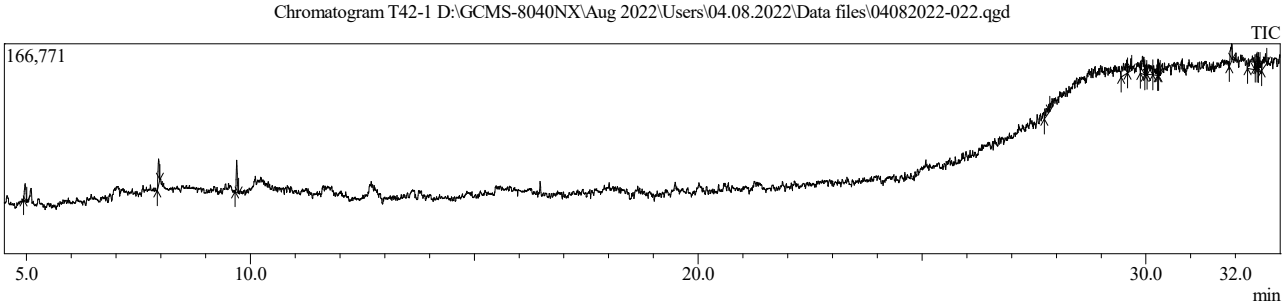
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 6:32:15 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T42-1
Sample ID	: T42-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 21
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-022.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-022.qgd
Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Org Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Report File	:
Tuning File	: D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 04082022.qgt
[Comment]	
Jerry samples	
Modified by	: Admin
Modified	: 05-Aug-22 4:42:00 PM

Chromatogram T42-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-022.qgd



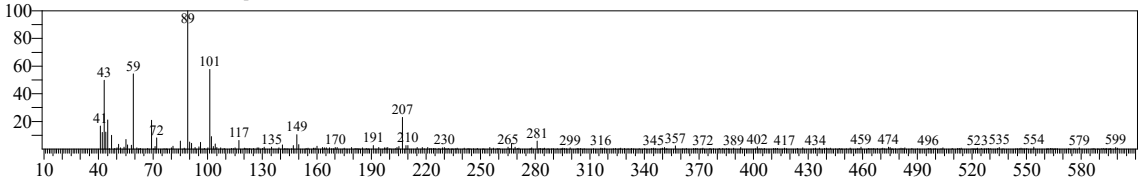
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.967	31501	5.86	13870	6.74	2.27	71	2-Propanol, 1,1'-oxybis-
2	7.948	39836	7.42	21081	10.24	1.89	86	Undecane
3	9.693	42089	7.84	25424	12.35	1.66	90	Dodecane
4	27.740	25973	4.84	6710	3.26	3.87	40	Epinephrine-3TMS
5	29.571	51833	9.65	10707	5.20	4.84	33	3,4-Dihydroxymandelic acid-4TMS
6	29.665	20962	3.90	9798	4.76	2.14	32	Hypoxanthine-2TMS
7	29.924	50923	9.48	13982	6.79	3.64	33	3,4-Dihydroxymandelic acid-4TMS
8	30.008	13511	2.52	8888	4.32	1.52	38	3,4-Dihydroxymandelic acid-4TMS
9	30.040	42415	7.90	6178	3.00	6.87	36	3,4-Dihydroxymandelic acid-4TMS
10	30.165	26813	4.99	6971	3.39	3.85	28	2-Phenyllactic acid-2TMS
11	30.272	14489	2.70	12842	6.24	1.13	34	Anthranilic acid-2TMS
12	30.305	11412	2.12	8774	4.26	1.30	41	Rhamnose-4TMS(2)
13	31.910	36567	6.81	13965	6.78	2.62	29	Glyceraldehyde 3-phosphate-meto-3TMS(2)
14	32.379	60150	11.20	10603	5.15	5.67	33	2-Deoxy-glucose-4TMS(1)
15	32.460	16795	3.13	10346	5.03	1.62	41	Epinephrine-3TMS
16	32.498	9067	1.69	8851	4.30	1.02	45	4-Hydroxybenzoic acid-2TMS
17	32.530	8207	1.53	7995	3.88	1.03	37	Anthranilic acid-2TMS
18	32.670	34566	6.44	8874	4.31	3.90	28	4-Hydroxybutyric acid-2TMS
		537109	100.00	205859	100.00			

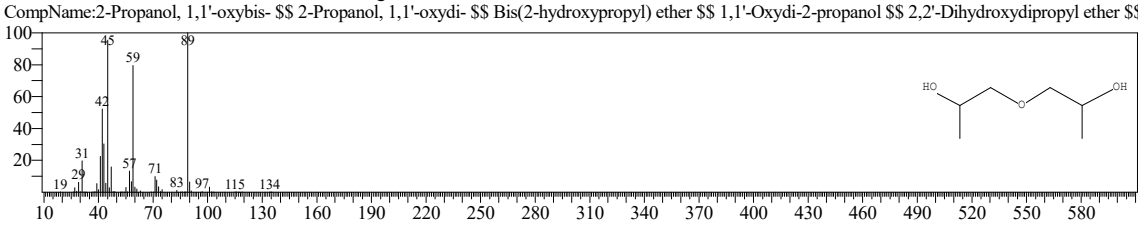
Library

TNAU

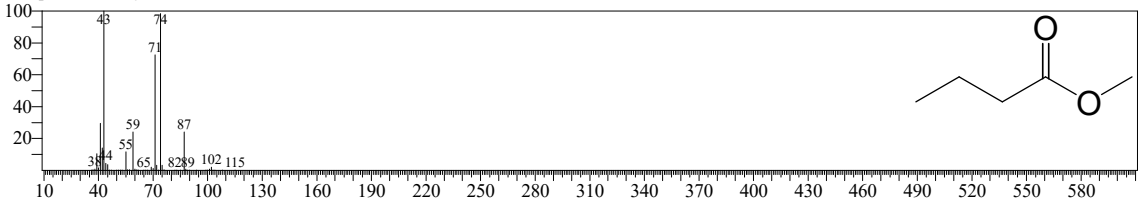
<< Target >>
Line#:1 R.Time:4.965(Scan#:94) MassPeaks:286
RawMode:Averaged 4.960-4.970(93-95) BasePeak:89.05(2793)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



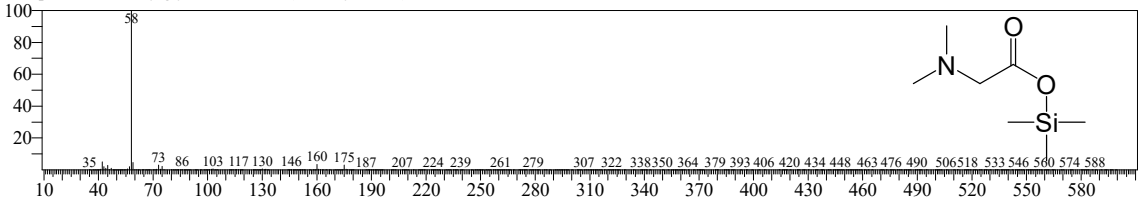
Hit#:1 Entry:7425 Library:NIST20R.lib
SI:71 Formula:C6H14O3 CAS:110-98-5 MolWeight:134 RetIndex:1018
CompName:2-Propanol, 1,1'-oxybis- $$ 2-Propanol, 1,1'-oxydi- $$ Bis(2-hydroxypropyl) ether $$ 1,1'-Oxydi-2-propanol $$ 2,2'-Dihydroxydipropyl ether $$



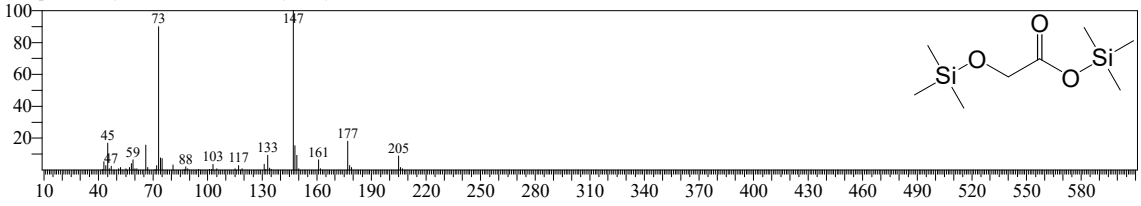
Hit#:2 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



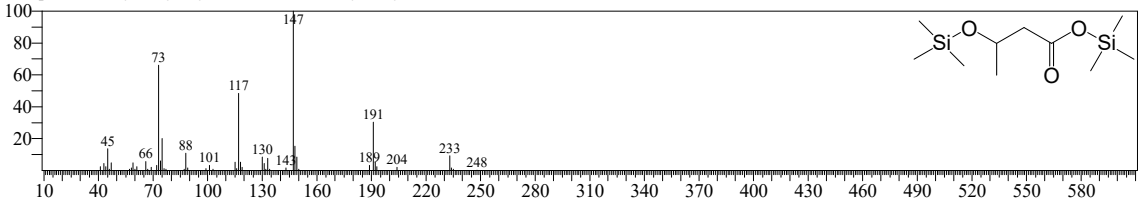
Hit#:3 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



Hit#:4 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

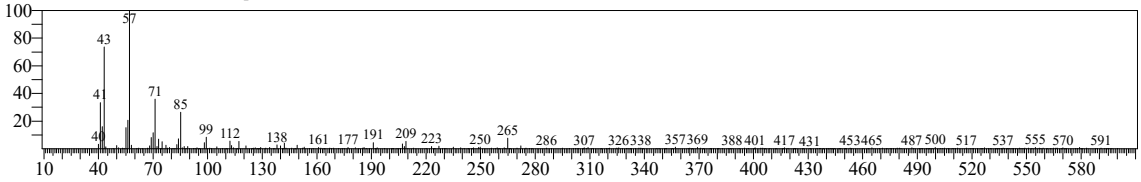


Hit#:5 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid

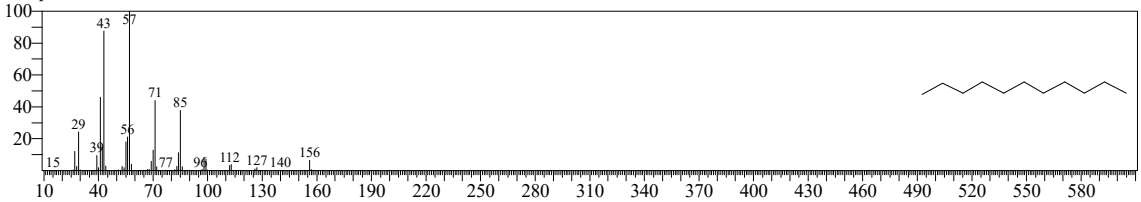


TNAU

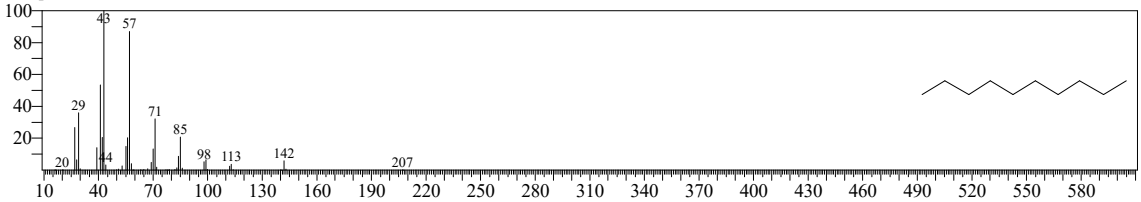
<< Target >>
Line#:2 R.Time:7.945(Scan#:690) MassPeaks:305
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(4812)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



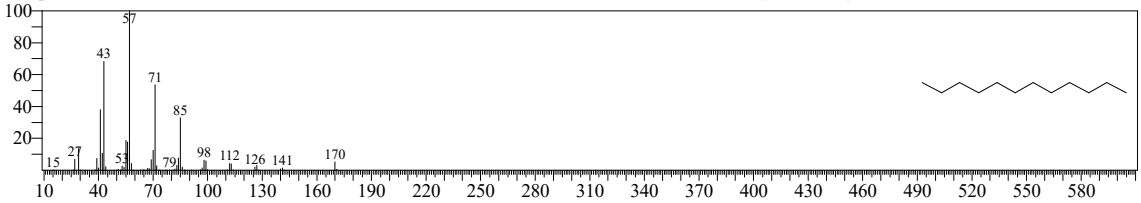
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



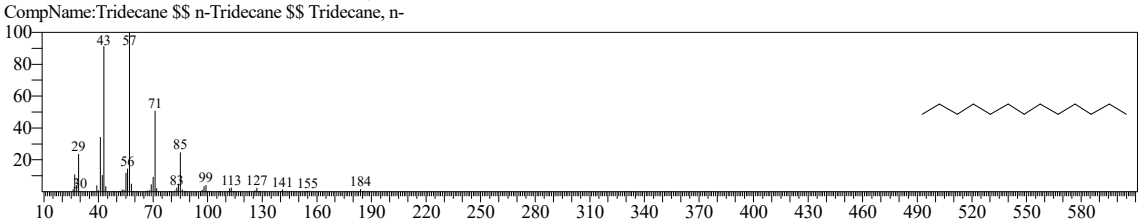
Hit#:2 Entry:9445 Library:NIST20R.lib
SI:86 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



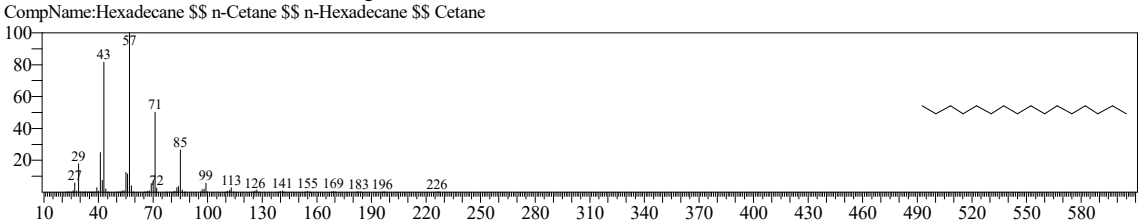
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:86 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:40226 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

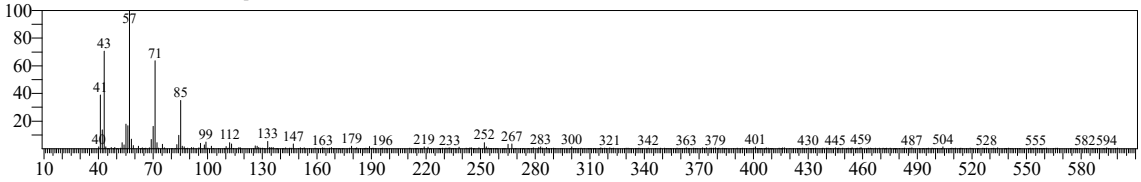


Hit#:5 Entry:27737 Library:NIST20R.lib
SI:85 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

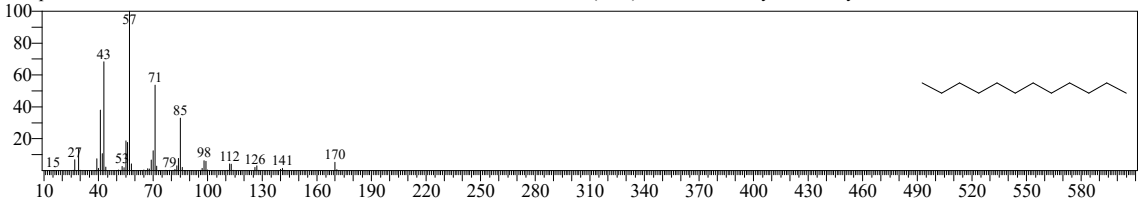


TNAU

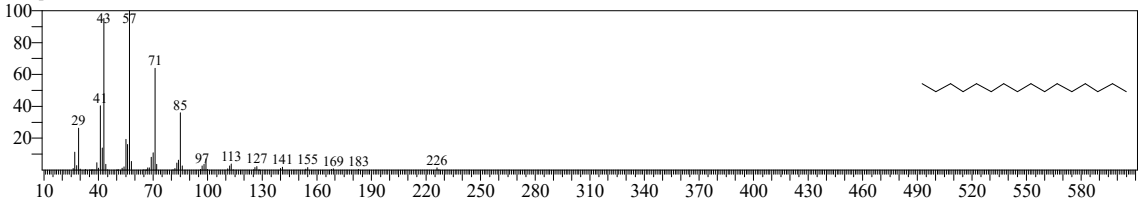
<< Target >>
Line#:3 R.Time:9.695(Scan#:1040) MassPeaks:351
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(4877)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



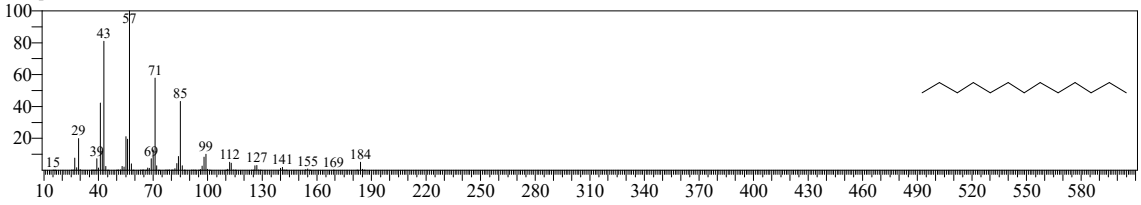
Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:90 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



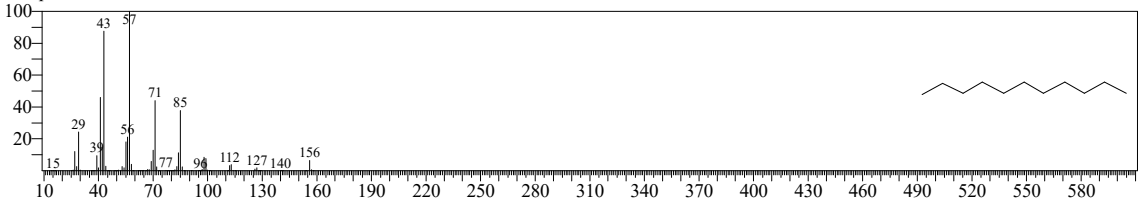
Hit#:2 Entry:27736 Library:NIST20R.lib
SI:90 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane



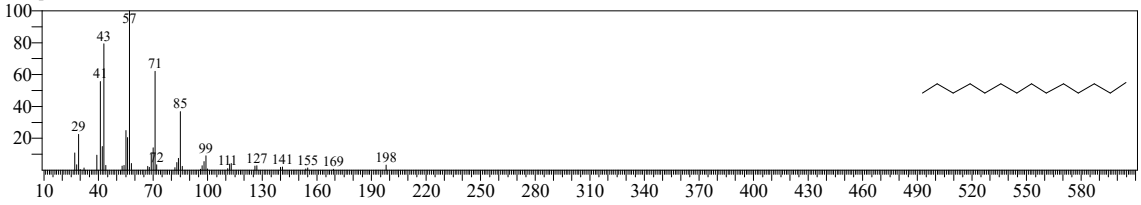
Hit#:3 Entry:19410 Library:NIST20R.lib
SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



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

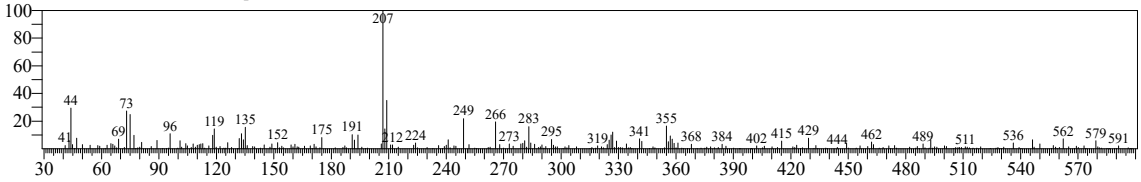


Hit#:5 Entry:22498 Library:NIST20R.lib
SI:89 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

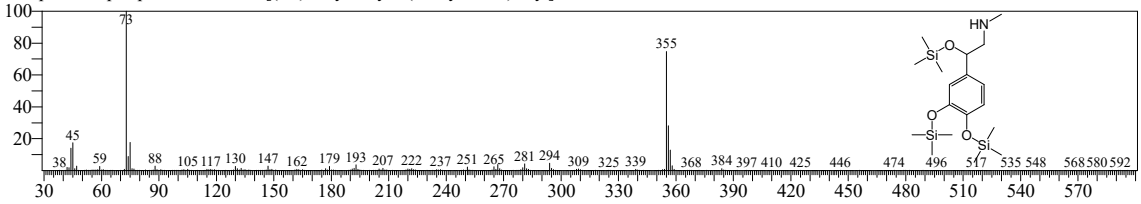


TNAU

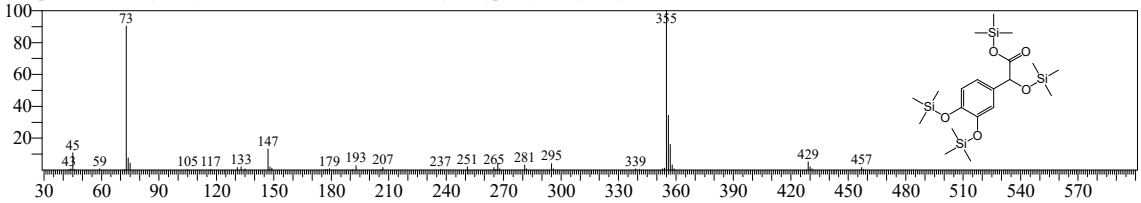
<< Target >>
Line#:4 R.Time:27.740(Scan#:4649) MassPeaks:283
RawMode:Averaged 27.735-27.745(4648-4650) BasePeak:207.05(1549)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



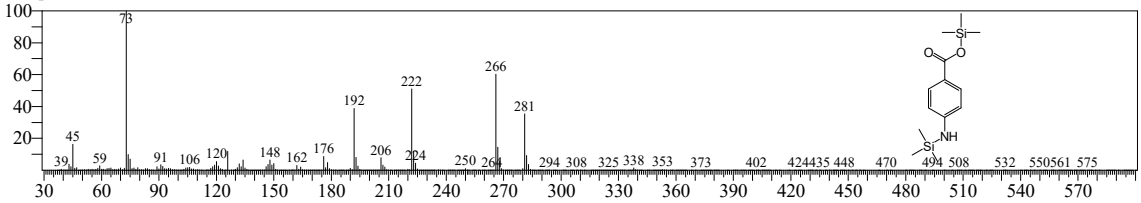
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



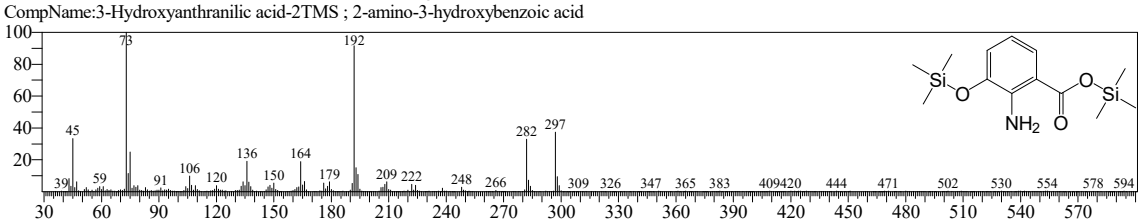
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



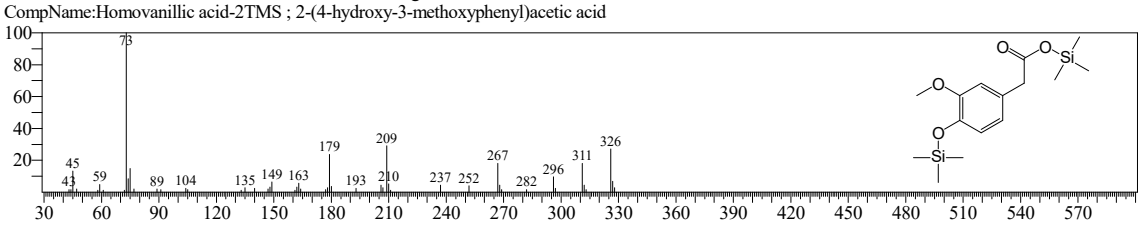
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

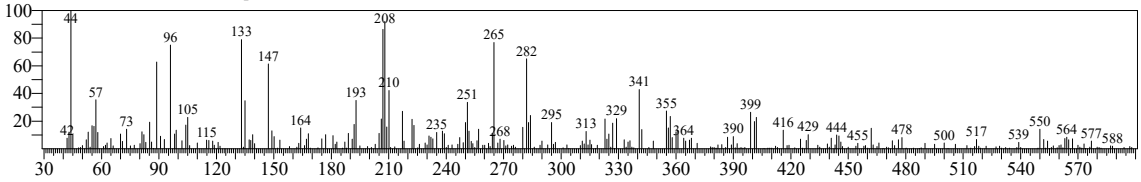


Hit#:5 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

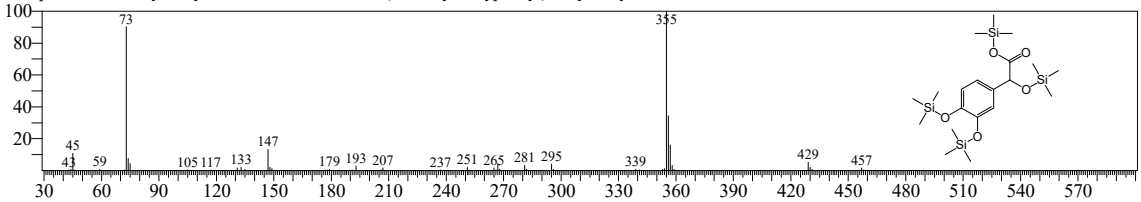


TNAU

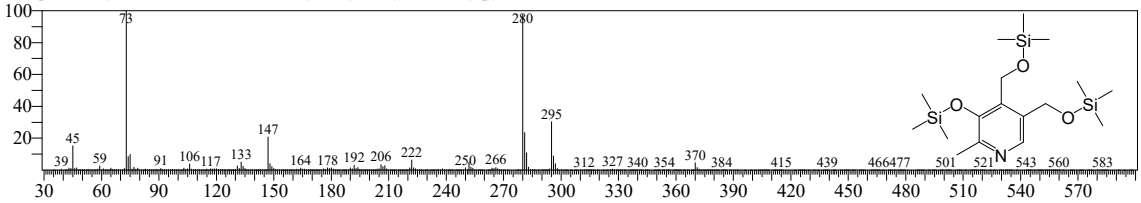
<< Target >>
Line#:5 R.Time:29.570(Scan#:5015) MassPeaks:302
RawMode:Averaged 29.565-29.575(5014-5016) BasePeak:44.00(797)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



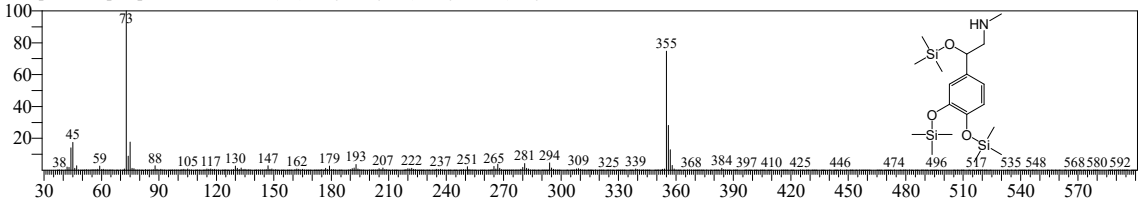
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



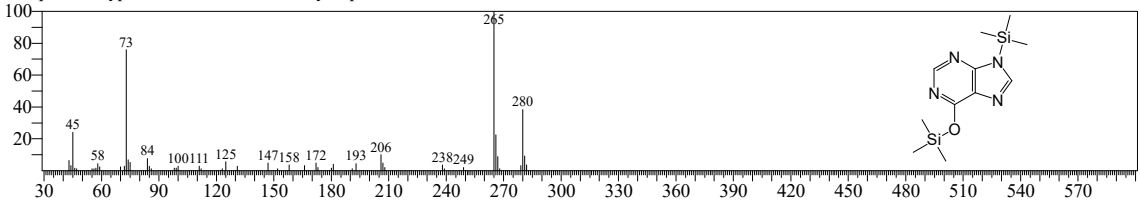
Hit#:2 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



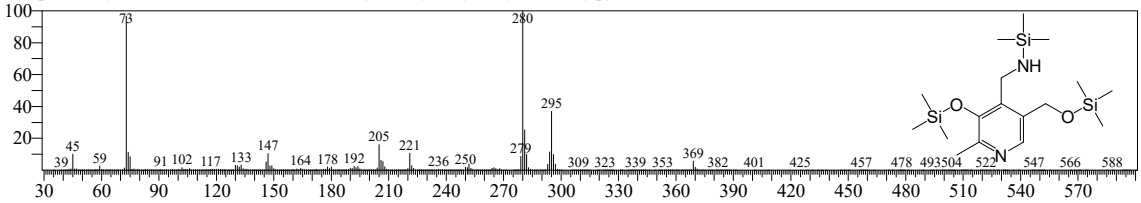
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

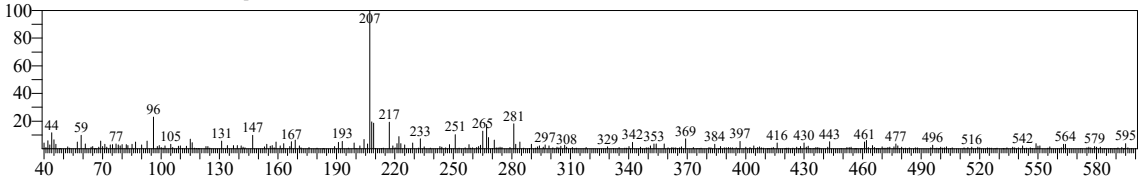


Hit#:5 Entry:418 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C17H36N2O2Si3 CAS:85-87-0 MolWeight:384 RetIndex:1964
CompName:Pyridoxamine-3TMS ; 4-(aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol

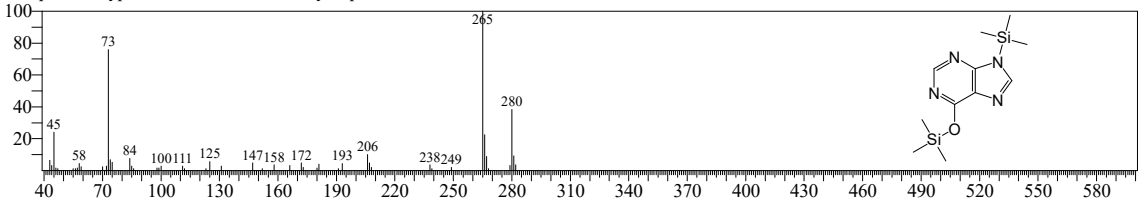


TNAU

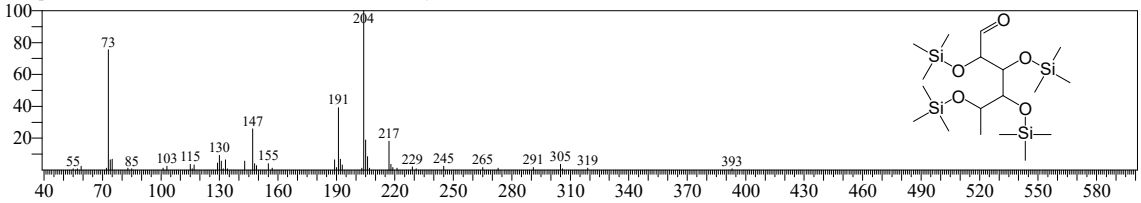
<< Target >>
Line#:6 R.Time:29.665(Scan#:5034) MassPeaks:303
RawMode:Averaged 29.660-29.670(5033-5035) BasePeak:207.05(2641)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



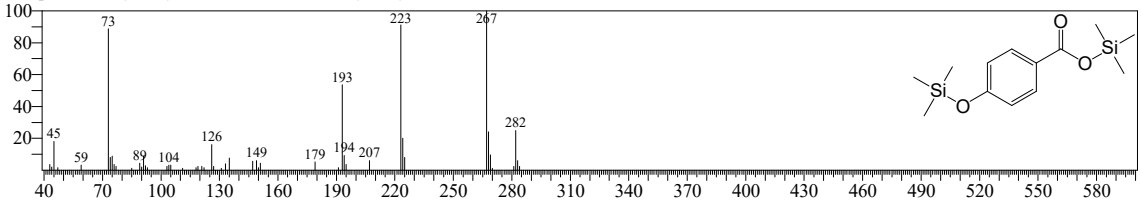
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



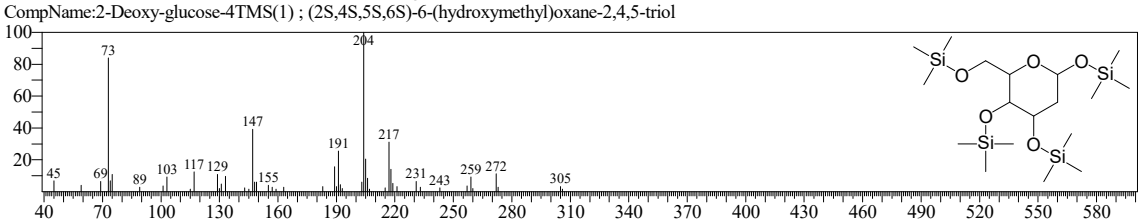
Hit#:2 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



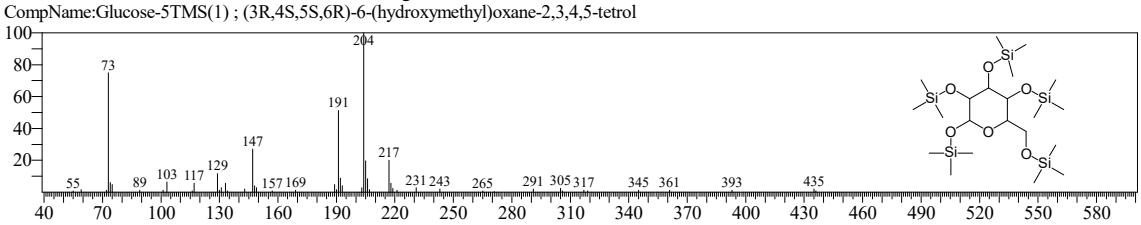
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

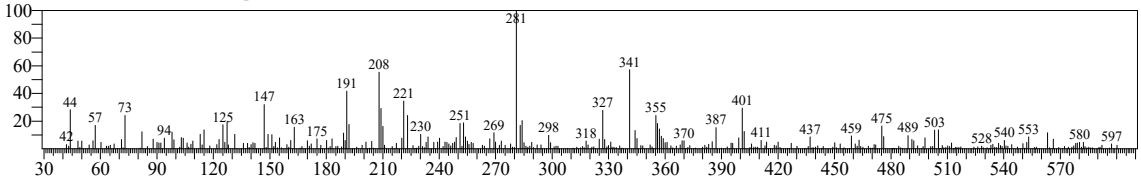


Hit#:5 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

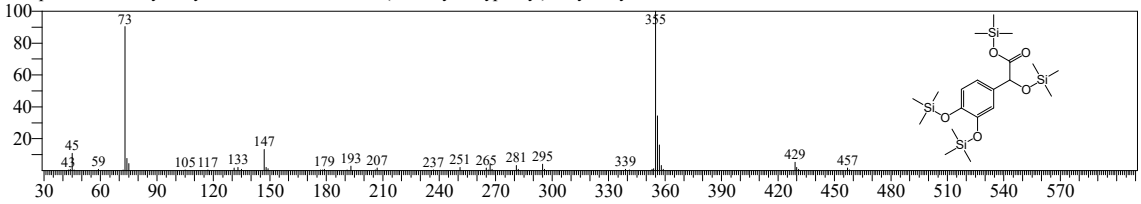


TNAU

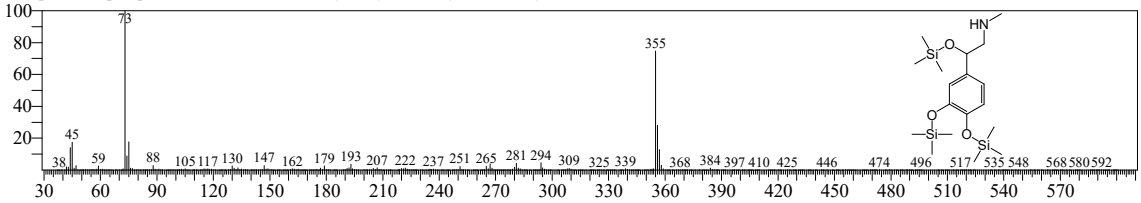
<< Target >>
Line#:7 R.Time:29.925(Scan#:5086) MassPeaks:337
RawMode:Averaged 29.920-29.930(5085-5087) BasePeak:281.05(1193)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



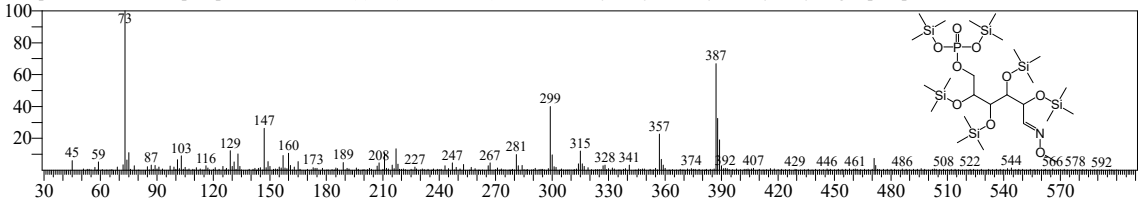
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



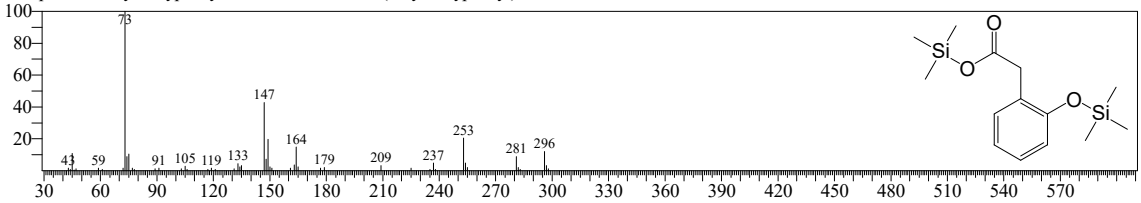
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



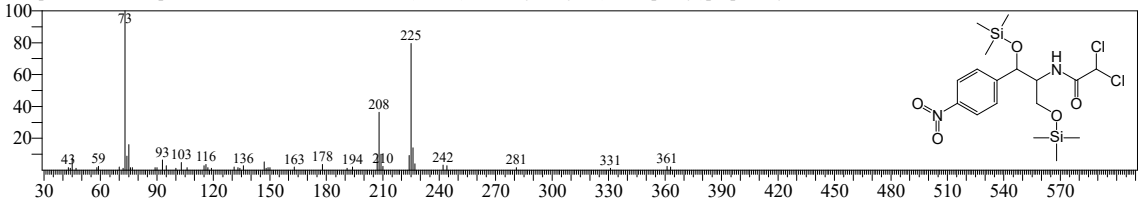
Hit#:3 Entry:507 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C25H64NO9PSi6 CAS:3672-15-9 MolWeight:721 RetIndex:2377
CompName:Mannose 6-phosphate-meto-6TMS(2) ; [(2R,3S,4S,5S)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl dihydrogen phosphate



Hit#:4 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

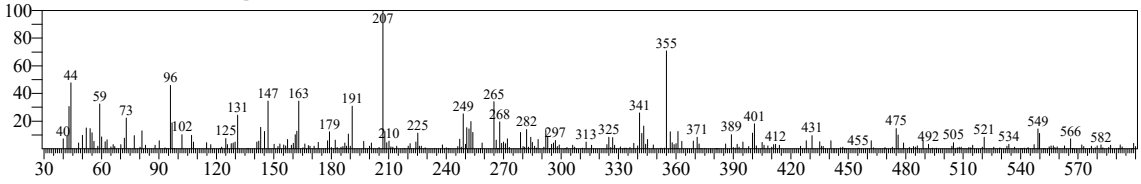


Hit#:5 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

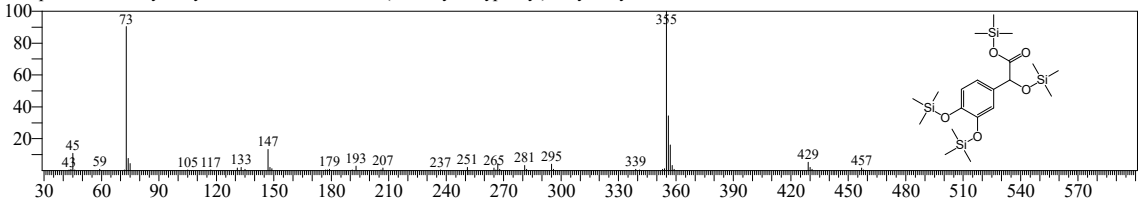


TNAU

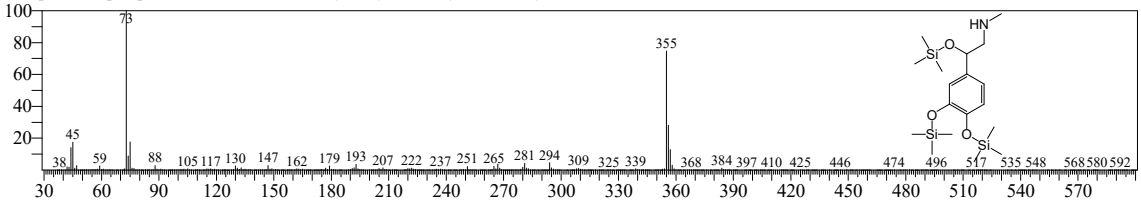
<< Target >>
Line#:8 R.Time:30.010(Scan#:5103) MassPeaks:274
RawMode:Averaged 30.005-30.015(5102-5104) BasePeak:207.05(960)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



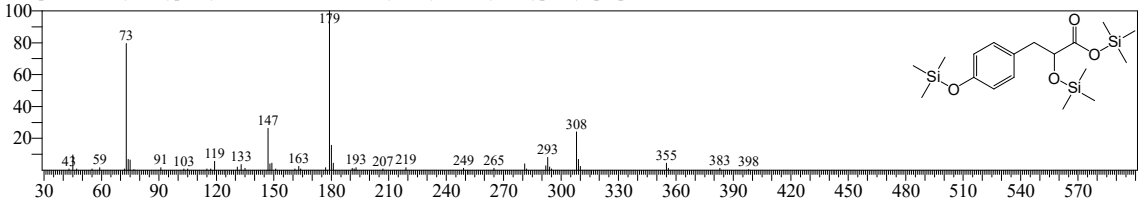
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



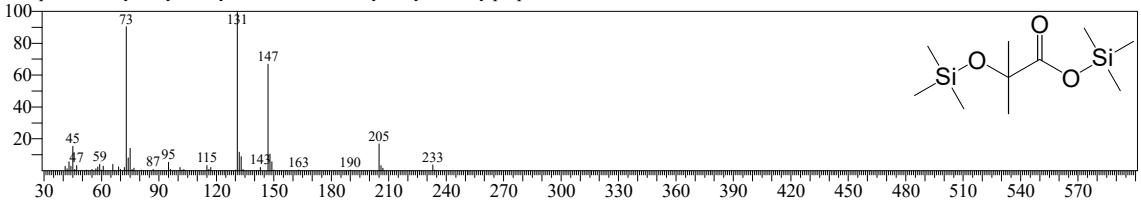
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



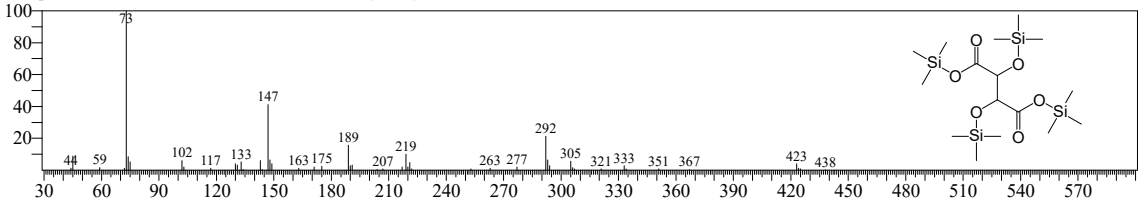
Hit#:3 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:4 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

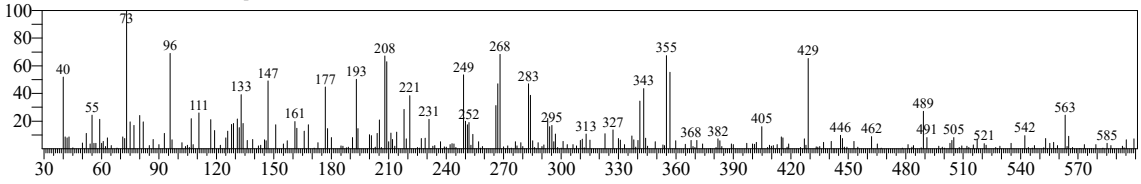


Hit#:5 Entry:224 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C16H38O6Si4 CAS:87-69-4 MolWeight:438 RetIndex:1654
CompName:Tartaric acid-4TMS ; (2R,3R)-2,3-dihydroxybutanedioic acid

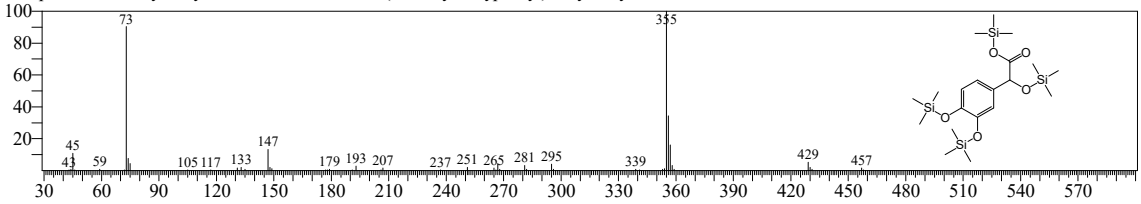


TNAU

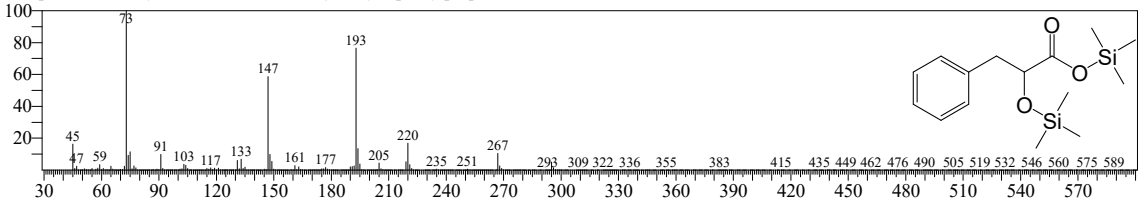
<< Target >>
Line#:9 R.Time:30.040(Scan#:5109) MassPeaks:264
RawMode:Averaged 30.035-30.045(5108-5110) BasePeak:73.05(718)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



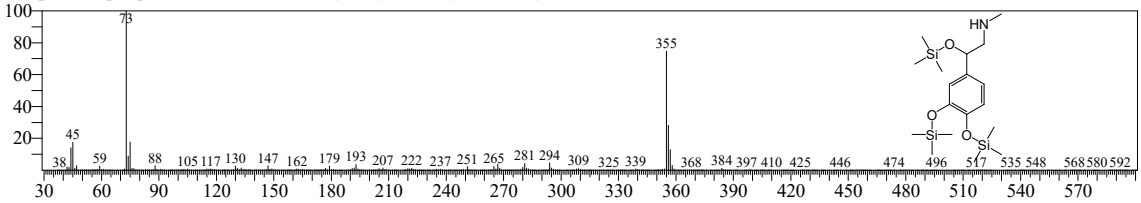
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



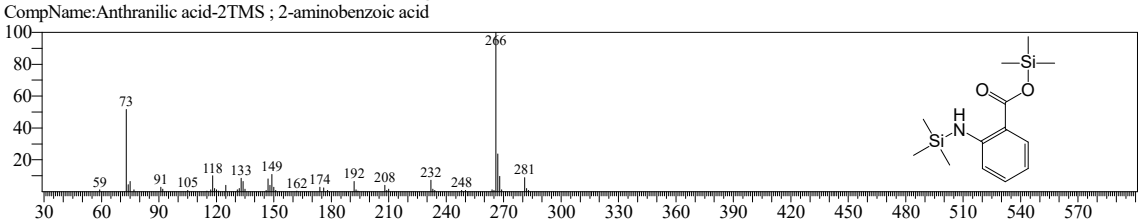
Hit#:2 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



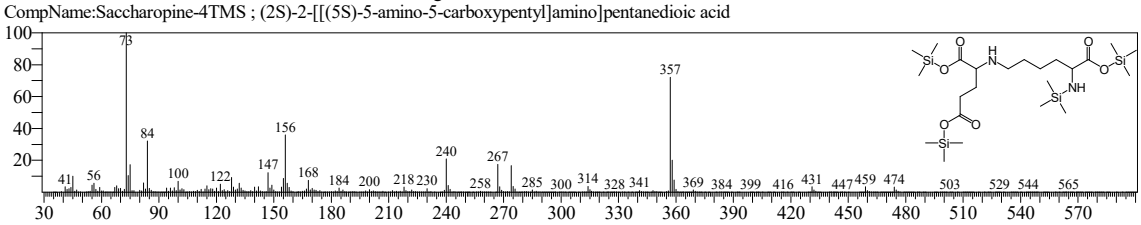
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

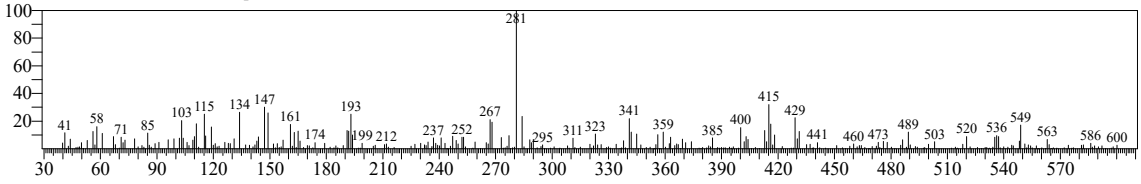


Hit#:5 Entry:526 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C23H52N2O6Si4 CAS:997-68-2 MolWeight:564 RetIndex:2497
CompName:Saccharopine-4TMS ; (2S)-2-[[(5S)-5-amino-5-carboxypentyl]amino]pentanedioic acid

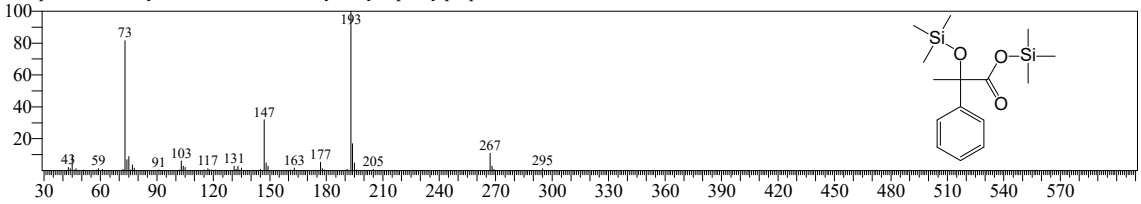


TNAU

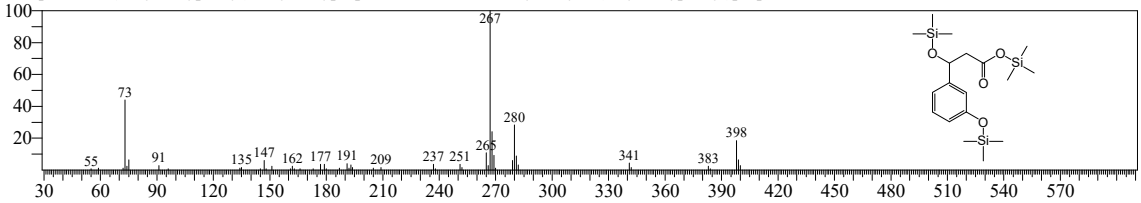
<< Target >>
Line#:10 R.Time:30.165(Scan#:5134) MassPeaks:308
RawMode:Averaged 30.160-30.170(5133-5135) BasePeak:281.00(1139)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



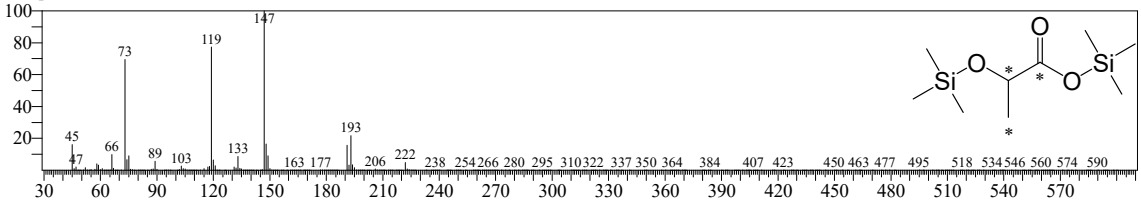
Hit#:1 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



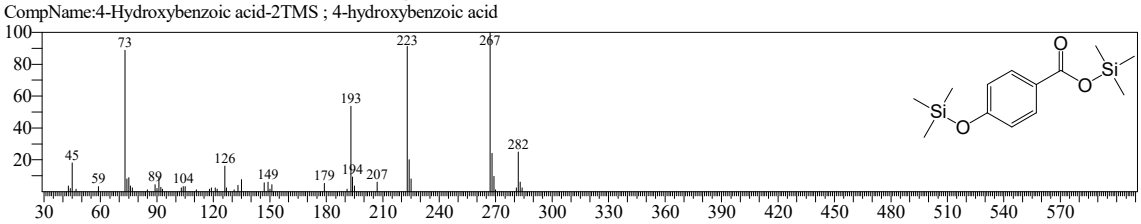
Hit#:2 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



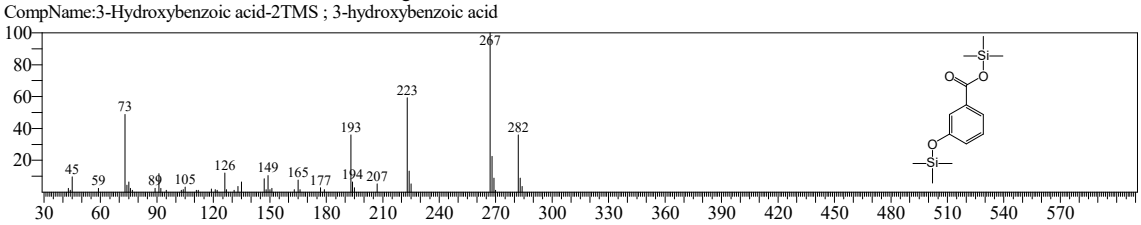
Hit#:3 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

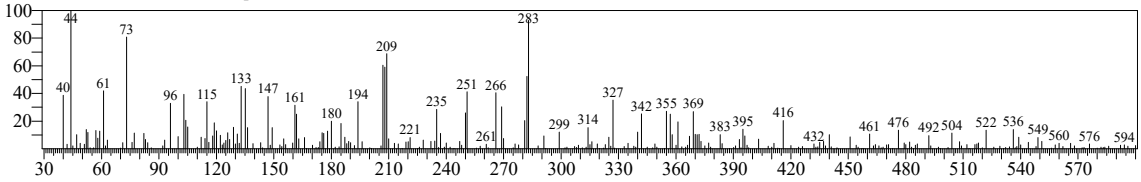


Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

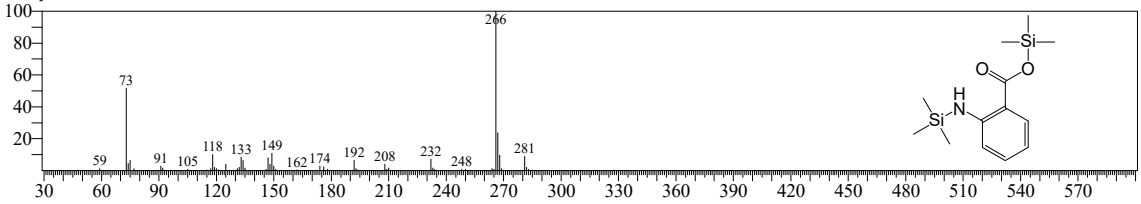


TNAU

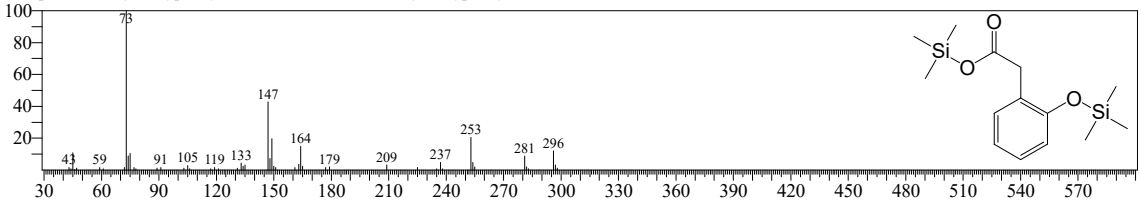
<< Target >>
Line#:11 R.Time:30.270(Scan#:5155) MassPeaks:280
RawMode:Averaged 30.265-30.275(5154-5156) BasePeak:44.00(651)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



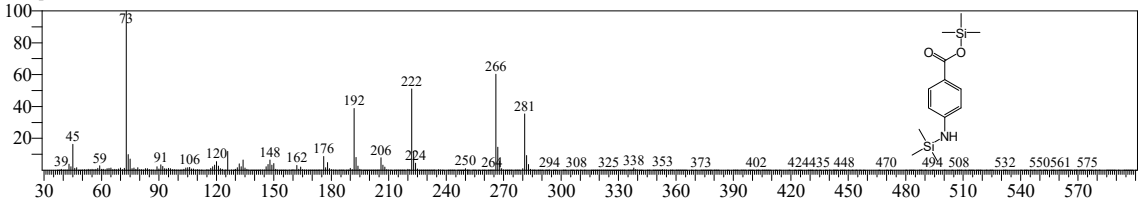
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



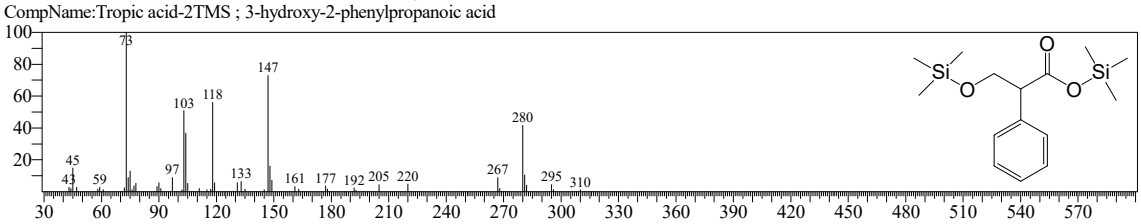
Hit#:2 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



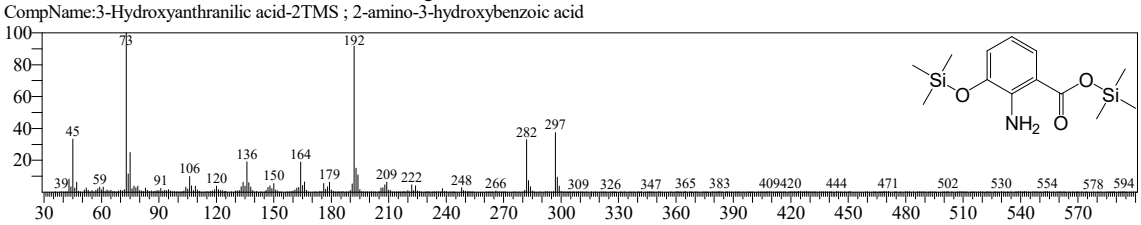
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid

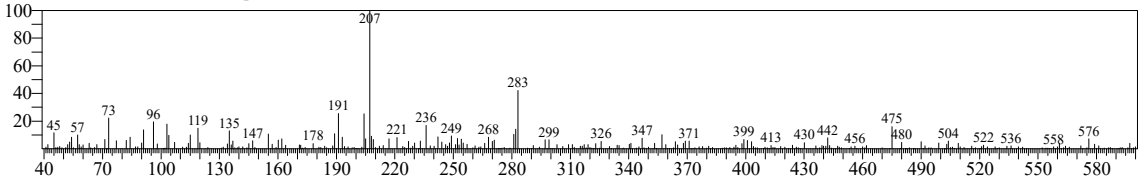


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

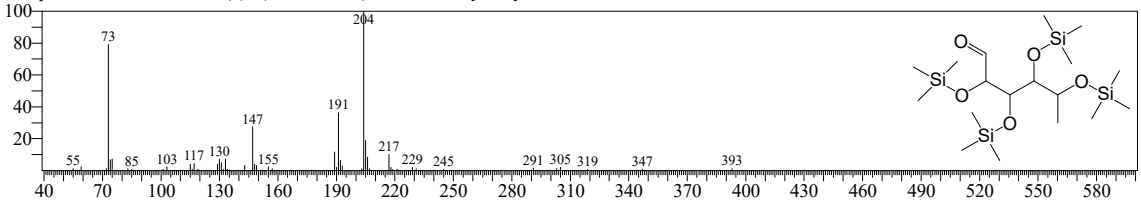


TNAU

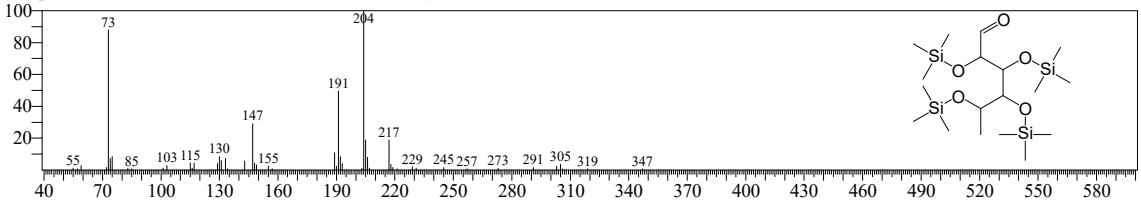
<< Target >>
Line#:12 R.Time:30.305(Scan#:5162) MassPeaks:311
RawMode:Averaged 30.300-30.310(5161-5163) BasePeak:207.05(1484)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



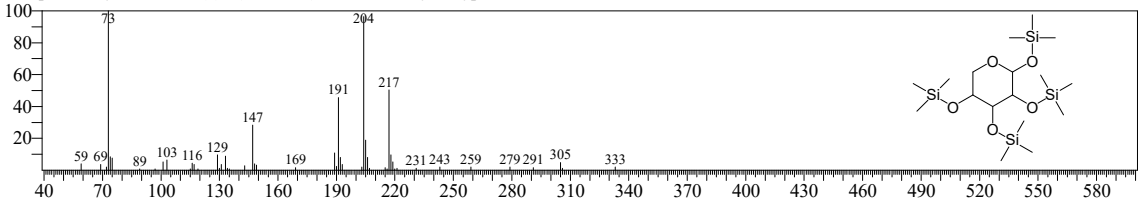
Hit#:1 Entry:261 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1719
CompName:Rhamnose-4TMS(2) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal



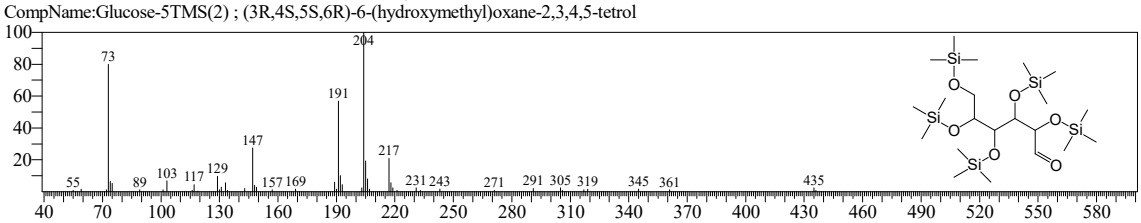
Hit#:2 Entry:271 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1738
CompName:Fucose-4TMS(2) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



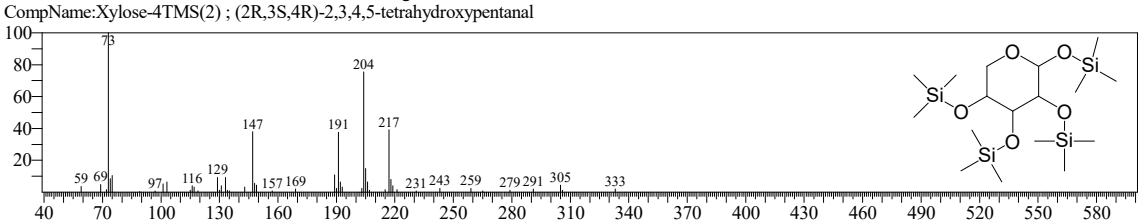
Hit#:3 Entry:205 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1624
CompName:Lyxose-4TMS(1) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:2002
CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

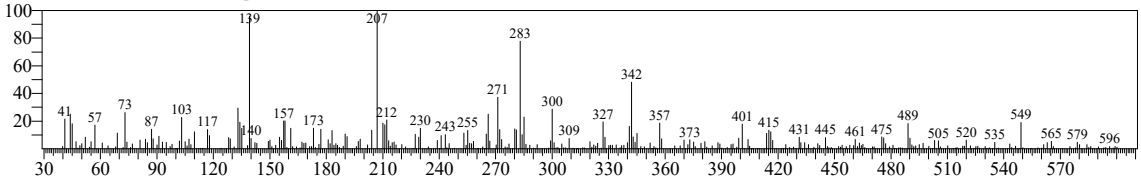


Hit#:5 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

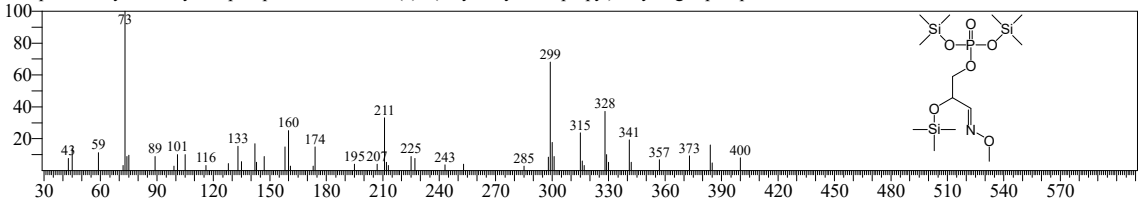


TNAU

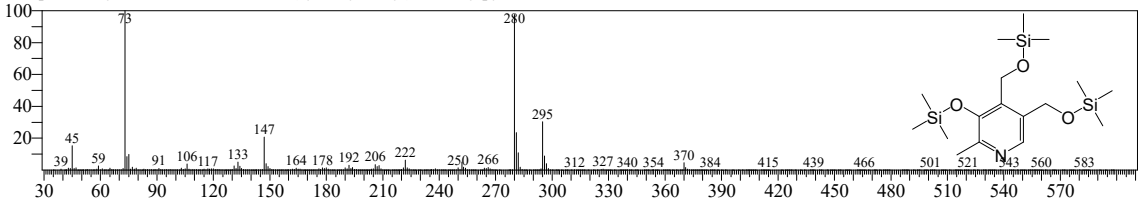
<< Target >>
Line#:13 R.Time:31.910(Scan#:5483) MassPeaks:317
RawMode:Averaged 31.905-31.915(5482-5484) BasePeak:207.05(1273)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



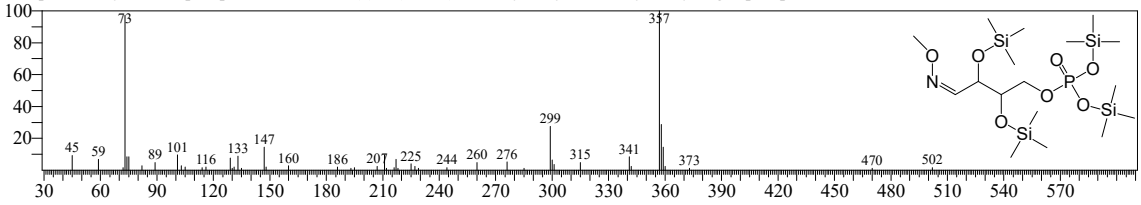
Hit#:1 Entry:269 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H34NO6PSi3 CAS:142-10-9 MolWeight:415 RetIndex:1734
CompName:Glyceraldehyde 3-phosphate-meto-3TMS(2) ; (2-hydroxy-3-oxopropyl) dihydrogen phosphate



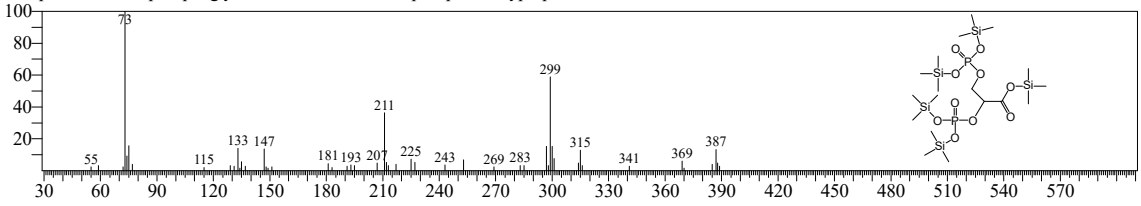
Hit#:2 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



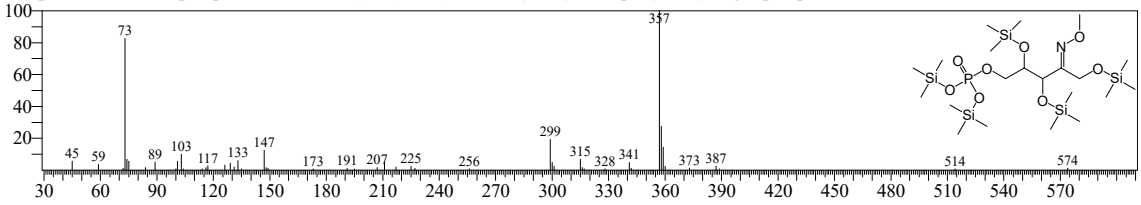
Hit#:3 Entry:394 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1935
CompName:Erythrose 4-phosphate-meto-4TMS(2) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate



Hit#:4 Entry:486 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H48O10P2Si5 CAS:138-81-8 MolWeight:626 RetIndex:2225
CompName:2,3-Bisphosphoglyceric acid-5TMS ; 2,3-diphosphonooxypropanoic acid

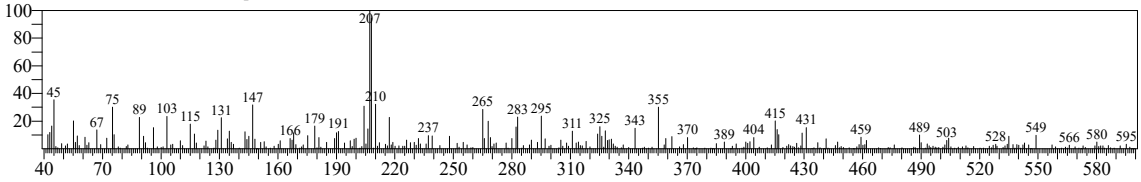


Hit#:5 Entry:468 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H54NO8PSi5 CAS:4151-19-3 MolWeight:619 RetIndex:2137
CompName:Ribulose 5-phosphate-meto-5TMS(1) ; [(2R,3R)-2,3,5-trihydroxy-4-oxopentyl] dihydrogen phosphate

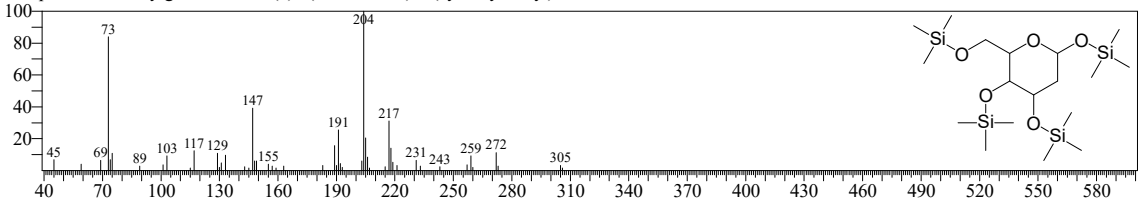


TNAU

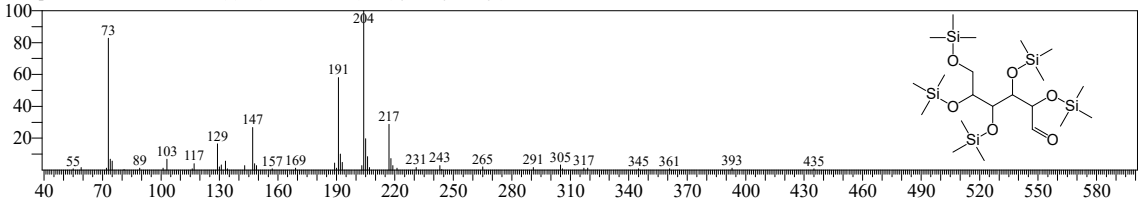
<< Target >>
Line#:14 R.Time:32.380(Scan#:5577) MassPeaks:314
RawMode:Averaged 32.375-32.385(5576-5578) BasePeak:207.05(1149)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



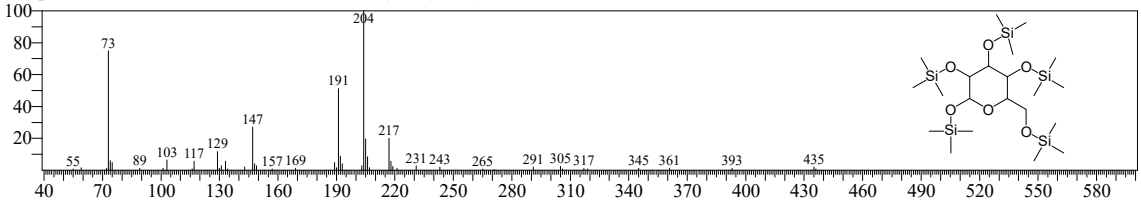
Hit#:1 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



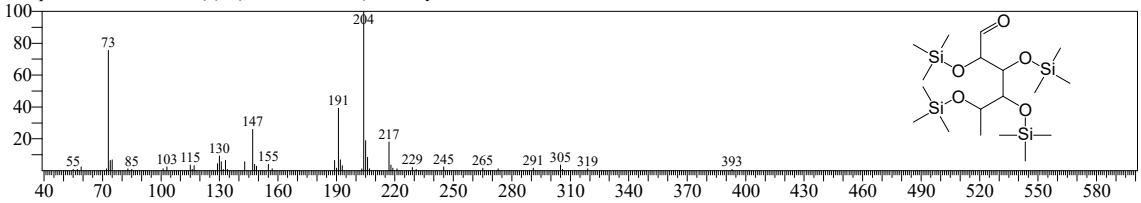
Hit#:2 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1824
CompName:Galactose-5TMS(1) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



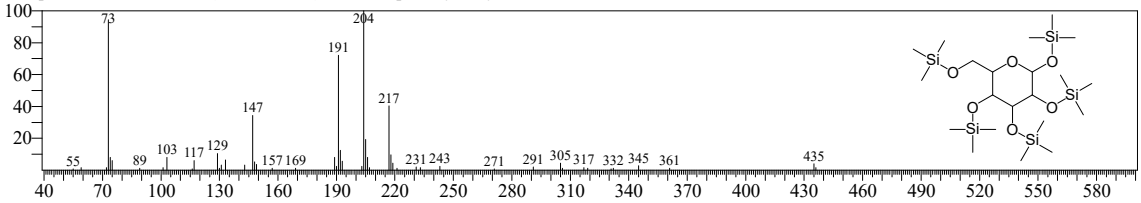
Hit#:3 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

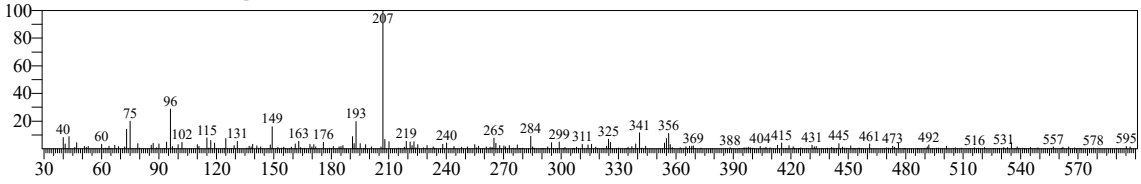


Hit#:5 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

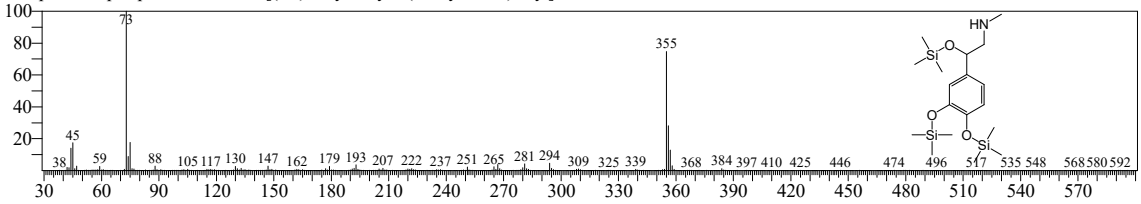


TNAU

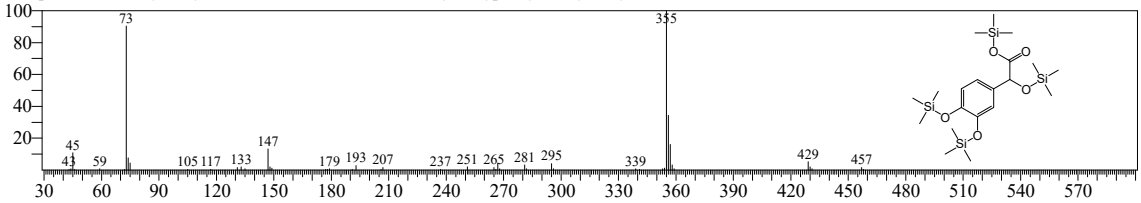
<< Target >>
Line#:15 R.Time:32.460(Scan#:5593) MassPeaks:249
RawMode:Averaged 32.455-32.465(5592-5594) BasePeak:207.00(3054)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



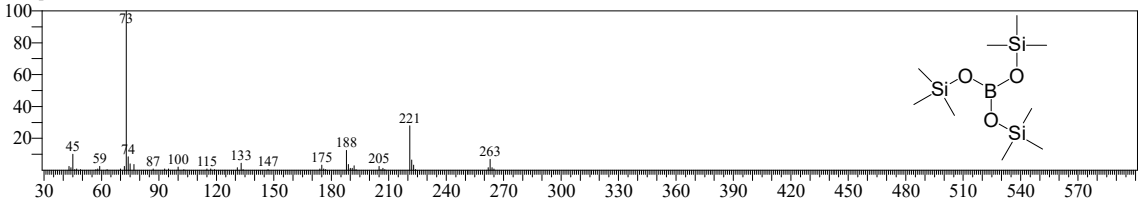
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



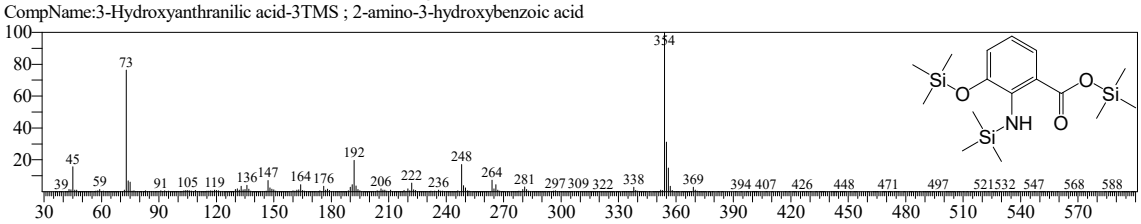
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



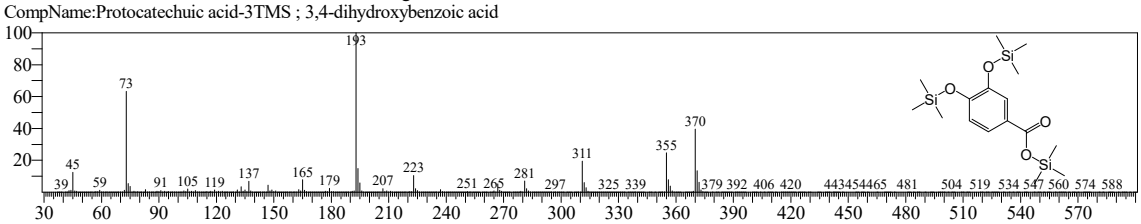
Hit#:3 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid



Hit#:4 Entry:354 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H31NO3Si3 CAS:548-93-6 MolWeight:369 RetIndex:1886
CompName:3-Hydroxyanthranilic acid-3TMS ; 2-amino-3-hydroxybenzoic acid

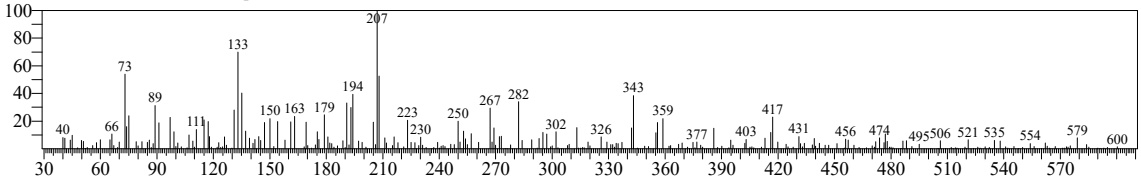


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

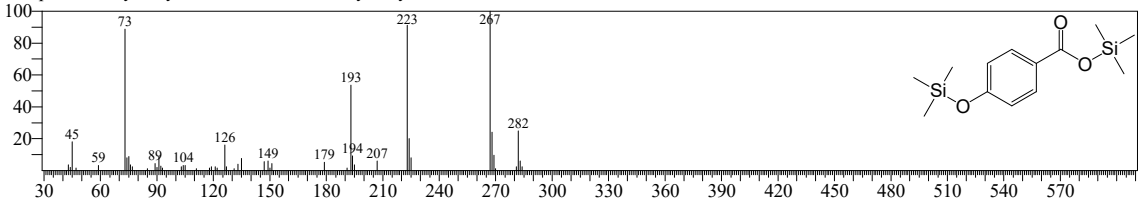


TNAU

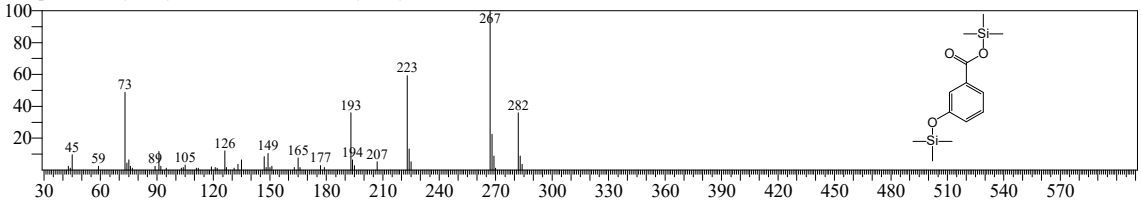
<< Target >>
Line#:16 R.Time:32.500(Scan#:5601) MassPeaks:273
RawMode:Averaged 32.495-32.505(5600-5602) BasePeak:207.05(827)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



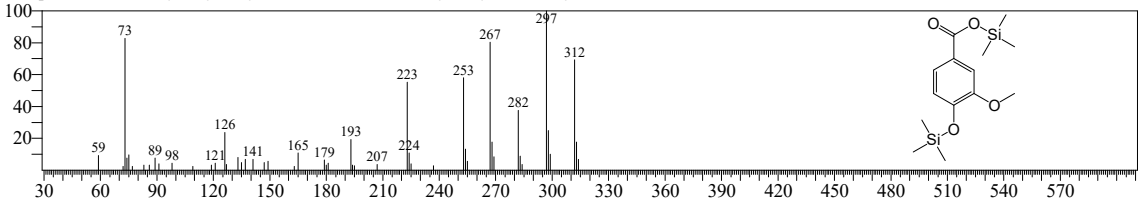
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



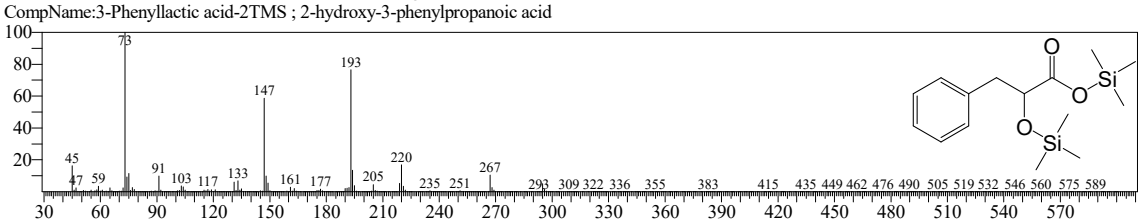
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



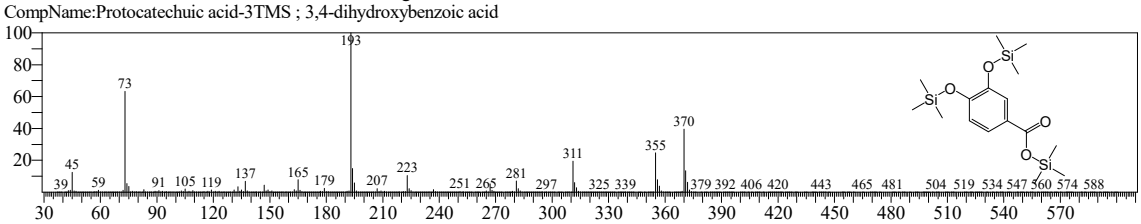
Hit#:3 Entry:291 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C14H24O4Si2 CAS:121-34-6 MolWeight:312 RetIndex:1775
CompName:3-Methoxy-4-hydroxybenzoic acid-2TMS ; 4-hydroxy-3-methoxybenzoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

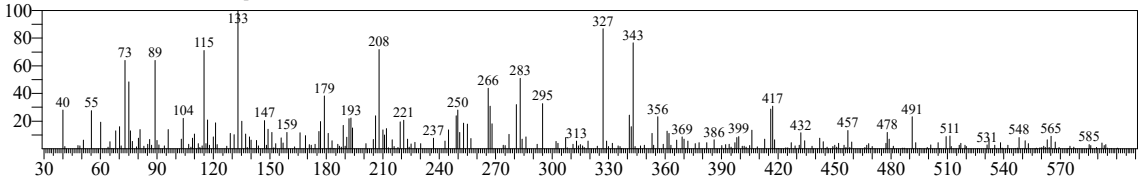


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

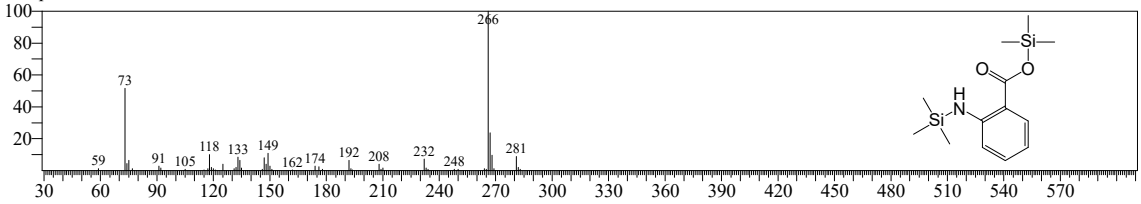


TNAU

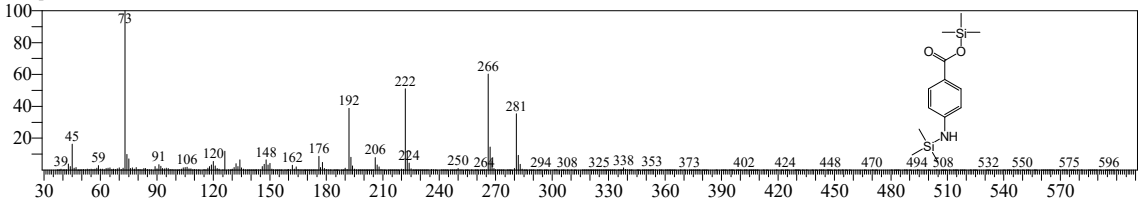
<< Target >>
Line#:17 R.Time:32.530(Scan#:5607) MassPeaks:266
RawMode:Averaged 32.525-32.535(5606-5608) BasePeak:133.05(716)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



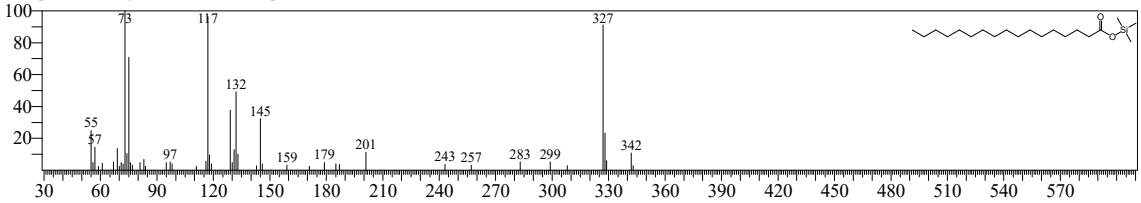
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



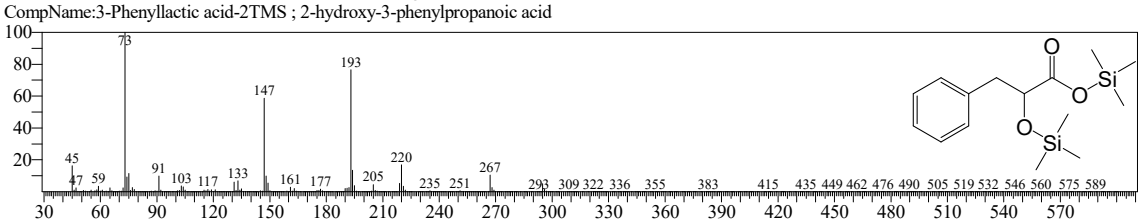
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



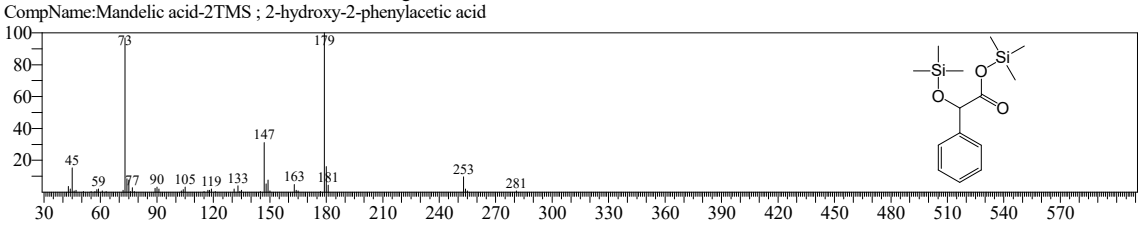
Hit#:3 Entry:472 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C20H42O2Si CAS:506-12-7 MolWeight:342 RetIndex:2146
CompName:Margaric acid-TMS ; heptadecanoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

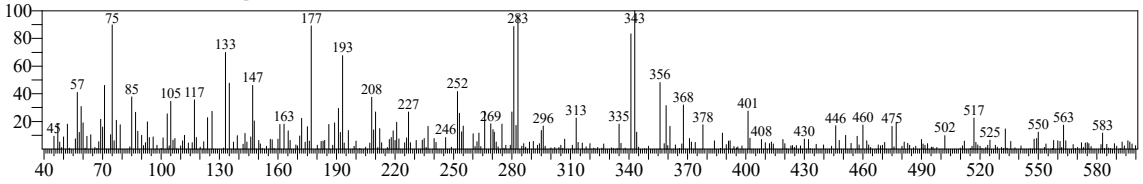


Hit#:5 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid

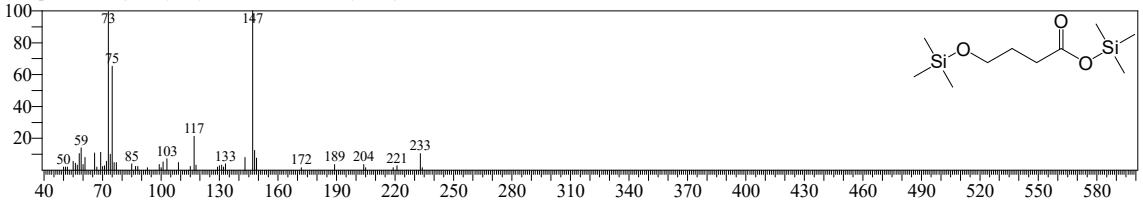


TNAU

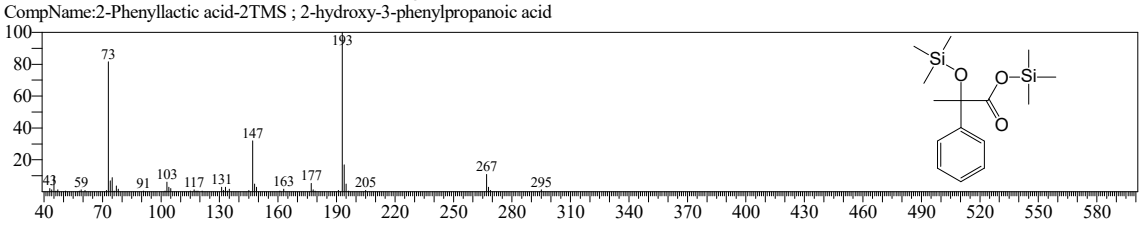
<< Target >>
Line#:18 R.Time:32.670(Scan#:5635) MassPeaks:325
RawMode:Averaged 32.665-32.675(5634-5636) BasePeak:343.05(557)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



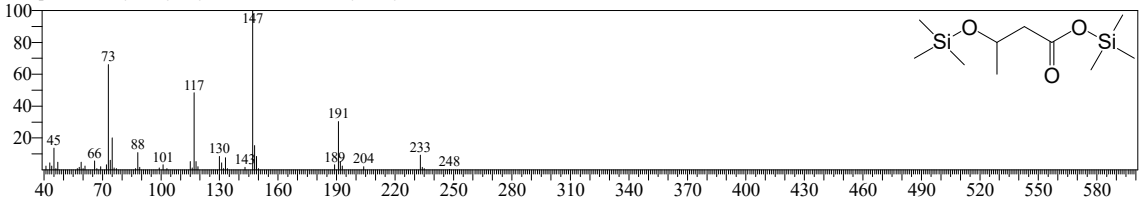
Hit#:1 Entry:60 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C10H24O3Si2 CAS:591-81-1 MolWeight:248 RetIndex:1240
CompName:4-Hydroxybutyric acid-2TMS ; 4-hydroxybutanoic acid



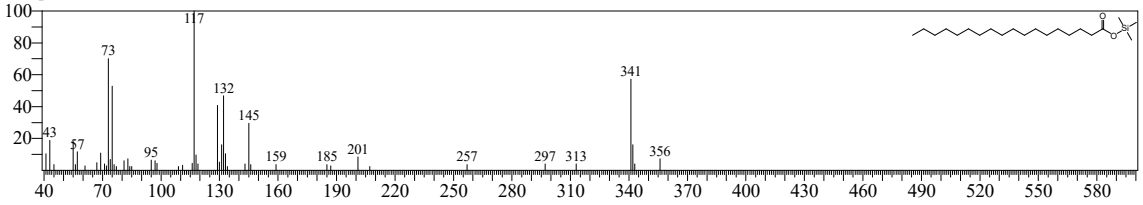
Hit#:2 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:3 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid



Hit#:4 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



Hit#:5 Entry:24 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula: CAS:0-00-0 MolWeight:236 RetIndex:1130
CompName:Oxalic acid-13C2-2TMS ;