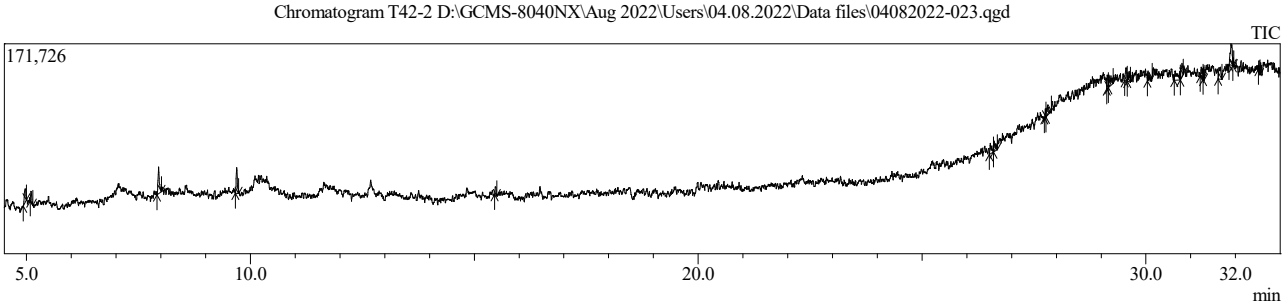
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 7:11:26 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T42-2
Sample ID	: T42-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 22
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-023.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-023.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 4:42:35 PM

Chromatogram T42-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-023.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.970	26467	5.35	11133	4.97	2.38	70	3,3-Dimethoxy-2-butanone
2	5.100	14142	2.86	9037	4.04	1.56	47	Hydroxylamine-3TMS
3	7.948	45890	9.28	21909	9.79	2.09	87	Undecane
4	9.693	39071	7.90	20986	9.38	1.86	87	Dodecane
5	15.471	10340	2.09	6615	2.96	1.56	70	2,4-Di-tert-butylphenol
6	26.520	20941	4.23	8595	3.84	2.44	36	2-Hydroxyisobutyric acid-2TMS
7	26.605	24040	4.86	8030	3.59	2.99	31	Stearic acid-TMS
8	27.753	6533	1.32	6990	3.12	0.93	31	2-Hydroxyphenylacetic acid-2TMS
9	27.780	21759	4.40	6523	2.91	3.34	35	Hypoxanthine-2TMS
10	29.135	13744	2.78	11163	4.99	1.23	46	3,4-Dihydroxymandelic acid-4TMS
11	29.170	31389	6.35	9831	4.39	3.19	25	Hippuric acid-TMS
12	29.560	22734	4.60	10605	4.74	2.14	33	2-Phenyllactic acid-2TMS
13	29.625	20286	4.10	8672	3.87	2.34	33	3-Hydroxybenzoic acid-2TMS
14	30.040	12905	2.61	6665	2.98	1.94	45	3-Hydroxyanthranilic acid-2TMS
15	30.645	34902	7.06	7354	3.29	4.75	34	3,4-Dihydroxymandelic acid-4TMS
16	30.785	25696	5.20	8448	3.77	3.04	39	Protocatechuic acid-3TMS
17	31.235	18653	3.77	8423	3.76	2.21	40	Chloramphenicol-2TMS
18	31.290	7725	1.56	10443	4.67	0.74	35	Glucose-5TMS(1)
19	31.664	29465	5.96	9780	4.37	3.01	39	4-Hydroxybenzoic acid-2TMS
20	31.900	53501	10.82	17270	7.72	3.10	30	4-Aminobenzoic acid-2TMS
21	31.950	4757	0.96	6185	2.76	0.77	22	3,4-Dihydroxymandelic acid-4TMS
22	32.526	9567	1.93	9172	4.10	1.04	34	Batyl alcohol-2TMS

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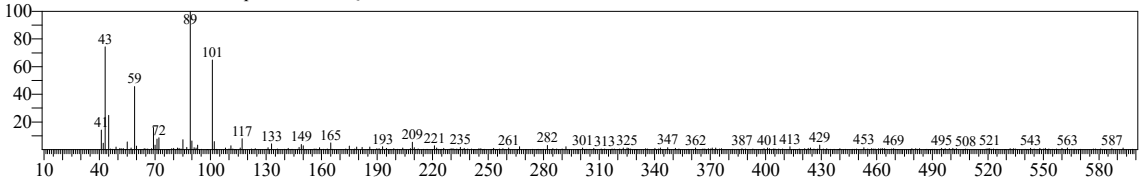
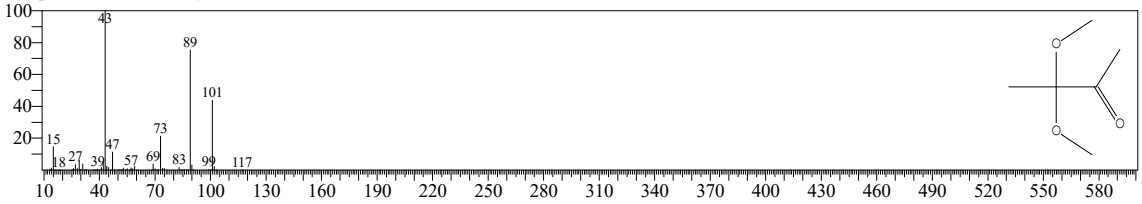
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
		494507	100.00	223829	100.00			

Library

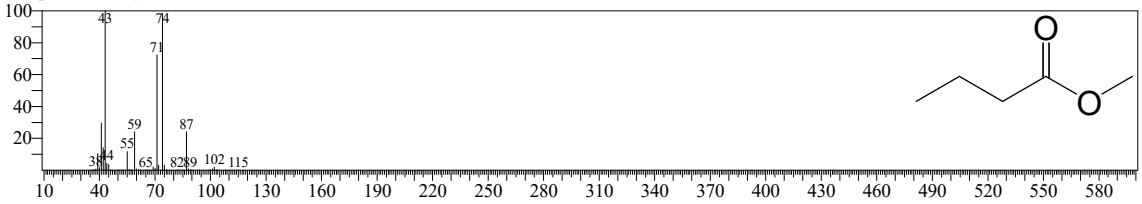
<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:276
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.05(2854)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



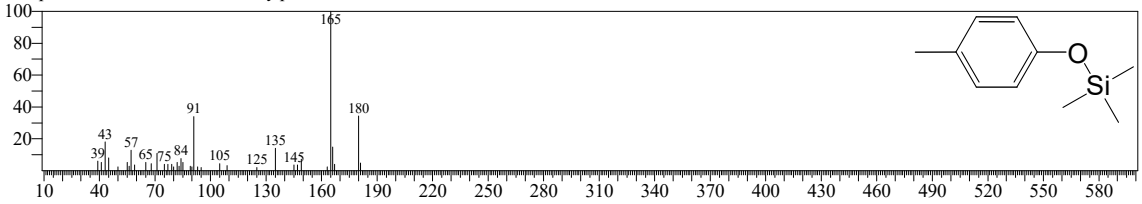
Hit#:1 Entry:9263 Library:NIST20M1.lib
SI:70 Formula:C6H12O3 CAS:21983-72-2 MolWeight:132 RetIndex:821
CompName:3,3-Dimethoxy-2-butanone



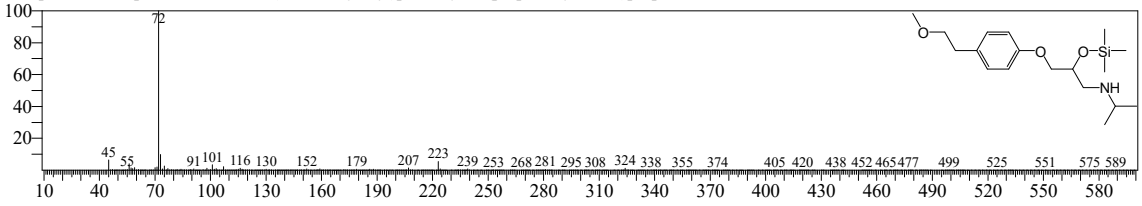
Hit#:2 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:56 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



Hit#:3 Entry:34 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C10H16OSi CAS:106-44-5 MolWeight:180 RetIndex:1160
CompName:4-Cresol-TMS ; 4-methylphenol

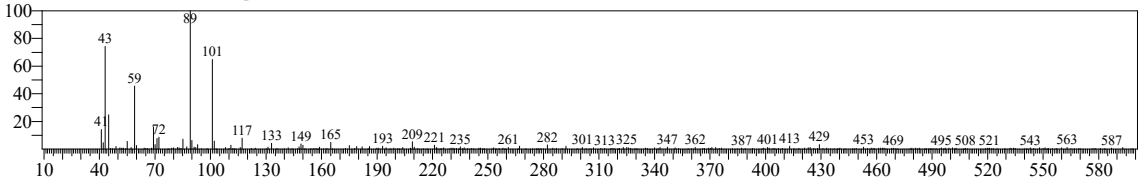


Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H33NO3Si CAS:37350-58-6 MolWeight:339 RetIndex:2094
CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol

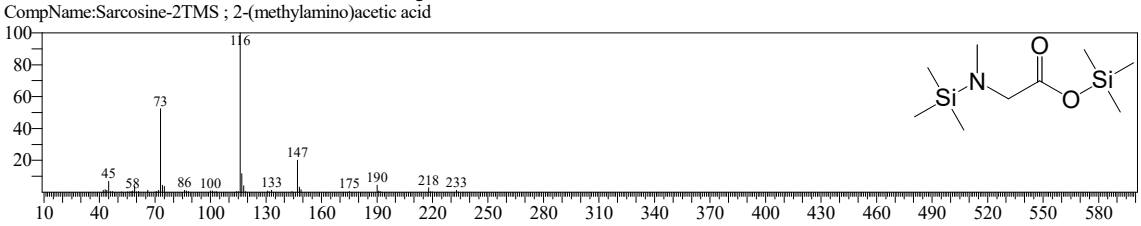


TNAU

<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:276
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.05(2854)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

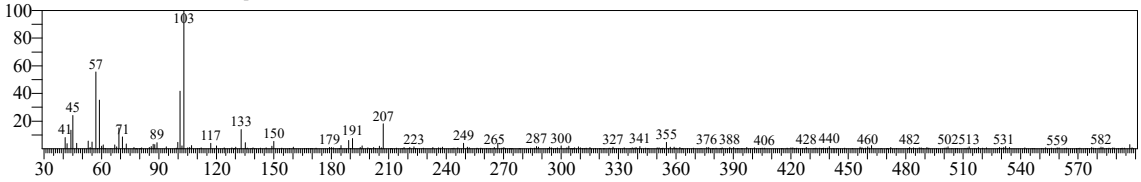


Hit#:5 Entry:29 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H23NO2Si2 CAS:107-97-1 MolWeight:233 RetIndex:1141
CompName:Sarcosine-2TMS ; 2-(methylamino)acetic acid

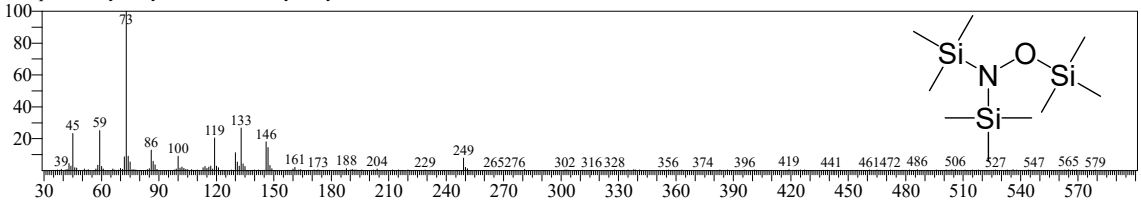


TNAU

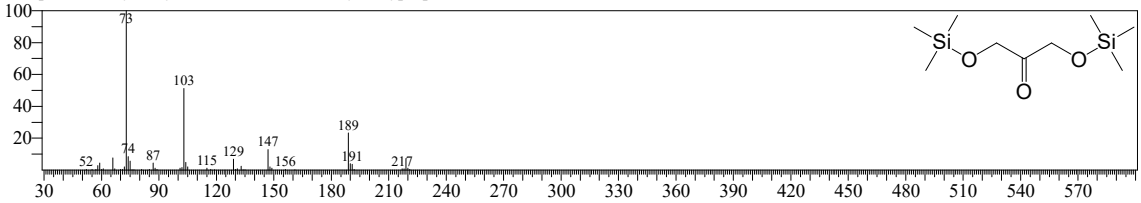
<< Target >>
Line#:2 R.Time:5.100(Scan#:121) MassPeaks:271
RawMode:Averaged 5.095-5.105(120-122) BasePeak:103.10(2407)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



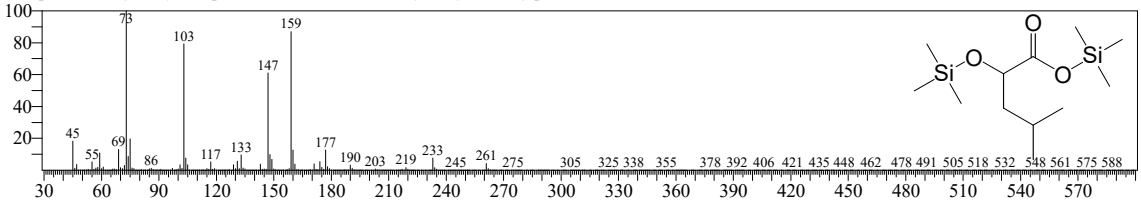
Hit#:1 Entry:20 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C9H27NOSi3 CAS:7803-49-8 MolWeight:249 RetIndex:1127
CompName:Hydroxylamine-3TMS ; hydroxylamine



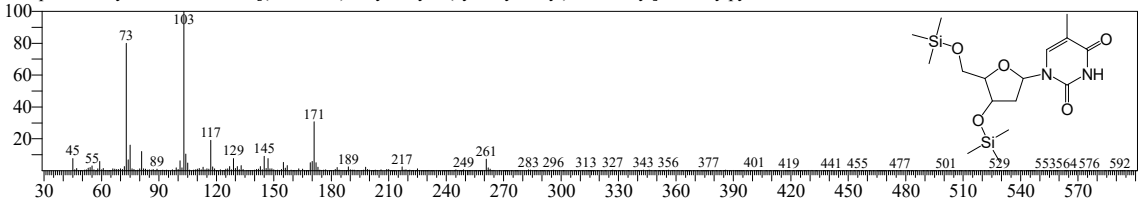
Hit#:2 Entry:57 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C9H22O3Si2 CAS:96-26-4 MolWeight:234 RetIndex:1224
CompName:Dihydroxyacetone-2TMS ; 1,3-dihydroxypropan-2-one



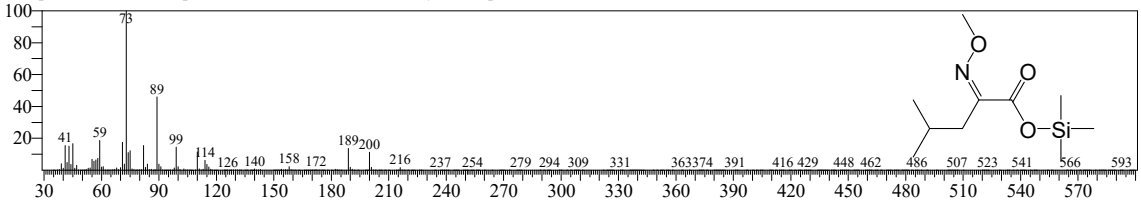
Hit#:3 Entry:62 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C12H28O3Si2 CAS:20312-37-2 MolWeight:276 RetIndex:1244
CompName:2-Hydroxyisocaproic acid-2TMS ; (2R)-2-hydroxy-4-methylpentanoic acid



Hit#:4 Entry:514 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C16H30N2O5Si2 CAS:50-89-5 MolWeight:386 RetIndex:2428
CompName:Thymidine-2TMS ; 1-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-methylpyrimidine-2,4-dione



Hit#:5 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid



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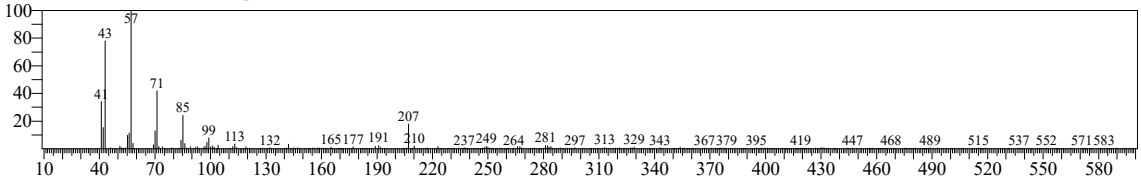
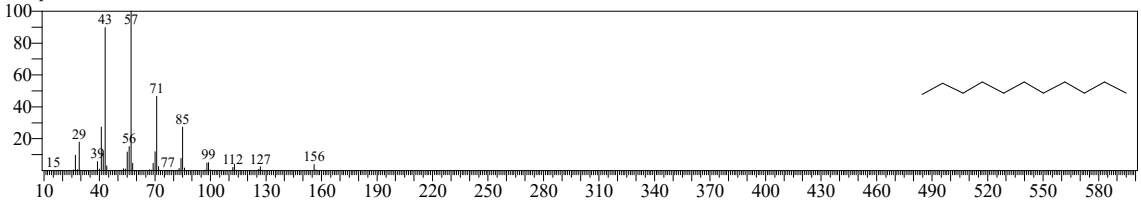
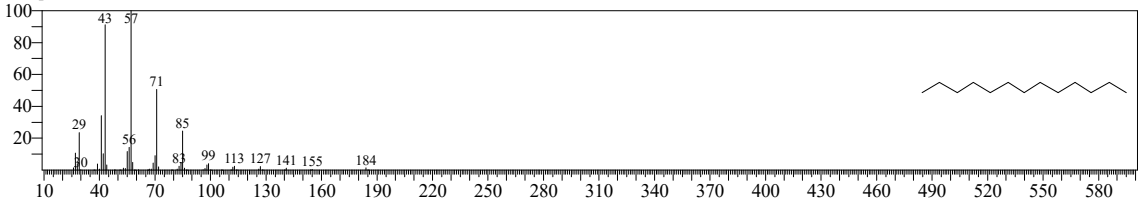
<< Target >>
Line#:3 R.Time:7.950(Scan#:691) MassPeaks:311
RawMode:Averaged 7.945-7.955(690-692) BasePeak:57.05(5246)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



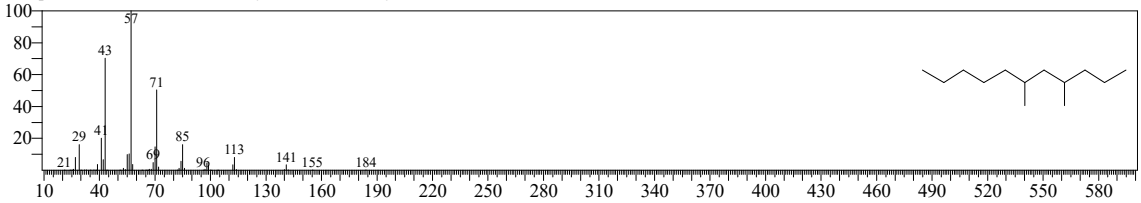
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



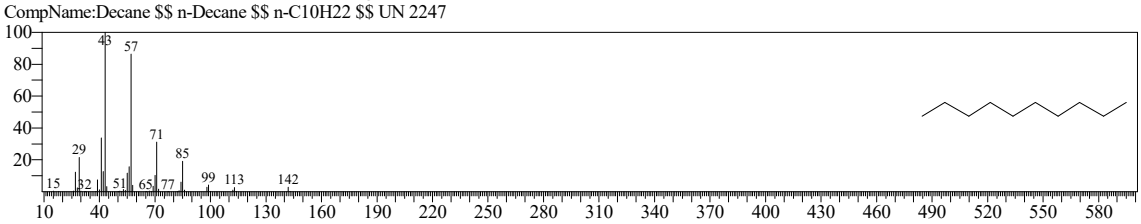
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



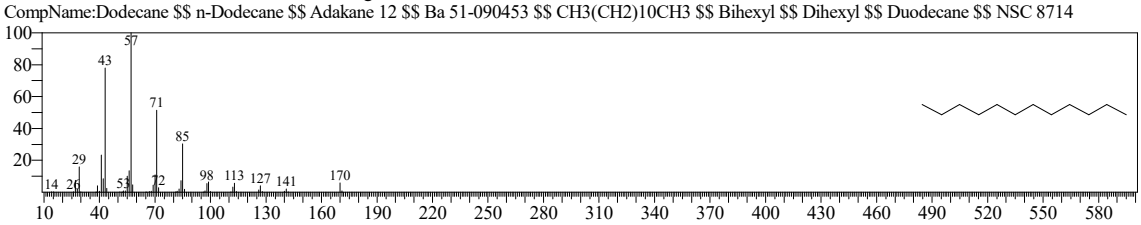
Hit#:3 Entry:40271 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:17312-82-2 MolWeight:184 RetIndex:1185
CompName:Undecane, 4,6-dimethyl- $$ 4,6-Dimethylundecane #



Hit#:4 Entry:9444 Library:NIST20R.lib
SI:87 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

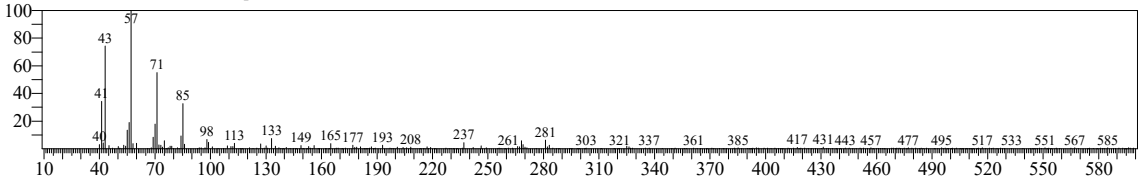


Hit#:5 Entry:16192 Library:NIST20R.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

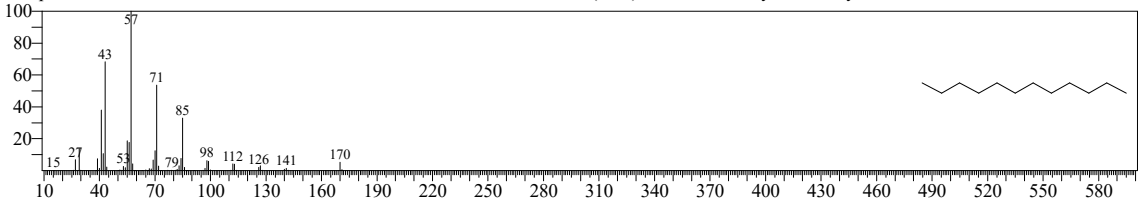


TNAU

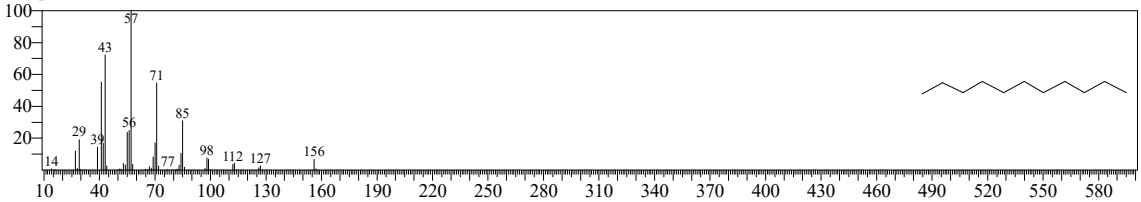
<< Target >>
Line#:4 R.Time:9.695(Scan#:1040) MassPeaks:291
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(4722)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



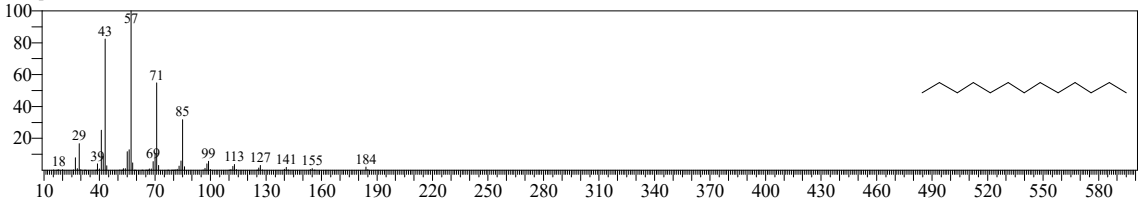
Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



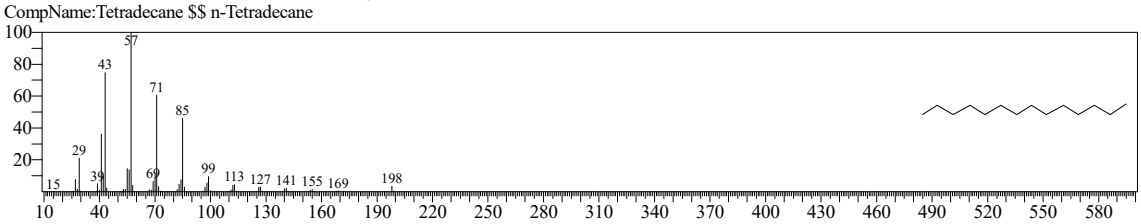
Hit#:2 Entry:12898 Library:NIST20R.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



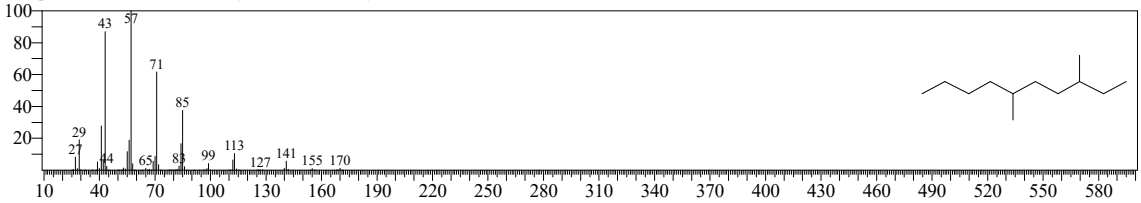
Hit#:3 Entry:19412 Library:NIST20R.lib
SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:22497 Library:NIST20R.lib
SI:86 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

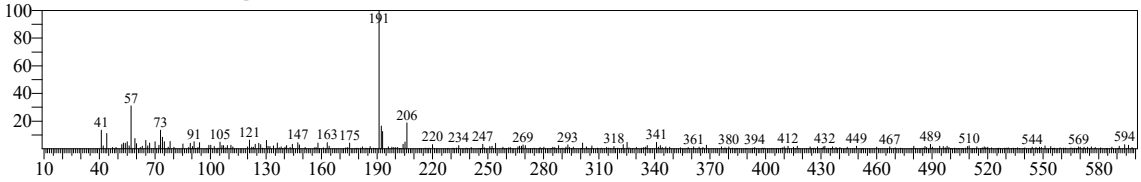


Hit#:5 Entry:30051 Library:NIST20M1.lib
SI:85 Formula:C12H26 CAS:17312-53-7 MolWeight:170 RetIndex:1086
CompName:Decane, 3,6-dimethyl- $$ 3,6-Dimethyldecane

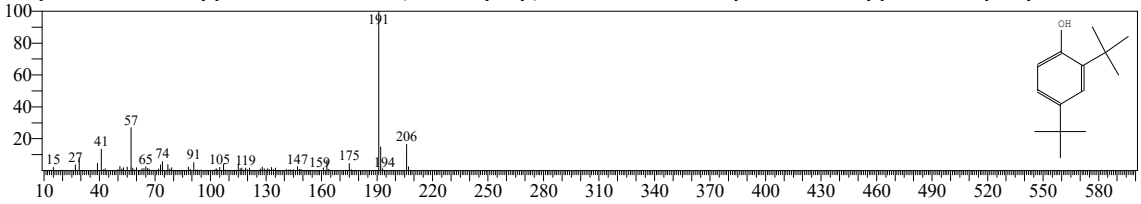


TNAU

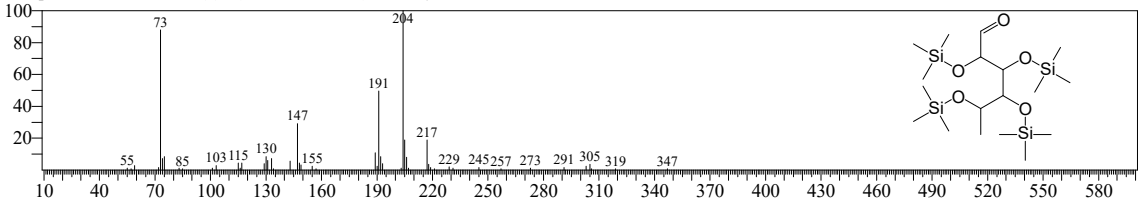
<< Target >>
Line#:5 R.Time:15.470(Scan#:2195) MassPeaks:295
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.10(1882)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



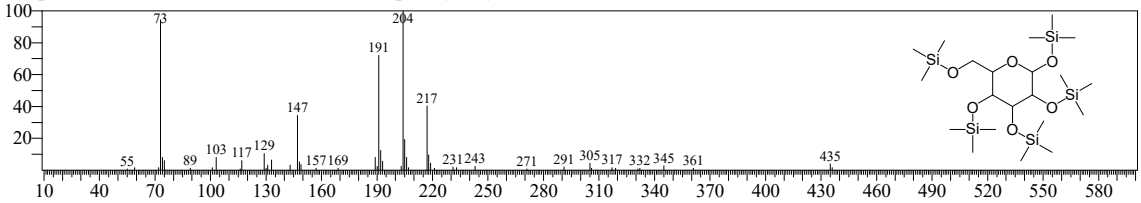
Hit#:1 Entry:24086 Library:NIST20R.lib
SI:70 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



