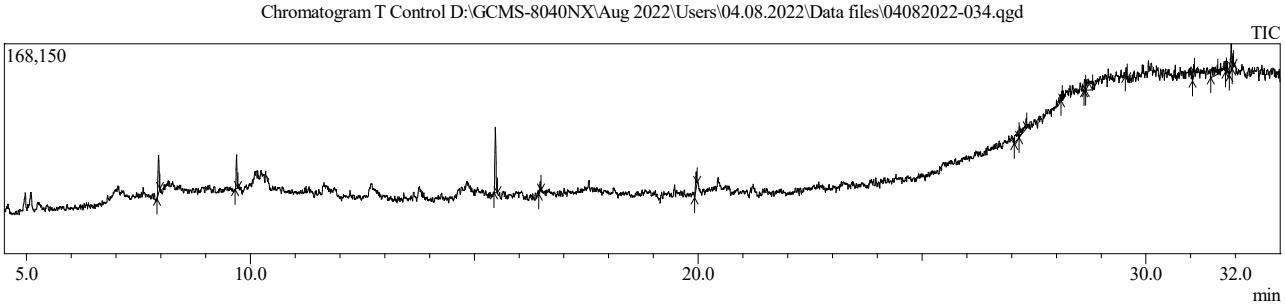
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 2:20:51 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T Control
Sample ID	: T Control
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 33
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-034.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-034.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 4:48:38 PM

Chromatogram T Control D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-034.qgd



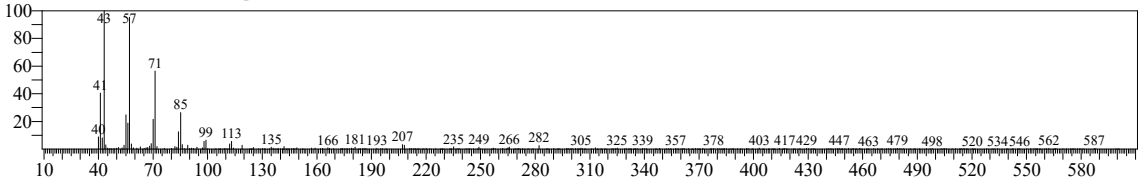
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.947	51490	10.87	30234	12.98	1.70	91	Dodecane
2	9.690	37024	7.82	27081	11.63	1.37	90	Dodecane
3	15.470	87902	18.56	52531	22.56	1.67	93	2,4-Di-tert-butylphenol
4	16.475	13202	2.79	7675	3.30	1.72	72	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
5	19.955	23634	4.99	12961	5.57	1.82	54	Dimethylglycine-TMS
6	27.070	26039	5.50	5388	2.31	4.83	32	3,4-Dihydroxymandelic acid-4TMS
7	27.325	39589	8.36	8003	3.44	4.95	35	Epinephrine-3TMS
8	28.123	6102	1.29	7460	3.20	0.82	40	4-Aminobenzoic acid-2TMS
9	28.625	11890	2.51	8498	3.65	1.40	38	Epinephrine-3TMS
10	28.708	56547	11.94	8898	3.82	6.36	42	4-Aminobenzoic acid-2TMS
11	29.558	7938	1.68	7863	3.38	1.01	28	2-Methylhippuric acid-TMS
12	31.066	12114	2.56	9256	3.97	1.31	34	Hypoxanthine-2TMS
13	31.593	41809	8.83	7606	3.27	5.50	38	3,4-Dihydroxymandelic acid-4TMS
14	31.786	6079	1.28	8942	3.84	0.68	36	3,4-Dihydroxymandelic acid-4TMS
15	31.905	43977	9.28	21601	9.28	2.04	28	3,4-Dihydroxymandelic acid-4TMS
16	31.935	8330	1.76	8862	3.81	0.94	34	2-Hydroxyphenylacetic acid-2TMS
		473666	100.00	232859	100.00			

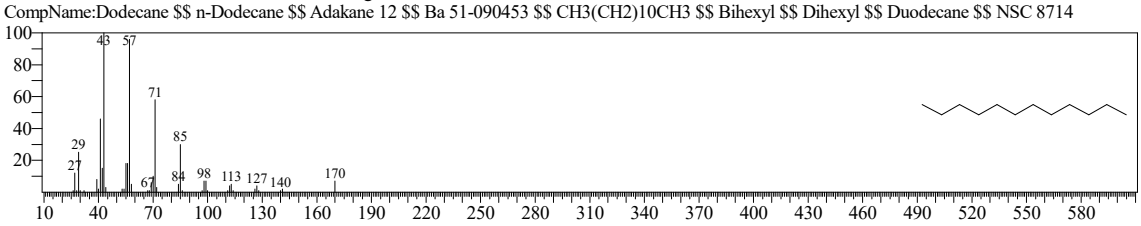
Library

TNAU

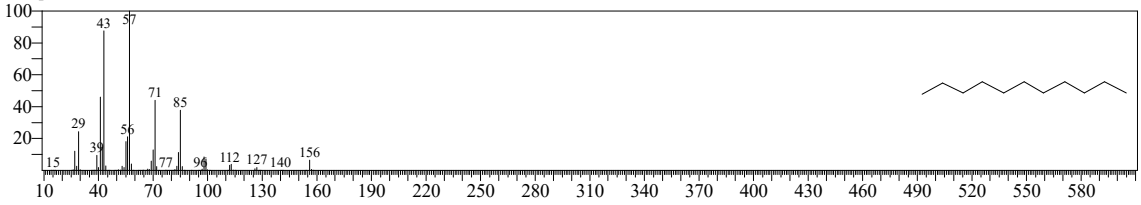
<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:305
RawMode:Averaged 7.940-7.950(689-691) BasePeak:43.05(6165)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



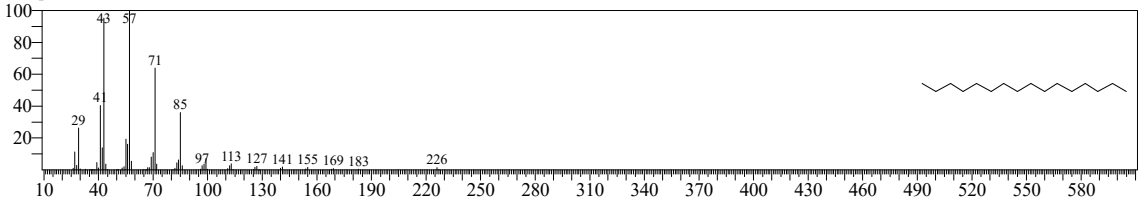
Hit#:1 Entry:16190 Library:NIST20R.lib
SI:91 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



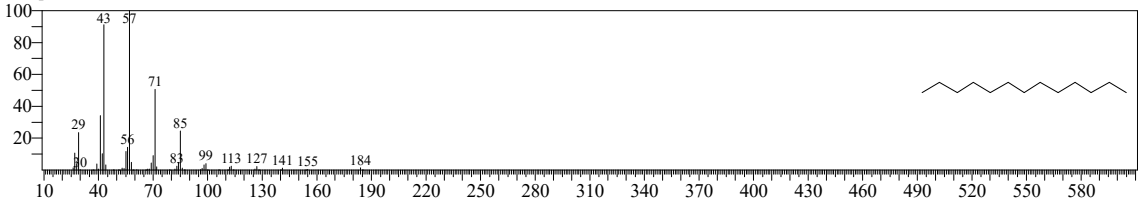
Hit#:2 Entry:12897 Library:NIST20R.lib
SI:90 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



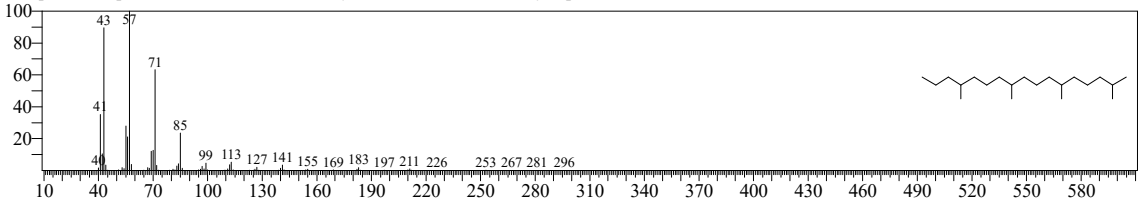
Hit#:3 Entry:27736 Library:NIST20R.lib
SI:90 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane



Hit#:4 Entry:40226 Library:NIST20M1.lib
SI:90 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

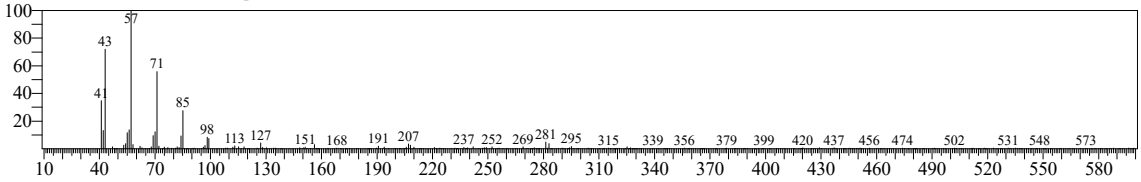


Hit#:5 Entry:159057 Library:NIST20M1.lib
SI:90 Formula:C21H44 CAS:18344-37-1 MolWeight:296 RetIndex:1852
CompName:Heptadecane, 2,6,10,14-tetramethyl- $$ 2,6,10,14-Tetramethylheptadecane

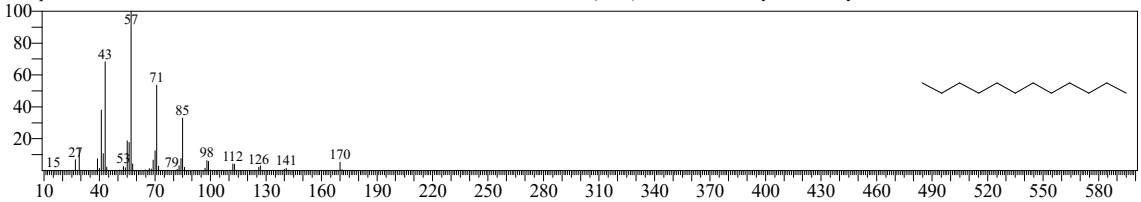


TNAU

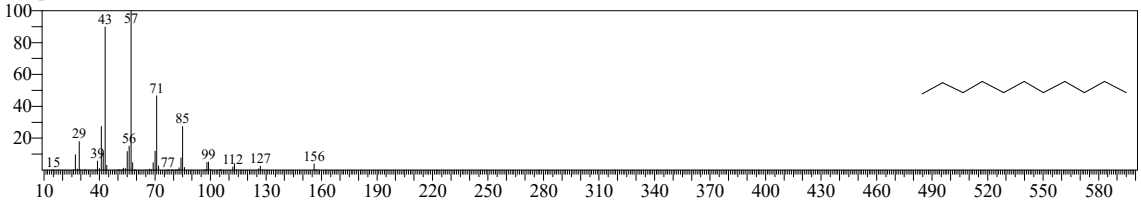
<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:260
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(6372)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



