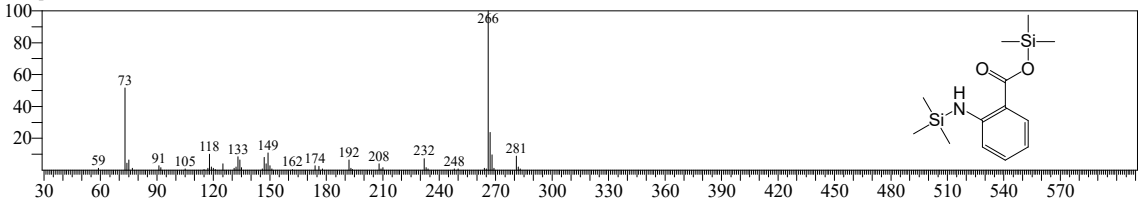
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

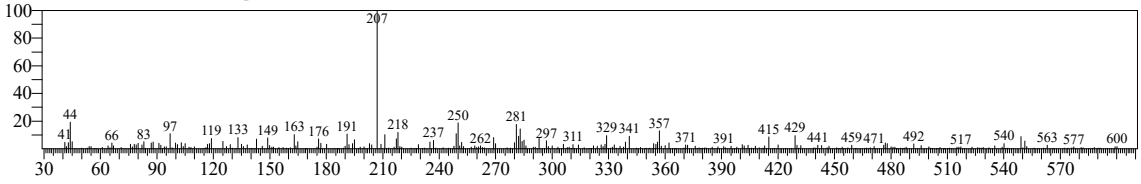


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

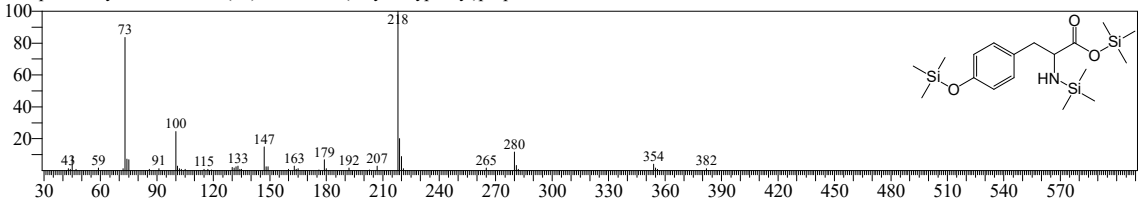


TNAU

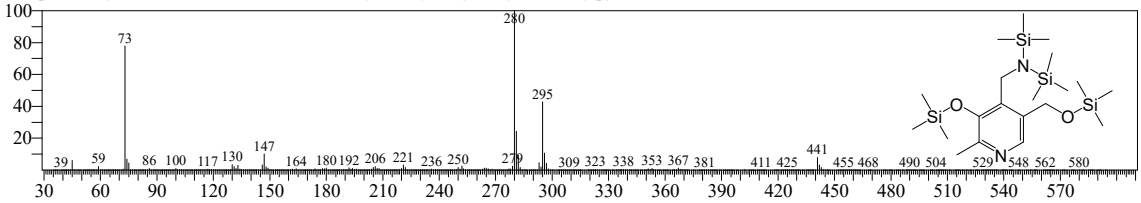
<< Target >>
Line#:18 R.Time:31.220(Scan#:5345) MassPeaks:300
RawMode:Averaged 31.215-31.225(5344-5346) BasePeak:207.05(2476)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



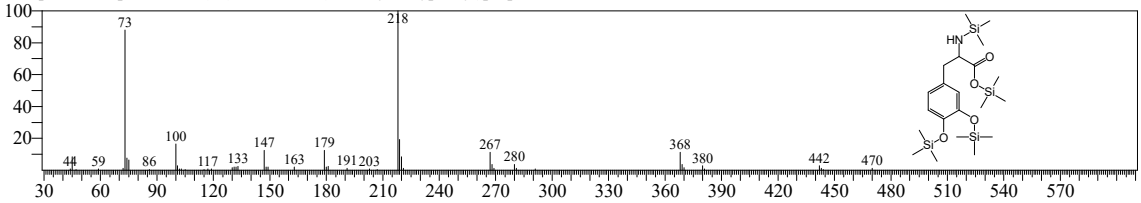
Hit#:1 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid



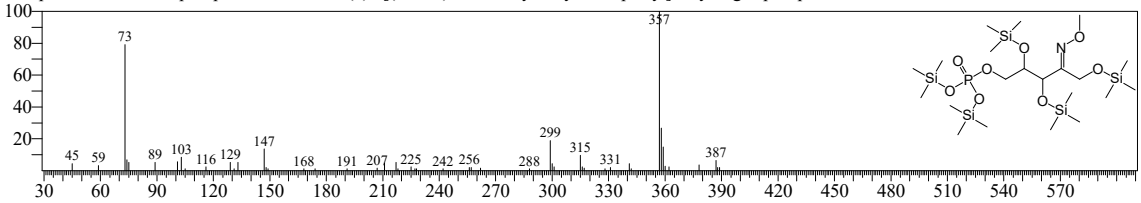
Hit#:2 Entry:469 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C20H44N2O2Si4 CAS:85-87-0 MolWeight:456 RetIndex:2139
CompName:Pyridoxamine-4TMS ; 4-(aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol



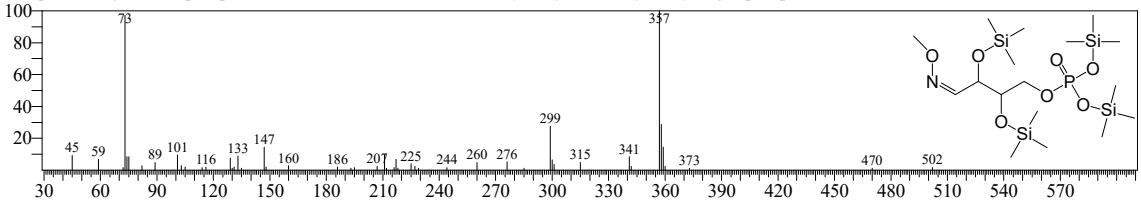
Hit#:3 Entry:463 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H43NO4Si4 CAS:59-92-7 MolWeight:485 RetIndex:2123
CompName:Dopa-4TMS ; (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid



Hit#:4 Entry:476 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C21H54NO8PSi5 CAS:4151-19-3 MolWeight:619 RetIndex:2152
CompName:Ribulose 5-phosphate-meto-5TMS(2) ; [(2R,3R)-2,3,5-trihydroxy-4-oxopentyl] dihydrogen phosphate

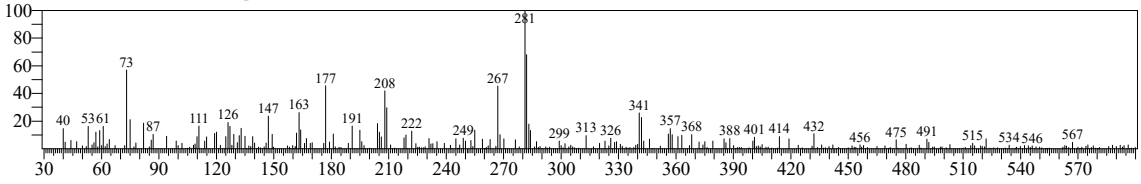


Hit#:5 Entry:394 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1935
CompName:Erythrose 4-phosphate-meto-4TMS(2) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate

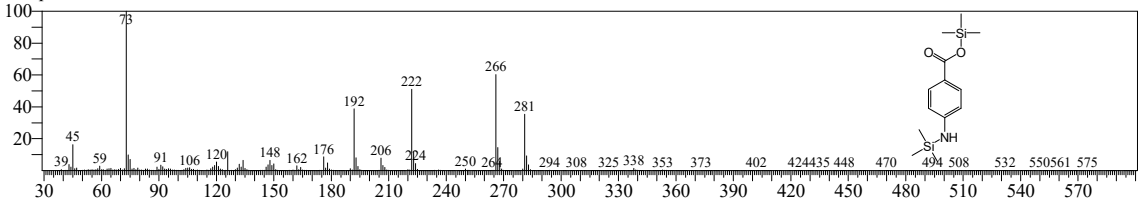


TNAU

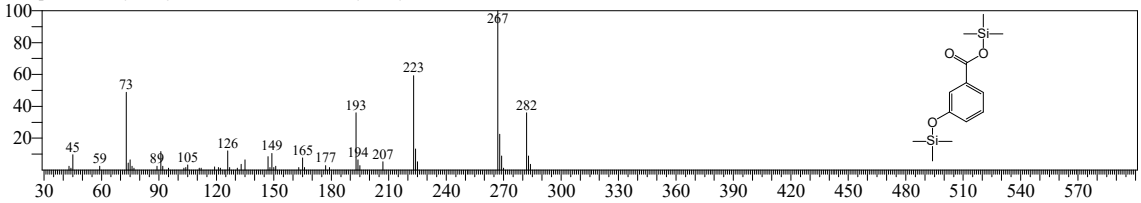
<< Target >>
Line#:19 R.Time:31.395(Scan#:5380) MassPeaks:297
RawMode:Averaged 31.390-31.400(5379-5381) BasePeak:281.10(1211)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



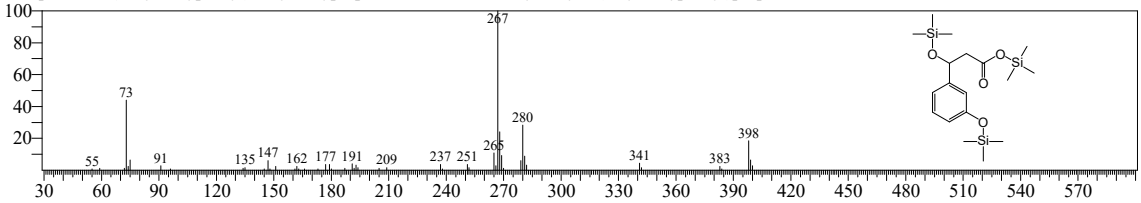
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



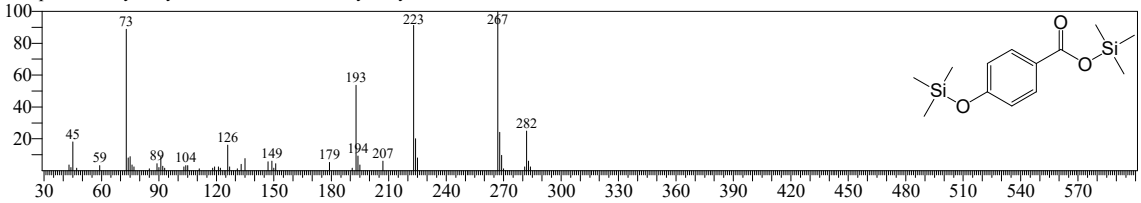
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



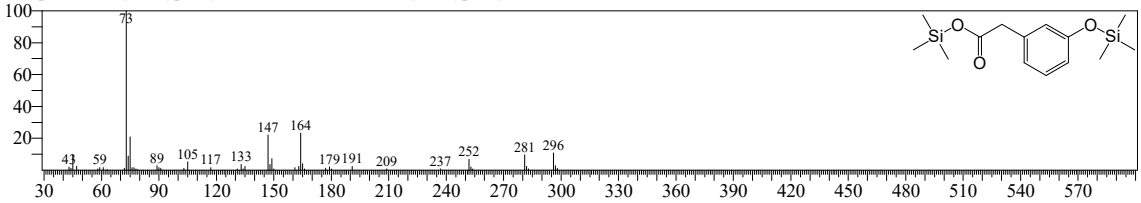
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

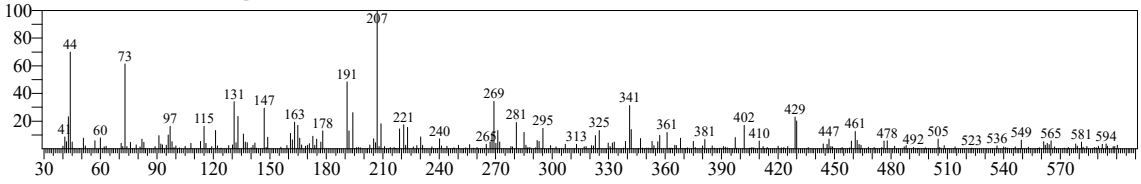


Hit#:5 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

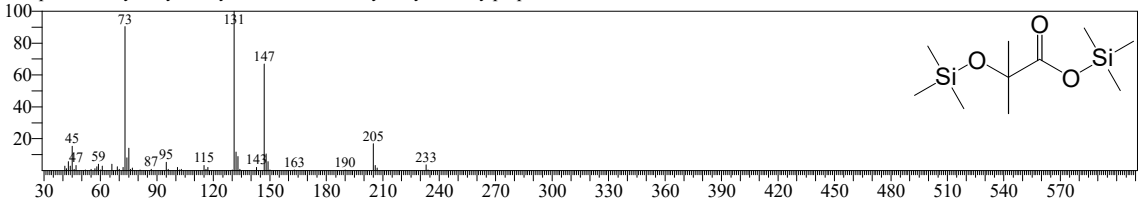


TNAU

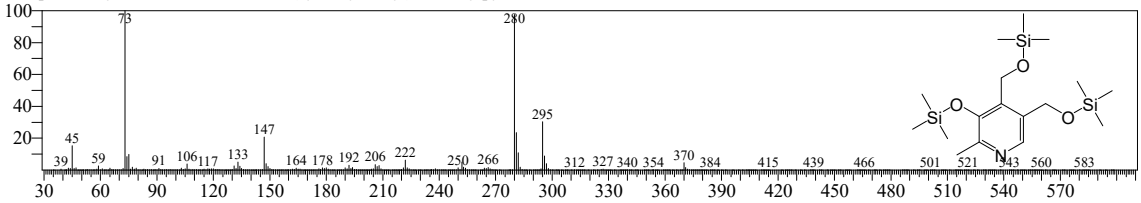
<< Target >>
Line#:20 R.Time:31.670(Scan#:5435) MassPeaks:267
RawMode:Averaged 31.665-31.675(5434-5436) BasePeak:207.05(1256)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



