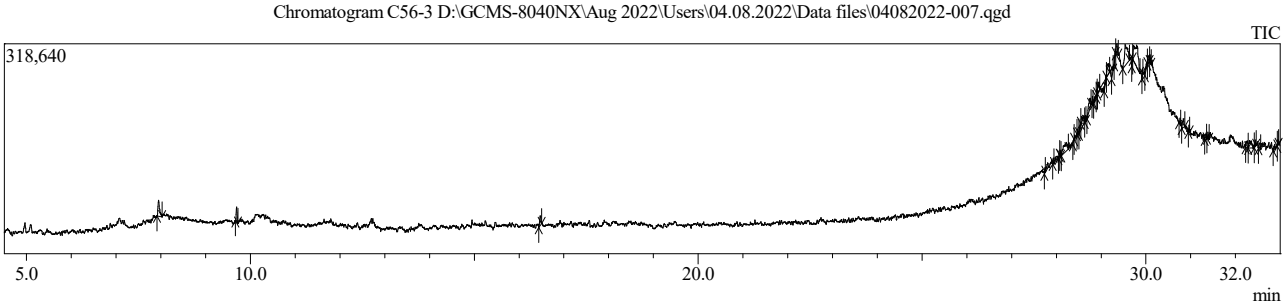
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 04-Aug-22 8:48:23 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C56-3
Sample ID	: C56-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 7
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-007.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-007.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 4:23:03 PM

Chromatogram C56-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-007.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.948	61909	5.40	24017	4.89	2.58	86	Decane
2	9.690	30853	2.69	22734	4.63	1.36	87	Undecane
3	16.467	28864	2.52	14990	3.06	1.93	80	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
4	27.745	7402	0.65	8659	1.76	0.85	27	Galactose-5TMS(2)
5	27.931	9469	0.83	9161	1.87	1.03	34	Allose-5TMS
6	28.055	5414	0.47	6039	1.23	0.90	28	Sucrose-8TMS
7	28.086	6708	0.59	9098	1.85	0.74	35	Isomaltose-meto-8TMS(2)
8	28.221	85719	7.48	13617	2.78	6.29	51	Sucrose-8TMS
9	28.375	4169	0.36	3743	0.76	1.11	26	4-Hydroxybenzoic acid-2TMS
10	28.405	4039	0.35	5232	1.07	0.77	26	Ribose-4TMS(1)
11	28.475	9561	0.83	7154	1.46	1.34	36	Trehalose-8TMS
12	28.535	11108	0.97	6099	1.24	1.82	36	Trehalose-8TMS
13	28.605	37331	3.26	10602	2.16	3.52	43	Trehalose-8TMS
14	28.646	7251	0.63	9788	1.99	0.74	29	Ribose-4TMS(1)
15	28.754	56676	4.95	14330	2.92	3.96	41	Lactitol-9TMS
16	28.807	9074	0.79	11515	2.35	0.79	34	3-Hydroxybenzoic acid-2TMS
17	28.855	10695	0.93	5831	1.19	1.83	27	Glucose-5TMS(2)
18	28.901	5911	0.52	9141	1.86	0.65	39	Arabinose-4TMS(1)
19	28.953	30313	2.64	12879	2.62	2.35	37	Sucrose-8TMS
20	29.100	16641	1.45	10415	2.12	1.60	39	Maltitol-9TMS
21	29.157	48547	4.24	16486	3.36	2.94	46	Sucrose-8TMS
22	29.250	16830	1.47	10870	2.22	1.55	35	3-Hydroxybenzoic acid-2TMS

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Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
23	29.315	15784	1.38	11383	2.32	1.39	36	Maltitol-9TMS
24	29.353	26481	2.31	15787	3.22	1.68	49	Trehalose-8TMS
25	29.538	152483	13.30	32062	6.53	4.76	59	Sucrose-8TMS
26	29.690	8688	0.76	8546	1.74	1.02	33	1,5-Anhydro-glucitol-4TMS
27	29.792	195569	17.06	33121	6.75	5.90	60	Sucrose-8TMS
28	29.921	8251	0.72	11327	2.31	0.73	37	Sucrose-8TMS
29	30.010	18533	1.62	8613	1.76	2.15	27	Ribose-4TMS(2)
30	30.064	20114	1.75	10724	2.19	1.88	37	Isomaltose-meto-8TMS(2)
31	30.091	12276	1.07	11956	2.44	1.03	47	Sucrose-8TMS
32	30.763	8677	0.76	9430	1.92	0.92	25	3-Hydroxy-kynurenine-3TMS
33	30.836	27755	2.42	13076	2.67	2.12	32	Trehalose-8TMS
34	30.964	7594	0.66	10433	2.13	0.73	36	Fructose-5TMS(3)
35	31.329	10345	0.90	6917	1.41	1.50	40	Inosine-4TMS
36	31.385	9693	0.85	9775	1.99	0.99	23	Hippuric acid-TMS
37	32.265	24875	2.17	10750	2.19	2.31	41	Chloramphenicol-2TMS
38	32.310	44490	3.88	11625	2.37	3.83	34	Boric acid-3TMS
39	32.443	11069	0.97	9443	1.92	1.17	38	Ribose-4TMS(4)
40	32.528	15940	1.39	8889	1.81	1.79	46	Epinephrine-3TMS
41	32.855	14777	1.29	5856	1.19	2.52	28	3,4-Dihydroxymandelic acid-4TMS
42	32.947	8234	0.72	8535	1.74	0.96	32	Maltitol-9TMS
		1146112	100.00	490648	100.00			

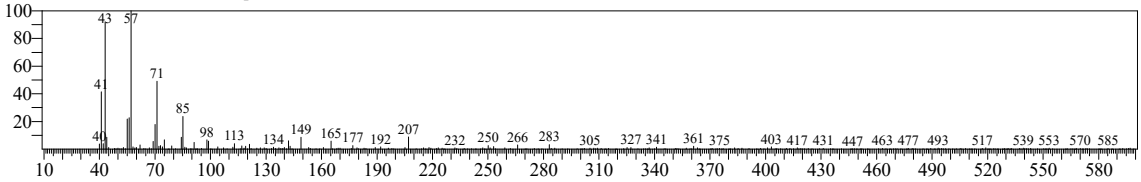
Library

<< Target >>

Line#:1 R.Time:7.945(Scan#:690) MassPeaks:288

RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(5029)

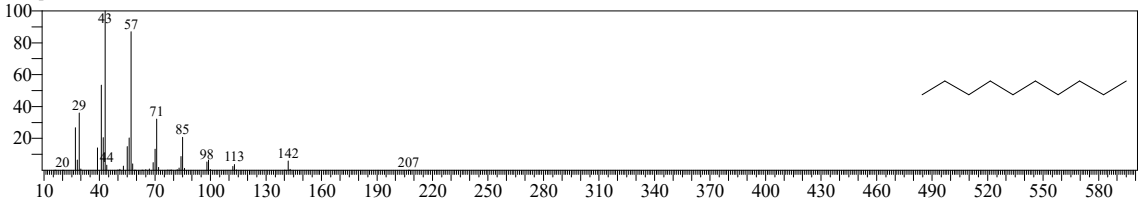
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:9445 Library:NIST20R.lib

SI:86 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000

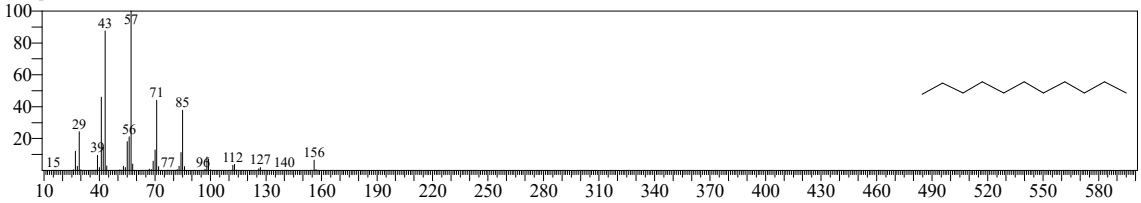
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



Hit#:2 Entry:12897 Library:NIST20R.lib

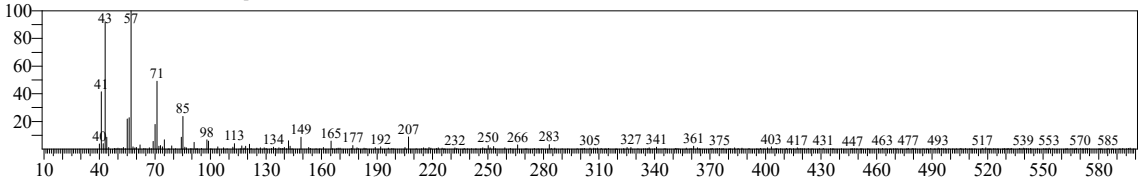
SI:85 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100

CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

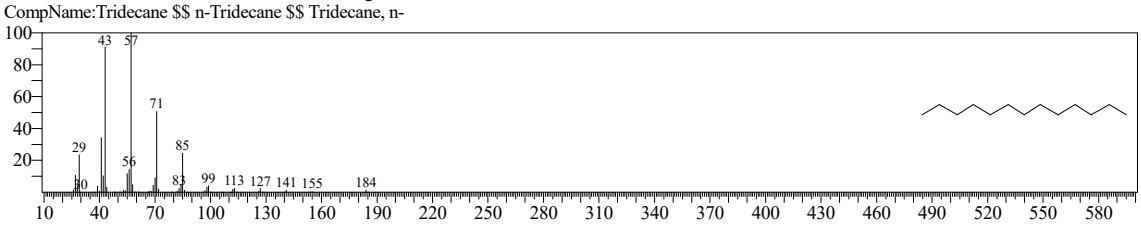


TNAU

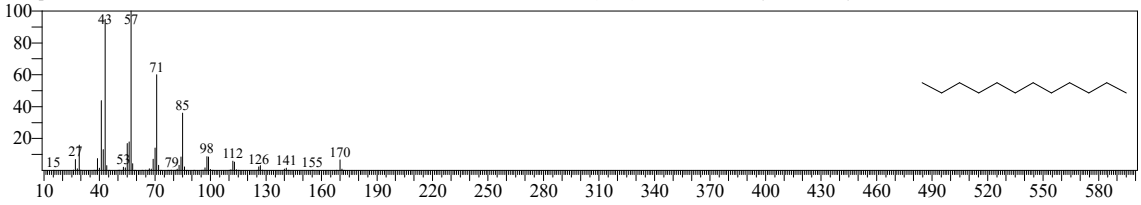
<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:288
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(5029)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



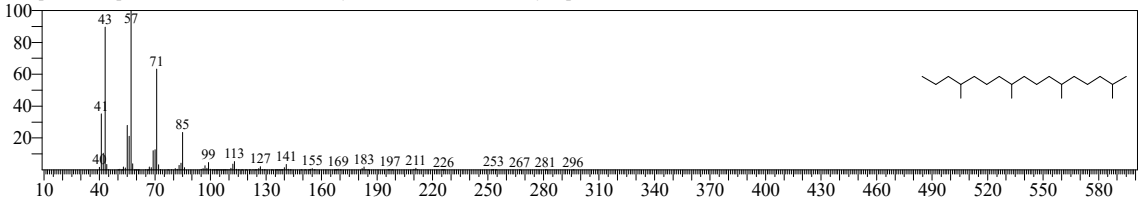
Hit#:3 Entry:40226 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:16191 Library:NIST20R.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

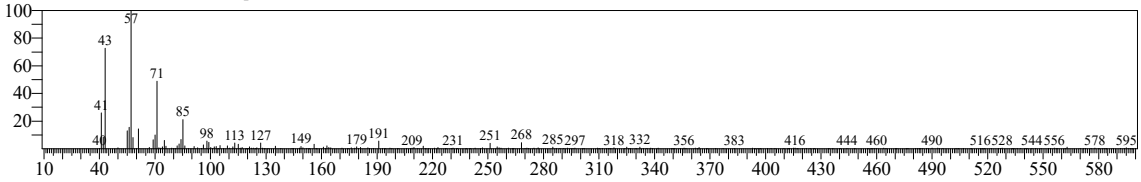


Hit#:5 Entry:159057 Library:NIST20M1.lib
SI:85 Formula:C21H44 CAS:18344-37-1 MolWeight:296 RetIndex:1852
CompName:Heptadecane, 2,6,10,14-tetramethyl- $$ 2,6,10,14-Tetramethylheptadecane

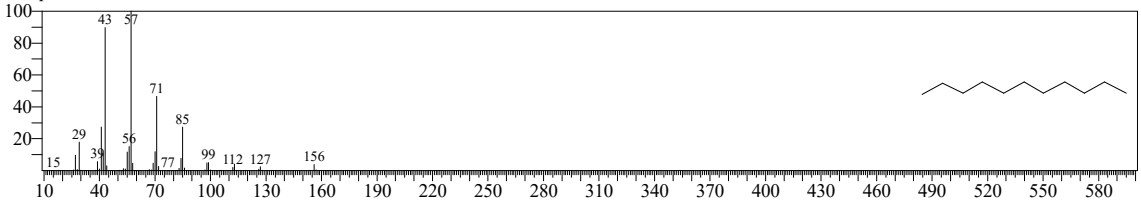


TNAU

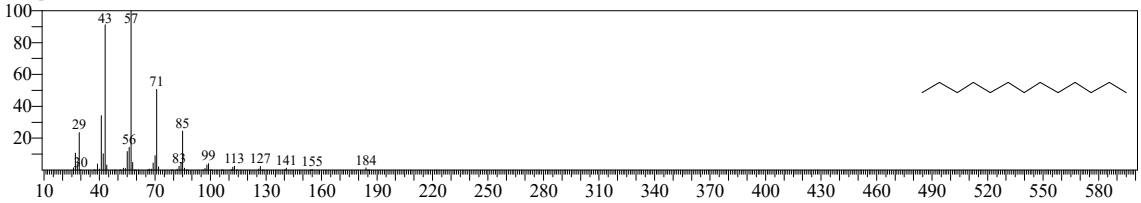
<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:253
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.05(5911)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



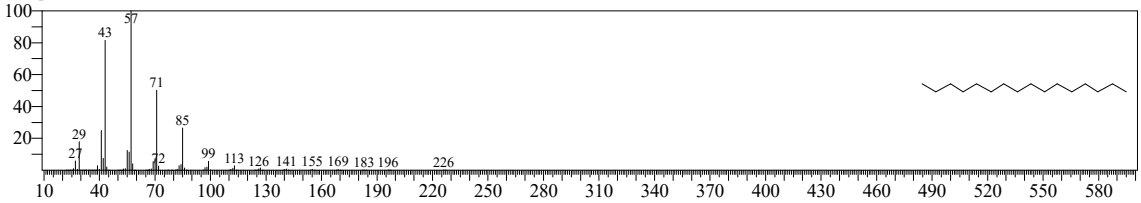
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



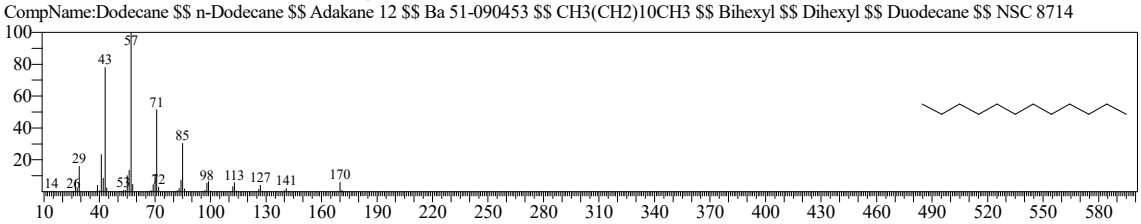
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



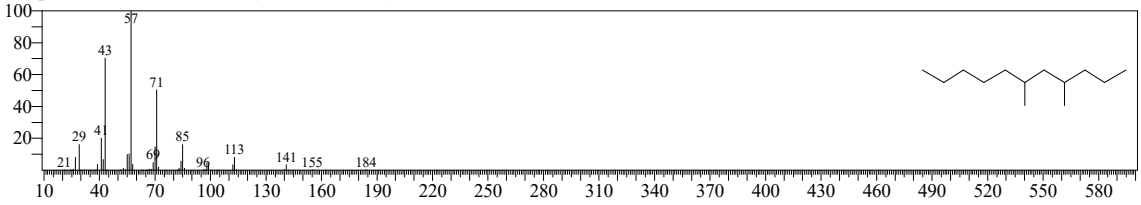
Hit#:3 Entry:27737 Library:NIST20R.lib
SI:86 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane



Hit#:4 Entry:16192 Library:NIST20R.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

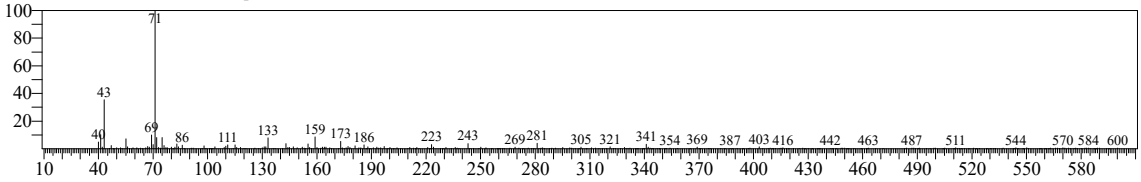


Hit#:5 Entry:40271 Library:NIST20M1.lib
SI:86 Formula:C13H28 CAS:17312-82-2 MolWeight:184 RetIndex:1185
CompName:Undecane, 4,6-dimethyl- $$ 4,6-Dimethylundecane #

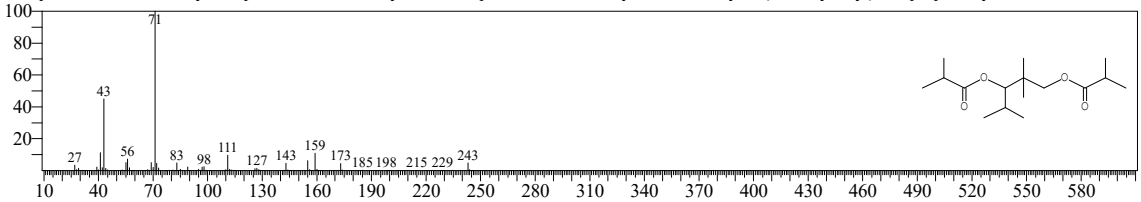


TNAU

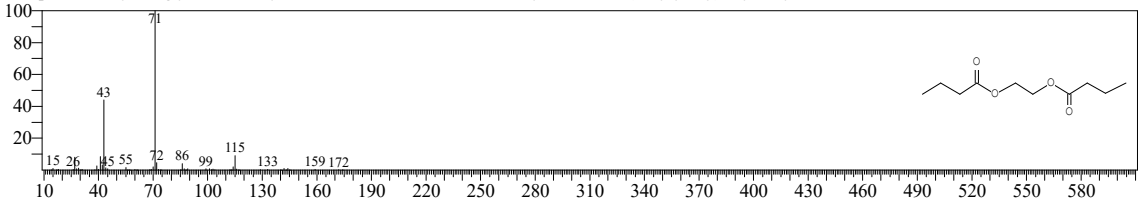
<< Target >>
Line#:3 R.Time:16.465(Scan#:2394) MassPeaks:297
RawMode:Averaged 16.460-16.470(2393-2395) BasePeak:71.05(5004)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



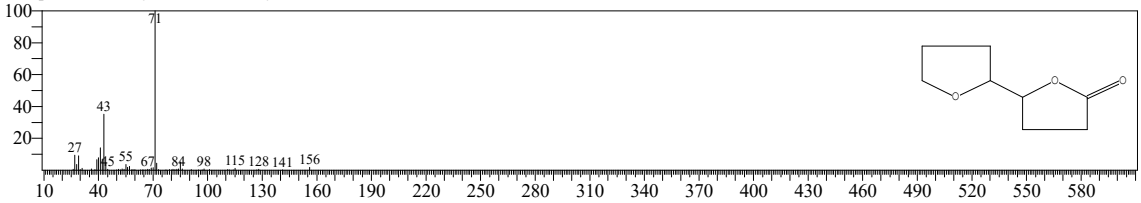
Hit#:1 Entry:34622 Library:NIST20R.lib
SI:80 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan



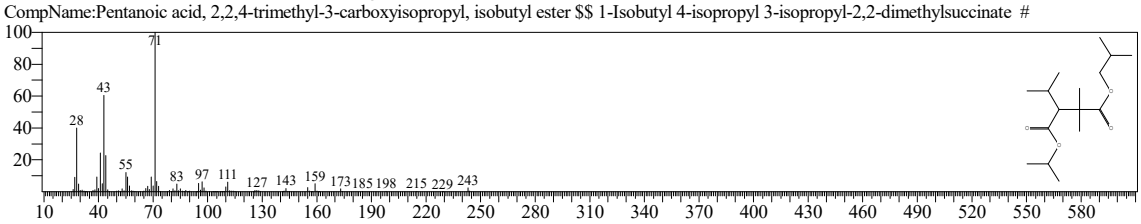
Hit#:2 Entry:54692 Library:NIST20M1.lib
SI:74 Formula:C10H18O4 CAS:105-72-6 MolWeight:202 RetIndex:1350
CompName:Ethylene glycol di-n-butyrate $$ Butanoic acid, 1,2-ethanediyl ester $$ 2-(Butyryloxy)ethyl butyrate #



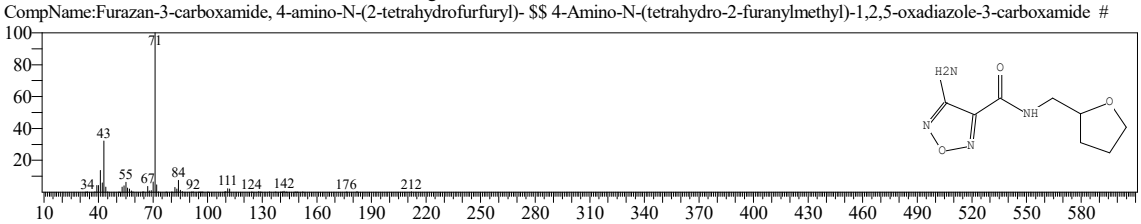
Hit#:3 Entry:20598 Library:NIST20M1.lib
SI:74 Formula:C8H12O3 CAS:19680-00-3 MolWeight:156 RetIndex:1316
CompName:Tetrahydro[2,2']bifuranyl-5-one



Hit#:4 Entry:146809 Library:NIST20M1.lib
SI:74 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 #

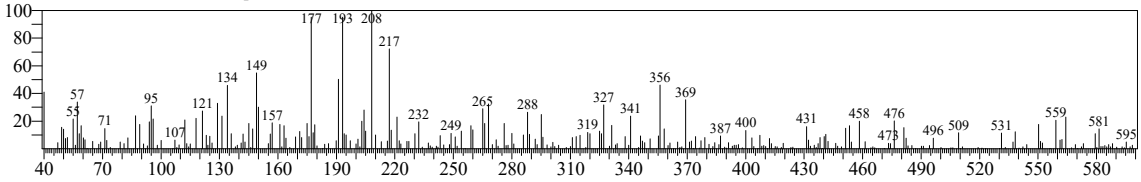


Hit#:5 Entry:64203 Library:NIST20M1.lib
SI:73 Formula:C8H12N4O3 CAS:309735-27-1 MolWeight:212 RetIndex:1980
CompName:Furazan-3-carboxamide, 4-amino-N-(2-tetrahydrofurfuryl)- $$ 4-Amino-N-(tetrahydro-2-furanylmethyl)-1,2,5-oxadiazole-3-carboxamide #

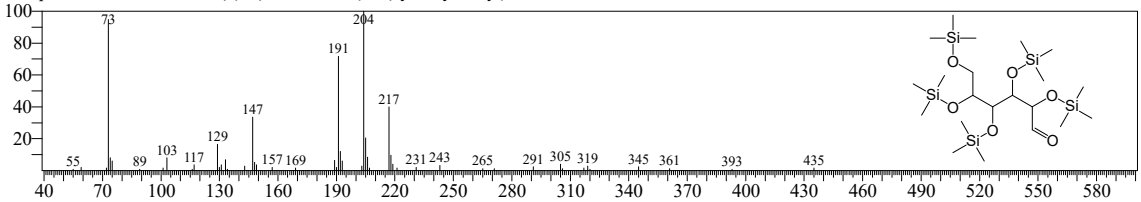


TNAU

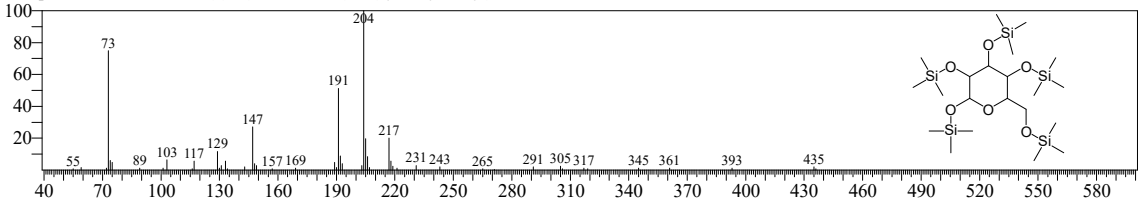
<< Target >>
Line#:4 R.Time:27.745(Scan#:4650) MassPeaks:296
RawMode:Averaged 27.740-27.750(4649-4651) BasePeak:208.05(610)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



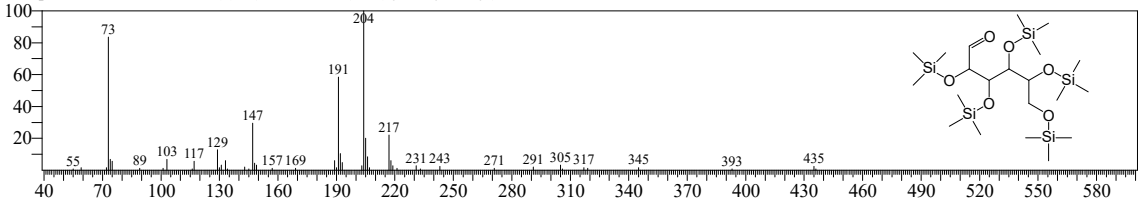
Hit#:1 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



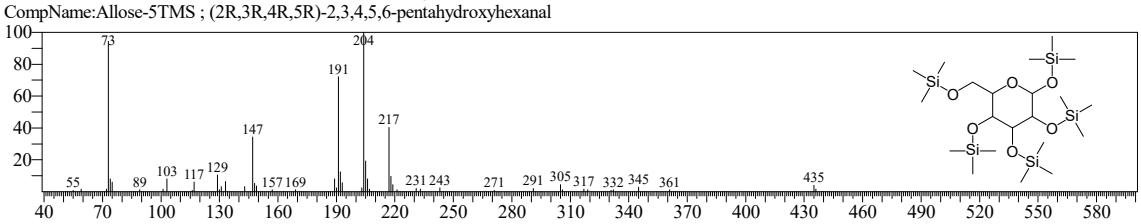
Hit#:2 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



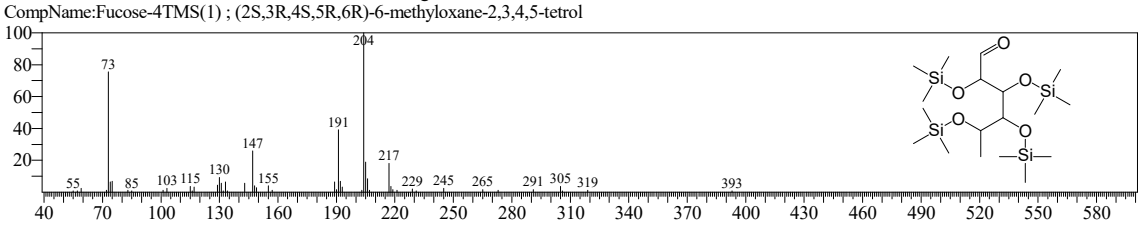
Hit#:3 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

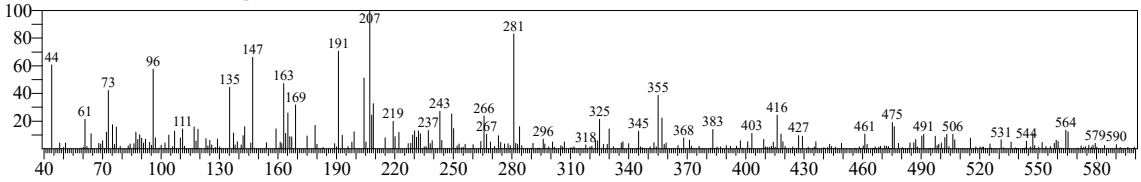


Hit#:5 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

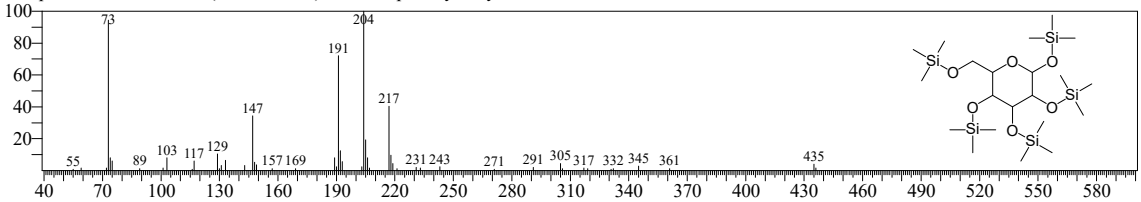


TNAU

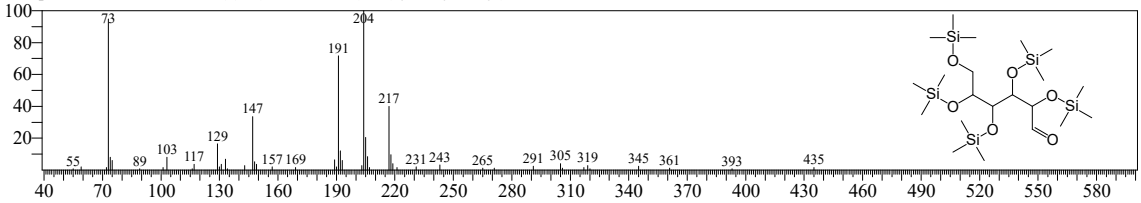
<< Target >>
Line#:5 R.Time:27.930(Scan#:4687) MassPeaks:297
RawMode:Averaged 27.925-27.935(4686-4688) BasePeak:207.05(927)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



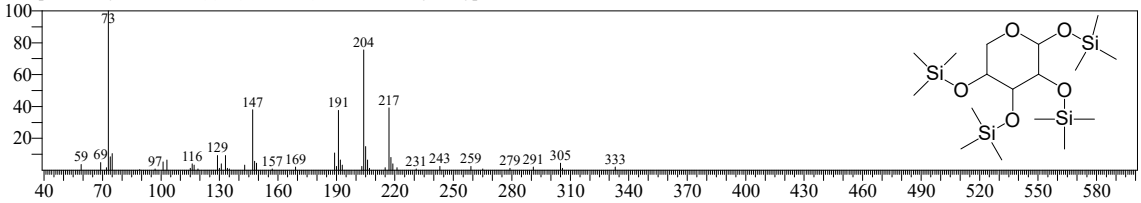
Hit#:1 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



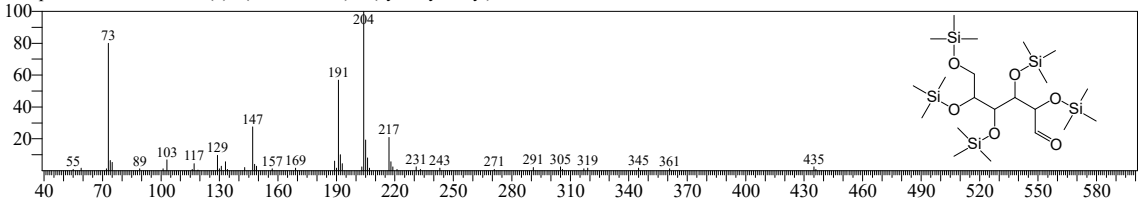
Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



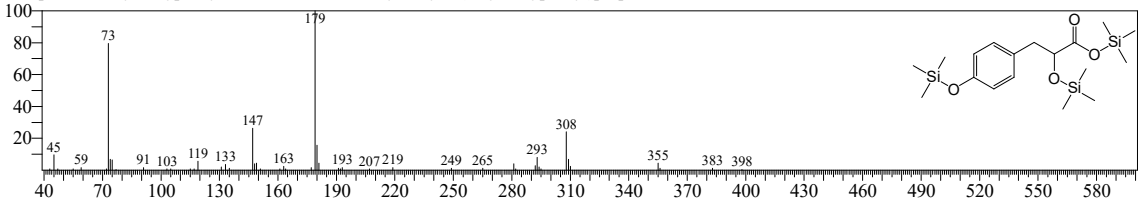
Hit#:3 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:33 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

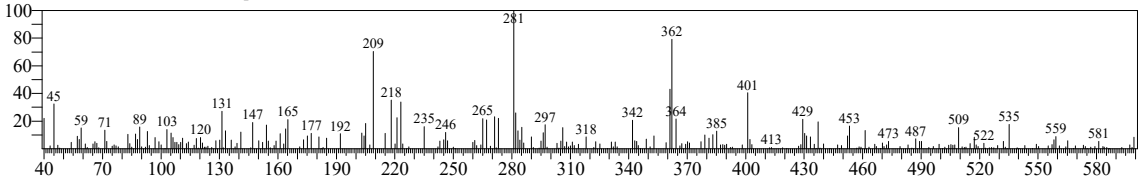


Hit#:5 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

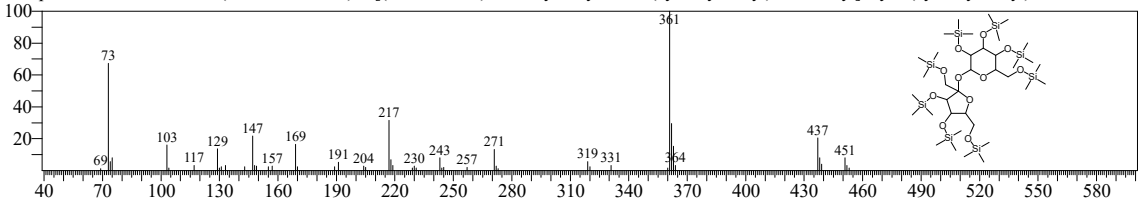


TNAU

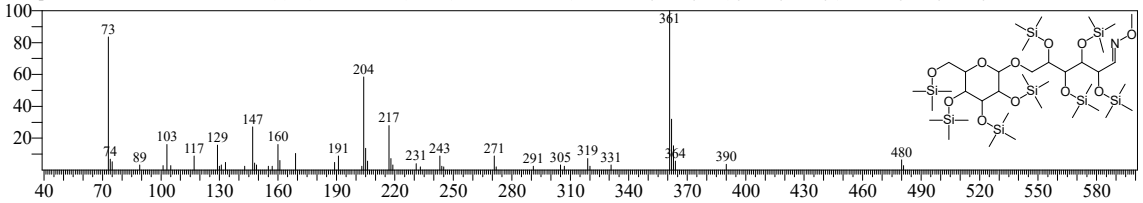
<< Target >>
Line#:6 R.Time:28.055(Scan#:4712) MassPeaks:276
RawMode:Averaged 28.050-28.060(4711-4713) BasePeak:281.00(901)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



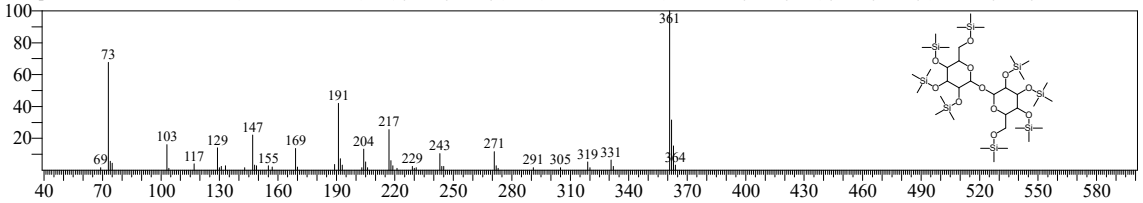
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



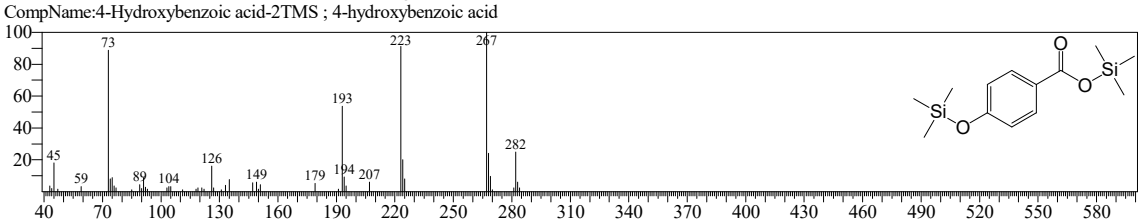
Hit#:2 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



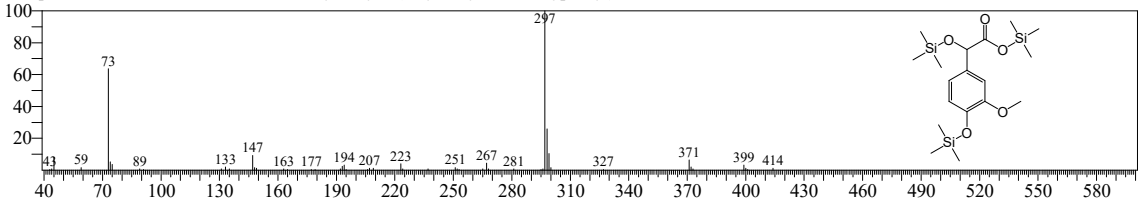
Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



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

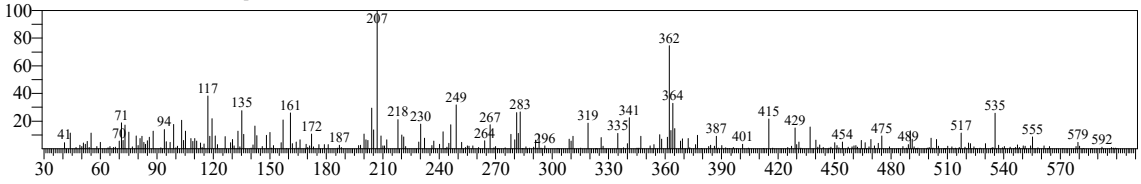


Hit#:5 Entry:359 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid

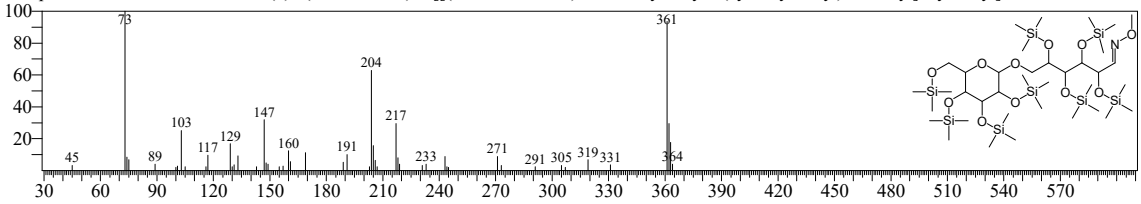


TNAU

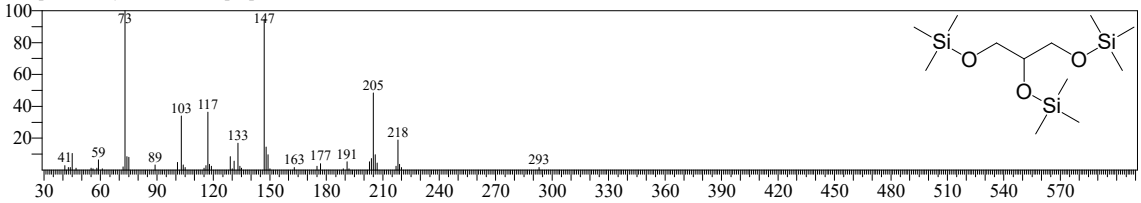
<< Target >>
Line#:7 R.Time:28.085(Scan#:4718) MassPeaks:283
RawMode:Averaged 28.080-28.090(4717-4719) BasePeak:207.05(1059)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



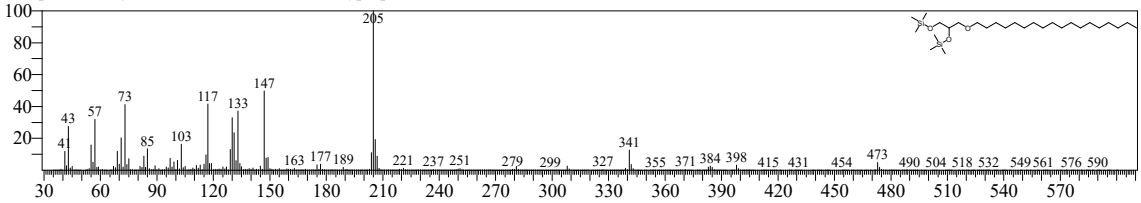
Hit#:1 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



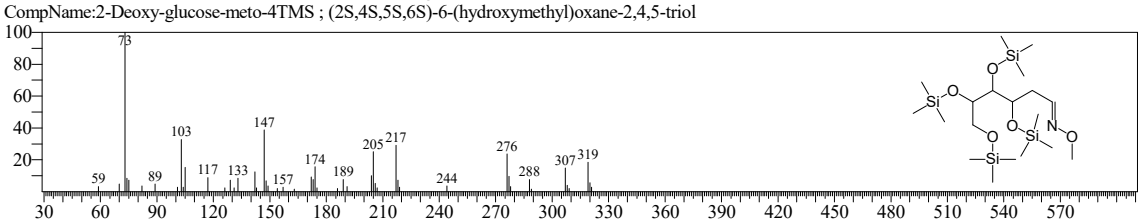
Hit#:2 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



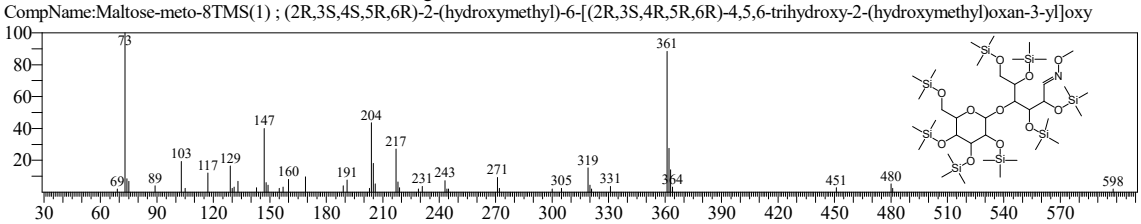
Hit#:3 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



Hit#:4 Entry:305 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C19H47NO5Si4 CAS:154-17-6 MolWeight:481 RetIndex:1814
CompName:2-Deoxy-glucose-meto-4TMS ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

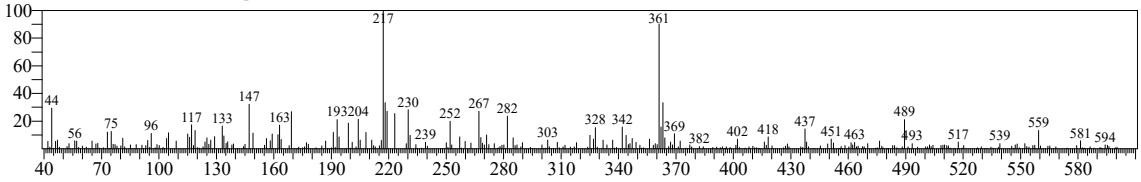


Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

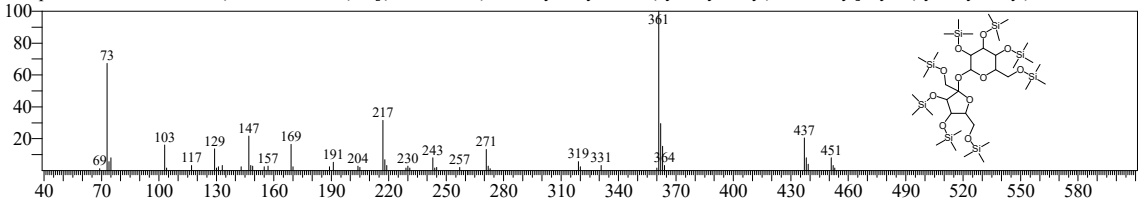


TNAU

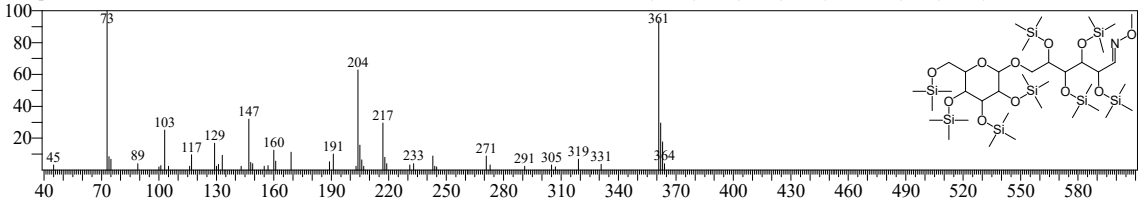
<< Target >>
Line#:8 R.Time:28.220(Scan#:4745) MassPeaks:307
RawMode:Averaged 28.215-28.225(4744-4746) BasePeak:217.15(1627)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



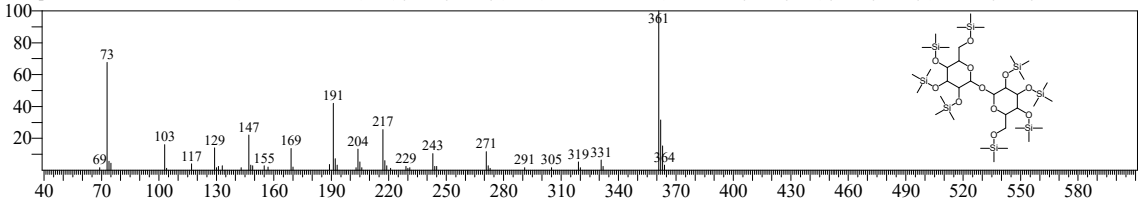
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:51 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



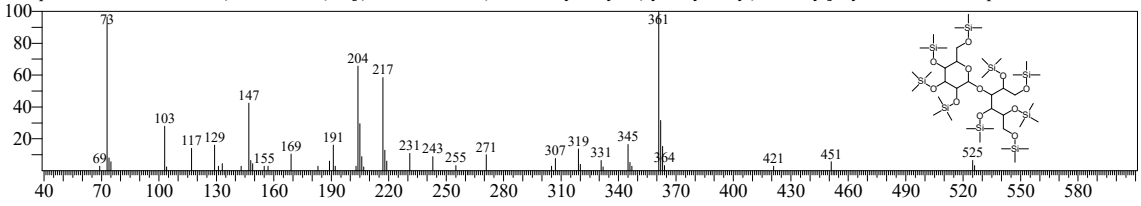
Hit#:2 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



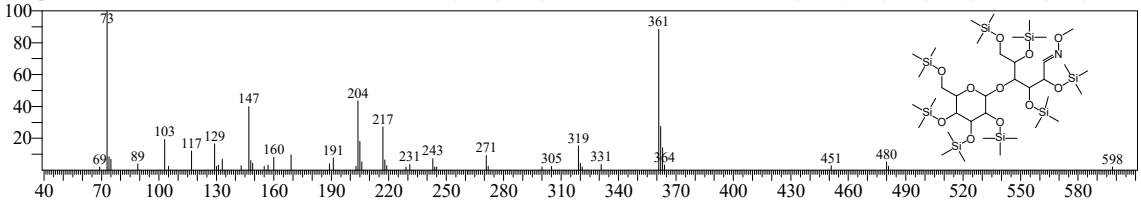
Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



Hit#:4 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

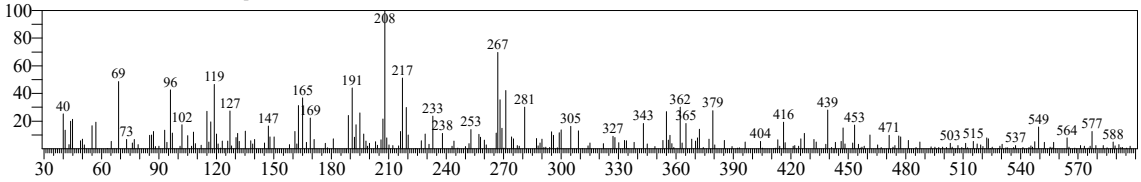


Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

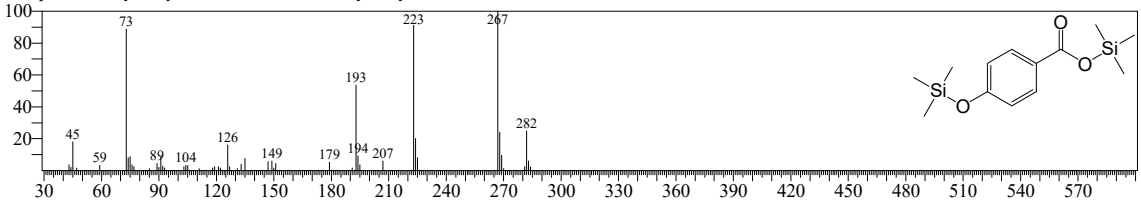


TNAU

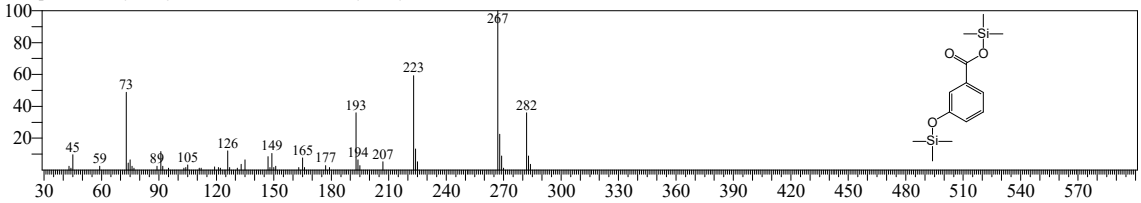
<< Target >>
Line#:9 R.Time:28.375(Scan#:4776) MassPeaks:260
RawMode:Averaged 28.370-28.380(4775-4777) BasePeak:208.05(727)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



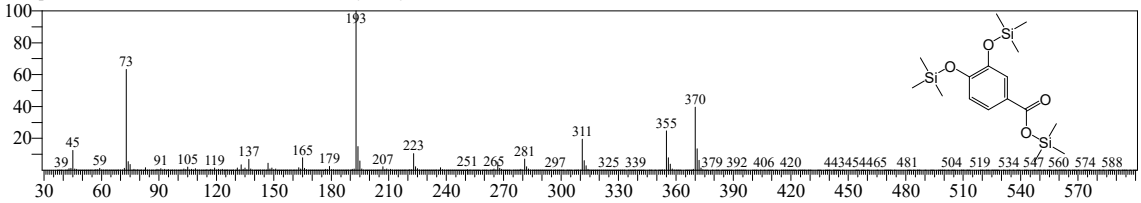
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



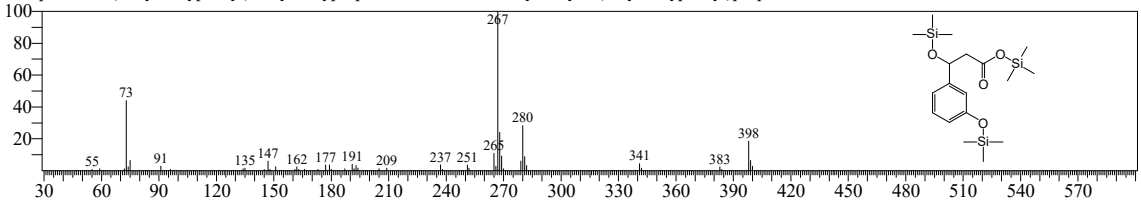
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



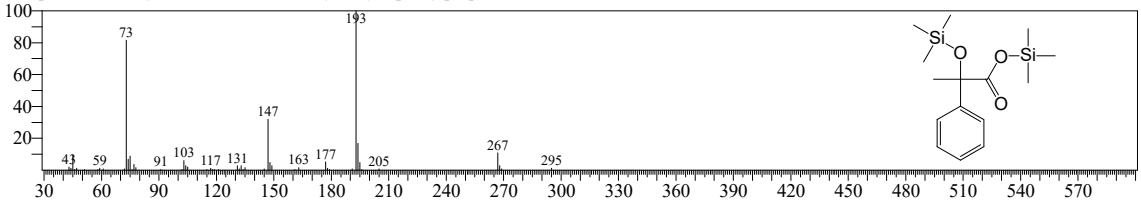
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:23 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

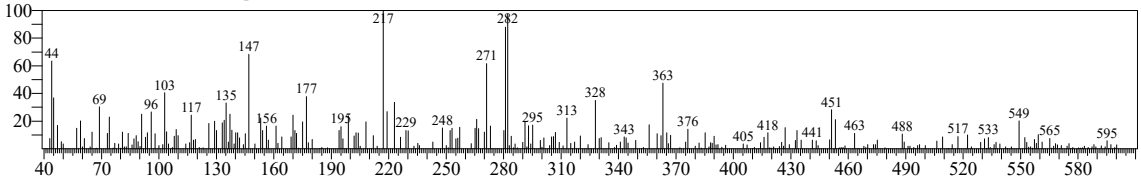


Hit#:5 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

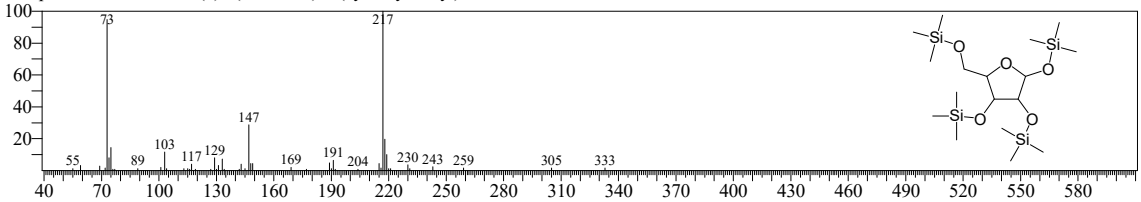


TNAU

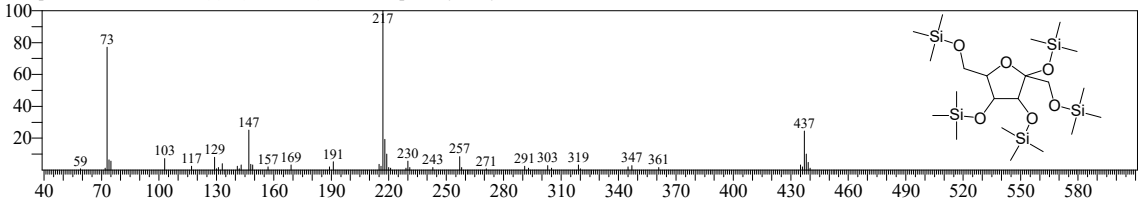
<< Target >>
Line#:10 R.Time:28.405(Scan#:4782) MassPeaks:285
RawMode:Averaged 28.400-28.410(4781-4783) BasePeak:217.10(677)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



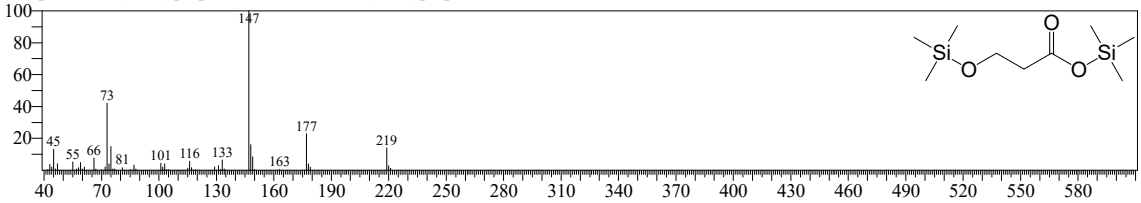
Hit#:1 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



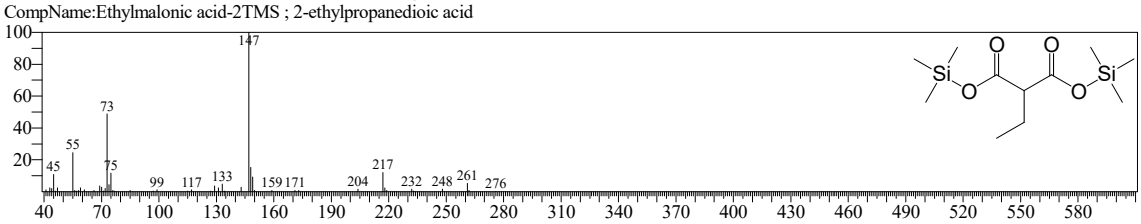
Hit#:2 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



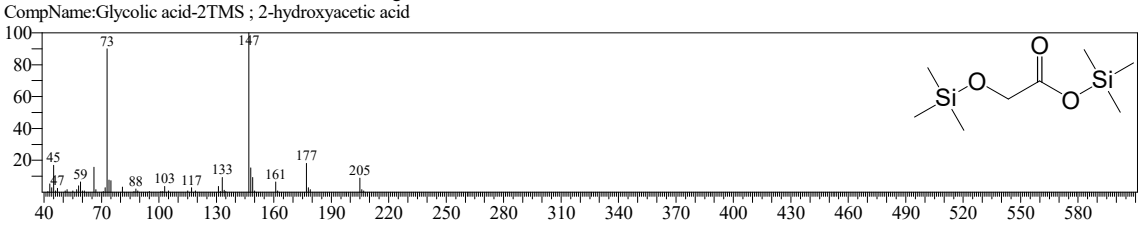
Hit#:3 Entry:30 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C9H22O3Si2 CAS:503-66-2 MolWeight:234 RetIndex:1145
CompName:3-Hydroxypropionic acid-2TMS ; 3-hydroxypropanoic acid



Hit#:4 Entry:80 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C11H24O4Si2 CAS:601-75-2 MolWeight:276 RetIndex:1284
CompName:Ethylmalonic acid-2TMS ; 2-ethylpropanedioic acid

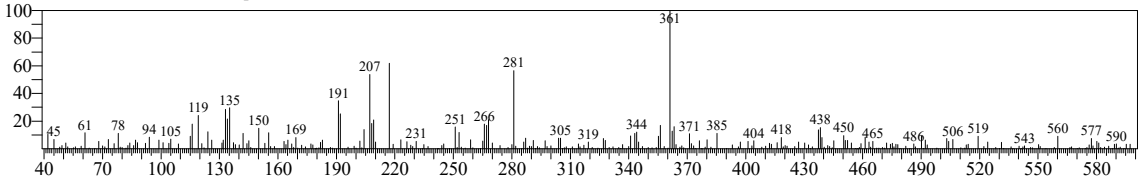


Hit#:5 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

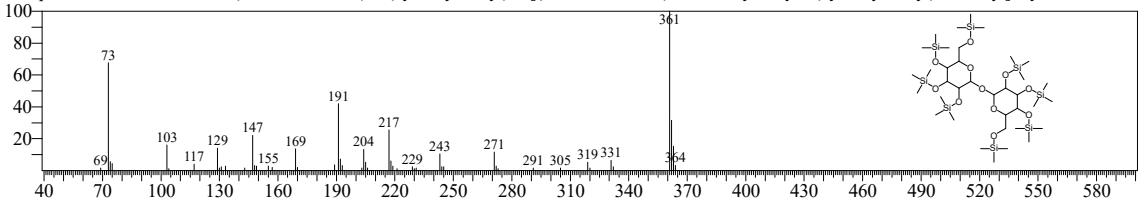


TNAU

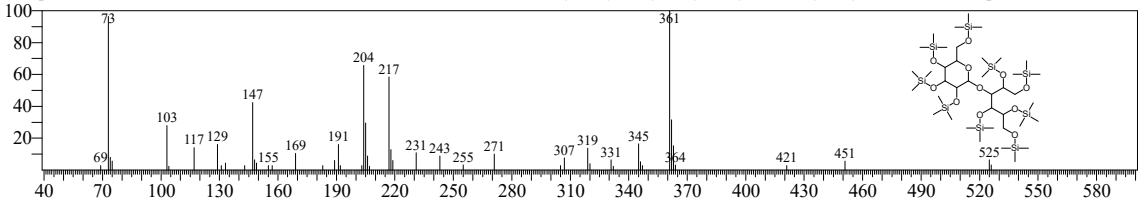
<< Target >>
Line#:11 R.Time:28.475(Scan#:4796) MassPeaks:293
RawMode:Averaged 28.470-28.480(4795-4797) BasePeak:361.20(1451)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



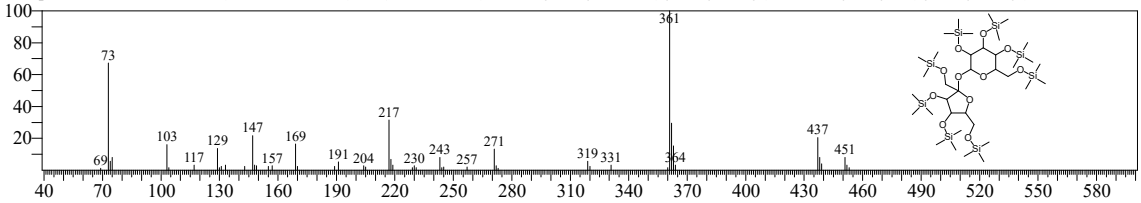
Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



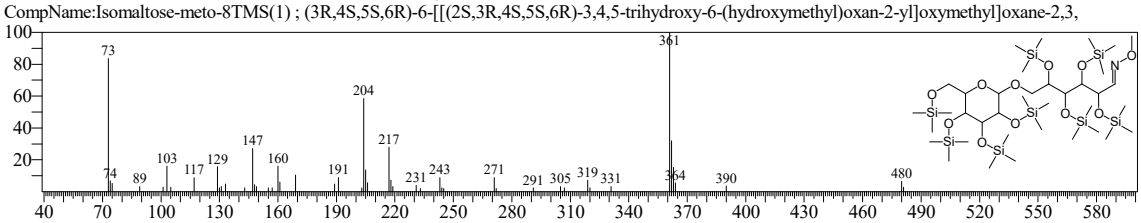
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



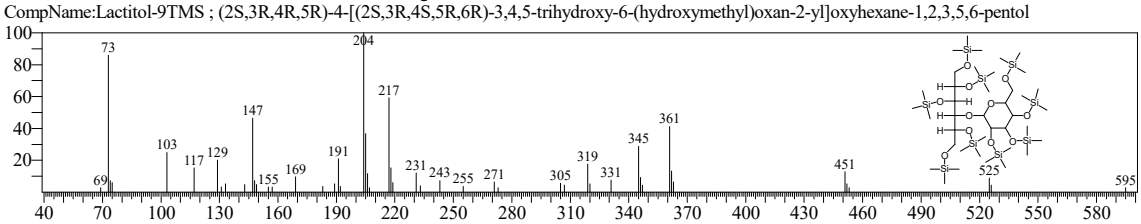
Hit#:3 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

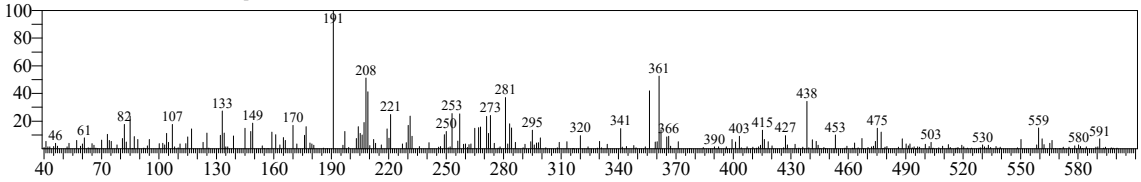


Hit#:5 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

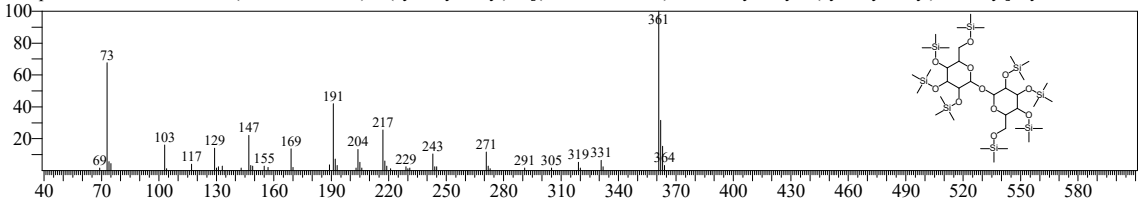


TNAU

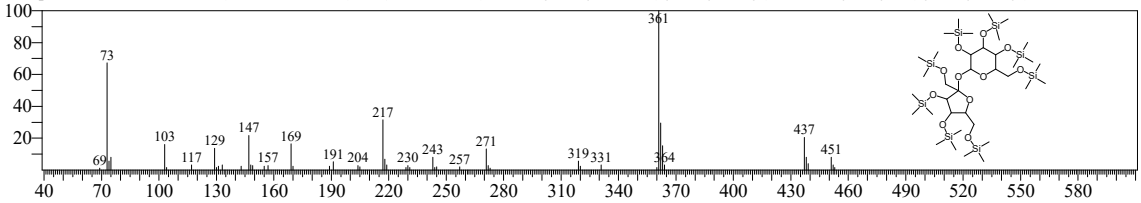
<< Target >>
Line#:12 R.Time:28.535(Scan#:4808) MassPeaks:270
RawMode:Averaged 28.530-28.540(4807-4809) BasePeak:191.00(1144)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



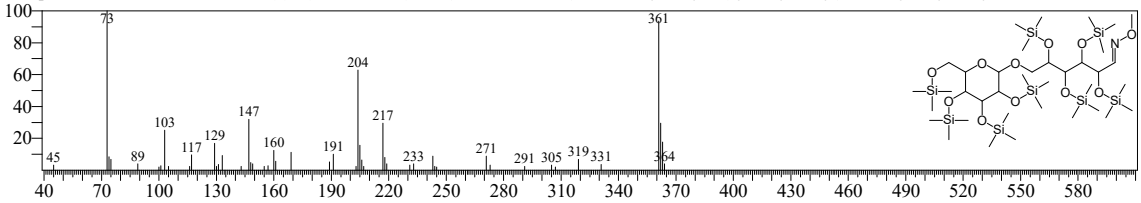
Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



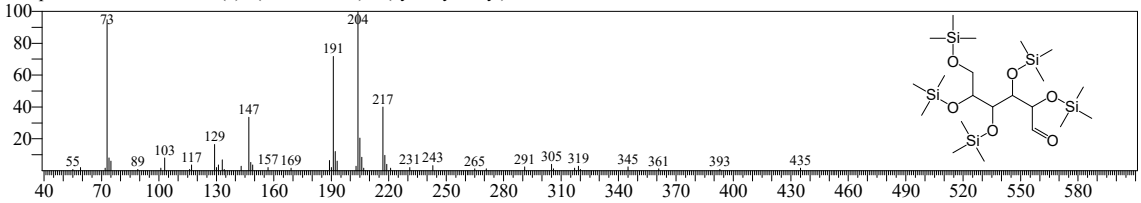
Hit#:2 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



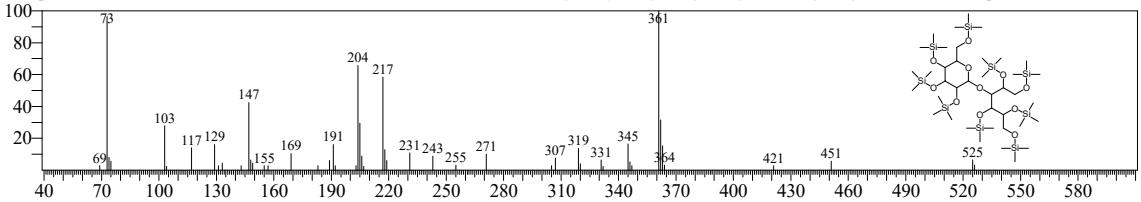
Hit#:3 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



Hit#:4 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:32 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

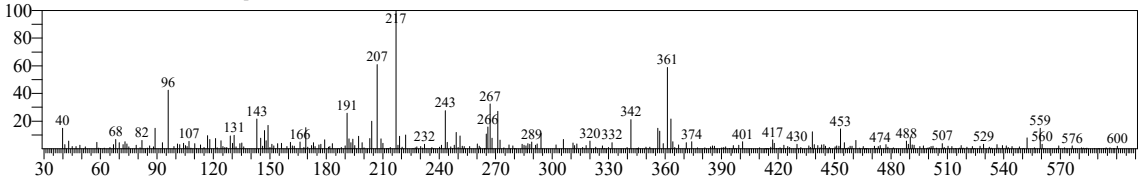


Hit#:5 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

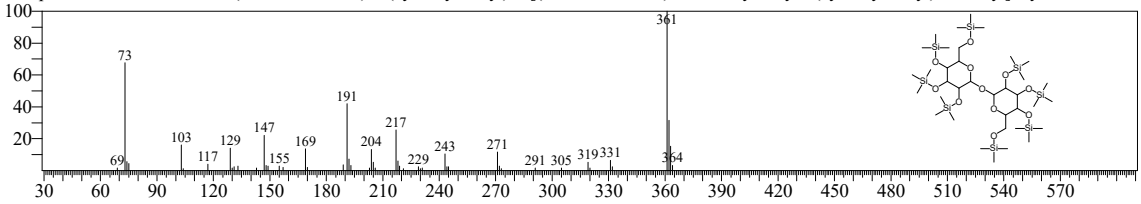


TNAU

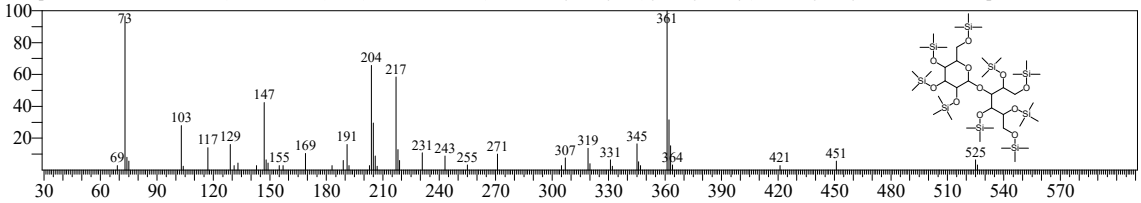
<< Target >>
Line#:13 R.Time:28.605(Scan#:4822) MassPeaks:295
RawMode:Averaged 28.600-28.610(4821-4823) BasePeak:217.10(2047)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



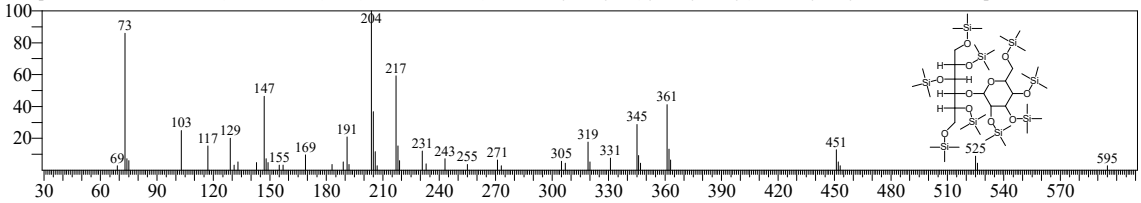
Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



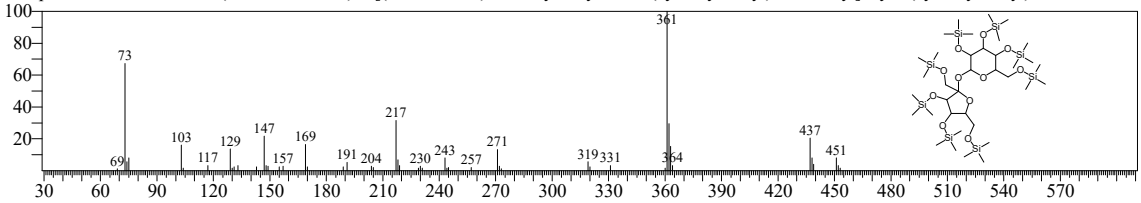
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



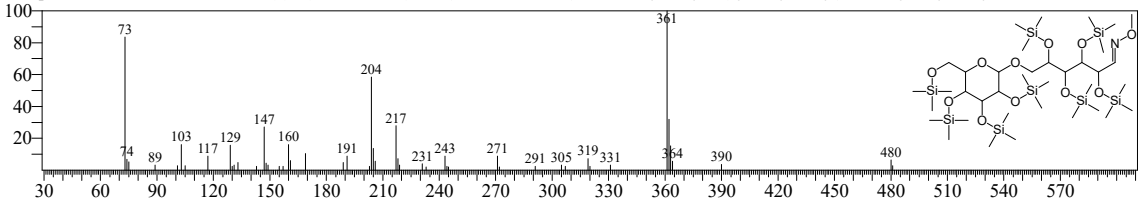
Hit#:3 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

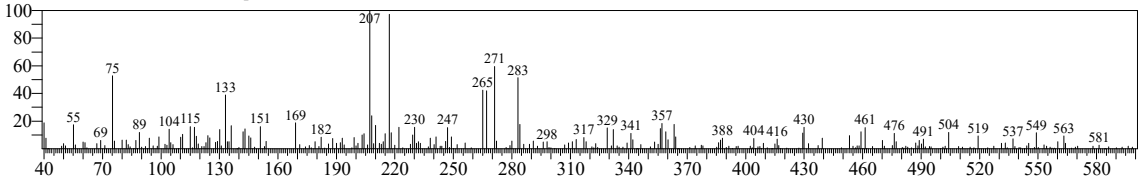


Hit#:5 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

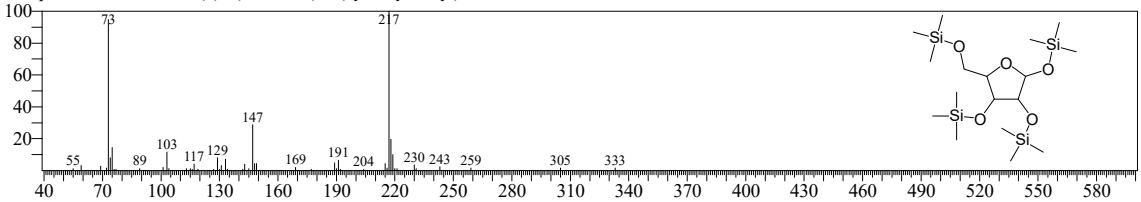


TNAU

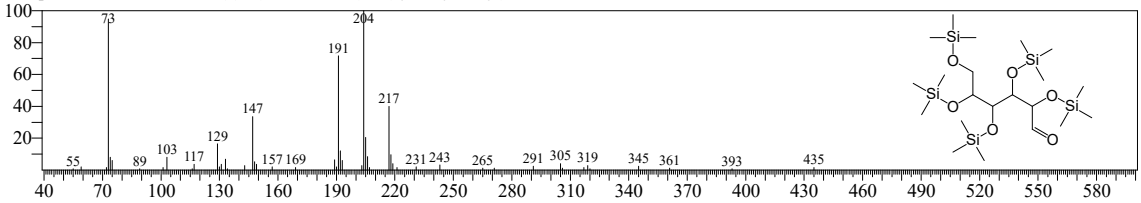
<< Target >>
Line#:14 R.Time:28.645(Scan#:4830) MassPeaks:278
RawMode:Averaged 28.640-28.650(4829-4831) BasePeak:207.05(1200)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



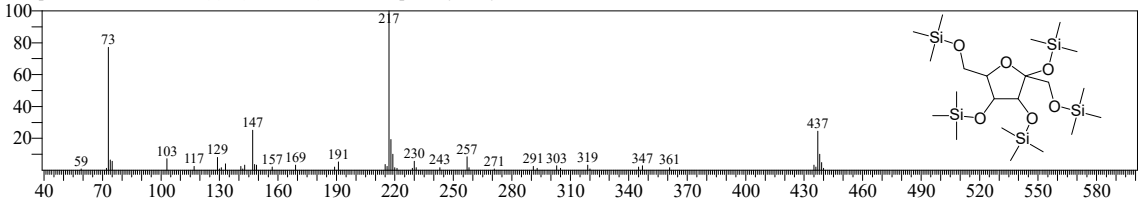
Hit#:1 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



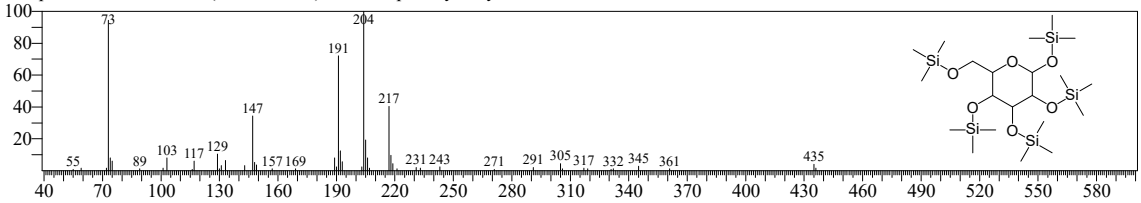
Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



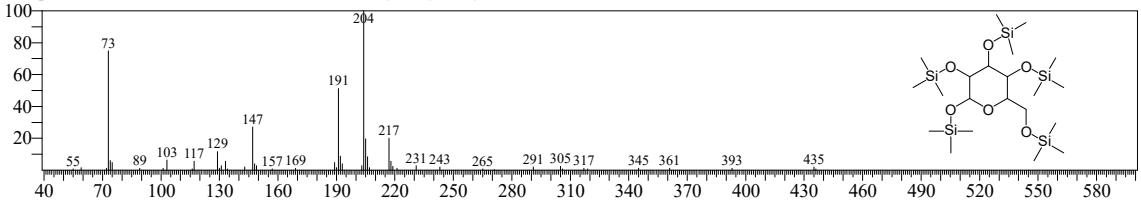
Hit#:3 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



Hit#:4 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

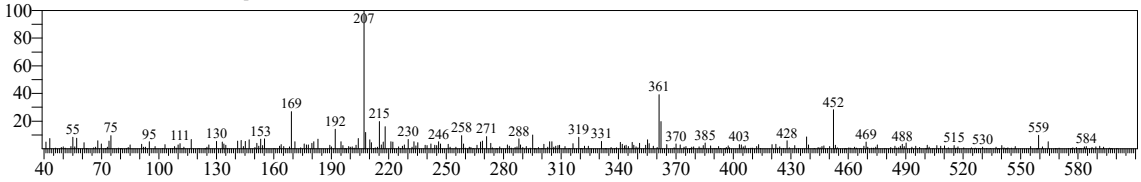


Hit#:5 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

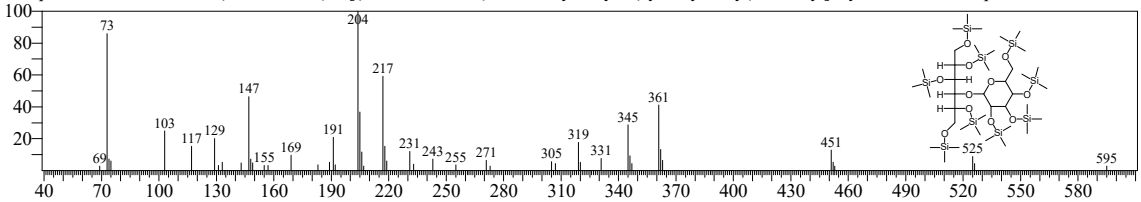


TNAU

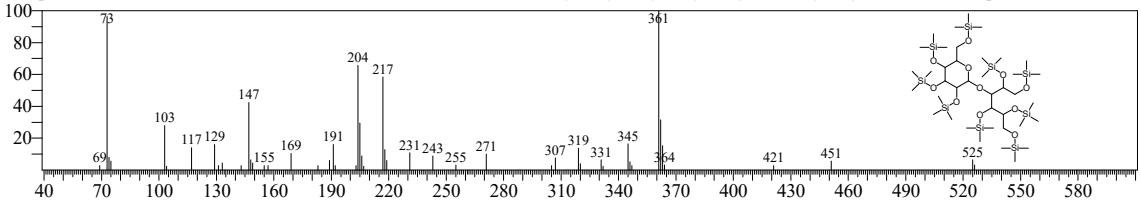
<< Target >>
Line#:15 R.Time:28.755(Scan#:4852) MassPeaks:312
RawMode:Averaged 28.750-28.760(4851-4853) BasePeak:207.05(3380)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



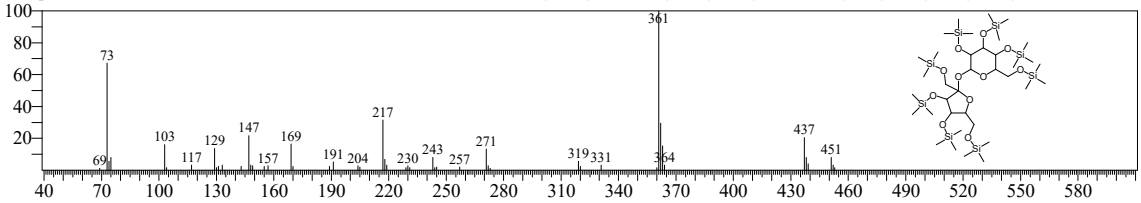
Hit#:1 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



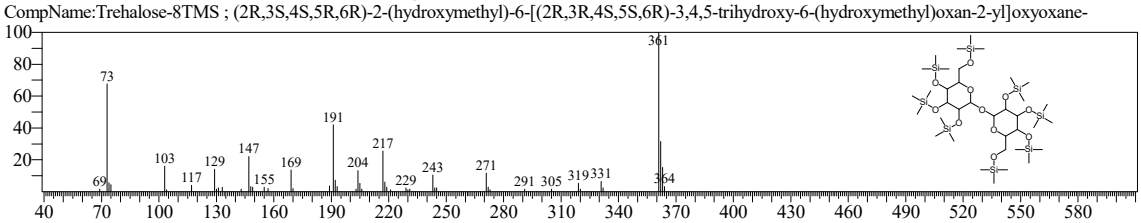
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



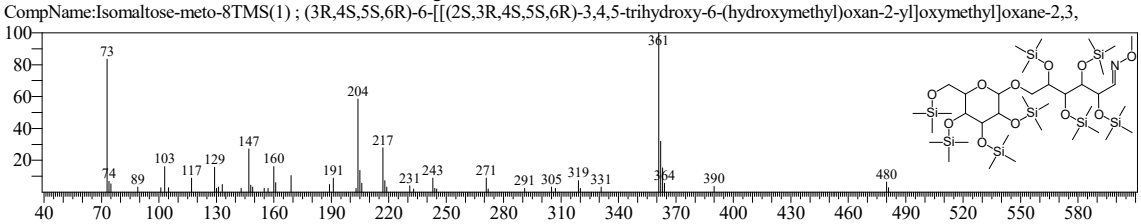
Hit#:3 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



Hit#:4 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

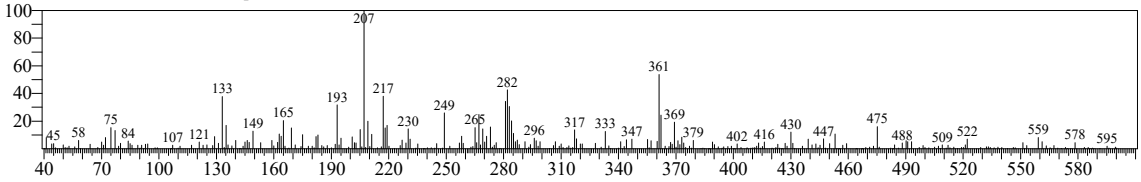


Hit#:5 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

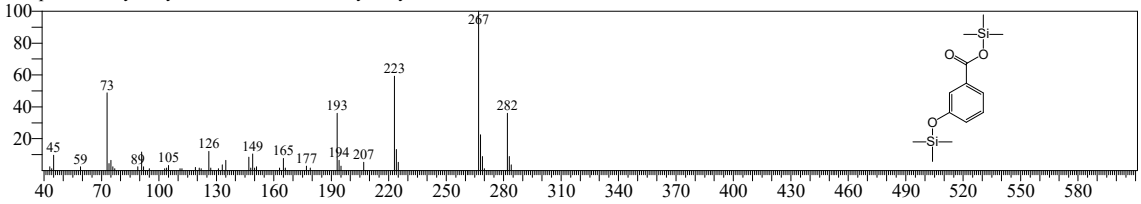


TNAU

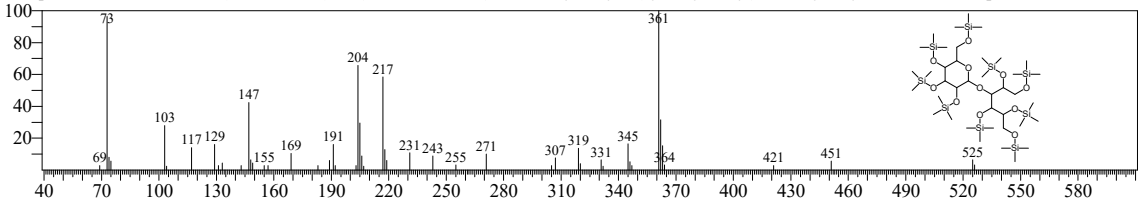
<< Target >>
Line#:16 R.Time:28.805(Scan#:4862) MassPeaks:303
RawMode:Averaged 28.800-28.810(4861-4863) BasePeak:207.05(1578)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



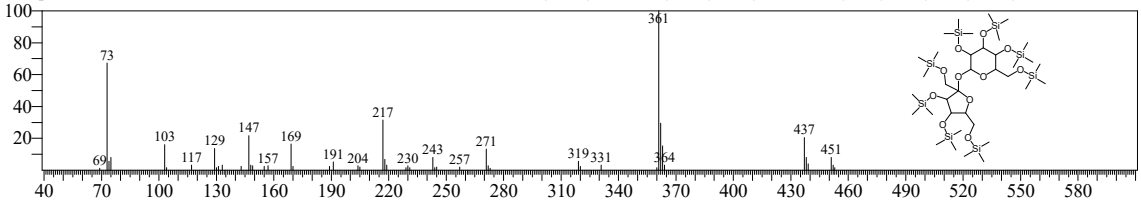
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



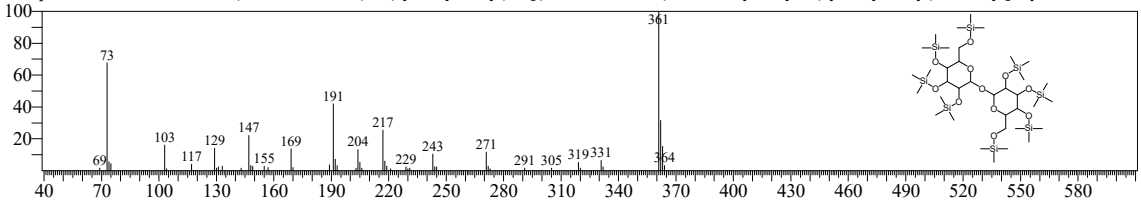
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



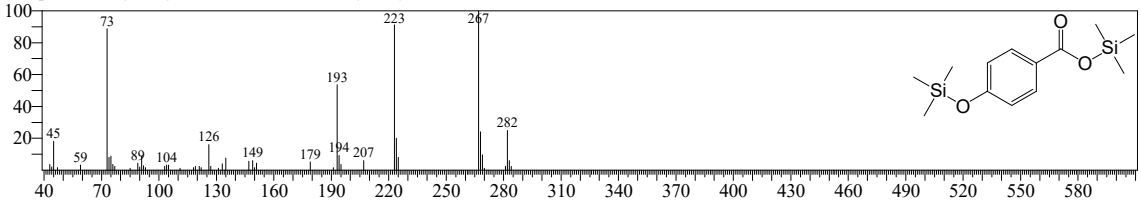
Hit#:3 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



Hit#:4 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

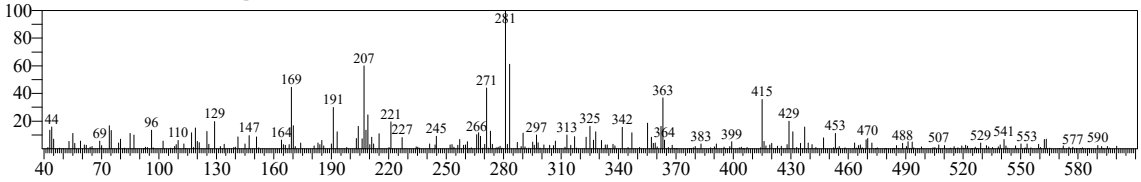


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

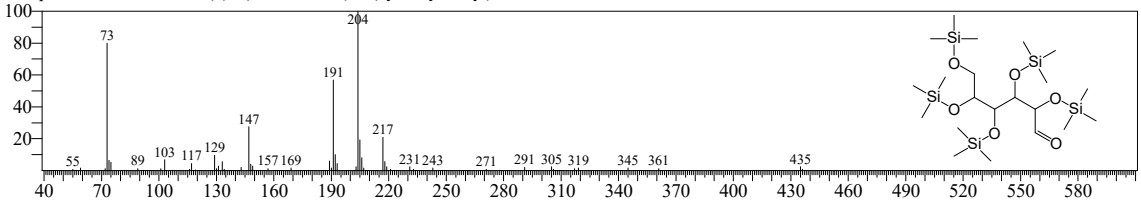


TNAU

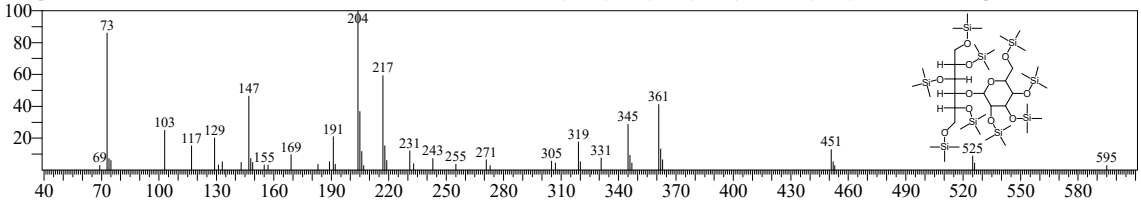
<< Target >>
Line#:17 R.Time:28.855(Scan#:4872) MassPeaks:268
RawMode:Averaged 28.850-28.860(4871-4873) BasePeak:281.05(1731)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



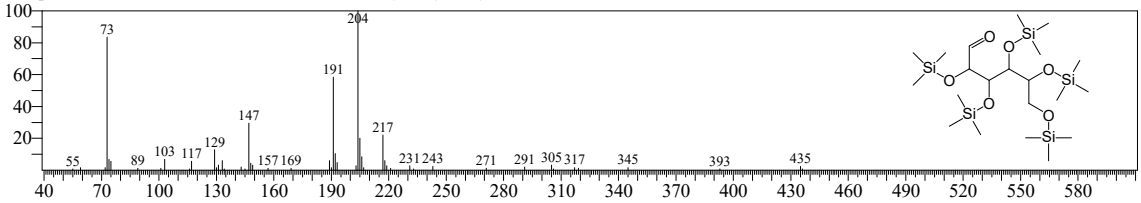
Hit#:1 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:2002
CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



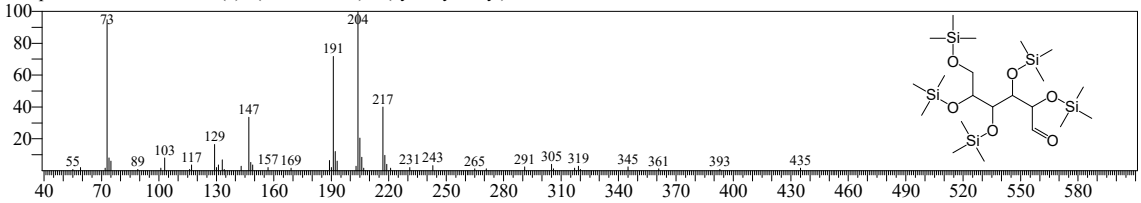
Hit#:2 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



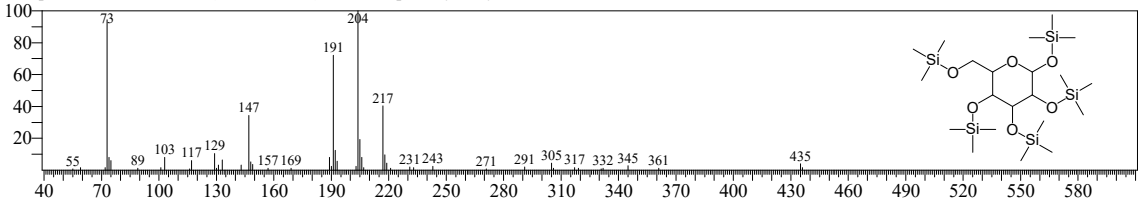
Hit#:3 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:26 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

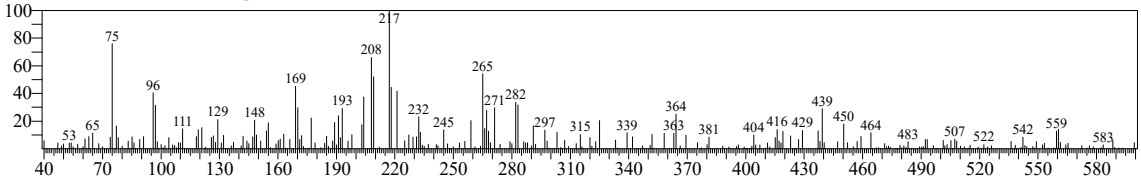


Hit#:5 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

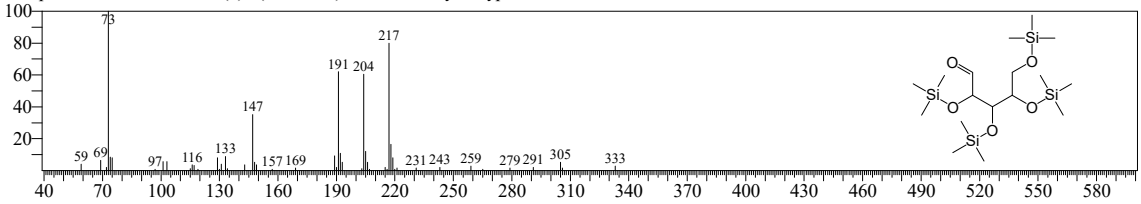


TNAU

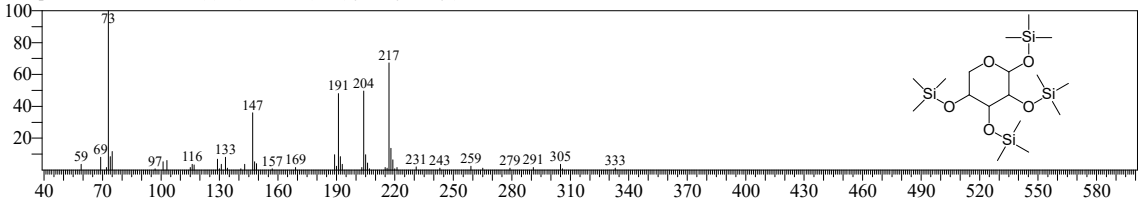
<< Target >>
Line#:18 R.Time:28.900(Scan#:4881) MassPeaks:266
RawMode:Averaged 28.895-28.905(4880-4882) BasePeak:217.10(936)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



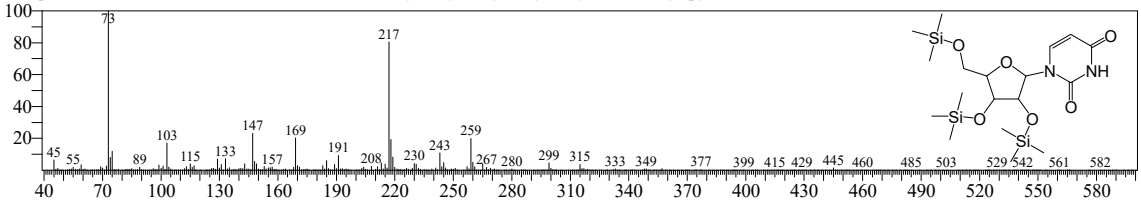
Hit#:1 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



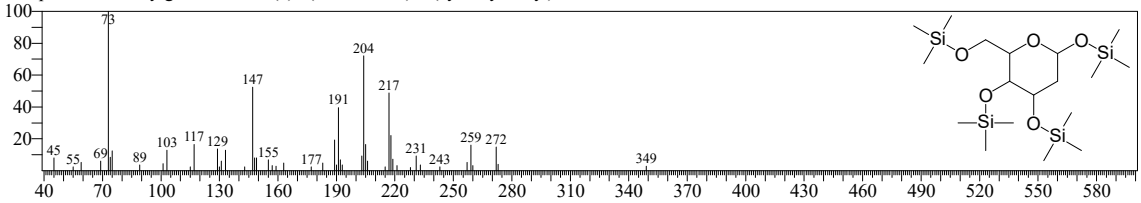
Hit#:2 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



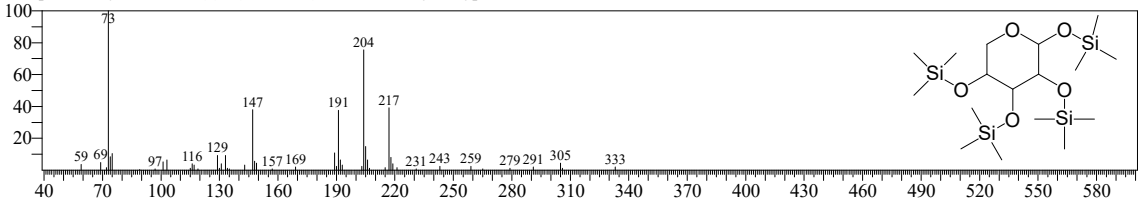
Hit#:3 Entry:523 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H36N2O6Si3 CAS:58-96-8 MolWeight:460 RetIndex:2483
CompName:Uridine-3TMS ; 1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione



Hit#:4 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:36 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

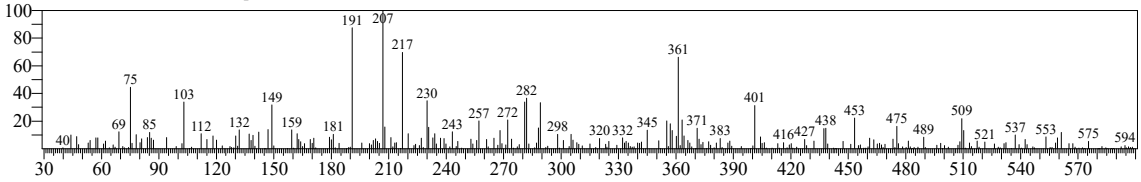


Hit#:5 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

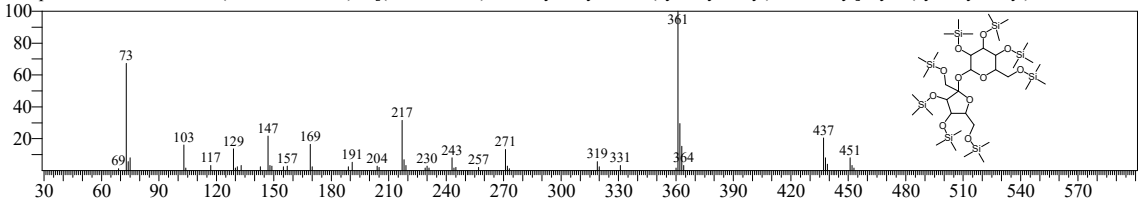


TNAU

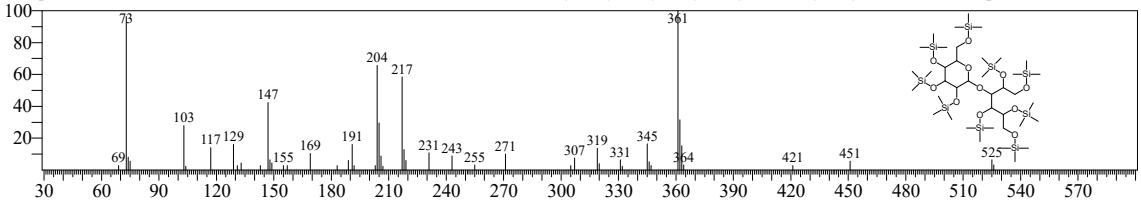
<< Target >>
Line#:19 R.Time:28.955(Scan#:4892) MassPeaks:296
RawMode:Averaged 28.950-28.960(4891-4893) BasePeak:207.05(1454)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



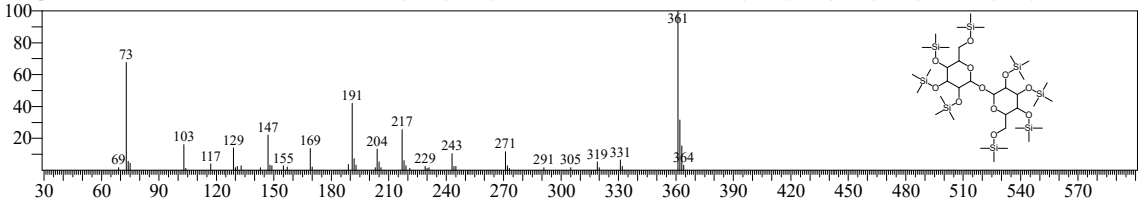
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



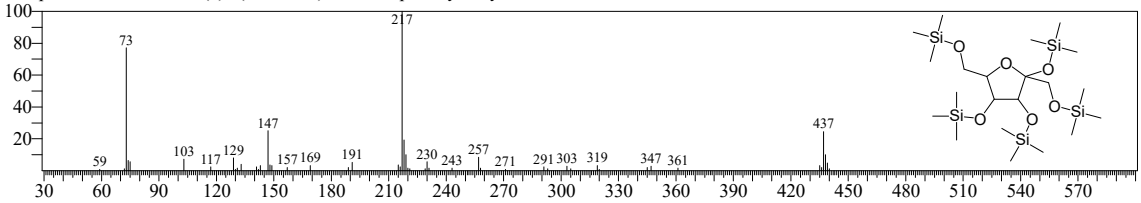
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



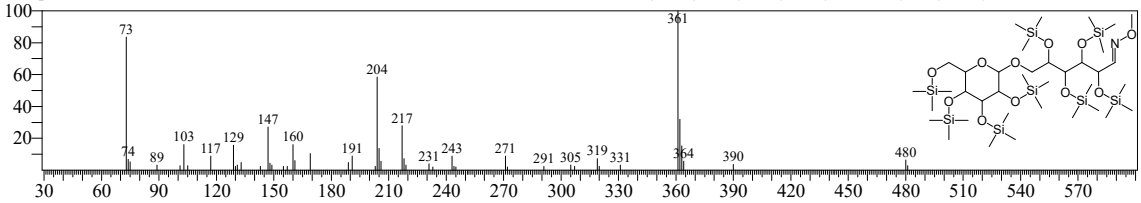
Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



Hit#:4 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:34 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

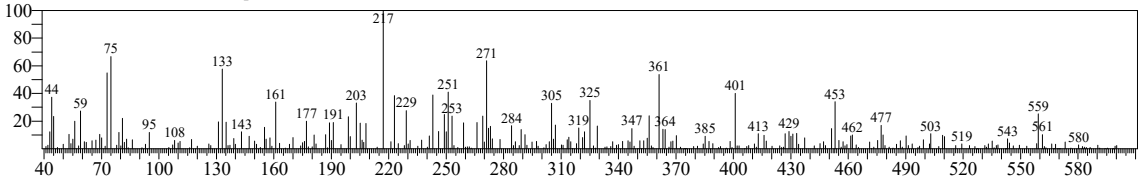


Hit#:5 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

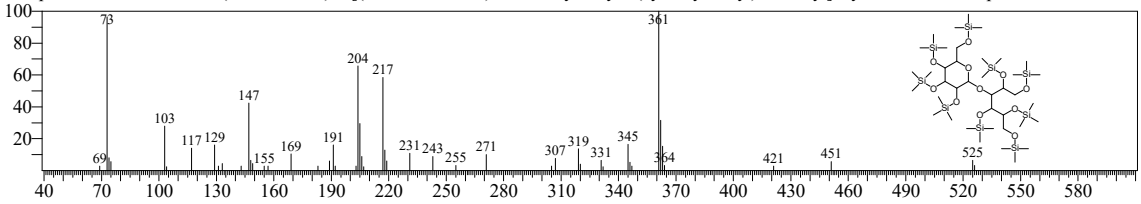


TNAU

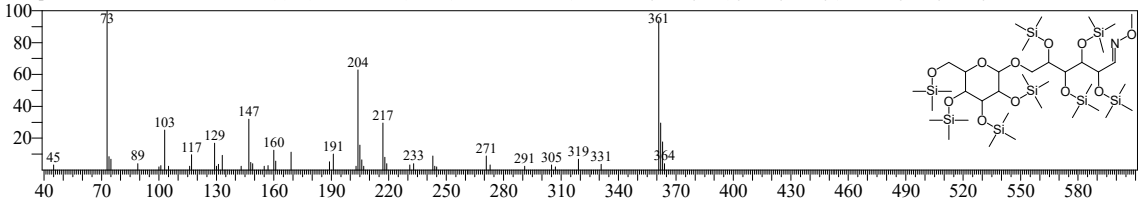
<< Target >>
Line#:20 R.Time:29.100(Scan#:4921) MassPeaks:293
RawMode:Averaged 29.095-29.105(4920-4922) BasePeak:217.10(1260)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



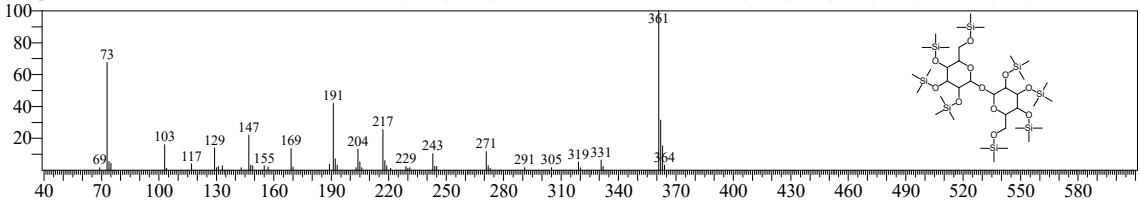
Hit#:1 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



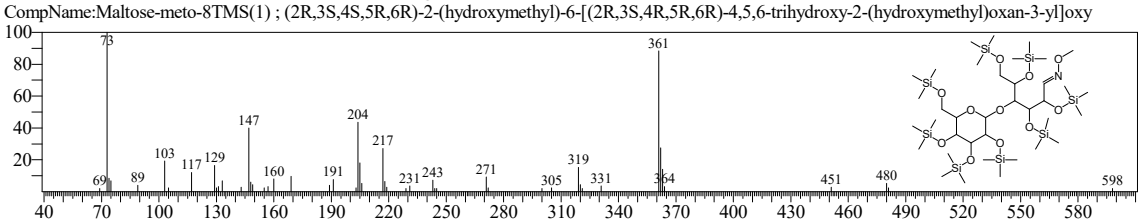
Hit#:2 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



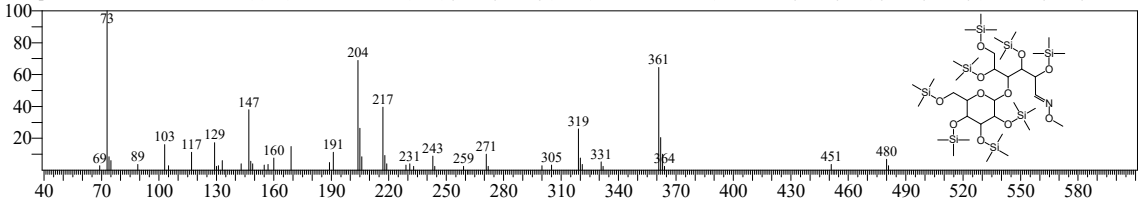
Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



Hit#:4 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

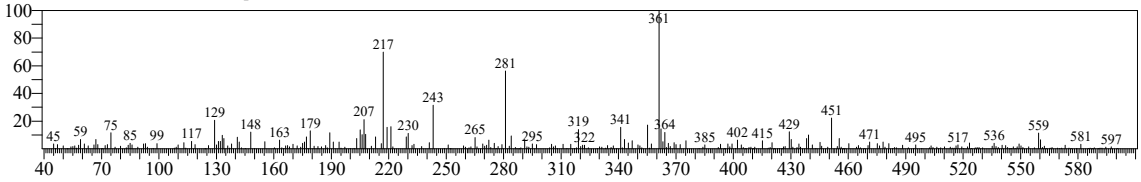


Hit#:5 Entry:545 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C37H89NO11Si8 CAS:63-42-3 MolWeight:947 RetIndex:2760
CompName:Lactose-meto-8TMS(1) ; (2R,3R,4S,5R,6S)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

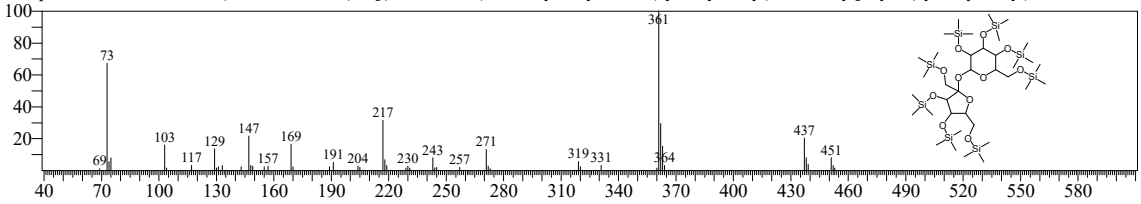


TNAU

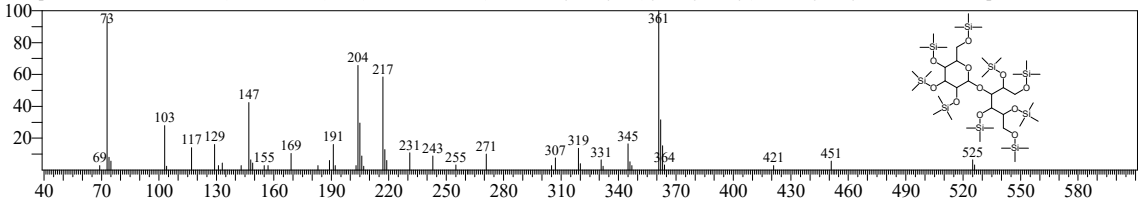
<< Target >>
Line#:21 R.Time:29.155(Scan#:4932) MassPeaks:308
RawMode:Averaged 29.150-29.160(4931-4933) BasePeak:361.20(2849)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



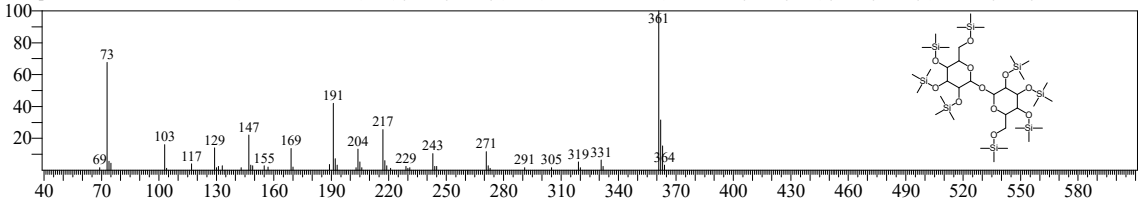
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



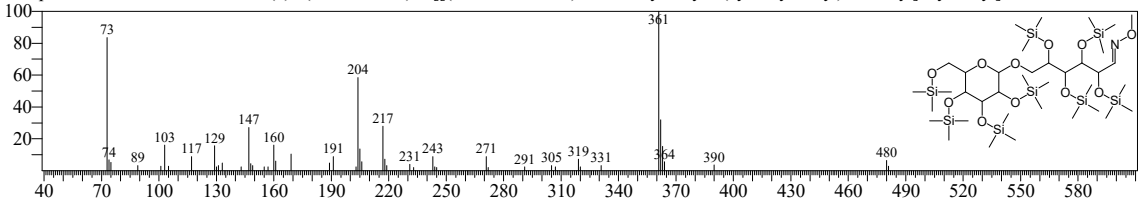
Hit#:2 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



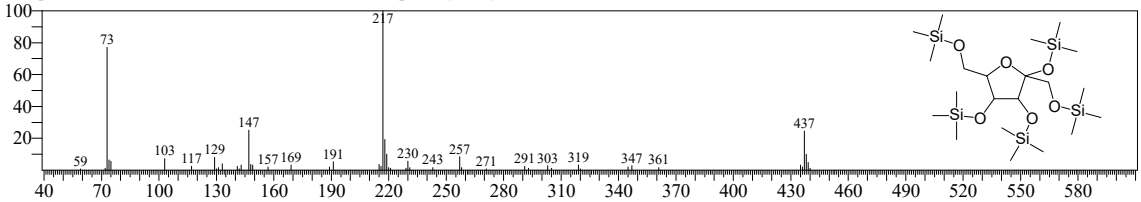
Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

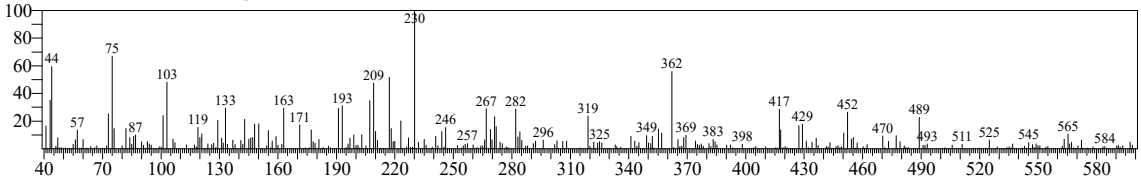


Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

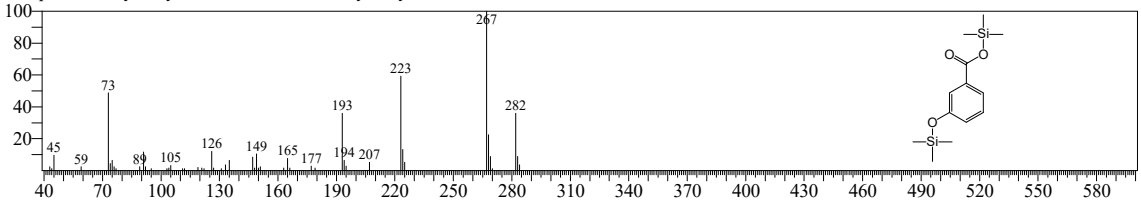


TNAU

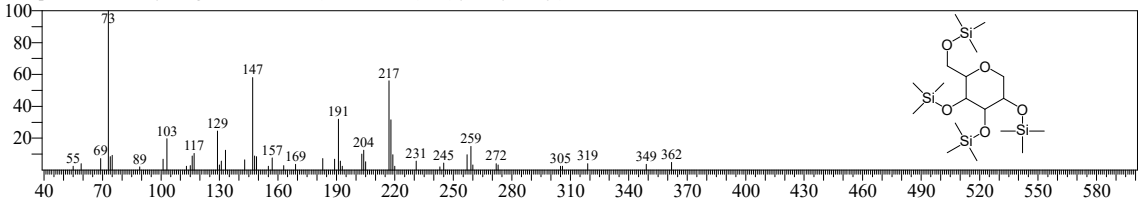
<< Target >>
Line#:22 R.Time:29.250(Scan#:4951) MassPeaks:291
RawMode:Averaged 29.245-29.255(4950-4952) BasePeak:230.10(1452)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



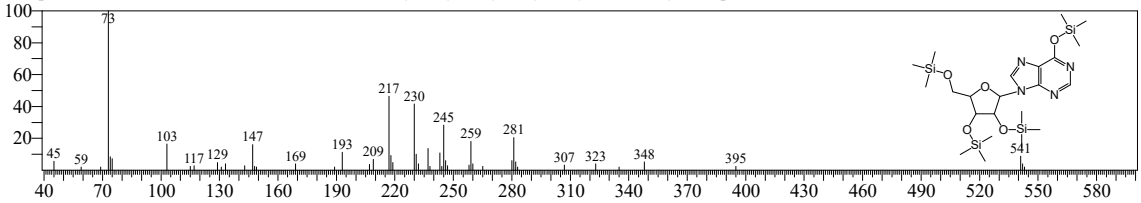
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



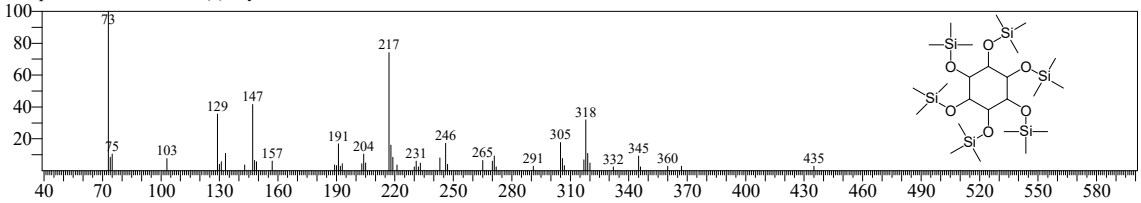
Hit#:2 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol



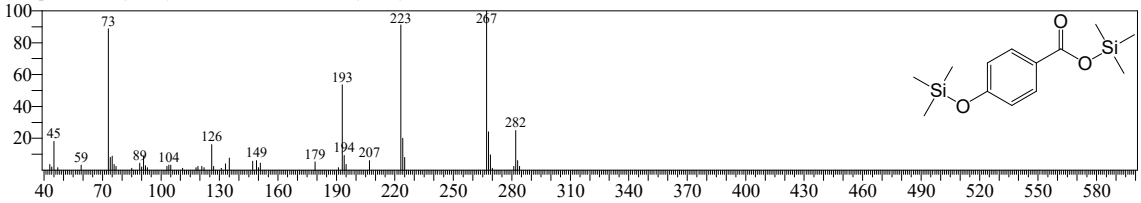
Hit#:3 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



Hit#:4 Entry:441 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C24H60O6Si6 CAS:87-89-8 MolWeight:612 RetIndex:2020
CompName:Inositol-6TMS(1) ; cyclohexane-1,2,3,4,5,6-hexol

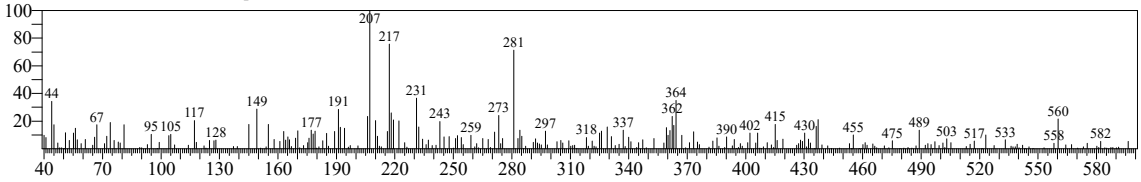


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

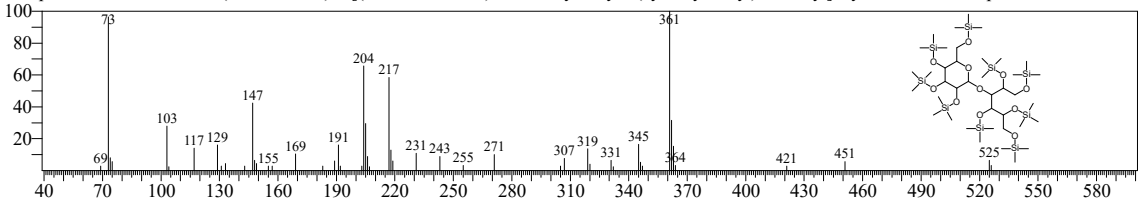


TNAU

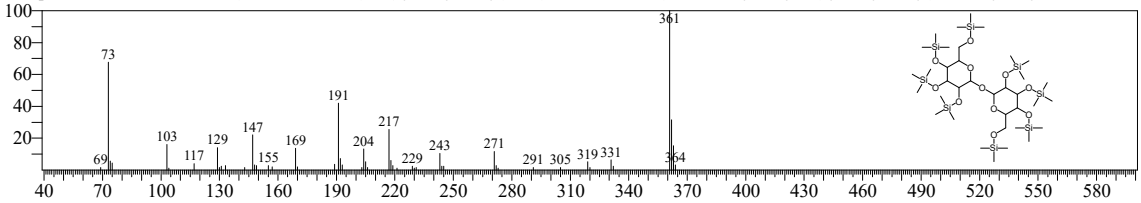
<< Target >>
Line#:23 R.Time:29.315(Scan#:4964) MassPeaks:274
RawMode:Averaged 29.310-29.320(4963-4965) BasePeak:207.05(1332)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



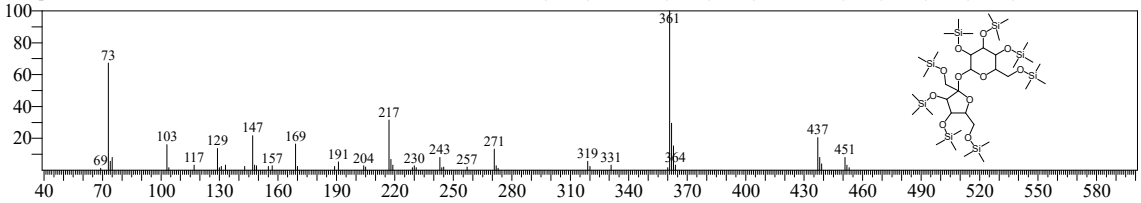
Hit#:1 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



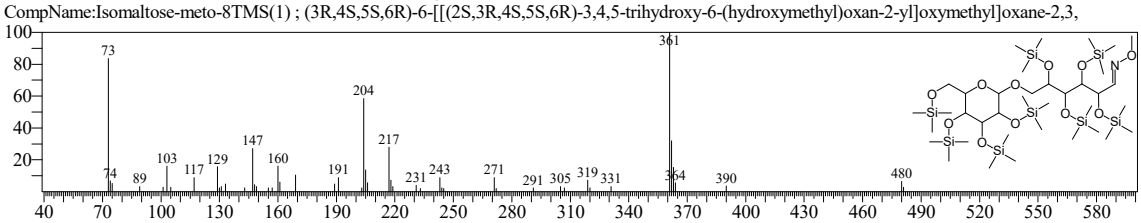
Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



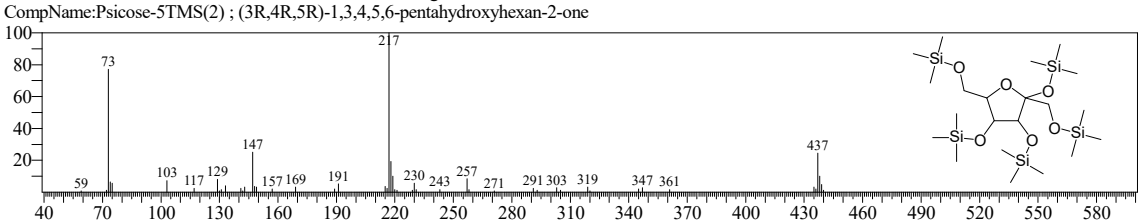
Hit#:3 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

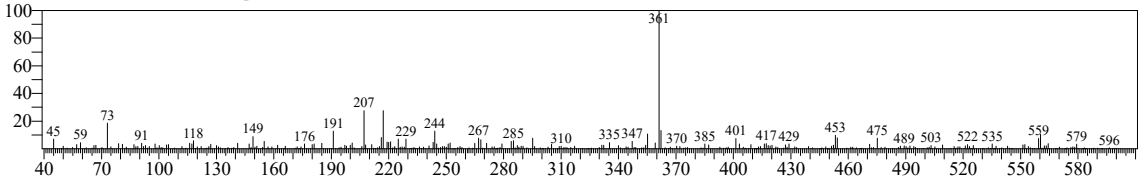


Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

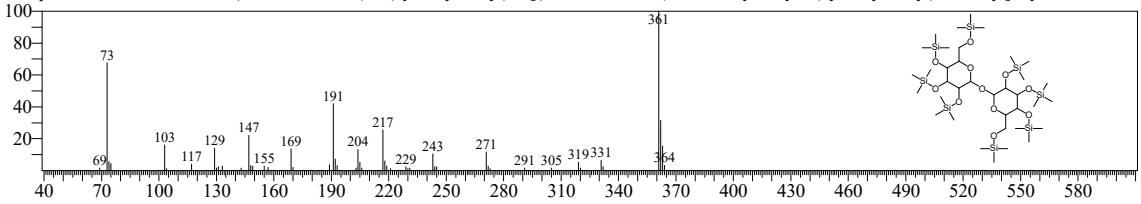


TNAU

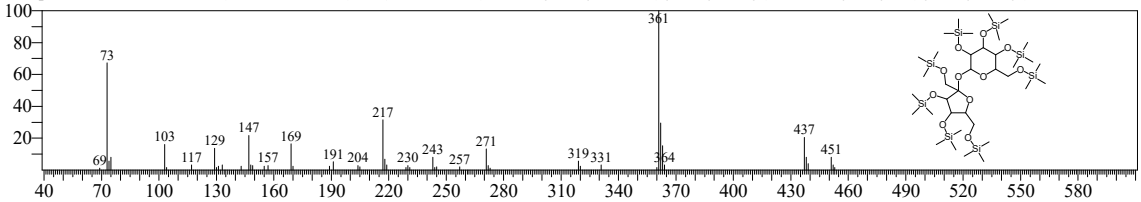
<< Target >>
Line#:24 R.Time:29.355(Scan#:4972) MassPeaks:311
RawMode:Averaged 29.350-29.360(4971-4973) BasePeak:361.20(4490)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



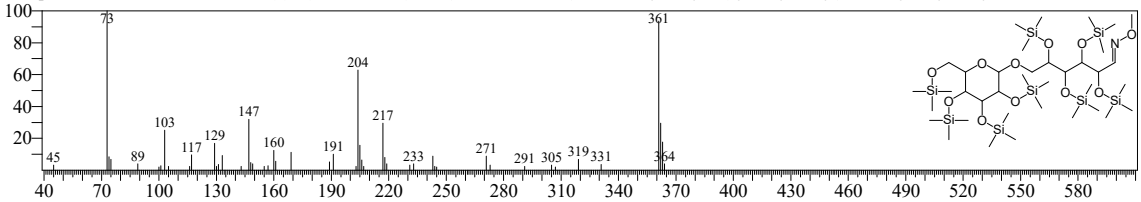
Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



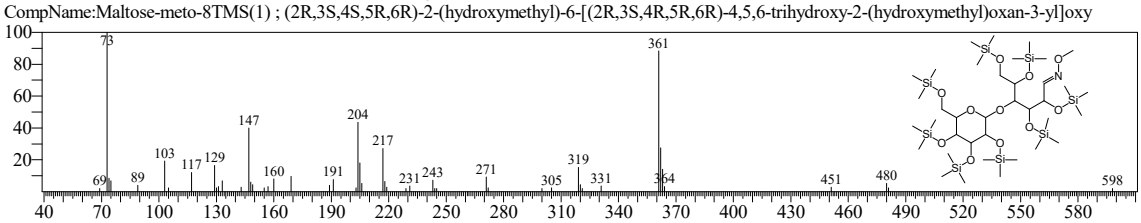
Hit#:2 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:48 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



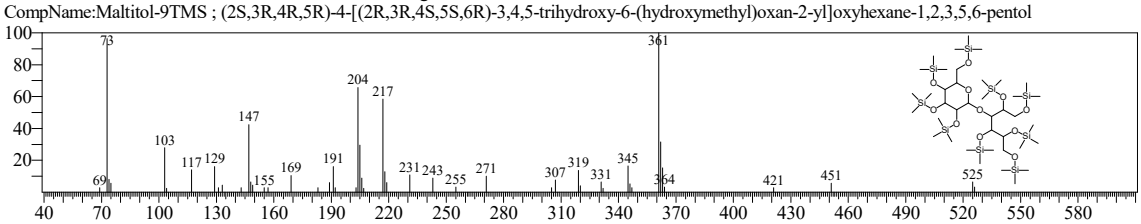
Hit#:3 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



Hit#:4 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

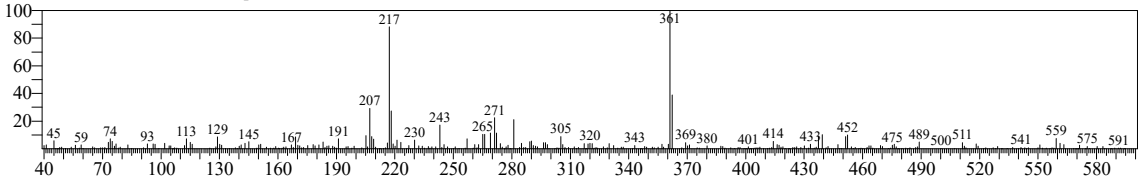


Hit#:5 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

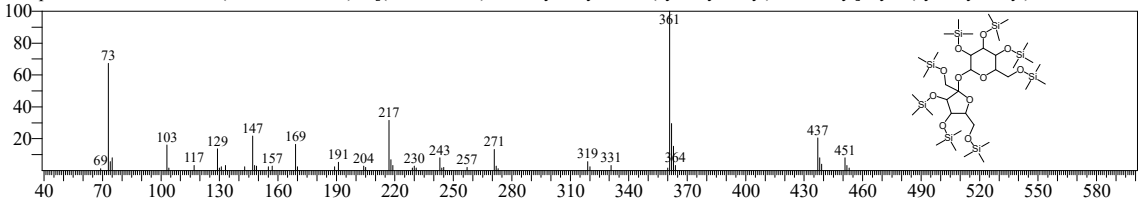


TNAU

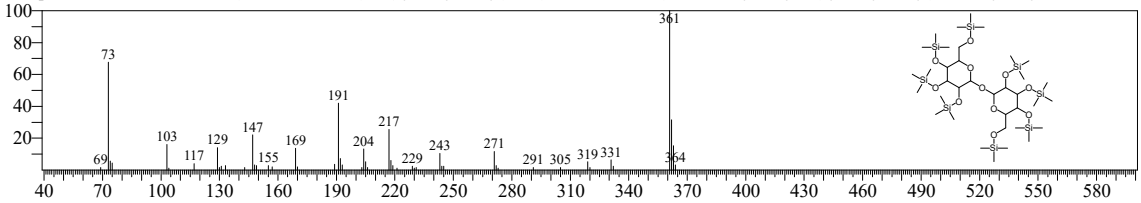
<< Target >>
Line#:25 R.Time:29.540(Scan#:5009) MassPeaks:316
RawMode:Averaged 29.535-29.545(5008-5010) BasePeak:361.20(5094)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



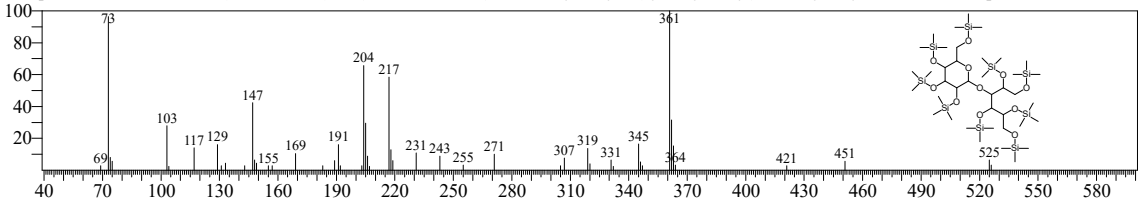
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:59 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



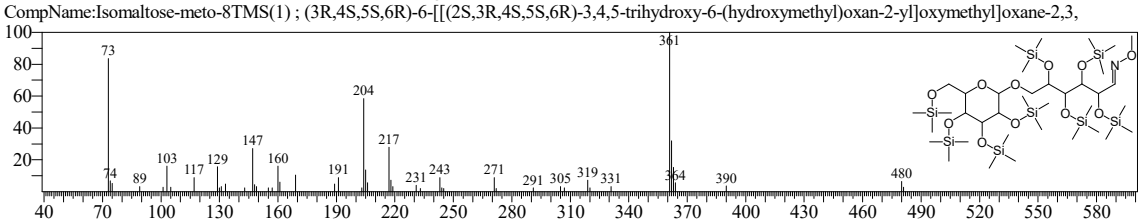
Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:55 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



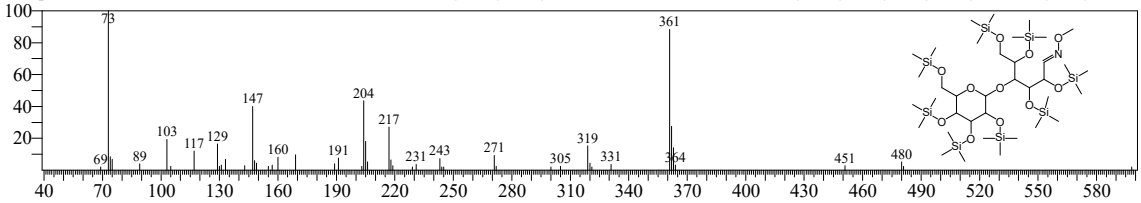
Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:52 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

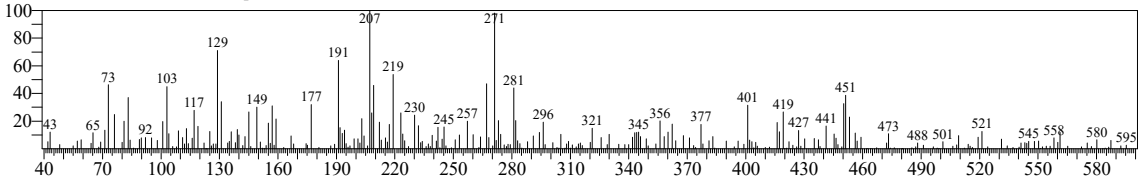


Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:50 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

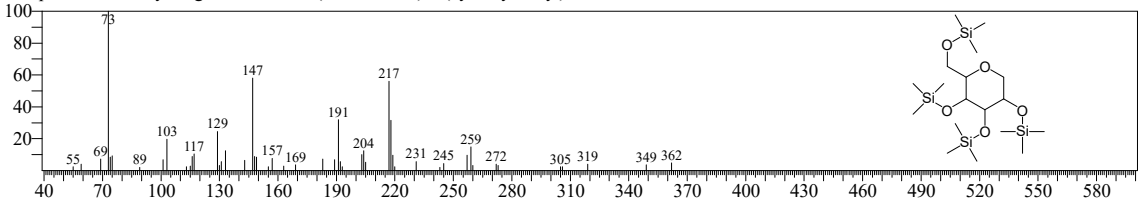


TNAU

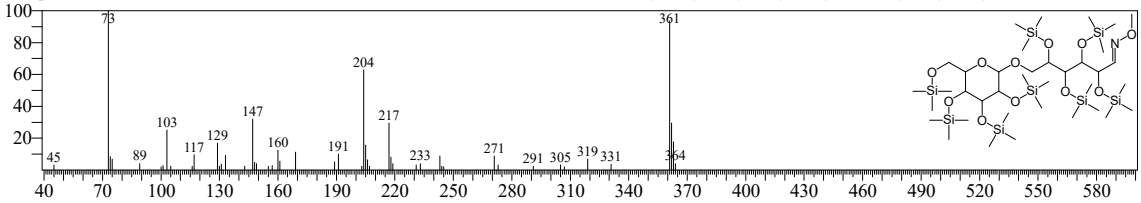
<< Target >>
Line#:26 R.Time:29.690(Scan#:5039) MassPeaks:275
RawMode:Averaged 29.685-29.695(5038-5040) BasePeak:207.05(873)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



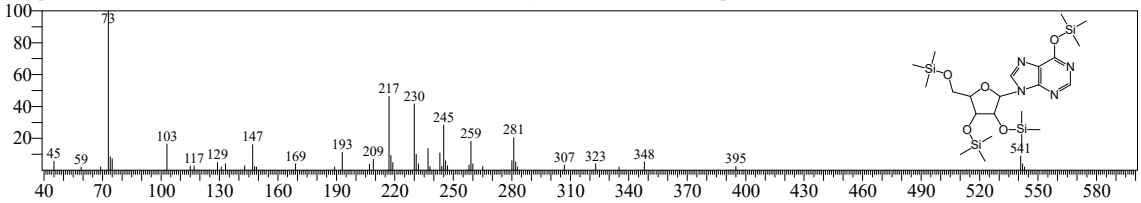
Hit#:1 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol



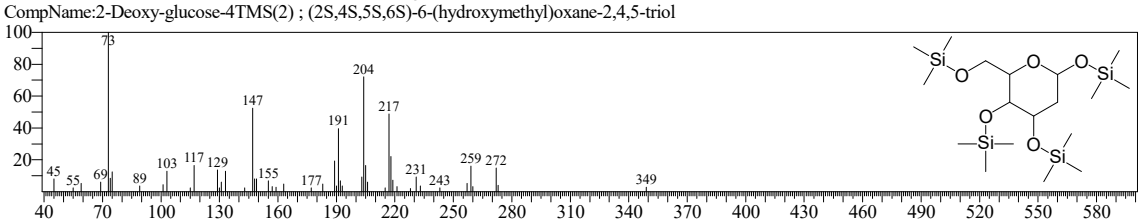
Hit#:2 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



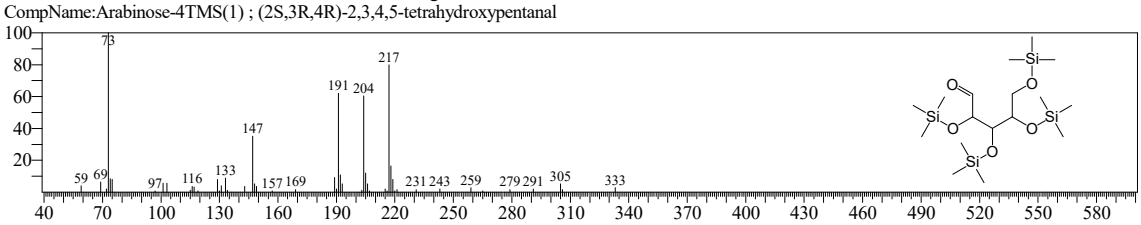
Hit#:3 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



Hit#:4 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:31 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

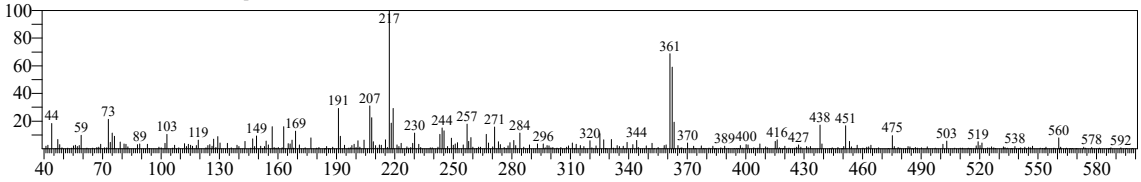


Hit#:5 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

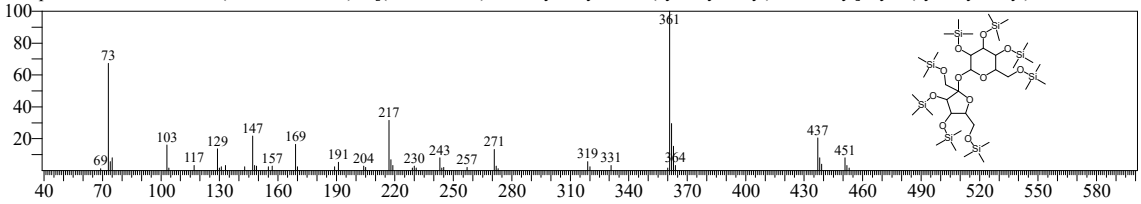


TNAU

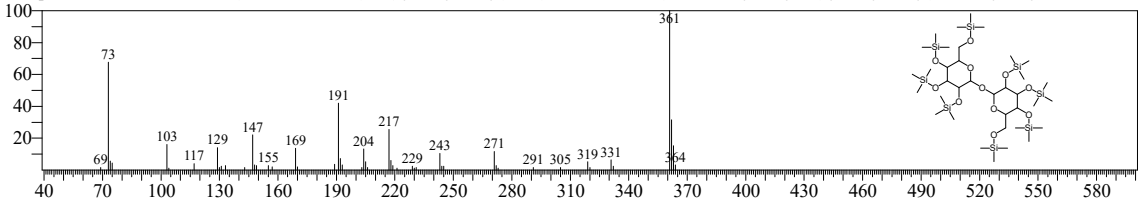
<< Target >>
Line#:27 R.Time:29.790(Scan#:5059) MassPeaks:319
RawMode:Averaged 29.785-29.795(5058-5060) BasePeak:217.10(3655)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



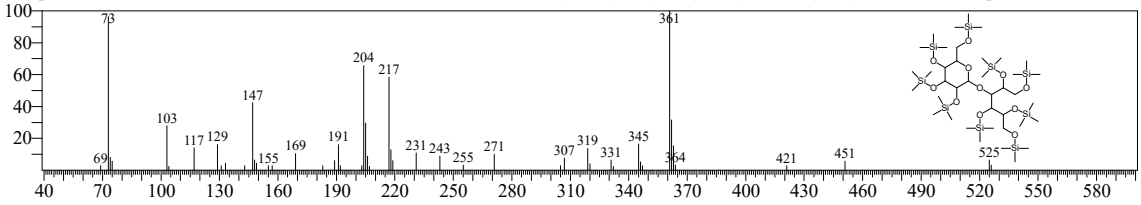
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:60 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



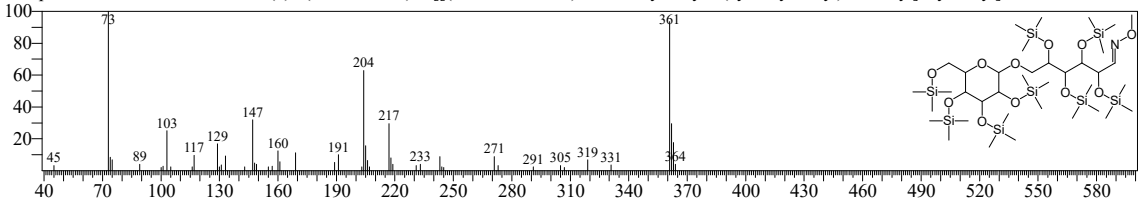
Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:59 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



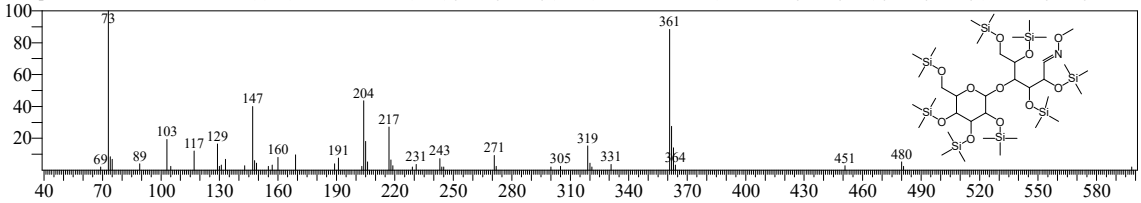
Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:56 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:55 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,

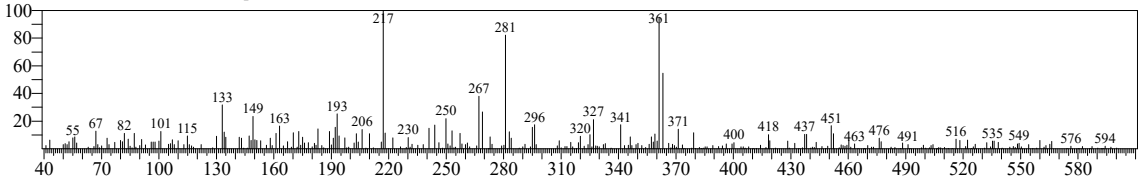


Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:54 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

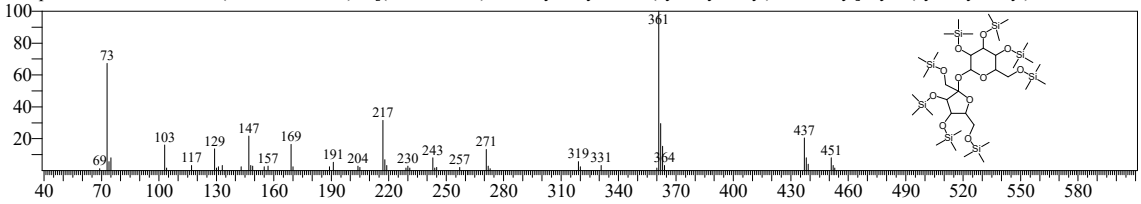


TNAU

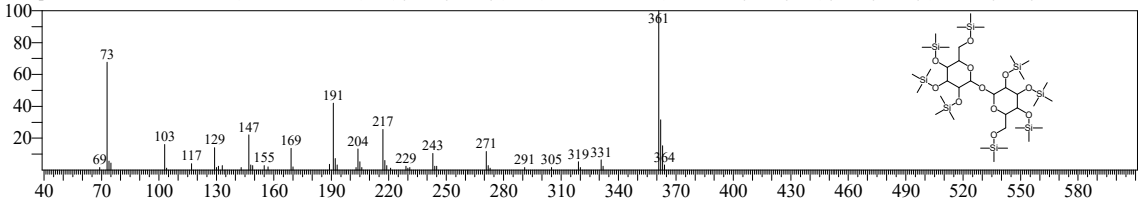
<< Target >>
Line#:28 R.Time:29.920(Scan#:5085) MassPeaks:302
RawMode:Averaged 29.915-29.925(5084-5086) BasePeak:217.10(1381)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



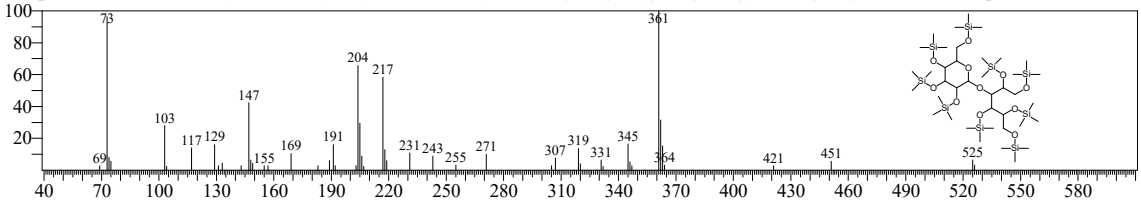
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



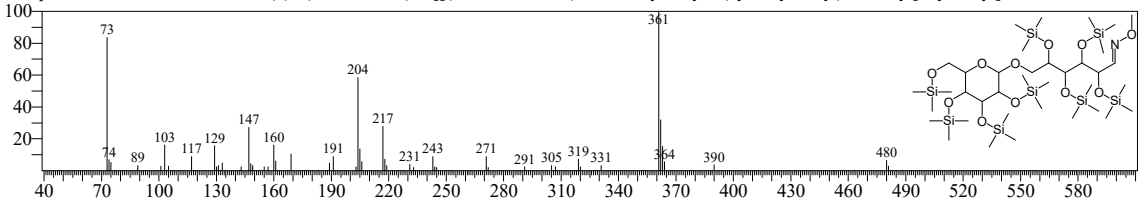
Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



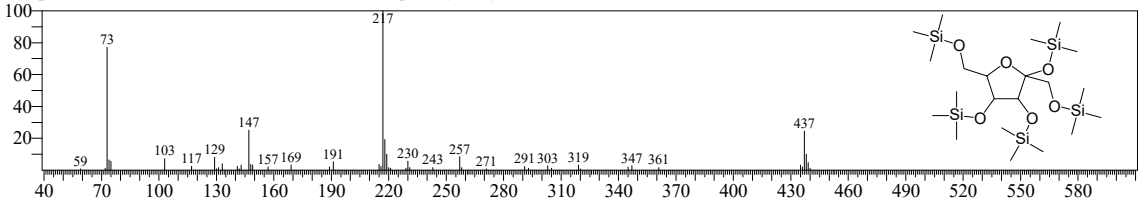
Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

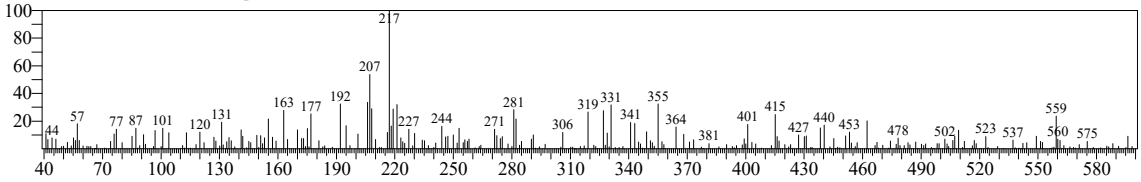


Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

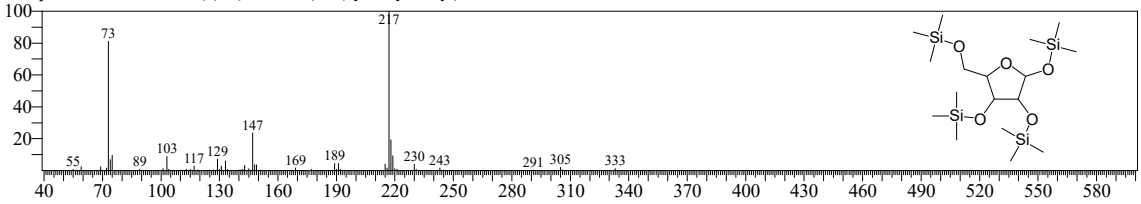


TNAU

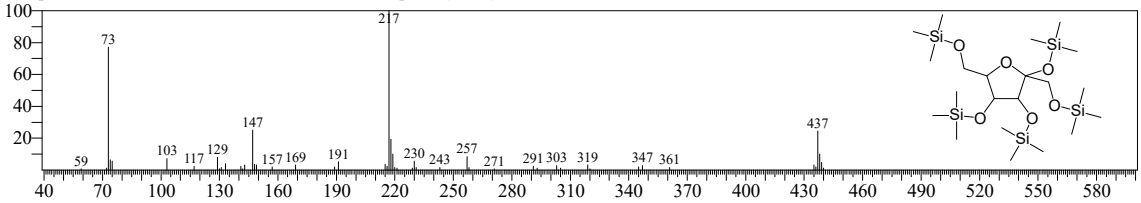
<< Target >>
Line#:29 R.Time:30.010(Scan#:5103) MassPeaks:279
RawMode:Averaged 30.005-30.015(5102-5104) BasePeak:217.10(1446)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



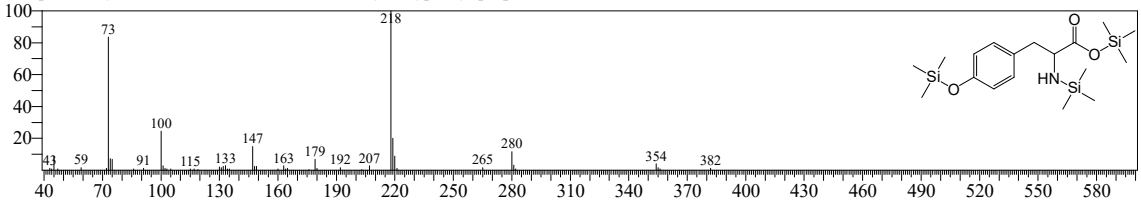
Hit#:1 Entry:230 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1666
CompName:Ribose-4TMS(2) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



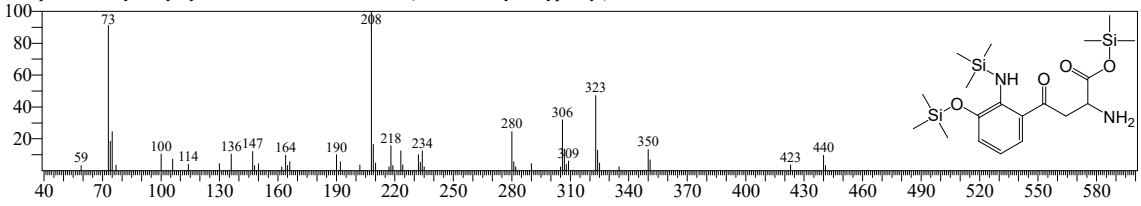
Hit#:2 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1841
CompName:Psicose-5TMS(2) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



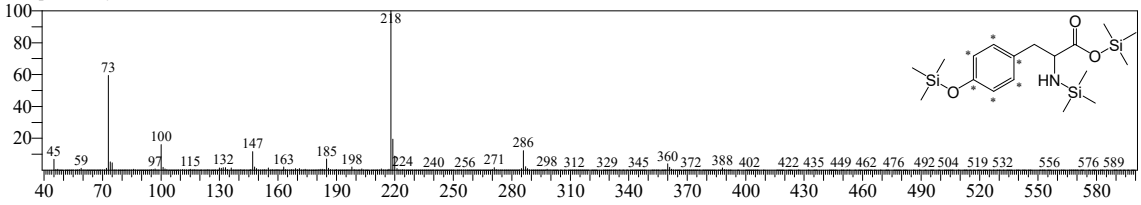
Hit#:3 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid



Hit#:4 Entry:506 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C19H36N2O4Si3 CAS:2147-61-7 MolWeight:440 RetIndex:2375
CompName:3-Hydroxy-kynurenine-3TMS ; 2-amino-4-(2-amino-3-hydroxyphenyl)-4-oxobutanoic acid

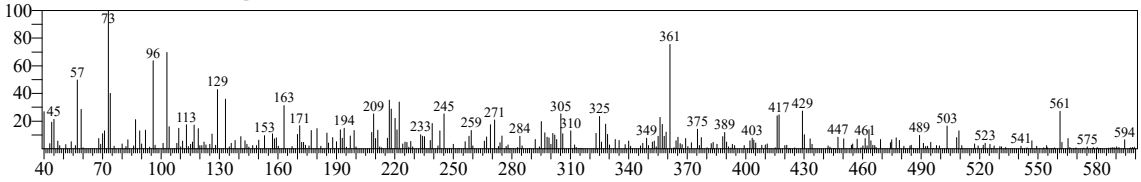


Hit#:5 Entry:412 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula: CAS:0-00-0 MolWeight:403 RetIndex:1957
CompName:Tyrosine-13C6-3TMS ;

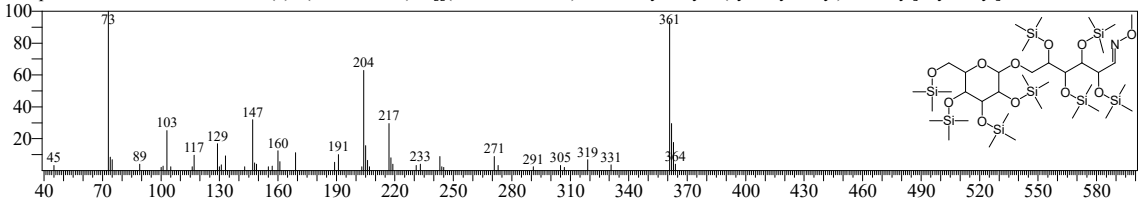


TNAU

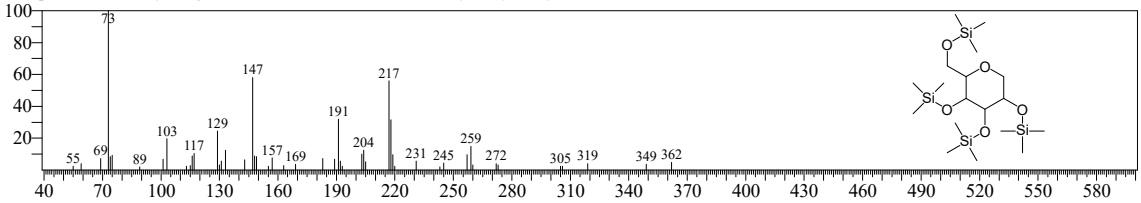
<< Target >>
Line#:30 R.Time:30.065(Scan#:5114) MassPeaks:297
RawMode:Averaged 30.060-30.070(5113-5115) BasePeak:73.05(1174)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



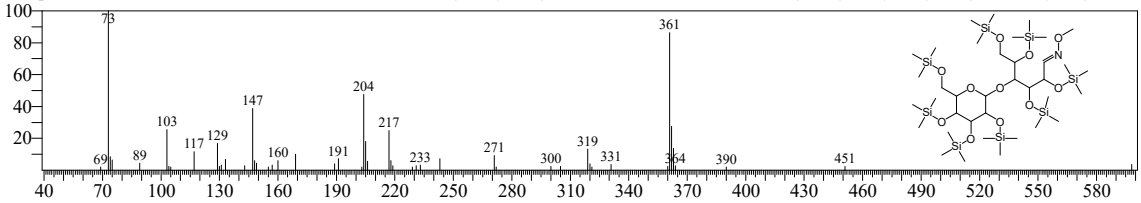
Hit#:1 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



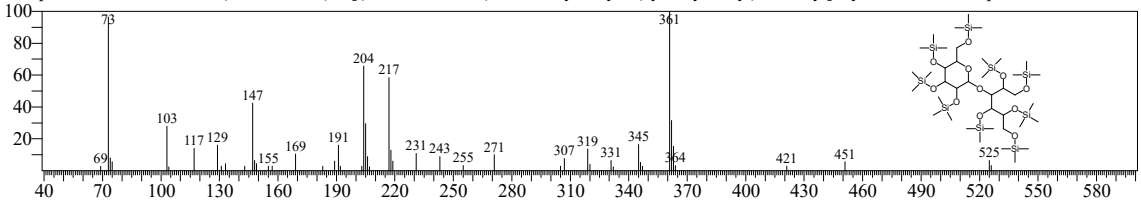
Hit#:2 Entry:351 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H44O5Si4 CAS:154-58-5 MolWeight:452 RetIndex:1876
CompName:1,5-Anhydro-glucitol-4TMS ; (2R,3S,4R,5S)-2-(hydroxymethyl)oxane-3,4,5-triol



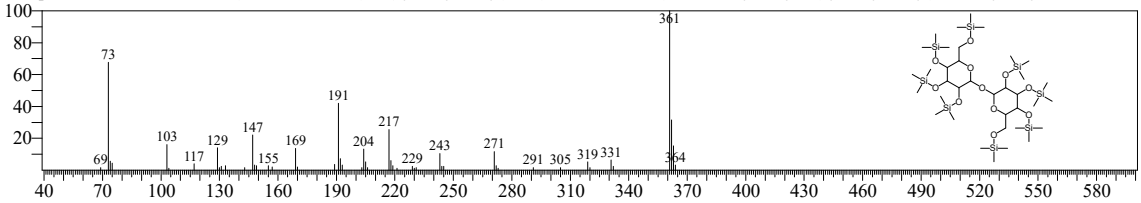
Hit#:3 Entry:556 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2846
CompName:Maltose-meto-8TMS(2) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy



Hit#:4 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

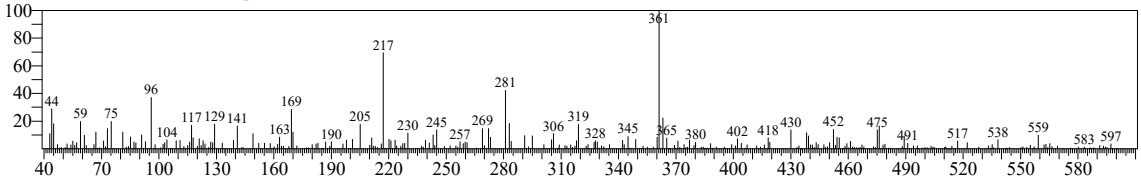


Hit#:5 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

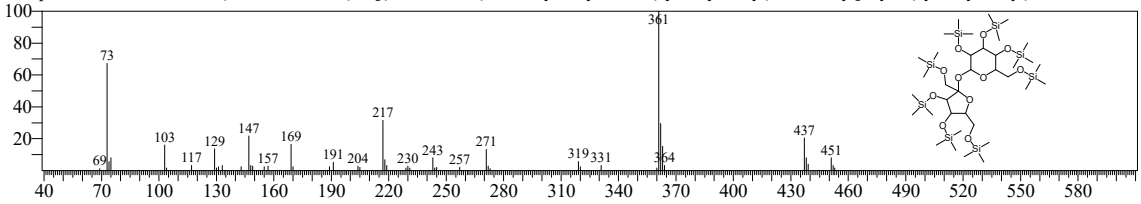


TNAU

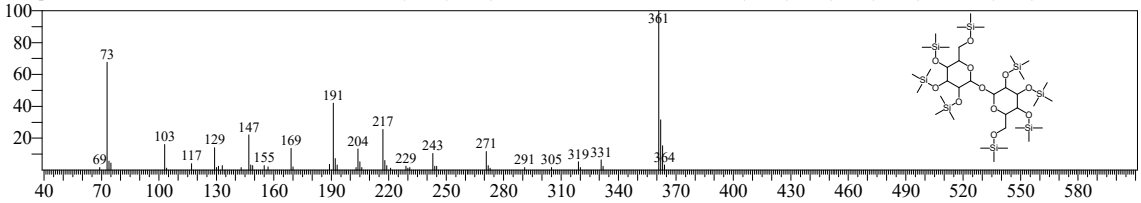
<< Target >>
Line#:31 R.Time:30.090(Scan#:5119) MassPeaks:298
RawMode:Averaged 30.085-30.095(5118-5120) BasePeak:361.20(1830)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



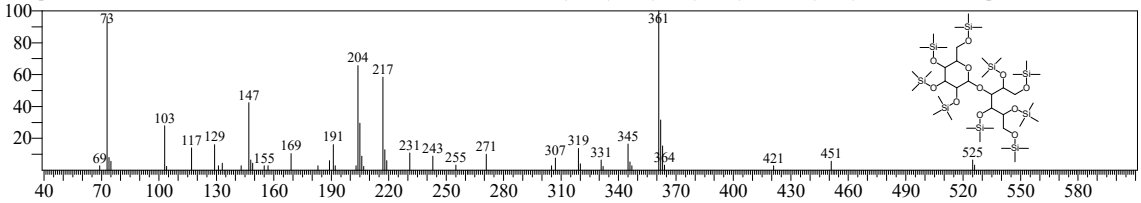
Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



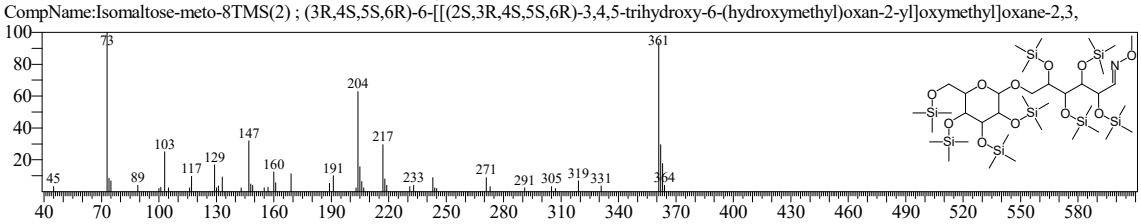
Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



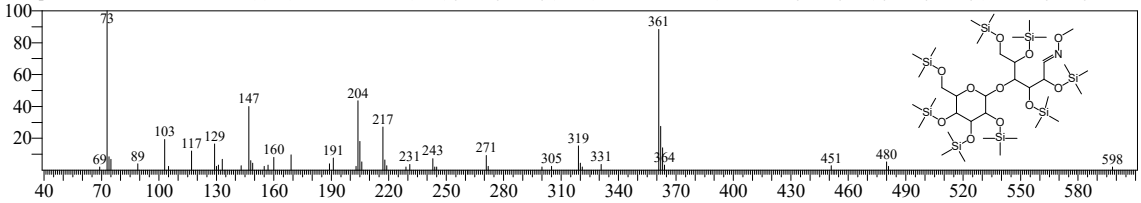
Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
SI:41 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,

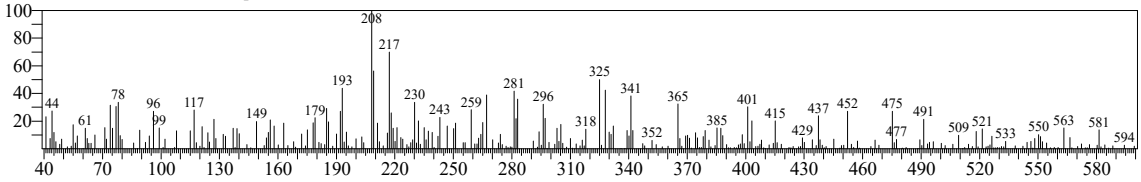


Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C37H89NO11Si8 CAS:69-79-4 MolWeight:947 RetIndex:2817
CompName:Maltose-meto-8TMS(1) ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3S,4R,5R,6R)-4,5,6-trihydroxy-2-(hydroxymethyl)oxan-3-yl]oxy

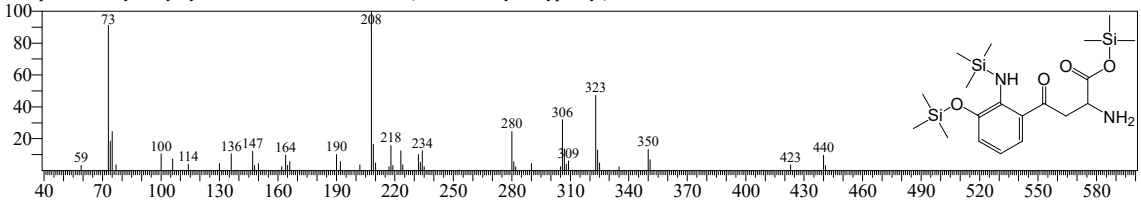


TNAU

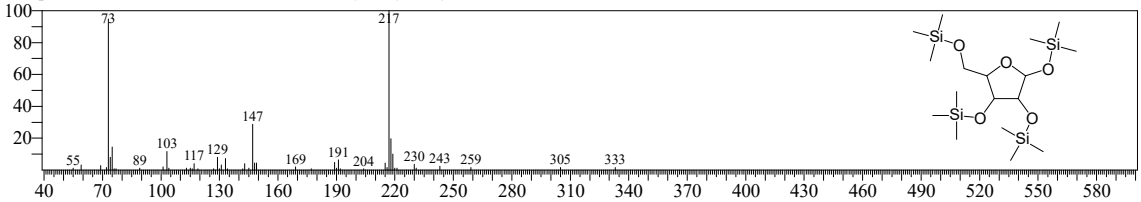
<< Target >>
Line#:32 R.Time:30.765(Scan#:5254) MassPeaks:308
RawMode:Averaged 30.760-30.770(5253-5255) BasePeak:208.05(781)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



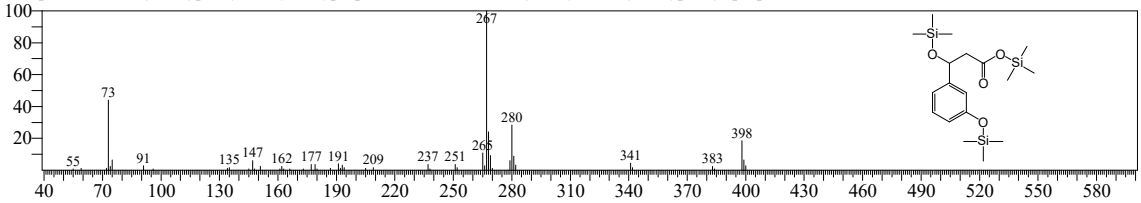
Hit#:1 Entry:506 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C19H36N2O4Si3 CAS:2147-61-7 MolWeight:440 RetIndex:2375
CompName:3-Hydroxy-kynurenine-3TMS ; 2-amino-4-(2-amino-3-hydroxyphenyl)-4-oxobutanoic acid



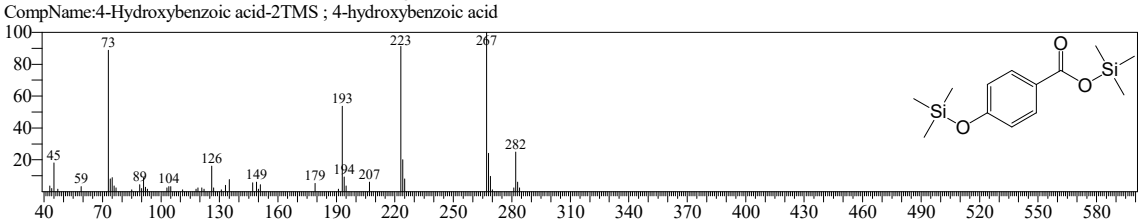
Hit#:2 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



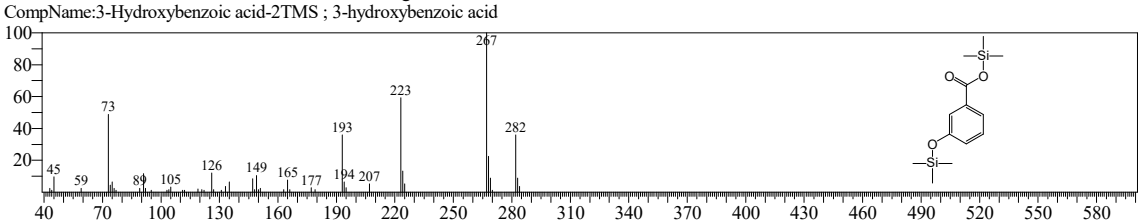
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

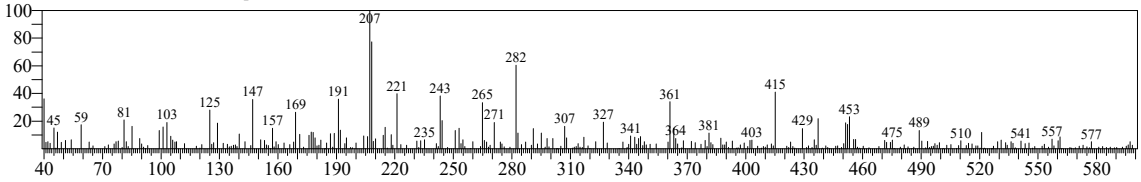


Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

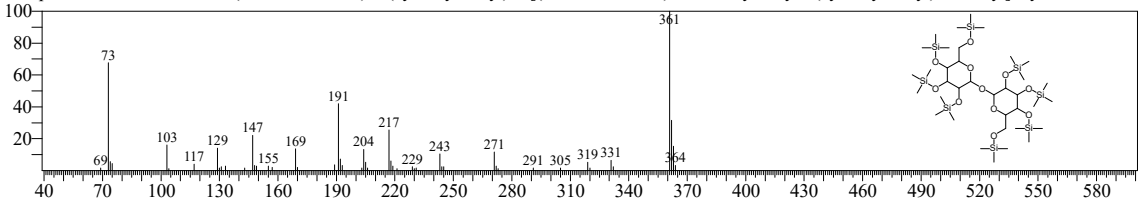


TNAU

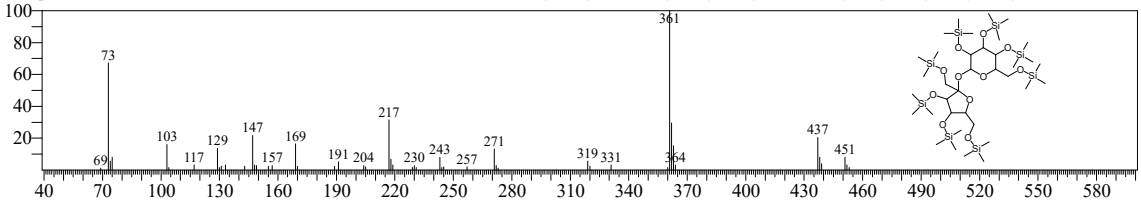
<< Target >>
Line#:33 R.Time:30.835(Scan#:5268) MassPeaks:314
RawMode:Averaged 30.830-30.840(5267-5269) BasePeak:207.05(1336)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



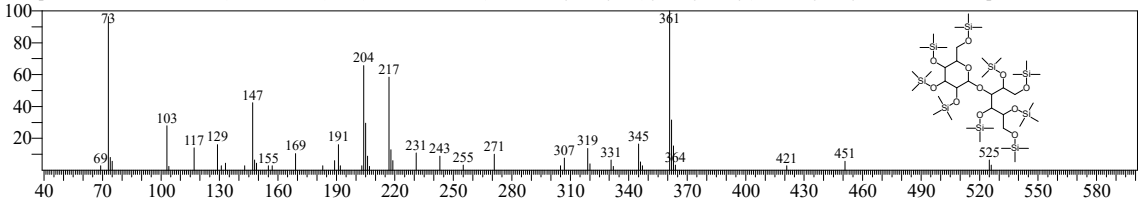
Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



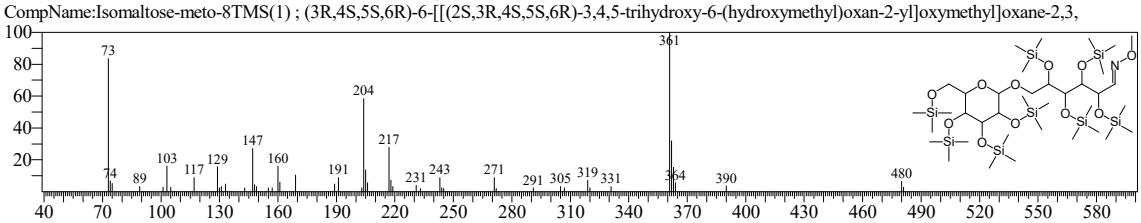
Hit#:2 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



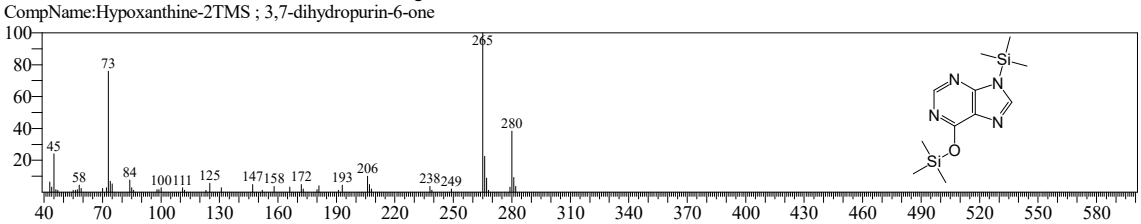
Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

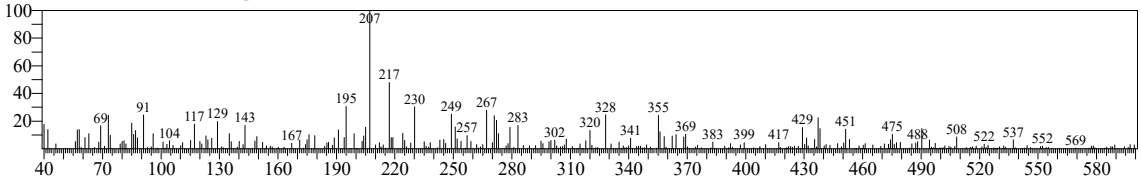


Hit#:5 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

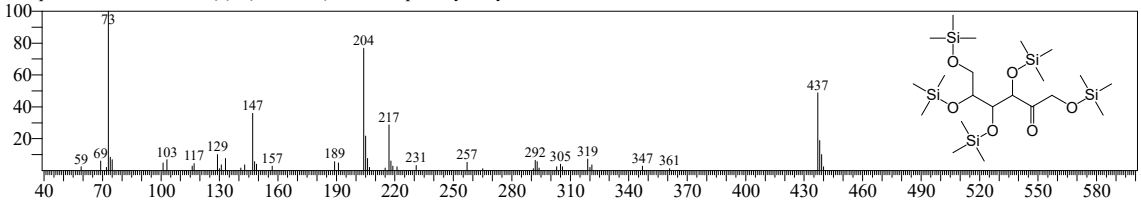


TNAU

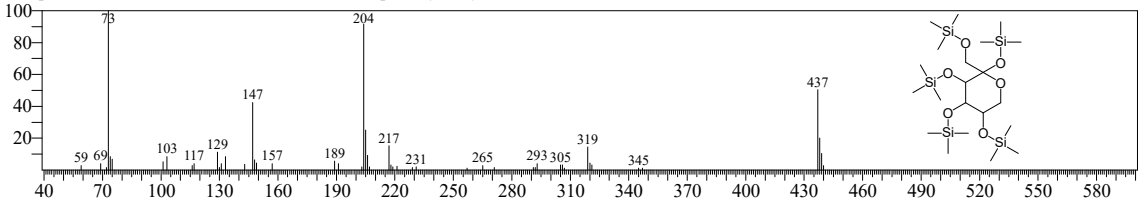
<< Target >>
Line#:34 R.Time:30.965(Scan#:5294) MassPeaks:290
RawMode:Averaged 30.960-30.970(5293-5295) BasePeak:207.05(1334)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



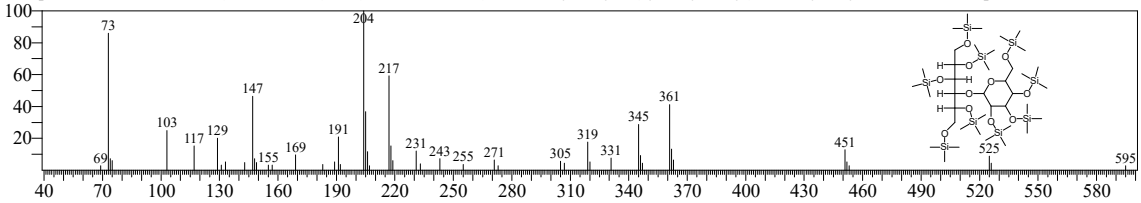
Hit#:1 Entry:334 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C21H52O6Si5 CAS:57-48-7 MolWeight:540 RetIndex:1852
CompName:Fructose-5TMS(3) ; (3S,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



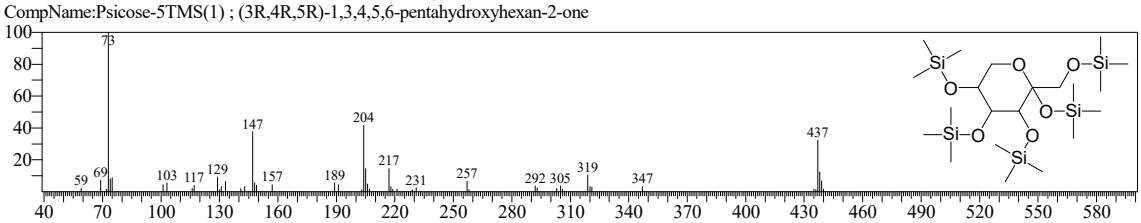
Hit#:2 Entry:360 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C21H52O6Si5 CAS:3615-56-3 MolWeight:540 RetIndex:1895
CompName:Sorbose-5TMS ; (3R,4S,5R)-1,3,4,5,6-pentahydroxyhexan-2-one



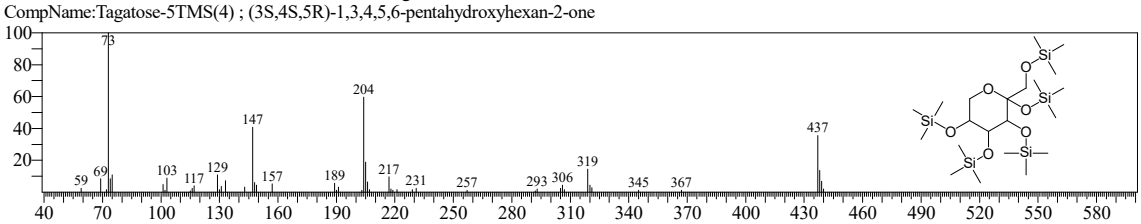
Hit#:3 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



Hit#:4 Entry:320 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1837
CompName:Psicose-5TMS(1) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

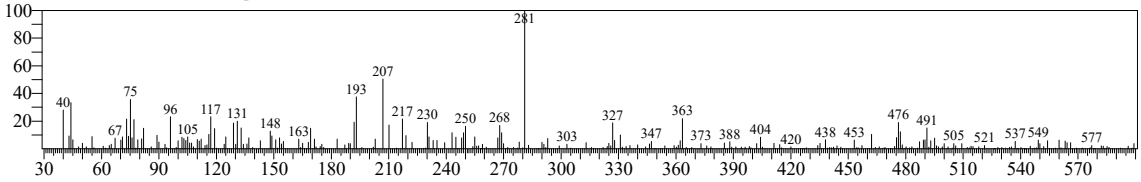


Hit#:5 Entry:380 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C21H52O6Si5 CAS:87-81-0 MolWeight:540 RetIndex:1914
CompName:Tagatose-5TMS(4) ; (3S,4S,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

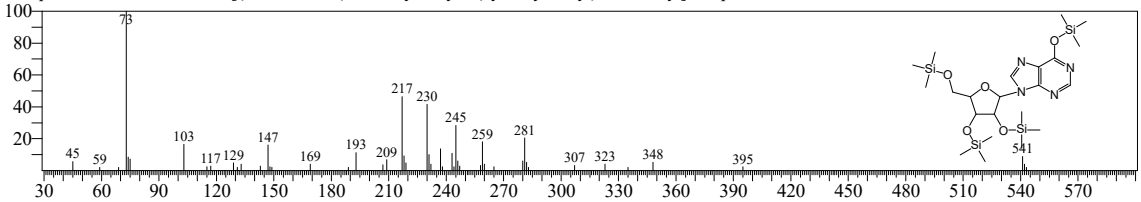


TNAU

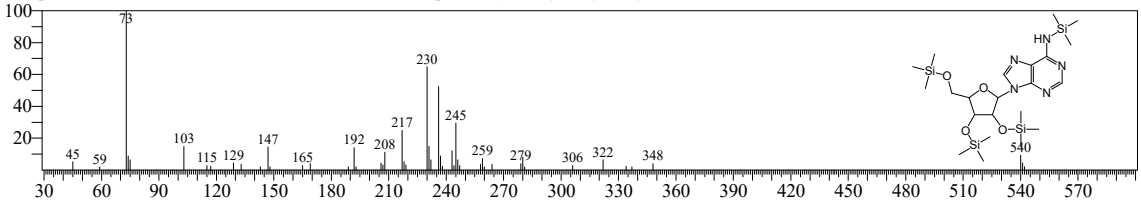
<< Target >>
Line#:35 R.Time:31.330(Scan#:5367) MassPeaks:273
RawMode:Averaged 31.325-31.335(5366-5368) BasePeak:281.05(1471)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



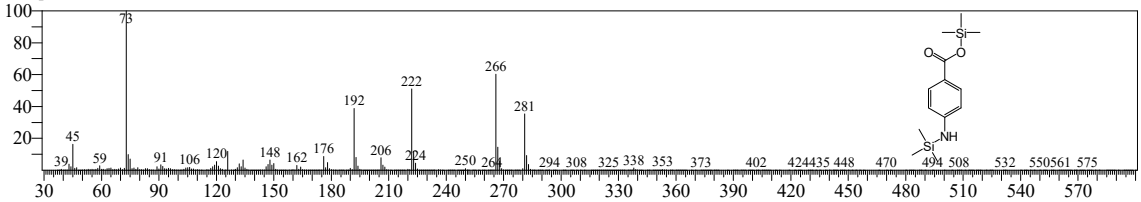
Hit#:1 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



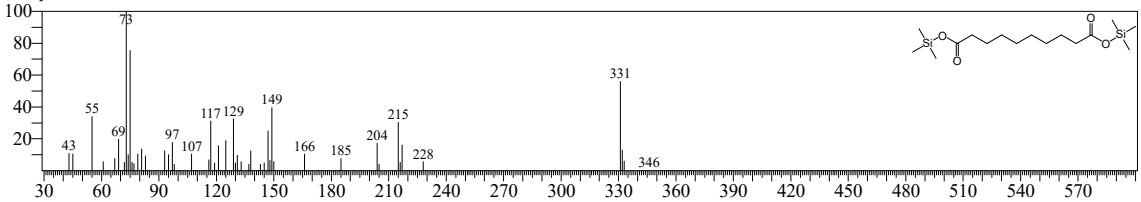
Hit#:2 Entry:538 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C22H45N5O4Si4 CAS:58-61-7 MolWeight:555 RetIndex:2670
CompName:Adenosine-4TMS ; (2R,3R,4S,5R)-2-(6-aminopurin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol



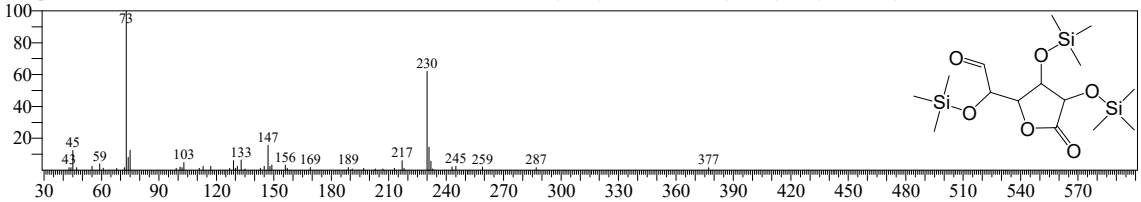
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:362 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C16H34O4Si2 CAS:111-20-6 MolWeight:346 RetIndex:1896
CompName:Sebacic acid-2TMS ; decanedioic acid

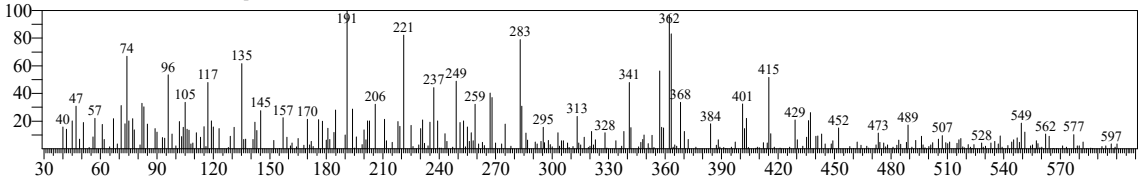


Hit#:5 Entry:336 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C15H32O6Si3 CAS:32449-92-6 MolWeight:392 RetIndex:1854
CompName:Glucuronic acid lactone-3TMS(2) ; (2R)-2-[(2S,3R,4S)-3,4-dihydroxy-5-oxooxolan-2-yl]-2-hydroxyacetaldehyde

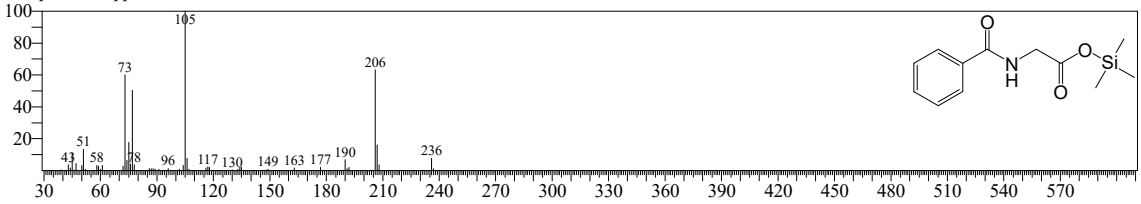


TNAU

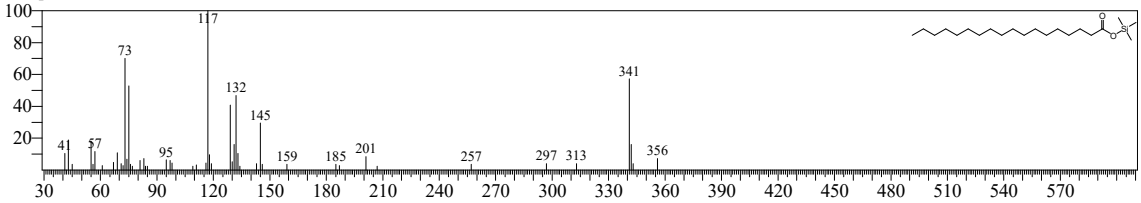
<< Target >>
Line#:36 R.Time:31.385(Scan#:5378) MassPeaks:299
RawMode:Averaged 31.380-31.390(5377-5379) BasePeak:191.05(738)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



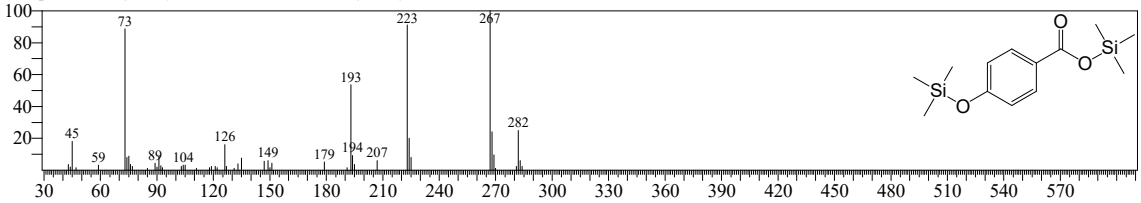
Hit#:1 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



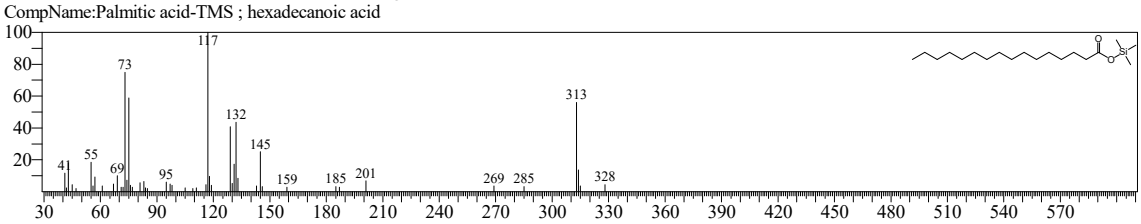
Hit#:2 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



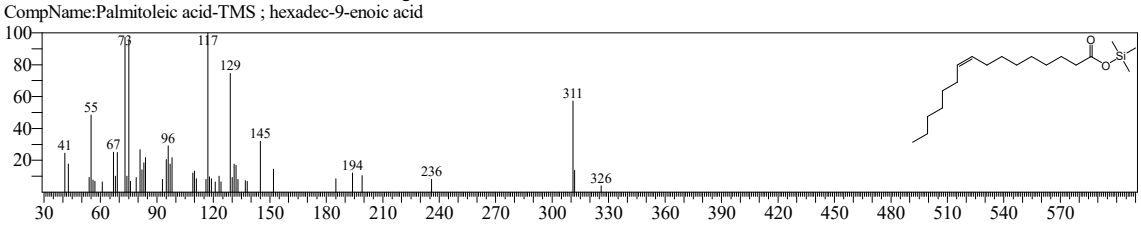
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:446 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C19H40O2Si CAS:57-10-3 MolWeight:328 RetIndex:2046
CompName:Palmitic acid-TMS ; hexadecanoic acid

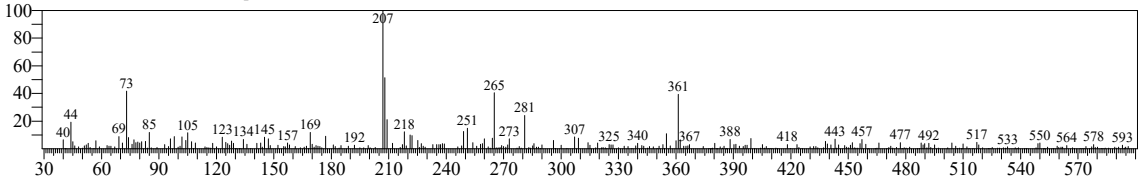


Hit#:5 Entry:442 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C19H38O2Si CAS:373-49-9 MolWeight:326 RetIndex:2028
CompName:Palmitoleic acid-TMS ; hexadec-9-enoic acid

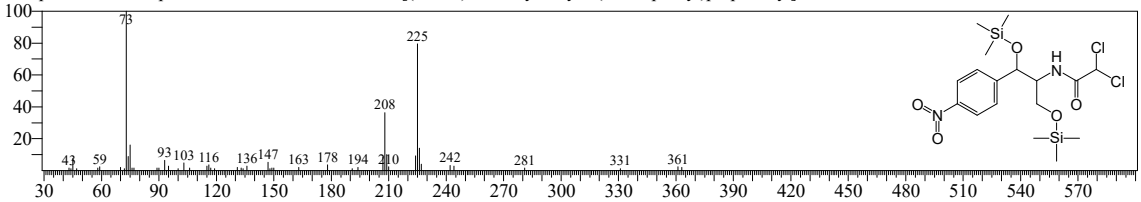


TNAU

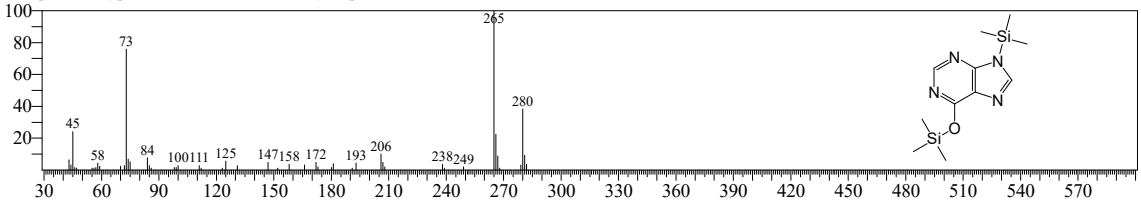
<< Target >>
Line#:37 R.Time:32.265(Scan#:5554) MassPeaks:330
RawMode:Averaged 32.260-32.270(5553-5555) BasePeak:207.05(2038)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



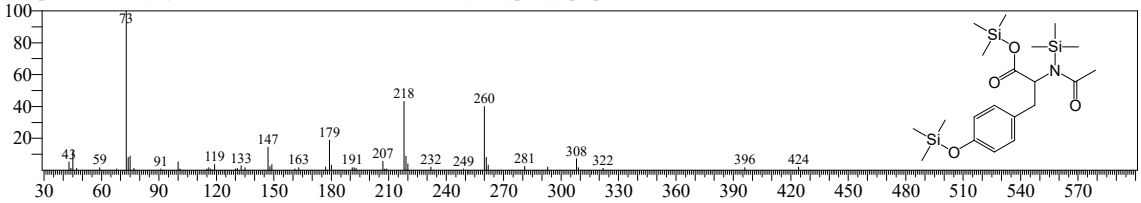
Hit#:1 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



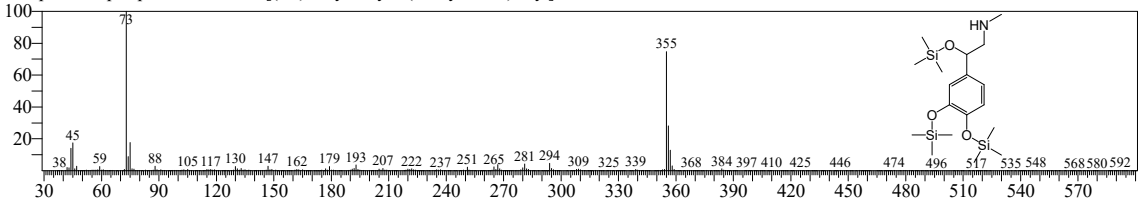
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



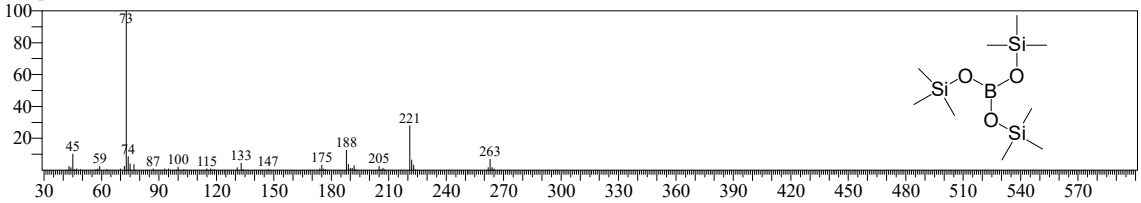
Hit#:3 Entry:461 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C20H37NO4Si3 CAS:537-55-3 MolWeight:439 RetIndex:2119
CompName:N-Acetyltyrosine-3TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid



Hit#:4 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

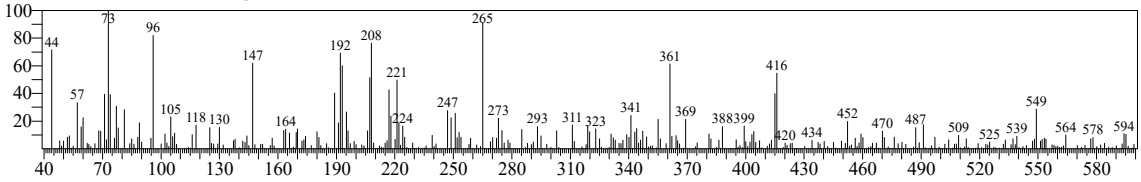


Hit#:5 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid

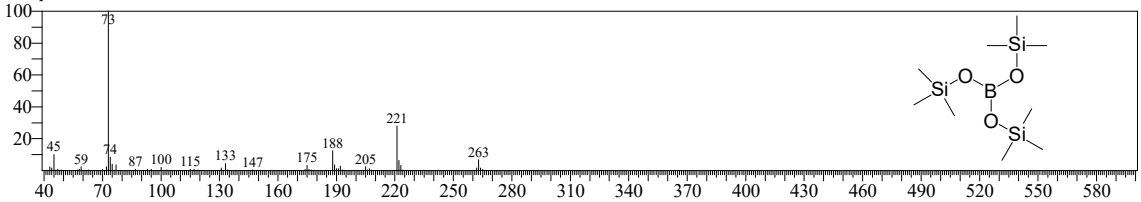


TNAU

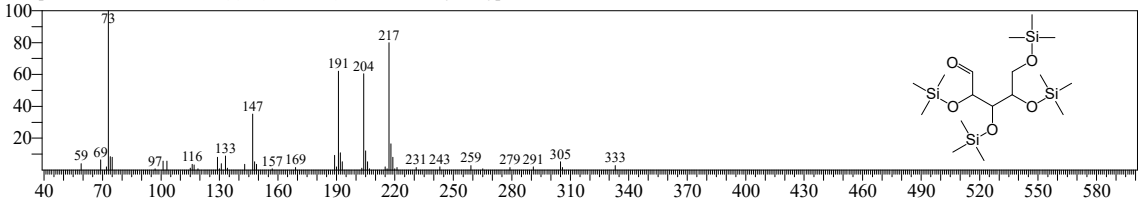
<< Target >>
Line#:38 R.Time:32.310(Scan#:5563) MassPeaks:325
RawMode:Averaged 32.305-32.315(5562-5564) BasePeak:73.05(797)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



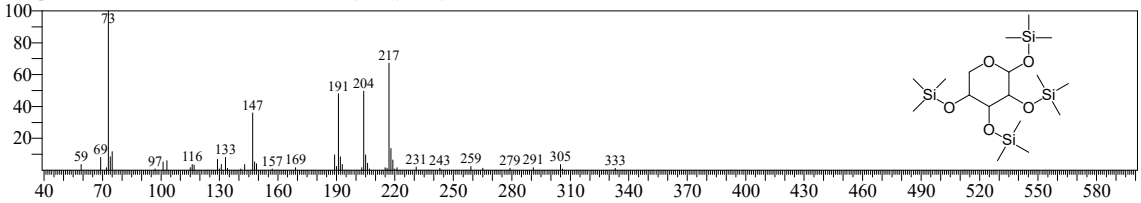
Hit#:1 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid



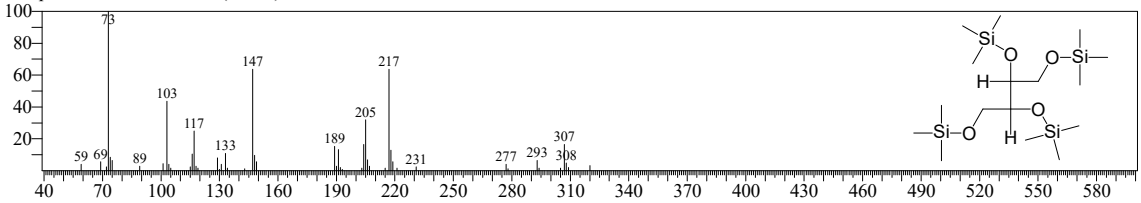
Hit#:2 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



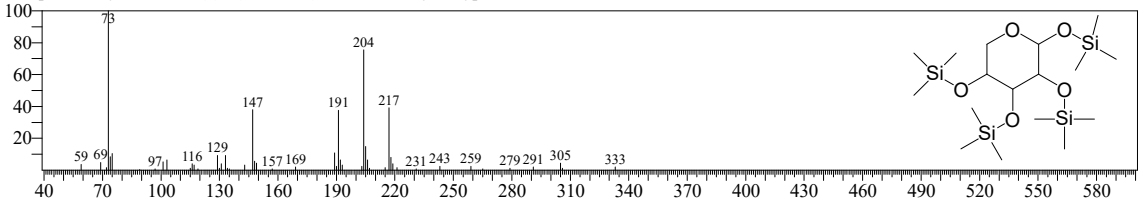
Hit#:3 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



Hit#:4 Entry:148 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C16H42O4Si4 CAS:2418-52-2 MolWeight:410 RetIndex:1512
CompName:Threitol-4TMS ; (2R,3R)-butane-1,2,3,4-tetrol

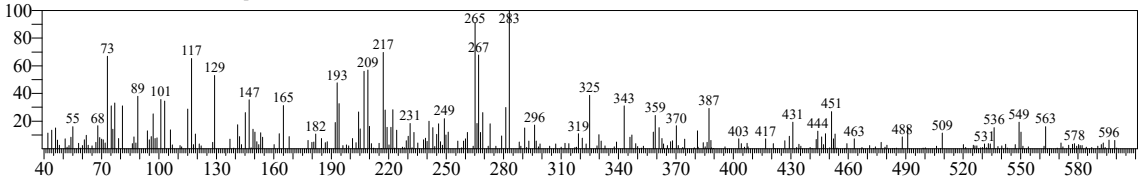


Hit#:5 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

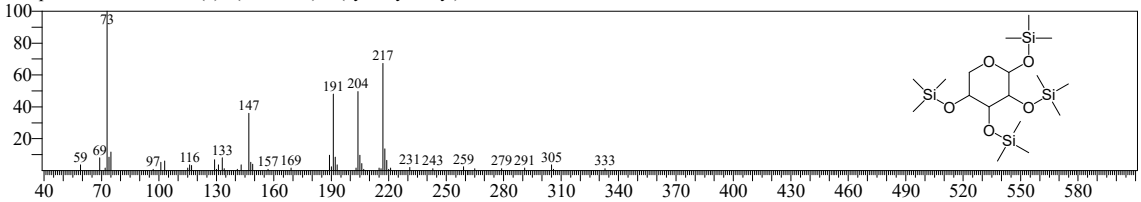


TNAU

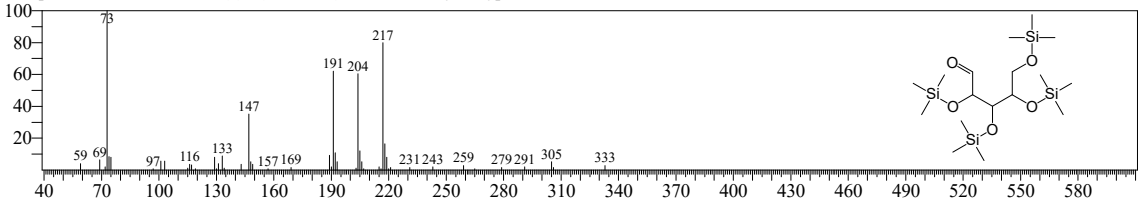
<< Target >>
Line#:39 R.Time:32.445(Scan#:5590) MassPeaks:289
RawMode:Averaged 32.440-32.450(5589-5591) BasePeak:283.05(801)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



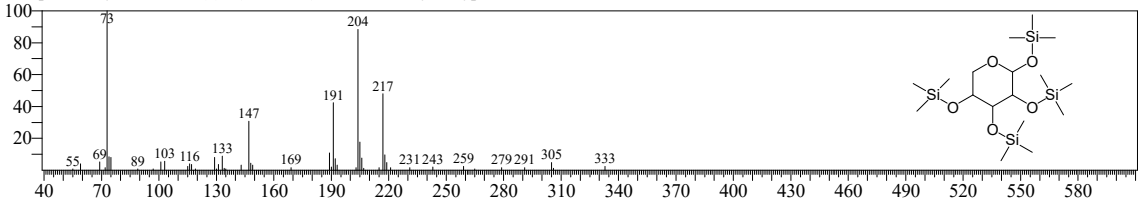
Hit#:1 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



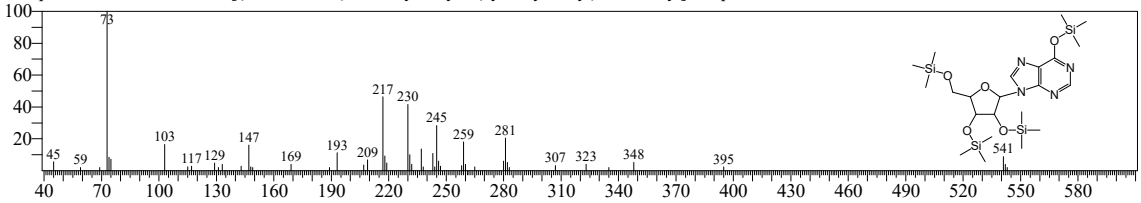
Hit#:2 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



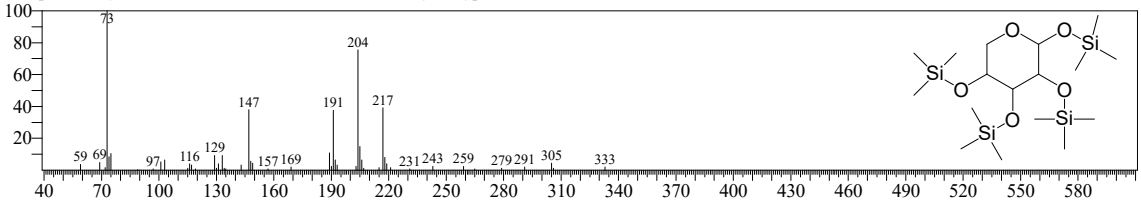
Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



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

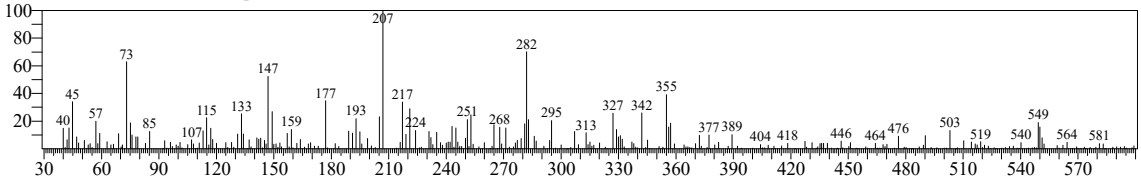


Hit#:5 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

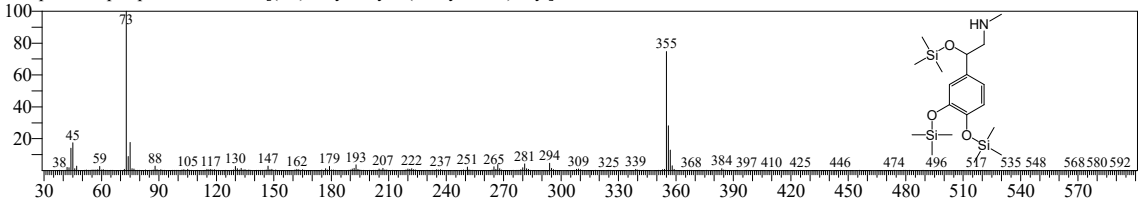


TNAU

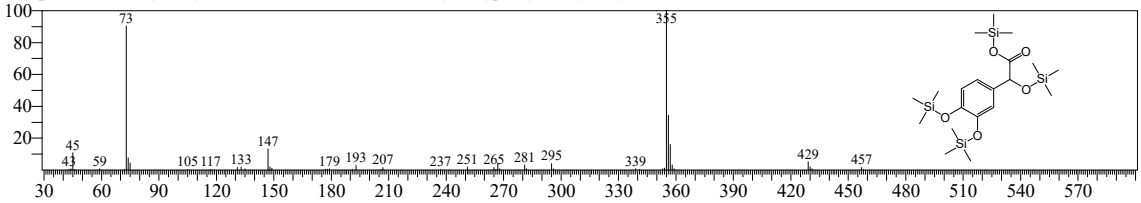
<< Target >>
Line#:40 R.Time:32.530(Scan#:5607) MassPeaks:301
RawMode:Averaged 32.525-32.535(5606-5608) BasePeak:207.05(1306)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



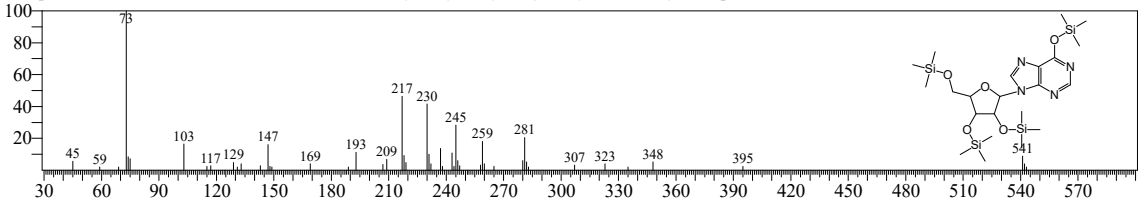
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



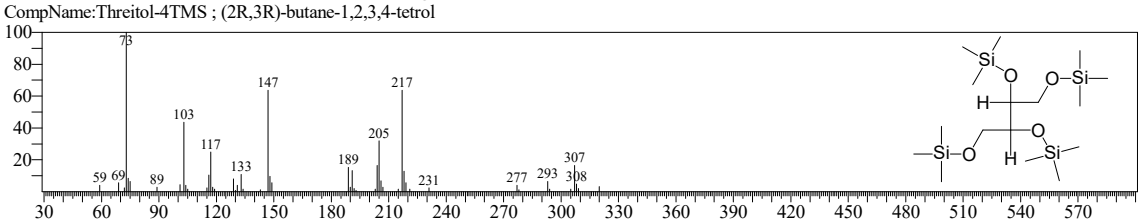
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



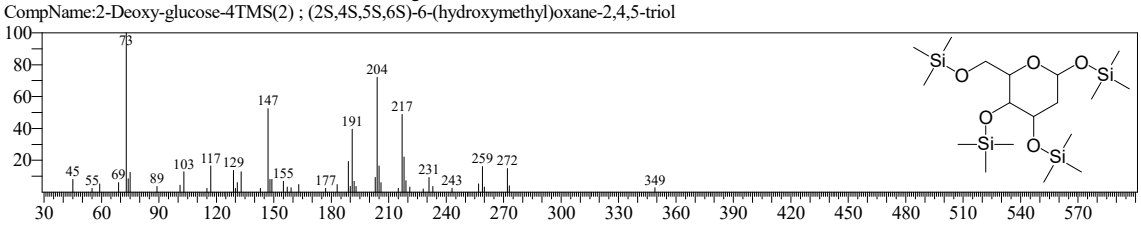
Hit#:3 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one



Hit#:4 Entry:148 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C16H42O4Si4 CAS:2418-52-2 MolWeight:410 RetIndex:1512
CompName:Threitol-4TMS ; (2R,3R)-butane-1,2,3,4-tetrol

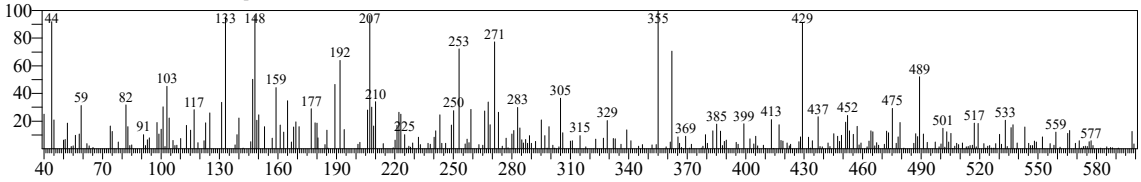


Hit#:5 Entry:306 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1816
CompName:2-Deoxy-glucose-4TMS(2) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

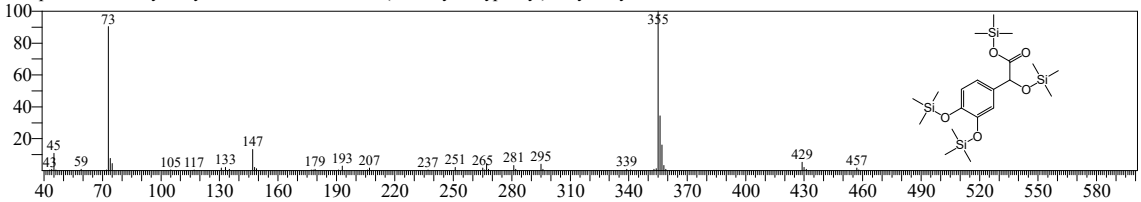


TNAU

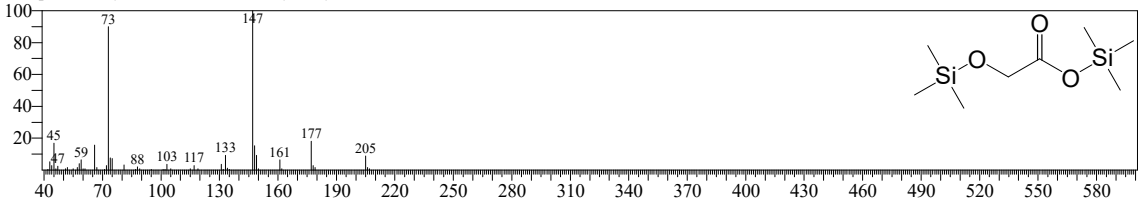
<< Target >>
Line#:41 R.Time:32.855(Scan#:5672) MassPeaks:298
RawMode:Averaged 32.850-32.860(5671-5673) BasePeak:355.10(544)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



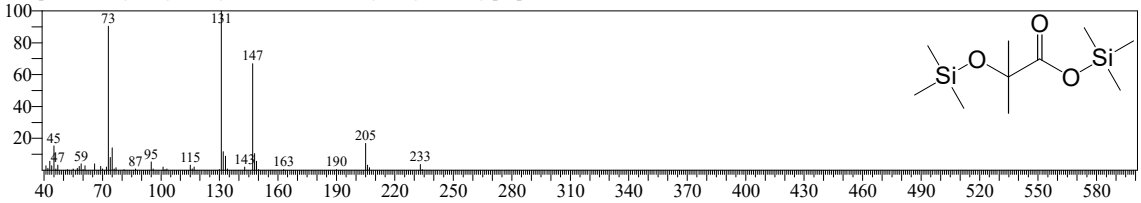
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



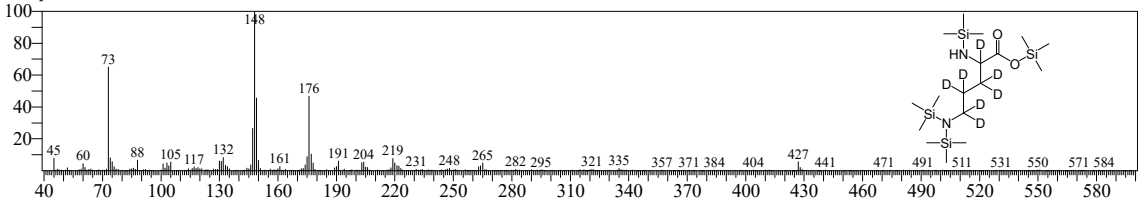
Hit#:2 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid



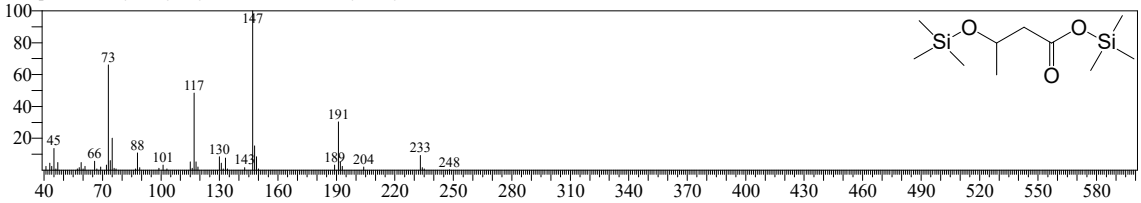
Hit#:3 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid



Hit#:4 Entry:313 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula: CAS:0-00-0 MolWeight:427 RetIndex:1831
CompName:Ornithine-d7-4TMS ;

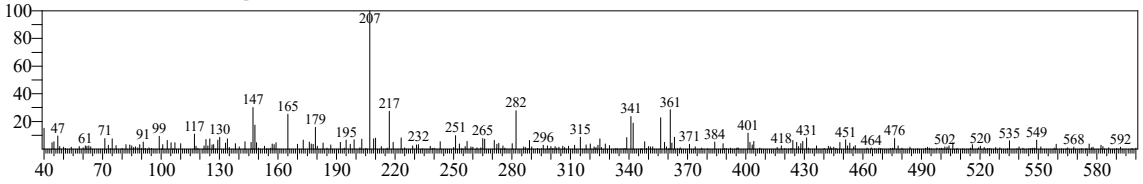


Hit#:5 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid

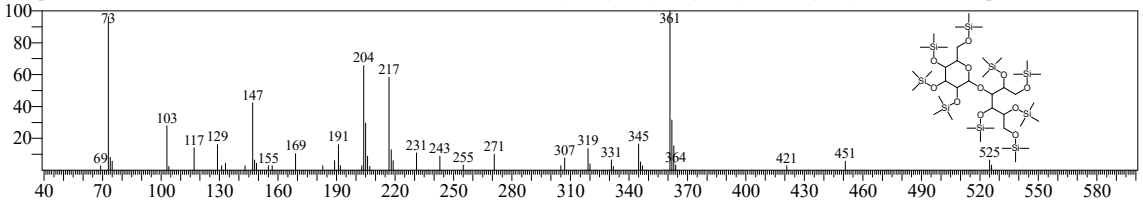


TNAU

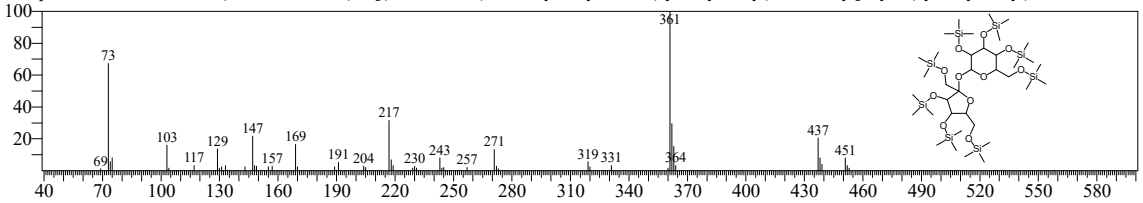
<< Target >>
Line#:42 R.Time:32.945(Scan#:5690) MassPeaks:283
RawMode:Averaged 32.940-32.950(5689-5691) BasePeak:207.05(1860)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



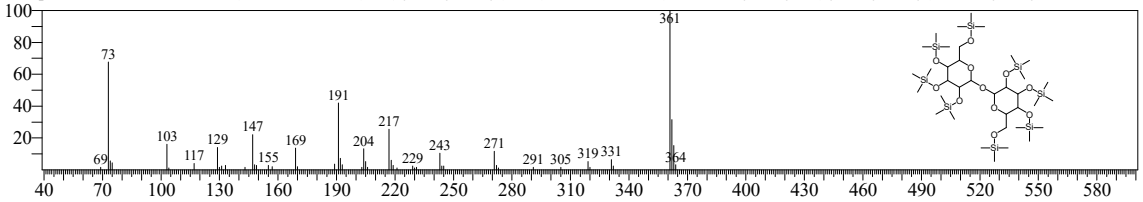
Hit#:1 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol



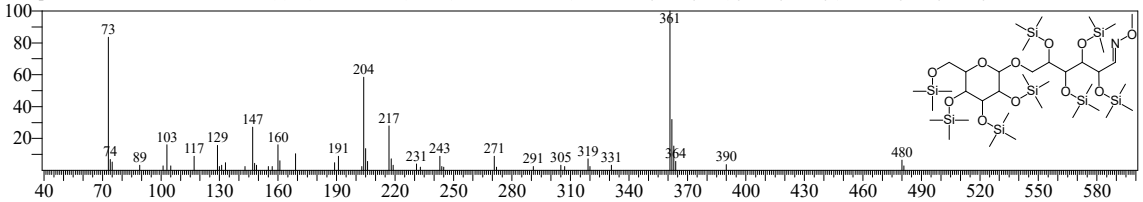
Hit#:2 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3



Hit#:3 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-



Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,



Hit#:5 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid