TNAU

Chromatogram C87-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-010.qgd

Peak Report TIC

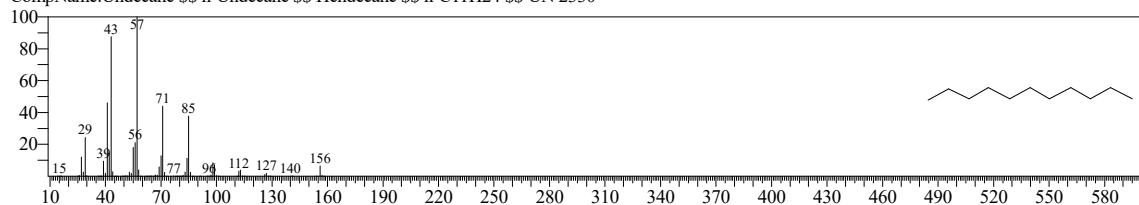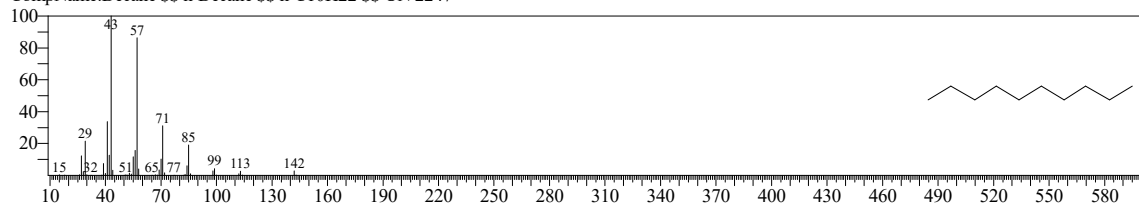| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.944	25607	4.53	19721	10.00	1.30	87	Undecane
2	9.688	46199	8.18	28517	14.47	1.62	88	Undecane
3	27.330	13578	2.40	8064	4.09	1.68	45	Trehalose-8TMS
4	27.792	40025	7.08	14159	7.18	2.83	48	Sucrose-8TMS
5	27.855	60563	10.72	8678	4.40	6.98	35	Tagatose-5TMS(4)
6	27.956	113346	20.06	25844	13.11	4.39	38	Sucrose-8TMS
7	29.216	13720	2.43	11210	5.69	1.22	35	Arabinose-4TMS(2)
8	29.439	11145	1.97	11556	5.86	0.96	41	Lyxose-4TMS(2)
9	30.040	40906	7.24	9851	5.00	4.15	42	4-Aminobenzoic acid-2TMS
10	30.165	8348	1.48	8798	4.46	0.95	38	Fucose-4TMS(1)
11	30.738	42131	7.46	8977	4.55	4.69	39	Epinephrine-3TMS
12	31.485	22536	3.99	8122	4.12	2.77	30	4-Hydroxybenzoic acid-2TMS
13	31.920	71254	12.61	21739	11.03	3.28	23	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
14	31.987	55713	9.86	11880	6.03	4.69	31	2-Phenyllactic acid-2TMS
		565071	100.00	197116	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:271
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5212)
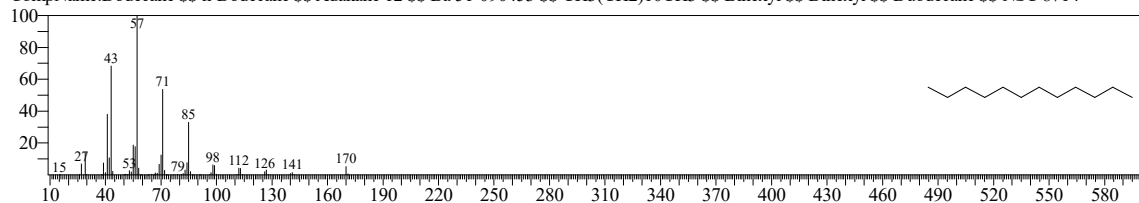BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:12897 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
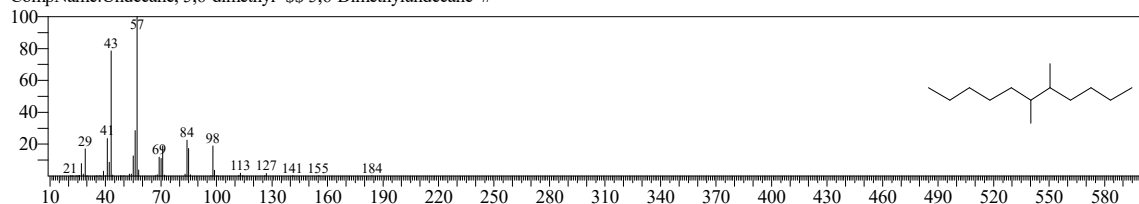CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:9444 Library:NIST20R.lib
SI:87 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
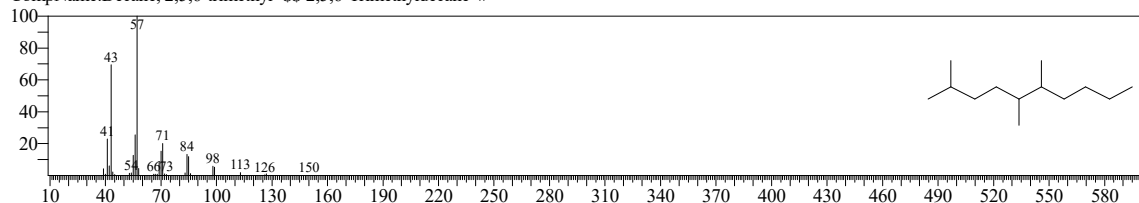CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:4 Entry:40266 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:17615-91-7 MolWeight:184 RetIndex:1185
CompName:Undecane, 5,6-dimethyl- $$ 5,6-Dimethylundecane #

Hit#:5 Entry:40218 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:62108-23-0 MolWeight:184 RetIndex:1121
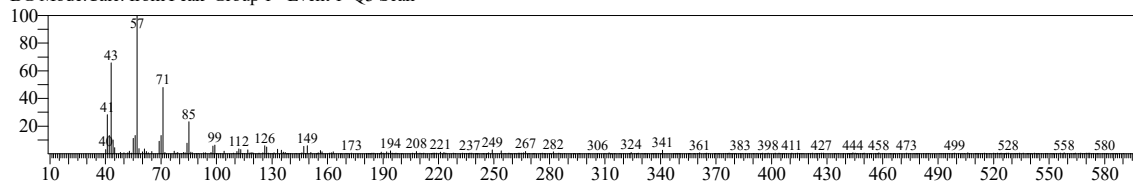CompName:Decane, 2,5,6-trimethyl- $$ 2,5,6-Trimethyldecane #

TNAU

<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:340
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.05(5958)
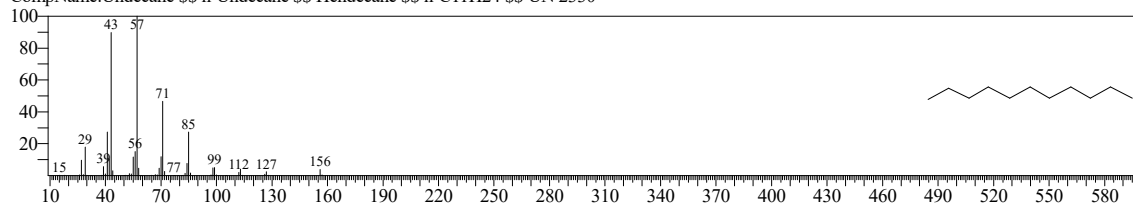BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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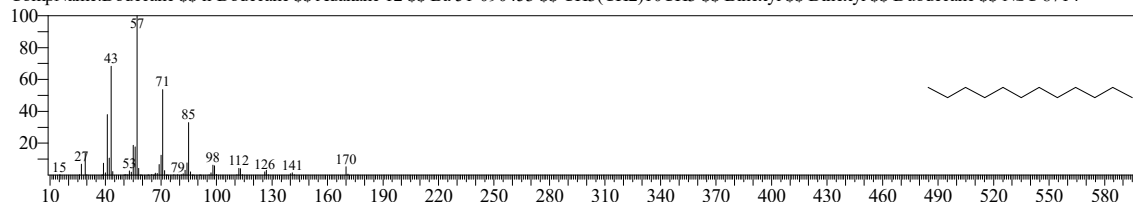CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
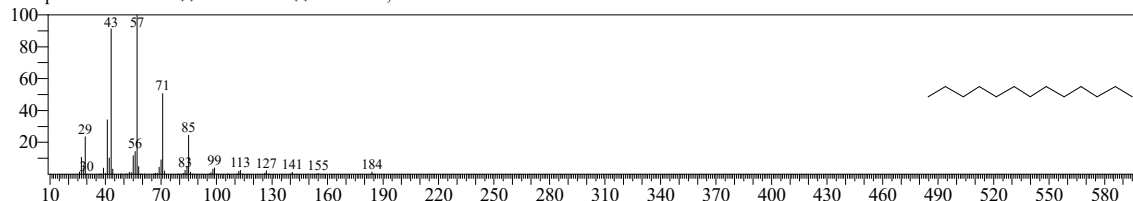CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:3 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
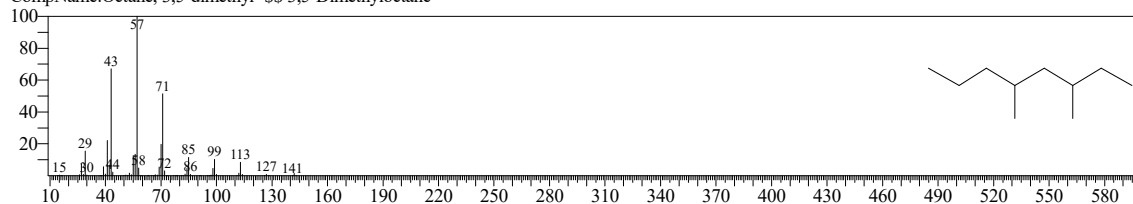CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:4 Entry:13631 Library:NIST20M1.lib
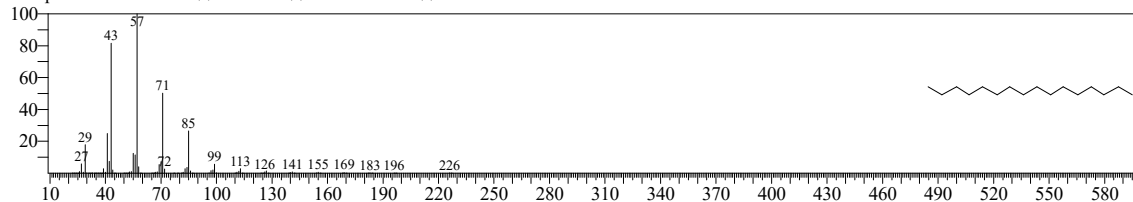SI:87 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

Hit#:5 Entry:27737 Library:NIST20R.lib
SI:86 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane
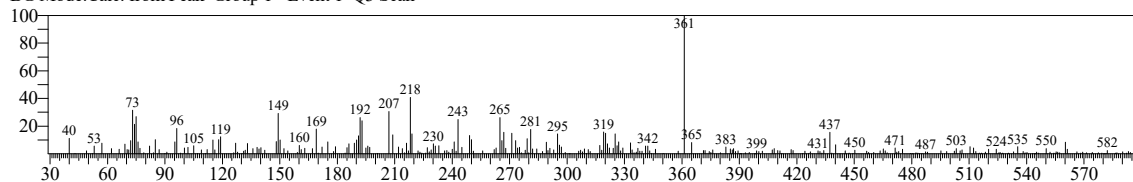
TNAU

<< Target >>
Line#:3 R.Time:27.330(Scan#:4567) MassPeaks:288
RawMode:Averaged 27.325-27.335(4566-4568) BasePeak:361.15(1501)
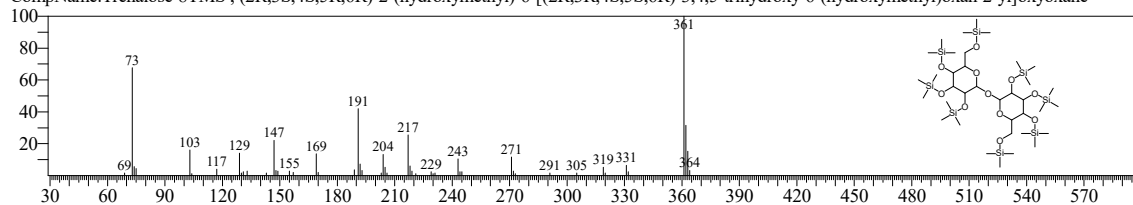BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
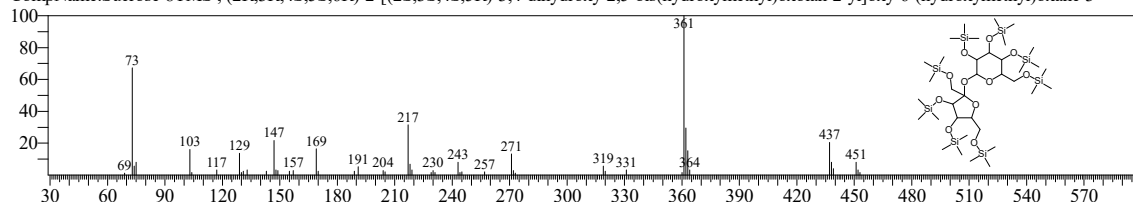SI:45 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

Hit#:2 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
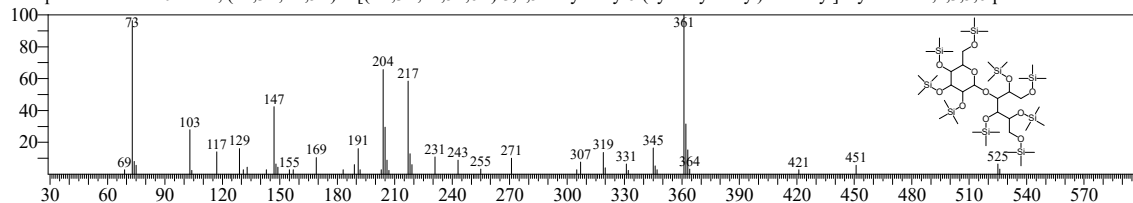SI:43 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

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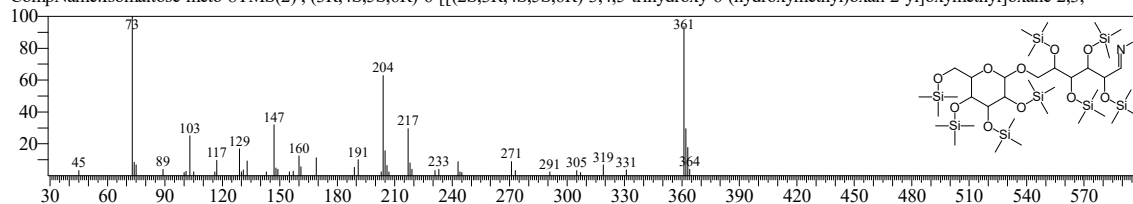SI:39 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:4 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
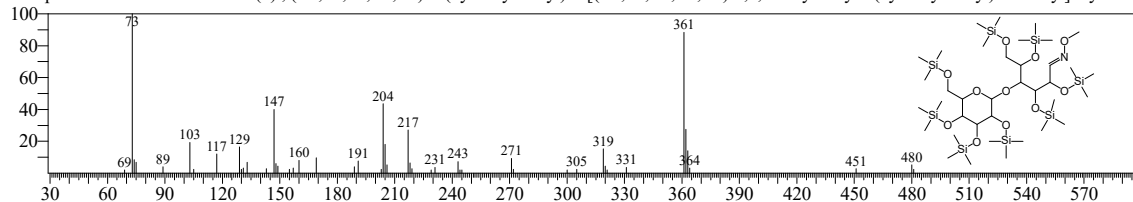SI:38 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

Hit#:5 Entry:553 Library:OA_TMS_DB5_67min_V3.lib
SI: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
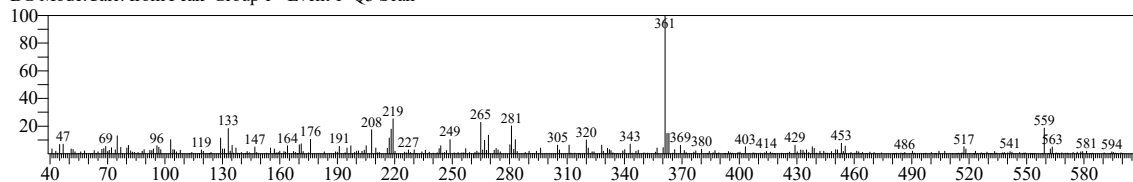
TNAU

<< Target >>
Line#:4 R.Time:27.790(Scan#:4659) MassPeaks:322
RawMode:Averaged 27.785-27.795(4658-4660) BasePeak:361.20(2908)
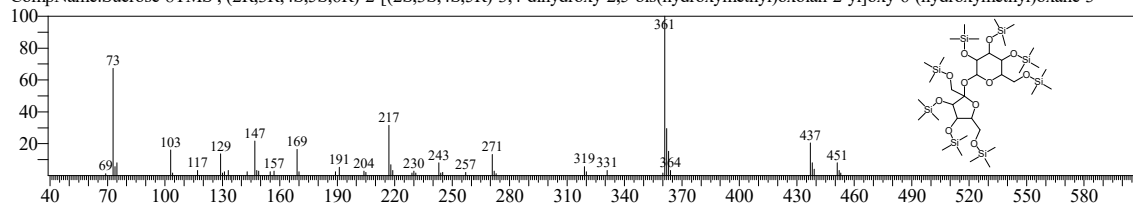BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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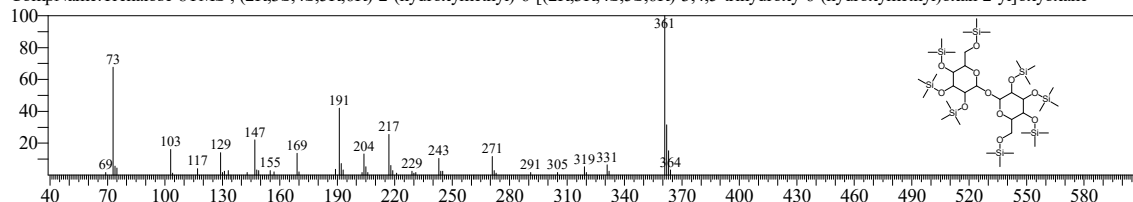SI:48 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
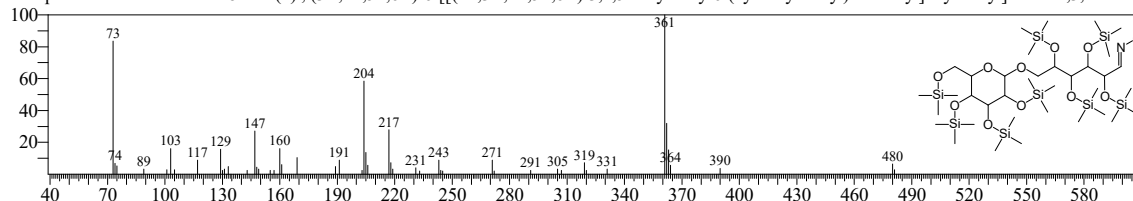SI:48 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

Hit#:3 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
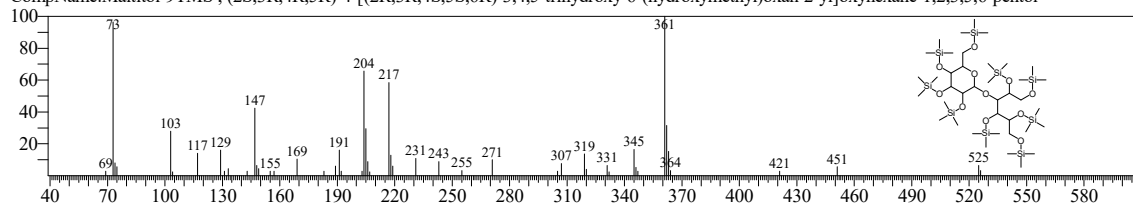CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

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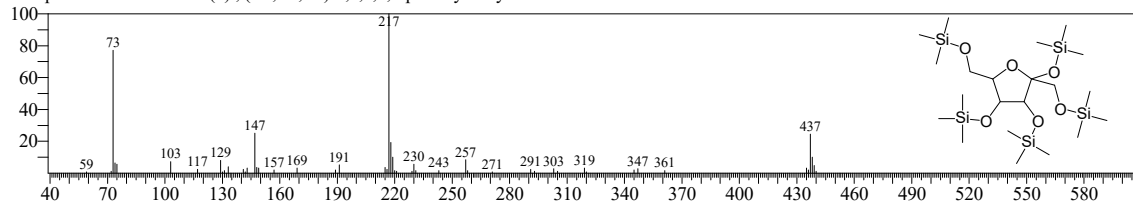SI:42 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:32 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
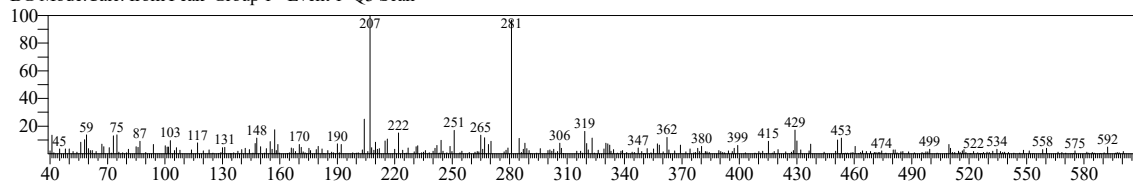
TNAU

<< Target >>
Line#:5   R.Time:27.855(Scan#:4672) MassPeaks:308
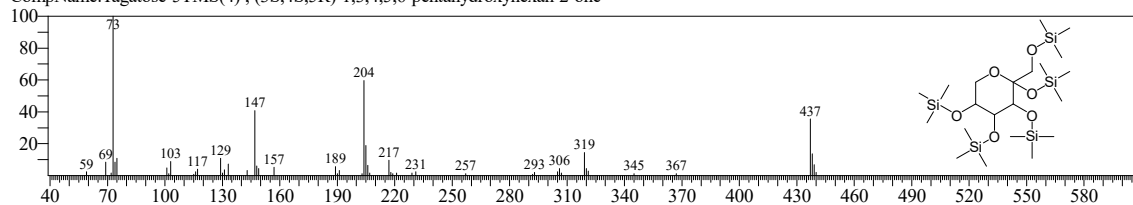RawMode:Averaged 27.850-27.860(4671-4673) BasePeak:207.05(1651)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:380 Library:OA_TMS_DB5_67min_V3.lib
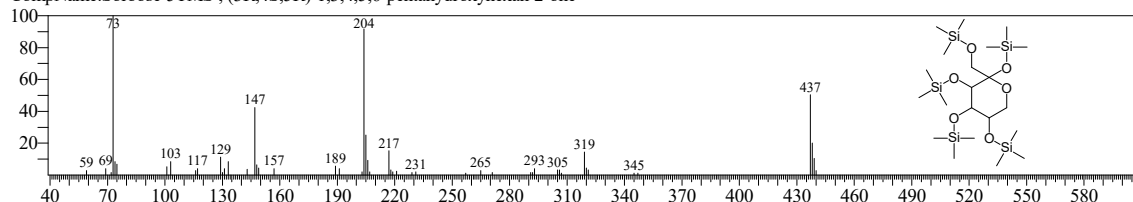SI:35 Formula:C21H52O6Si5 CAS:87-81-0 MolWeight:540 RetIndex:1914
CompName:Tagatose-5TMS(4) ; (3S,4S,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

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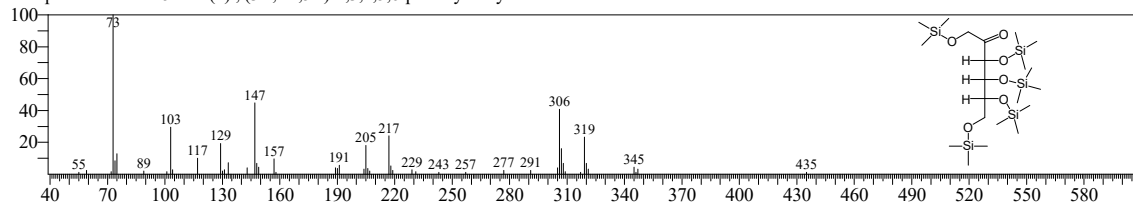SI:35 Formula:C21H52O6Si5 CAS:3615-56-3 MolWeight:540 RetIndex:1895
CompName:Sorbose-5TMS ; (3R,4S,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

Hit#:3 Entry:387 Library:OA_TMS_DB5_67min_V3.lib
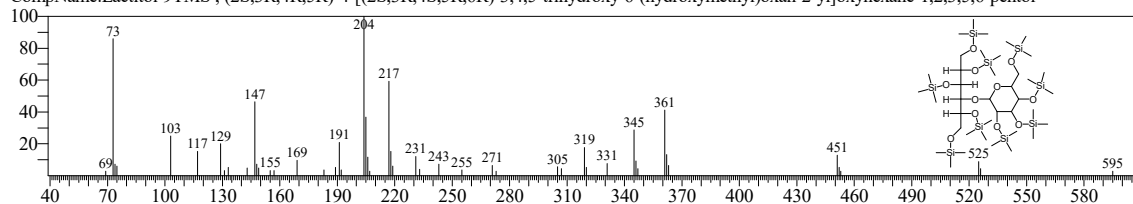SI:33 Formula:C21H52O6Si5 CAS:23140-52-5 MolWeight:540 RetIndex:1923
CompName:Psicose-5TMS(4) ; (3R,4R,5R)-1,3,4,5,6-pentahydroxyhexan-2-one

Hit#:4 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
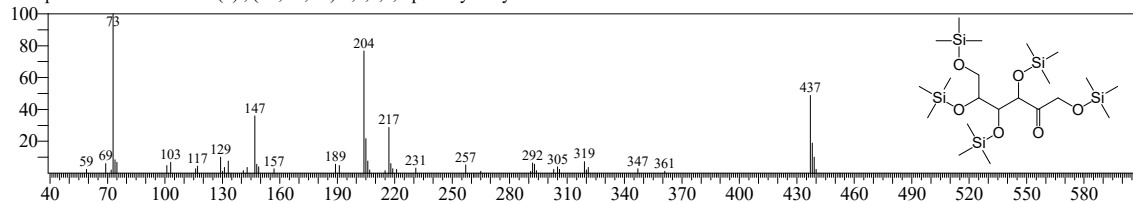SI:33 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:5 Entry:334 Library:OA_TMS_DB5_67min_V3.lib
SI:33 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
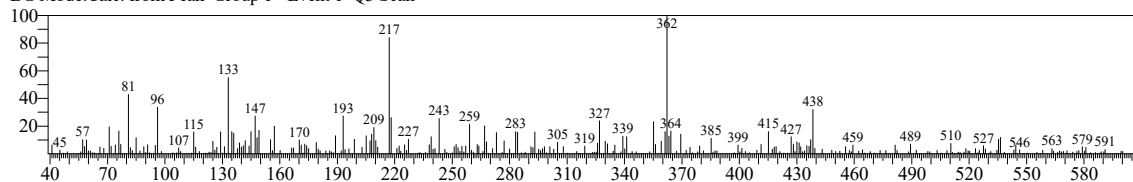
TNAU

<< Target >>
Line#:6   R.Time:27.955(Scan#:4692) MassPeaks:302
RawMode:Averaged 27.950-27.960(4691-4693) BasePeak:362.15(1406)
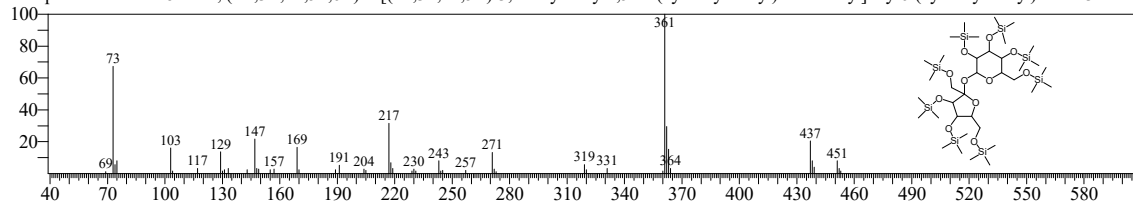BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
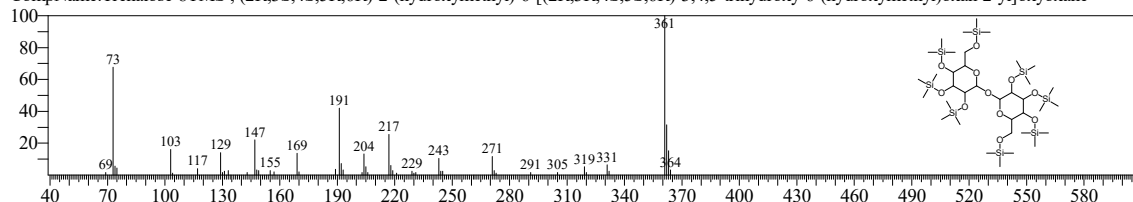SI:38 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

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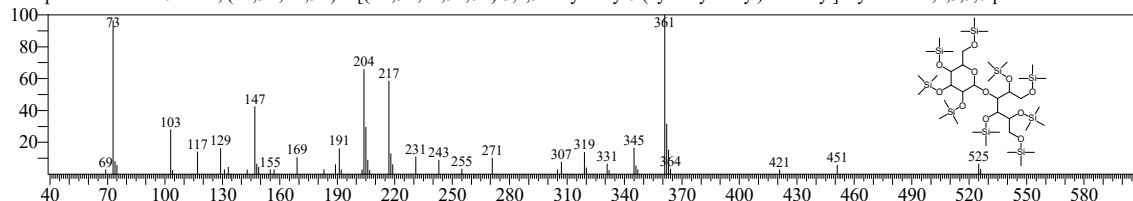SI:36 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

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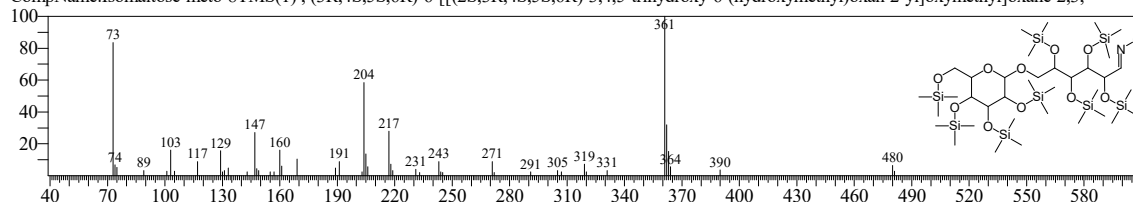CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:4 Entry:560 Library:OA_TMS_DB5_67min_V3.lib
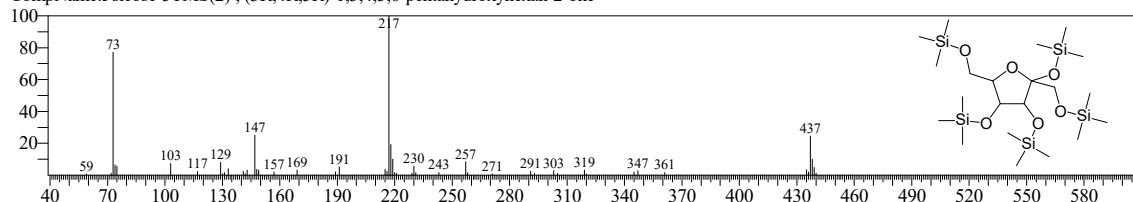SI:34 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2947
CompName:Isomaltose-meto-8TMS(1) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

Hit#:5 Entry:326 Library:OA_TMS_DB5_67min_V3.lib
SI:32 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
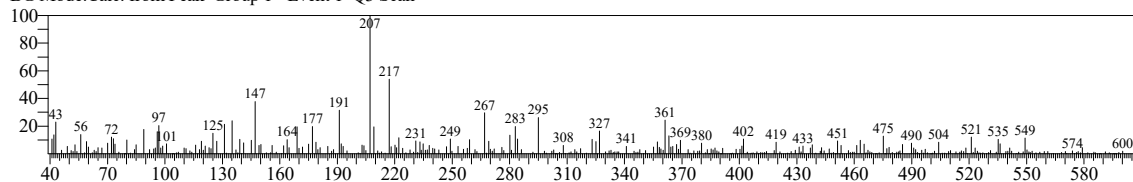
TNAU

<< Target >>
Line#:7 R.Time:29.215(Scan#:4944) MassPeaks:335
RawMode:Averaged 29.210-29.220(4943-4945) BasePeak:207.05(1381)
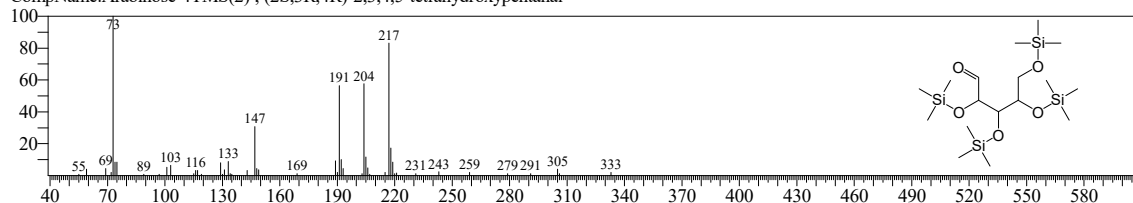BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
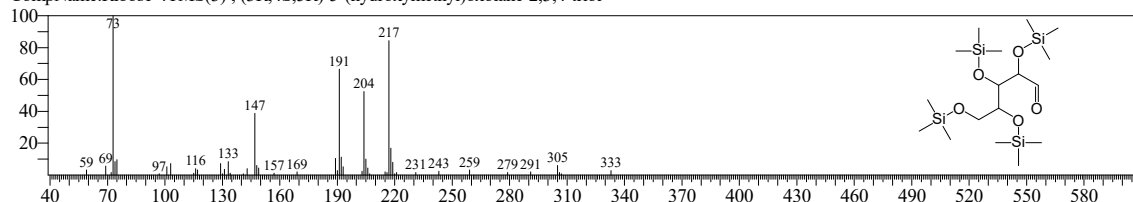SI:35 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:2 Entry:236 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1673
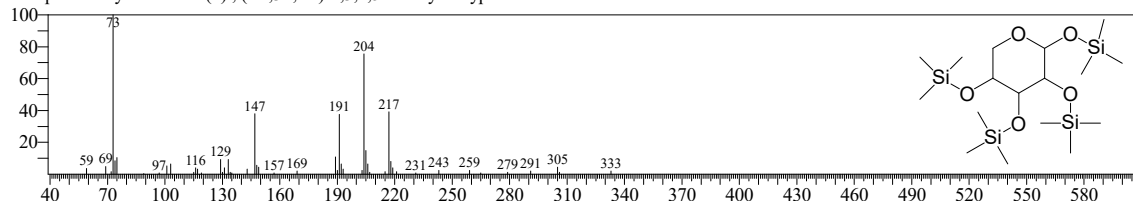CompName:Ribose-4TMS(3) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

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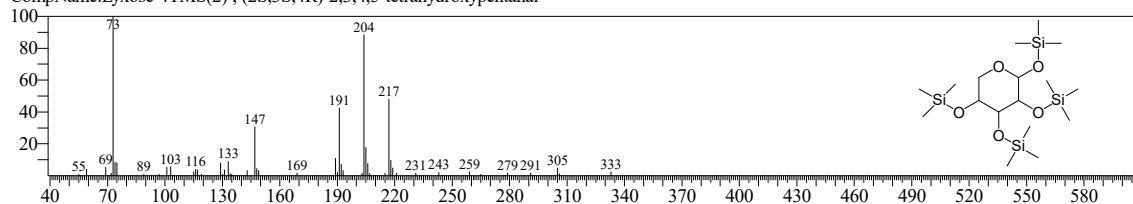SI:34 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

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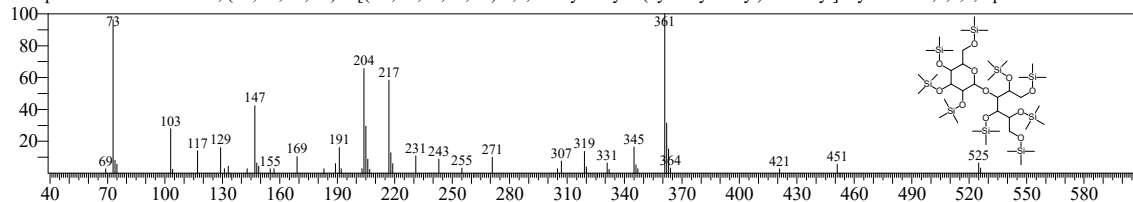CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:5 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
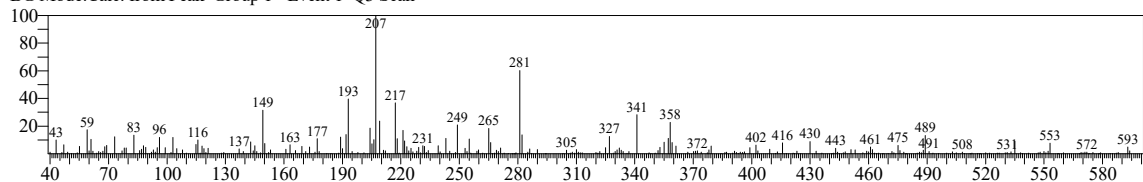
TNAU

<< Target >>
Line#:8   R.Time:29.440(Scan#:4989) MassPeaks:274
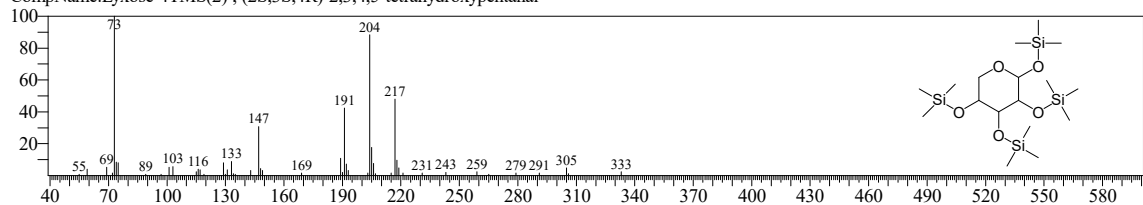RawMode:Averaged 29.435-29.445(4988-4990) BasePeak:207.05(1986)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
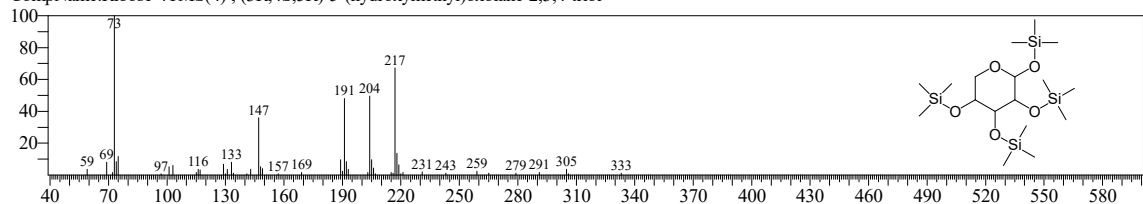SI:41 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:2 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
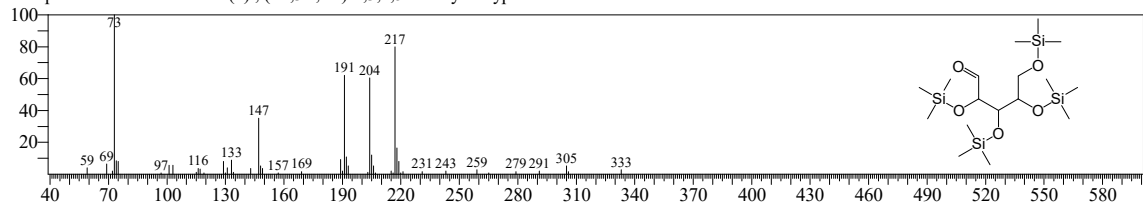CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

Hit#:3 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
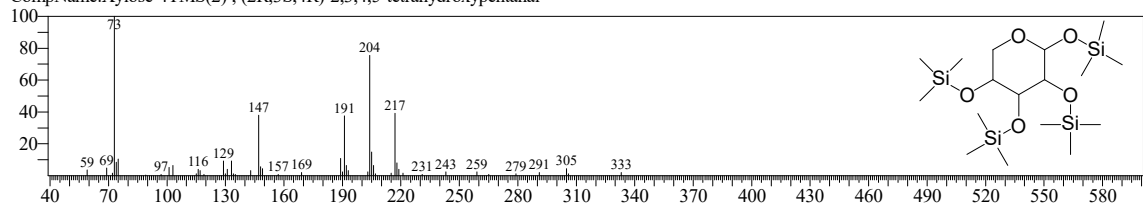SI:40 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:4 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
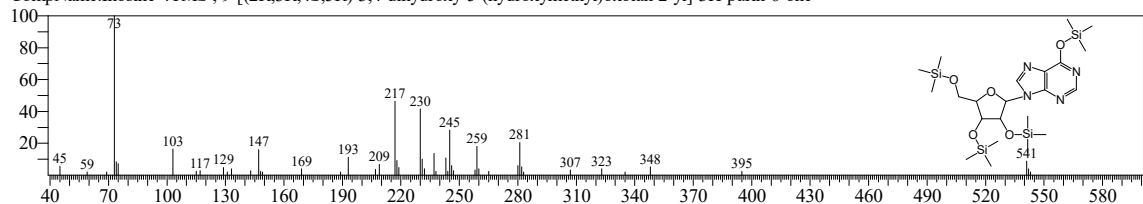CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:5 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
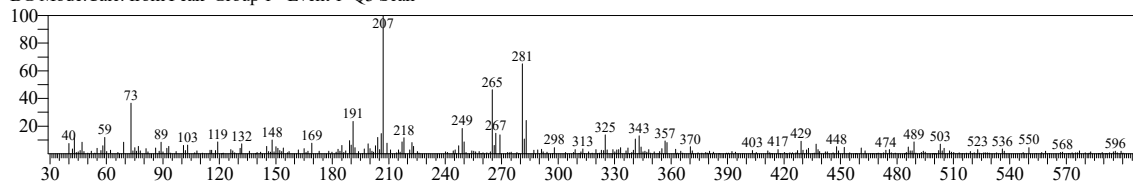CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

TNAU

<< Target >>
Line#:9 R.Time:30.040(Scan#:5109) MassPeaks:304
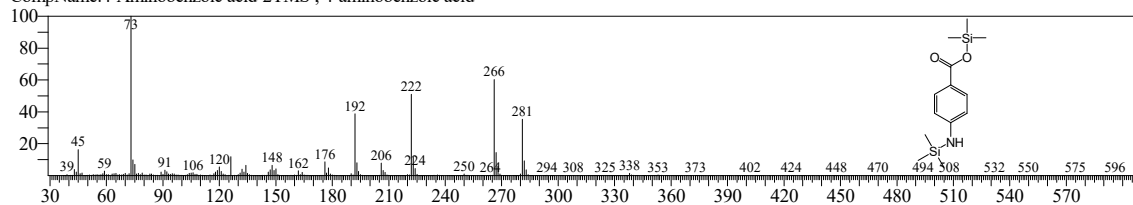RawMode:Averaged 30.035-30.045(5108-5110) BasePeak:207.05(1829)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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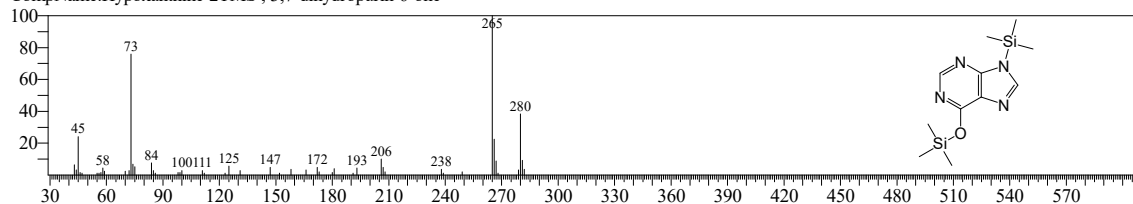SI:42 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
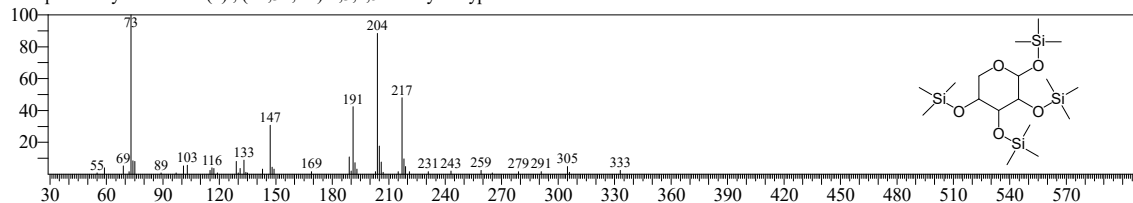SI:42 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
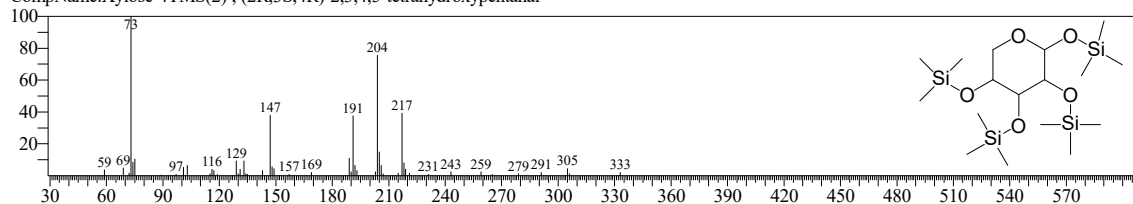SI:41 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:4 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
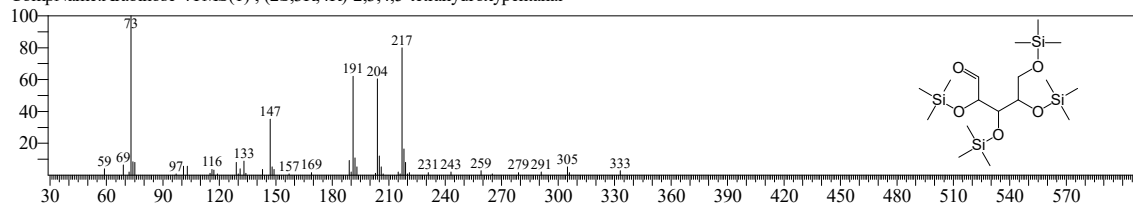CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

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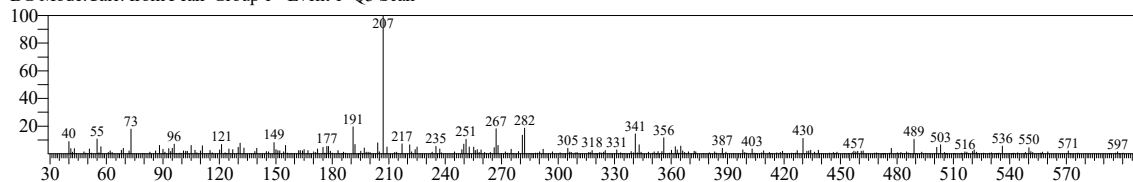
TNAU

<< Target >>
Line#:10   R.Time:30.165(Scan#:5134) MassPeaks:280
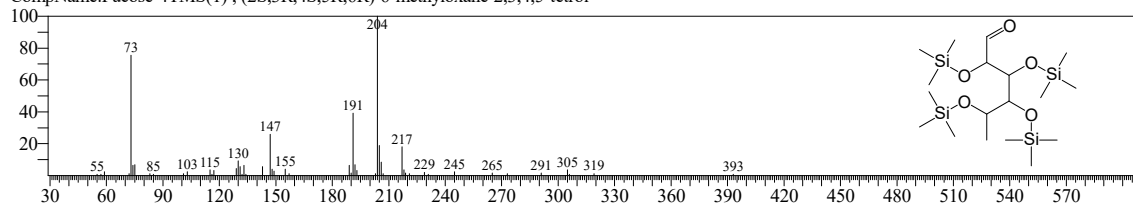RawMode:Averaged 30.160-30.170(5133-5135) BasePeak:207.05(2665)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
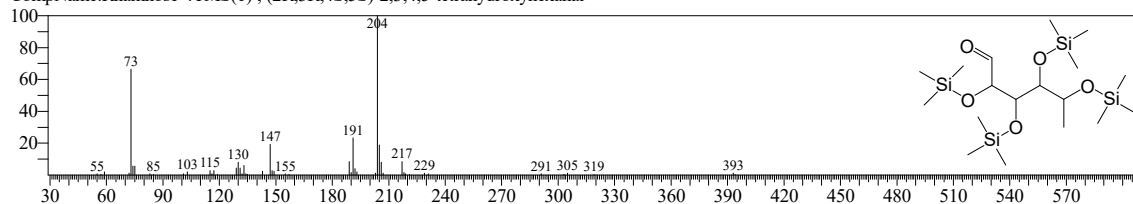SI:38 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

Hit#:2 Entry:219 Library:OA_TMS_DB5_67min_V3.lib
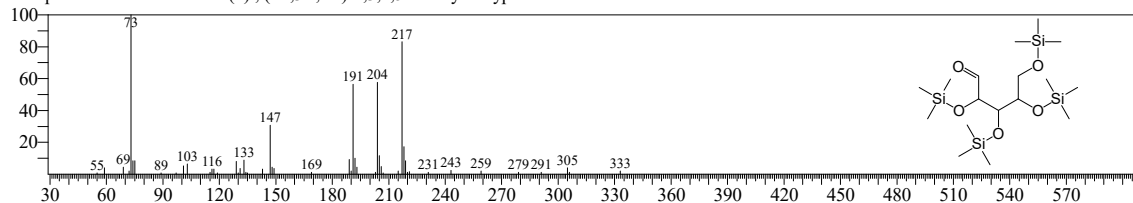SI:37 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1646
CompName:Rhamnose-4TMS(1) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

Hit#:3 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
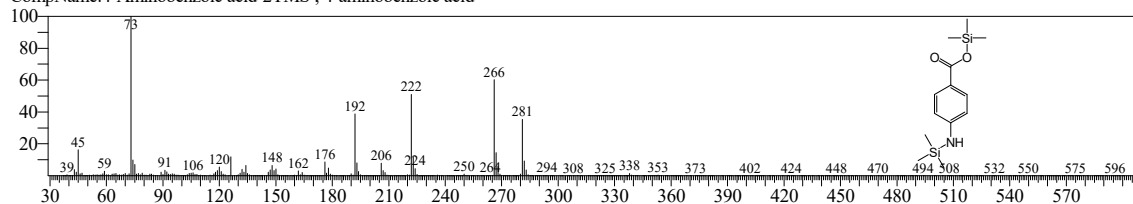SI:36 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

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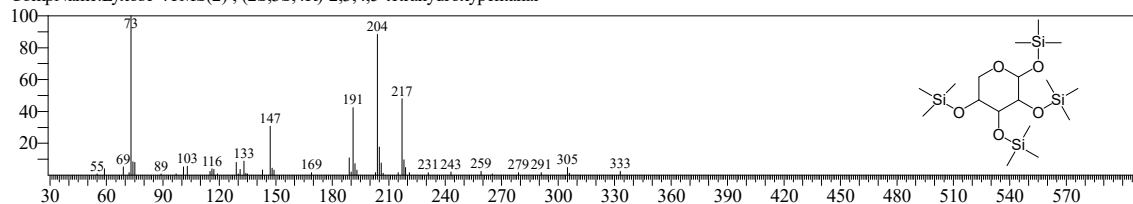SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:5 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal
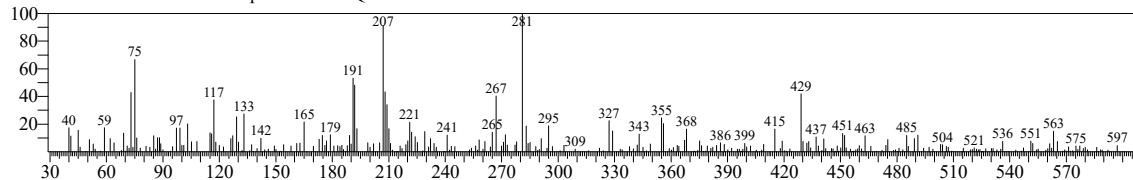
TNAU

<< Target >>
Line#:11 R.Time:30.740(Scan#:5249) MassPeaks:298
RawMode:Averaged 30.735-30.745(5248-5250) BasePeak:281.05(1083)
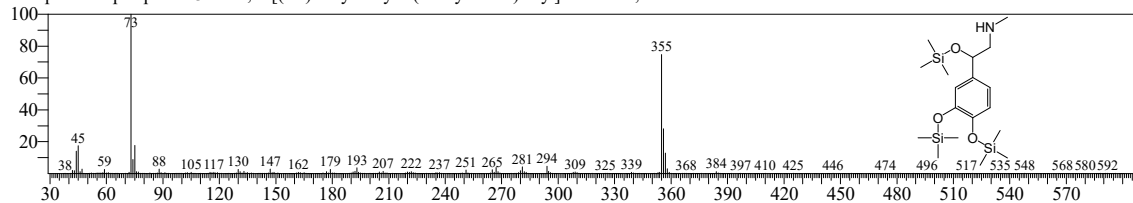BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
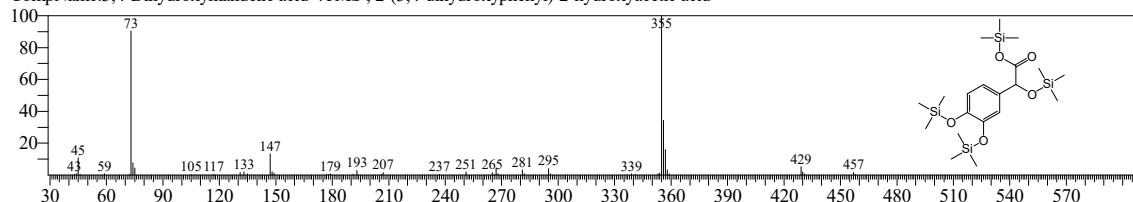SI:39 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

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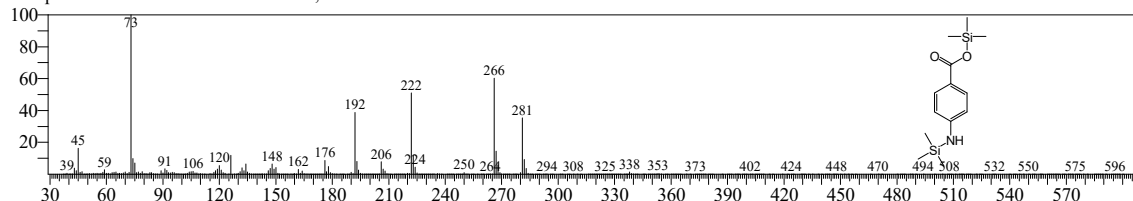SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

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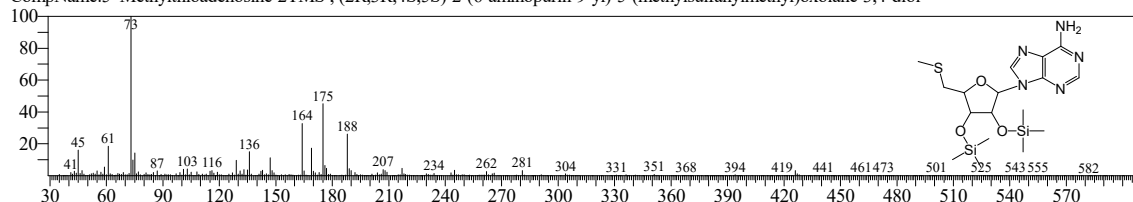CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

Hit#:4 Entry:548 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787
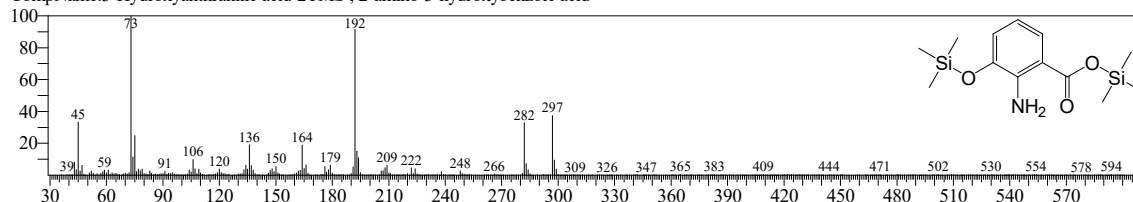CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol

Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid
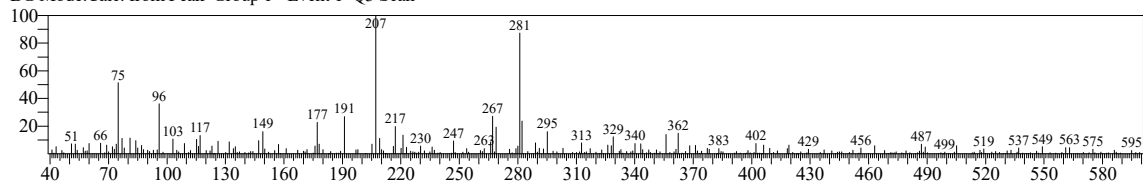
TNAU

<< Target >>
Line#:12 R.Time:31.485(Scan#:5398) MassPeaks:287
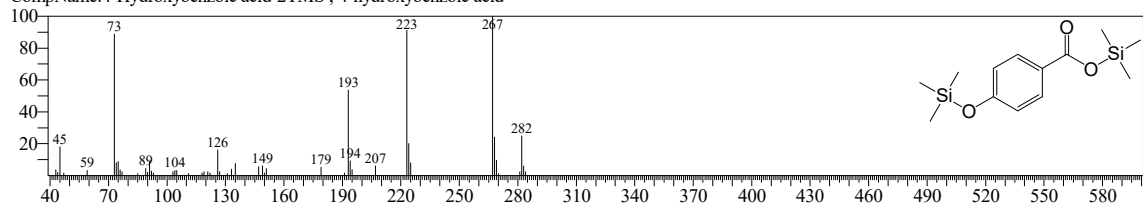RawMode:Averaged 31.480-31.490(5397-5399) BasePeak:207.05(1841)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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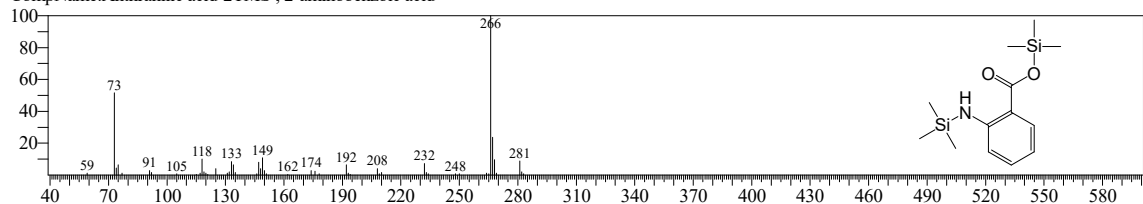SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:2 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
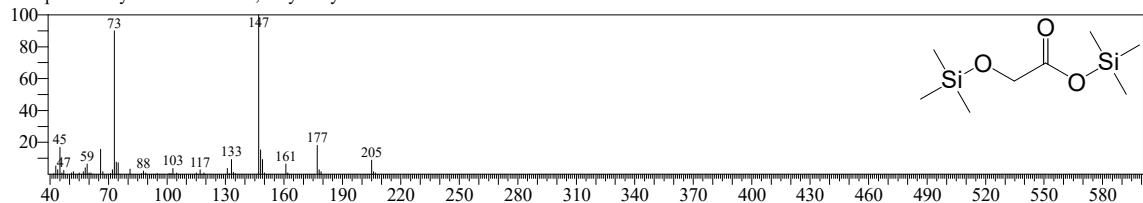CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

Hit#:3 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
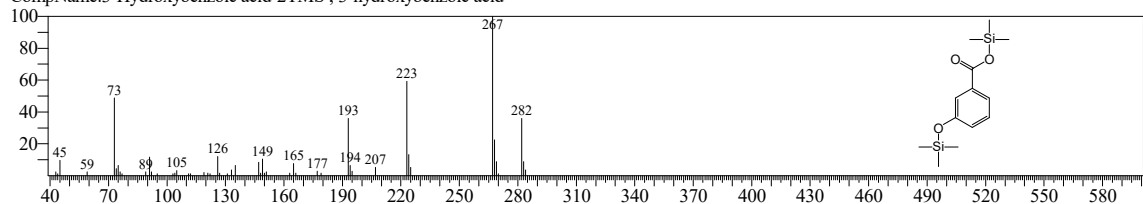SI:29 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
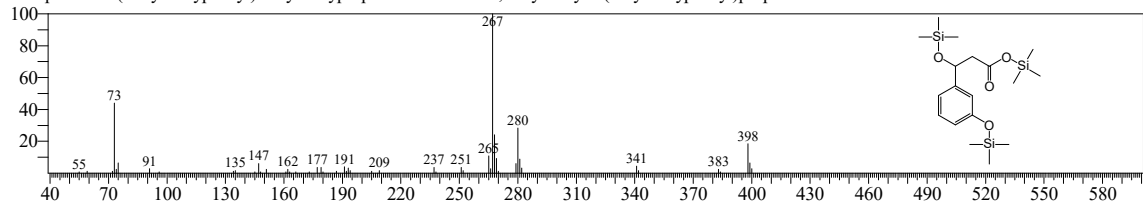SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid
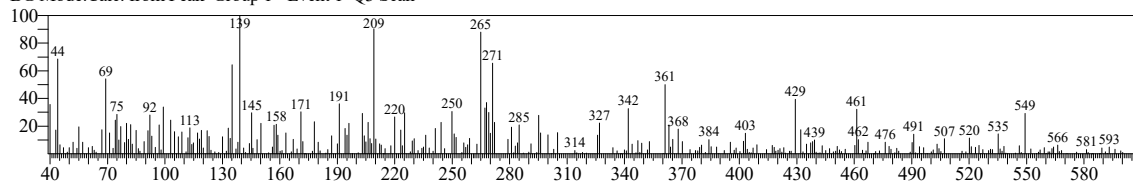
TNAU

<< Target >>
Line#:13 R.Time:31.920(Scan#:5485) MassPeaks:317
RawMode:Averaged 31.915-31.925(5484-5486) BasePeak:139.15(888)
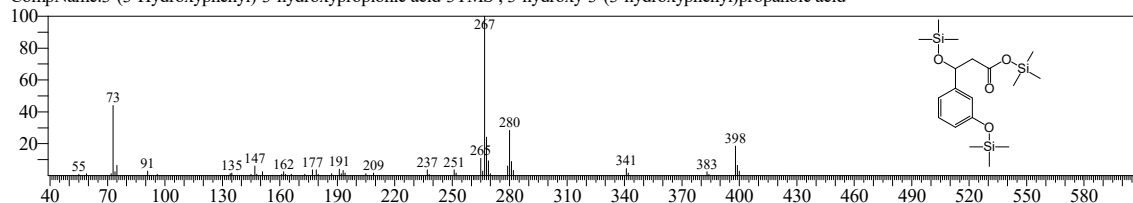BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
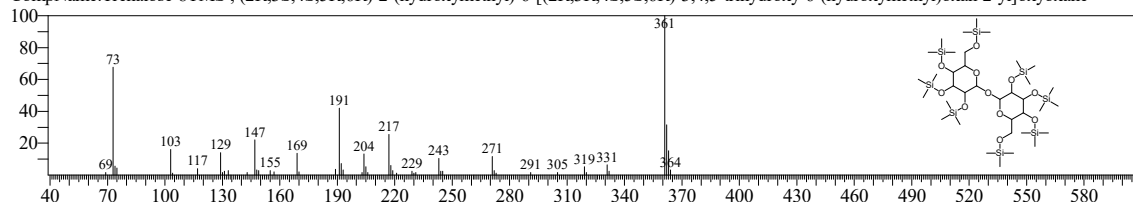SI:23 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

Hit#:2 Entry:552 Library:OA_TMS_DB5_67min_V3.lib
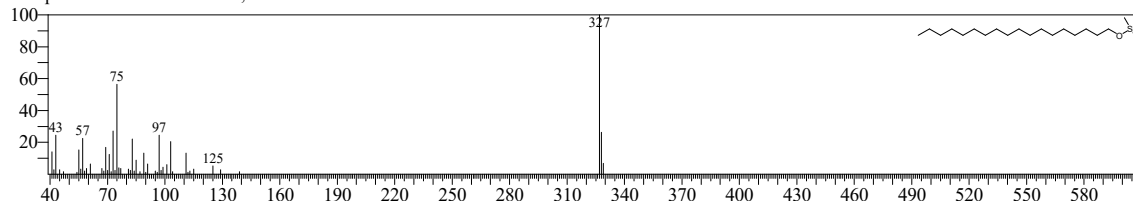SI:22 Formula:C36H86O11Si8 CAS:99-20-7 MolWeight:918 RetIndex:2812
CompName:Trehalose-8TMS ; (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxane-

Hit#:3 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
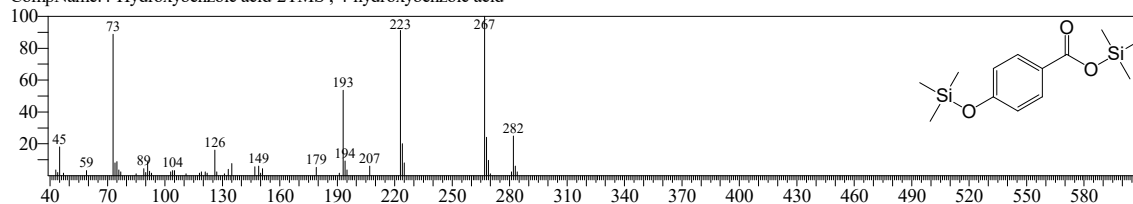CompName:Octadecanol-TMS ; octadecan-1-ol

Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
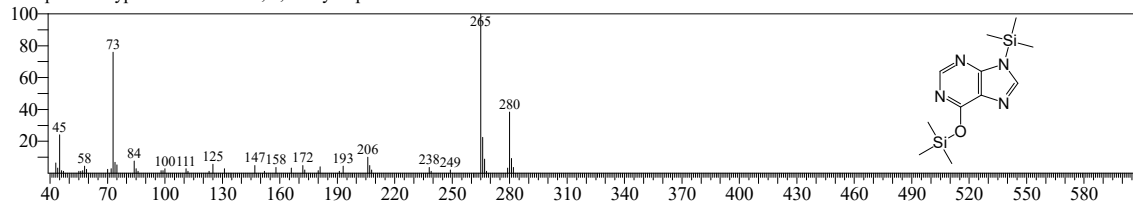SI:21 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:5 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
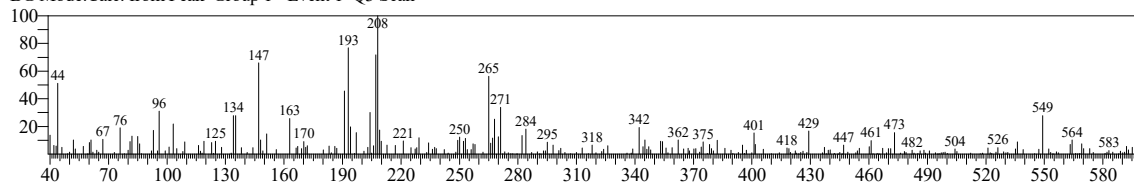CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

TNAU

<< Target >>
Line#:14 R.Time:31.985(Scan#:5498) MassPeaks:275
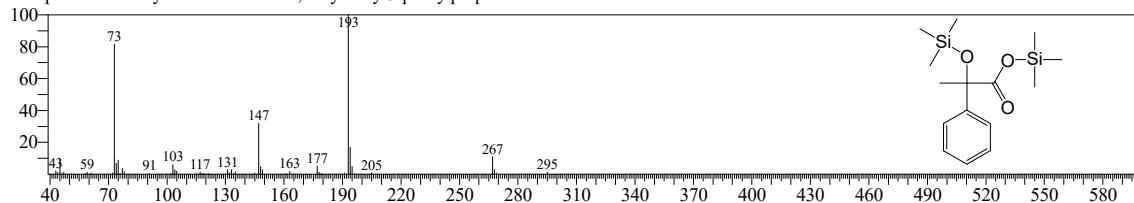RawMode:Averaged 31.980-31.990(5497-5499) BasePeak:208.00(1198)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
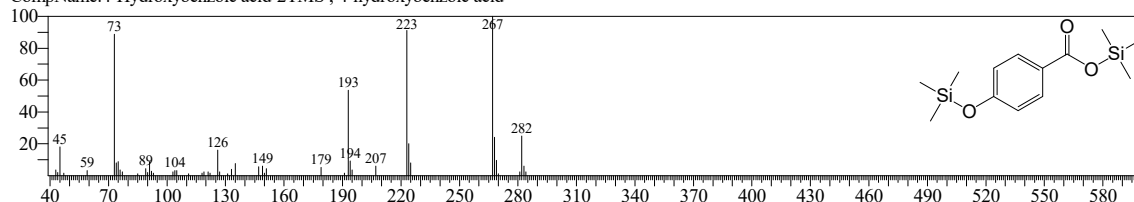SI:31 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

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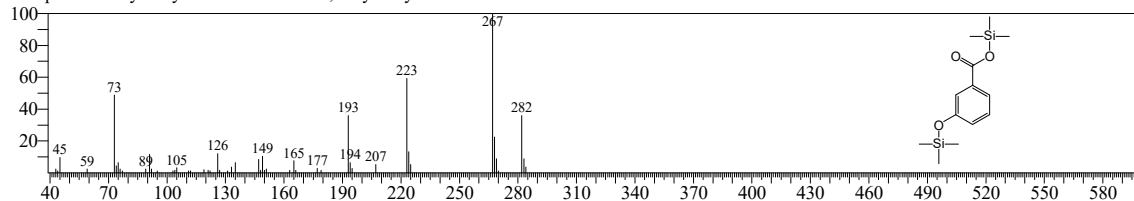CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

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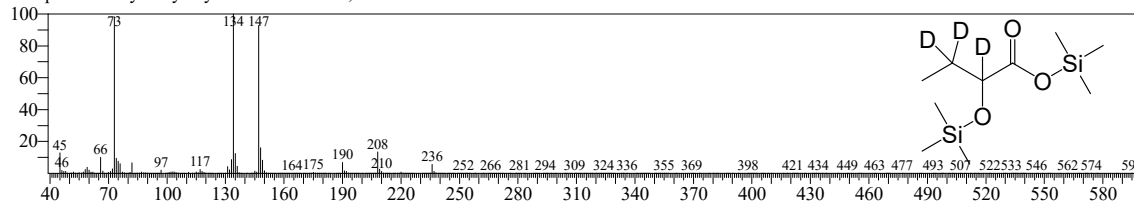SI:30 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:4 Entry:25 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula: CAS:0-00-0 MolWeight:251 RetIndex:1130
CompName:2-Hydroxybutyric acid-d3-2TMS ;

Hit#:5 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:29 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