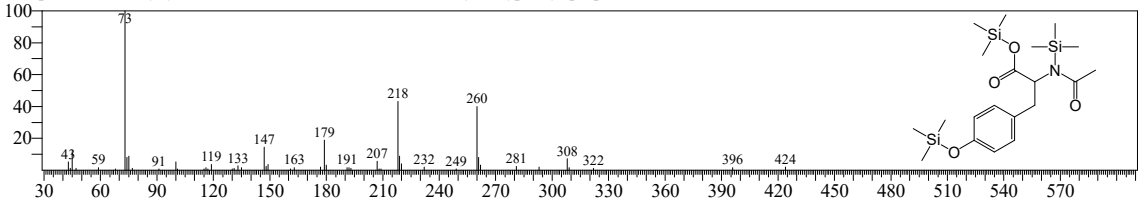
Hit#:1 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid



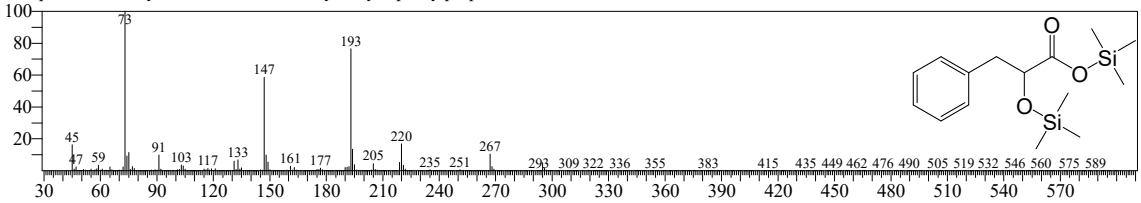
Hit#:2 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



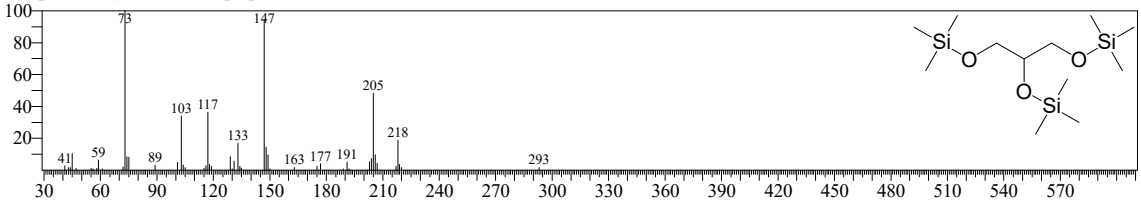
Hit#:3 Entry:461 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C20H37NO4Si3 CAS:537-55-3 MolWeight:439 RetIndex:2119
CompName:N-Acetyltyrosine-3TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

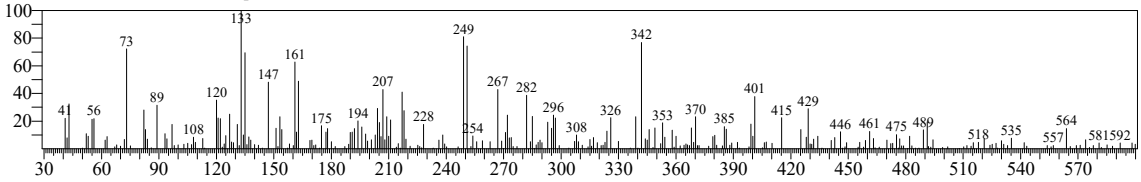


Hit#:5 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol

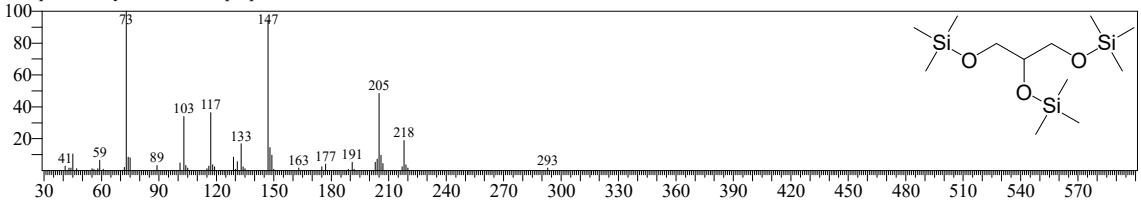


TNAU

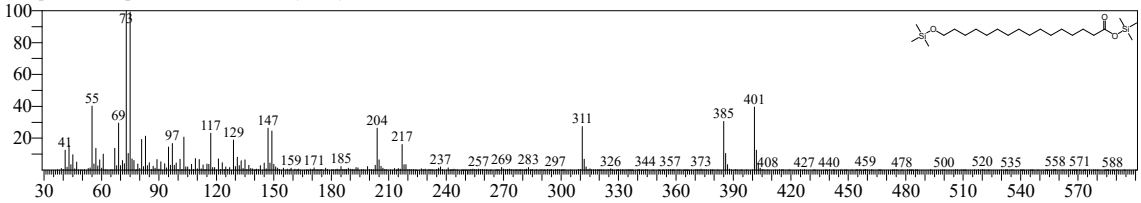
<< Target >>
Line#:21 R.Time:31.745(Scan#:5450) MassPeaks:276
RawMode:Averaged 31.740-31.750(5449-5451) BasePeak:133.00(537)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



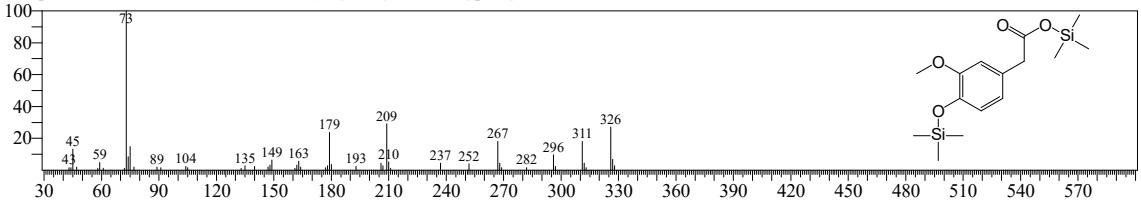
Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



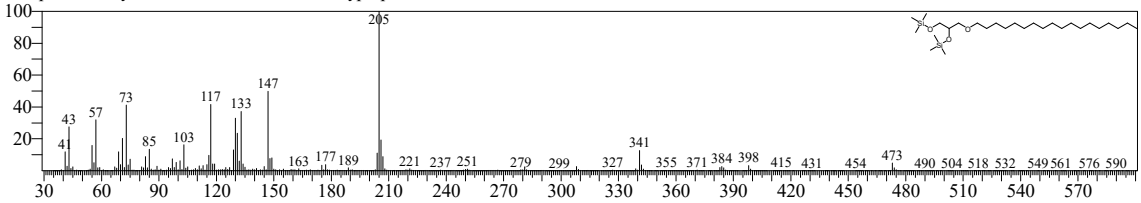
Hit#:2 Entry:511 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C22H48O3Si2 CAS:506-13-8 MolWeight:416 RetIndex:2396
CompName:Juniperic acid-2TMS ; 16-hydroxyhexadecanoic acid



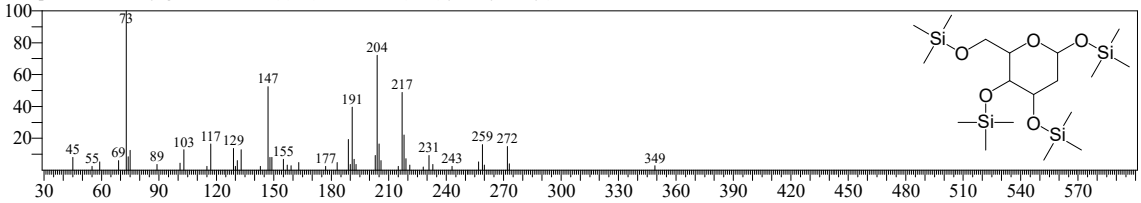
Hit#:3 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

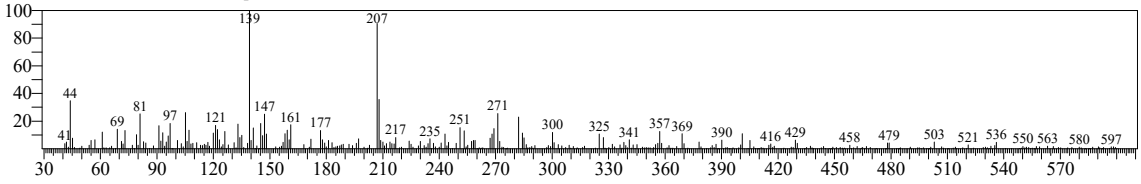


Hit#:5 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1816
CompName:2-Deoxy-glucose-4TMS(2) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

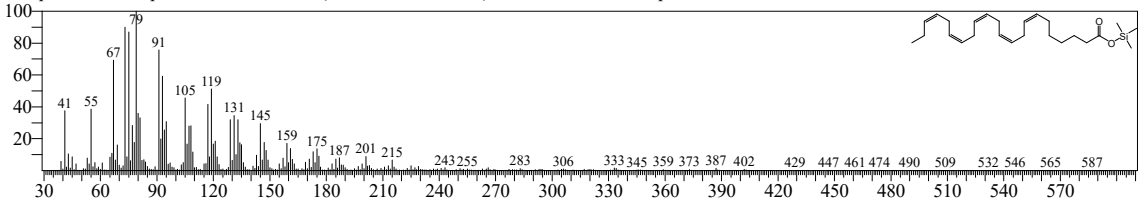


TNAU

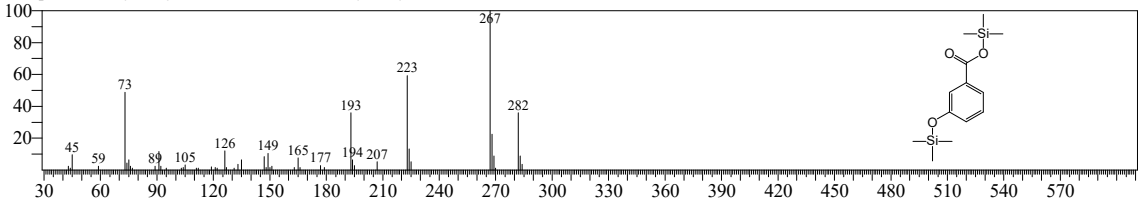
<< Target >>
Line#:22 R.Time:31.895(Scan#:5480) MassPeaks:342
RawMode:Averaged 31.890-31.900(5479-5481) BasePeak:139.15(2062)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



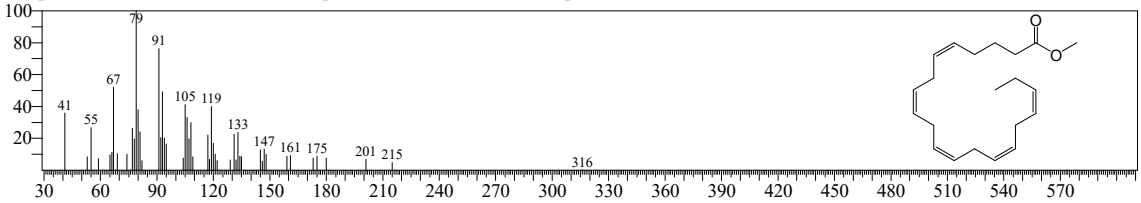
Hit#:1 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



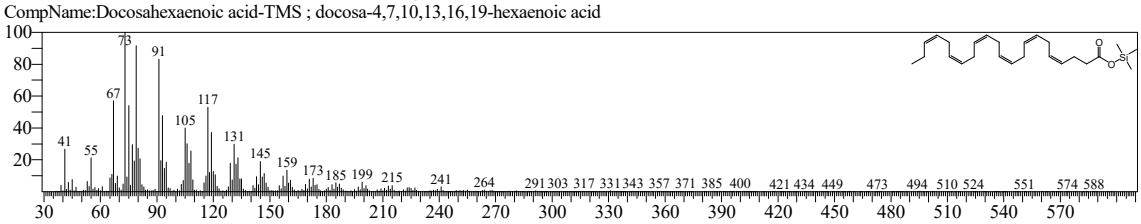
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



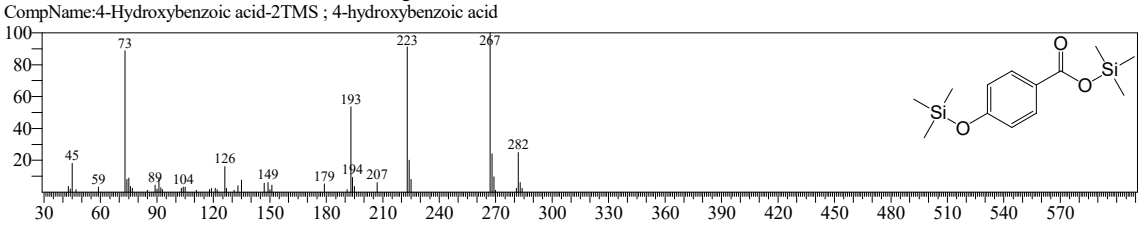
Hit#:3 Entry:36 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C21H32O2 CAS:10417-94-4 MolWeight:316 RetIndex:3232
CompName:Methyl cis-5,8,11,14,17-Eicosapentaenoate ; Icosa-5,8,11,14,17-pentaenoic acid



Hit#:4 Entry:533 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C25H40O2Si CAS:6217-54-5 MolWeight:400 RetIndex:2576
CompName:Docosahexaenoic acid-TMS ; docosa-4,7,10,13,16,19-hexaenoic acid

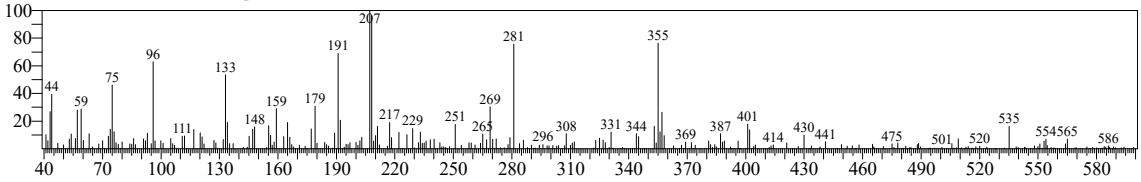


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

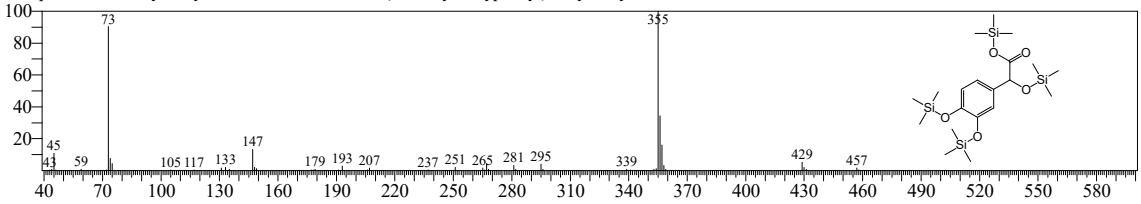


TNAU

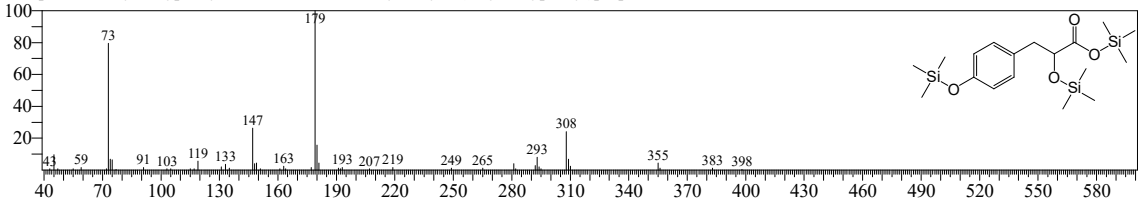
<< Target >>
Line#:23 R.Time:32.015(Scan#:5504) MassPeaks:276
RawMode:Averaged 32.010-32.020(5503-5505) BasePeak:207.05(932)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



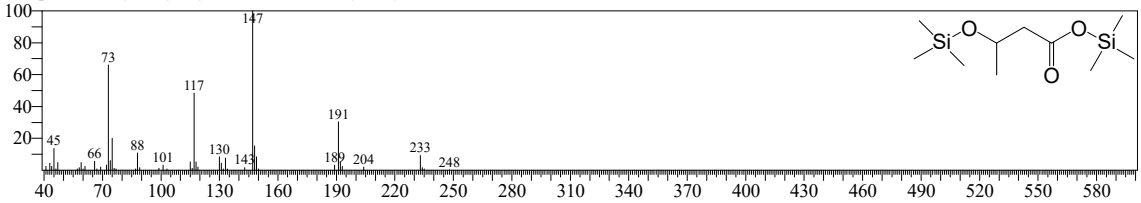
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



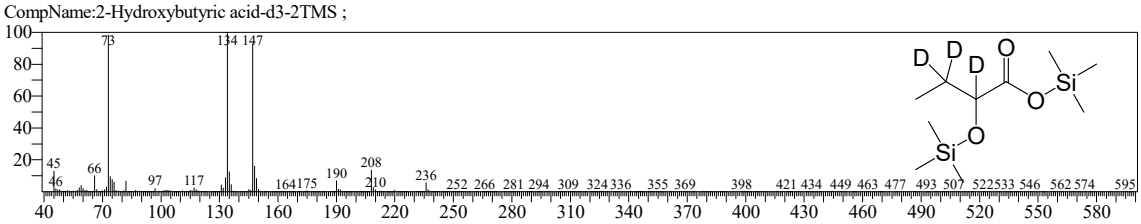
Hit#:2 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



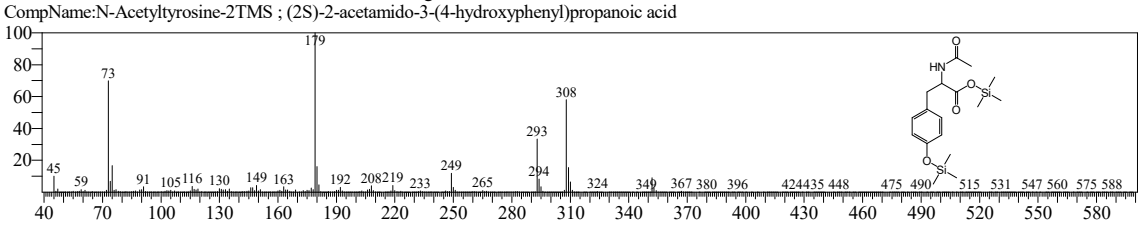
Hit#:3 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid



Hit#:4 Entry:25 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula: CAS:0-00-0 MolWeight:251 RetIndex:1130
CompName:2-Hydroxybutyric acid-d3-2TMS ;

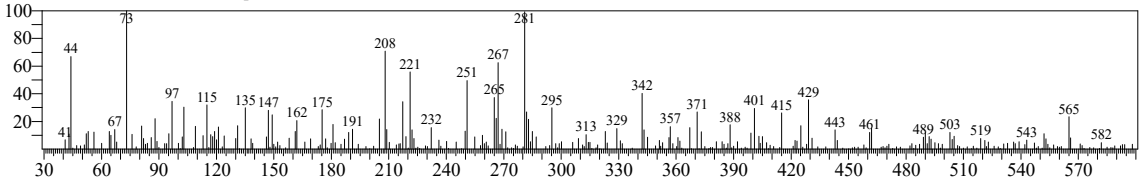


Hit#:5 Entry:474 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C17H29NO4Si2 CAS:537-55-3 MolWeight:367 RetIndex:2148
CompName:N-Acetyltyrosine-2TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid

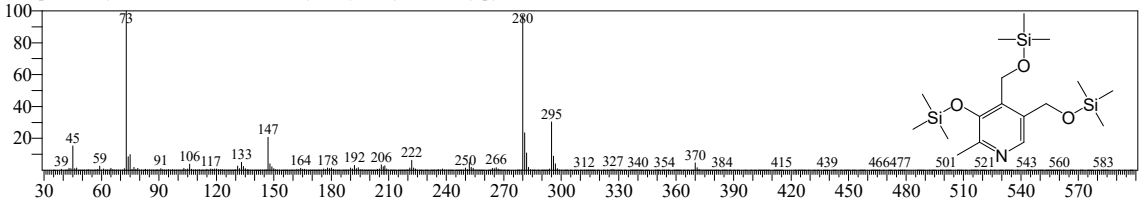


TNAU

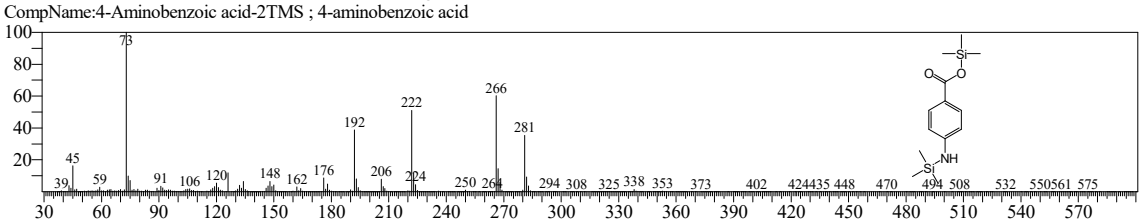
<< Target >>
Line#:24 R.Time:32.505(Scan#:5602) MassPeaks:299
RawMode:Averaged 32.500-32.510(5601-5603) BasePeak:73.05(782)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



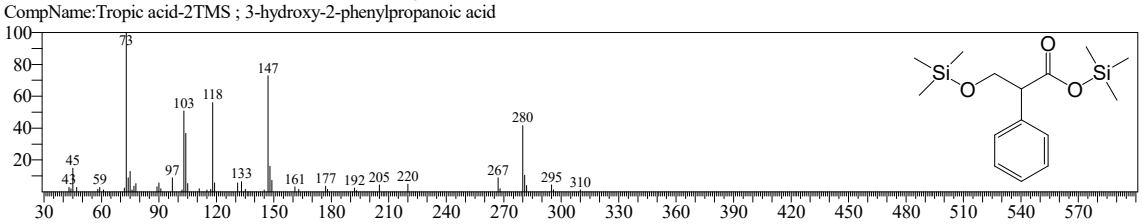
Hit#:1 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



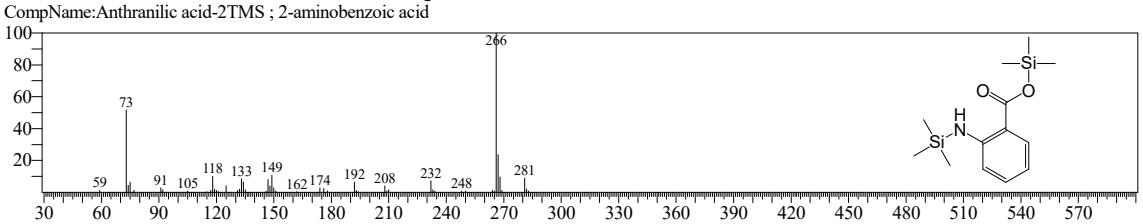
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:3 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



Hit#:5 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid