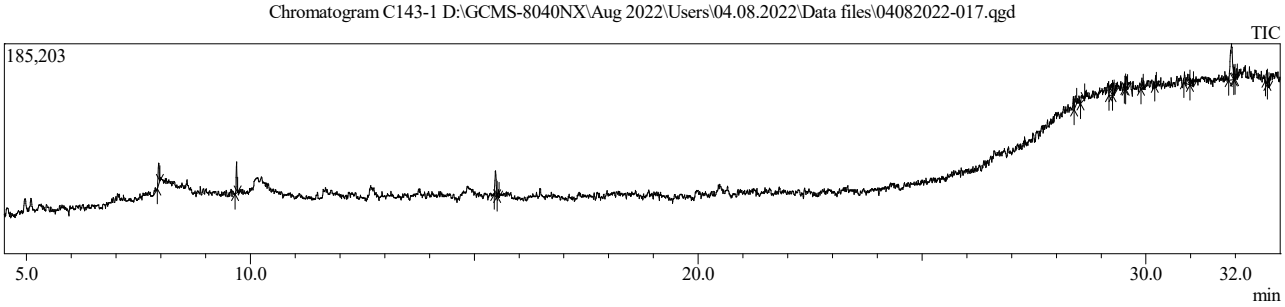
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 3:18:21 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C143-1
Sample ID	: C143-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 17
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-017.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-017.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 4:33:13 PM

Chromatogram C143-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-017.qgd



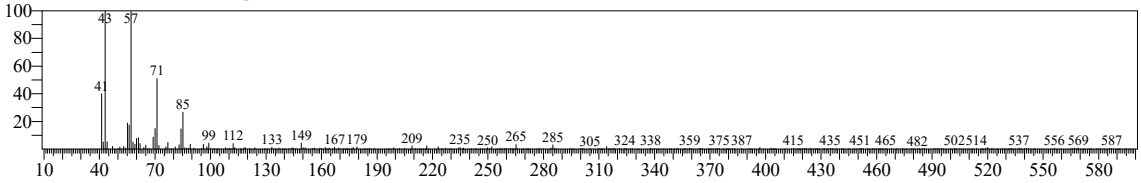
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.950	35358	7.57	18948	8.19	1.87	88	Octane, 3,4,5,6-tetramethyl-
2	9.690	35277	7.56	27532	11.90	1.28	90	Tridecane
3	15.473	39330	8.42	21206	9.17	1.85	89	2,4-Di-tert-butylphenol
4	15.540	7077	1.52	6278	2.71	1.13	37	Juniperic acid-2TMS
5	28.428	17455	3.74	8663	3.74	2.01	33	Shikimic acid-4TMS
6	28.550	17699	3.79	5355	2.31	3.31	39	Juniperic acid-2TMS
7	29.234	30507	6.53	10294	4.45	2.96	41	4-Aminobenzoic acid-2TMS
8	29.278	16426	3.52	10967	4.74	1.50	35	Epinephrine-3TMS
9	29.536	12720	2.72	10878	4.70	1.17	36	3-Hydroxybenzoic acid-2TMS
10	29.575	15700	3.36	9805	4.24	1.60	31	3,4-Dihydroxymandelic acid-4TMS
11	29.900	13790	2.95	6031	2.61	2.29	42	Protocatechuic acid-3TMS
12	30.215	8884	1.90	9962	4.31	0.89	34	Isomaltose-meto-8TMS(2)
13	30.861	34917	7.48	9613	4.15	3.63	40	2-Hydroxyisobutyric acid-2TMS
14	31.045	17490	3.75	6912	2.99	2.53	39	4-Hydroxybenzoic acid-2TMS
15	31.910	112027	24.00	31623	13.67	3.54	36	Methyl cis-4,7,10,13,16,19-Docosahexaenoate
16	31.980	14694	3.15	9814	4.24	1.50	33	Glucose-5TMS(1)
17	32.030	14328	3.07	8937	3.86	1.60	27	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
18	32.695	13717	2.94	11166	4.83	1.23	27	3,4-Dihydroxymandelic acid-4TMS
19	32.735	9465	2.03	7395	3.20	1.28	40	Batyl alcohol-2TMS
		466861	100.00	231379	100.00			

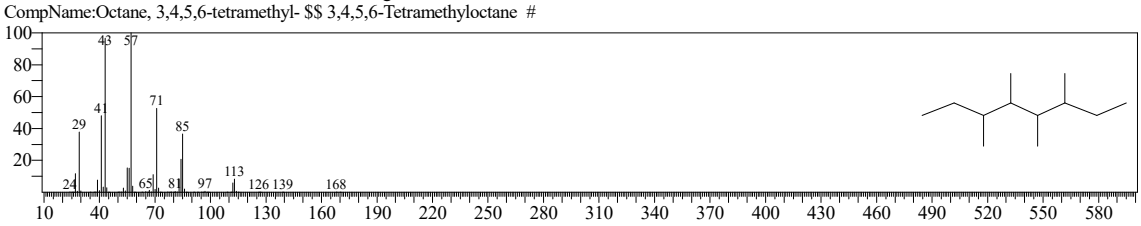
Library

TNAU

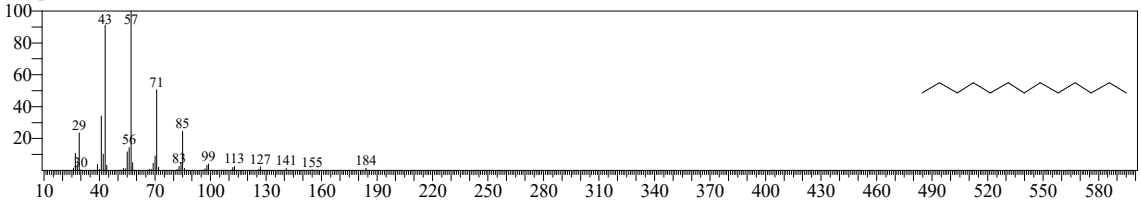
<< Target >>
Line#:1 R.Time:7.950(Scan#:691) MassPeaks:289
RawMode:Averaged 7.945-7.955(690-692) BasePeak:43.05(4404)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



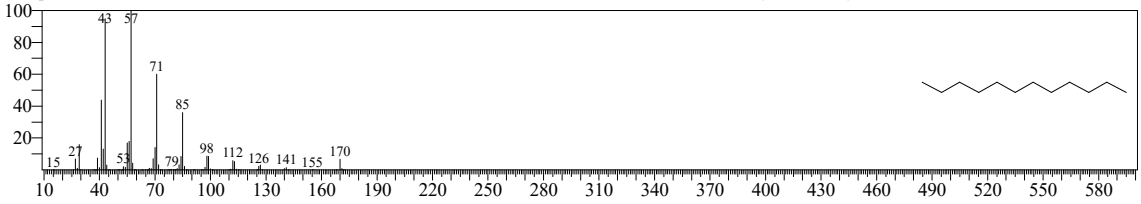
Hit#:1 Entry:30049 Library:NIST20M1.lib
SI:88 Formula:C12H26 CAS:62185-21-1 MolWeight:170 RetIndex:958
CompName:Octane, 3,4,5,6-tetramethyl- $$ 3,4,5,6-Tetramethyloctane #



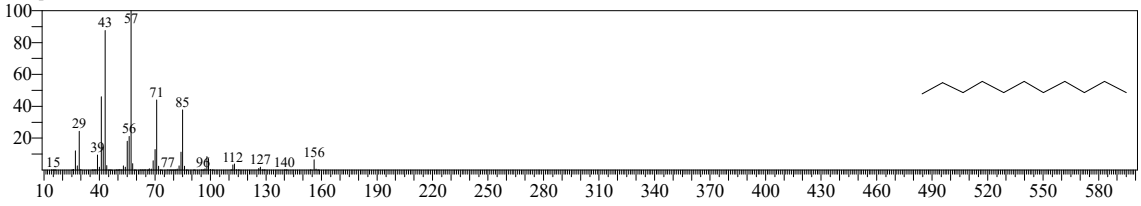
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:88 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



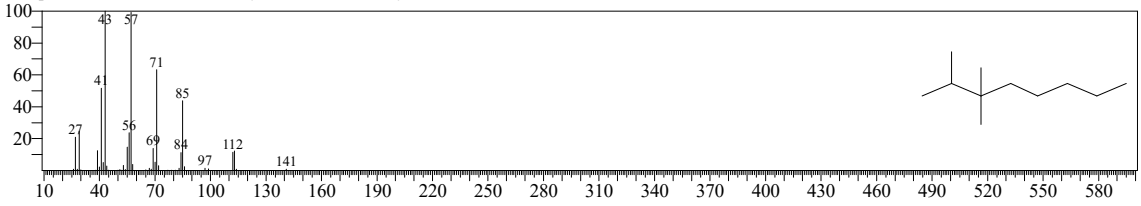
Hit#:3 Entry:16191 Library:NIST20R.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:12897 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

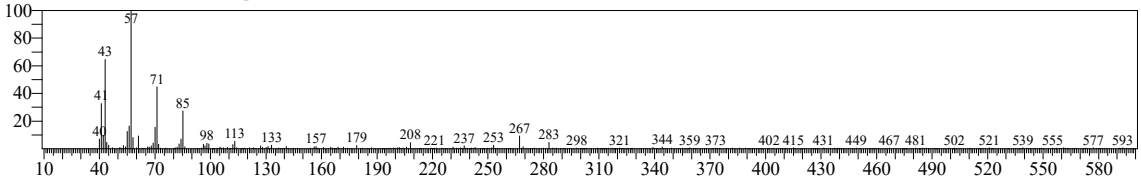


Hit#:5 Entry:21035 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:62016-30-2 MolWeight:156 RetIndex:966
CompName:Octane, 2,3,3-trimethyl- $$ 2,3,3-Trimethyloctane #

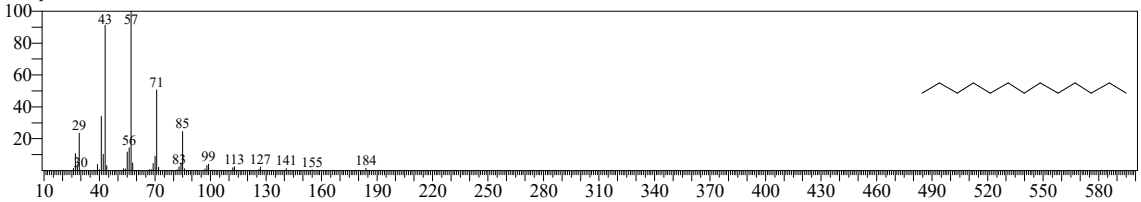


TNAU

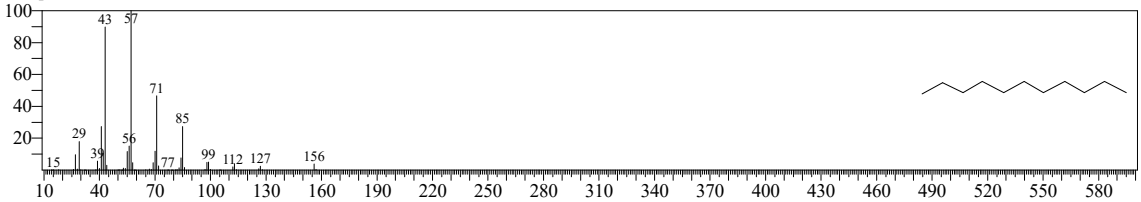
<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:288
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(5841)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



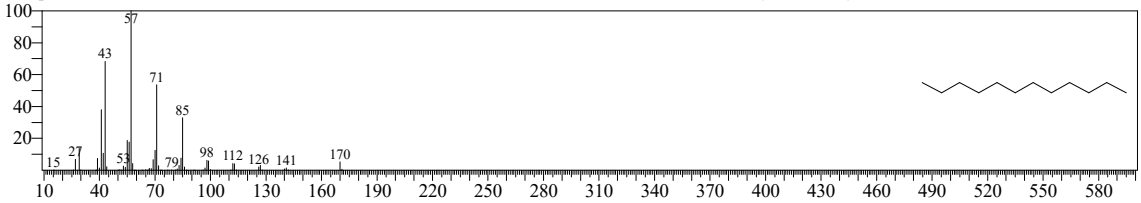
Hit#:1 Entry:40226 Library:NIST20M1.lib
SI:90 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



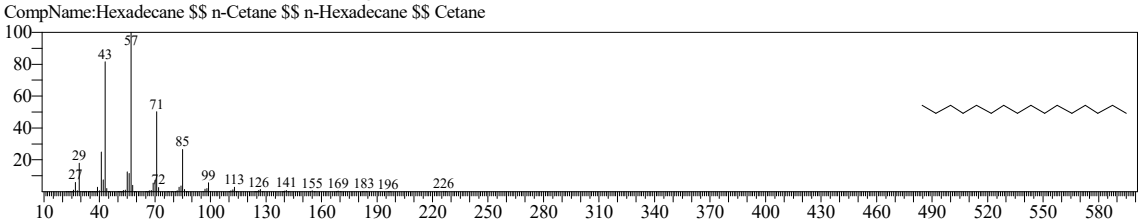
Hit#:2 Entry:21042 Library:NIST20M1.lib
SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



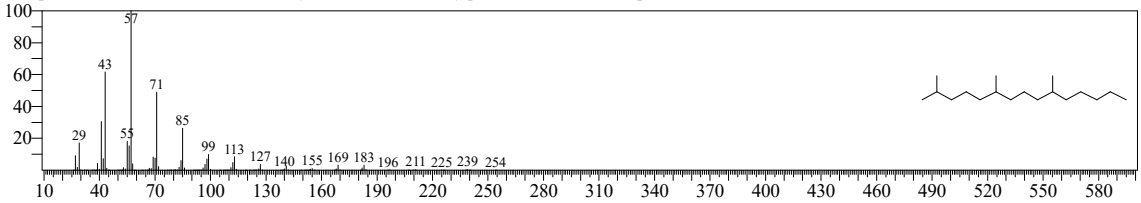
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:89 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



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

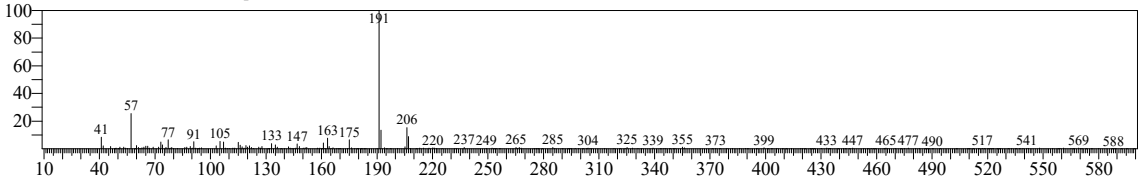


Hit#:5 Entry:109863 Library:NIST20M1.lib
SI:88 Formula:C18H38 CAS:3892-00-0 MolWeight:254 RetIndex:1618
CompName:Pentadecane, 2,6,10-trimethyl- $$ 2,6,10-Trimethylpentadecane # $$ Nor-pristane

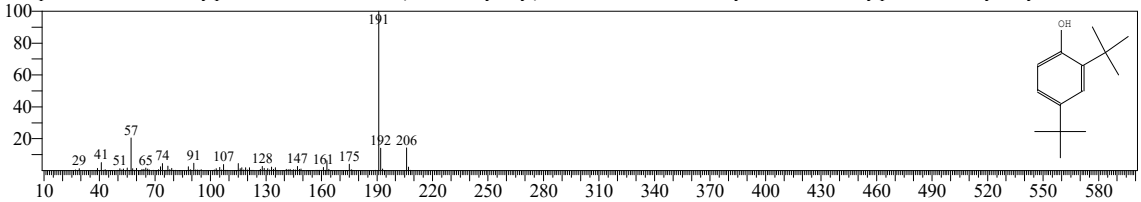


TNAU

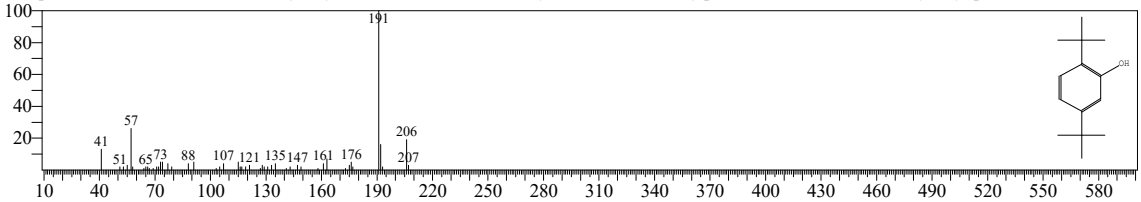
<< Target >>
Line#:3 R.Time:15.475(Scan#:2196) MassPeaks:254
RawMode:Averaged 15.470-15.480(2195-2197) BasePeak:191.15(8013)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



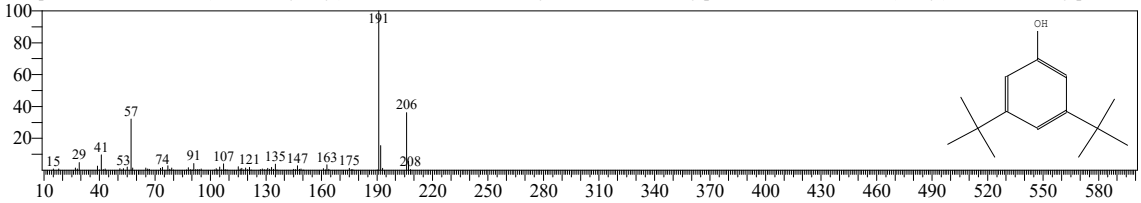
Hit#:1 Entry:24088 Library:NIST20R.lib
SI:89 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



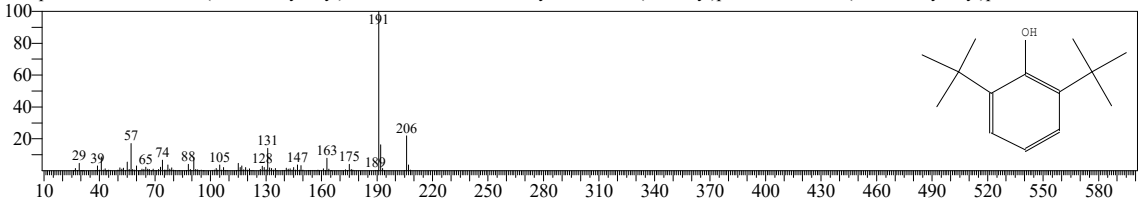
Hit#:2 Entry:24098 Library:NIST20R.lib
SI:86 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



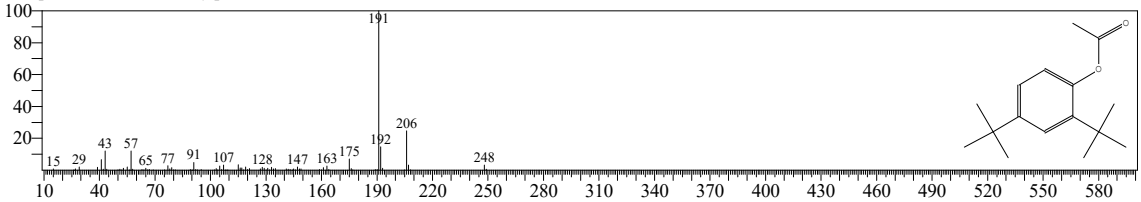
Hit#:3 Entry:24110 Library:NIST20R.lib
SI:86 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



Hit#:4 Entry:24081 Library:NIST20R.lib
SI:84 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

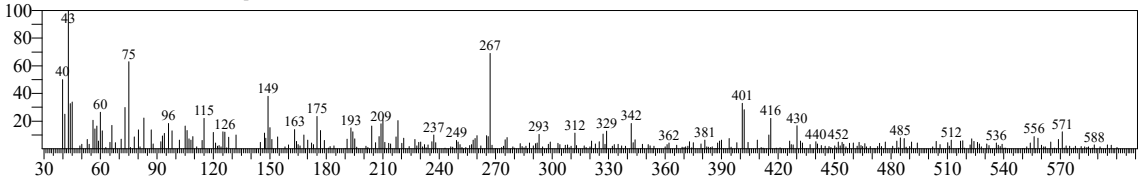


Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:82 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
CompName:2,4-Di-tert-butylphenol, acetate

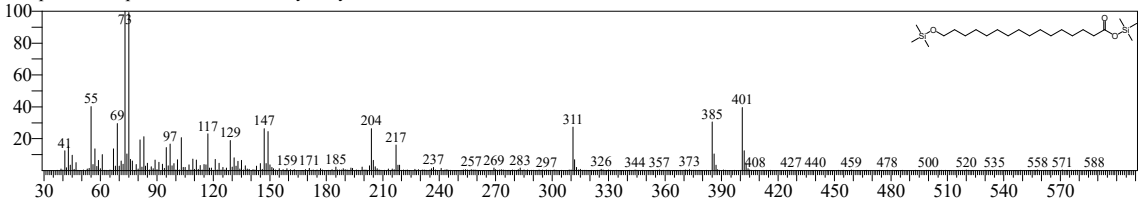


TNAU

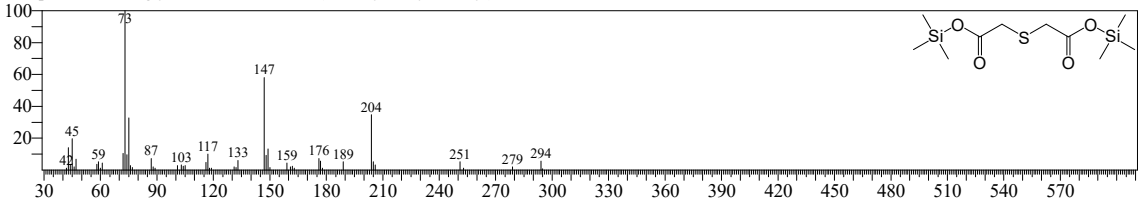
<< Target >>
Line#:4 R.Time:15.540(Scan#:2209) MassPeaks:307
RawMode:Averaged 15.535-15.545(2208-2210) BasePeak:43.00(467)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



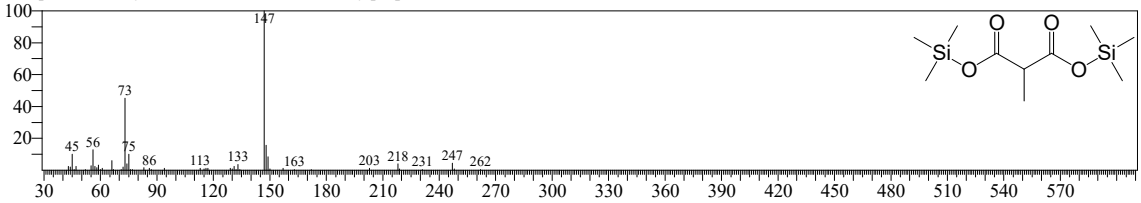
Hit#:1 Entry:511 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C22H48O3Si2 CAS:506-13-8 MolWeight:416 RetIndex:2396
CompName:Juniperic acid-2TMS ; 16-hydroxyhexadecanoic acid



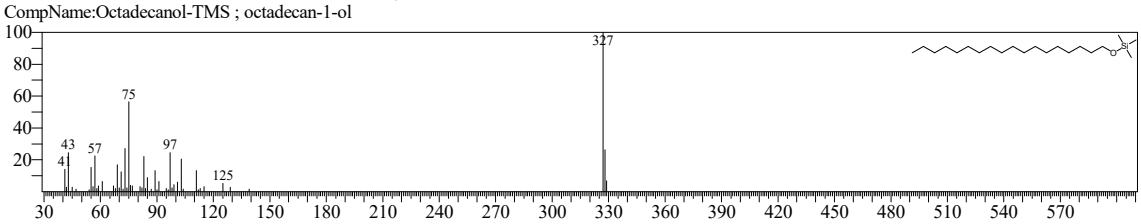
Hit#:2 Entry:163 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C10H22O4SSi2 CAS:123-93-3 MolWeight:294 RetIndex:1537
CompName:Thiodiglycolic acid-2TMS ; 2-(carboxymethylsulfanyl)acetic acid



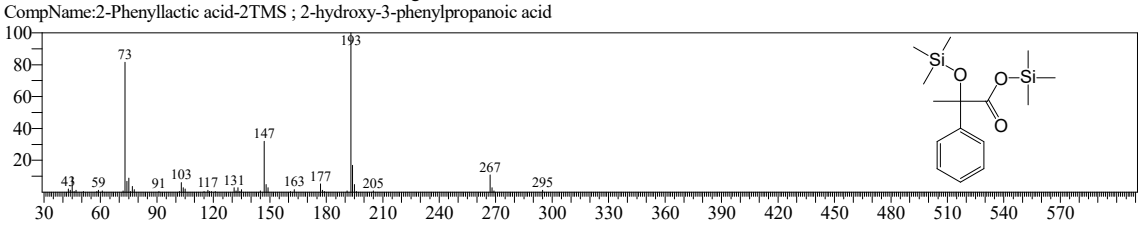
Hit#:3 Entry:52 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C10H22O4Si2 CAS:516-05-2 MolWeight:262 RetIndex:1218
CompName:Methylmalonic acid-2TMS ; 2-methylpropanedioic acid



Hit#:4 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol

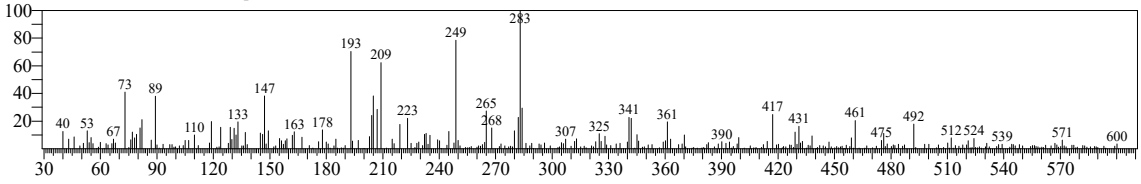


Hit#:5 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

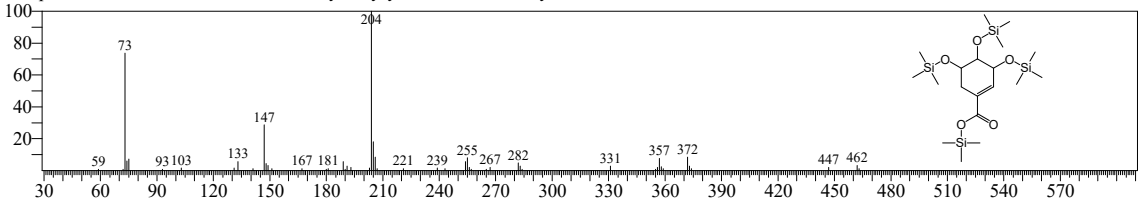


TNAU

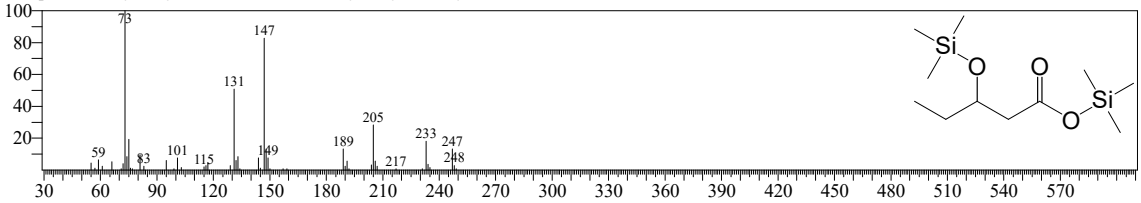
<< Target >>
Line#:5 R.Time:28.430(Scan#:4787) MassPeaks:338
RawMode:Averaged 28.425-28.435(4786-4788) BasePeak:283.00(1005)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



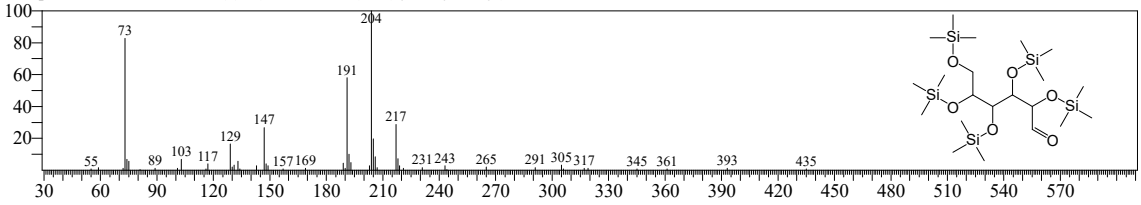
Hit#:1 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid



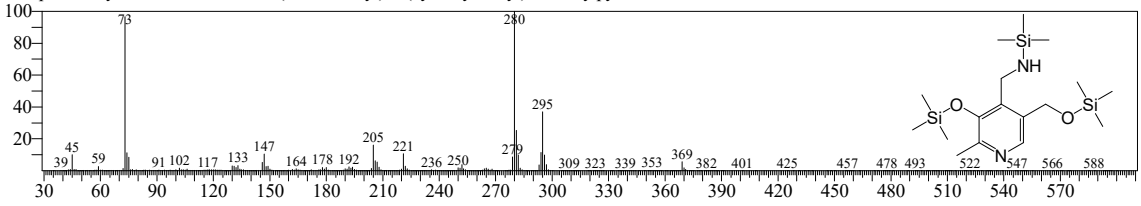
Hit#:2 Entry:61 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H26O3Si2 CAS:10237-77-1 MolWeight:262 RetIndex:1244
CompName:3-Hydroxyvaleric acid-2TMS ; 3-hydroxy-3-methylbutanoic acid



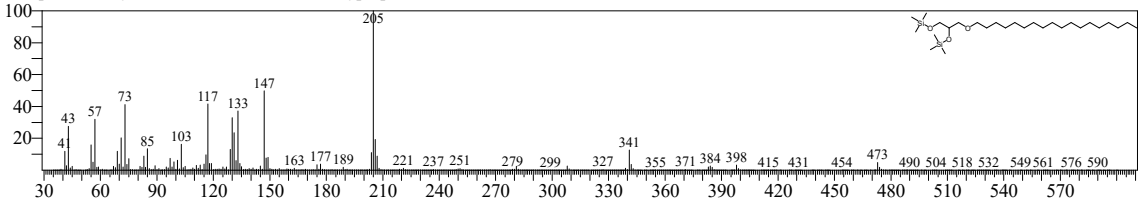
Hit#:3 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1824
CompName:Galactose-5TMS(1) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:418 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H36N2O2Si3 CAS:85-87-0 MolWeight:384 RetIndex:1964
CompName:Pyridoxamine-3TMS ; 4-(aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol

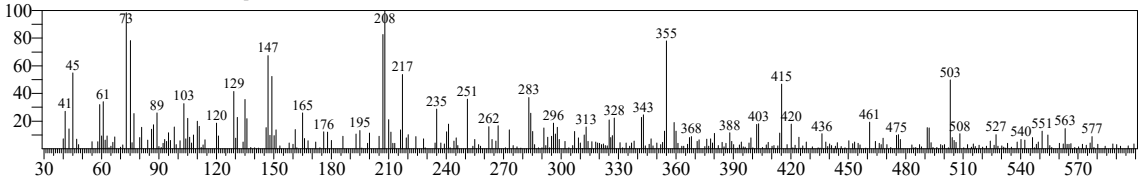


Hit#:5 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

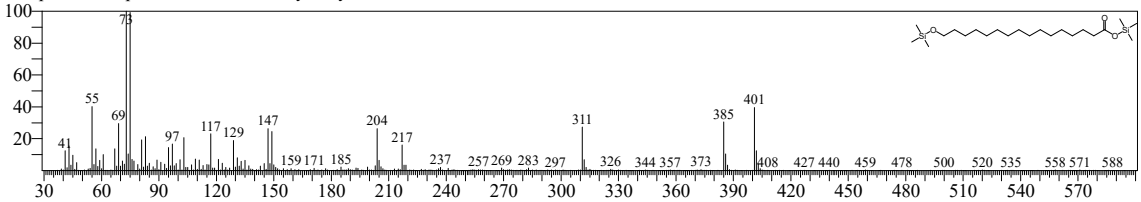


TNAU

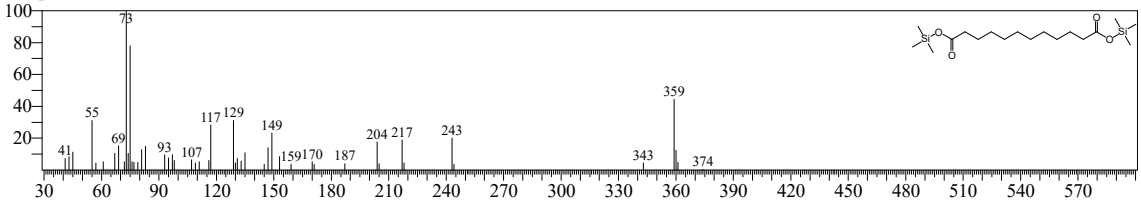
<< Target >>
Line#:6 R.Time:28.550(Scan#:4811) MassPeaks:325
RawMode:Averaged 28.545-28.555(4810-4812) BasePeak:208.00(515)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



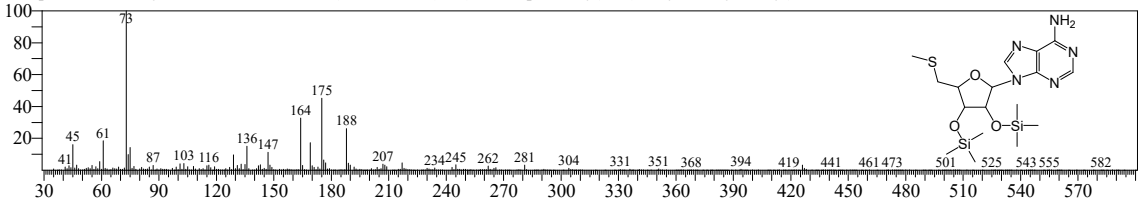
Hit#:1 Entry:511 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C22H48O3Si2 CAS:506-13-8 MolWeight:416 RetIndex:2396
CompName:Juniperic acid-2TMS ; 16-hydroxyhexadecanoic acid



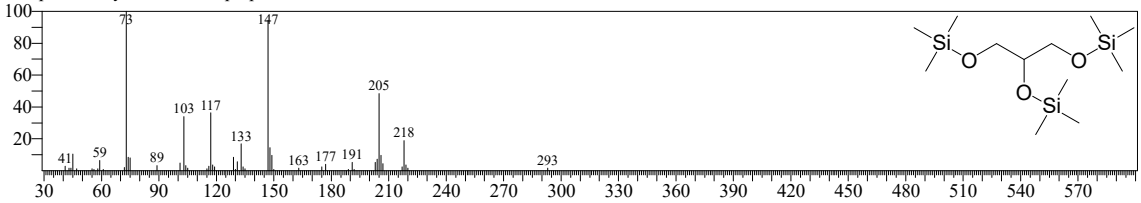
Hit#:2 Entry:455 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H38O4Si2 CAS:693-23-2 MolWeight:374 RetIndex:2092
CompName:Dodecanedioic acid-2TMS ; dodecanedioic acid



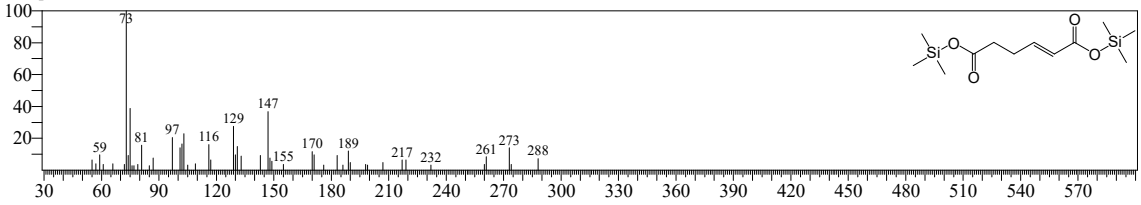
Hit#:3 Entry:548 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787
CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol



Hit#:4 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol

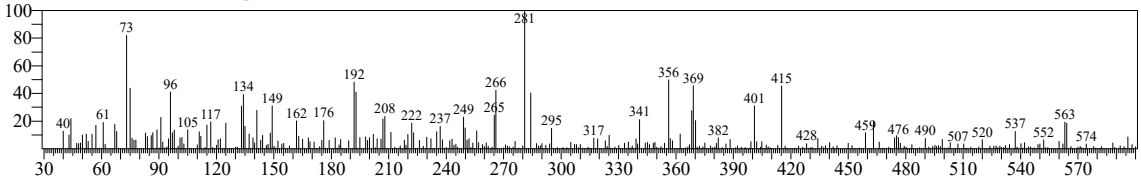


Hit#:5 Entry:156 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C12H24O4Si2 CAS:4440-68-0 MolWeight:288 RetIndex:1522
CompName:2-Hexenedioic acid-2TMS ; hex-2-enedioic acid

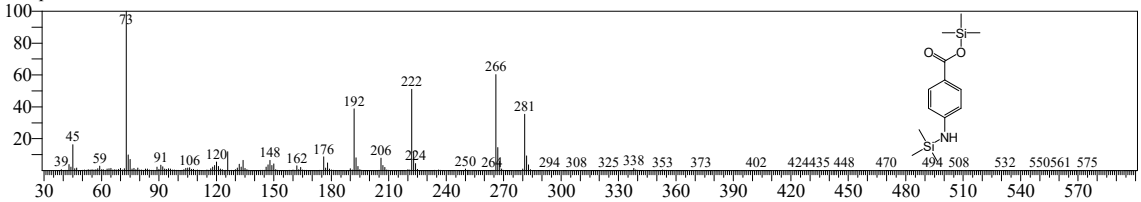


TNAU

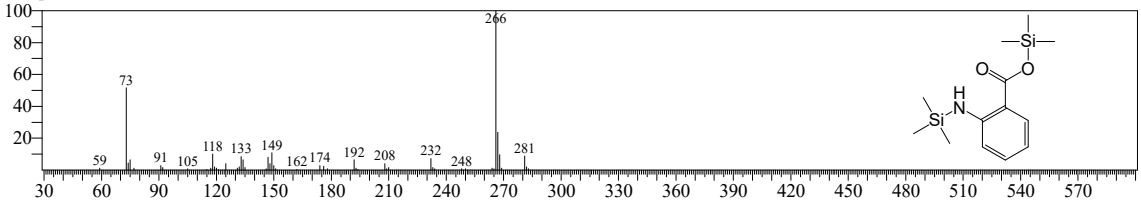
<< Target >>
Line#:7 R.Time:29.235(Scan#:4948) MassPeaks:322
RawMode:Averaged 29.230-29.240(4947-4949) BasePeak:281.00(828)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



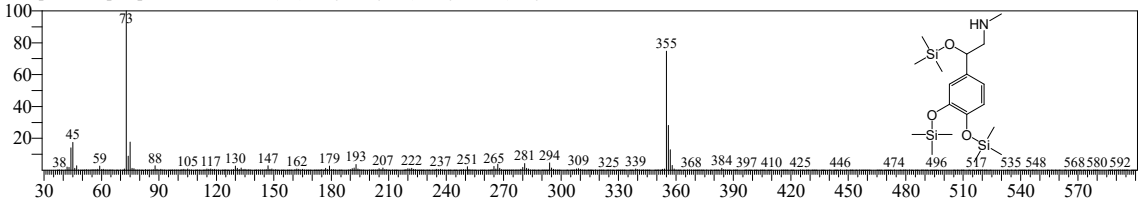
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



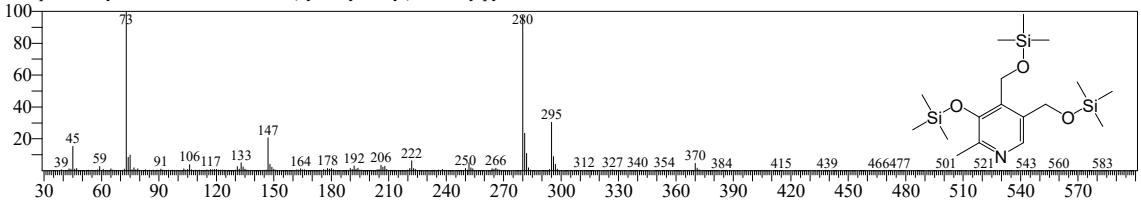
Hit#:2 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



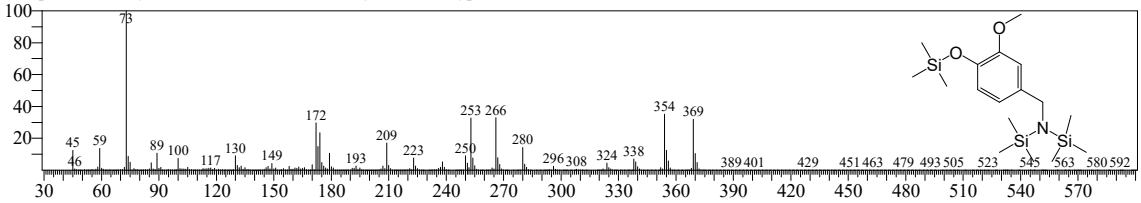
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

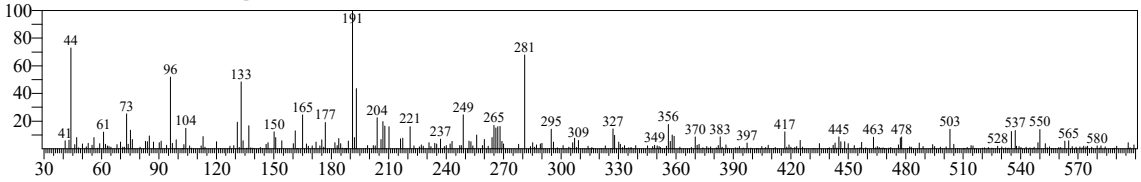


Hit#:5 Entry:368 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H35NO2Si3 CAS:1196-92-5 MolWeight:369 RetIndex:1899
CompName:Vanillylamine-3TMS ; 4-(aminomethyl)-2-methoxyphenol

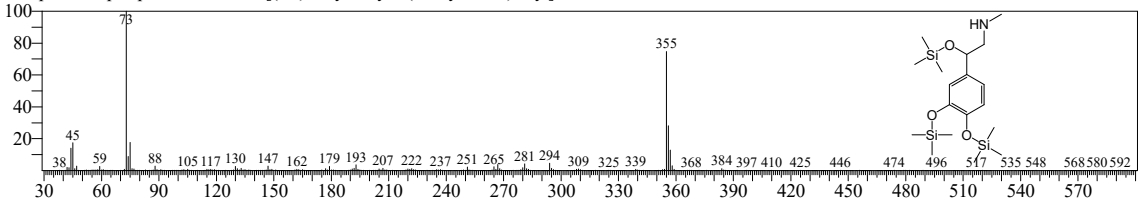


TNAU

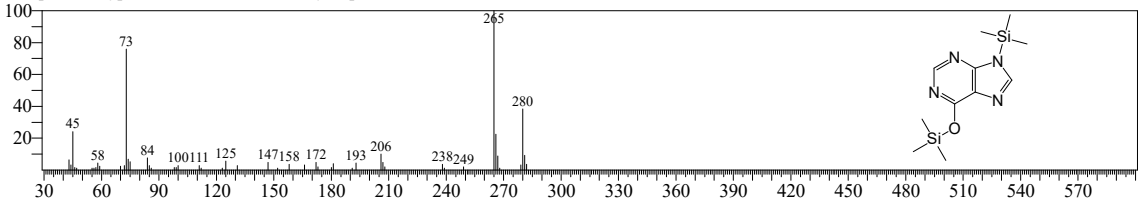
<< Target >>
Line#:8 R.Time:29.280(Scan#:4957) MassPeaks:306
RawMode:Averaged 29.275-29.285(4956-4958) BasePeak:191.05(1113)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



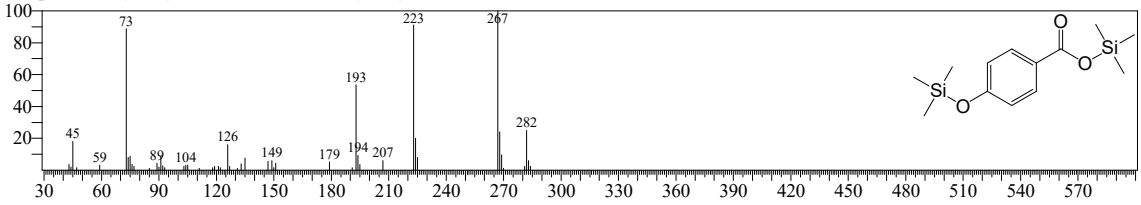
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



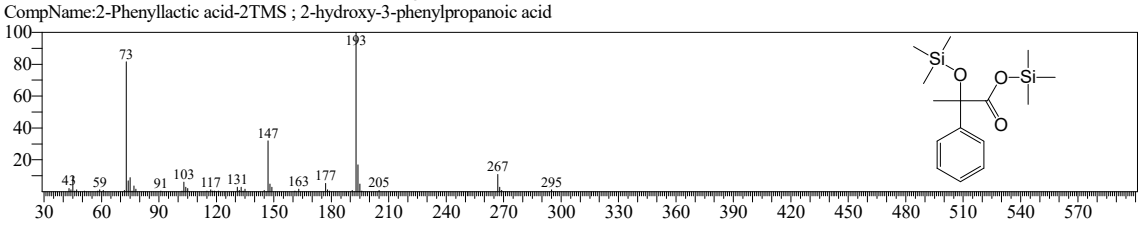
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



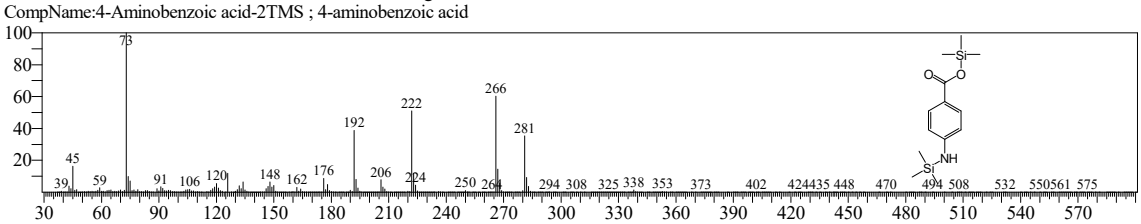
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

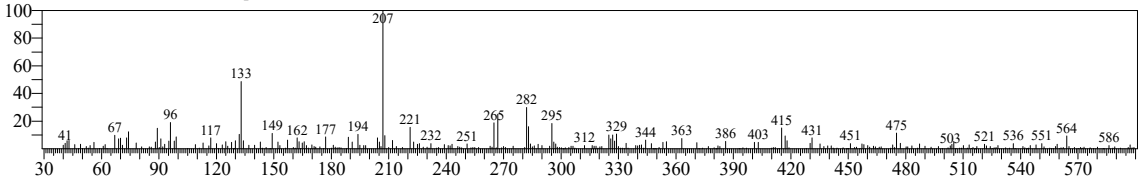


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

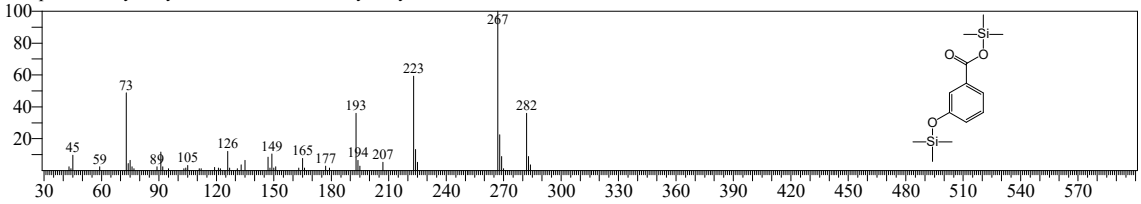


TNAU

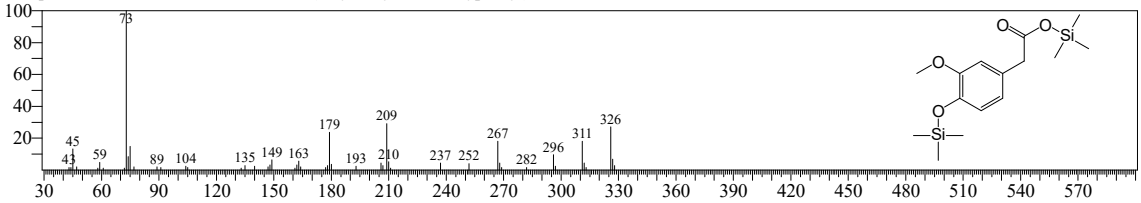
<< Target >>
Line#:9 R.Time:29.535(Scan#:5008) MassPeaks:305
RawMode:Averaged 29.530-29.540(5007-5009) BasePeak:207.05(1737)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



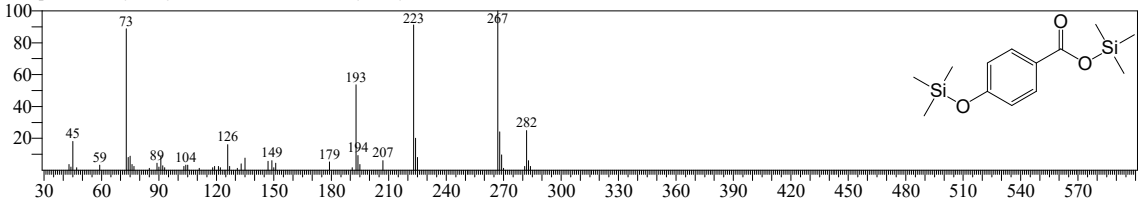
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



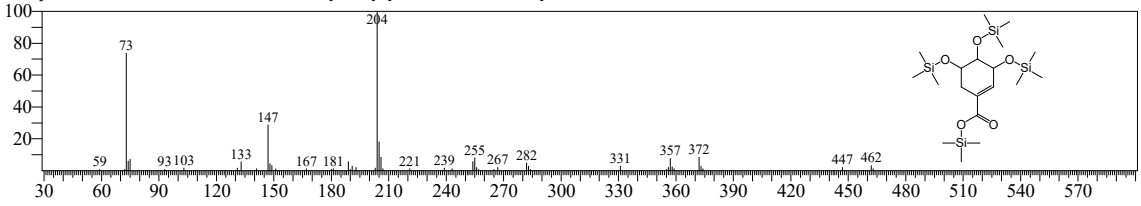
Hit#:2 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



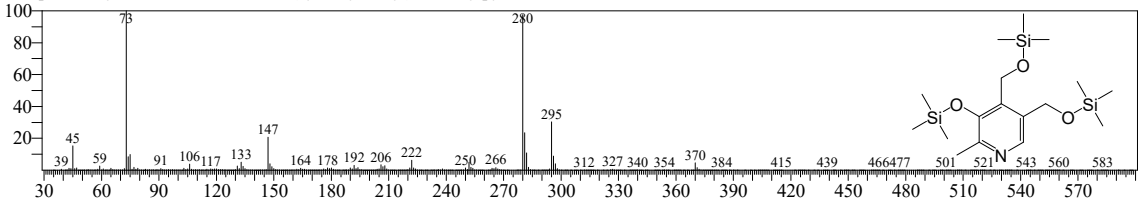
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid

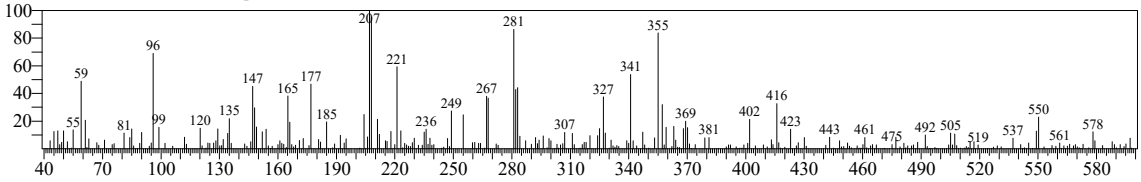


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

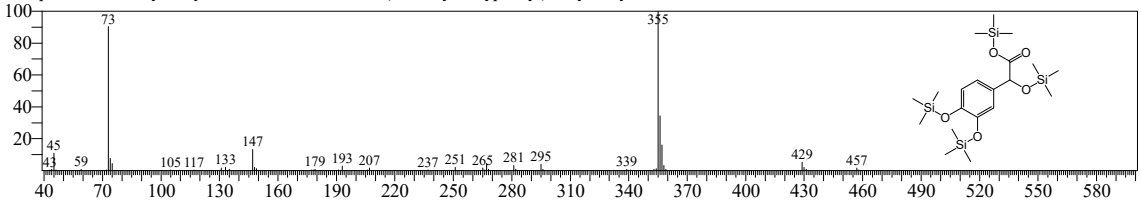


TNAU

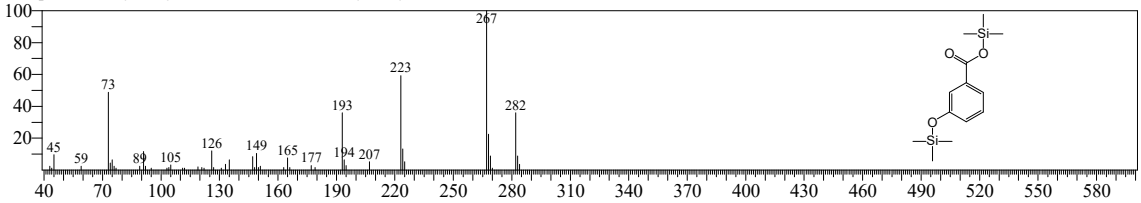
<< Target >>
Line#:10 R.Time:29.575(Scan#:5016) MassPeaks:300
RawMode:Averaged 29.570-29.580(5015-5017) BasePeak:207.00(781)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



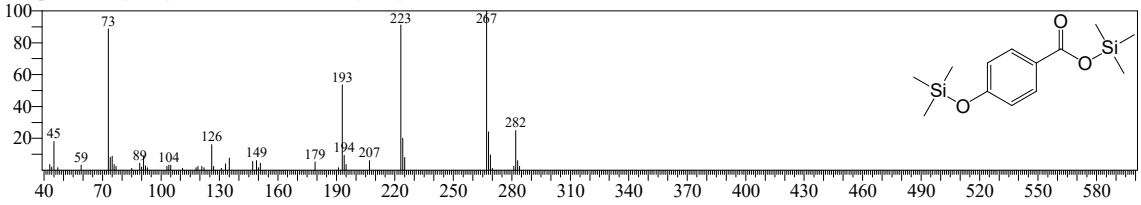
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



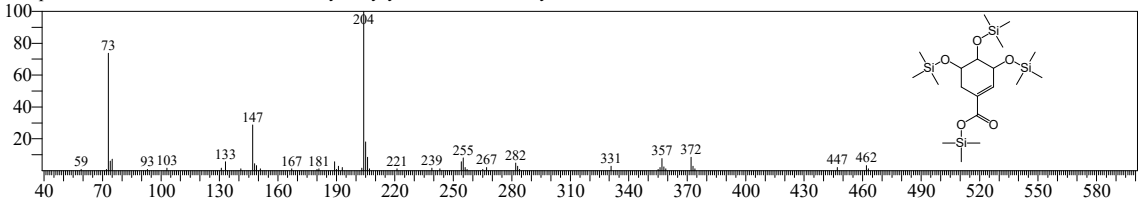
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



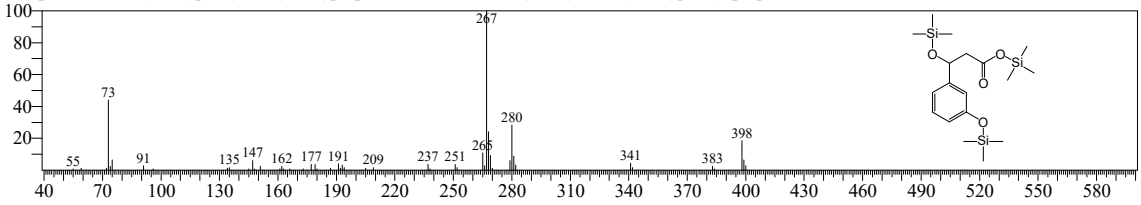
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid

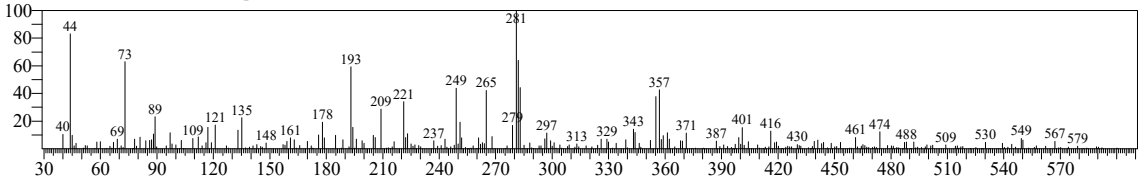


Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

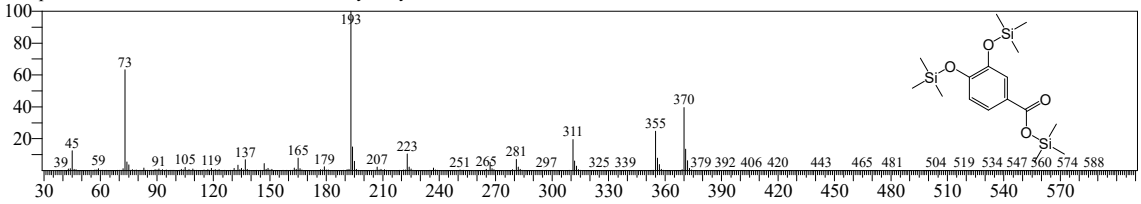


TNAU

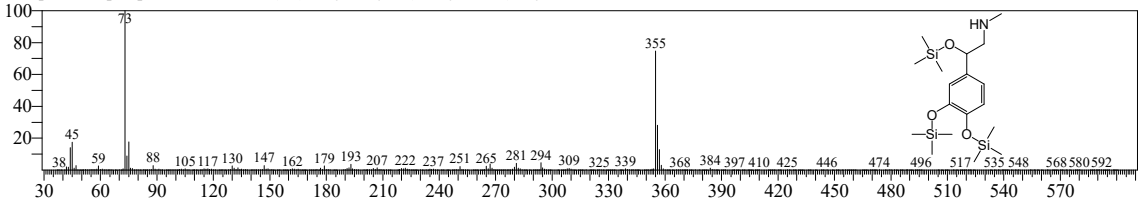
<< Target >>
Line#:11 R.Time:29.900(Scan#:5081) MassPeaks:277
RawMode:Averaged 29.895-29.905(5080-5082) BasePeak:281.05(1094)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



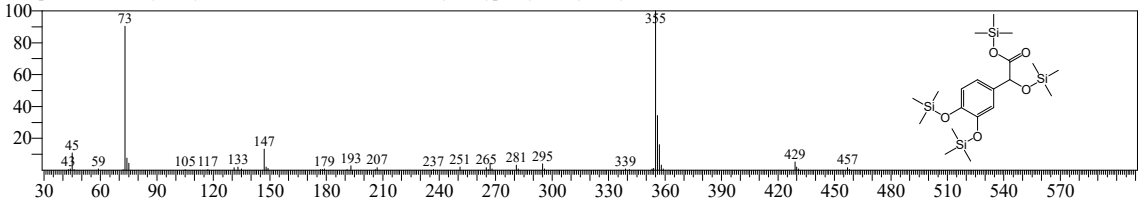
Hit#:1 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



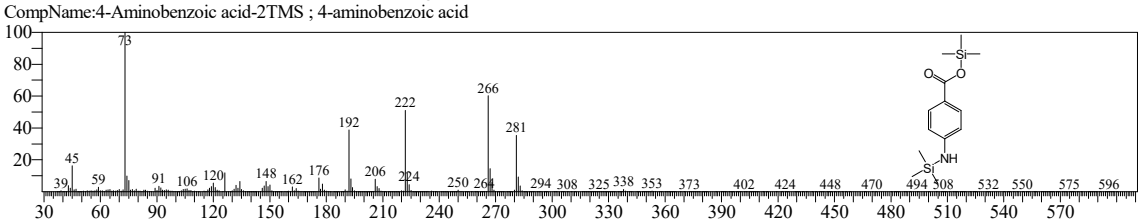
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



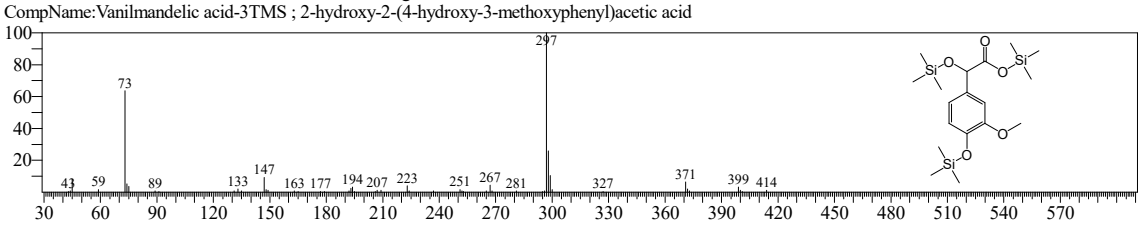
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

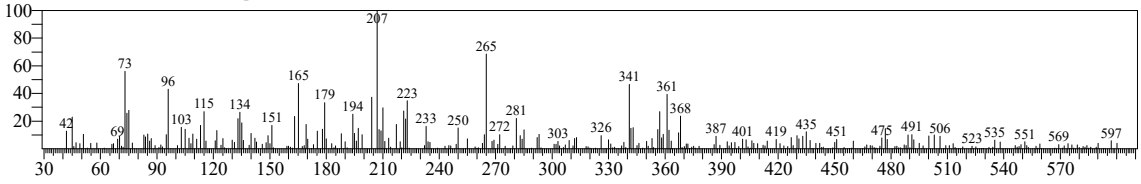


Hit#:5 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

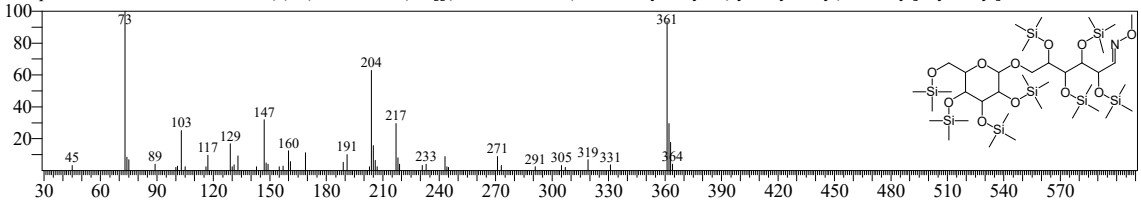


TNAU

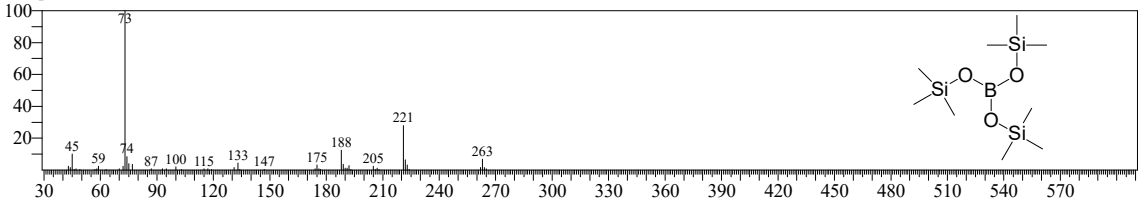
<< Target >>
Line#:12 R.Time:30.215(Scan#:5144) MassPeaks:303
RawMode:Averaged 30.210-30.220(5143-5145) BasePeak:207.05(841)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



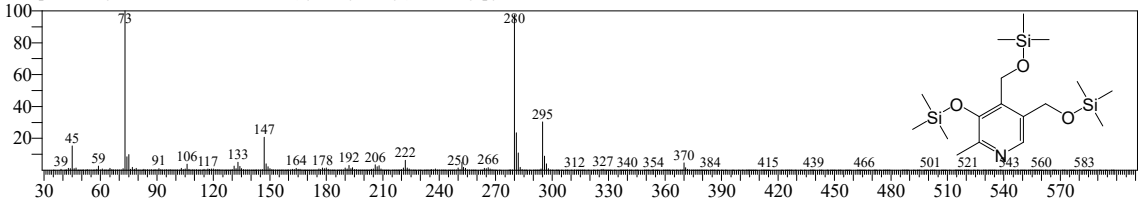
Hit#:1 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



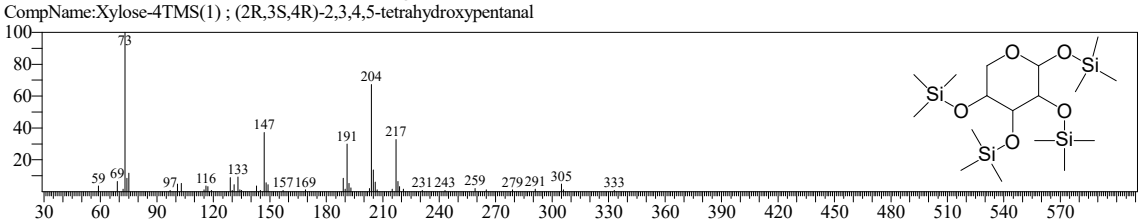
Hit#:2 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid



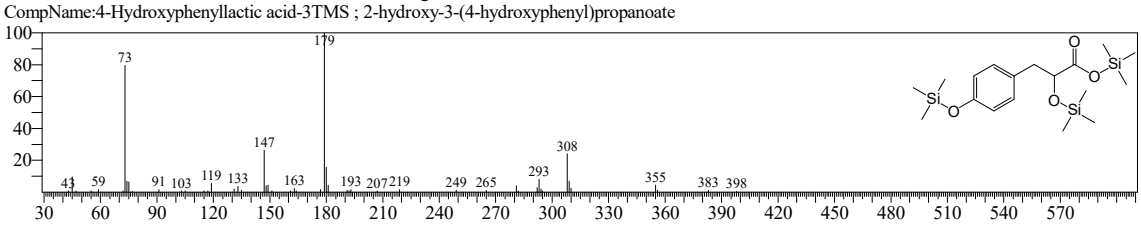
Hit#:3 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



Hit#:4 Entry:267 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

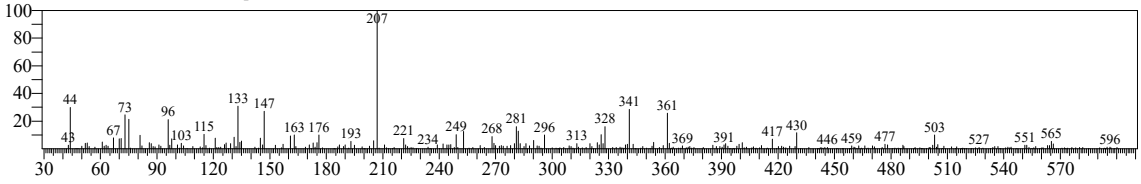


Hit#:5 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

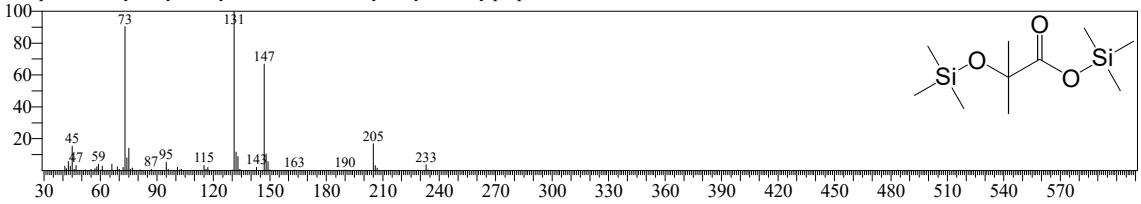


TNAU

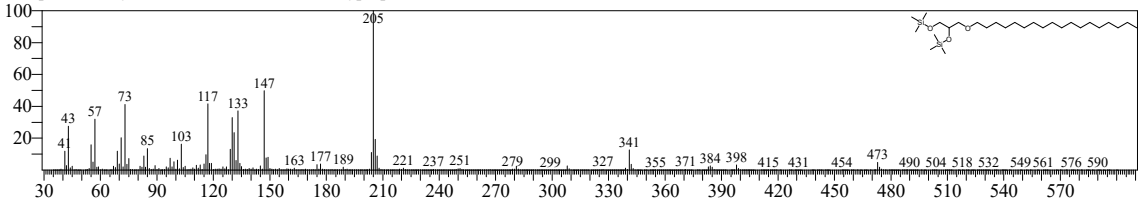
<< Target >>
Line#:13 R.Time:30.860(Scan#:5273) MassPeaks:310
RawMode:Averaged 30.855-30.865(5272-5274) BasePeak:207.05(1965)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



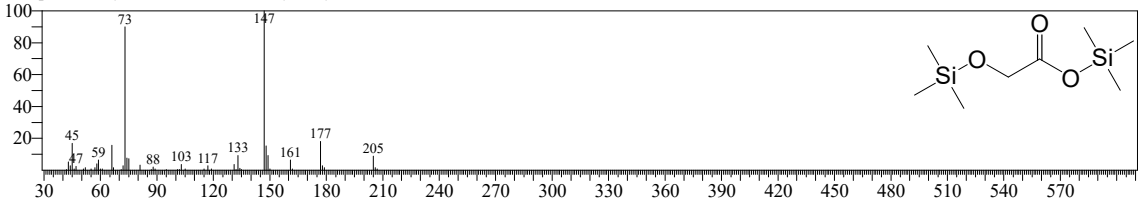
Hit#:1 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid



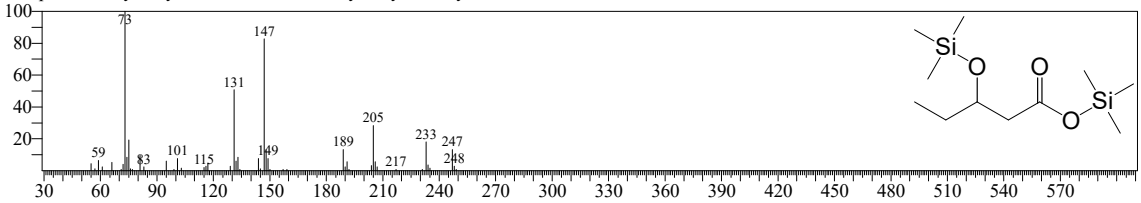
Hit#:2 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



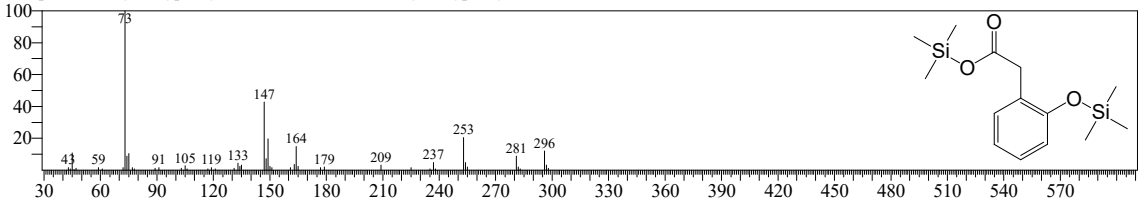
Hit#:3 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid



Hit#:4 Entry:61 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C11H26O3Si2 CAS:10237-77-1 MolWeight:262 RetIndex:1244
CompName:3-Hydroxyvaleric acid-2TMS ; 3-hydroxy-3-methylbutanoic acid

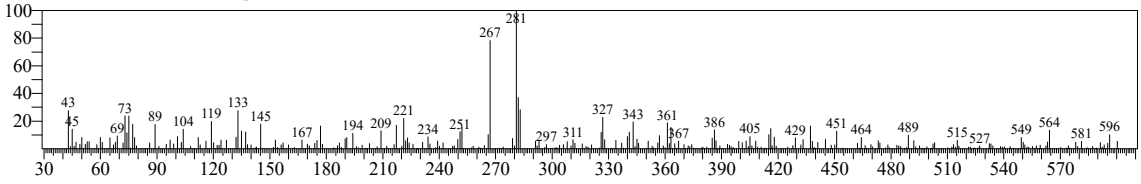


Hit#:5 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

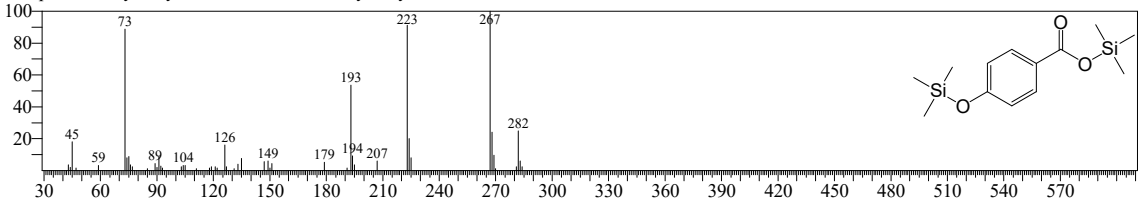


TNAU

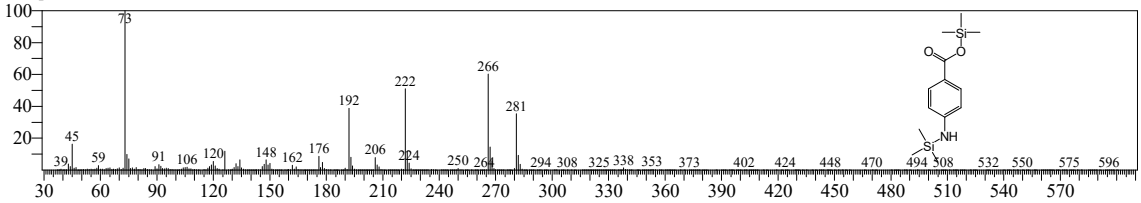
<< Target >>
Line#:14 R.Time:31.045(Scan#:5310) MassPeaks:292
RawMode:Averaged 31.040-31.050(5309-5311) BasePeak:281.05(1148)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



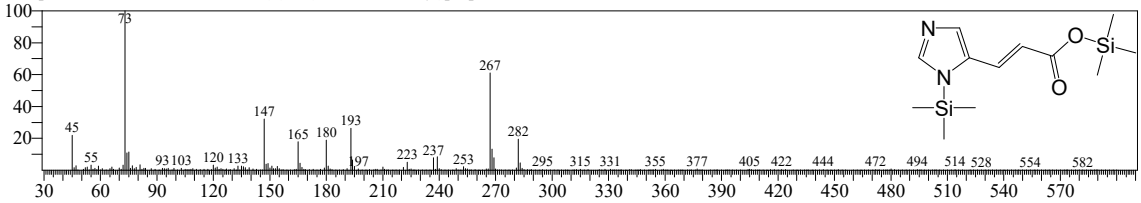
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



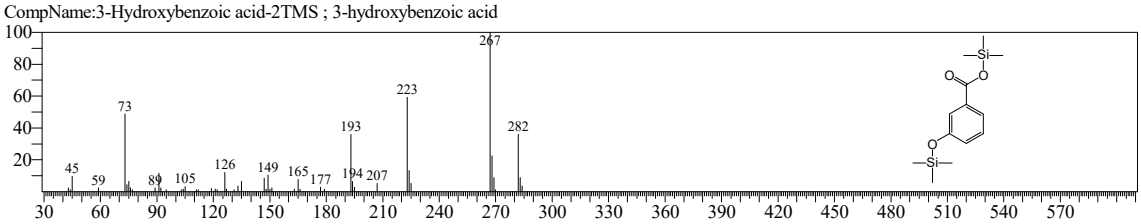
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



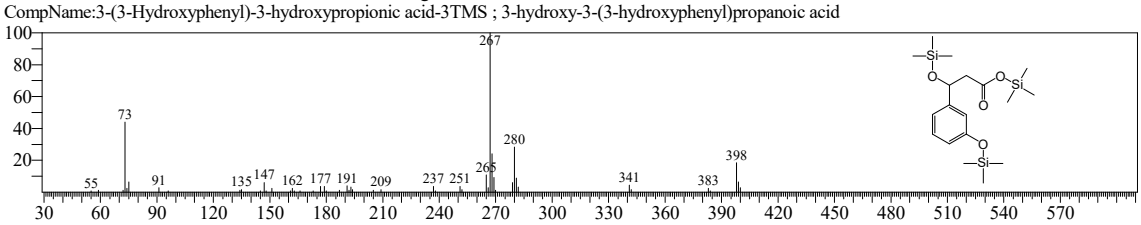
Hit#:3 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

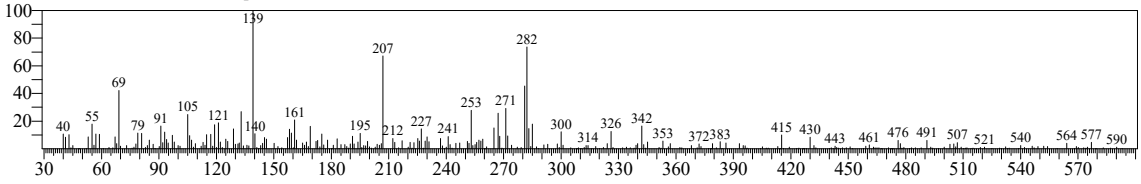


Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

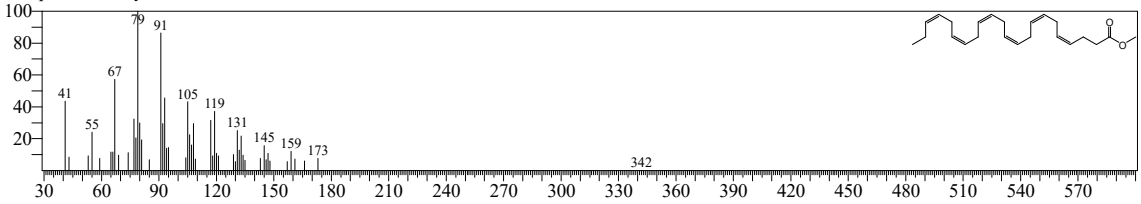


TNAU

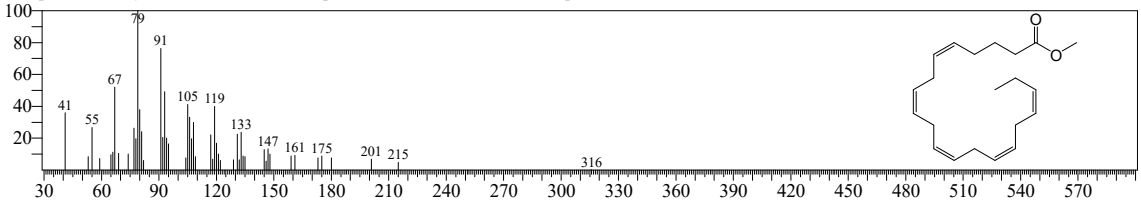
<< Target >>
Line#:15 R.Time:31.910(Scan#:5483) MassPeaks:312
RawMode:Averaged 31.905-31.915(5482-5484) BasePeak:139.10(2546)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



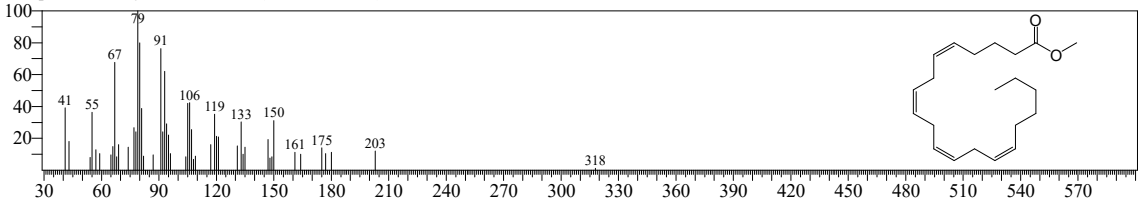
Hit#:1 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C23H34O2 CAS:6217-54-5 MolWeight:342 RetIndex:3514
CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid



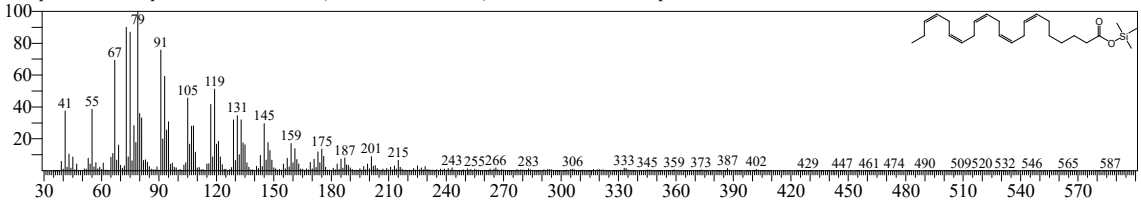
Hit#:2 Entry:36 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C21H32O2 CAS:10417-94-4 MolWeight:316 RetIndex:3232
CompName:Methyl cis-5,8,11,14,17-Eicosapentaenoate ; Icosa-5,8,11,14,17-pentaenoic acid



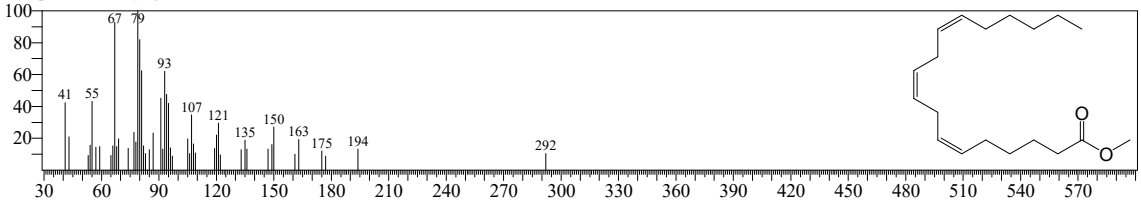
Hit#:3 Entry:33 Library:FA_ME_SP2560_EI_V3.lib
SI:35 Formula:C21H34O2 CAS:506-32-1 MolWeight:318 RetIndex:3109
CompName:Methyl arachidonate ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid



Hit#:4 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

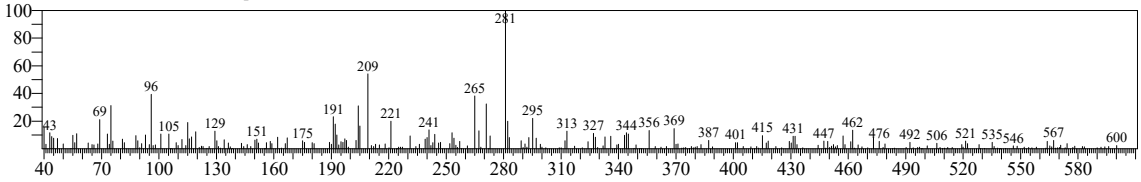


Hit#:5 Entry:23 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C19H32O2 CAS:506-26-3 MolWeight:292 RetIndex:2852
CompName:Methyl ganma-linolenate ; ; Octadeca-6,9,12-trienoic acid

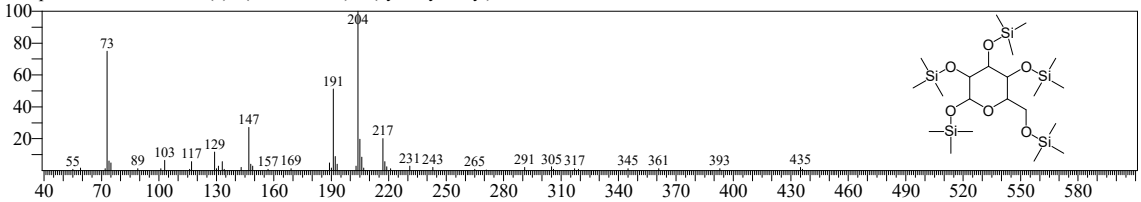


TNAU

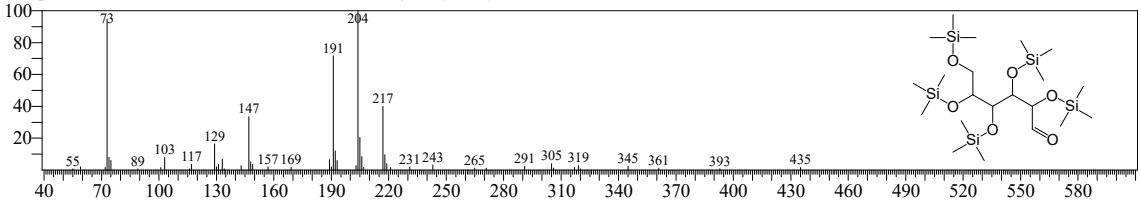
<< Target >>
Line#:16 R.Time:31.980(Scan#:5497) MassPeaks:271
RawMode:Averaged 31.975-31.985(5496-5498) BasePeak:281.05(1181)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



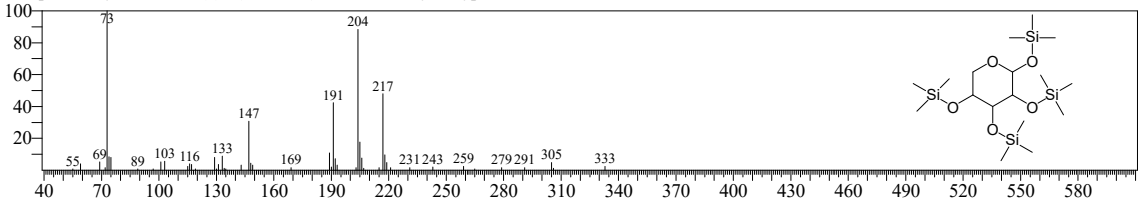
Hit#:1 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



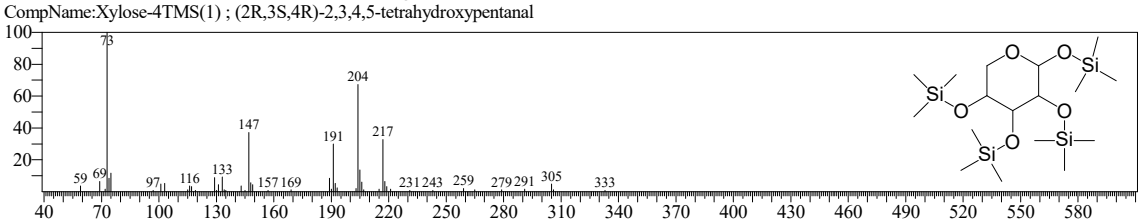
Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



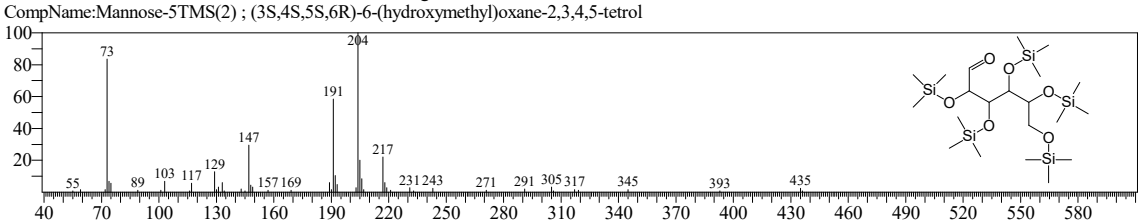
Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:267 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

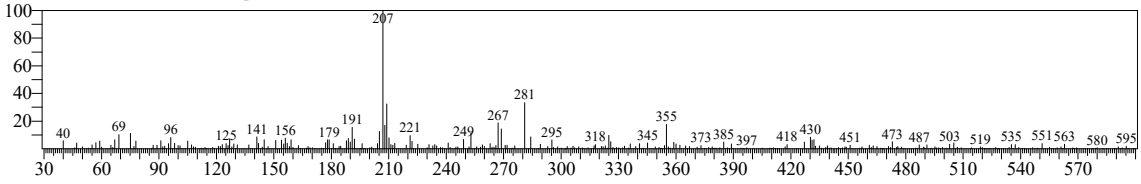


Hit#:5 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

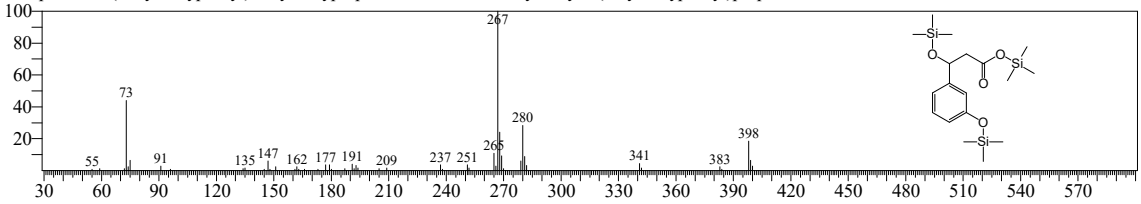


TNAU

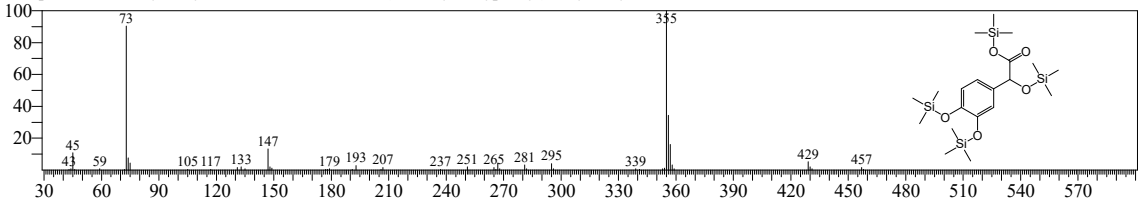
<< Target >>
Line#:17 R.Time:32.030(Scan#:5507) MassPeaks:291
RawMode:Averaged 32.025-32.035(5506-5508) BasePeak:207.05(2041)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



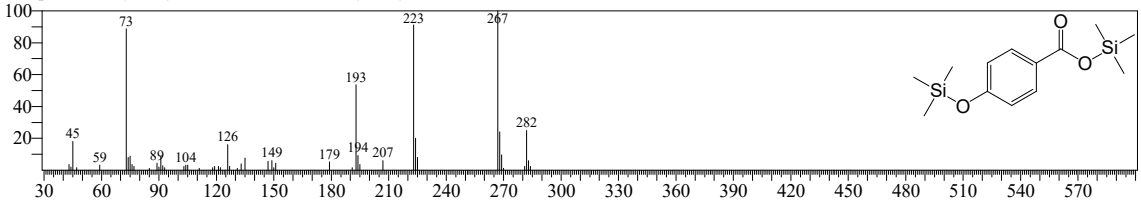
Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



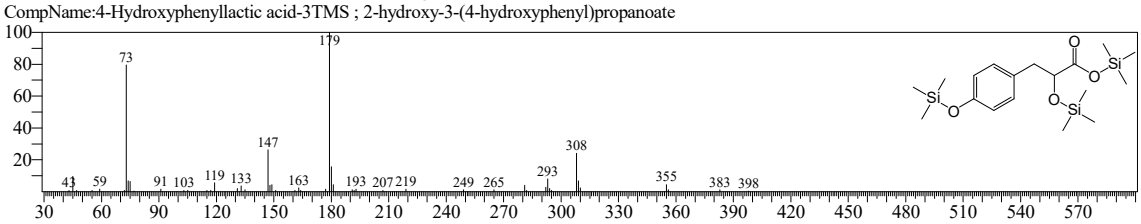
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



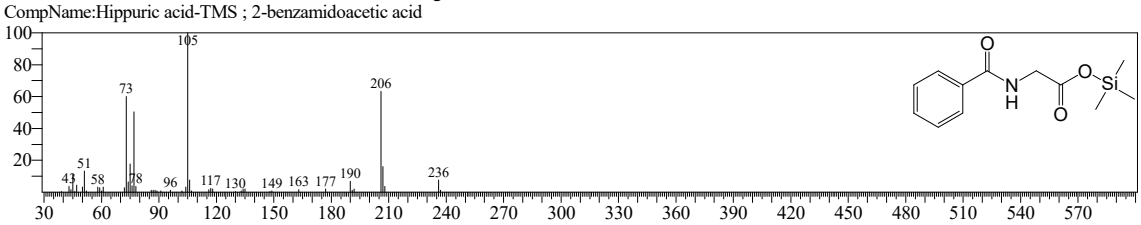
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

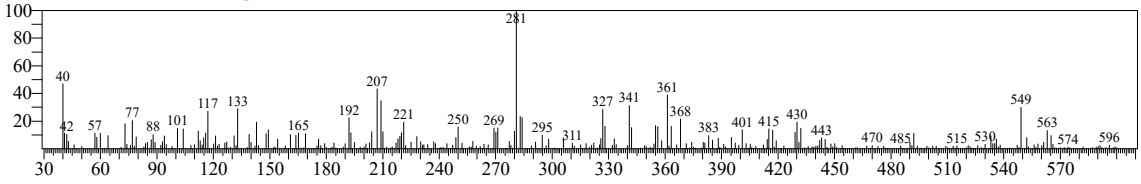


Hit#:5 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid

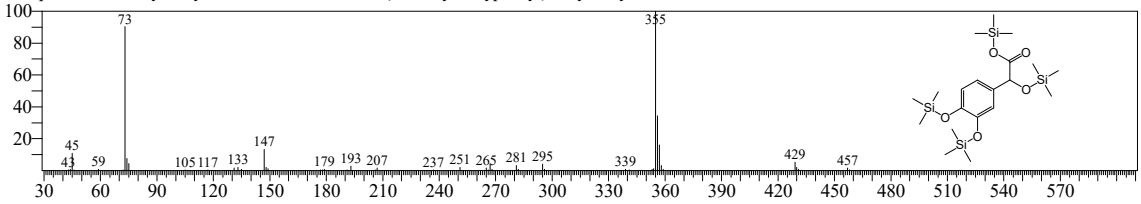


TNAU

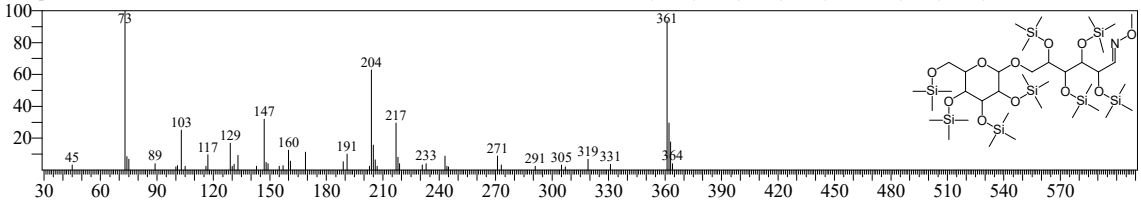
<< Target >>
Line#:18 R.Time:32.695(Scan#:5640) MassPeaks:304
RawMode:Averaged 32.690-32.700(5639-5641) BasePeak:281.05(1077)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



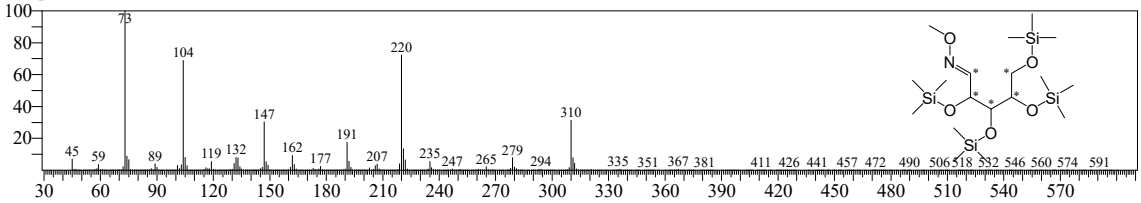
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



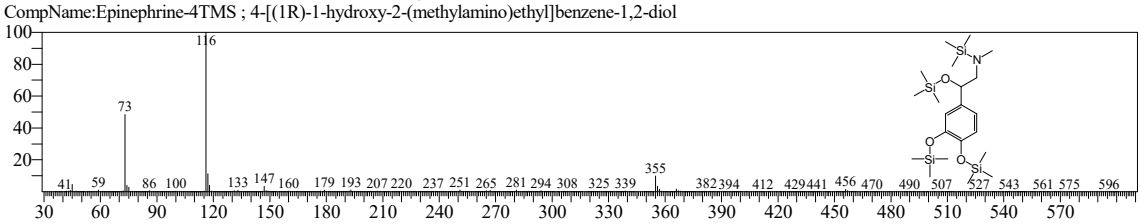
Hit#:2 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



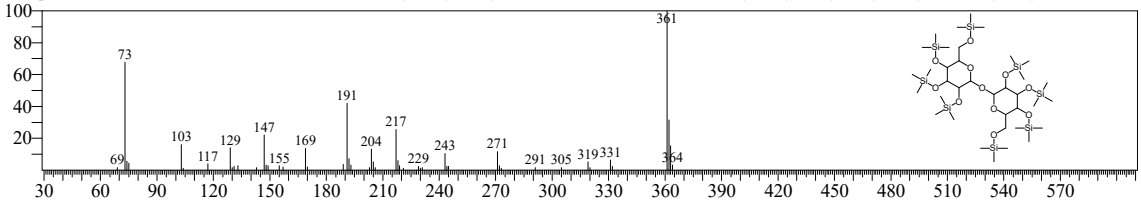
Hit#:3 Entry:256 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula: CAS:0-00-0 MolWeight:472 RetIndex:1698
CompName:Ribose-13C5-meto-4TMS ;



Hit#:4 Entry:431 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H45NO3Si4 CAS:51-43-4 MolWeight:471 RetIndex:1989
CompName:Epinephrine-4TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

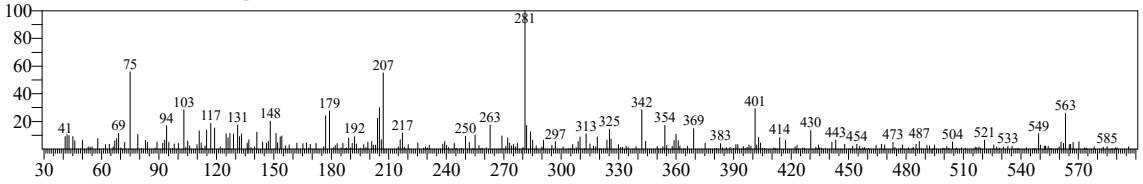


Hit#:5 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

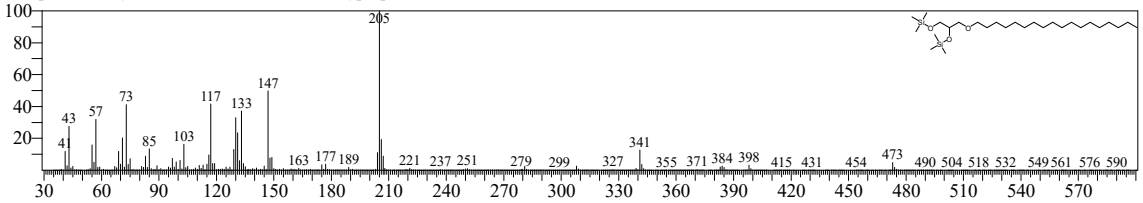


TNAU

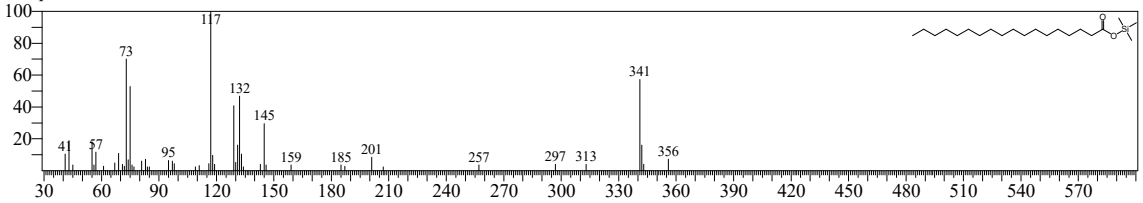
<< Target >>
Line#:19 R.Time:32.735(Scan#:5648) MassPeaks:300
RawMode:Averaged 32.730-32.740(5647-5649) BasePeak:281.05(1115)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



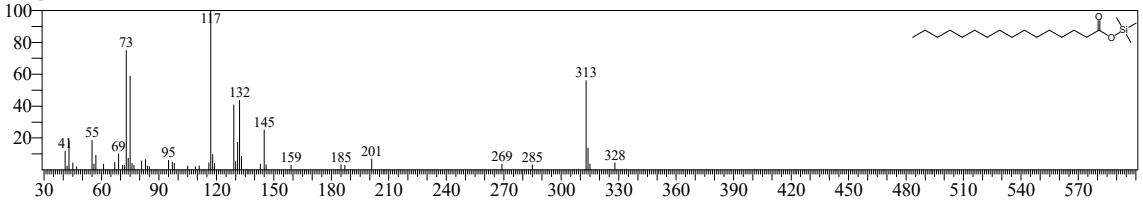
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



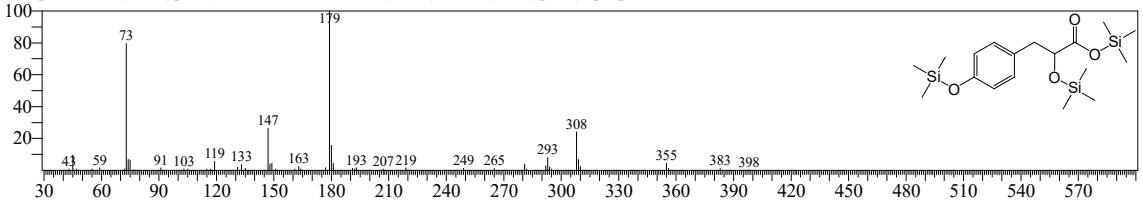
Hit#:2 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



Hit#:3 Entry:446 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C19H40O2Si CAS:57-10-3 MolWeight:328 RetIndex:2046
CompName:Palmitic acid-TMS ; hexadecanoic acid



Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:5 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:29 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