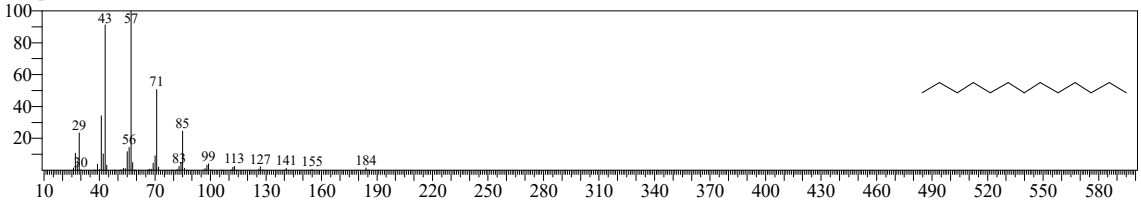
Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:90 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



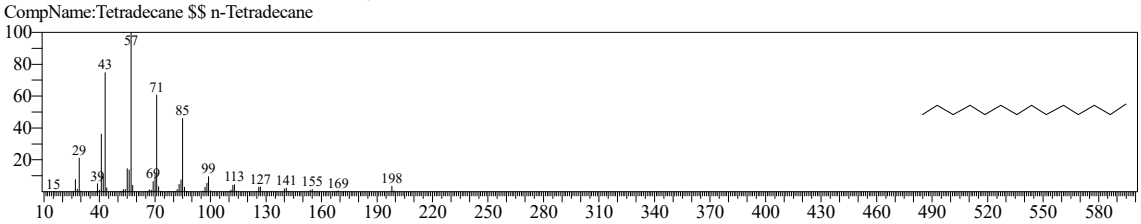
Hit#:2 Entry:21042 Library:NIST20M1.lib
SI:90 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



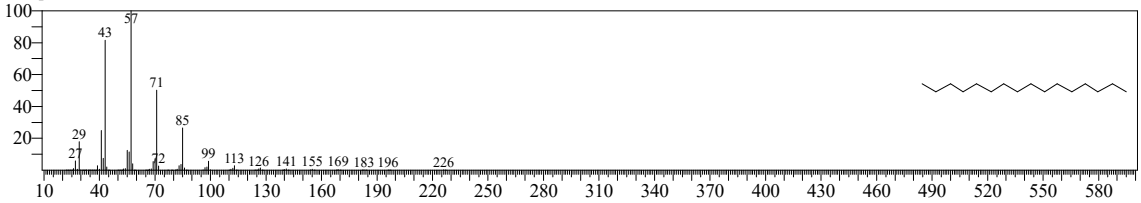
Hit#:3 Entry:40226 Library:NIST20M1.lib
SI:90 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:22497 Library:NIST20R.lib
SI:89 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

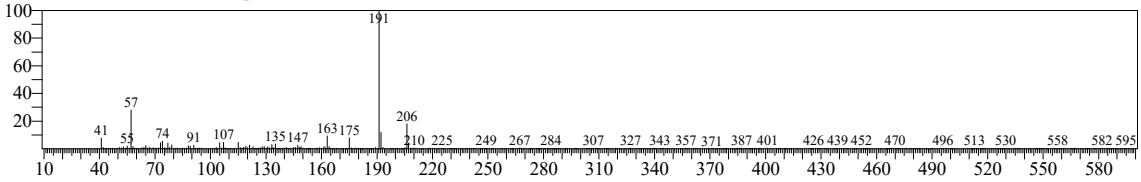


Hit#:5 Entry:27737 Library:NIST20R.lib
SI:89 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

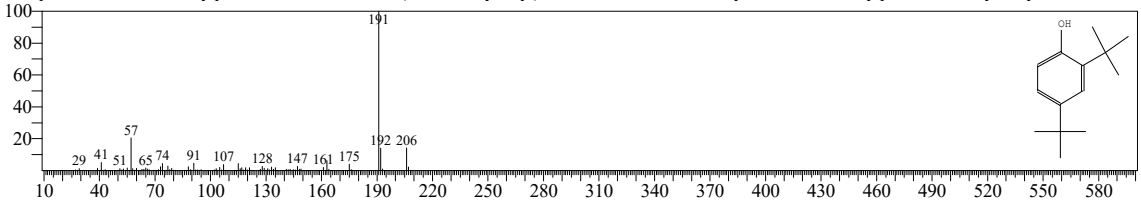


TNAU

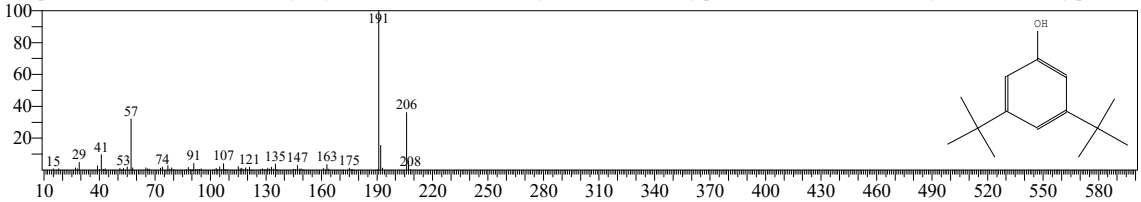
<< Target >>
Line#:3 R.Time:15.470(Scan#:2195) MassPeaks:328
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.15(17010)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



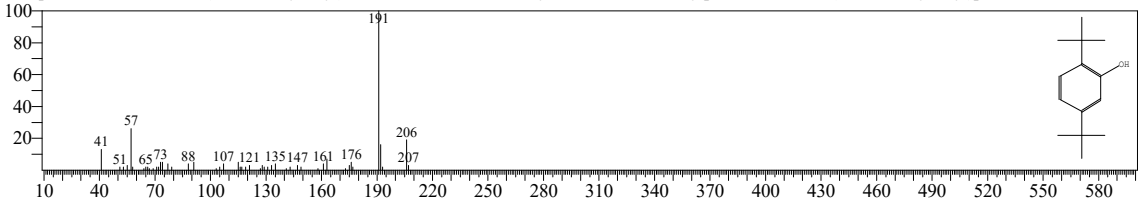
Hit#:1 Entry:24088 Library:NIST20R.lib
SI:93 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



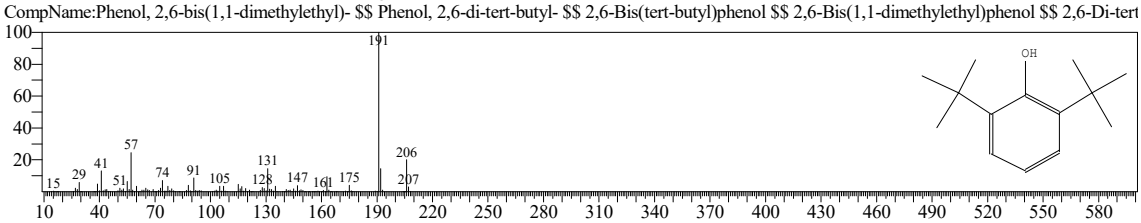
Hit#:2 Entry:24110 Library:NIST20R.lib
SI:91 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



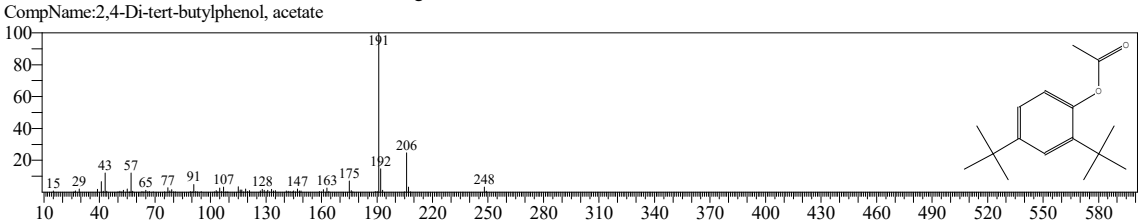
Hit#:3 Entry:24098 Library:NIST20R.lib
SI:90 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



Hit#:4 Entry:59031 Library:NIST20M1.lib
SI:89 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

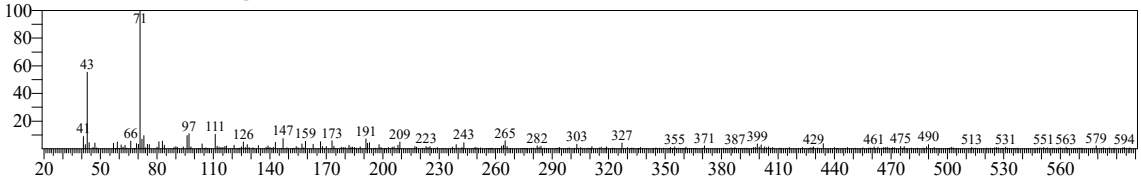


Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:87 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
CompName:2,4-Di-tert-butylphenol, acetate

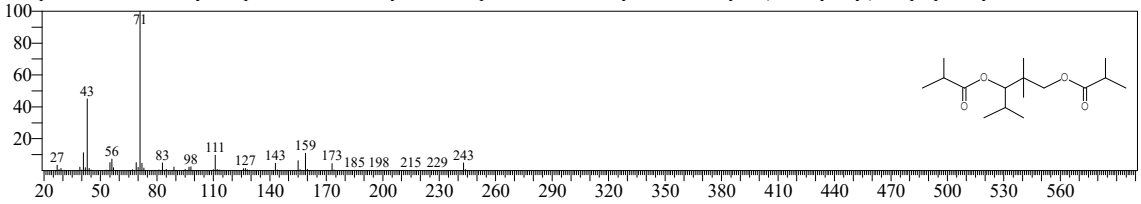


TNAU

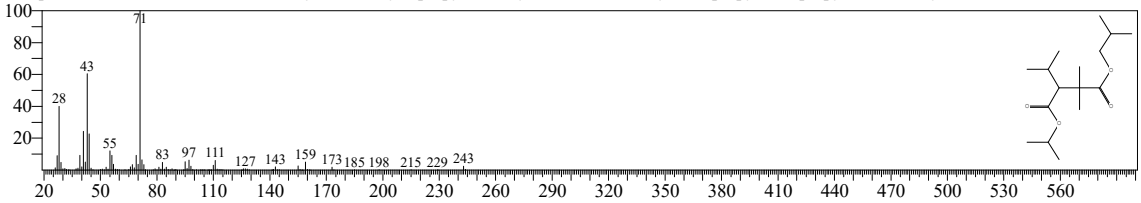
<< Target >>
Line#:4 R.Time:16.475(Scan#:2396) MassPeaks:297
RawMode:Averaged 16.470-16.480(2395-2397) BasePeak:71.05(2316)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



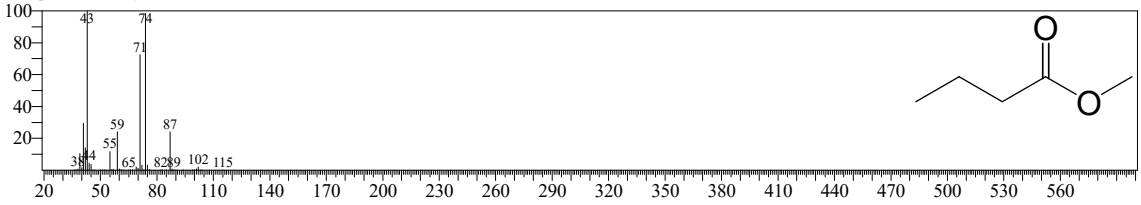
Hit#:1 Entry:34622 Library:NIST20R.lib
SI:72 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan



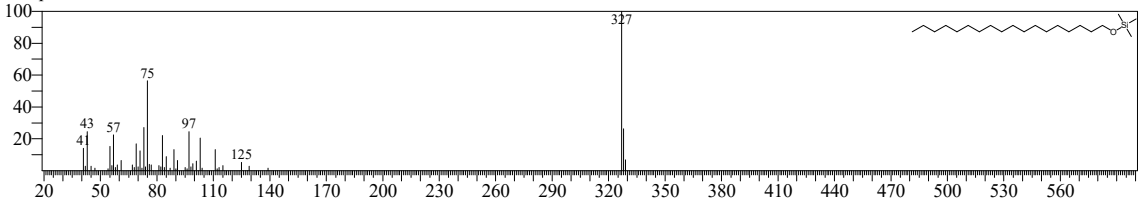
Hit#:2 Entry:146809 Library:NIST20M1.lib
SI:72 Formula:C16H30O4 CAS:0-00-0 MolWeight:286 RetIndex:1605
CompName:Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester $$ 1-Isobutyl 4-isopropyl 3-isopropyl-2,2-dimethylsuccinate #



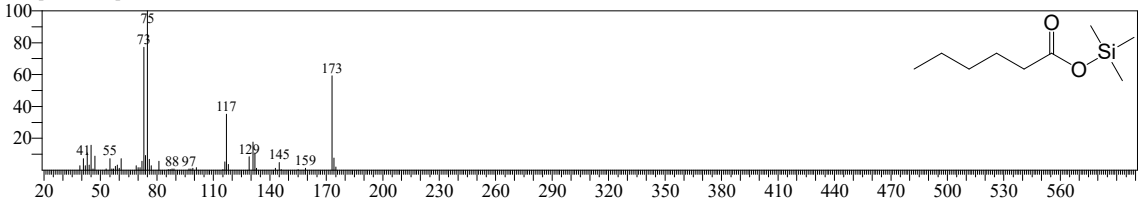
Hit#:3 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



Hit#:4 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol

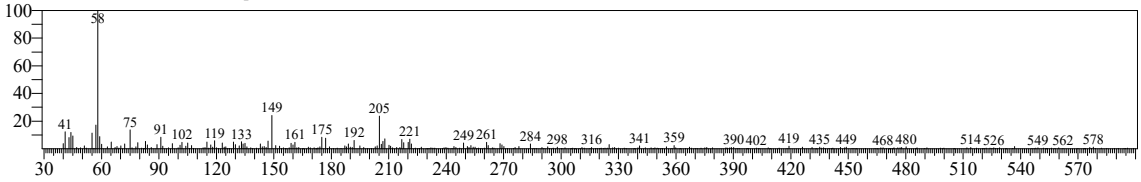


Hit#:5 Entry:11 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid

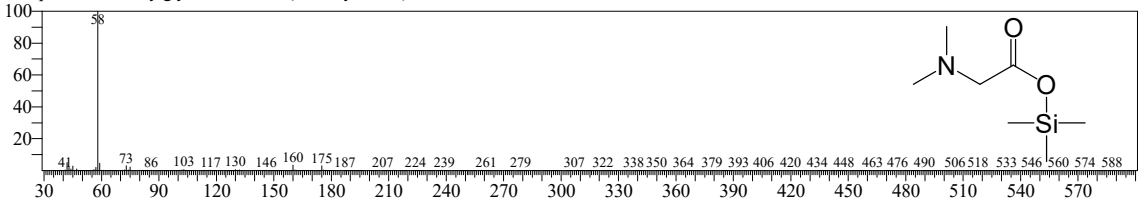


TNAU

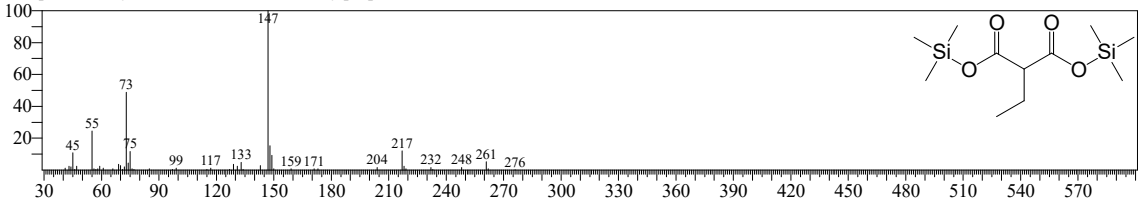
<< Target >>
Line#:5 R.Time:19.955(Scan#:3092) MassPeaks:315
RawMode:Averaged 19.950-19.960(3091-3093) BasePeak:58.10(2929)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



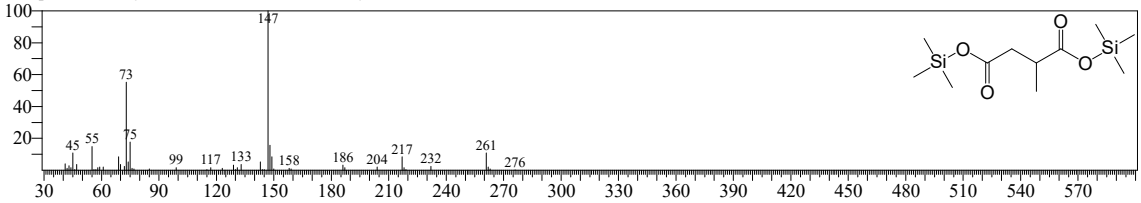
Hit#:1 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:54 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



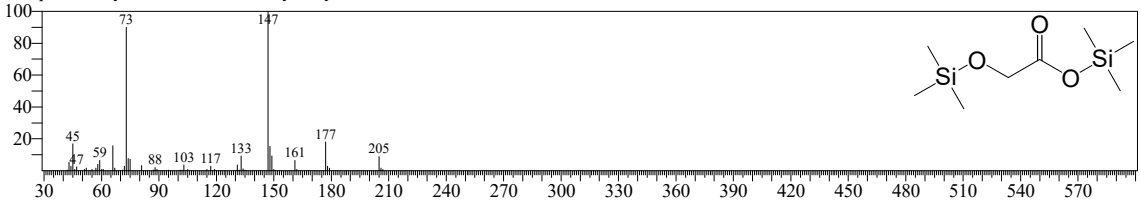
Hit#:2 Entry:80 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C11H24O4Si2 CAS:601-75-2 MolWeight:276 RetIndex:1284
CompName:Ethylmalonic acid-2TMS ; 2-ethylpropanedioic acid



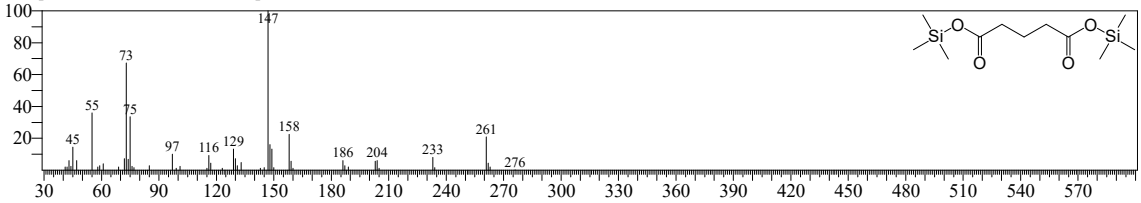
Hit#:3 Entry:95 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C11H24O4Si2 CAS:498-21-5 MolWeight:276 RetIndex:1327
CompName:Methylsuccinic acid-2TMS ; 2-methylbutanedioic acid



Hit#:4 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

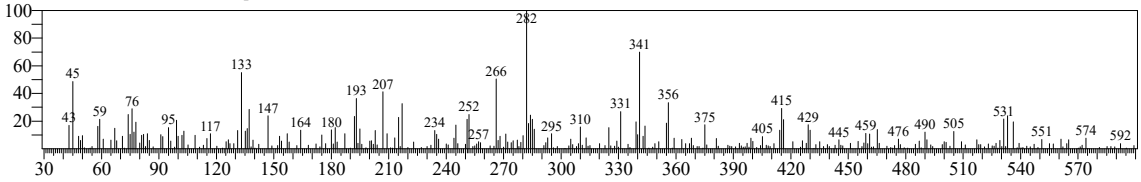


Hit#:5 Entry:115 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C11H24O4Si2 CAS:110-94-1 MolWeight:276 RetIndex:1403
CompName:Glutaric acid-2TMS ; pentanedioic acid

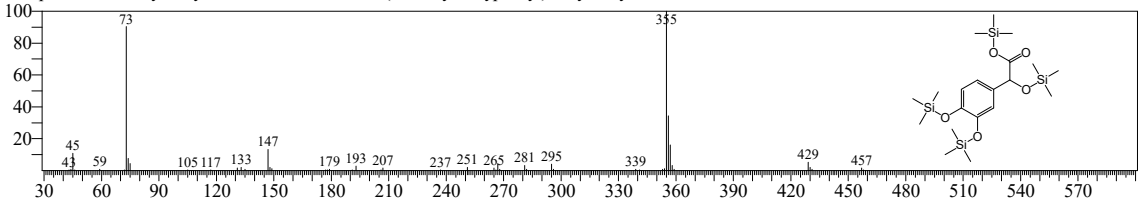


TNAU

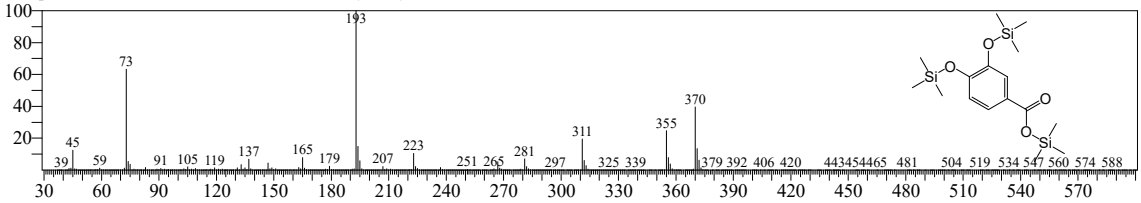
<< Target >>
Line#:6 R.Time:27.070(Scan#:4515) MassPeaks:302
RawMode:Averaged 27.065-27.075(4514-4516) BasePeak:282.05(527)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



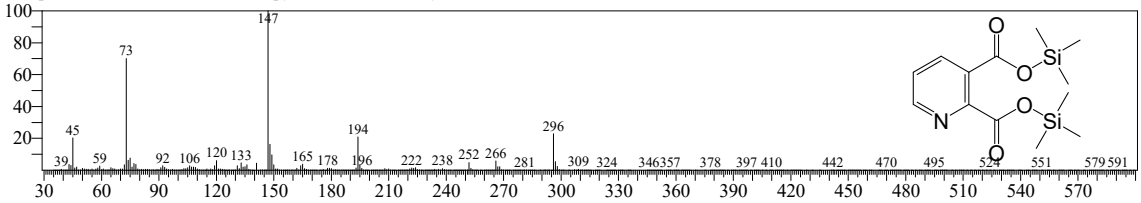
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



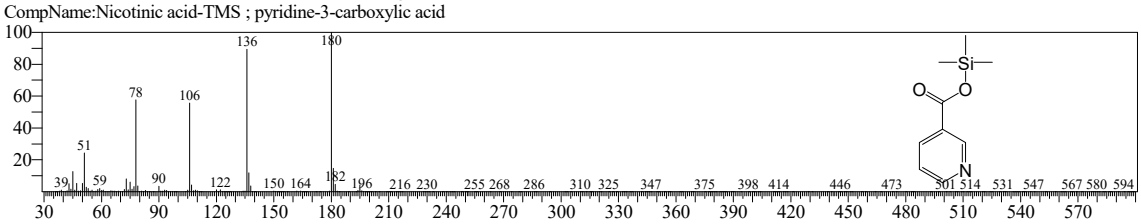
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



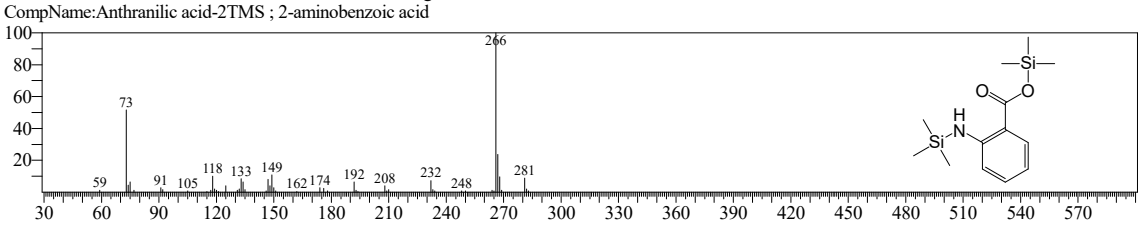
Hit#:3 Entry:272 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C13H21NO4Si2 CAS:89-00-9 MolWeight:311 RetIndex:1743
CompName:Quinolinic acid-2TMS ; pyridine-2,3-dicarboxylic acid



Hit#:4 Entry:84 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C9H13NO2Si CAS:59-67-6 MolWeight:195 RetIndex:1300
CompName:Nicotinic acid-TMS ; pyridine-3-carboxylic acid

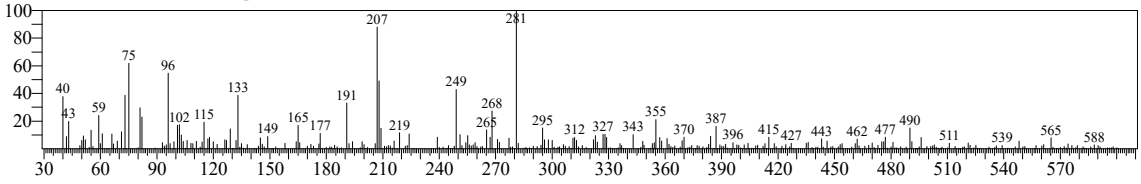


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

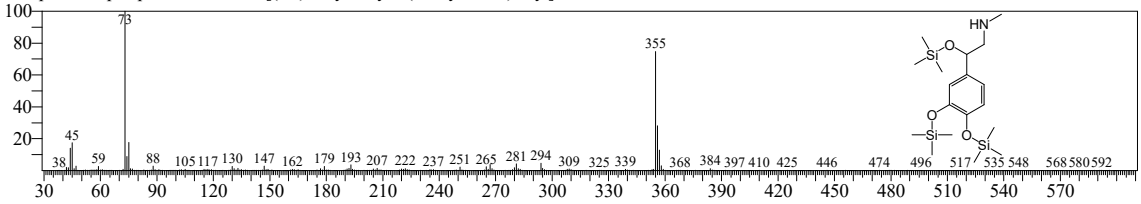


TNAU

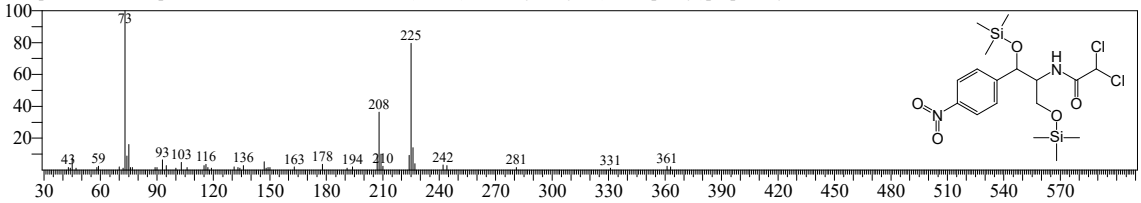
<< Target >>
Line#:7 R.Time:27.325(Scan#:4566) MassPeaks:319
RawMode:Averaged 27.320-27.330(4565-4567) BasePeak:281.00(947)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



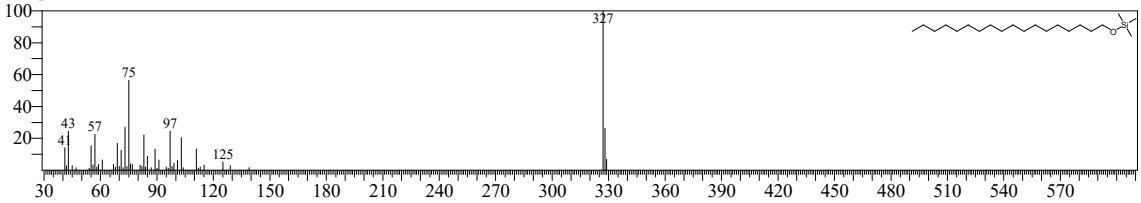
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



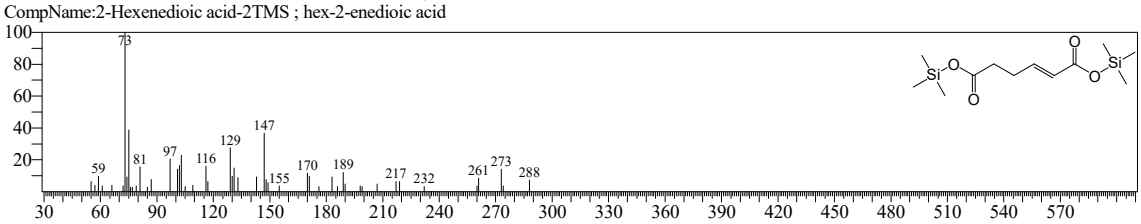
Hit#:2 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



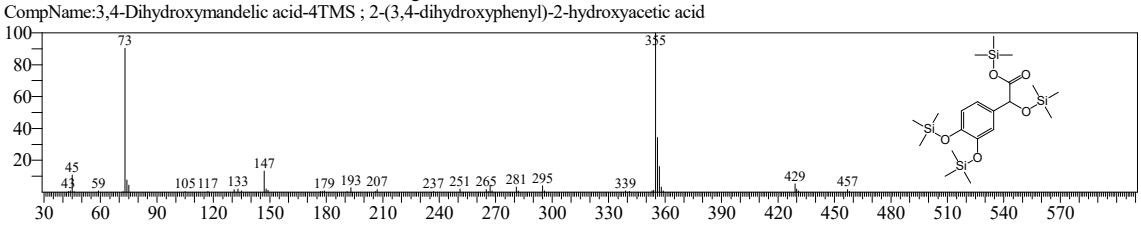
Hit#:3 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol



Hit#:4 Entry:156 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C12H24O4Si2 CAS:4440-68-0 MolWeight:288 RetIndex:1522
CompName:2-Hexenedioic acid-2TMS ; hex-2-enedioic acid

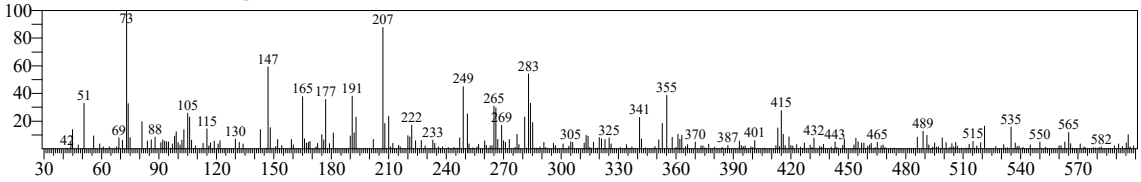


Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

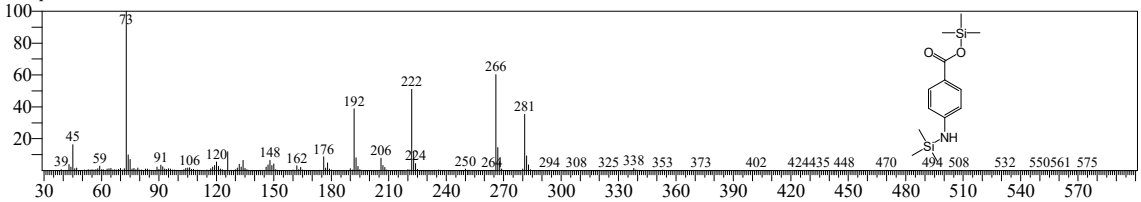


TNAU

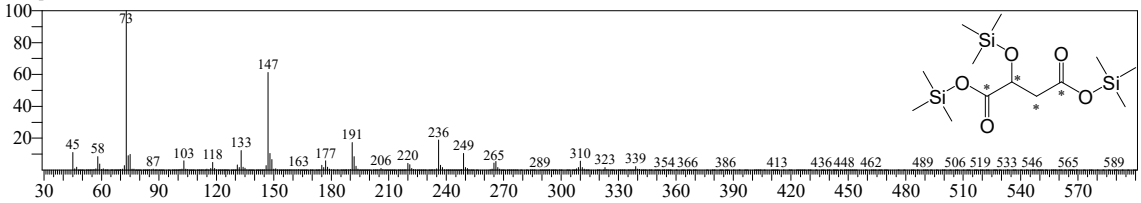
<< Target >>
Line#:8 R.Time:28.125(Scan#:4726) MassPeaks:275
RawMode:Averaged 28.120-28.130(4725-4727) BasePeak:73.10(704)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



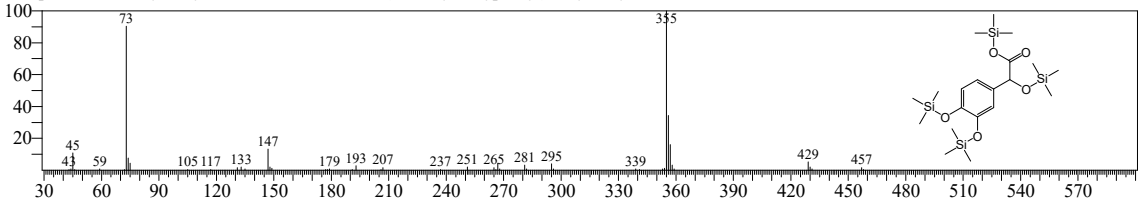
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



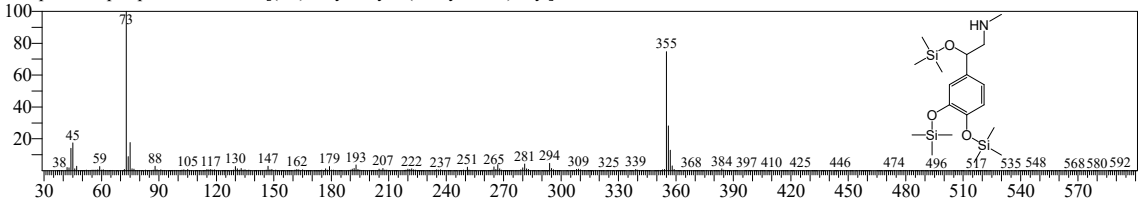
Hit#:2 Entry:143 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula: CAS:0-00-0 MolWeight:354 RetIndex:1495
CompName:Malic acid-13C4-3TMS ;



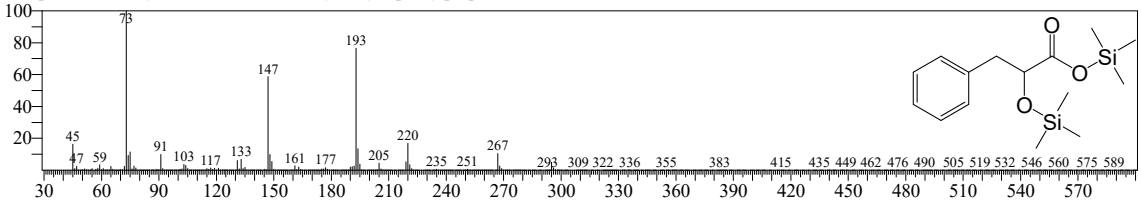
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

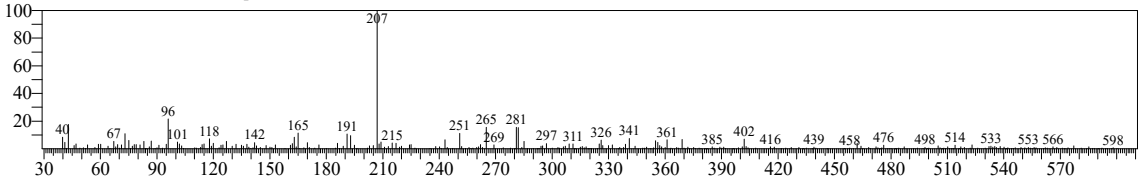


Hit#:5 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

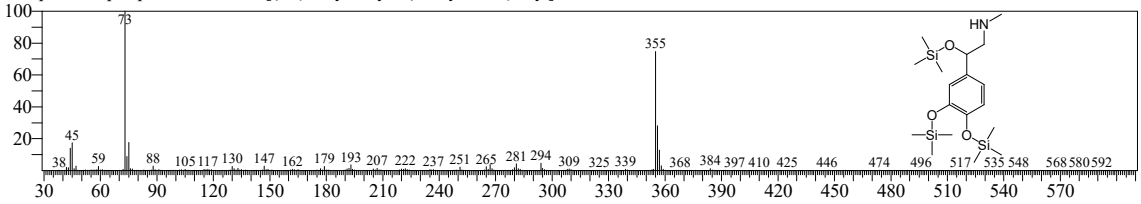


TNAU

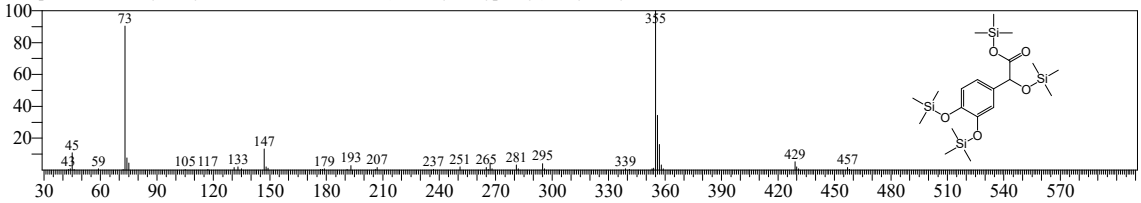
<< Target >>
Line#:9 R.Time:28.625(Scan#:4826) MassPeaks:298
RawMode:Averaged 28.620-28.630(4825-4827) BasePeak:207.05(2342)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



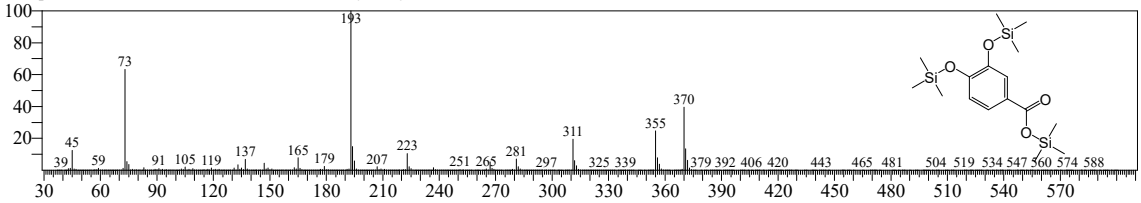
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



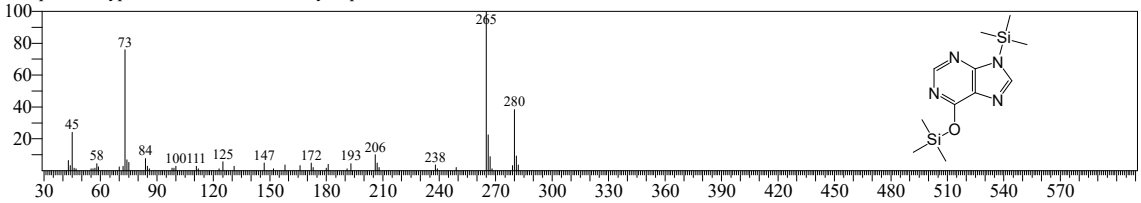
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



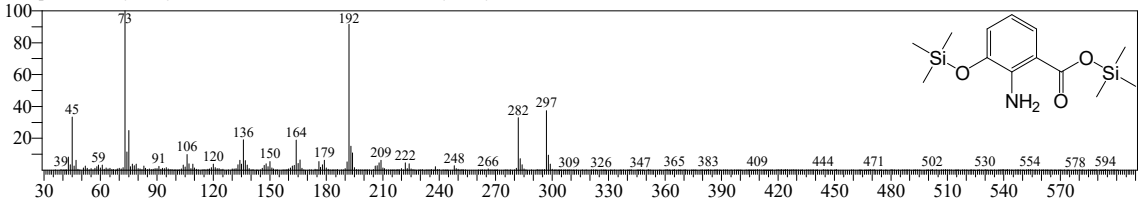
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

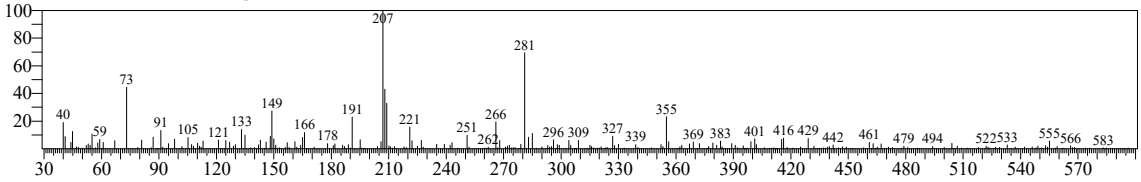


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

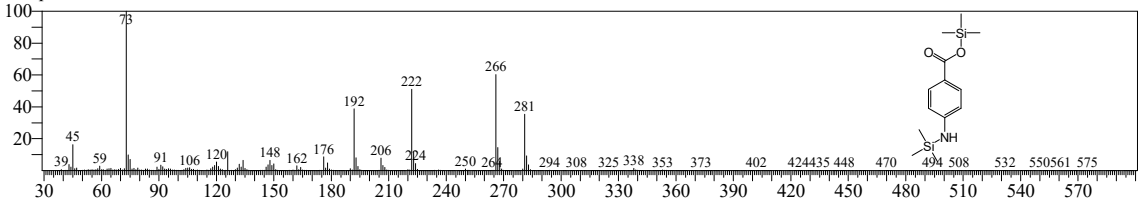


TNAU

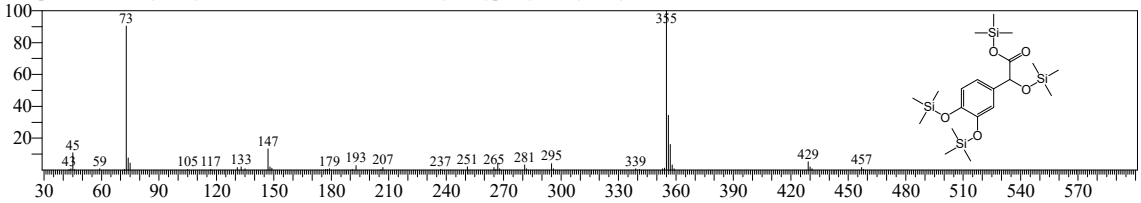
<< Target >>
Line#:10 R.Time:28.710(Scan#:4843) MassPeaks:258
RawMode:Averaged 28.705-28.715(4842-4844) BasePeak:207.05(1807)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



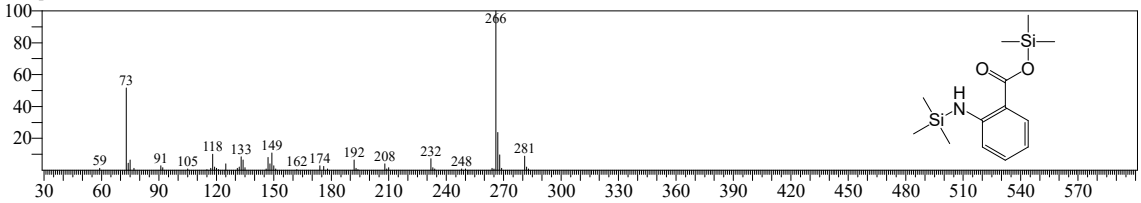
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



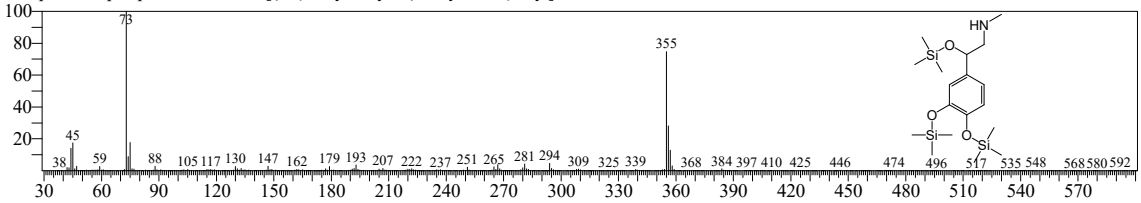
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



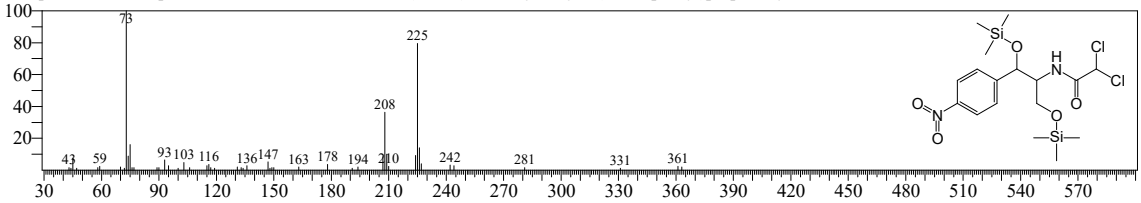
Hit#:3 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



Hit#:4 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

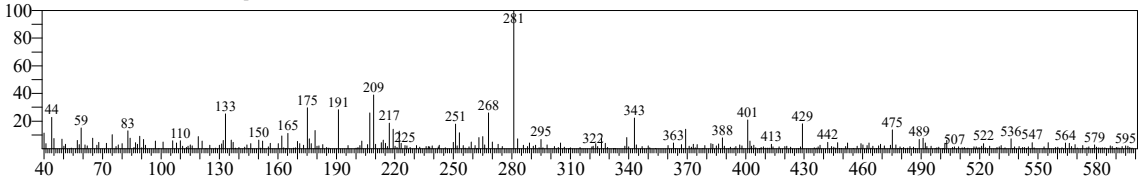


Hit#:5 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

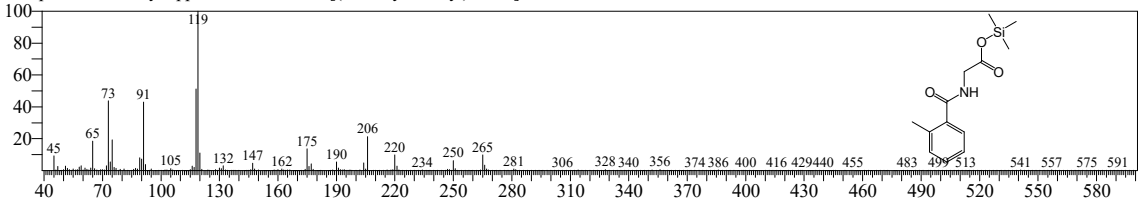


TNAU

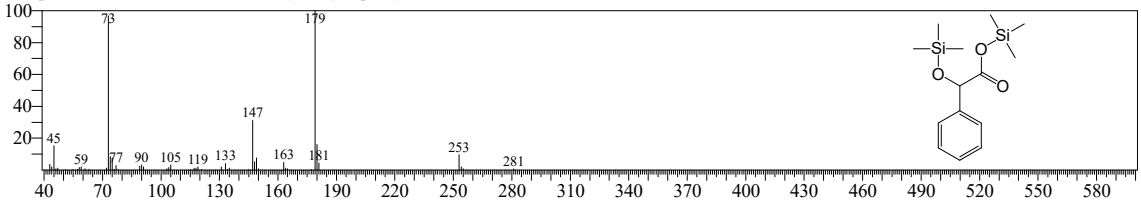
<< Target >>
Line#:11 R.Time:29.560(Scan#:5013) MassPeaks:318
RawMode:Averaged 29.555-29.565(5012-5014) BasePeak:281.05(1483)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



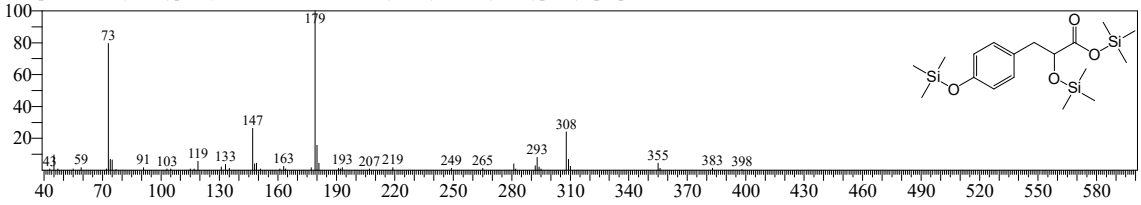
Hit#:1 Entry:365 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H19NO3Si CAS:42013-20-7 MolWeight:265 RetIndex:1898
CompName:2-Methylhippuric acid-TMS ; 2-[(2-methylbenzoyl)amino]acetic acid



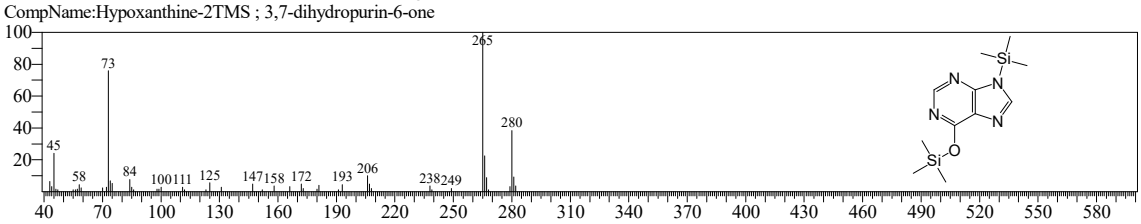
Hit#:2 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



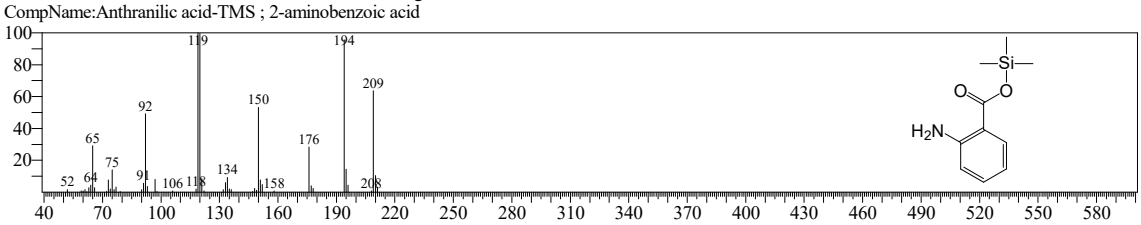
Hit#:3 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:4 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

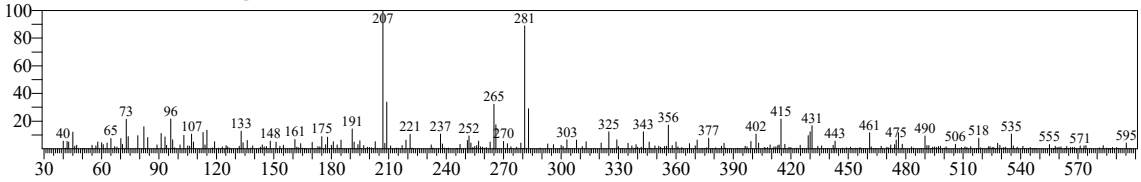


Hit#:5 Entry:142 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C10H15NO2Si CAS:118-92-3 MolWeight:209 RetIndex:1495
CompName:Anthranilic acid-TMS ; 2-aminobenzoic acid

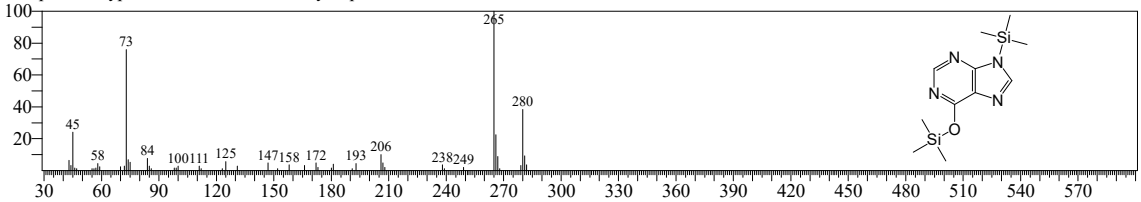


TNAU

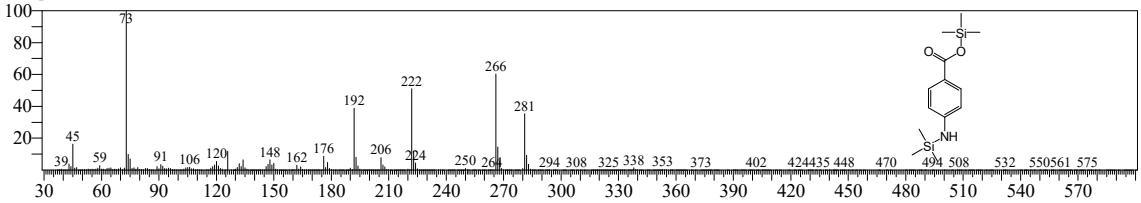
<< Target >>
Line#:12 R.Time:31.065(Scan#:5314) MassPeaks:288
RawMode:Averaged 31.060-31.070(5313-5315) BasePeak:207.05(1473)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



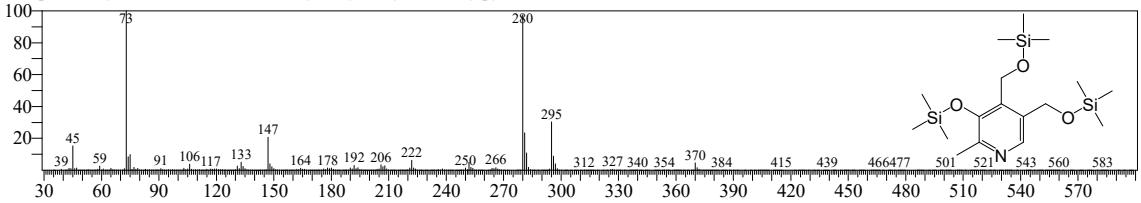
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



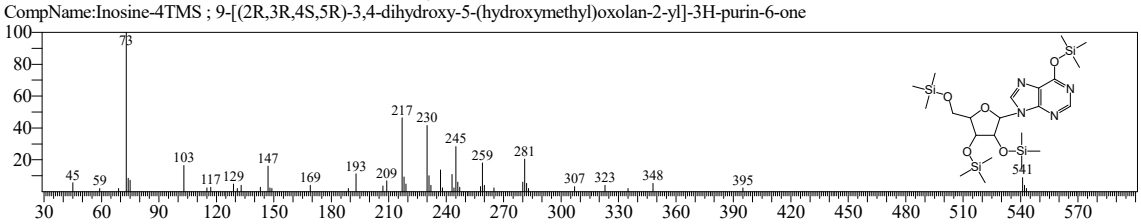
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



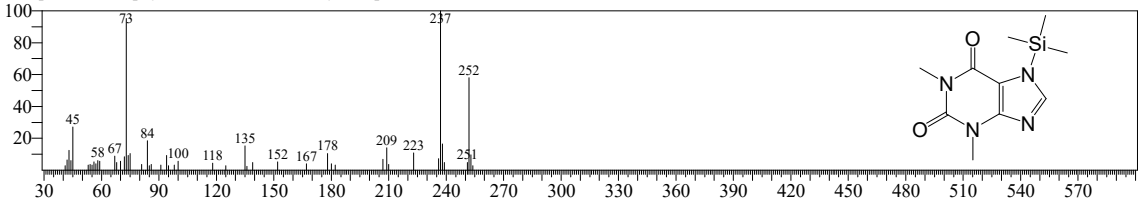
Hit#:3 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



Hit#:4 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:31 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

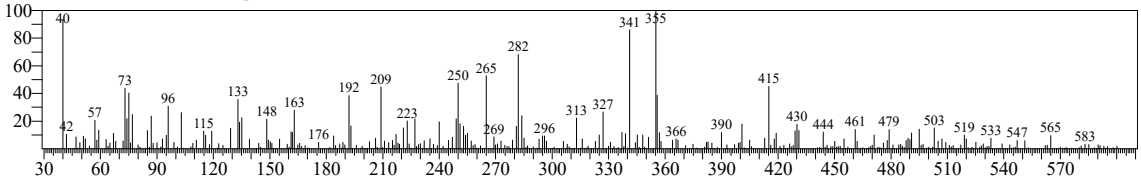


Hit#:5 Entry:395 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C10H16N4O2Si CAS:58-55-9 MolWeight:252 RetIndex:1936
CompName:Theophylline-TMS ; 1,3-dimethyl-7H-purine-2,6-dione

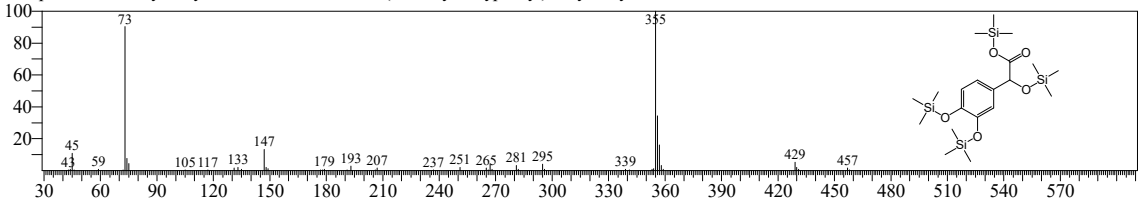


TNAU

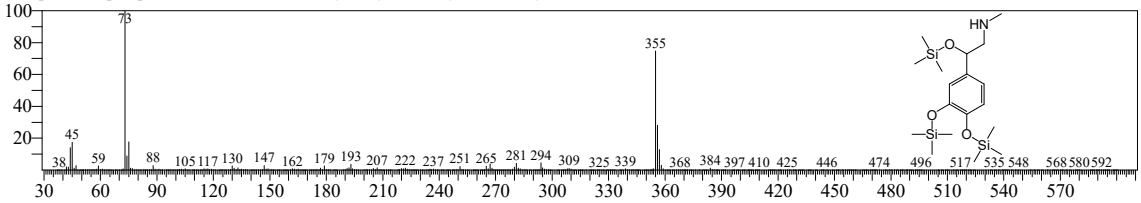
<< Target >>
Line#:13 R.Time:31.595(Scan#:5420) MassPeaks:308
RawMode:Averaged 31.590-31.600(5419-5421) BasePeak:355.10(727)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



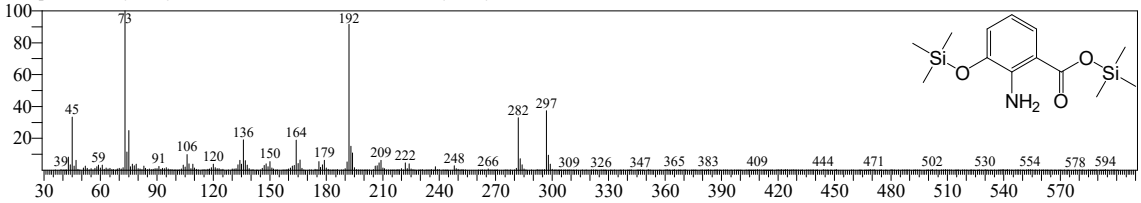
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



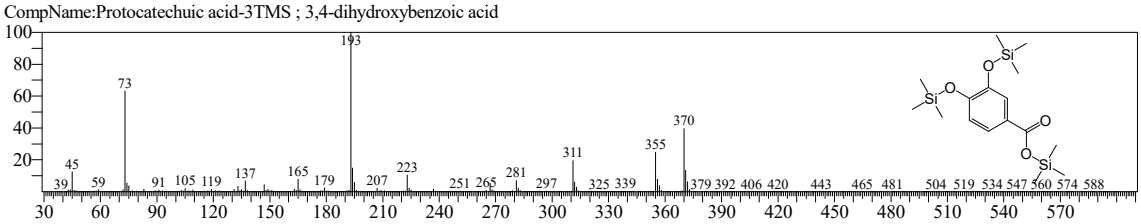
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



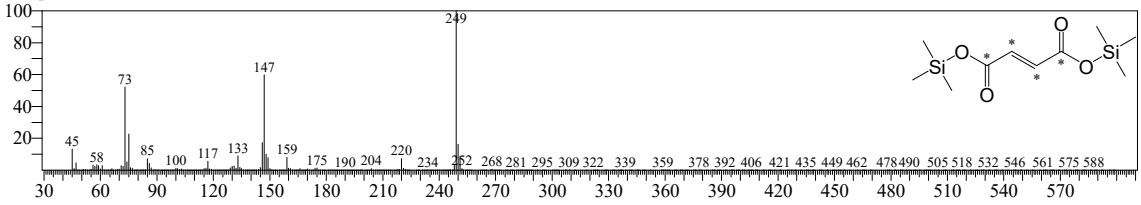
Hit#:3 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

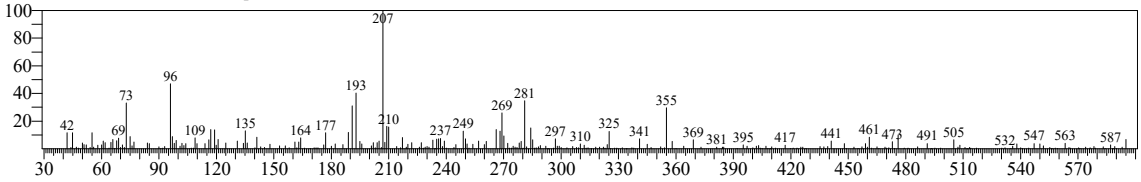


Hit#:5 Entry:100 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula: CAS:0-00-0 MolWeight:264 RetIndex:1346
CompName:Fumaric acid-13C4-2TMS ;

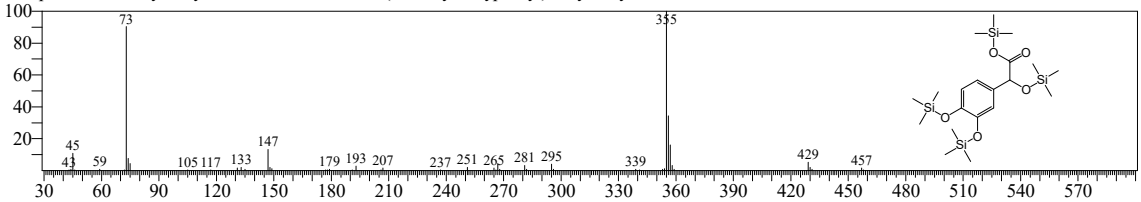


TNAU

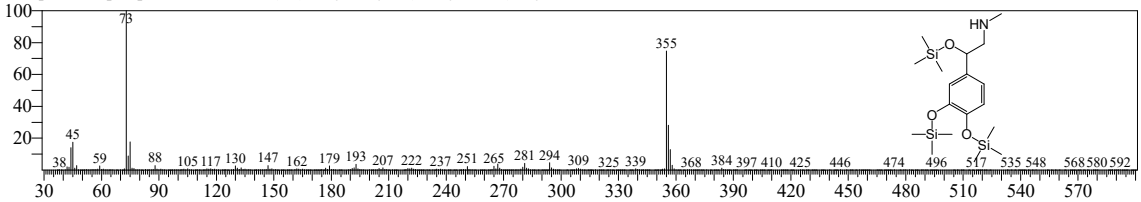
<< Target >>
Line#:14 R.Time:31.785(Scan#:5458) MassPeaks:276
RawMode:Averaged 31.780-31.790(5457-5459) BasePeak:207.05(1439)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



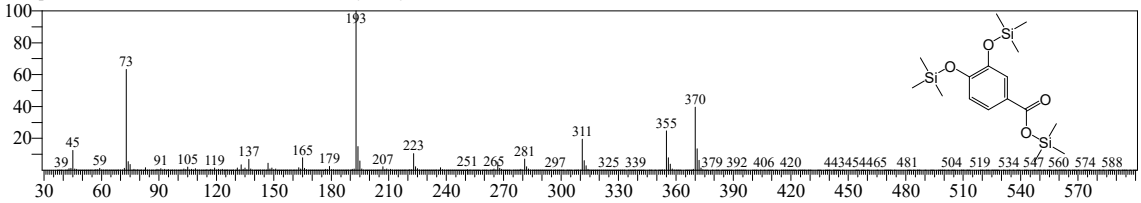
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



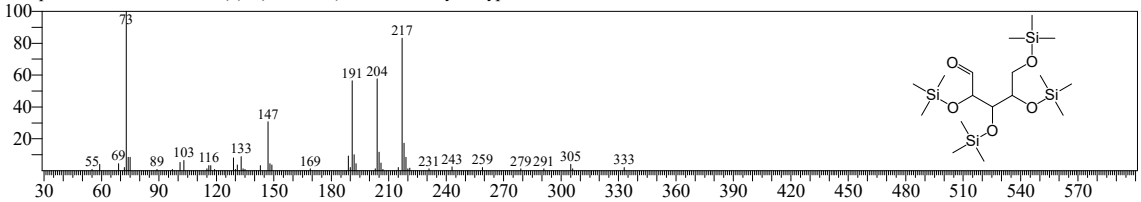
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



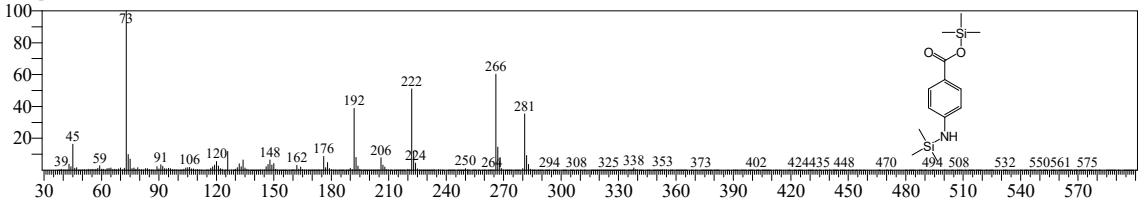
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

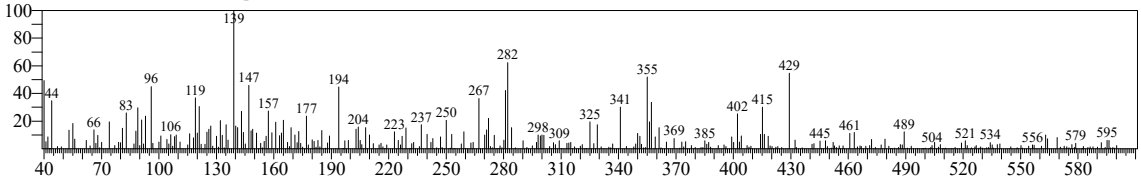


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

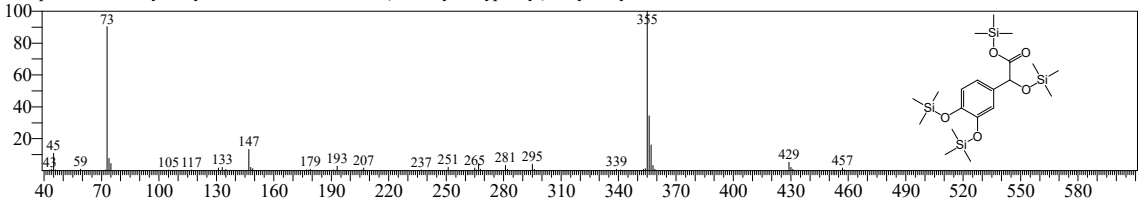


TNAU

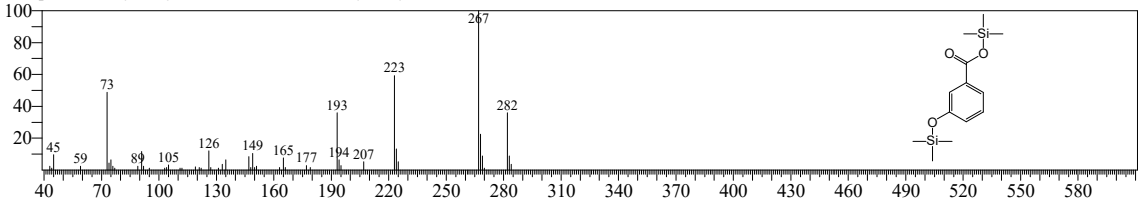
<< Target >>
Line#:15 R.Time:31.905(Scan#:5482) MassPeaks:331
RawMode:Averaged 31.900-31.910(5481-5483) BasePeak:139.10(1014)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



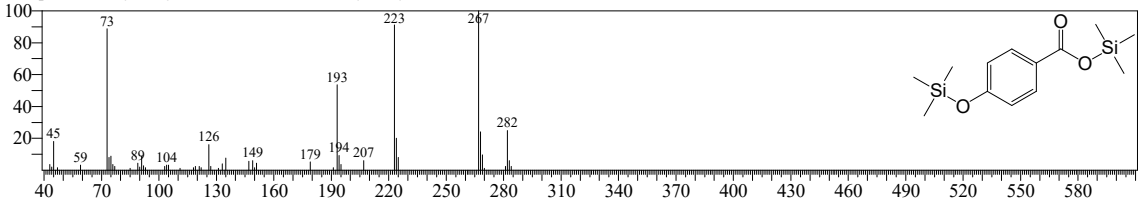
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



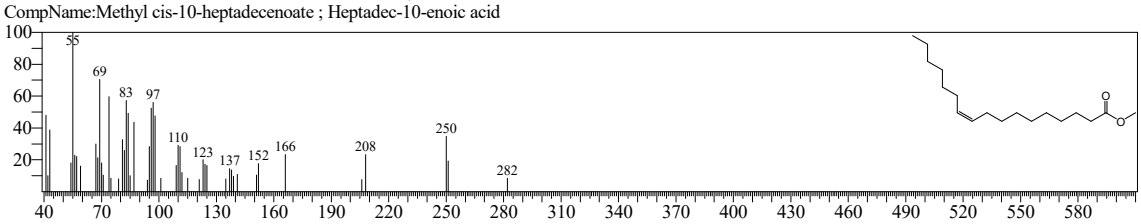
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



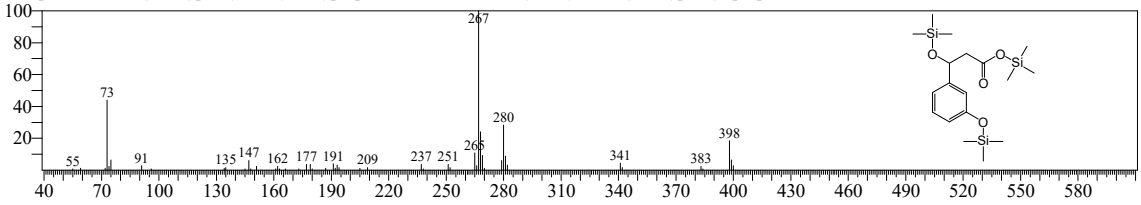
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:23 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

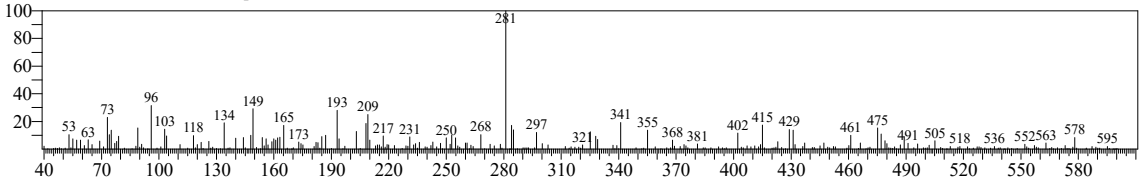


Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

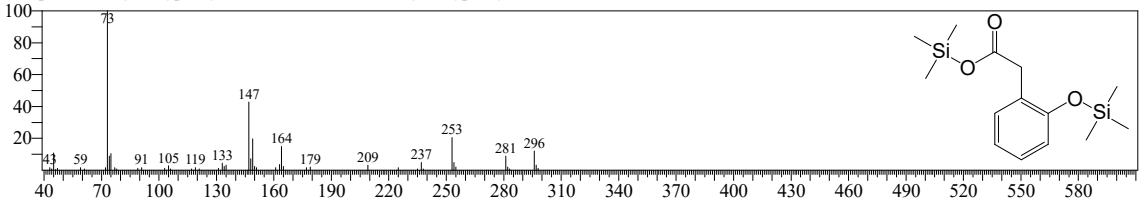


TNAU

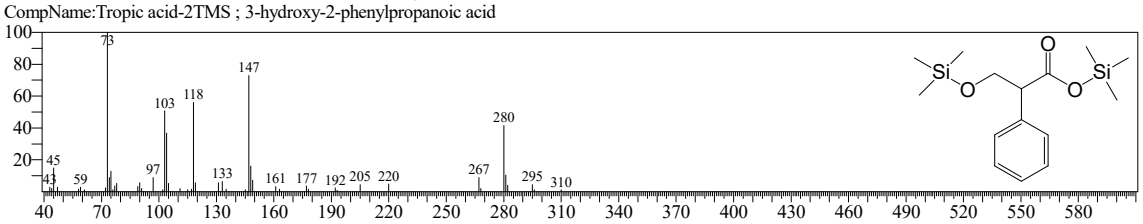
<< Target >>
Line#:16 R.Time:31.935(Scan#:5488) MassPeaks:287
RawMode:Averaged 31.930-31.940(5487-5489) BasePeak:281.05(1175)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



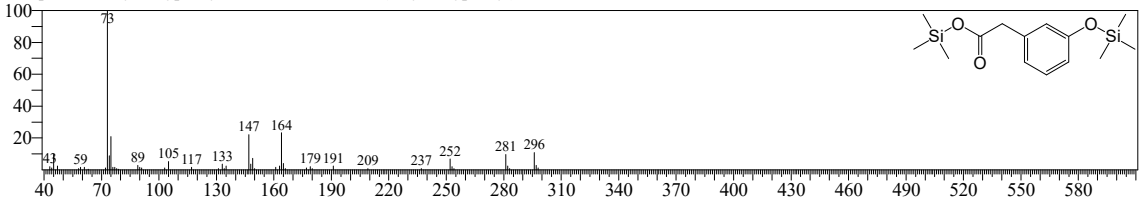
Hit#:1 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



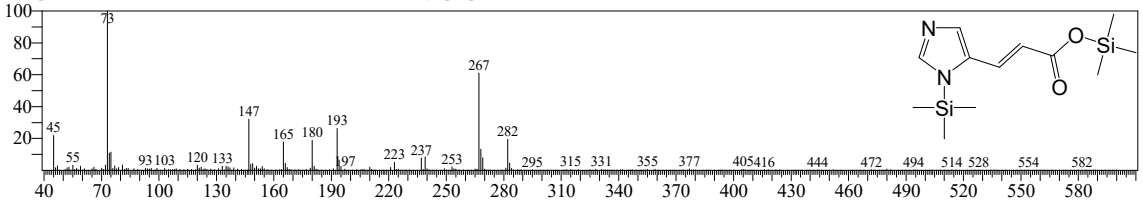
Hit#:2 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid



Hit#:3 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid



Hit#:4 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:5 Entry: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