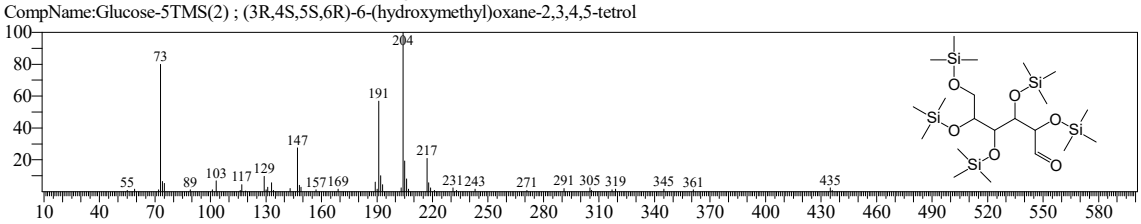
Hit#:2 Entry:271 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1738
CompName:Fucose-4TMS(2) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



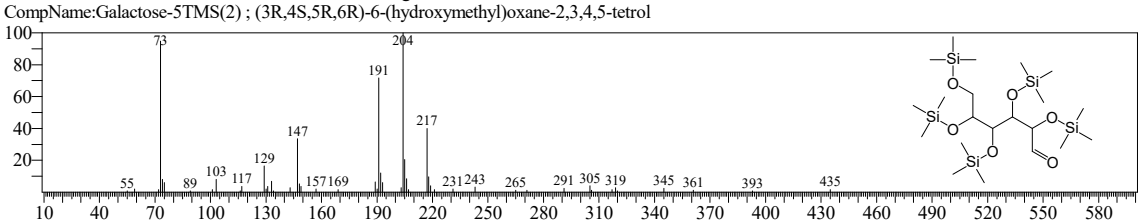
Hit#:3 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:48 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:4 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:48 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:2002
CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

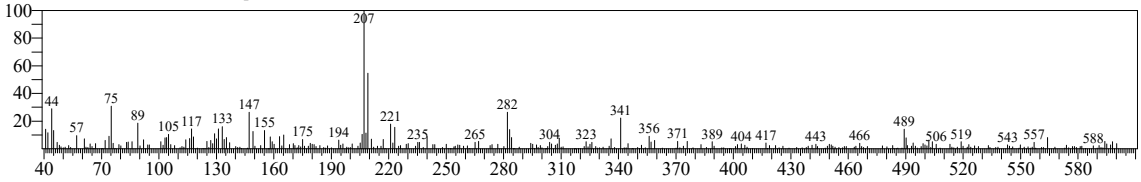


Hit#:5 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:48 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

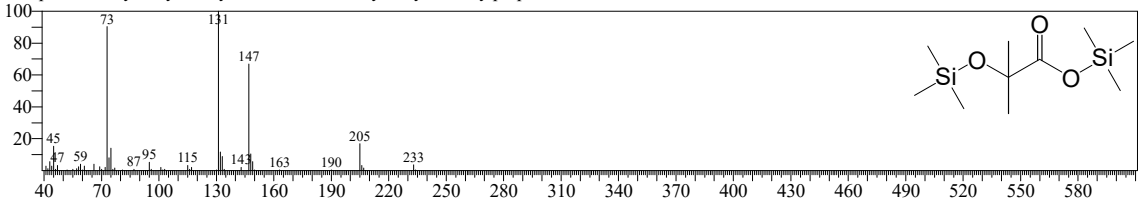


TNAU

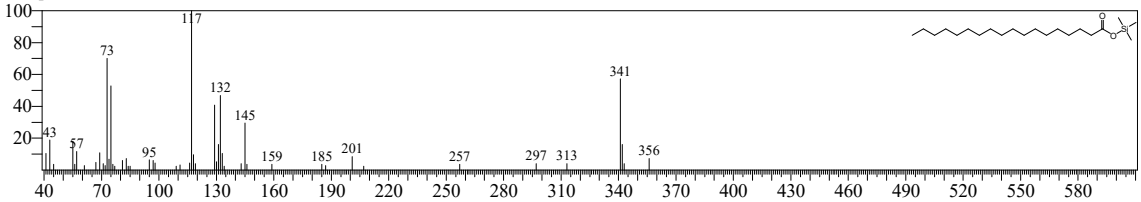
<< Target >>
Line#:6 R.Time:26.520(Scan#:4405) MassPeaks:320
RawMode:Averaged 26.515-26.525(4404-4406) BasePeak:207.05(1182)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



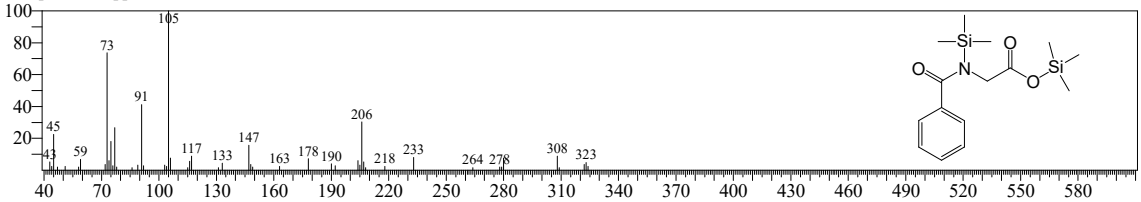
Hit#:1 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid



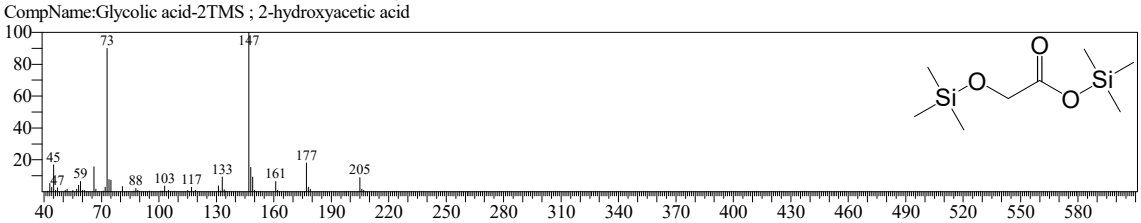
Hit#:2 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



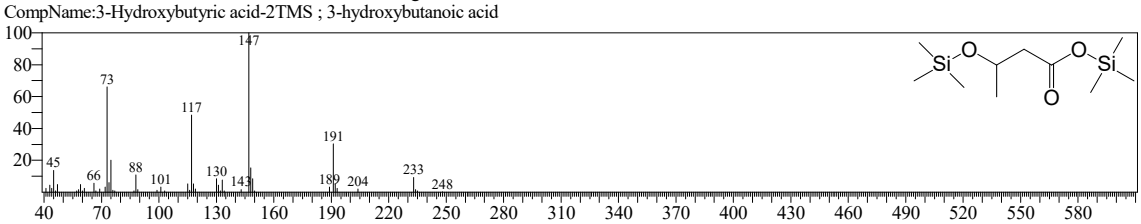
Hit#:3 Entry:307 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C15H25NO3Si2 CAS:66407-11-2 MolWeight:323 RetIndex:1819
CompName:Hippuric acid-2TMS ; 2-benzamidoacetic acid



Hit#:4 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

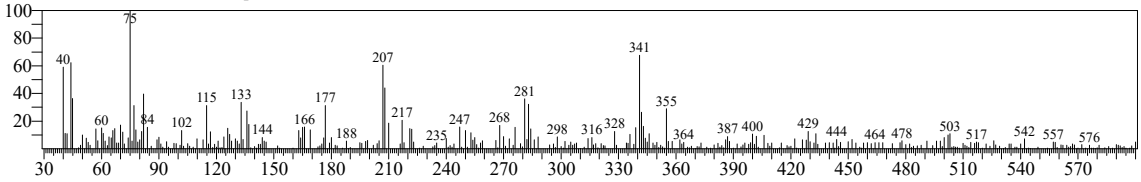


Hit#:5 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid

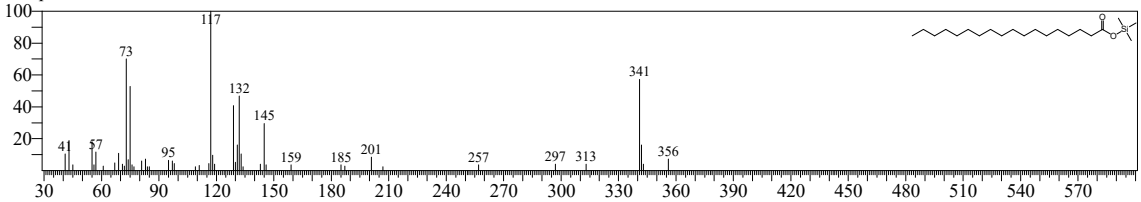


TNAU

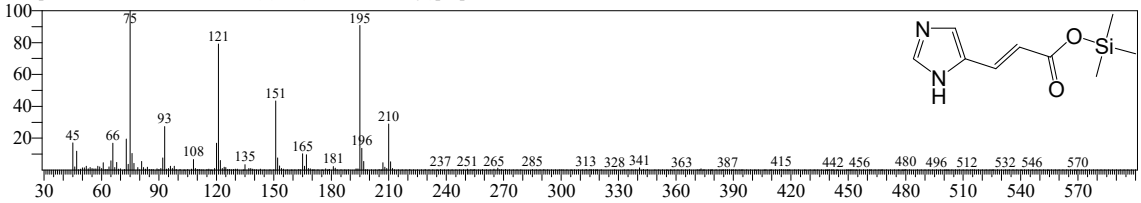
<< Target >>
Line#:7 R.Time:26.605(Scan#:4422) MassPeaks:350
RawMode:Averaged 26.600-26.610(4421-4423) BasePeak:75.00(565)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



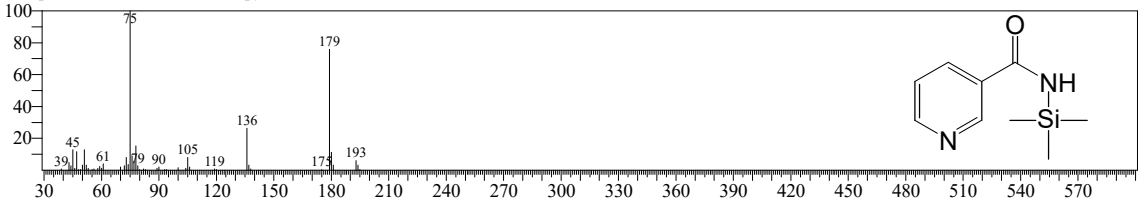
Hit#:1 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



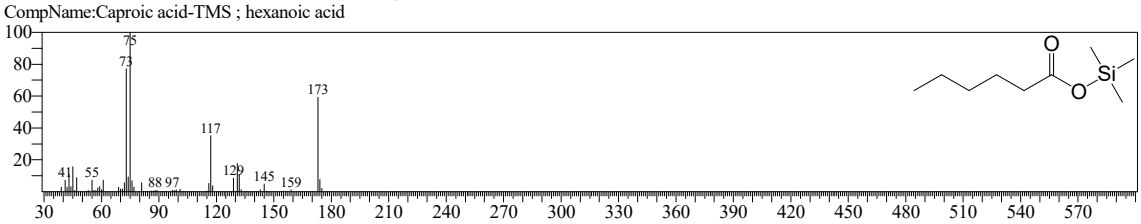
Hit#:2 Entry:361 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C9H14N2O2Si CAS:104-98-3 MolWeight:210 RetIndex:1896
CompName:Urocanic acid-TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



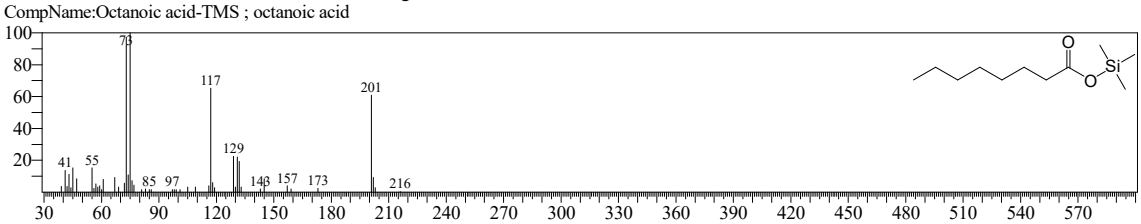
Hit#:3 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide



Hit#:4 Entry:11 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid

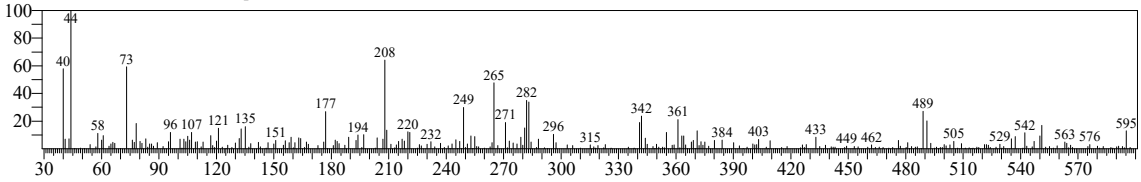


Hit#:5 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
CompName:Octanoic acid-TMS ; octanoic acid

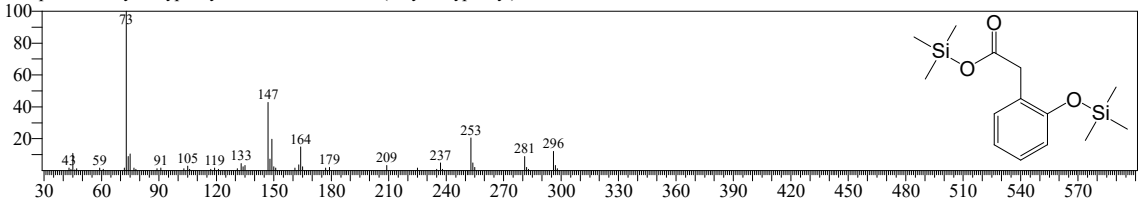


TNAU

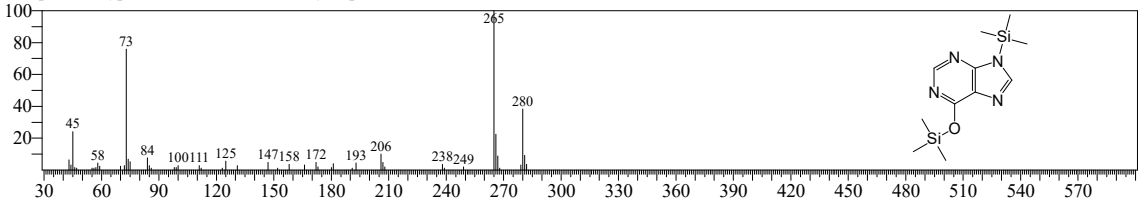
<< Target >>
Line#:8 R.Time:27.755(Scan#:4652) MassPeaks:294
RawMode:Averaged 27.750-27.760(4651-4653) BasePeak:44.00(817)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



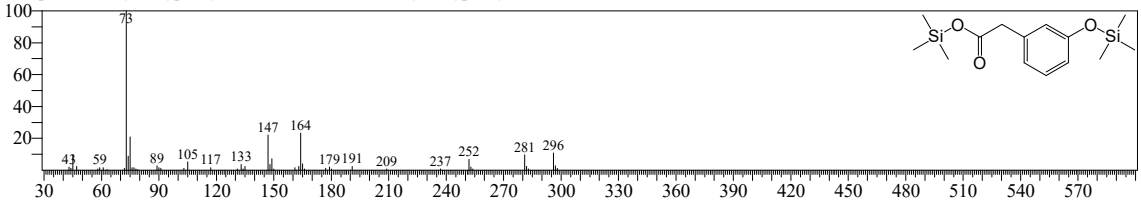
Hit#:1 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



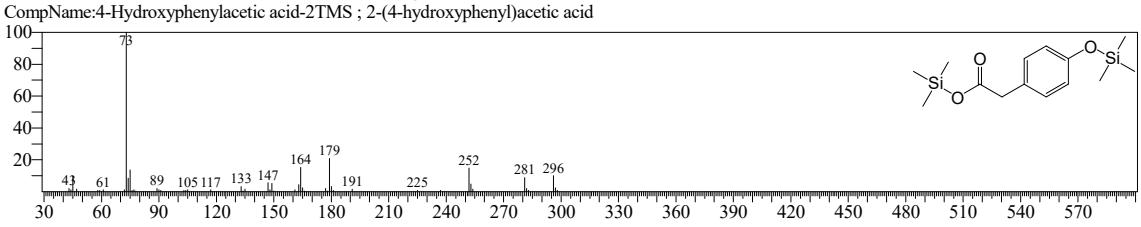
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



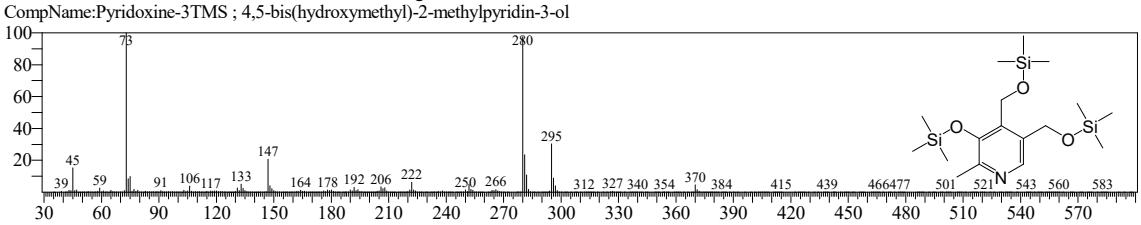
Hit#:3 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid



Hit#:4 Entry:220 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C14H24O3Si2 CAS:156-38-7 MolWeight:296 RetIndex:1647
CompName:4-Hydroxyphenylacetic acid-2TMS ; 2-(4-hydroxyphenyl)acetic acid

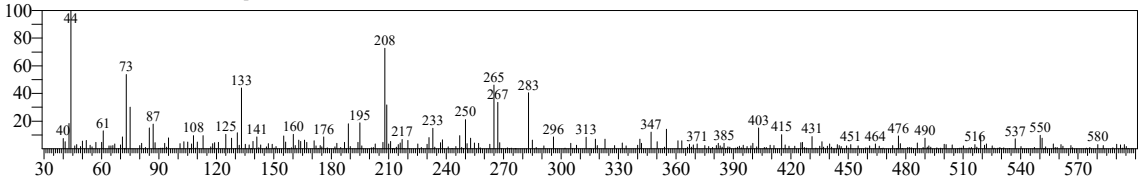


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

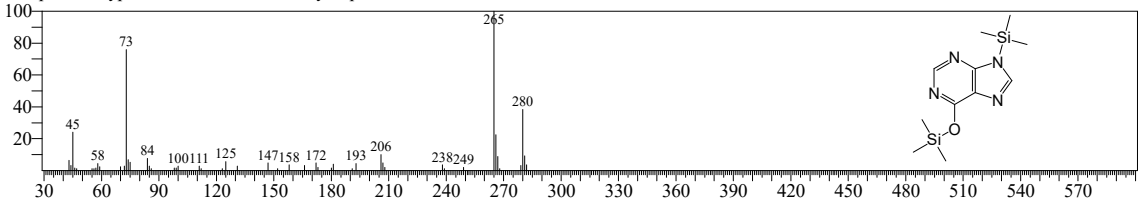


TNAU

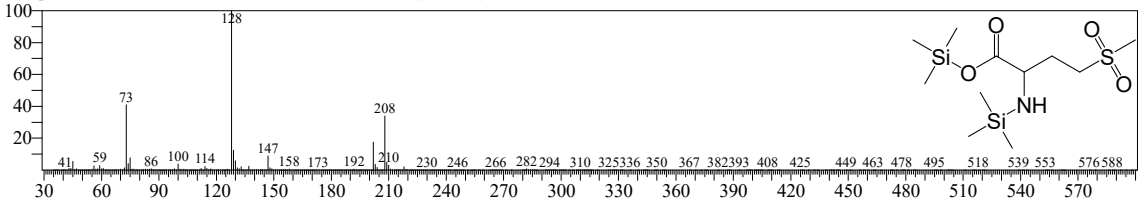
<< Target >>
Line#:9 R.Time:27.780(Scan#:4657) MassPeaks:289
RawMode:Averaged 27.775-27.785(4656-4658) BasePeak:44.00(970)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



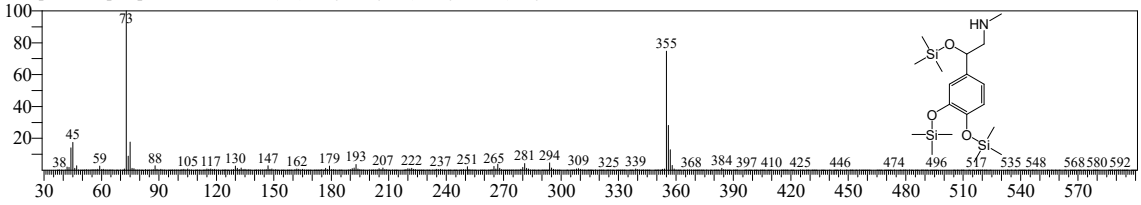
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



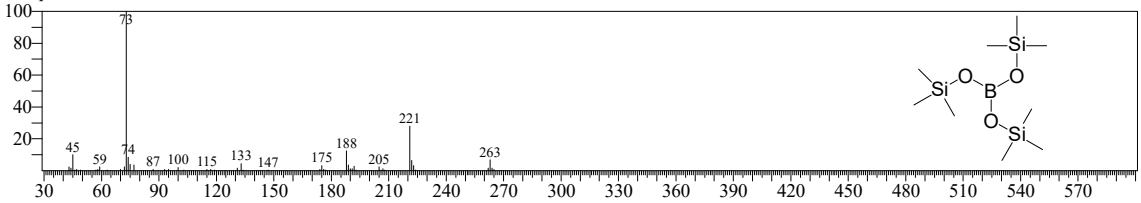
Hit#:2 Entry:329 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C11H27NO4SSi2 CAS:820-10-0 MolWeight:325 RetIndex:1848
CompName:Methionine sulfone-2TMS ; 2-amino-4-methylsulfonylbutanoic acid



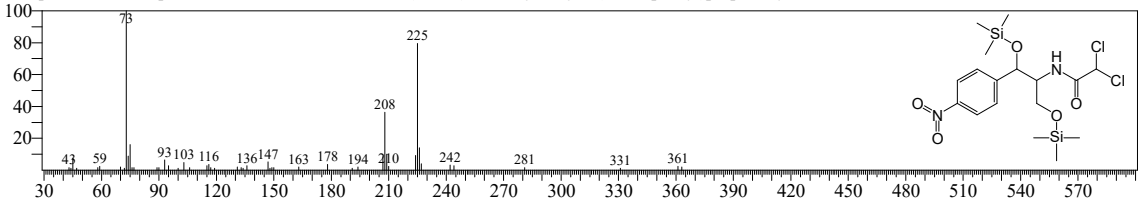
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid

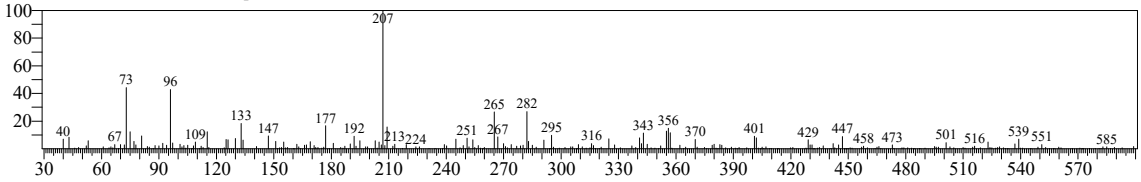


Hit#:5 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

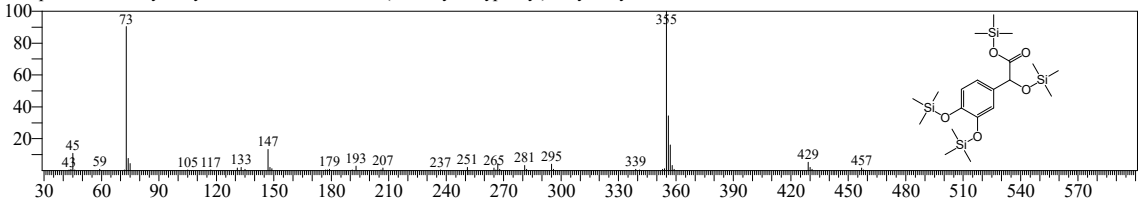


TNAU

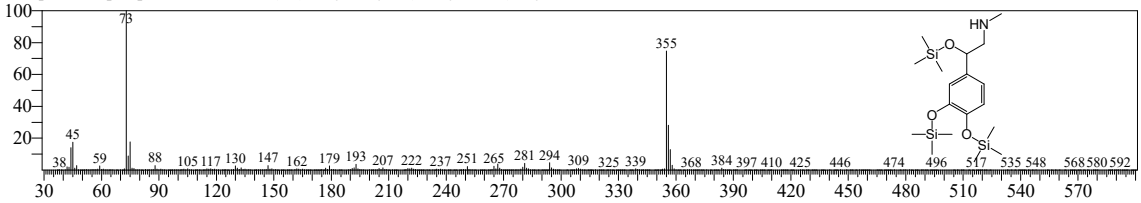
<< Target >>
Line#:10 R.Time:29.135(Scan#:4928) MassPeaks:268
RawMode:Averaged 29.130-29.140(4927-4929) BasePeak:207.05(1957)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



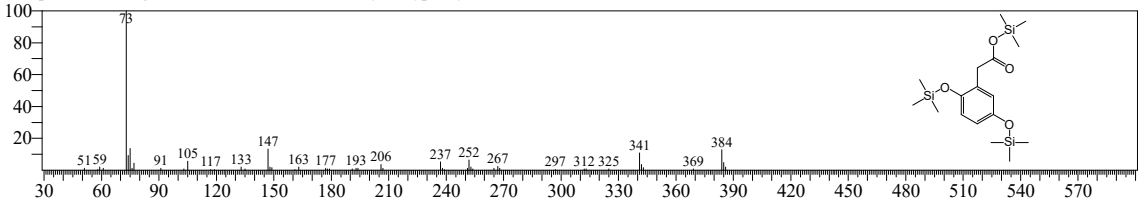
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



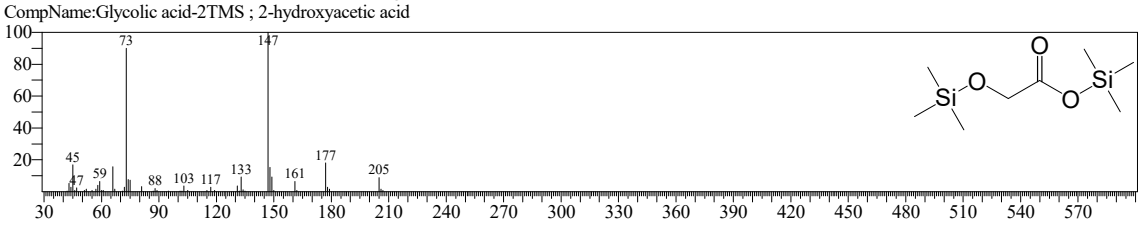
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



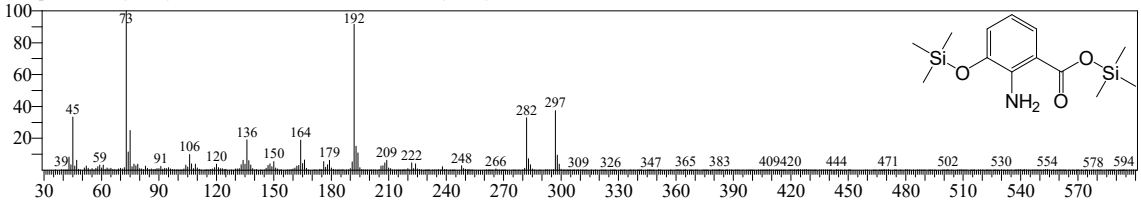
Hit#:3 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid



Hit#:4 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

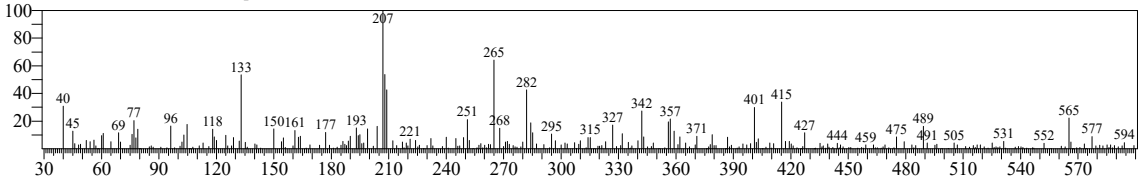


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

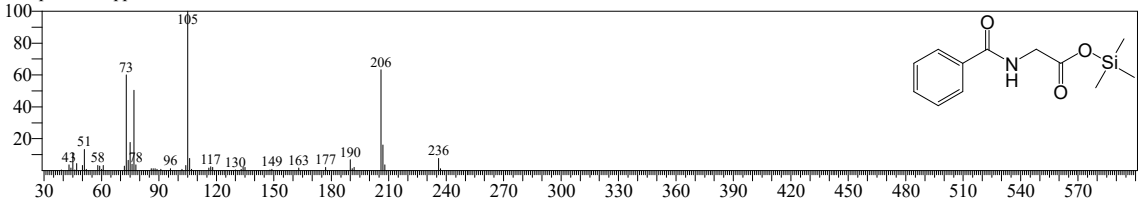


TNAU

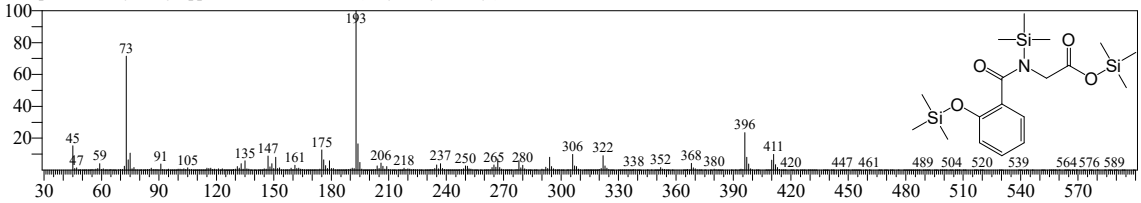
<< Target >>
Line#:11 R.Time:29.170(Scan#:4935) MassPeaks:293
RawMode:Averaged 29.165-29.175(4934-4936) BasePeak:207.05(1012)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



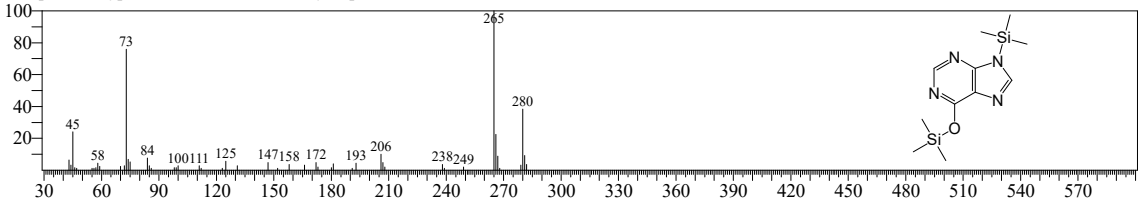
Hit#:1 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



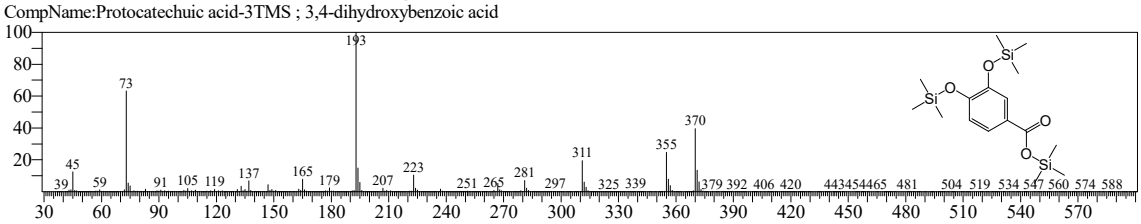
Hit#:2 Entry:420 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973
CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid



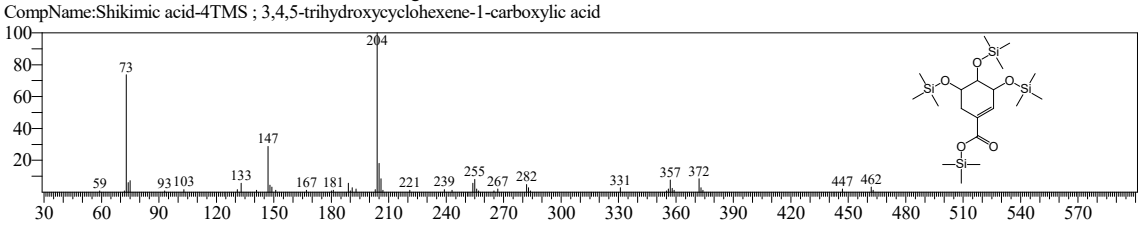
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

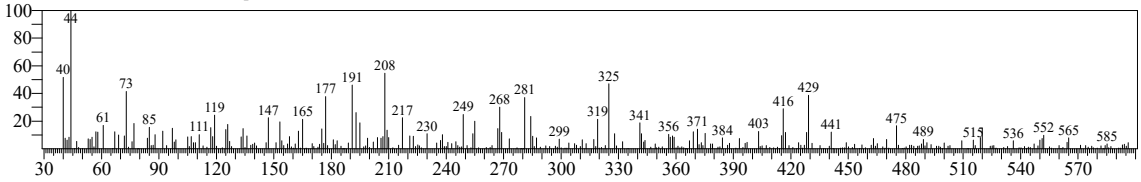


Hit#:5 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid

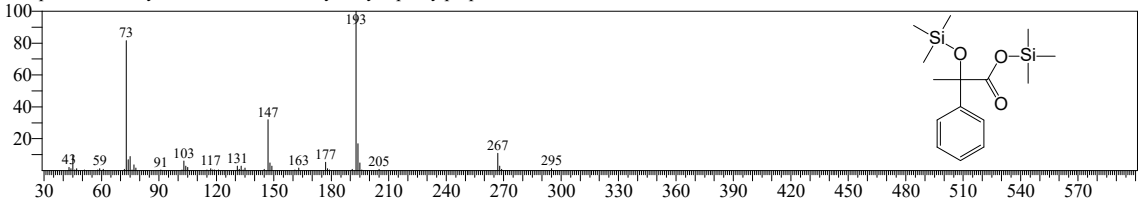


TNAU

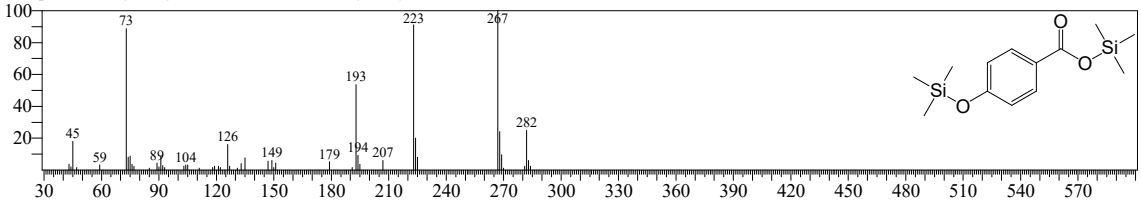
<< Target >>
Line#:12 R.Time:29.560(Scan#:5013) MassPeaks:328
RawMode:Averaged 29.555-29.565(5012-5014) BasePeak:44.00(982)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



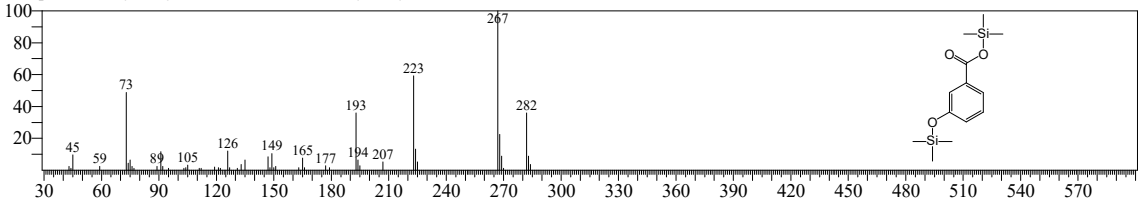
Hit#:1 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



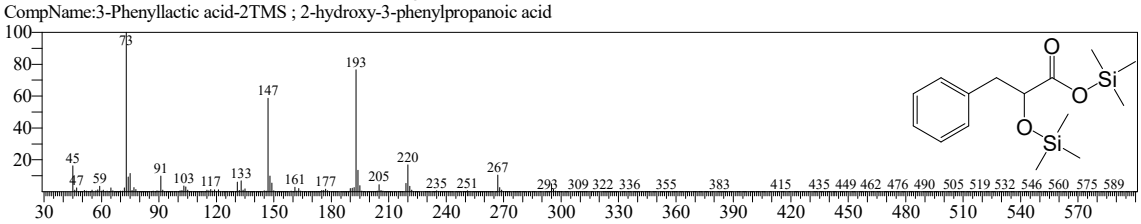
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



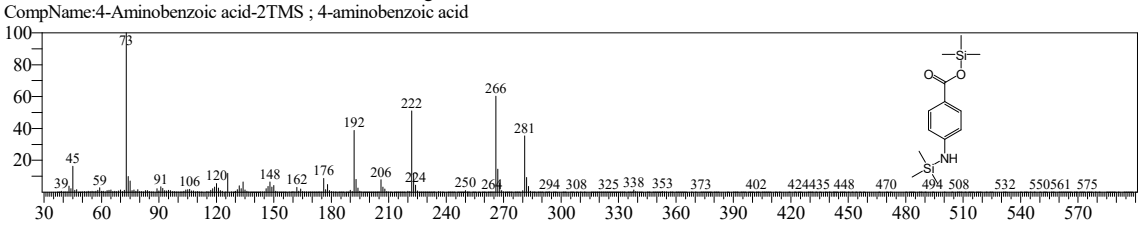
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

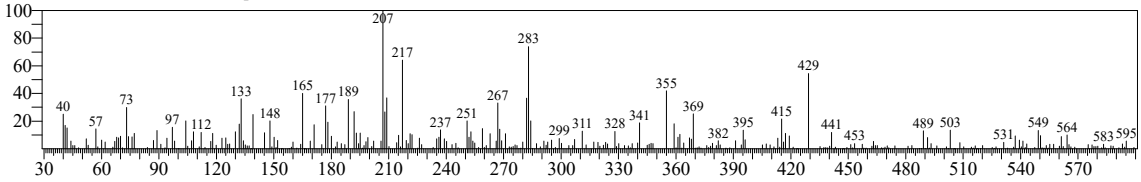


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

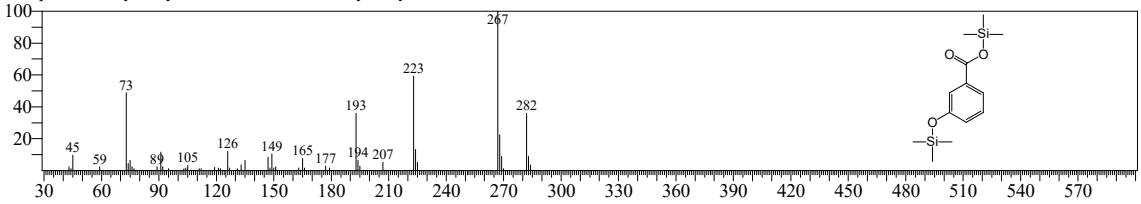


TNAU

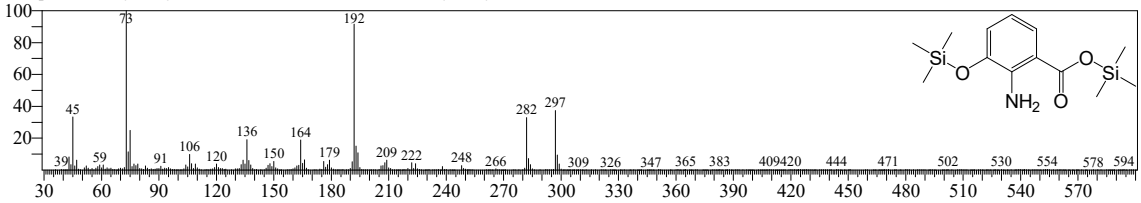
<< Target >>
Line#:13 R.Time:29.625(Scan#:5026) MassPeaks:305
RawMode:Averaged 29.620-29.630(5025-5027) BasePeak:207.05(885)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



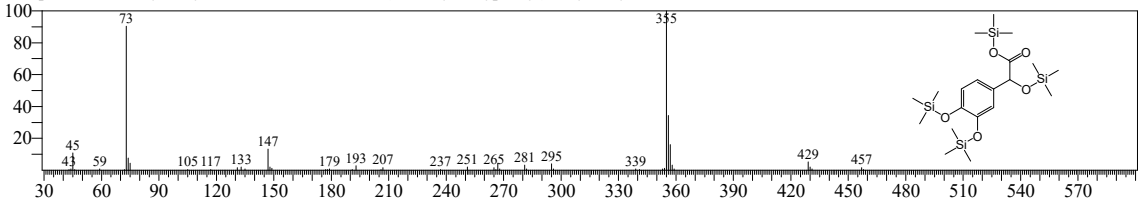
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



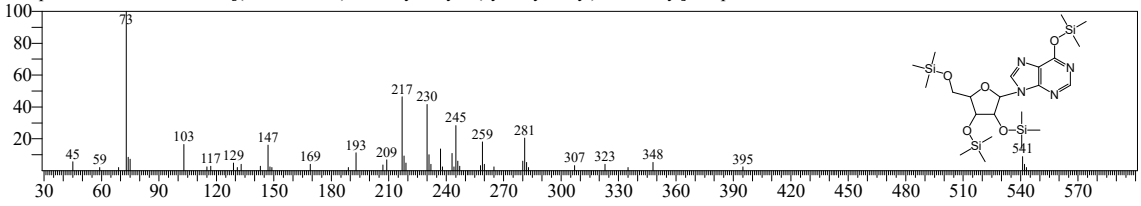
Hit#:2 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



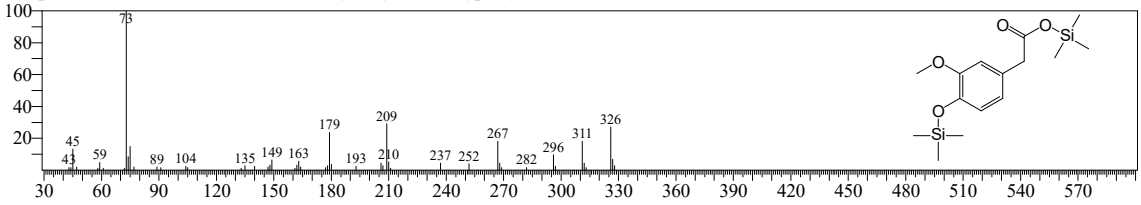
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

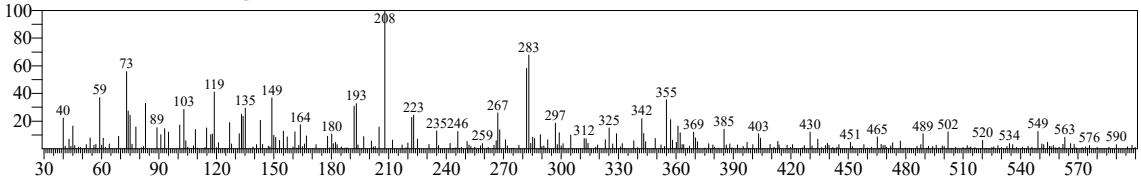


Hit#:5 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

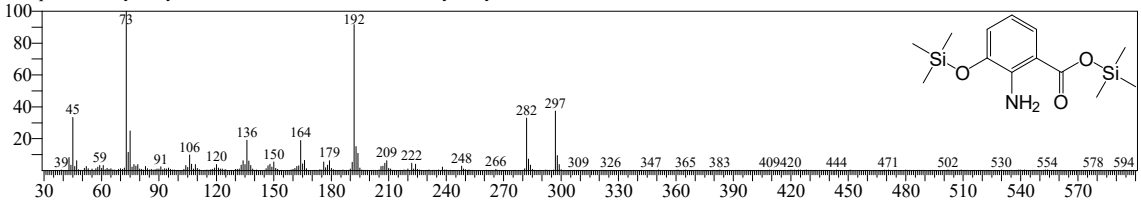


TNAU

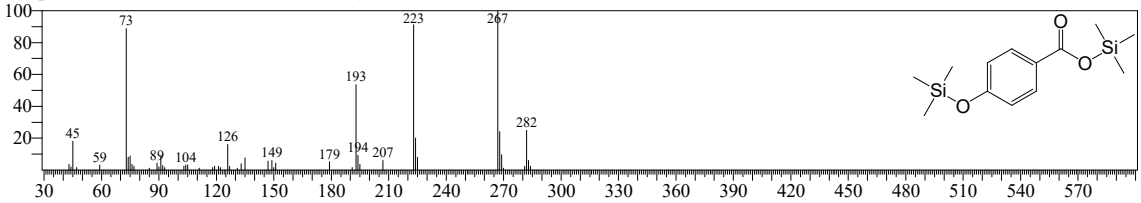
<< Target >>
Line#:14 R.Time:30.040(Scan#:5109) MassPeaks:288
RawMode:Averaged 30.035-30.045(5108-5110) BasePeak:208.00(843)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



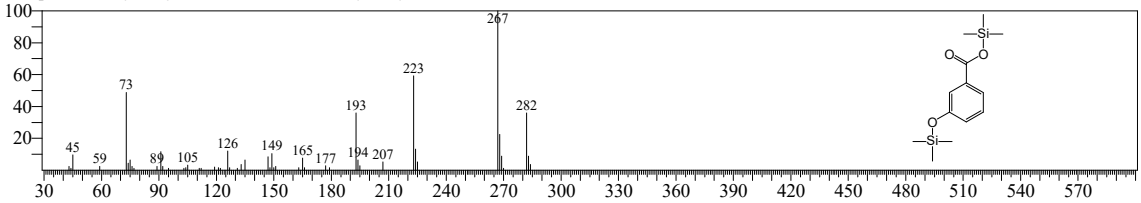
Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



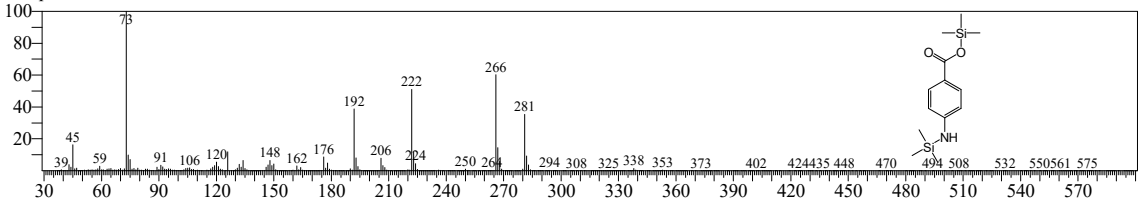
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



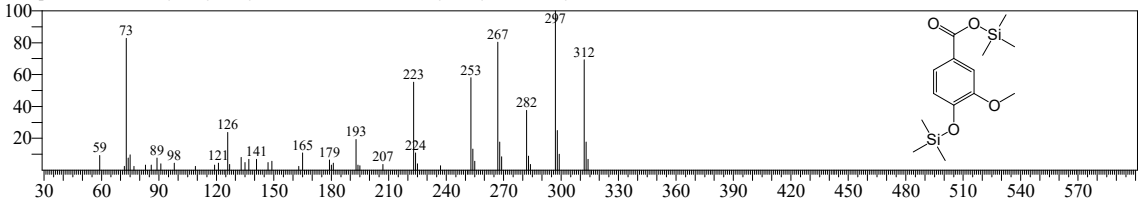
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

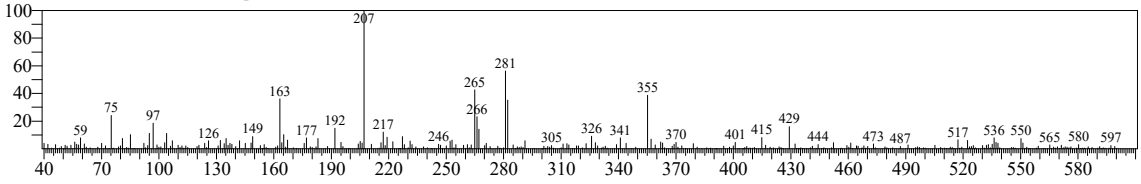


Hit#:5 Entry:291 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C14H24O4Si2 CAS:121-34-6 MolWeight:312 RetIndex:1775
CompName:3-Methoxy-4-hydroxybenzoic acid-2TMS ; 4-hydroxy-3-methoxybenzoic acid

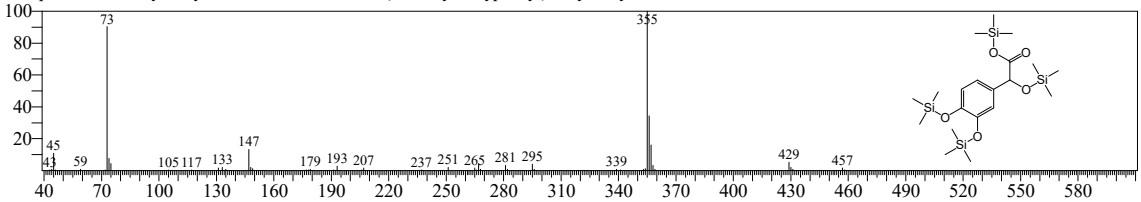


TNAU

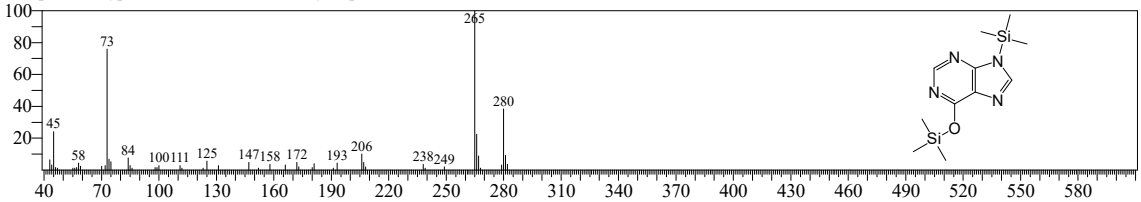
<< Target >>
Line#:15 R.Time:30.645(Scan#:5230) MassPeaks:312
RawMode:Averaged 30.640-30.650(5229-5231) BasePeak:207.05(1617)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



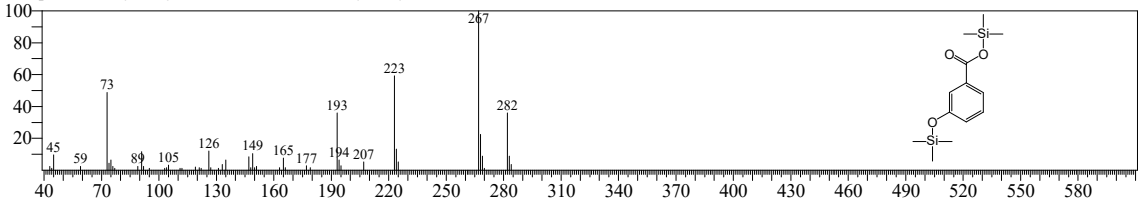
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



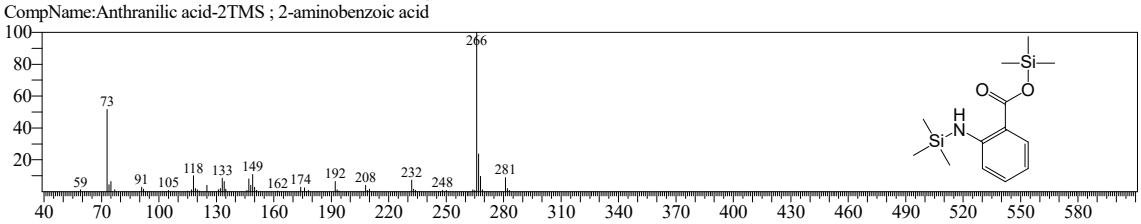
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



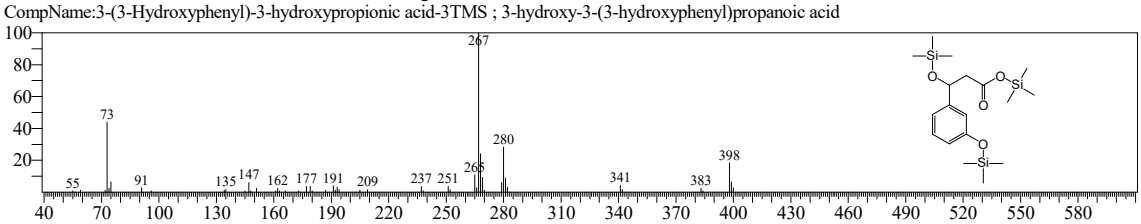
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

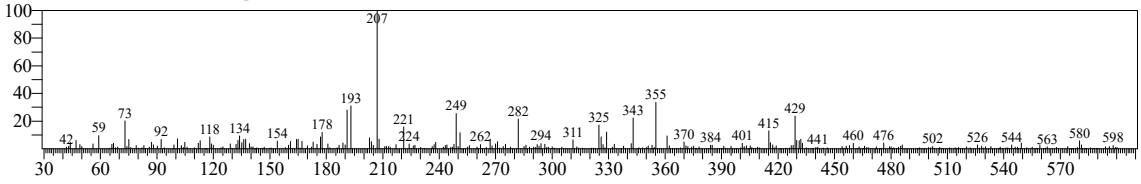


Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

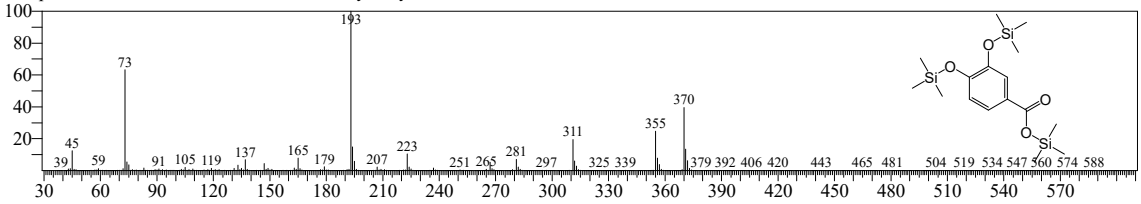


TNAU

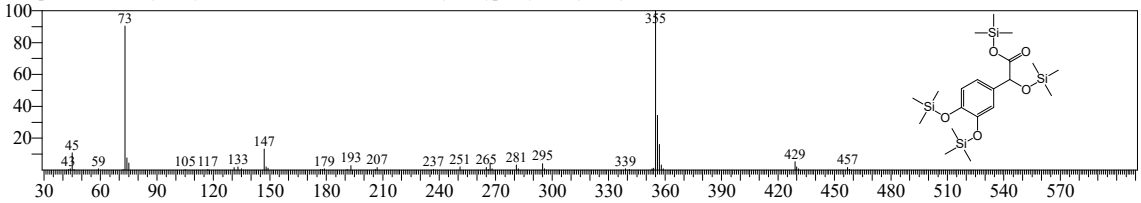
<< Target >>
Line#:16 R.Time:30.785(Scan#:5258) MassPeaks:303
RawMode:Averaged 30.780-30.790(5257-5259) BasePeak:207.05(1874)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



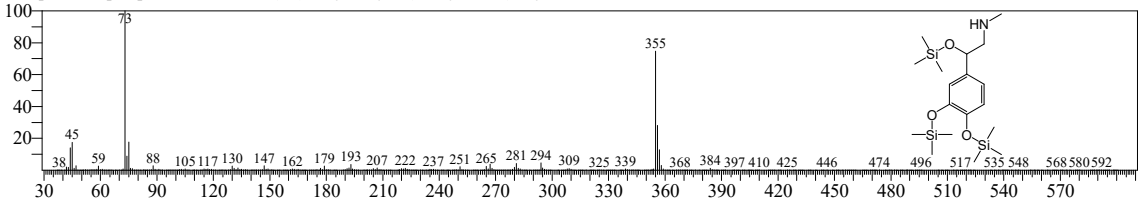
Hit#:1 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



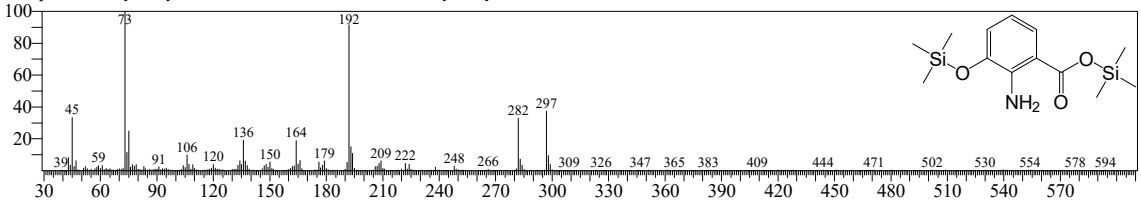
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



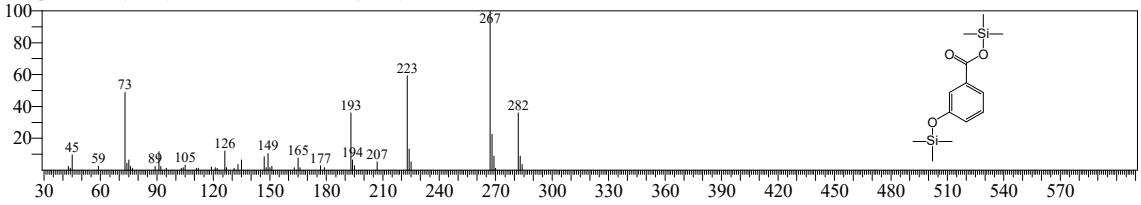
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

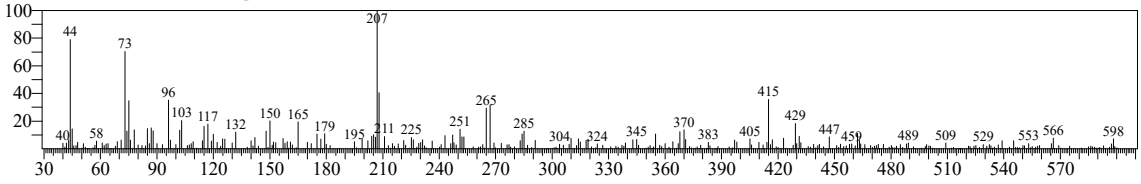


Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

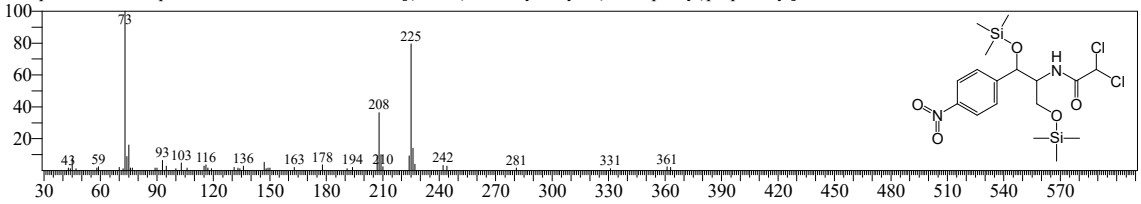


TNAU

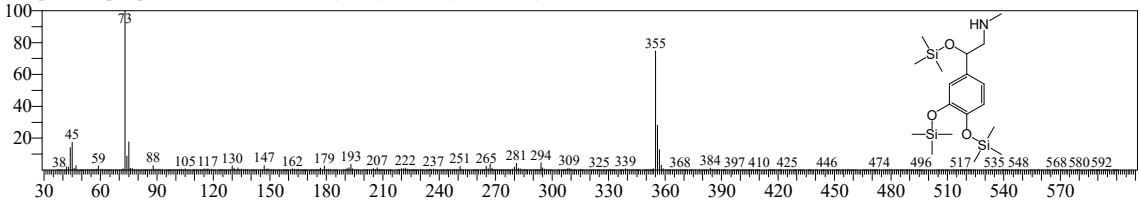
<< Target >>
Line#:17 R.Time:31.235(Scan#:5348) MassPeaks:313
RawMode:Averaged 31.230-31.240(5347-5349) BasePeak:207.05(1085)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



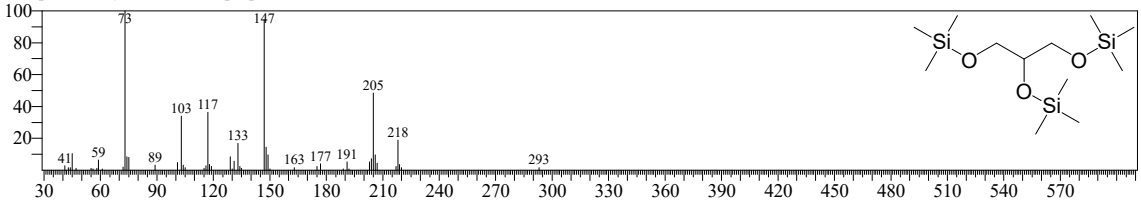
Hit#:1 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



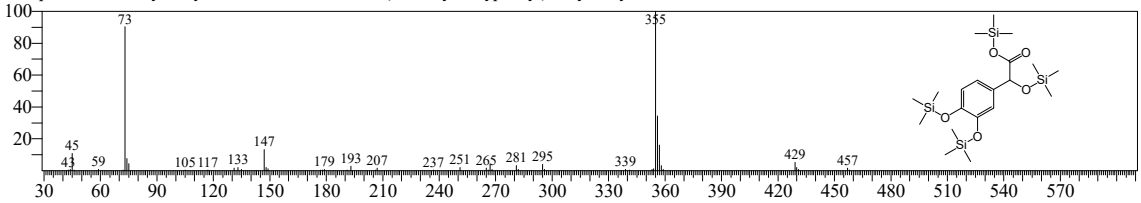
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



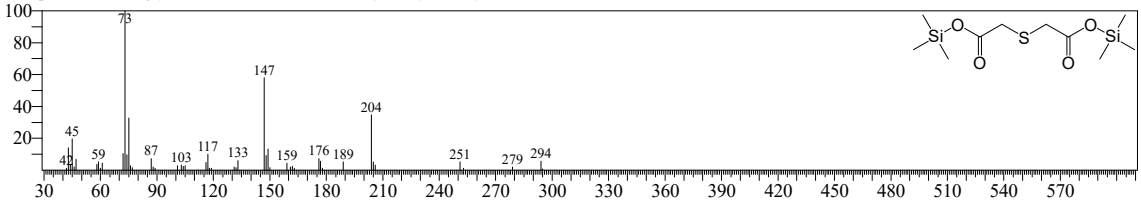
Hit#:3 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

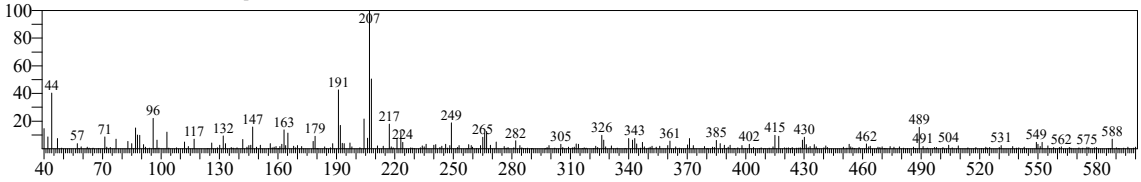


Hit#:5 Entry:163 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C10H22O4SSi2 CAS:123-93-3 MolWeight:294 RetIndex:1537
CompName:Thiodiglycolic acid-2TMS ; 2-(carboxymethylsulfanyl)acetic acid

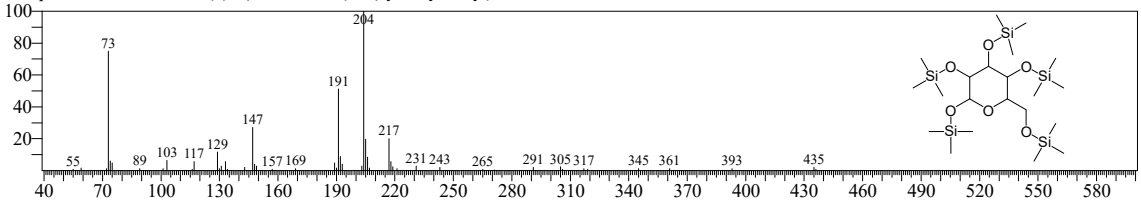


TNAU

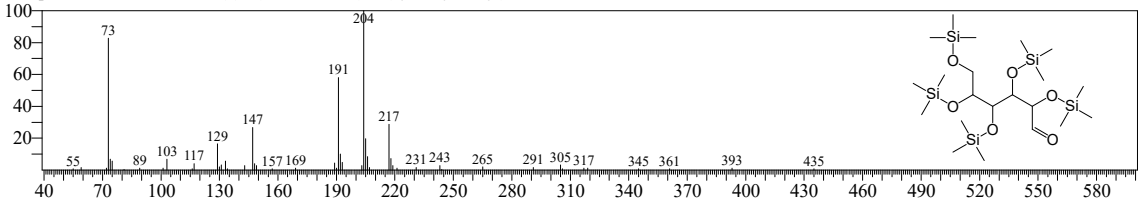
<< Target >>
Line#:18 R.Time:31.290(Scan#:5359) MassPeaks:283
RawMode:Averaged 31.285-31.295(5358-5360) BasePeak:207.00(1682)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



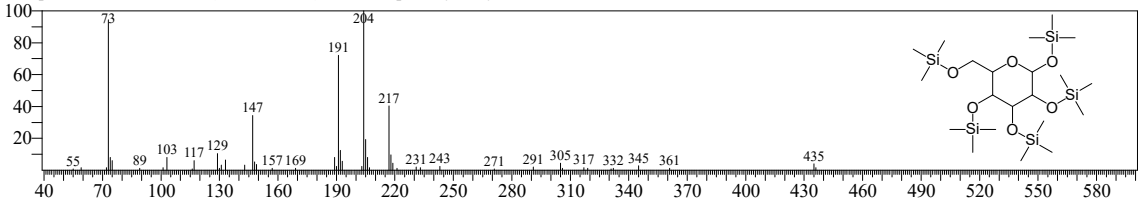
Hit#:1 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



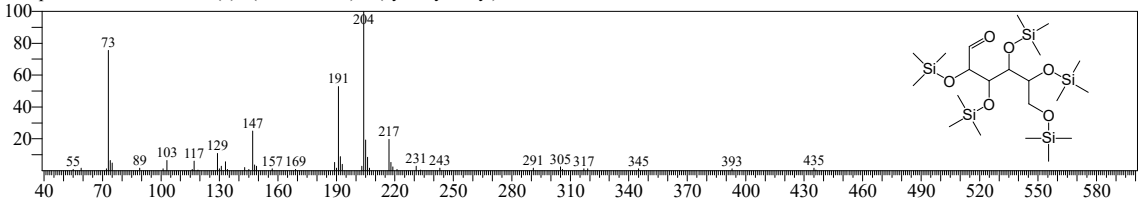
Hit#:2 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1824
CompName:Galactose-5TMS(1) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



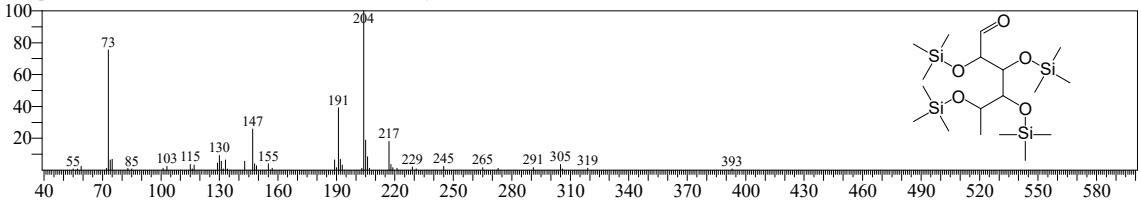
Hit#:3 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:4 Entry:288 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1771
CompName:Mannose-5TMS(1) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

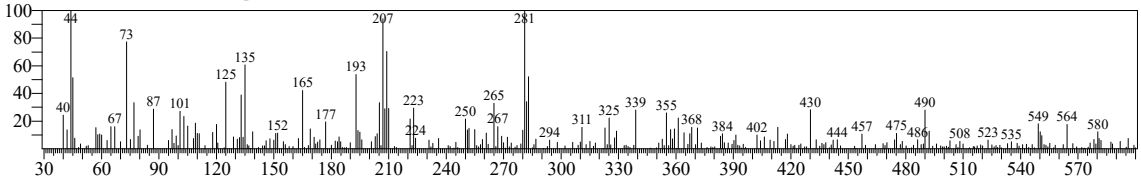


Hit#:5 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

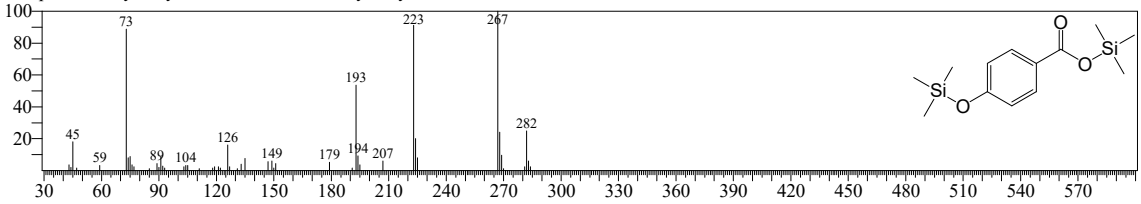


TNAU

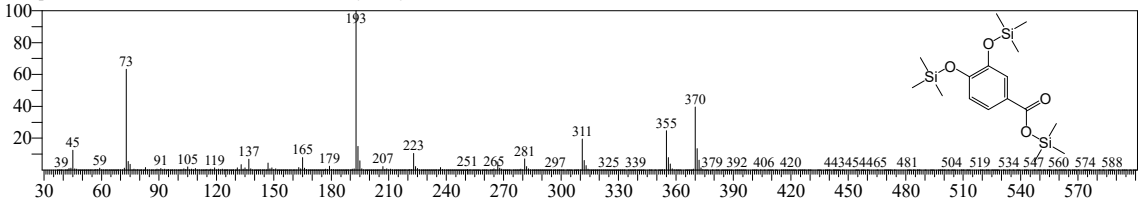
<< Target >>
Line#:19 R.Time:31.665(Scan#:5434) MassPeaks:315
RawMode:Averaged 31.660-31.670(5433-5435) BasePeak:44.00(680)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



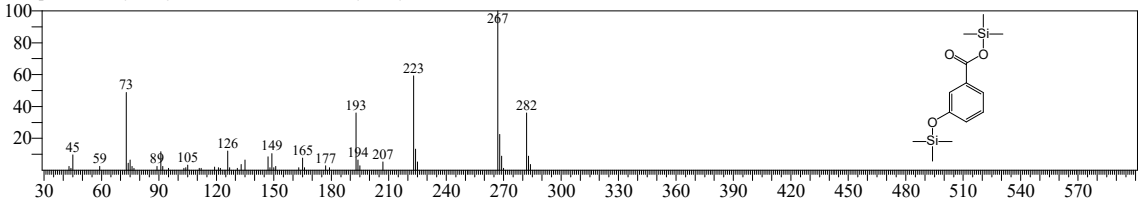
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



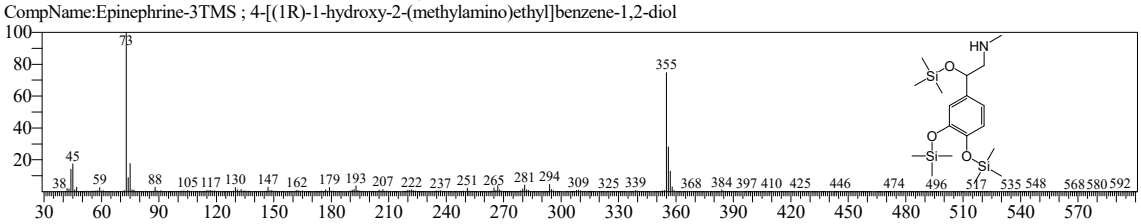
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



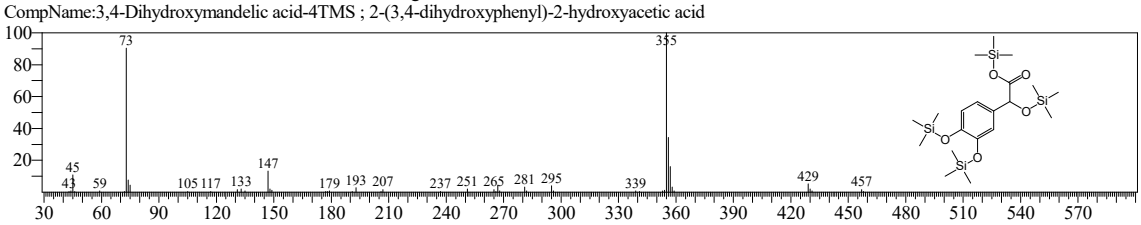
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

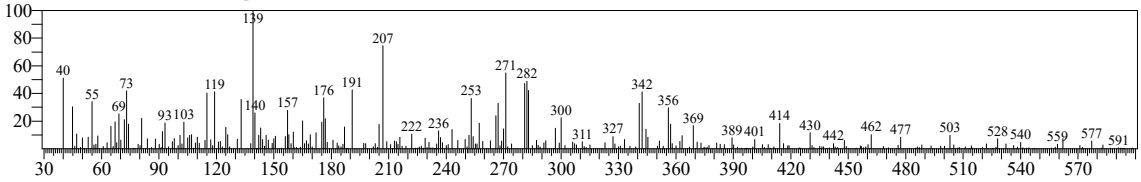


Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

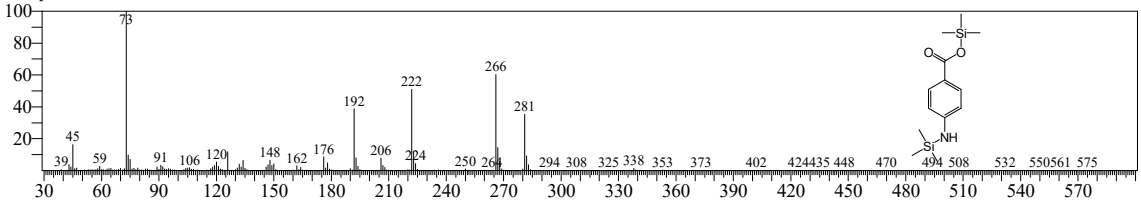


TNAU

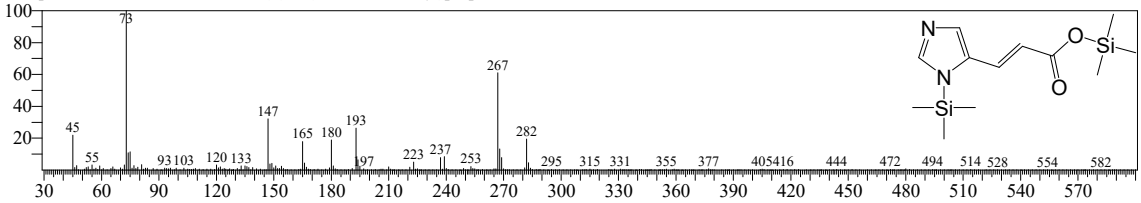
<< Target >>
Line#:20 R.Time:31.900(Scan#:5481) MassPeaks:305
RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.10(1082)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



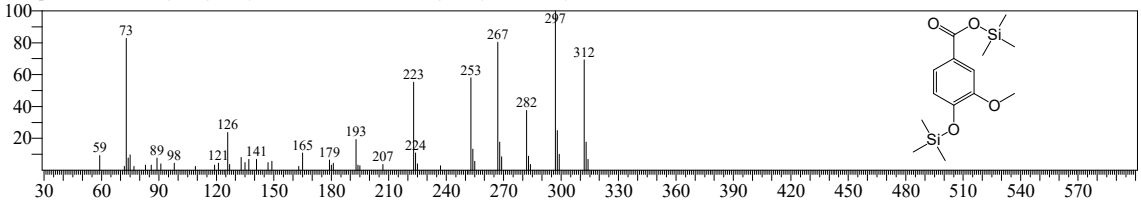
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



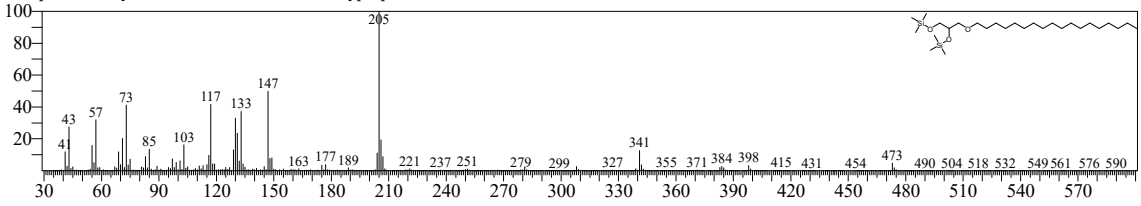
Hit#:2 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



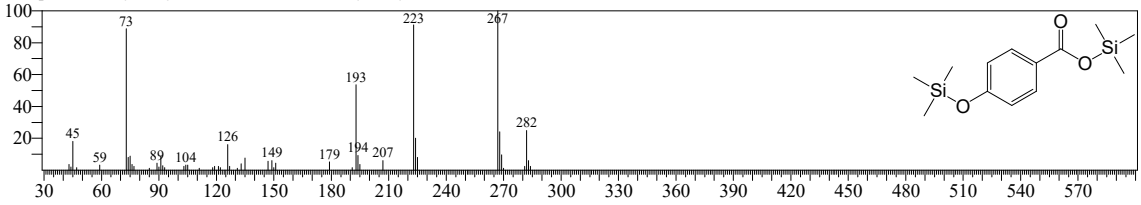
Hit#:3 Entry:291 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C14H24O4Si2 CAS:121-34-6 MolWeight:312 RetIndex:1775
CompName:3-Methoxy-4-hydroxybenzoic acid-2TMS ; 4-hydroxy-3-methoxybenzoic acid



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

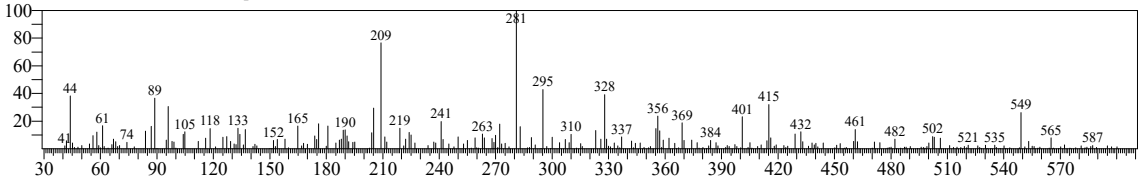


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

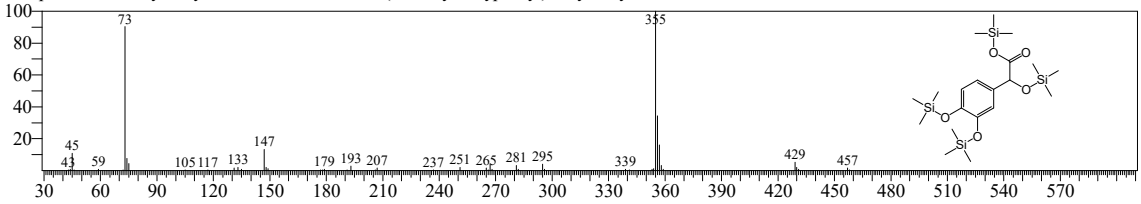


TNAU

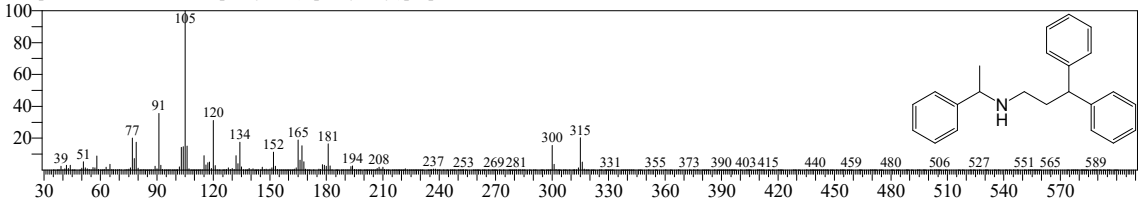
<< Target >>
Line#:21 R.Time:31.950(Scan#:5491) MassPeaks:271
RawMode:Averaged 31.945-31.955(5490-5492) BasePeak:281.00(811)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



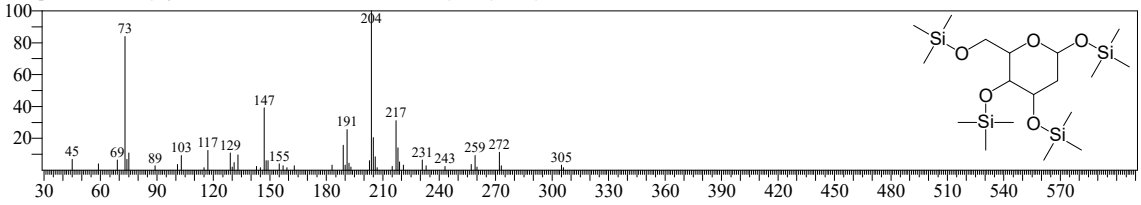
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



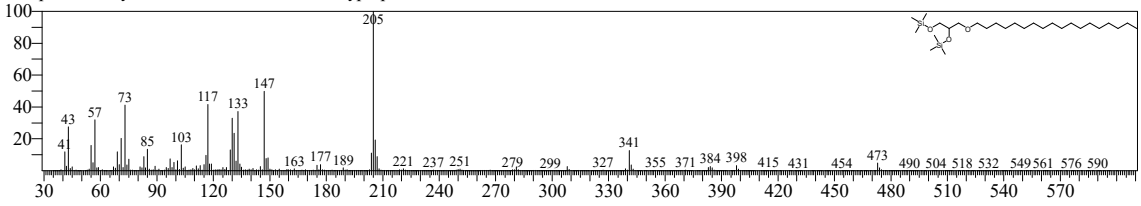
Hit#:2 Entry:530 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C23H25N CAS:13042-18-7 MolWeight:315 RetIndex:2545
CompName:Fendiline ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine



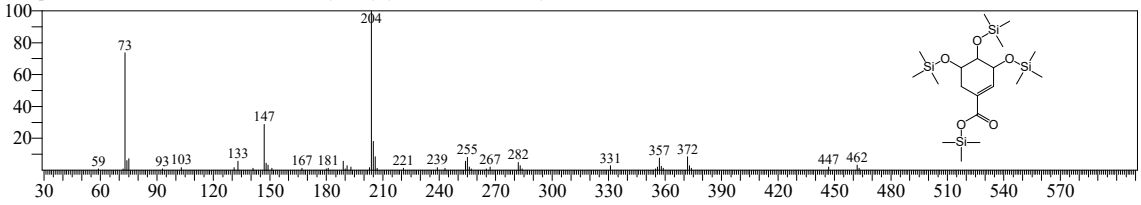
Hit#:3 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:17 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:17 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

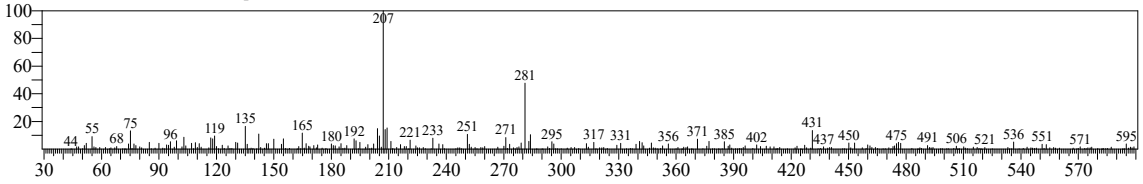


Hit#:5 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid

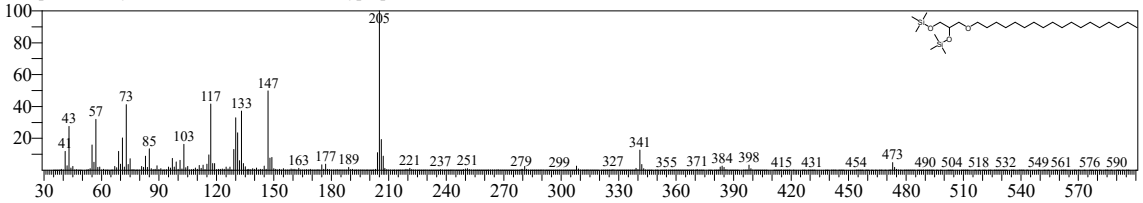


TNAU

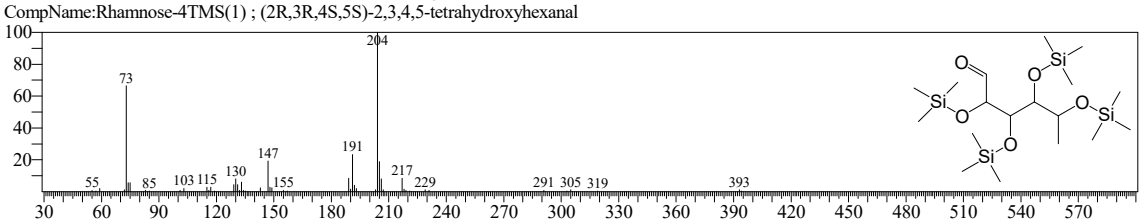
<< Target >>
Line#:22 R.Time:32.525(Scan#:5606) MassPeaks:324
RawMode:Averaged 32.520-32.530(5605-5607) BasePeak:207.00(2145)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



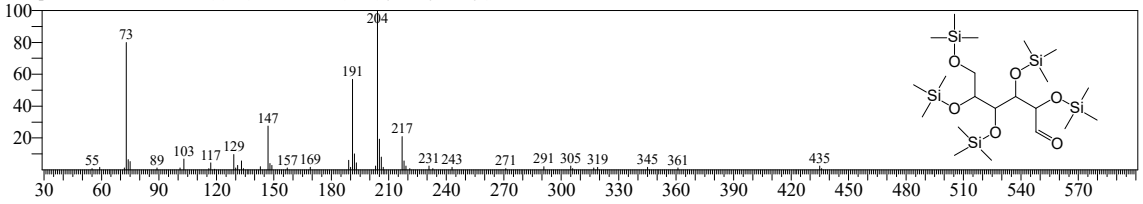
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



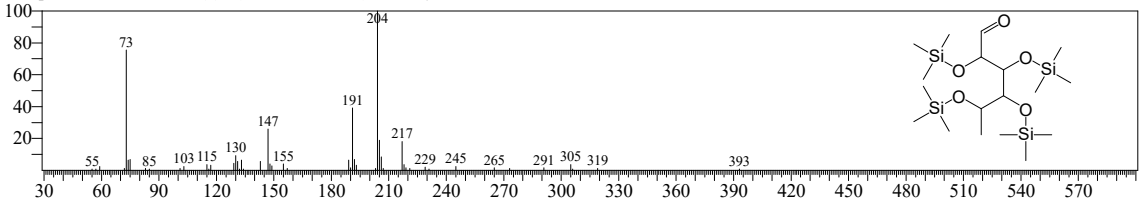
Hit#:2 Entry:219 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1646
CompName:Rhamnose-4TMS(1) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal



Hit#:3 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:2002
CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



Hit#:5 Entry:288 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1771
CompName:Mannose-5TMS(1) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol