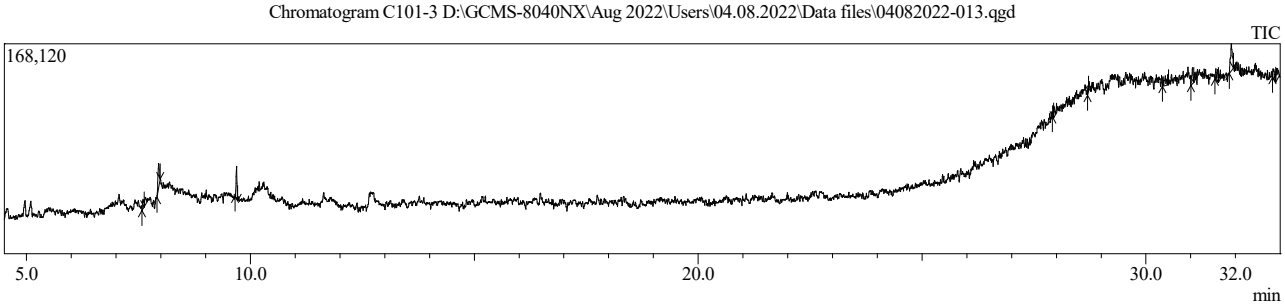
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 12:42:45 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C101-3
Sample ID	: C101-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 13
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-013.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-013.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 4:29:58 PM

Chromatogram C101-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-013.qgd



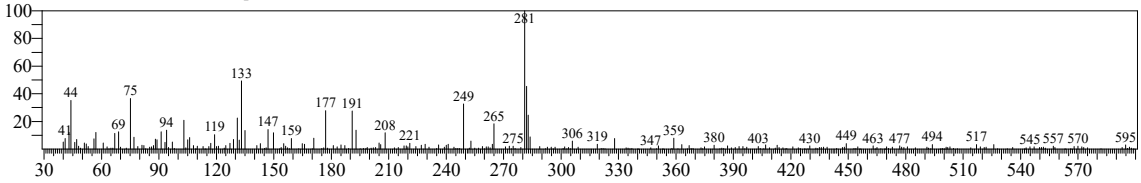
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.590	15409	5.61	6584	5.24	2.34	41	Batyl alcohol-2TMS
2	7.950	41151	14.99	19315	15.36	2.13	83	Undecane
3	9.690	37196	13.55	25742	20.47	1.44	88	Undecane
4	27.923	7419	2.70	9615	7.65	0.77	41	Epinephrine-3TMS
5	28.705	5338	1.95	5605	4.46	0.95	40	Chloramphenicol-2TMS
6	30.489	34607	12.61	8525	6.78	4.06	30	Stearic acid-TMS
7	31.041	25962	9.46	13017	10.35	1.99	41	Batyl alcohol-2TMS
8	31.562	23725	8.64	8898	7.08	2.67	34	3-Hydroxybenzoic acid-2TMS
9	31.907	63116	23.00	21713	17.27	2.91	37	Inosine-4TMS
10	32.835	20518	7.48	6728	5.35	3.05	28	Tyrosine-3TMS
		274441	100.00	125742	100.00			

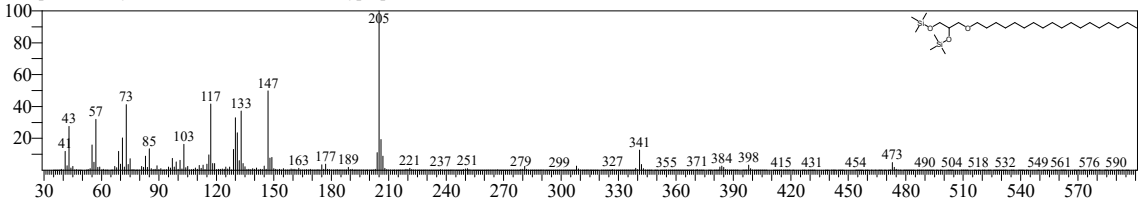
Library

TNAU

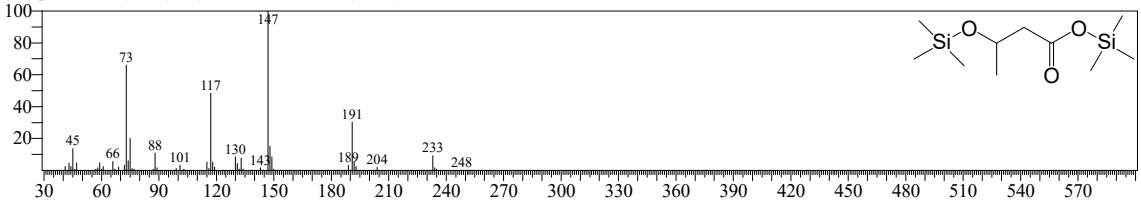
<< Target >>
Line#:1 R.Time:7.590(Scan#:619) MassPeaks:279
RawMode:Averaged 7.585-7.595(618-620) BasePeak:281.00(959)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



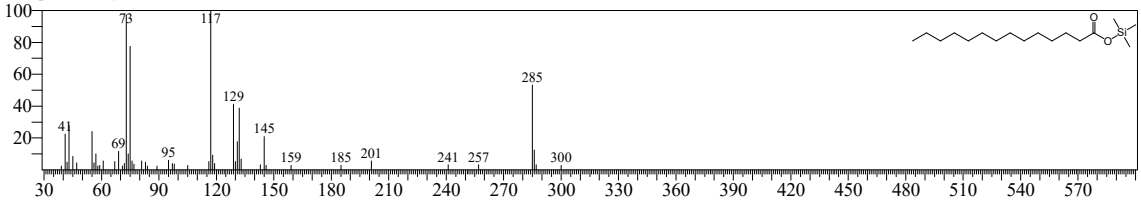
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



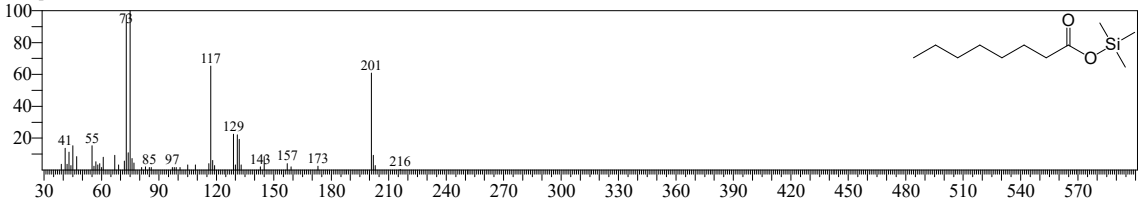
Hit#:2 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid



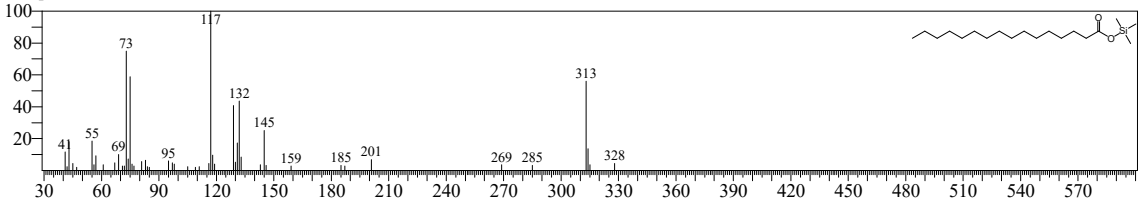
Hit#:3 Entry:331 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C17H36O2Si CAS:544-63-8 MolWeight:300 RetIndex:1850
CompName:Myristic acid-TMS ; tetradecanoic acid



Hit#:4 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
CompName:Octanoic acid-TMS ; octanoic acid

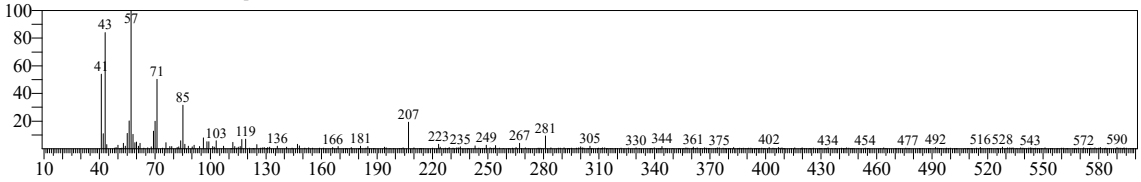


Hit#:5 Entry:446 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C19H40O2Si CAS:57-10-3 MolWeight:328 RetIndex:2046
CompName:Palmitic acid-TMS ; hexadecanoic acid

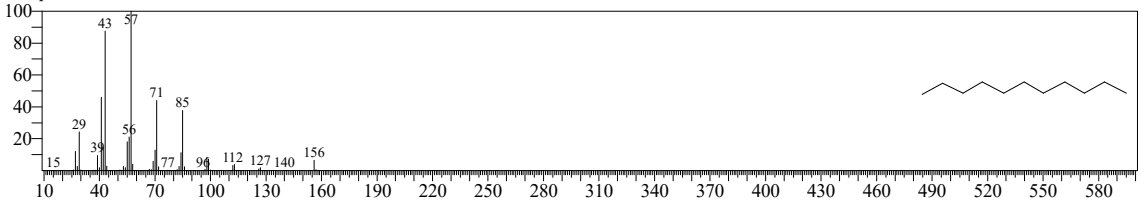


TNAU

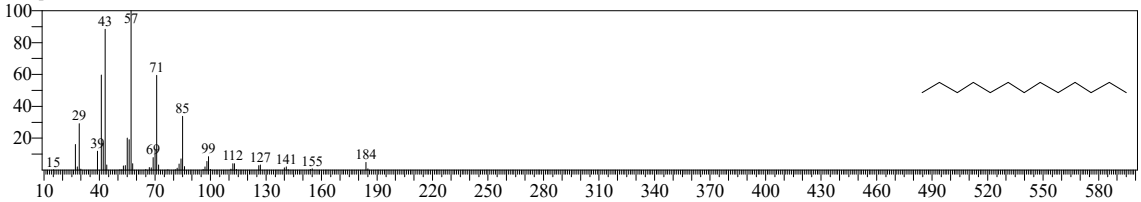
<< Target >>
Line#:2 R.Time:7.950(Scan#:691) MassPeaks:320
RawMode:Averaged 7.945-7.955(690-692) BasePeak:57.10(3539)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



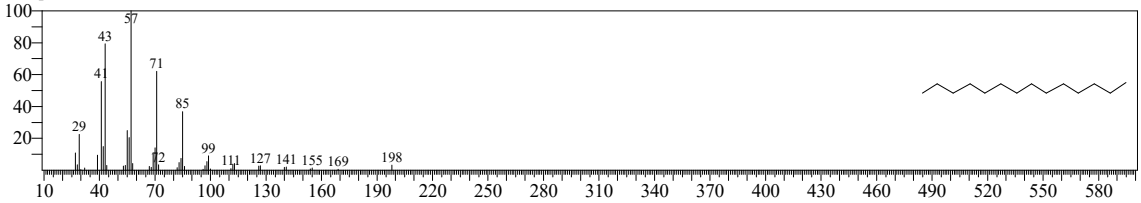
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:83 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



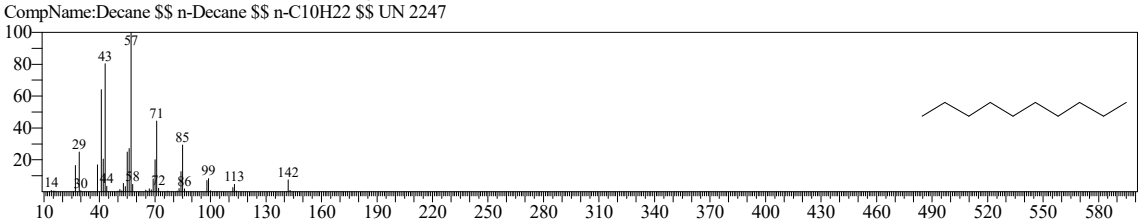
Hit#:2 Entry:19411 Library:NIST20R.lib
SI:83 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



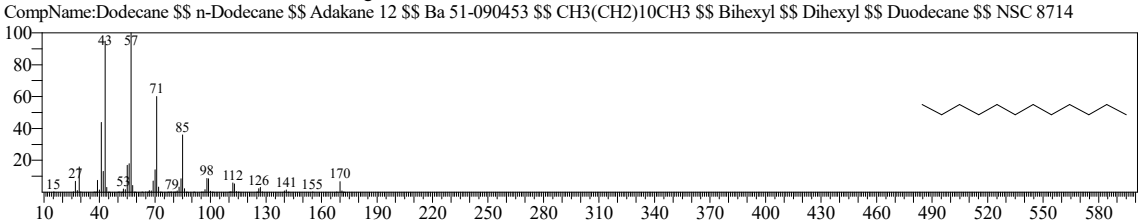
Hit#:3 Entry:22498 Library:NIST20R.lib
SI:83 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane



Hit#:4 Entry:13604 Library:NIST20M1.lib
SI:82 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

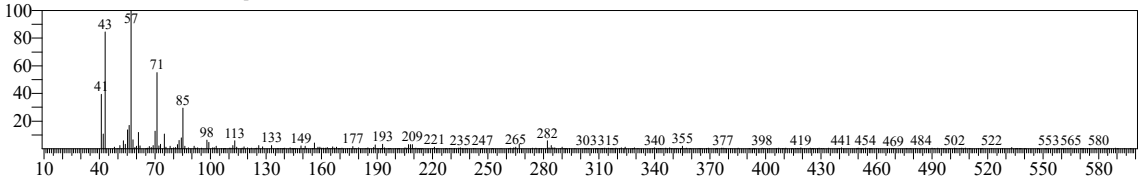


Hit#:5 Entry:16191 Library:NIST20R.lib
SI:82 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

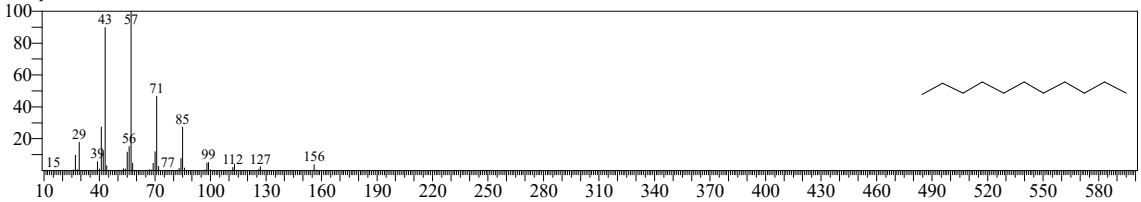


TNAU

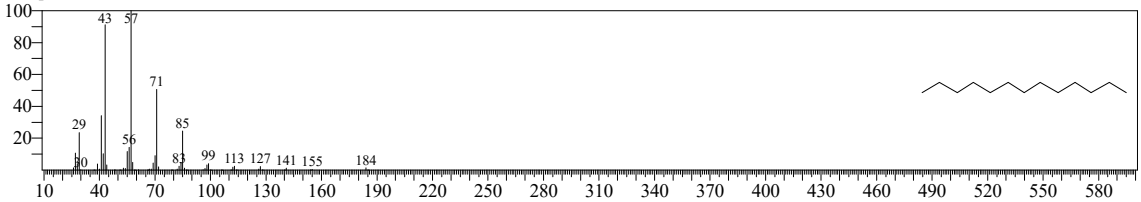
<< Target >>
Line#:3 R.Time:9.690(Scan#:1039) MassPeaks:294
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(4873)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



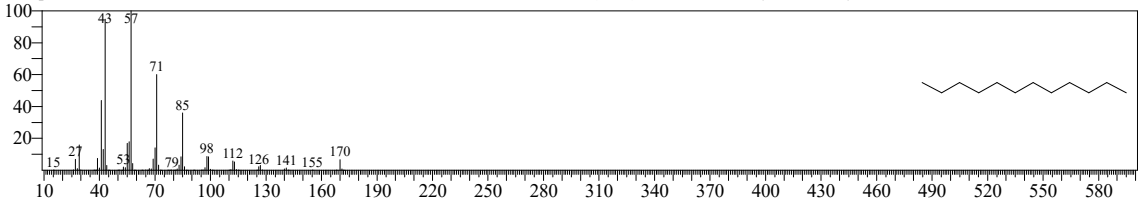
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



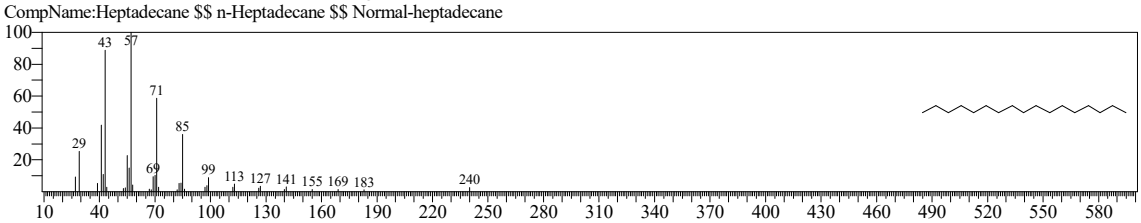
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



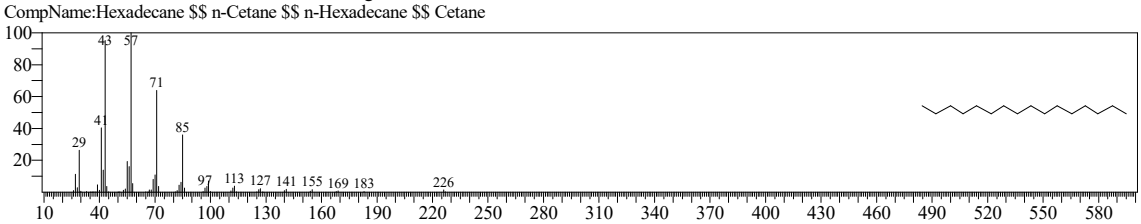
Hit#:3 Entry:16191 Library:NIST20R.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:29663 Library:NIST20R.lib
SI:86 Formula:C17H36 CAS:629-78-7 MolWeight:240 RetIndex:1700
CompName:Heptadecane $$ n-Heptadecane $$ Normal-heptadecane

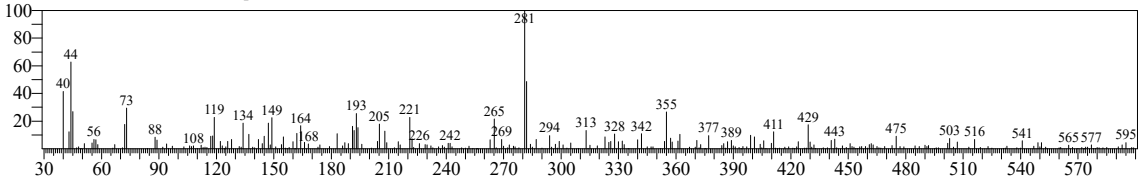


Hit#:5 Entry:27736 Library:NIST20R.lib
SI:86 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

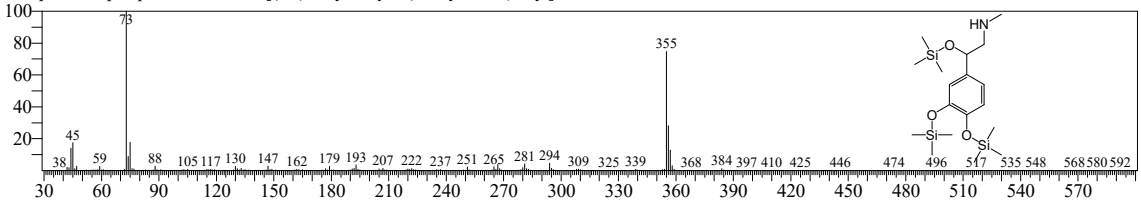


TNAU

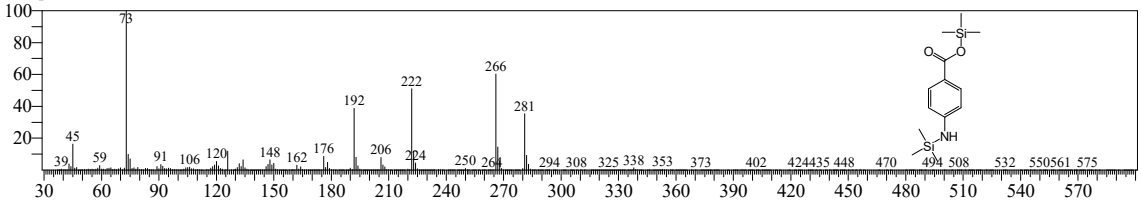
<< Target >>
Line#:4 R.Time:27.925(Scan#:4686) MassPeaks:274
RawMode:Averaged 27.920-27.930(4685-4687) BasePeak:281.05(1162)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



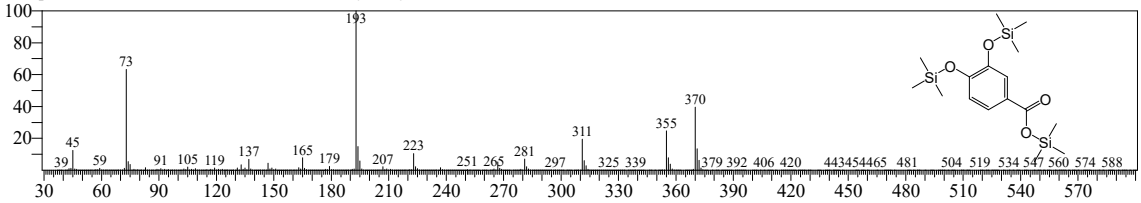
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



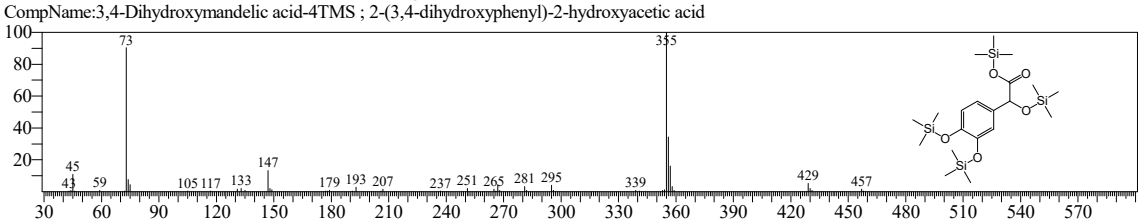
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



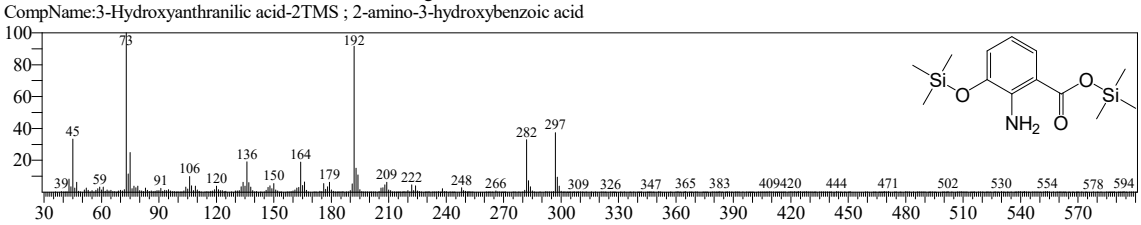
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



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

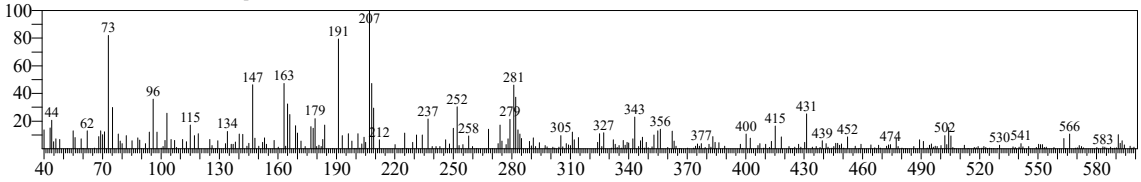


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

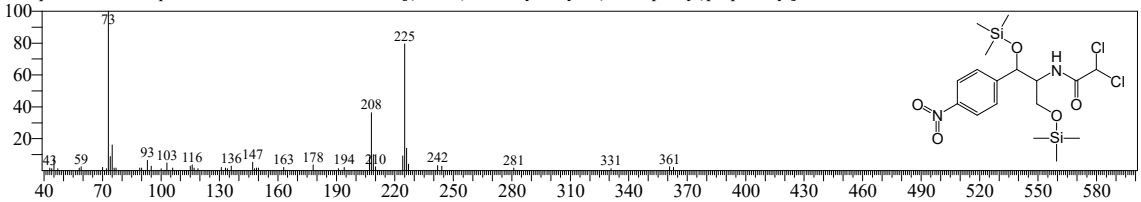


TNAU

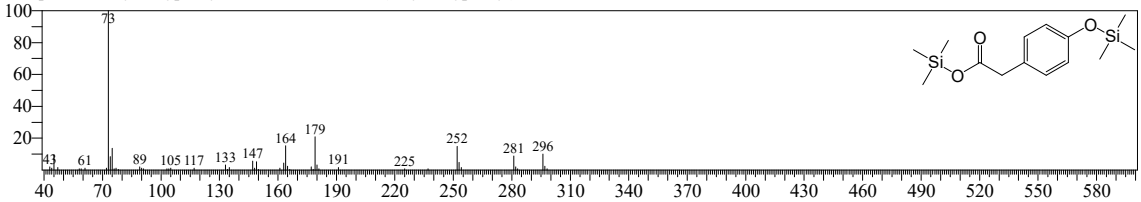
<< Target >>
Line#:5 R.Time:28.705(Scan#:4842) MassPeaks:307
RawMode:Averaged 28.700-28.710(4841-4843) BasePeak:207.00(721)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



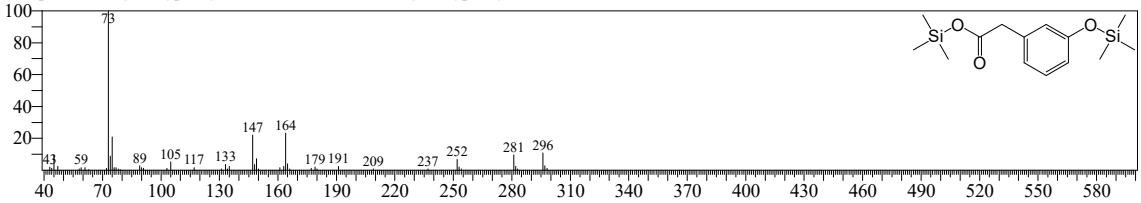
Hit#:1 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



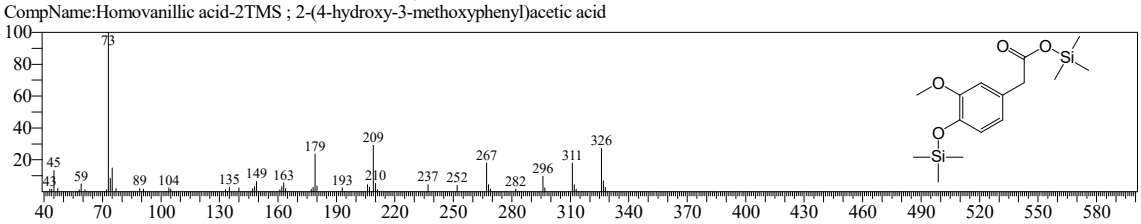
Hit#:2 Entry:220 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C14H24O3Si2 CAS:156-38-7 MolWeight:296 RetIndex:1647
CompName:4-Hydroxyphenylacetic acid-2TMS ; 2-(4-hydroxyphenyl)acetic acid



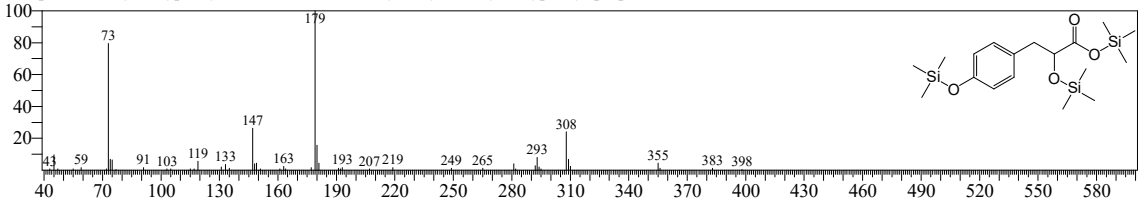
Hit#:3 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid



Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

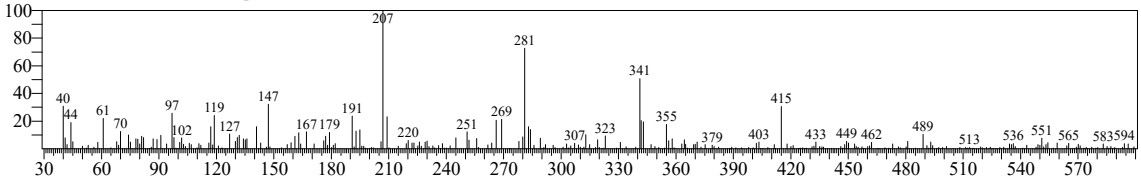


Hit#:5 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

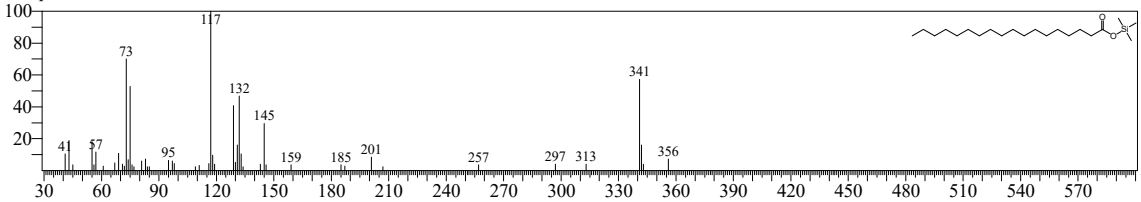


TNAU

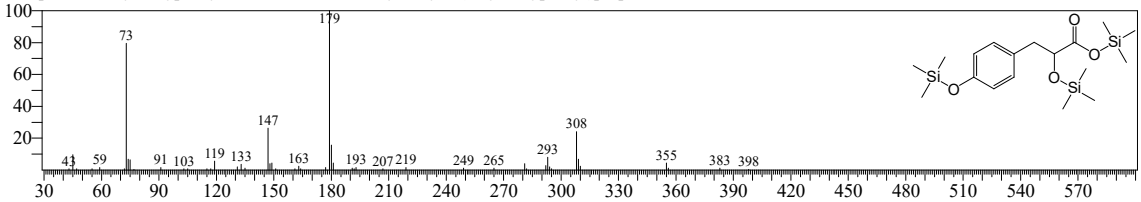
<< Target >>
Line#:6 R.Time:30.490(Scan#:5199) MassPeaks:283
RawMode:Averaged 30.485-30.495(5198-5200) BasePeak:207.05(1579)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



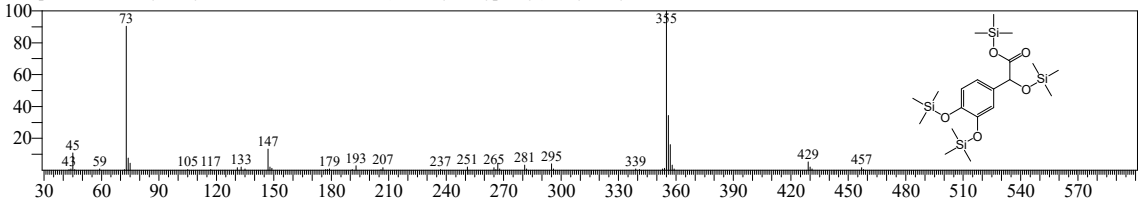
Hit#:1 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



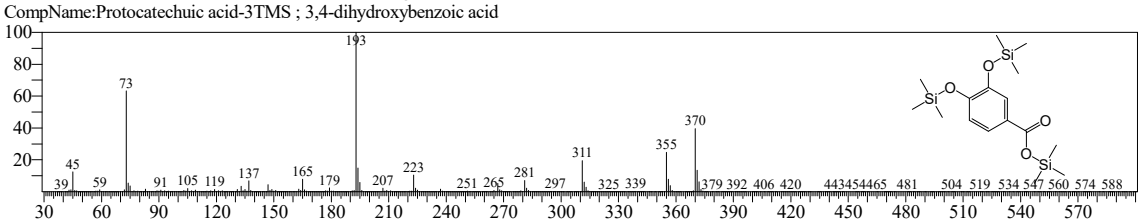
Hit#:2 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



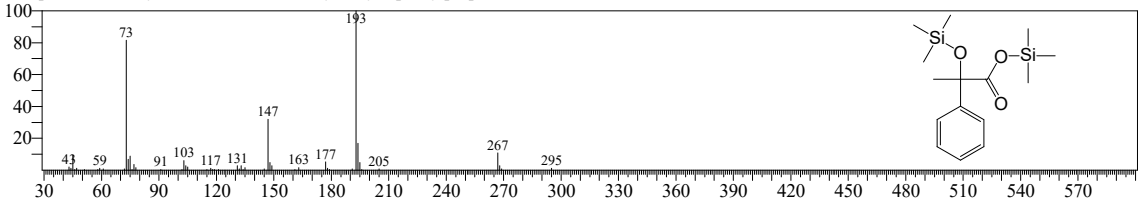
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



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

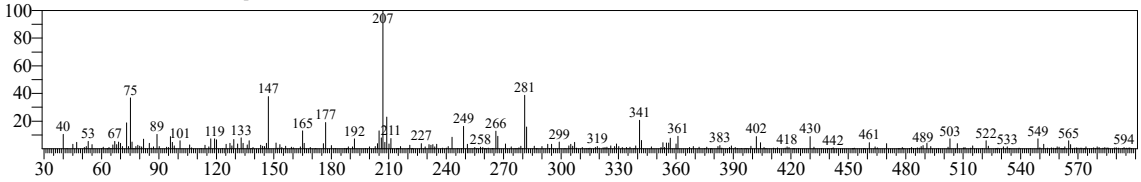


Hit#:5 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

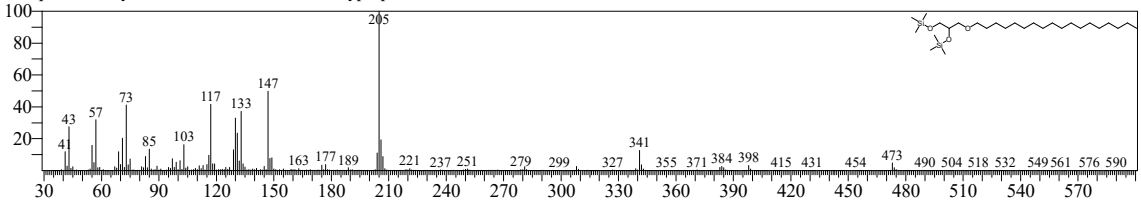


TNAU

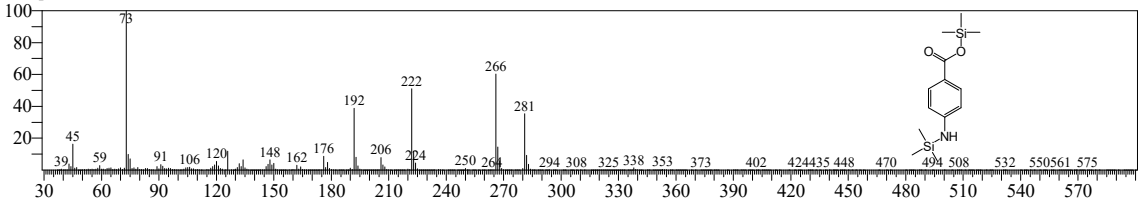
<< Target >>
Line#:7 R.Time:31.040(Scan#:5309) MassPeaks:293
RawMode:Averaged 31.035-31.045(5308-5310) BasePeak:207.05(2620)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



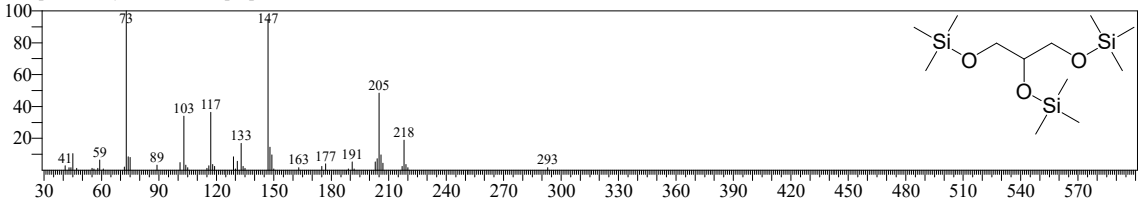
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



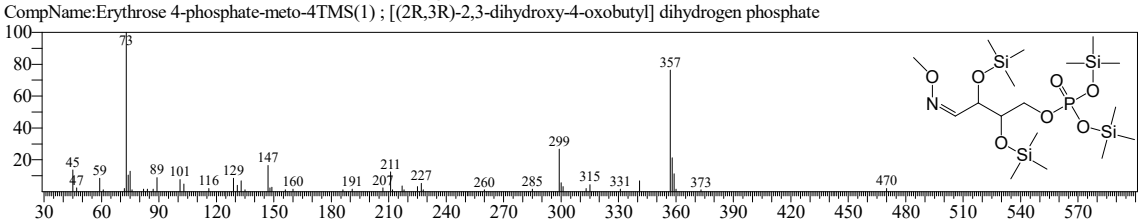
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



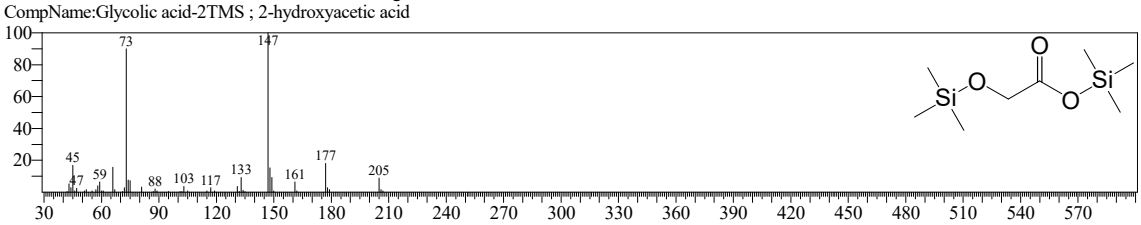
Hit#:3 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



Hit#:4 Entry:389 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1928
CompName:Erythrose 4-phosphate-meto-4TMS(1) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate

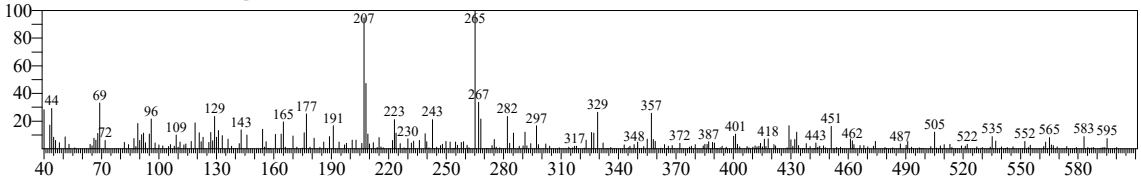


Hit#:5 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

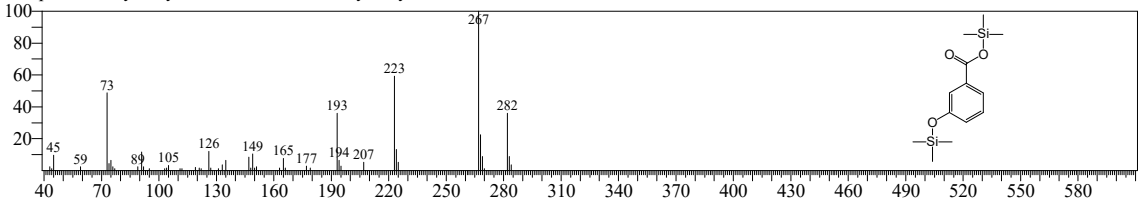


TNAU

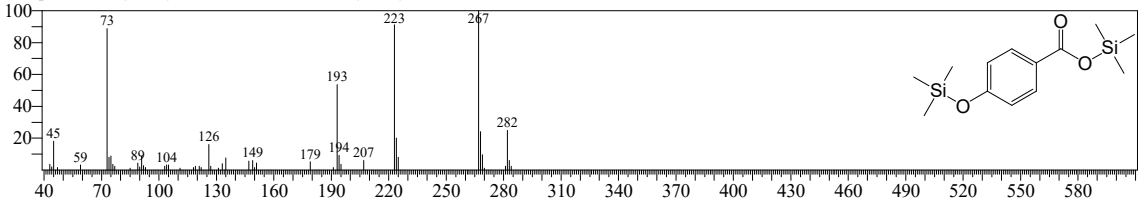
<< Target >>
Line#:8 R.Time:31.560(Scan#:5413) MassPeaks:282
RawMode:Averaged 31.555-31.565(5412-5414) BasePeak:265.05(1196)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



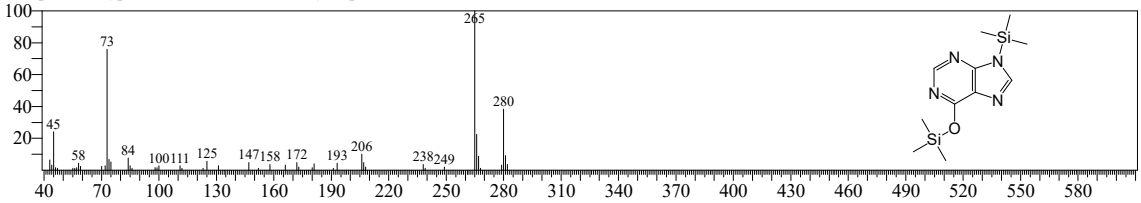
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



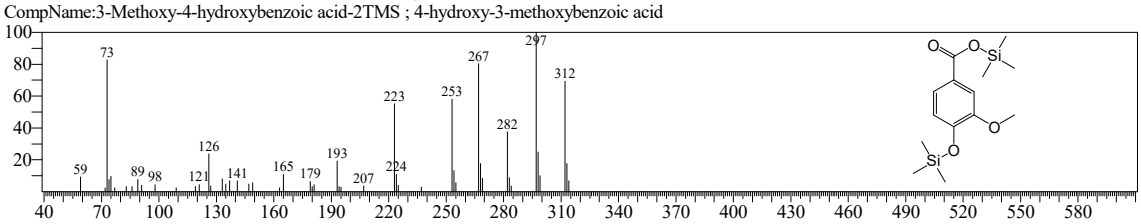
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



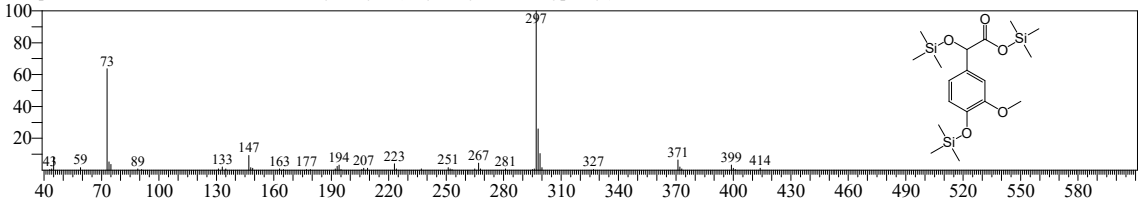
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



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

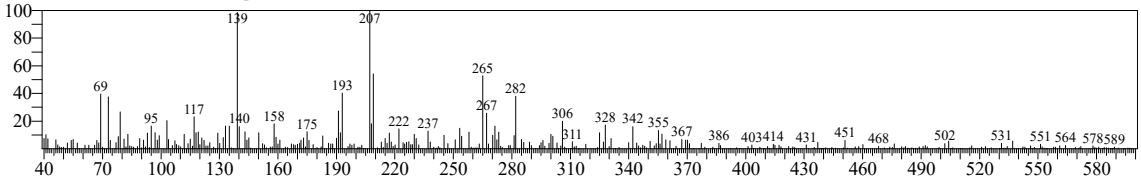


Hit#:5 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

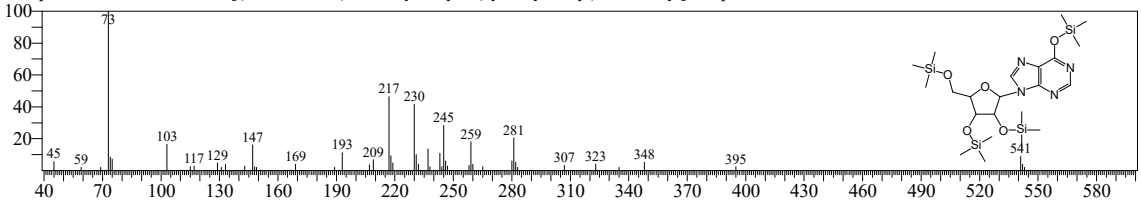


TNAU

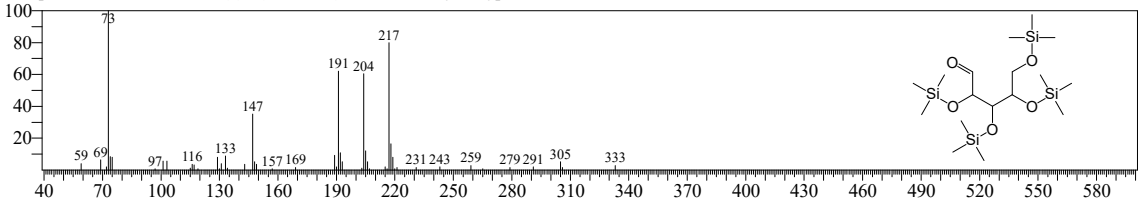
<< Target >>
Line#:9 R.Time:31.905(Scan#:5482) MassPeaks:330
RawMode:Averaged 31.900-31.910(5481-5483) BasePeak:207.05(1669)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



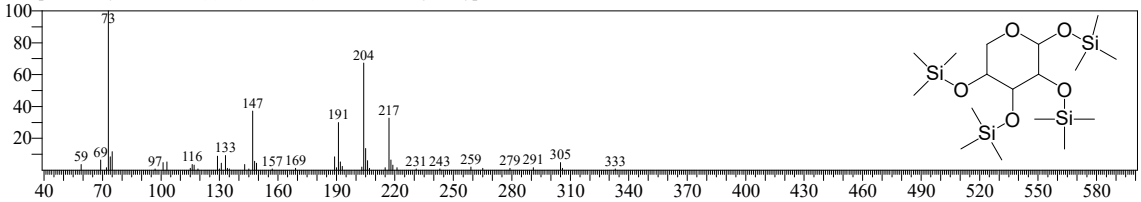
Hit#:1 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



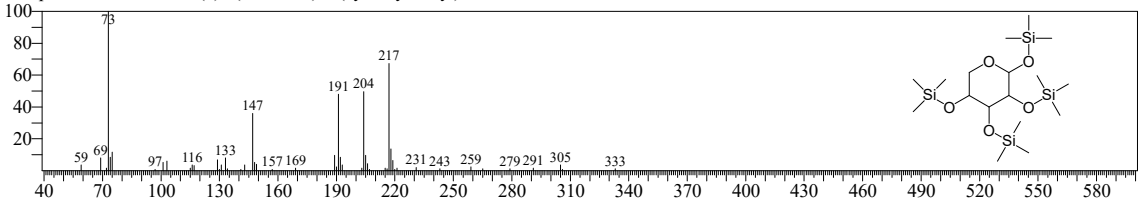
Hit#:2 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



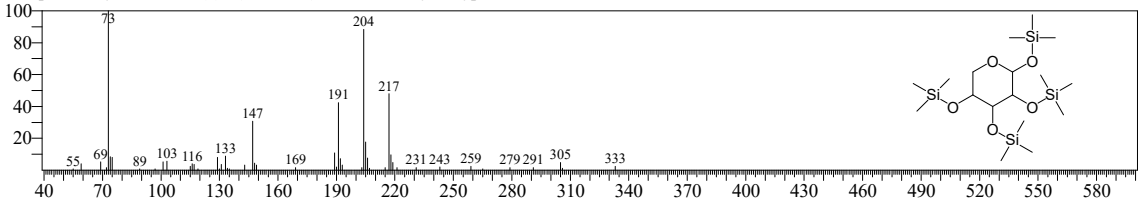
Hit#:3 Entry:267 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

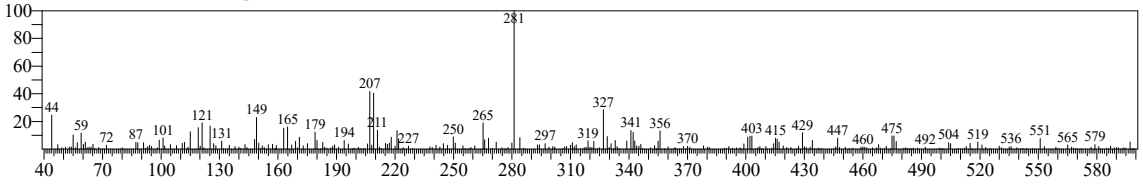


Hit#:5 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

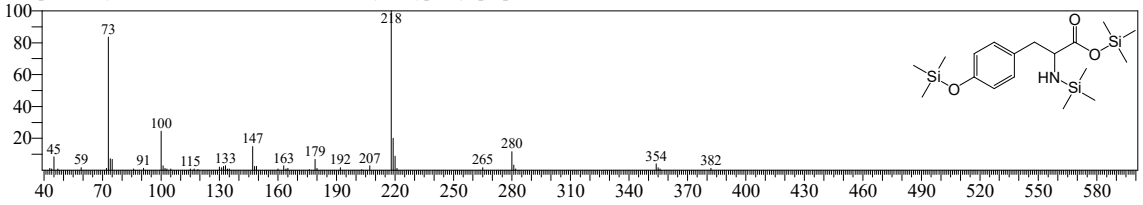


TNAU

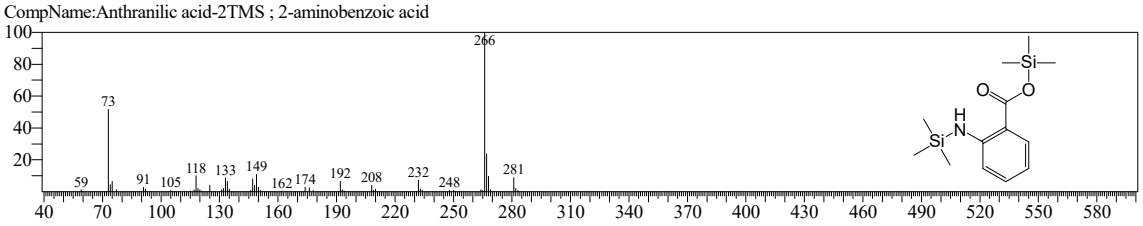
<< Target >>
Line#:10 R.Time:32.835(Scan#:5668) MassPeaks:299
RawMode:Averaged 32.830-32.840(5667-5669) BasePeak:281.05(1612)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



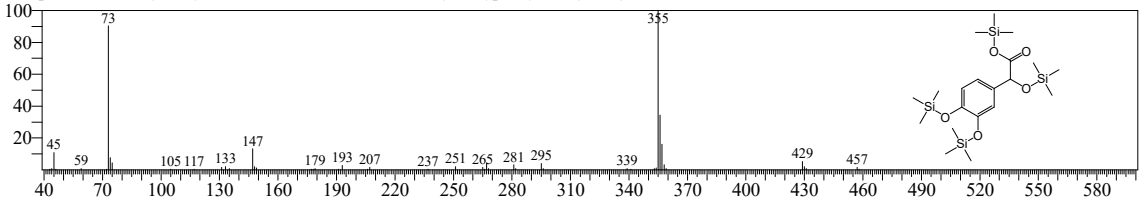
Hit#:1 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid



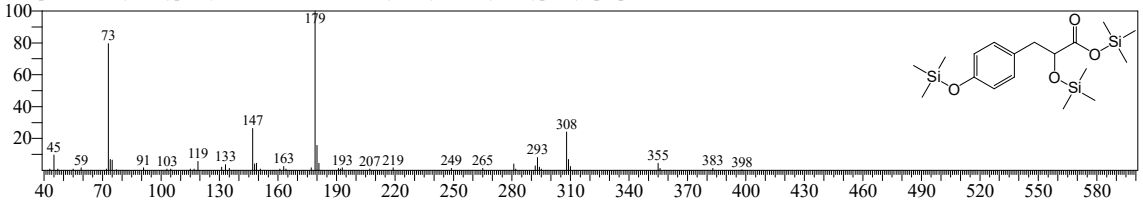
Hit#:2 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



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



Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:5 Entry:463 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C21H43NO4Si4 CAS:59-92-7 MolWeight:485 RetIndex:2123
CompName:Dopa-4TMS ; (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid