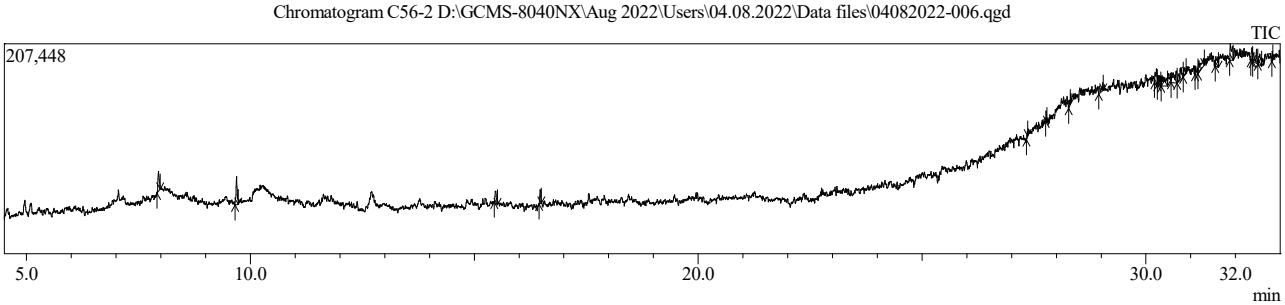
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 04-Aug-22 8:09:19 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C56-2
Sample ID	: C56-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 6
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-006.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-006.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 4:20:47 PM

Chromatogram C56-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-006.qgd



Peak Report TIC

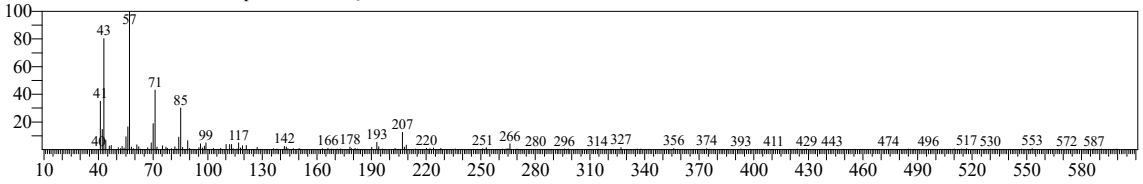
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.945	38567	5.87	19767	7.81	1.95	86	Tridecane
2	9.690	52192	7.94	27840	10.99	1.87	88	Dodecane
3	15.472	25618	3.90	11690	4.62	2.19	38	Lactic acid-13C3-2TMS
4	16.472	21349	3.25	13567	5.36	1.57	82	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
5	27.350	5249	0.80	5712	2.26	0.92	24	3,4-Dihydroxymandelic acid-4TMS
6	27.771	6594	1.00	10735	4.24	0.61	38	Epinephrine-3TMS
7	28.285	7613	1.16	5562	2.20	1.37	30	4-Hydroxybenzoic acid-2TMS
8	29.033	23469	3.57	7966	3.15	2.95	32	4-Hydroxybenzoic acid-2TMS
9	30.235	33541	5.10	14859	5.87	2.26	28	Phosphoric acid-3TMS
10	30.303	30187	4.59	10060	3.97	3.00	35	Glycerol-3TMS
11	30.357	50679	7.71	10042	3.97	5.05	42	3-Hydroxybenzoic acid-2TMS
12	30.684	58513	8.90	11675	4.61	5.01	34	Lactitol-9TMS
13	30.765	47783	7.27	11226	4.43	4.26	38	2-Deoxy-glucose-4TMS(2)
14	30.845	17273	2.63	6745	2.66	2.56	38	2-Methyl-3-hydroxyvaleric acid-2TMS
15	31.115	13758	2.09	8243	3.25	1.67	40	4-Aminobenzoic acid-2TMS
16	31.283	53084	8.08	7781	3.07	6.82	28	Batyl alcohol-2TMS
17	31.560	27568	4.19	9537	3.77	2.89	32	Lactitol-9TMS
18	31.886	46181	7.03	16107	6.36	2.87	36	5'-Methylthioadenosine-2TMS
19	32.367	23393	3.56	13008	5.14	1.80	37	3-Hydroxybenzoic acid-2TMS
20	32.470	35670	5.43	13878	5.48	2.57	41	Arabinose-4TMS(1)
21	32.520	30777	4.68	7872	3.11	3.91	27	Psicose-5TMS(2)
22	32.821	8313	1.26	9383	3.70	0.89	30	2-Deoxy-glucose-4TMS(1)

TNAU

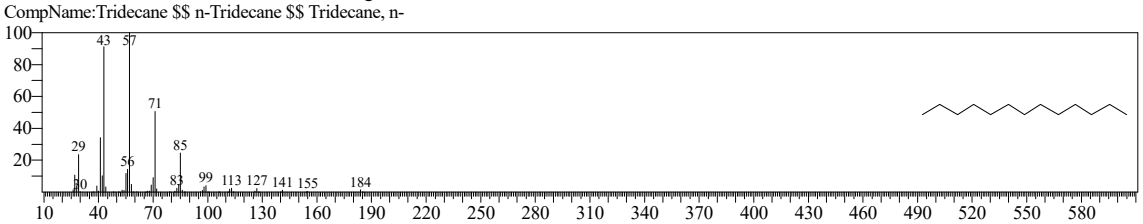
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
		657371	100.00	253255	100.00			

Library

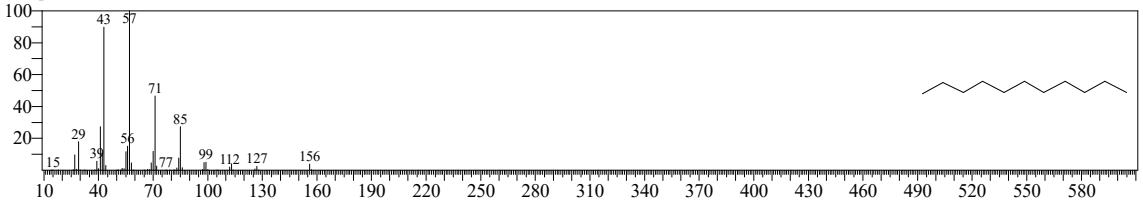
<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:237
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(4895)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



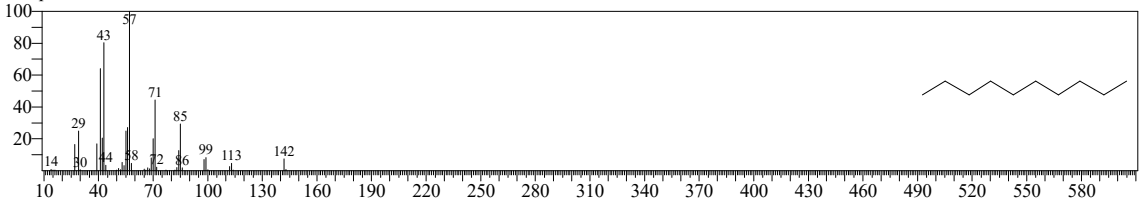
Hit#:1 Entry:40226 Library:NIST20M1.lib
SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



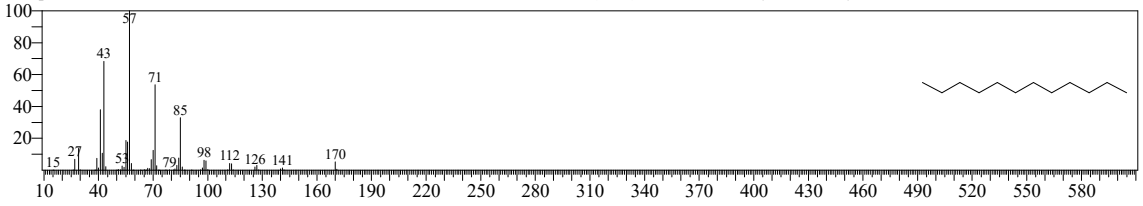
Hit#:2 Entry:21042 Library:NIST20M1.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



Hit#:3 Entry:13604 Library:NIST20M1.lib
SI:86 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

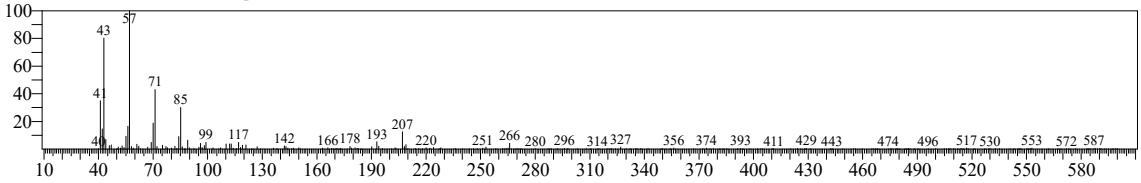


Hit#:4 Entry:30057 Library:NIST20M1.lib
SI:85 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

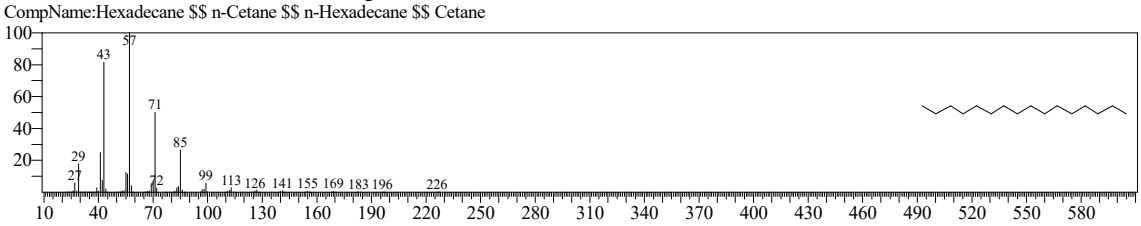


TNAU

<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:237
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(4895)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

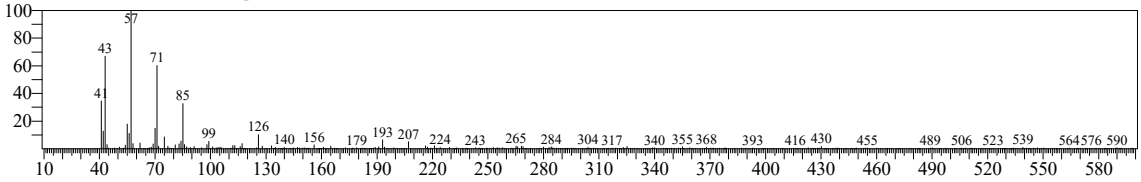


Hit#:5 Entry:27737 Library:NIST20R.lib
SI:85 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

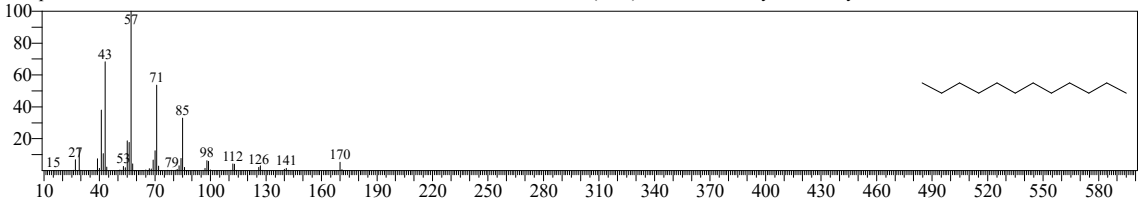


TNAU

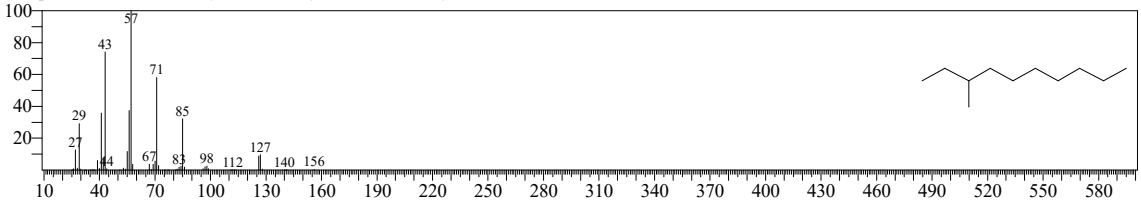
<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:313
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(5470)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



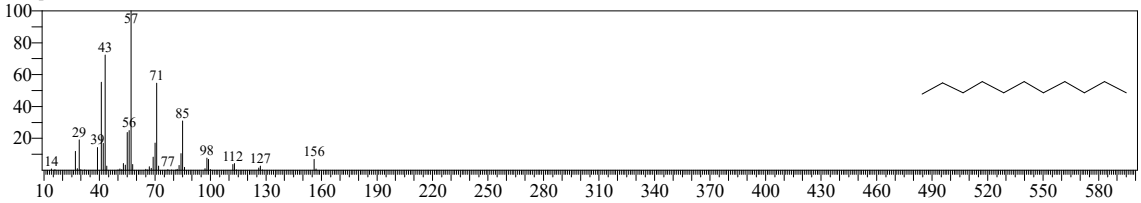
Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:88 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



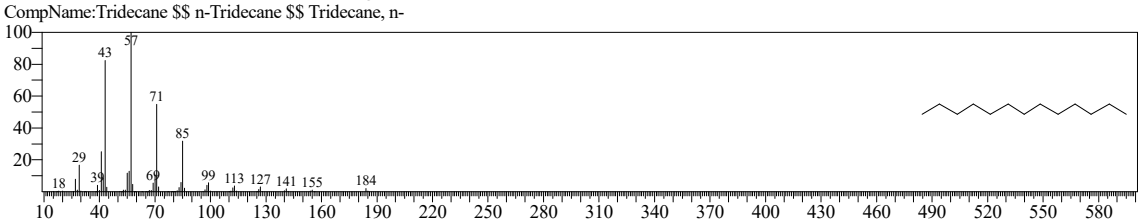
Hit#:2 Entry:12893 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:13151-34-3 MolWeight:156 RetIndex:1051
CompName:Decane, 3-methyl- $$ 3-Methyldecane $$ 2-Ethylnonane



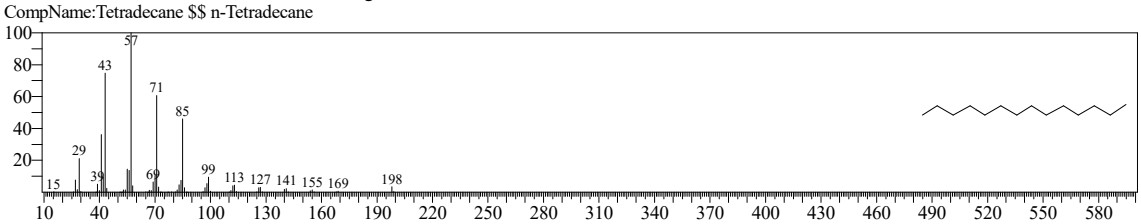
Hit#:3 Entry:12898 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



Hit#:4 Entry:19412 Library:NIST20R.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

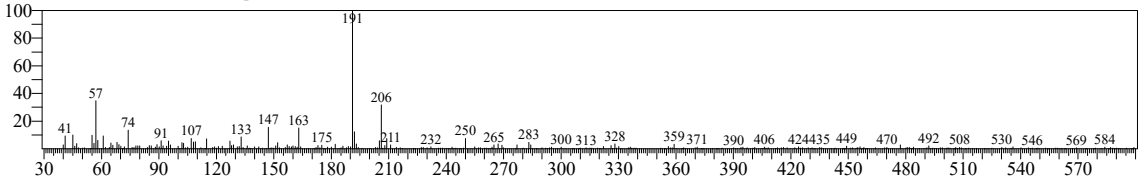


Hit#:5 Entry:22497 Library:NIST20R.lib
SI:87 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

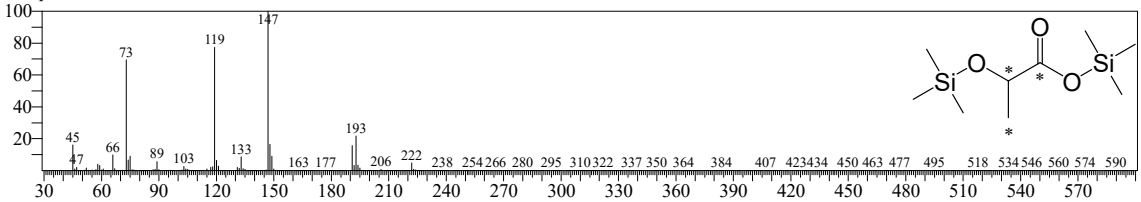


TNAU

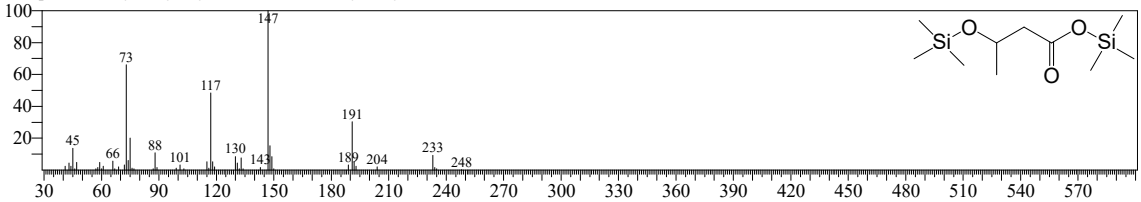
<< Target >>
Line#:3 R.Time:15.470(Scan#:2195) MassPeaks:314
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.10(2752)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



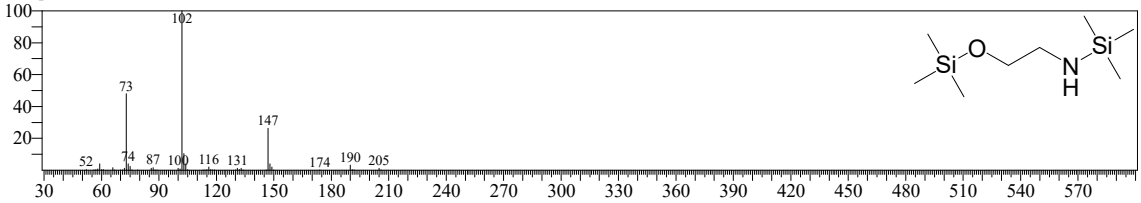
Hit#:1 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;



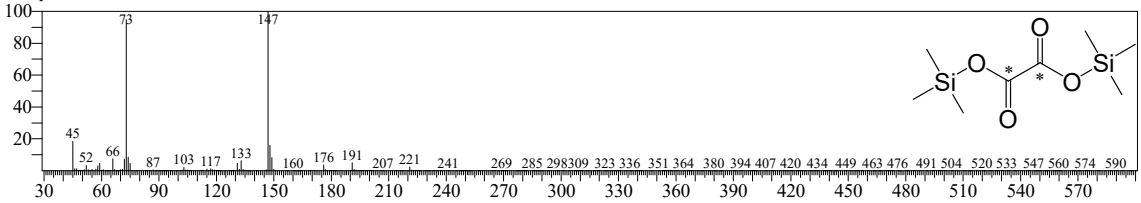
Hit#:2 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid



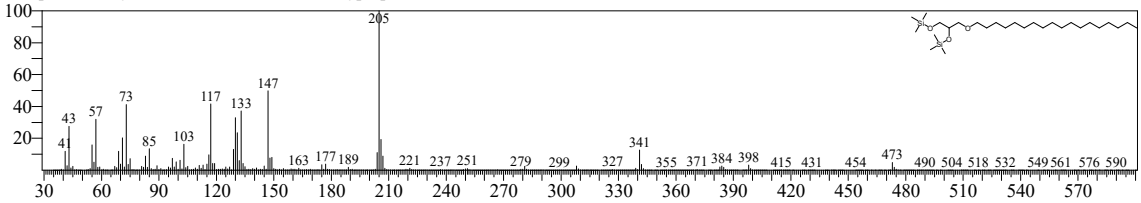
Hit#:3 Entry:4 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C8H23NOSi2 CAS:141-43-5 MolWeight:205 RetIndex:1029
CompName:2-Aminoethanol-2TMS ; 2-aminoethanol



Hit#:4 Entry:24 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula: CAS:0-00-0 MolWeight:236 RetIndex:1130
CompName:Oxalic acid-13C2-2TMS ;

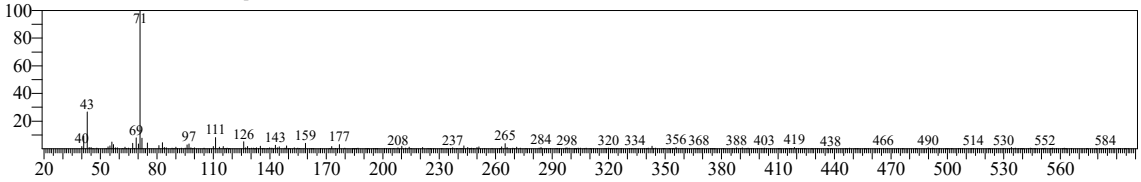


Hit#:5 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

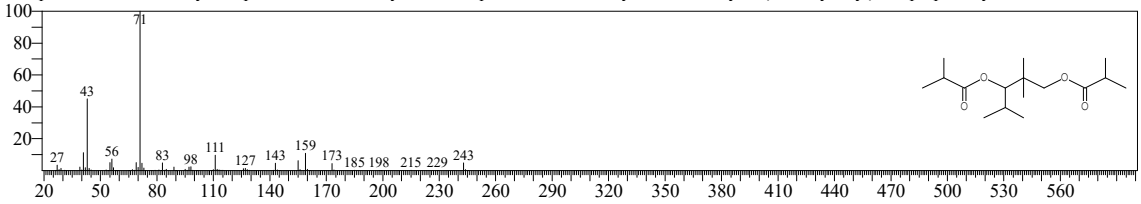


TNAU

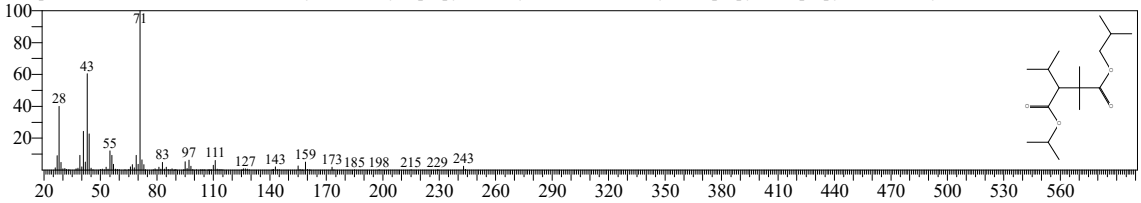
<< Target >>
Line#:4 R.Time:16.470(Scan#:2395) MassPeaks:270
RawMode:Averaged 16.465-16.475(2394-2396) BasePeak:71.05(6519)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



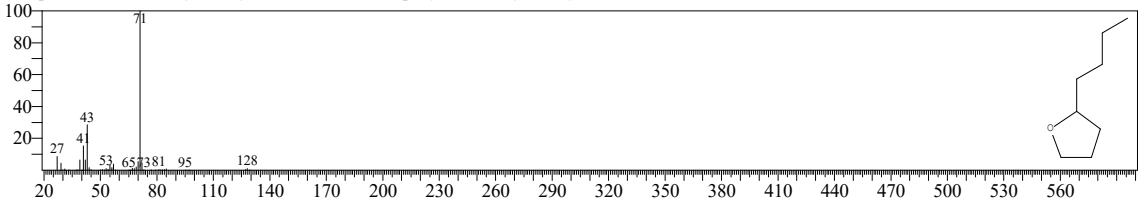
Hit#:1 Entry:34622 Library:NIST20R.lib
SI:82 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan



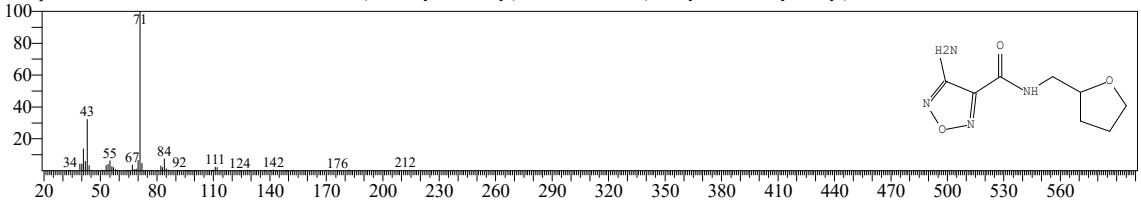
Hit#:2 Entry:146809 Library:NIST20M1.lib
SI:79 Formula:C16H30O4 CAS:0-00-0 MolWeight:286 RetIndex:1605
CompName:Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester $$ 1-Isobutyl 4-isopropyl 3-isopropyl-2,2-dimethylsuccinate #



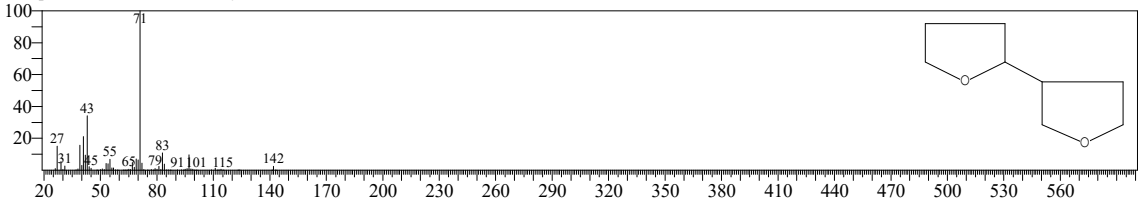
Hit#:3 Entry:6356 Library:NIST20R.lib
SI:78 Formula:C8H16O CAS:1004-29-1 MolWeight:128 RetIndex:948
CompName:Furan, 2-butyltetrahydro- $$ Octane, 1,4-epoxy- $$ 2-Butyltetrahydrofuran



Hit#:4 Entry:64203 Library:NIST20M1.lib
SI:77 Formula:C8H12N4O3 CAS:309735-27-1 MolWeight:212 RetIndex:1980
CompName:Furazan-3-carboxamide, 4-amino-N-(2-tetrahydrofurfuryl)- $$ 4-Amino-N-(tetrahydro-2-furanylmethyl)-1,2,5-oxadiazole-3-carboxamide #

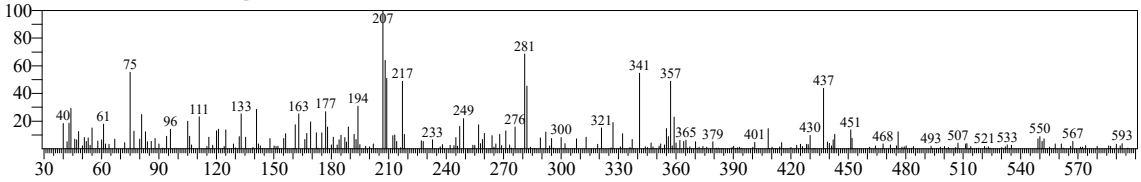


Hit#:5 Entry:13419 Library:NIST20M1.lib
SI:77 Formula:C8H14O2 CAS:73373-15-6 MolWeight:142 RetIndex:1079
CompName:2,3'-Bifuran, octahydro-

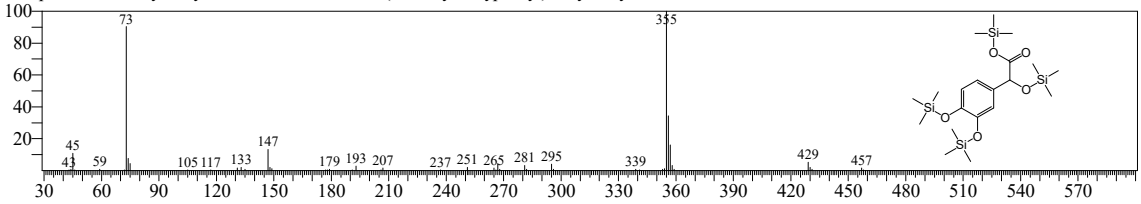


TNAU

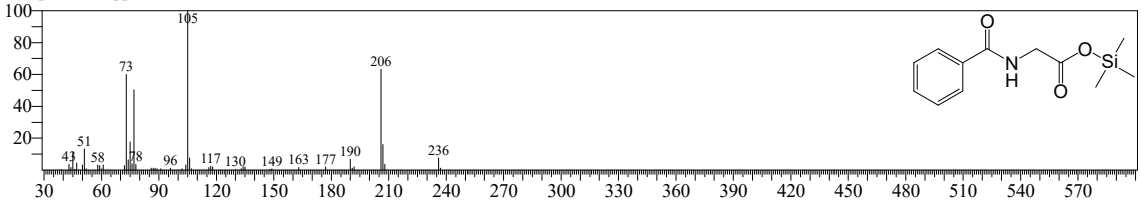
<< Target >>
Line#:5 R.Time:27.350(Scan#:4571) MassPeaks:258
RawMode:Averaged 27.345-27.355(4570-4572) BasePeak:207.05(736)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



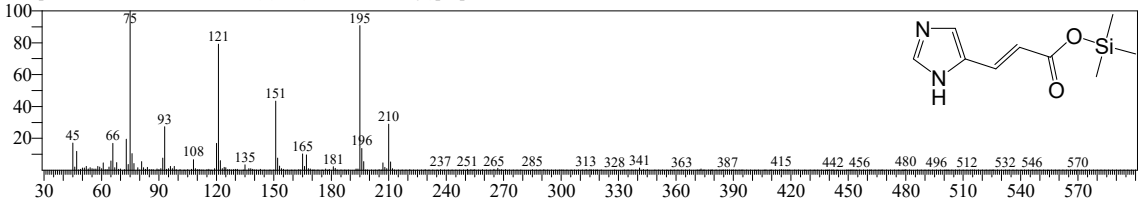
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



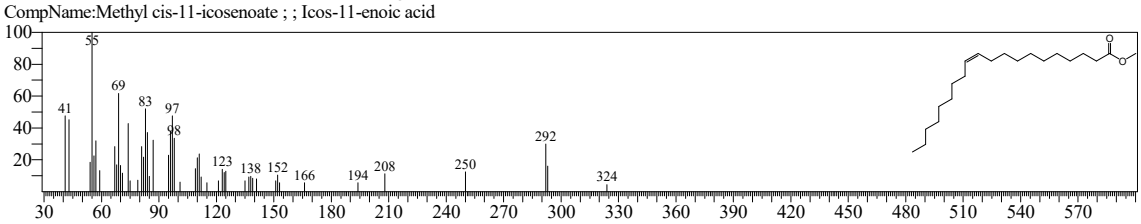
Hit#:2 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



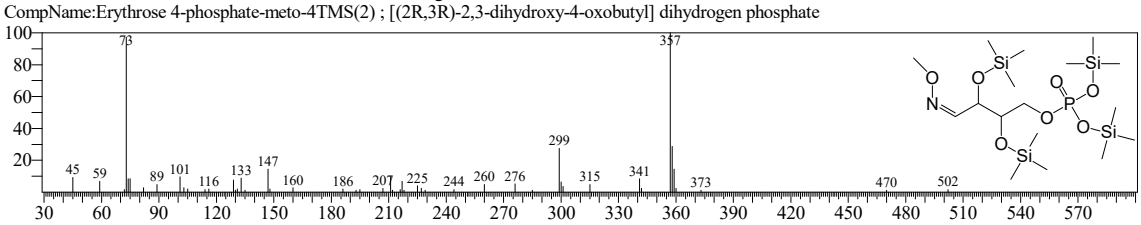
Hit#:3 Entry:361 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C9H14N2O2Si CAS:104-98-3 MolWeight:210 RetIndex:1896
CompName:Urocanic acid-TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:4 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:22 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid

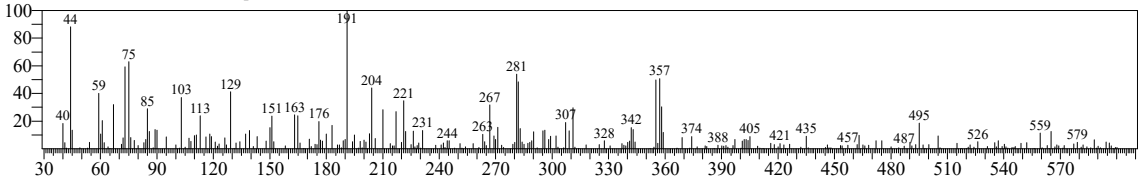


Hit#:5 Entry:394 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1935
CompName:Erythrose 4-phosphate-meto-4TMS(2) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate

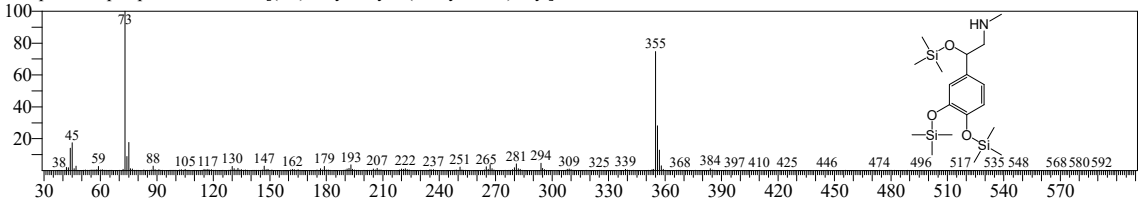


TNAU

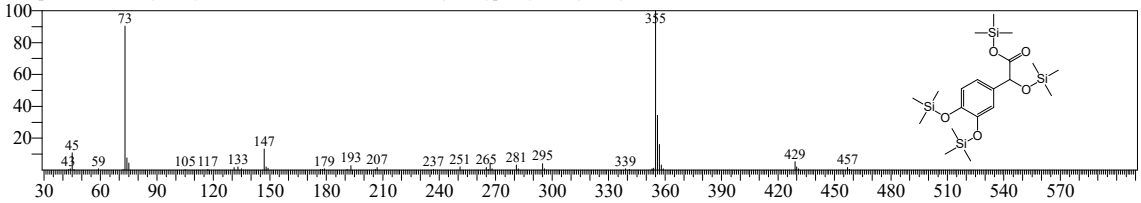
<< Target >>
Line#:6 R.Time:27.770(Scan#:4655) MassPeaks:275
RawMode:Averaged 27.765-27.775(4654-4656) BasePeak:191.00(807)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



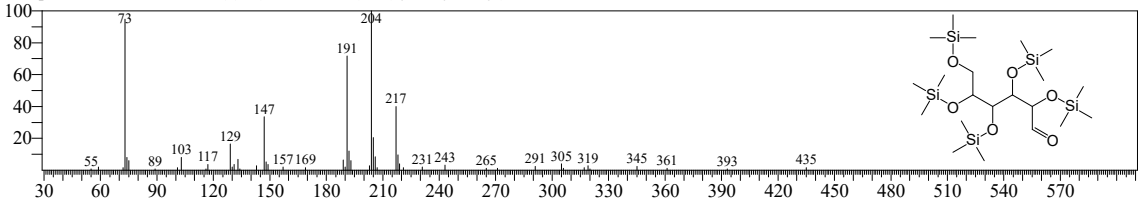
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



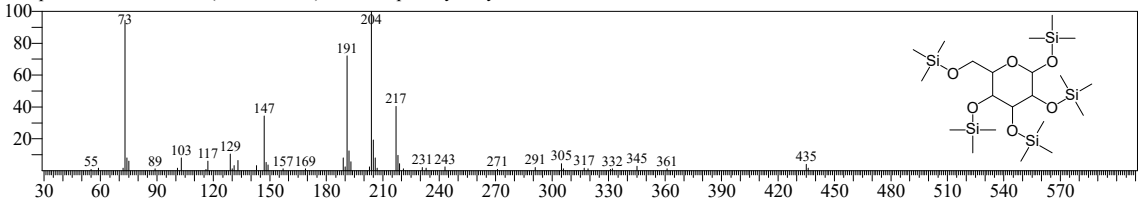
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



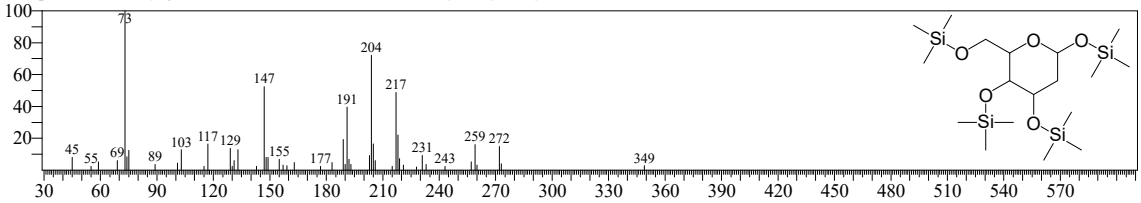
Hit#:3 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



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

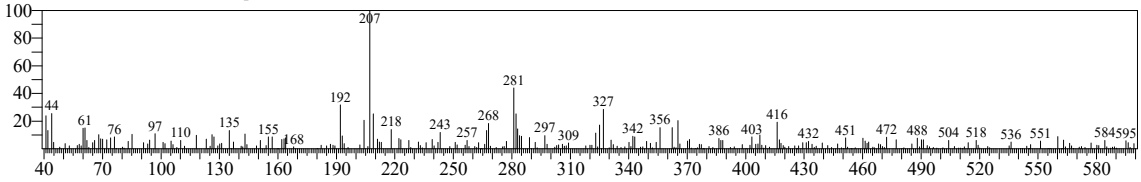


Hit#:5 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1816
CompName:2-Deoxy-glucose-4TMS(2) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

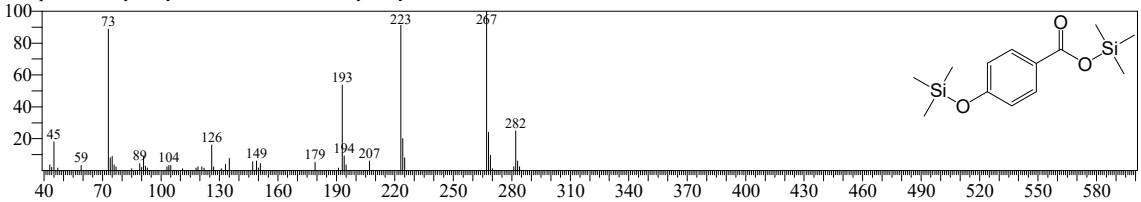


TNAU

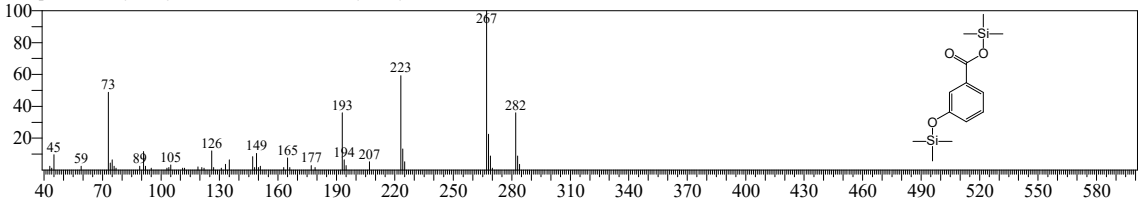
<< Target >>
Line#:7 R.Time:28.285(Scan#:4758) MassPeaks:282
RawMode:Averaged 28.280-28.290(4757-4759) BasePeak:207.05(1166)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



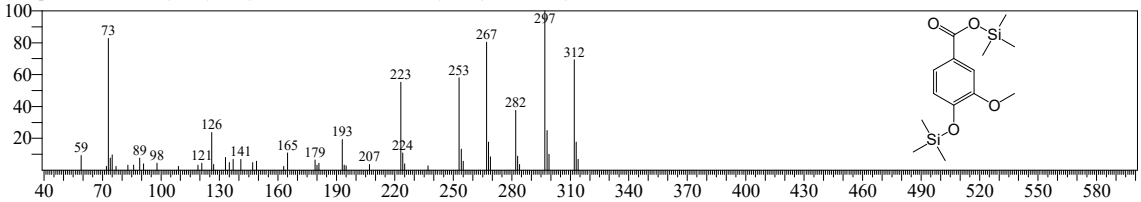
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



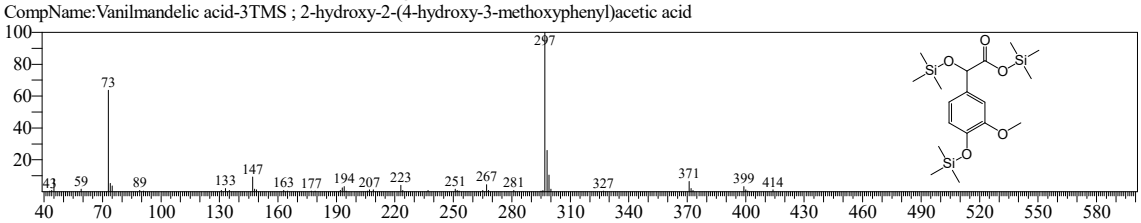
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



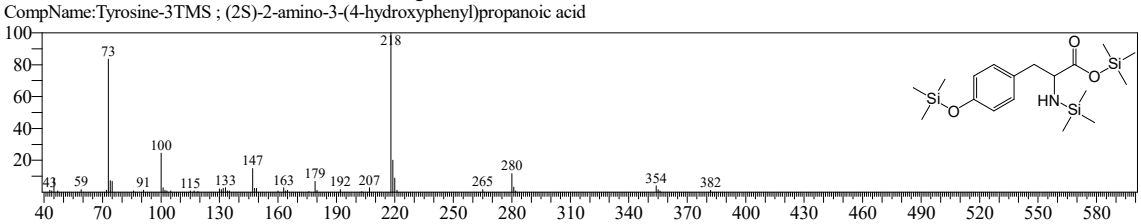
Hit#:3 Entry:291 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C14H24O4Si2 CAS:121-34-6 MolWeight:312 RetIndex:1775
CompName:3-Methoxy-4-hydroxybenzoic acid-2TMS ; 4-hydroxy-3-methoxybenzoic acid



Hit#:4 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

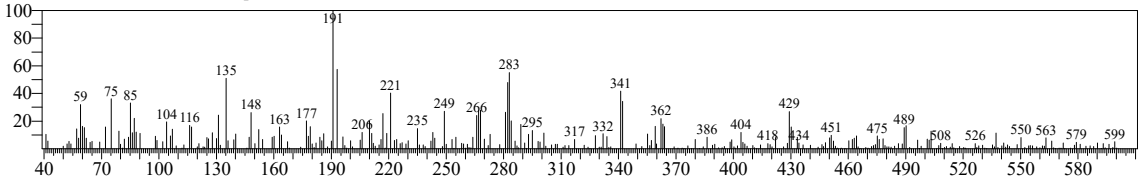


Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

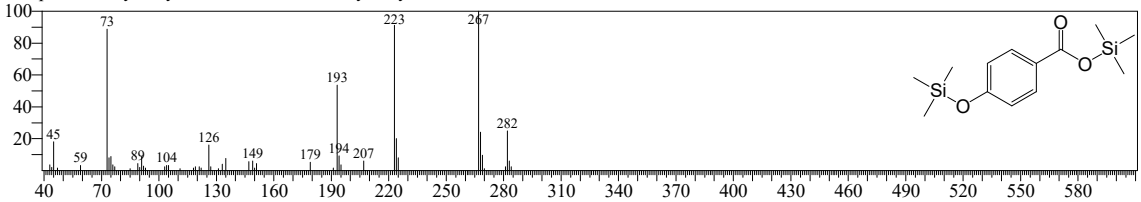


TNAU

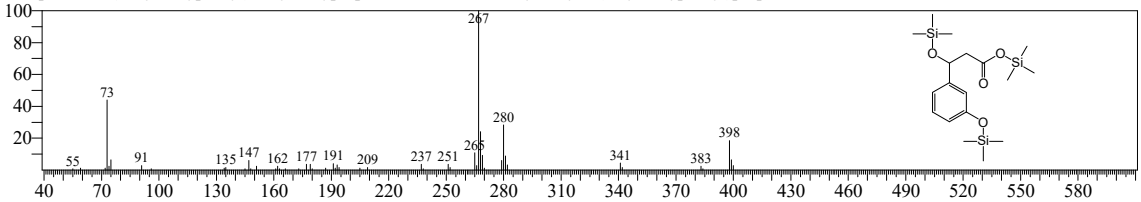
<< Target >>
Line#:8 R.Time:29.035(Scan#:4908) MassPeaks:318
RawMode:Averaged 29.030-29.040(4907-4909) BasePeak:190.95(844)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



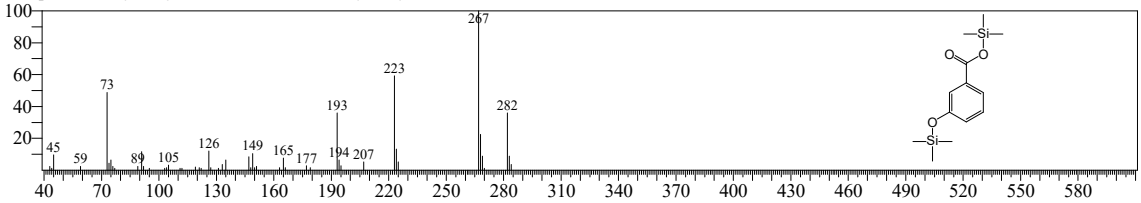
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



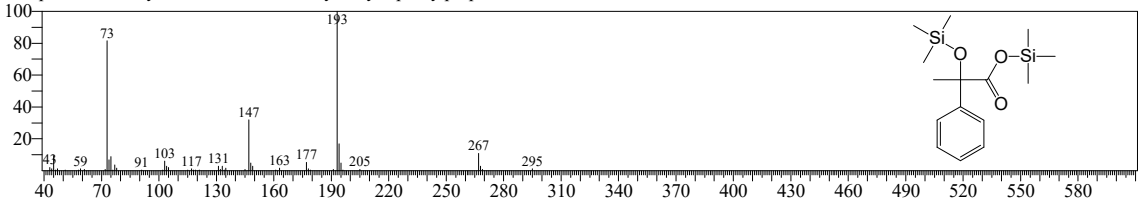
Hit#:2 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



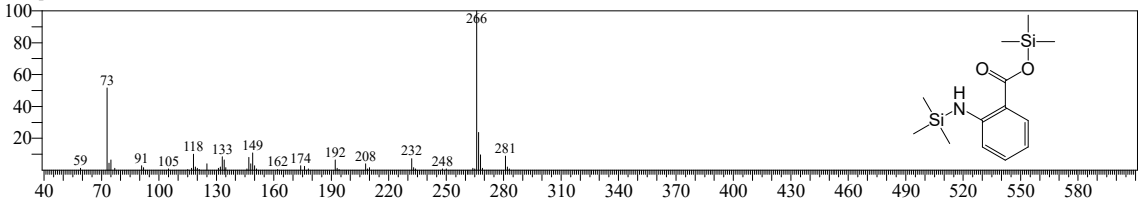
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry: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

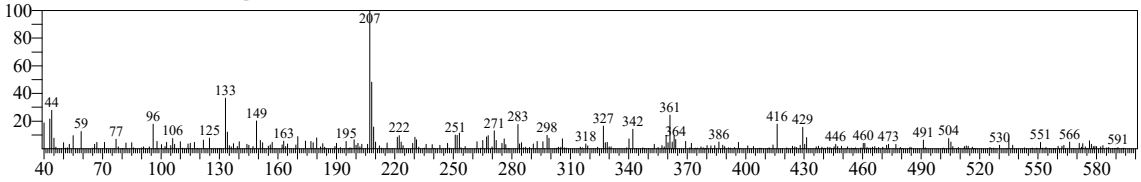


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

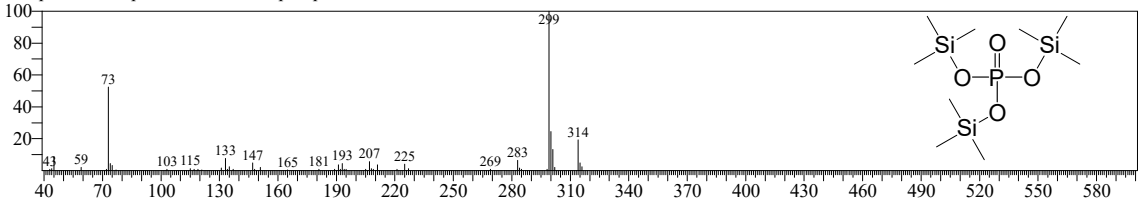


TNAU

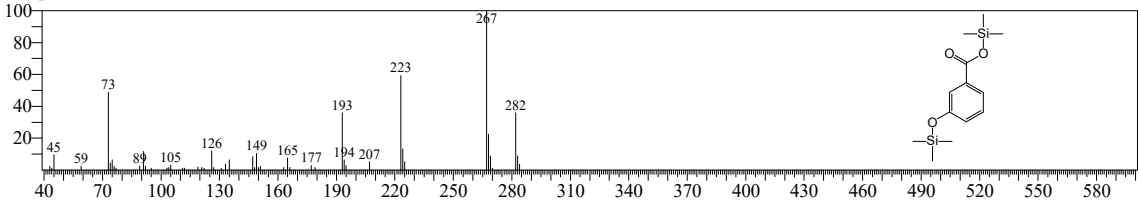
<< Target >>
Line#:9 R.Time:30.235(Scan#:5148) MassPeaks:289
RawMode:Averaged 30.230-30.240(5147-5149) BasePeak:207.05(1855)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



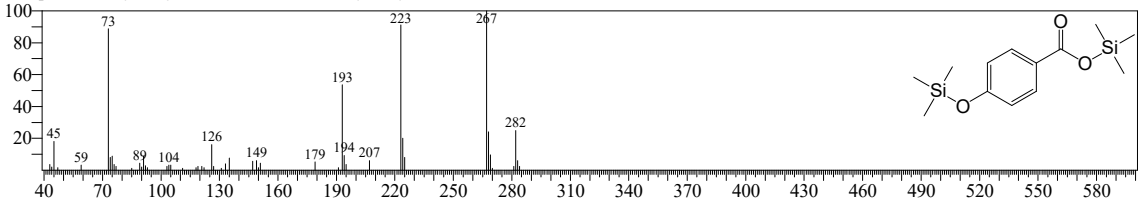
Hit#:1 Entry:79 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C9H27O4PSi3 CAS:7664-38-2 MolWeight:314 RetIndex:1280
CompName:Phosphoric acid-3TMS ; phosphoric acid



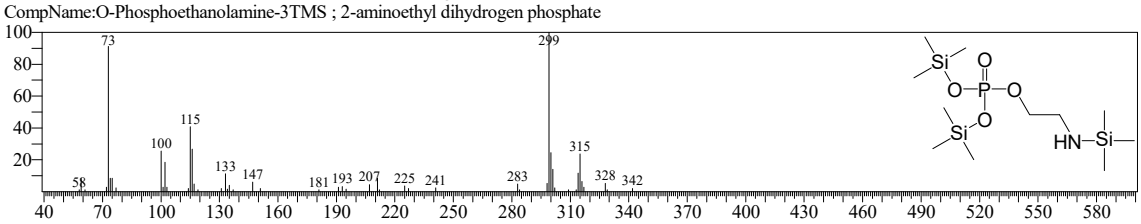
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



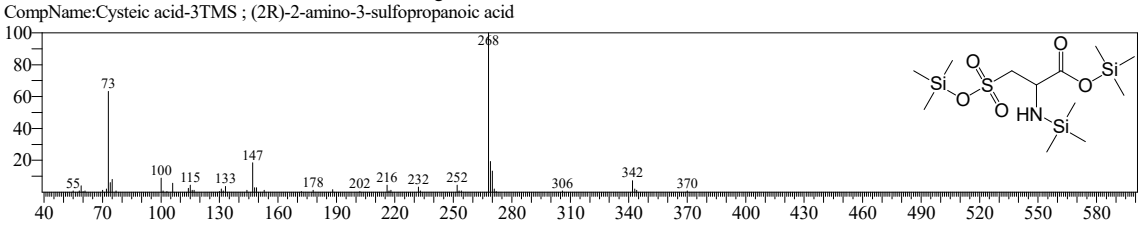
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:189 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C11H32NO4PSi3 CAS:1071-23-4 MolWeight:357 RetIndex:1587
CompName:O-Phosphoethanolamine-3TMS ; 2-aminoethyl dihydrogen phosphate

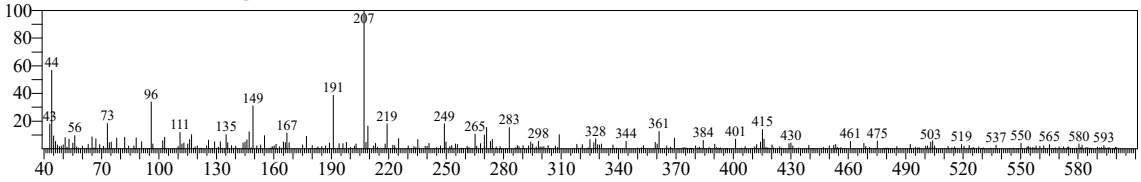


Hit#:5 Entry:277 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C12H31NO5SSi3 CAS:498-40-8 MolWeight:385 RetIndex:1749
CompName:Cysteic acid-3TMS ; (2R)-2-amino-3-sulfopropanoic acid

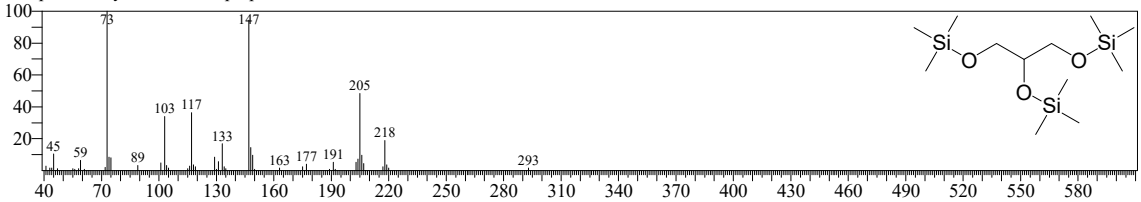


TNAU

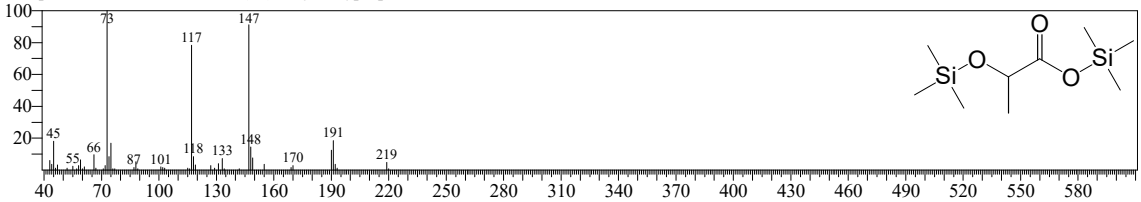
<< Target >>
Line#:10 R.Time:30.305(Scan#:5162) MassPeaks:295
RawMode:Averaged 30.300-30.310(5161-5163) BasePeak:207.05(1710)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



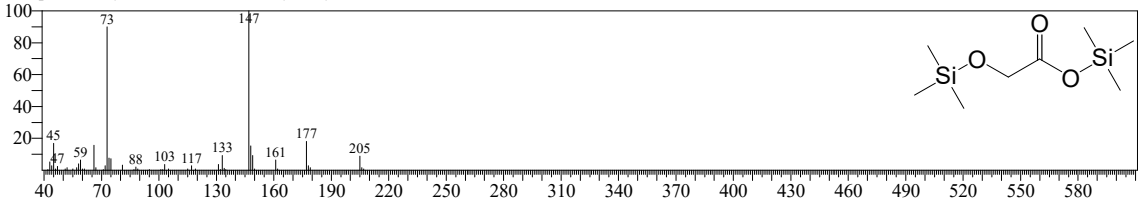
Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



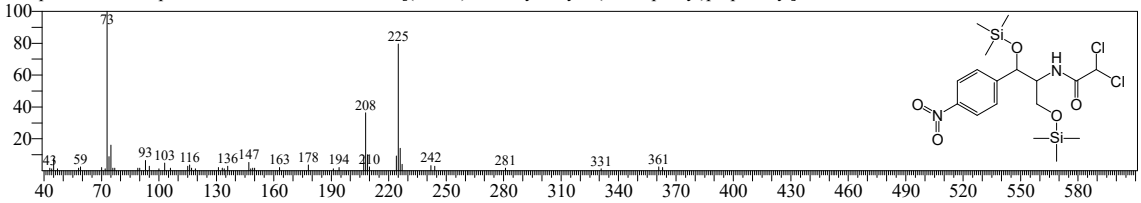
Hit#:2 Entry:8 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C9H22O3Si2 CAS:79-33-4 MolWeight:234 RetIndex:1061
CompName:Lactic acid-2TMS ; (2S)-2-hydroxypropanoic acid



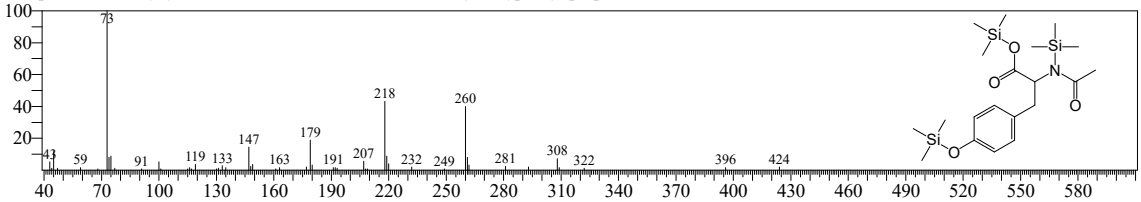
Hit#:3 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid



Hit#:4 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

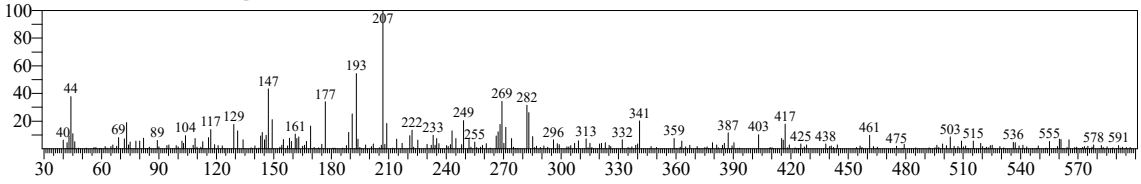


Hit#:5 Entry:461 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H37NO4Si3 CAS:537-55-3 MolWeight:439 RetIndex:2119
CompName:N-Acetyltyrosine-3TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid

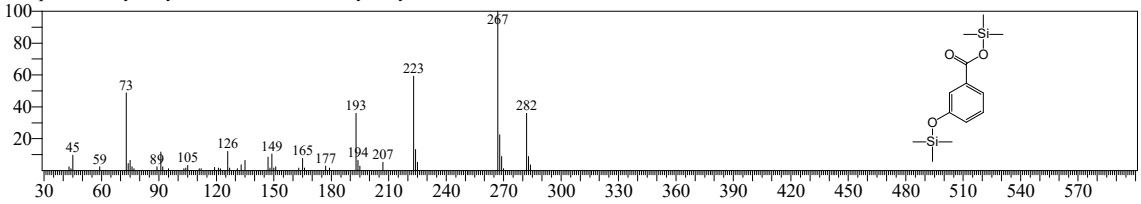


TNAU

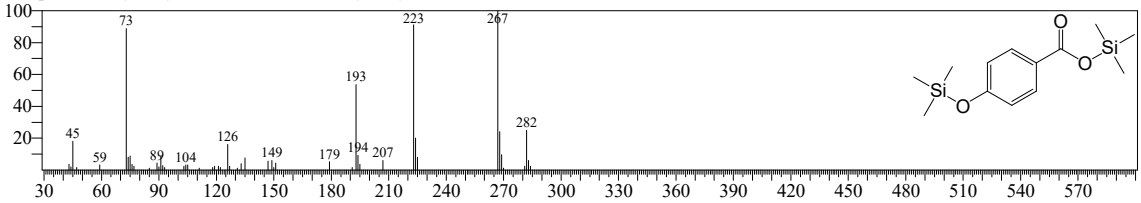
<< Target >>
Line#:11 R.Time:30.355(Scan#:5172) MassPeaks:280
RawMode:Averaged 30.350-30.360(5171-5173) BasePeak:207.05(1671)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



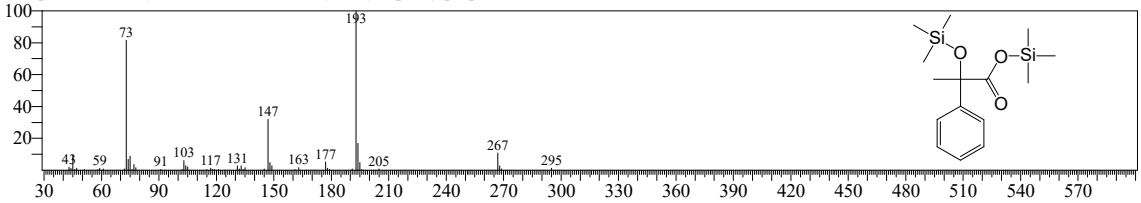
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



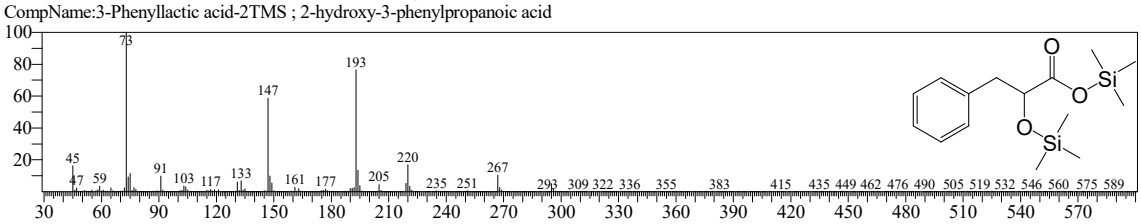
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



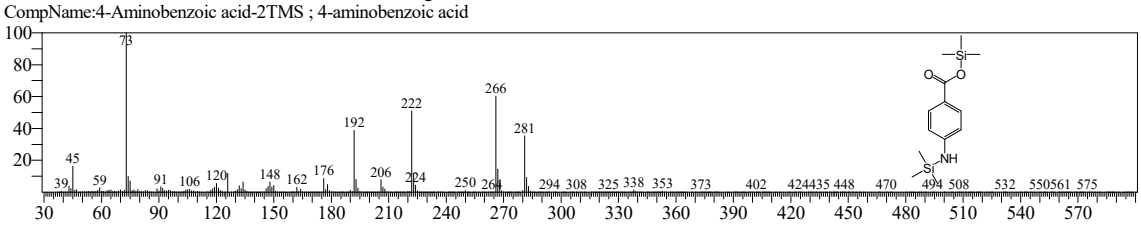
Hit#:3 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

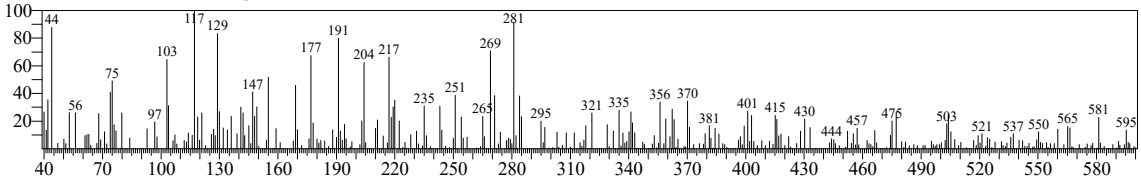


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

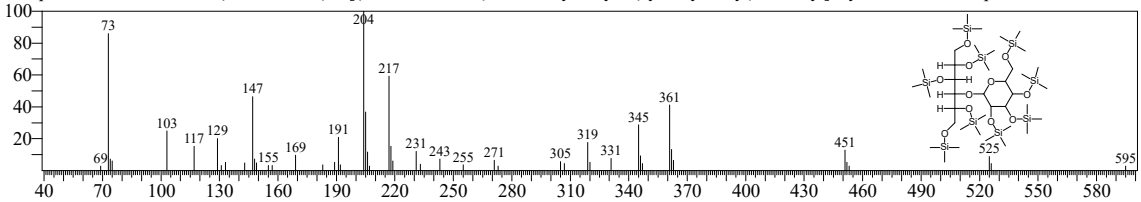


TNAU

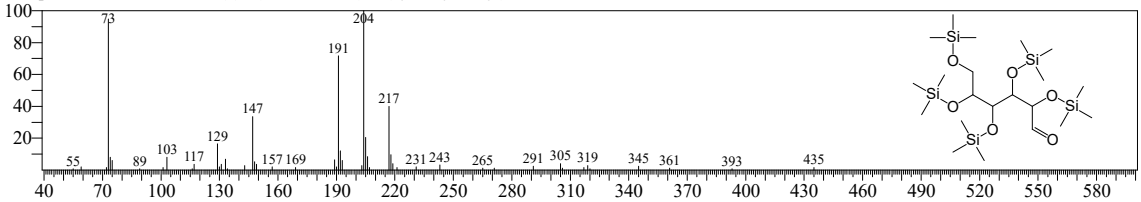
<< Target >>
Line#:12 R.Time:30.685(Scan#:5238) MassPeaks:330
RawMode:Averaged 30.680-30.690(5237-5239) BasePeak:117.10(584)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



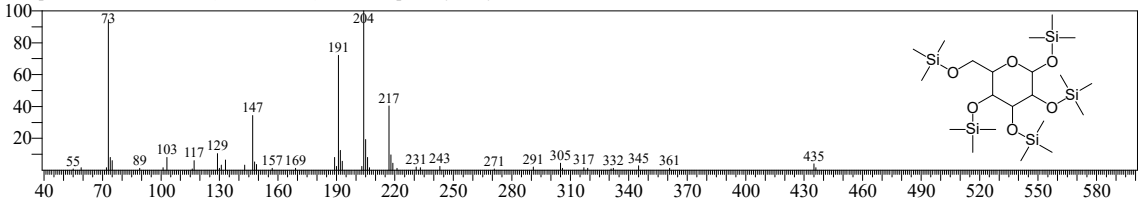
Hit#:1 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



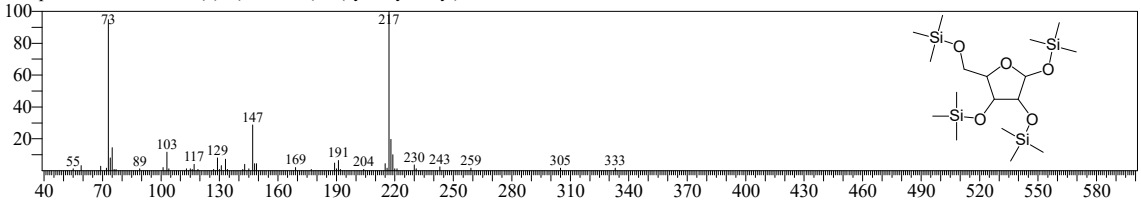
Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



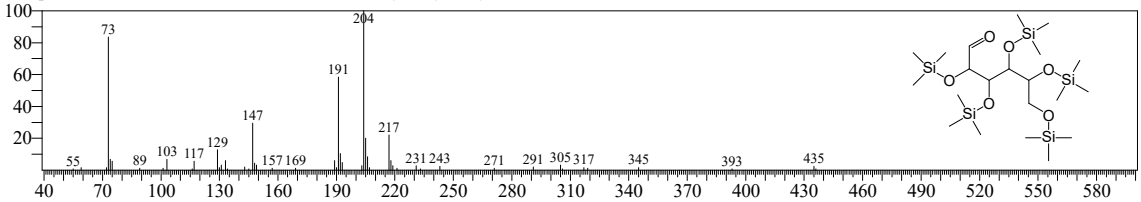
Hit#:3 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:4 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

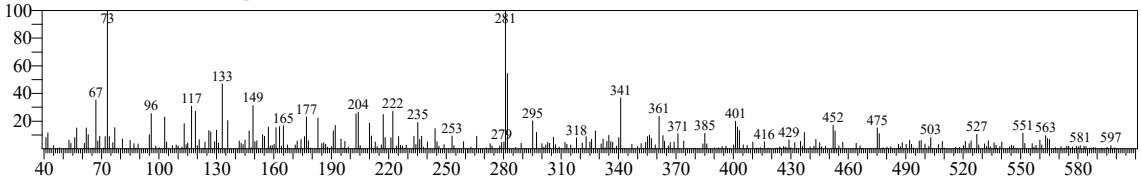


Hit#:5 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

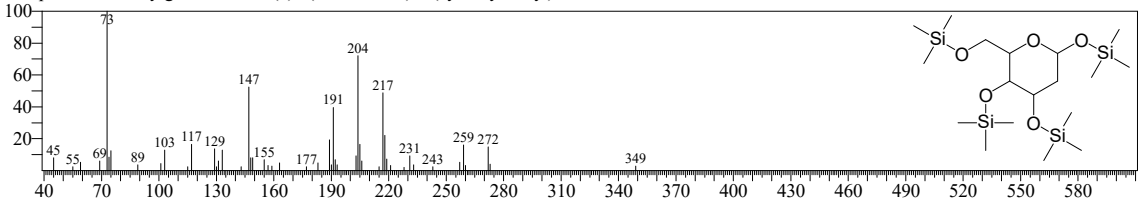


TNAU

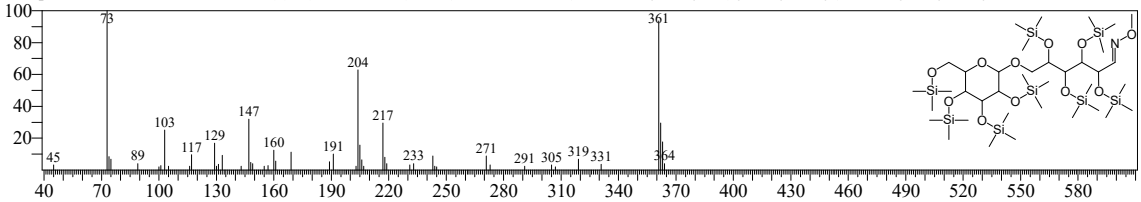
<< Target >>
Line#:13 R.Time:30.765(Scan#:5254) MassPeaks:306
RawMode:Averaged 30.760-30.770(5253-5255) BasePeak:281.05(1120)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



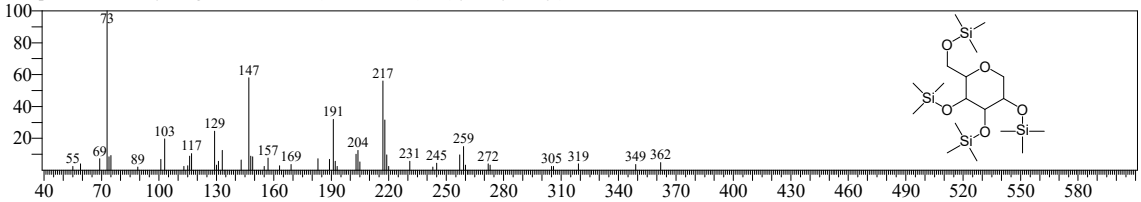
Hit#:1 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1816
CompName:2-Deoxy-glucose-4TMS(2) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



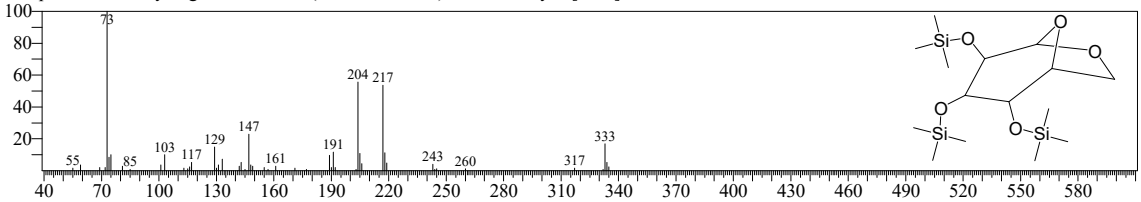
Hit#:2 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



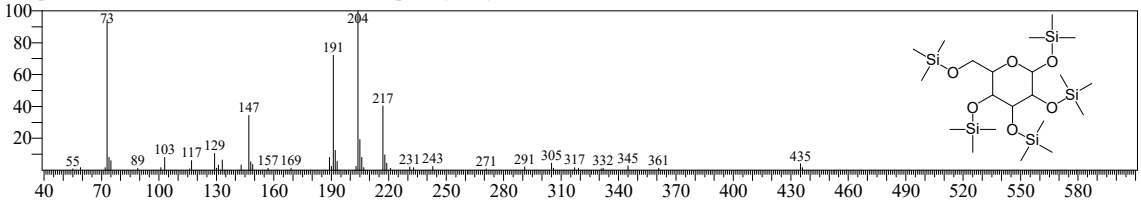
Hit#:3 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol



Hit#:4 Entry:264 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C15H34O5Si3 CAS:498-07-7 MolWeight:378 RetIndex:1725
CompName:1,6-Anhydroglucose-3TMS ; (1R,2S,3S,4R,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol

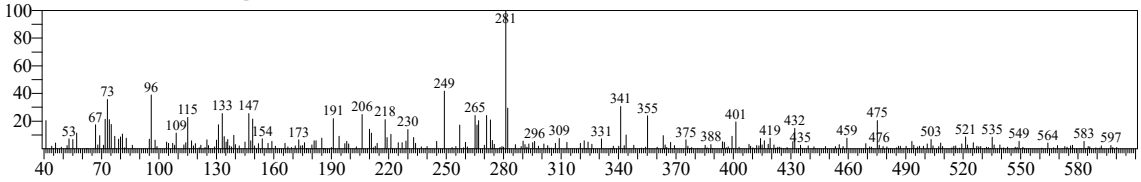


Hit#:5 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

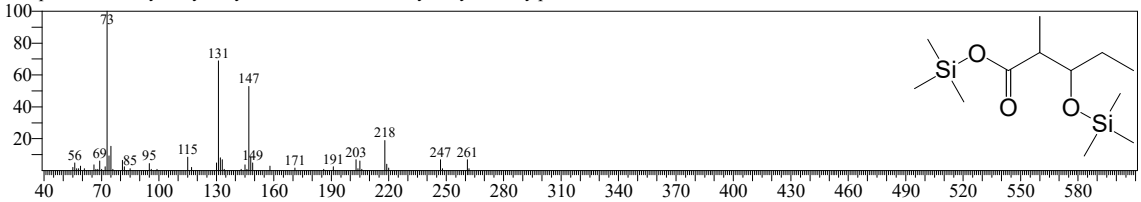


TNAU

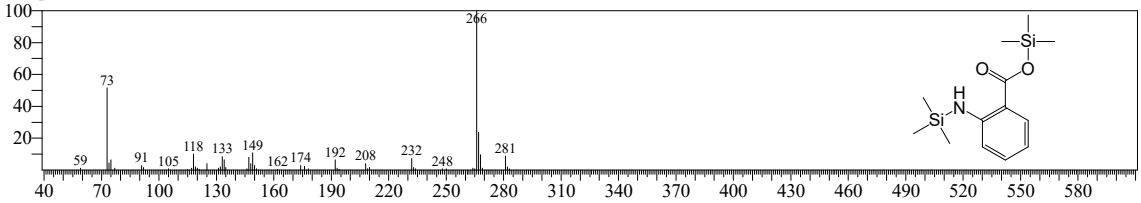
<< Target >>
Line#:14 R.Time:30.845(Scan#:5270) MassPeaks:283
RawMode:Averaged 30.840-30.850(5269-5271) BasePeak:281.10(1187)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



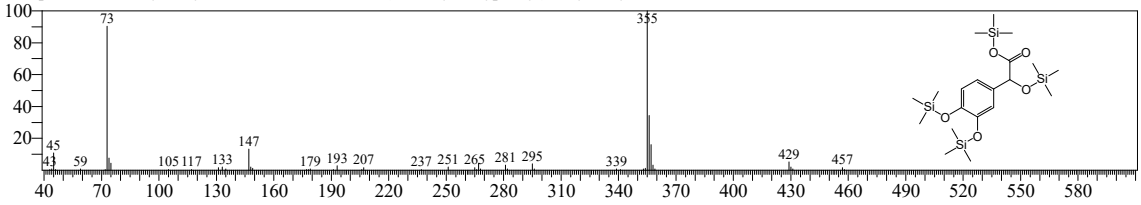
Hit#:1 Entry:74 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C12H28O3Si2 CAS:28892-73-1 MolWeight:276 RetIndex:1277
CompName:2-Methyl-3-hydroxyvaleric acid-2TMS ; 3-hydroxy-2-methylpentanoic acid



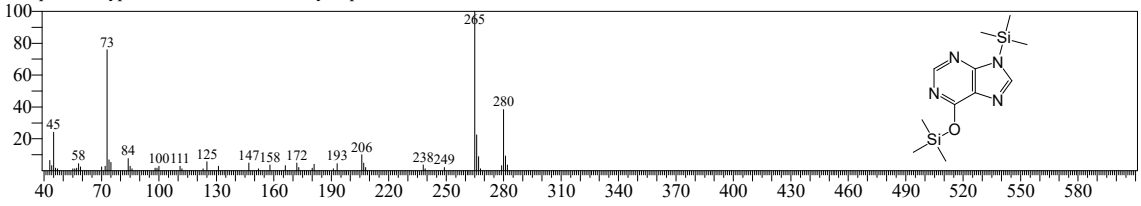
Hit#:2 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



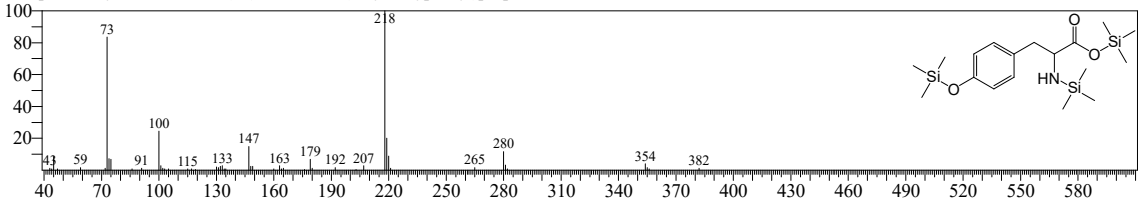
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

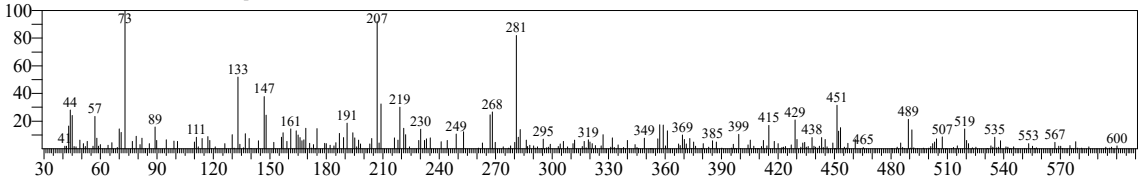


Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

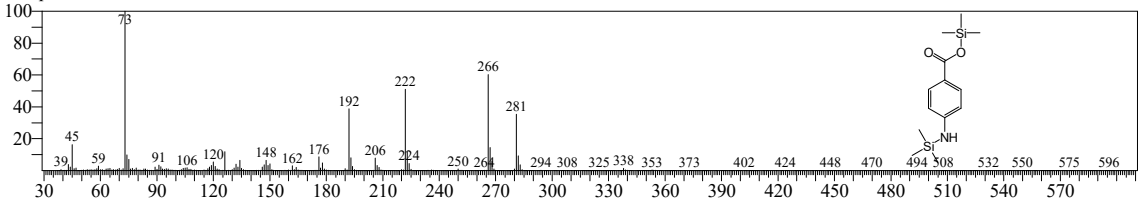


TNAU

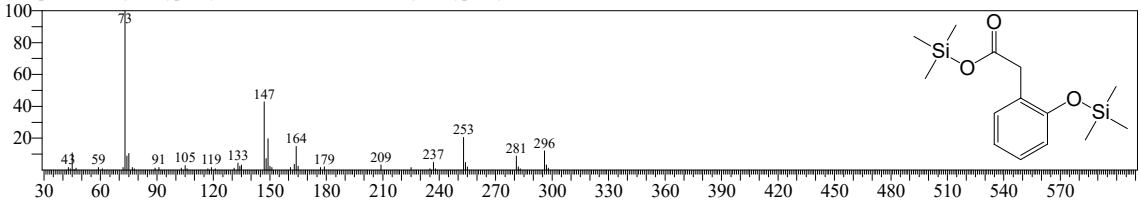
<< Target >>
Line#:15 R.Time:31.115(Scan#:5324) MassPeaks:275
RawMode:Averaged 31.110-31.120(5323-5325) BasePeak:73.00(1233)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



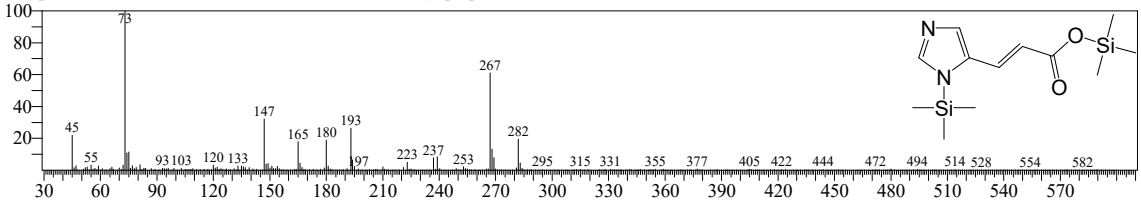
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



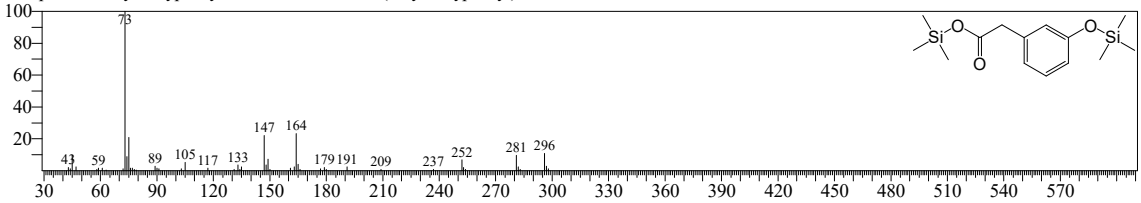
Hit#:2 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



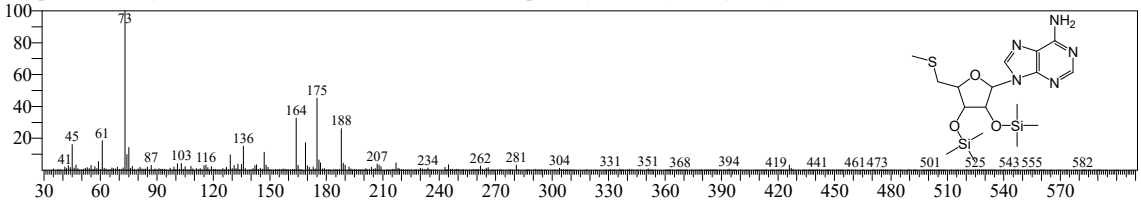
Hit#:3 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:4 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

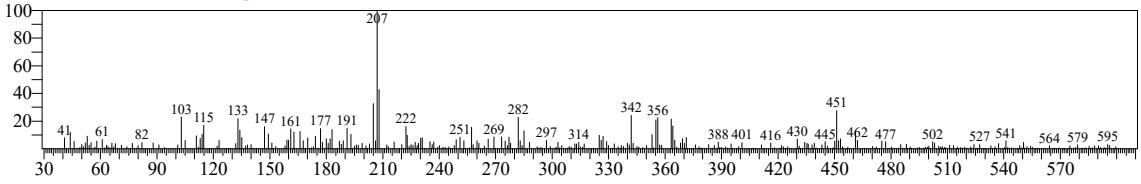


Hit#:5 Entry:548 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787
CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol

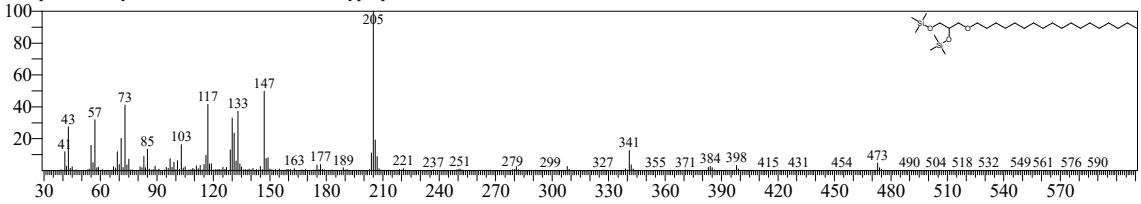


TNAU

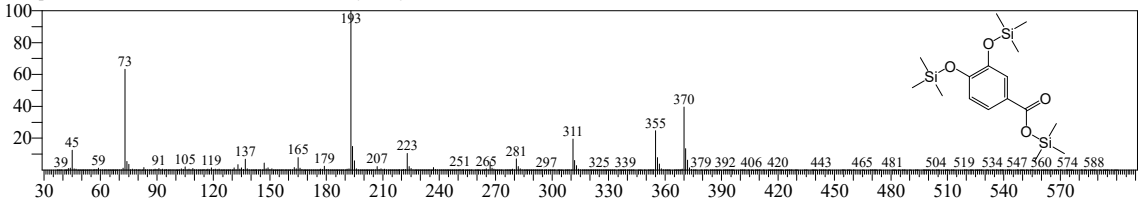
<< Target >>
Line#:16 R.Time:31.285(Scan#:5358) MassPeaks:313
RawMode:Averaged 31.280-31.290(5357-5359) BasePeak:207.05(1756)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



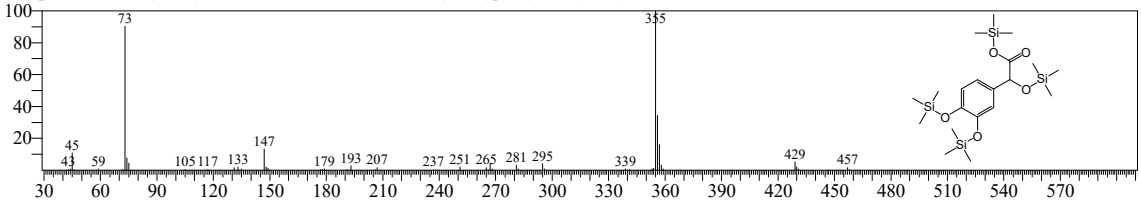
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



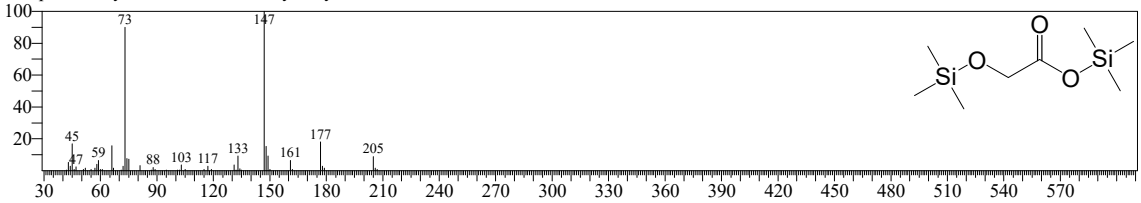
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



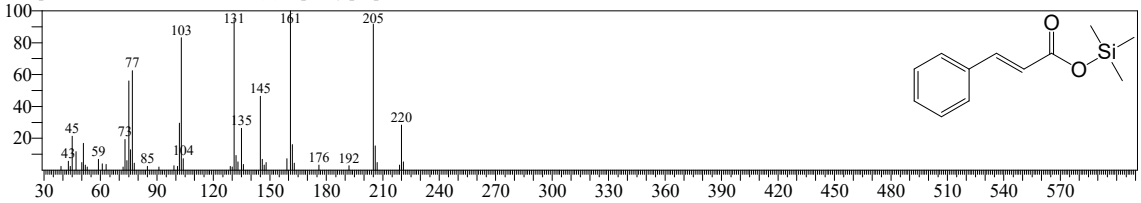
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

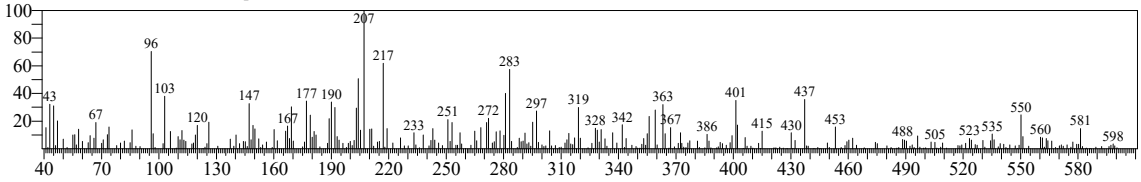


Hit#:5 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid

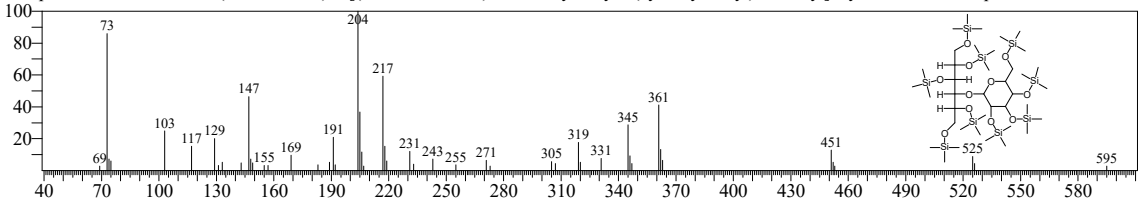


TNAU

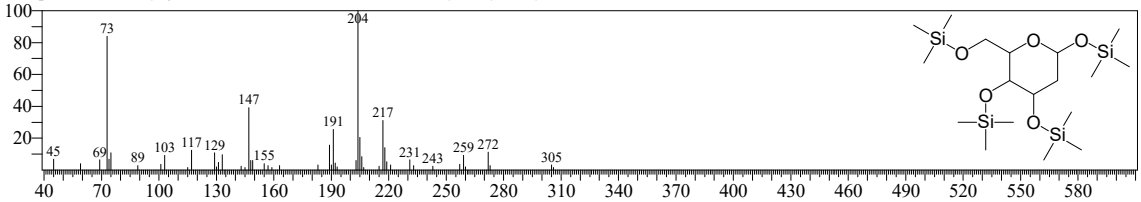
<< Target >>
Line#:17 R.Time:31.560(Scan#:5413) MassPeaks:325
RawMode:Averaged 31.555-31.565(5412-5414) BasePeak:207.05(820)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



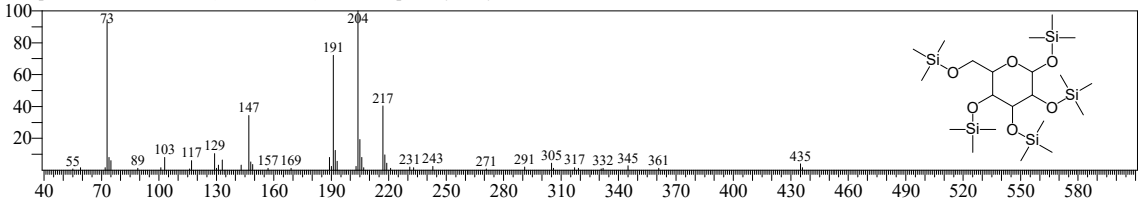
Hit#:1 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



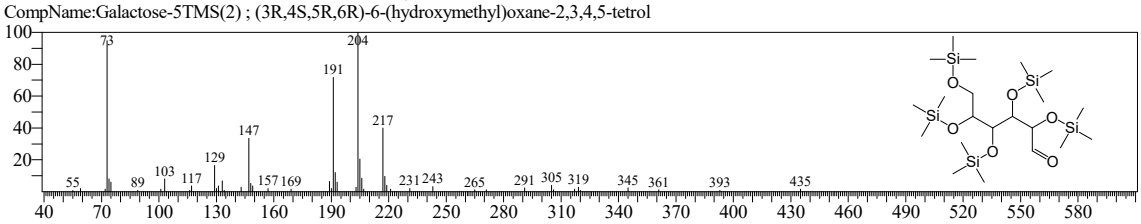
Hit#:2 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



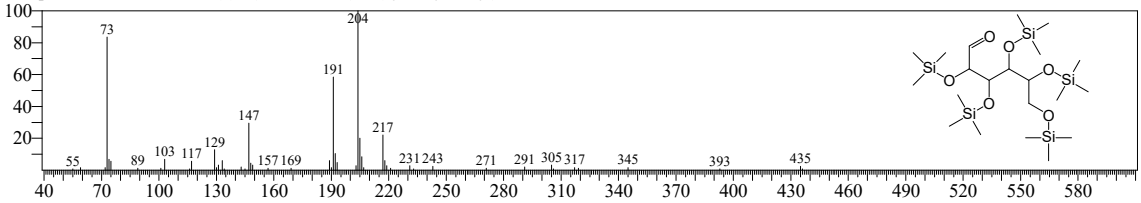
Hit#:3 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:4 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

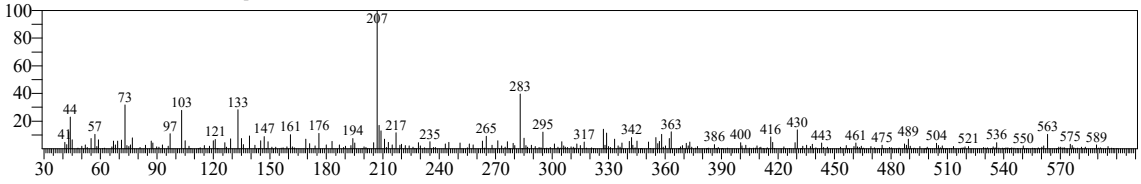


Hit#:5 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

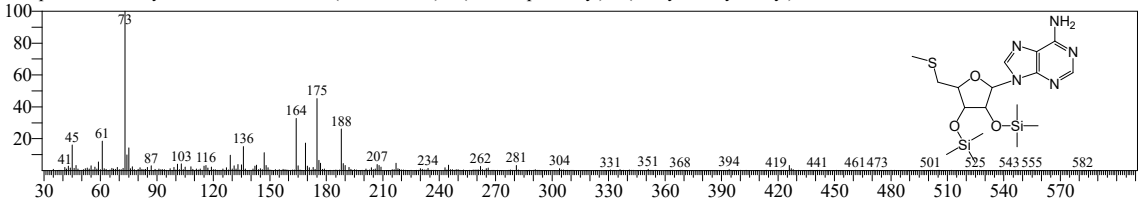


TNAU

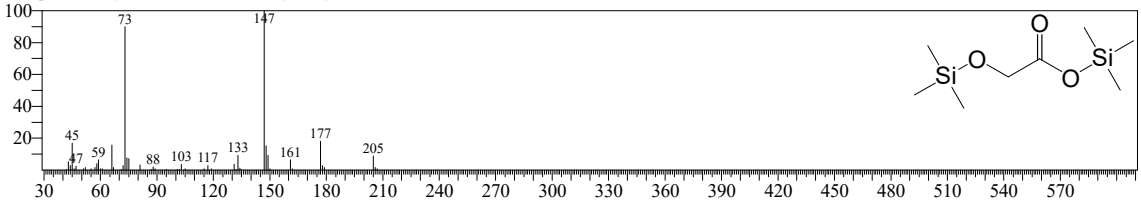
<< Target >>
Line#:18 R.Time:31.885(Scan#:5478) MassPeaks:300
RawMode:Averaged 31.880-31.890(5477-5479) BasePeak:207.05(2682)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



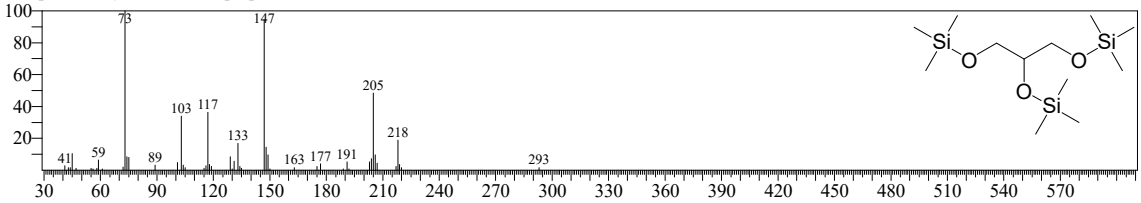
Hit#:1 Entry:548 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787
CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol



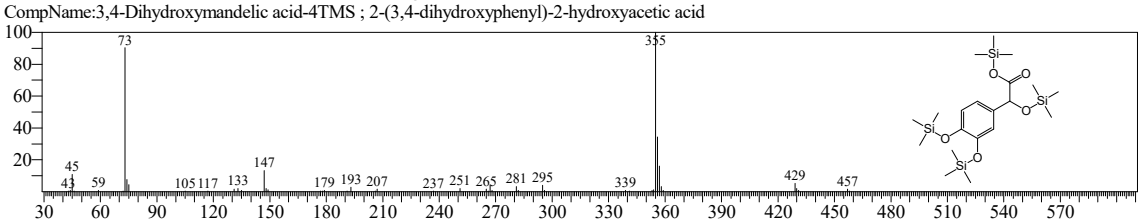
Hit#:2 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid



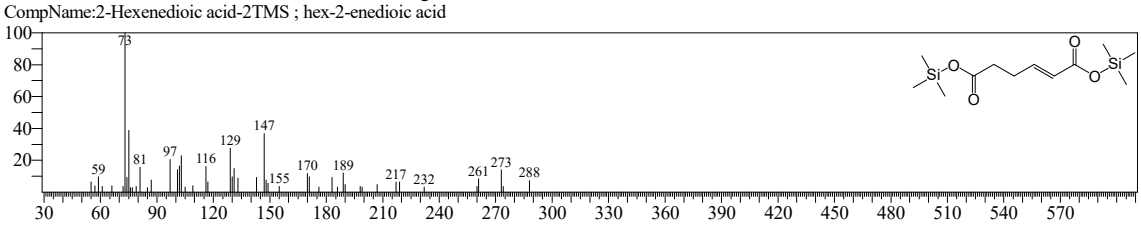
Hit#:3 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



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

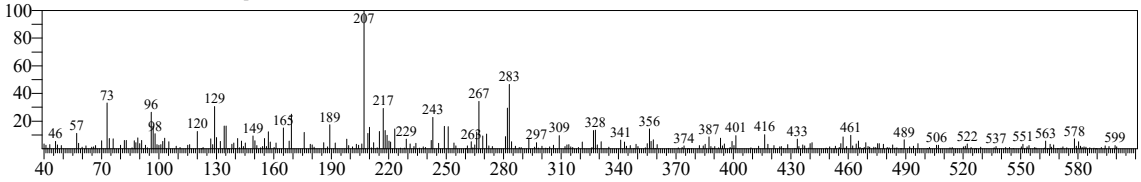


Hit#:5 Entry:156 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C12H24O4Si2 CAS:4440-68-0 MolWeight:288 RetIndex:1522
CompName:2-Hexenedioic acid-2TMS ; hex-2-enedioic acid

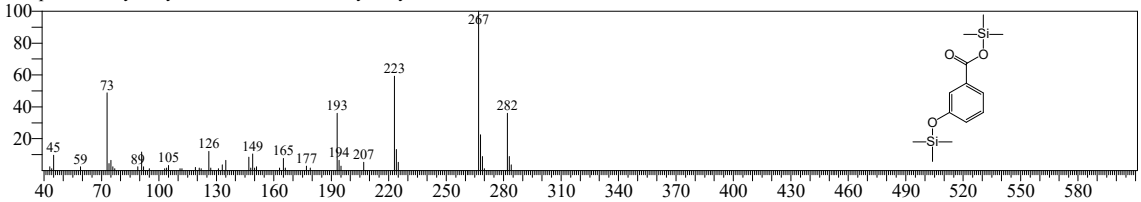


TNAU

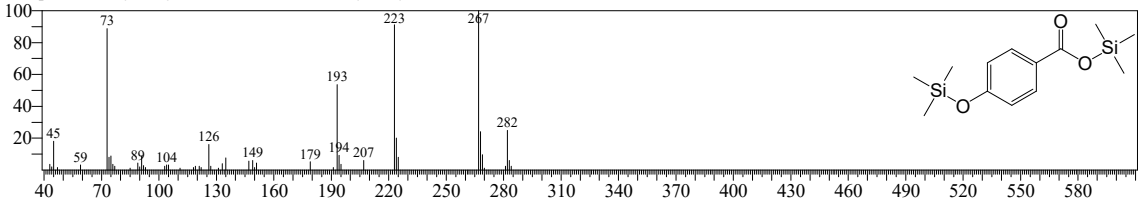
<< Target >>
Line#:19 R.Time:32.365(Scan#:5574) MassPeaks:293
RawMode:Averaged 32.360-32.370(5573-5575) BasePeak:207.05(1745)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



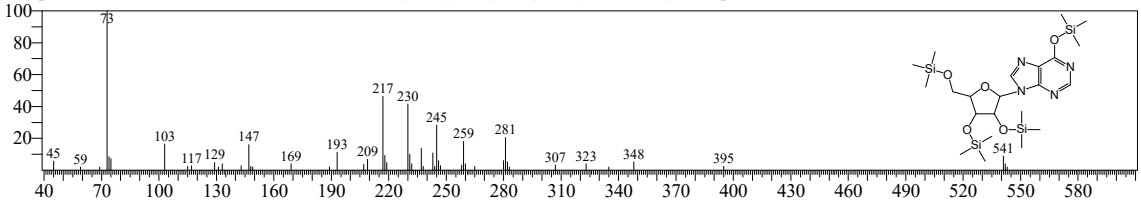
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



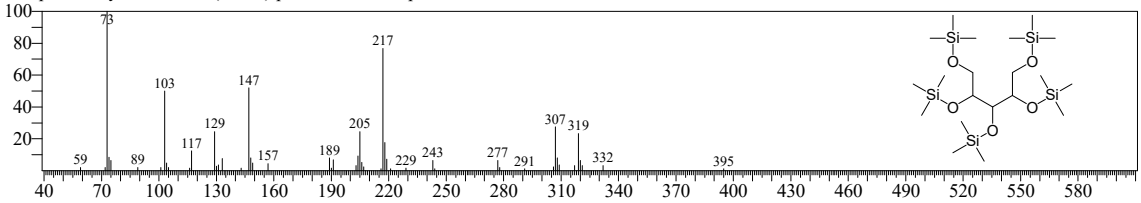
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



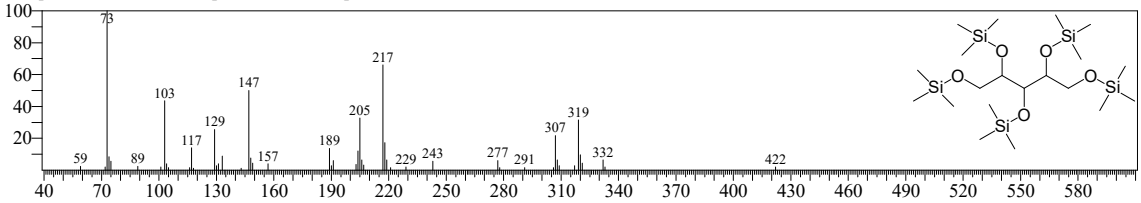
Hit#:3 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



Hit#:4 Entry:268 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C20H52O5Si5 CAS:87-99-0 MolWeight:512 RetIndex:1732
CompName:Xylitol-5TMS ; (2S,4R)-pentane-1,2,3,4,5-pentol

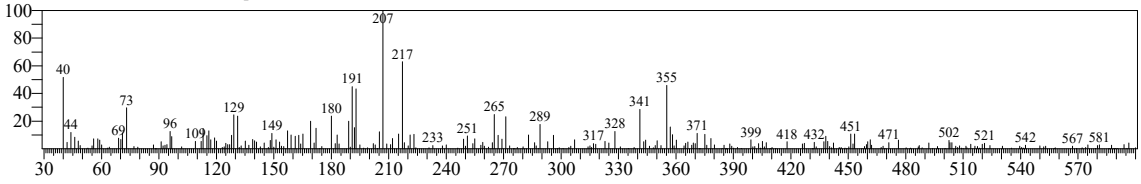


Hit#:5 Entry:279 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C20H52O5Si5 CAS:488-81-3 MolWeight:512 RetIndex:1750
CompName:Ribitol-5TMS ; pentane-1,2,3,4,5-pentol

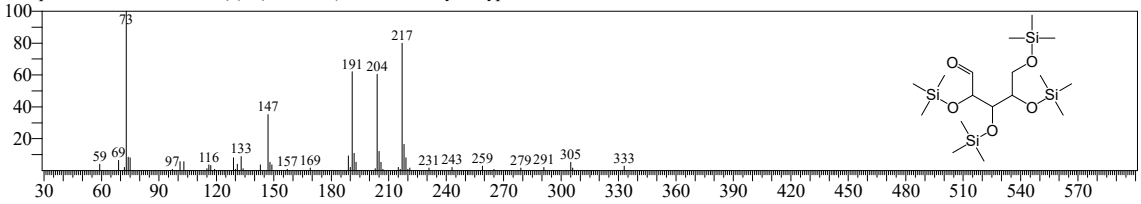


TNAU

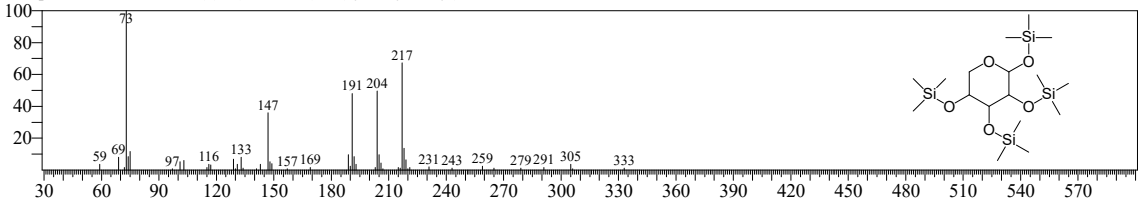
<< Target >>
Line#:20 R.Time:32.470(Scan#:5595) MassPeaks:278
RawMode:Averaged 32.465-32.475(5594-5596) BasePeak:207.05(1555)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



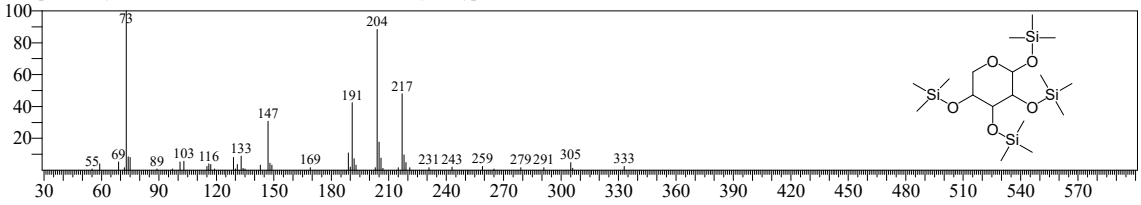
Hit#:1 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



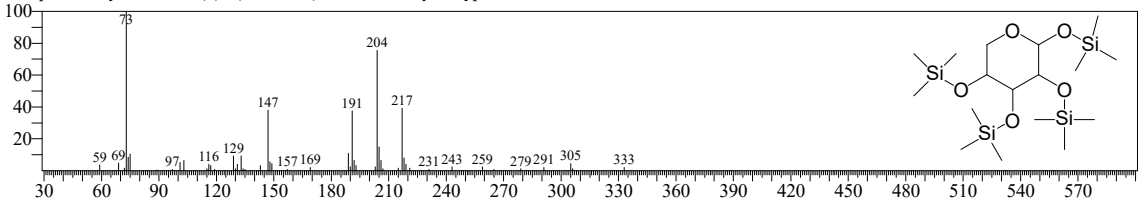
Hit#:2 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



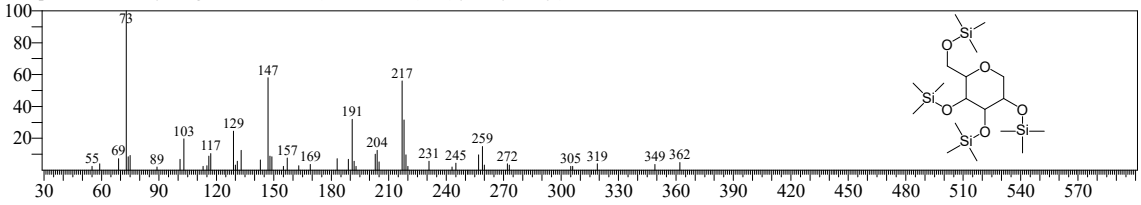
Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

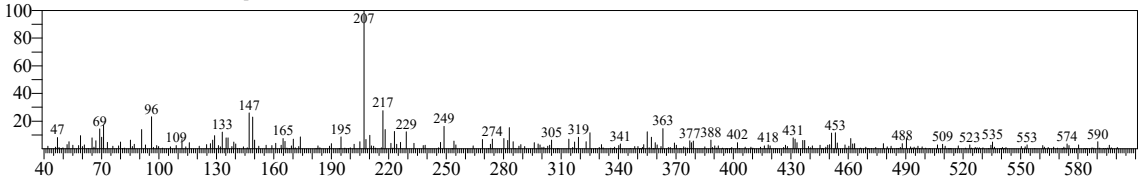


Hit#:5 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol

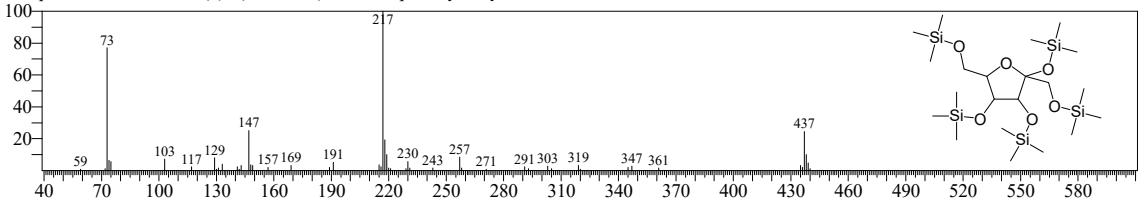


TNAU

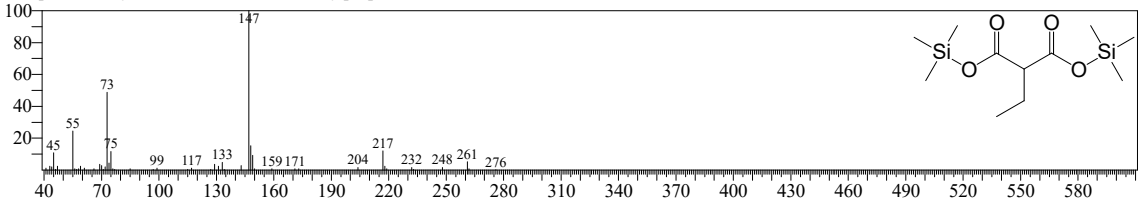
<< Target >>
Line#:21 R.Time:32.520(Scan#:5605) MassPeaks:290
RawMode:Averaged 32.515-32.525(5604-5606) BasePeak:207.05(2001)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



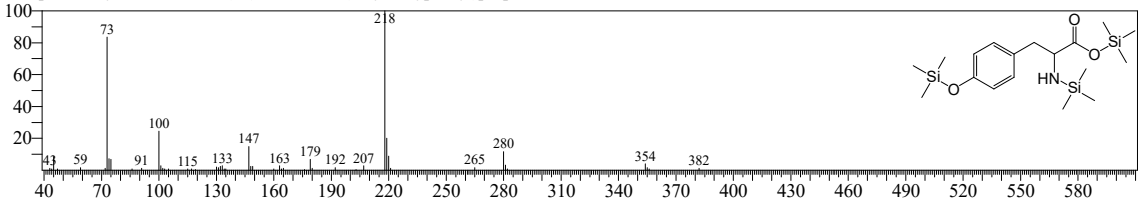
Hit#:1 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



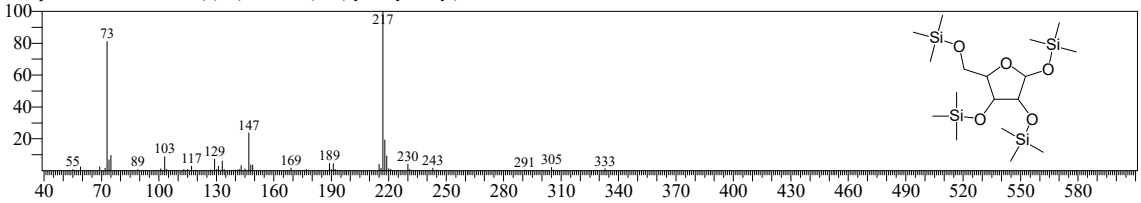
Hit#:2 Entry:80 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C11H24O4Si2 CAS:601-75-2 MolWeight:276 RetIndex:1284
CompName:Ethylmalonic acid-2TMS ; 2-ethylpropanedioic acid



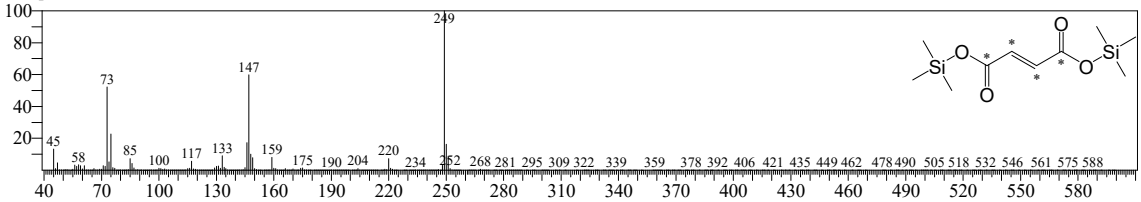
Hit#:3 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid



Hit#:4 Entry:230 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1666
CompName:Ribose-4TMS(2) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

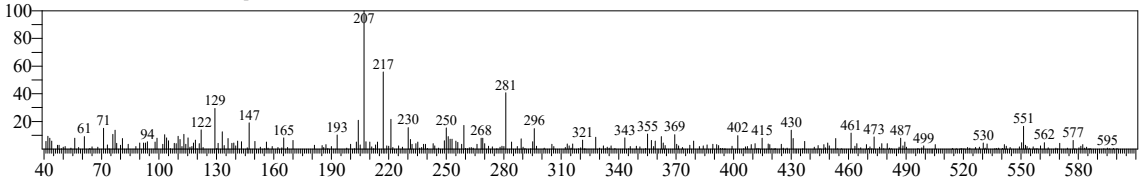


Hit#:5 Entry:100 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula: CAS:0-00-0 MolWeight:264 RetIndex:1346
CompName:Fumaric acid-13C4-2TMS ;

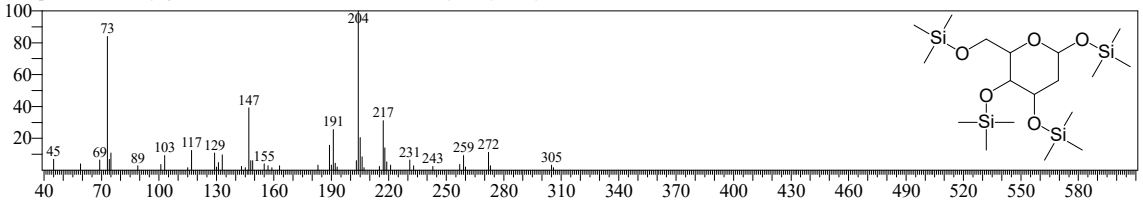


TNAU

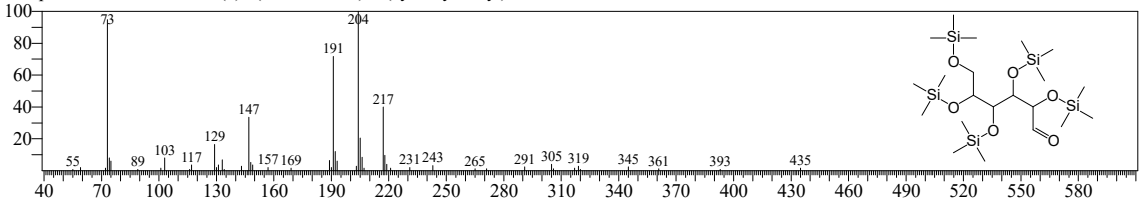
<< Target >>
Line#:22 R.Time:32.820(Scan#:5665) MassPeaks:305
RawMode:Averaged 32.815-32.825(5664-5666) BasePeak:207.05(1534)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



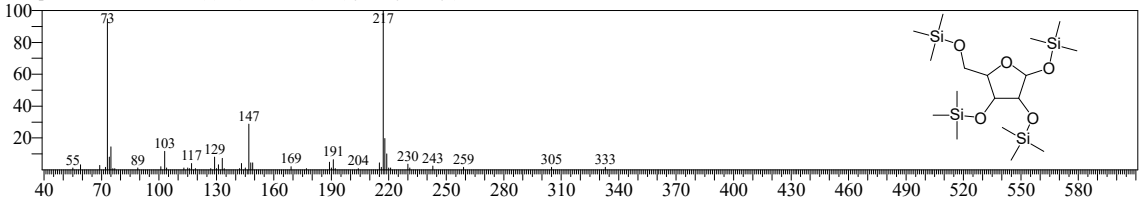
Hit#:1 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



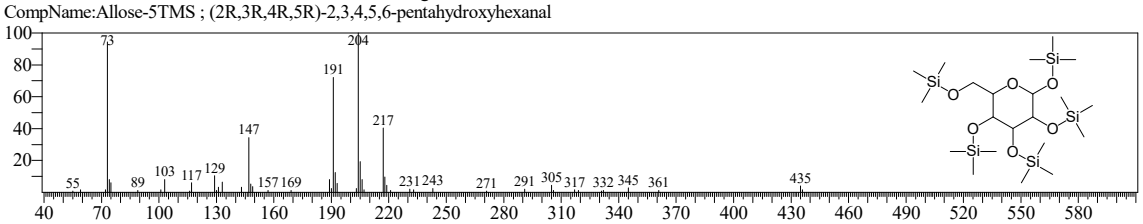
Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:3 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



Hit#:4 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:5 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol