TNAU

Chromatogram C101-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-012.qgd

Peak Report TIC

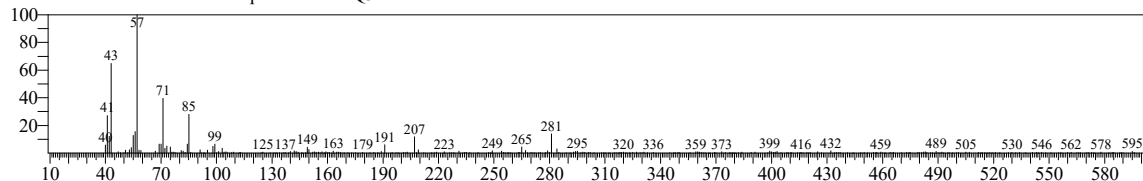| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.949	53559	23.22	22826	21.32	2.35	83	Undecane, 3-methyl-
2	7.995	6582	2.85	8069	7.54	0.82	43	Juniperic acid-2TMS
3	9.689	37360	16.20	22272	20.80	1.68	88	Dodecane
4	28.110	23187	10.05	9416	8.79	2.46	31	3,4-Dihydroxymandelic acid-4TMS
5	29.110	16039	6.95	6698	6.26	2.39	38	Batyl alcohol-2TMS
6	29.553	47317	20.52	11895	11.11	3.98	33	4-Aminobenzoic acid-2TMS
7	31.917	28981	12.57	13903	12.98	2.08	35	Arabinose-4TMS(1)
8	32.480	17597	7.63	12002	11.21	1.47	29	Isomaltose-meto-8TMS(2)
		230622	100.00	107081	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:7.950(Scan#:691) MassPeaks:295
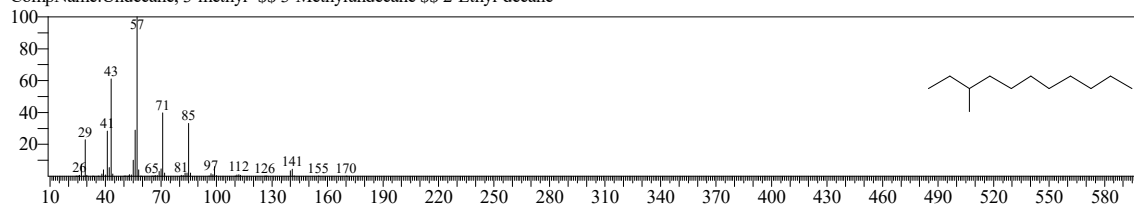RawMode:Averaged 7.945-7.955(690-692) BasePeak:57.10(4542)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:16184 Library:NIST20R.lib
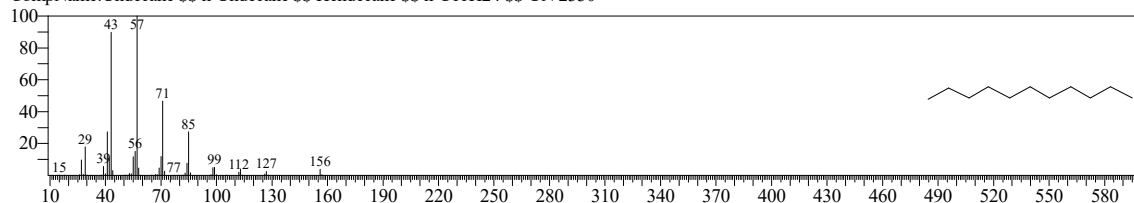SI:83 Formula:C12H26 CAS:1002-43-3 MolWeight:170 RetIndex:1150
CompName:Undecane, 3-methyl- $$ 3-Methylundecane $$ 2-Ethyl-decane

Hit#:2 Entry:21042 Library:NIST20M1.lib
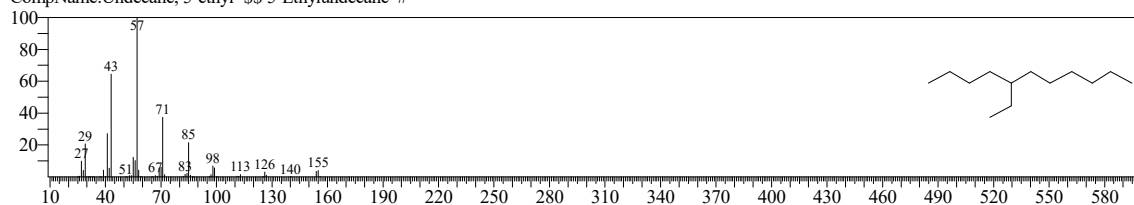SI:83 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:3 Entry:40233 Library:NIST20M1.lib
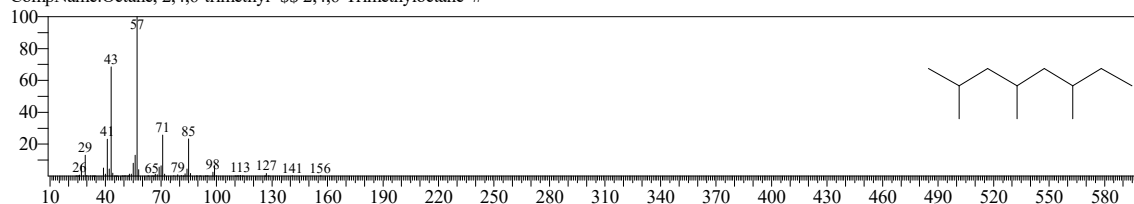SI:83 Formula:C13H28 CAS:17453-94-0 MolWeight:184 RetIndex:1249
CompName:Undecane, 5-ethyl- $$ 5-Ethylundecane #

Hit#:4 Entry:21045 Library:NIST20M1.lib
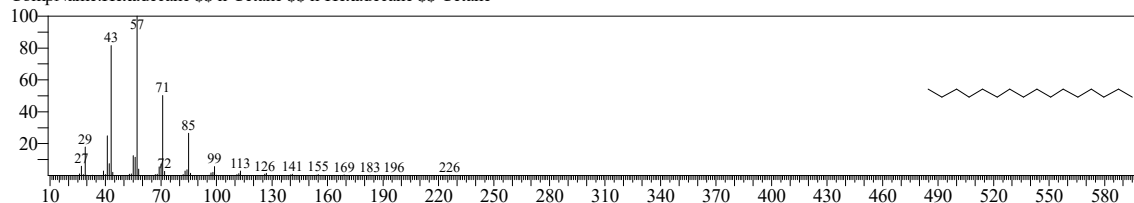SI:83 Formula:C11H24 CAS:62016-37-9 MolWeight:156 RetIndex:922
CompName:Octane, 2,4,6-trimethyl- $$ 2,4,6-Trimethyloctane #

Hit#:5 Entry:27737 Library:NIST20R.lib
SI:83 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
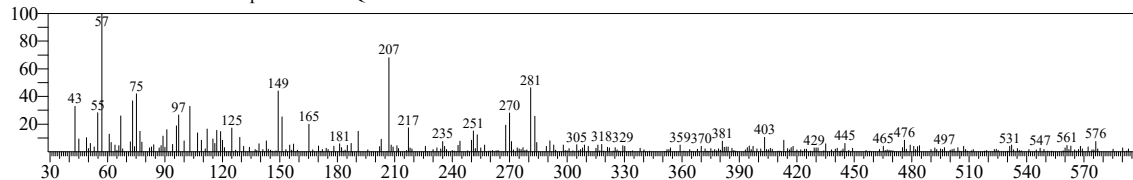CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

TNAU

<< Target >>
Line#:2 R.Time:7.995(Scan#:700) MassPeaks:302
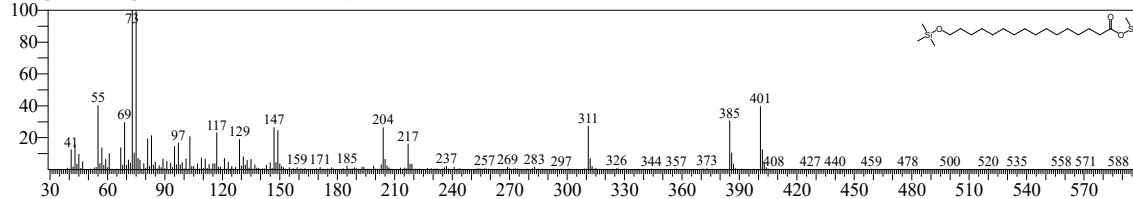RawMode:Averaged 7.990-8.000(699-701) BasePeak:57.05(523)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:511 Library:OA_TMS_DB5_67min_V3.lib
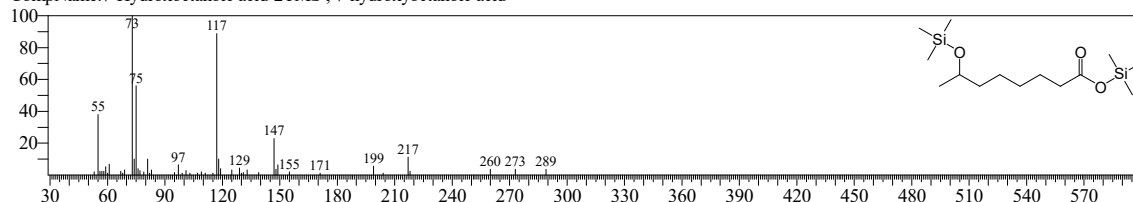SI:43 Formula:C22H48O3Si2 CAS:506-13-8 MolWeight:416 RetIndex:2396
CompName:Juniperic acid-2TMS ; 16-hydroxyhexadecanoic acid

Hit#:2 Entry:169 Library:OA_TMS_DB5_67min_V3.lib
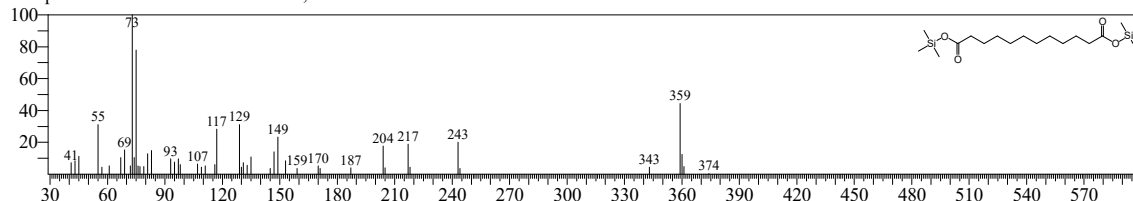SI:40 Formula:C14H32O3Si2 CAS:17173-14-7 MolWeight:304 RetIndex:1551
CompName:7-Hydroxoctanoic acid-2TMS ; 7-hydroxyoctanoic acid

Hit#:3 Entry:455 Library:OA_TMS_DB5_67min_V3.lib
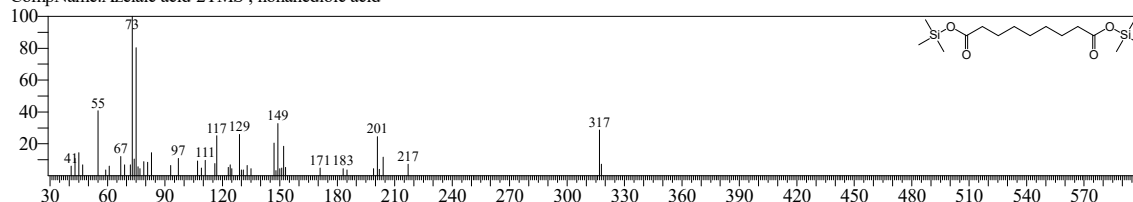SI:40 Formula:C18H38O4Si2 CAS:693-23-2 MolWeight:374 RetIndex:2092
CompName:Dodecanedioic acid-2TMS ; dodecanedioic acid

Hit#:4 Entry:300 Library:OA_TMS_DB5_67min_V3.lib
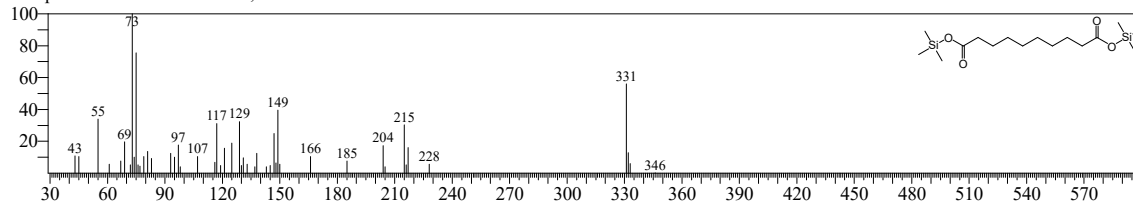SI:40 Formula:C15H32O4Si2 CAS:123-99-9 MolWeight:332 RetIndex:1799
CompName:Azelaic acid-2TMS ; nonanedioic acid

Hit#:5 Entry:362 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C16H34O4Si2 CAS:111-20-6 MolWeight:346 RetIndex:1896
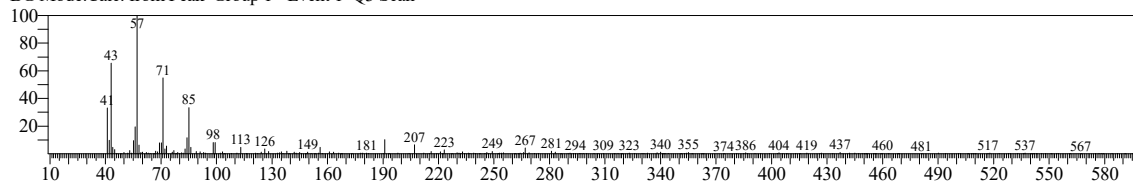CompName:Sebacic acid-2TMS ; decanedioic acid

TNAU

<< Target >>
Line#:3 R.Time:9.690(Scan#:1039) MassPeaks:228
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(5564)
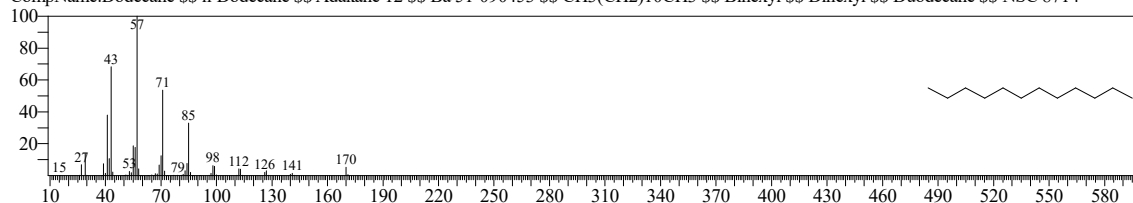BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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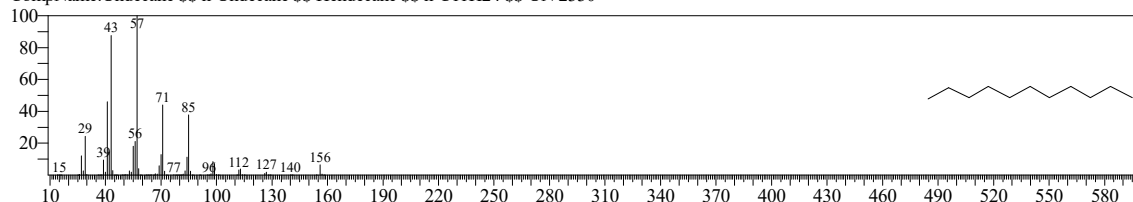CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:2 Entry:12897 Library:NIST20R.lib
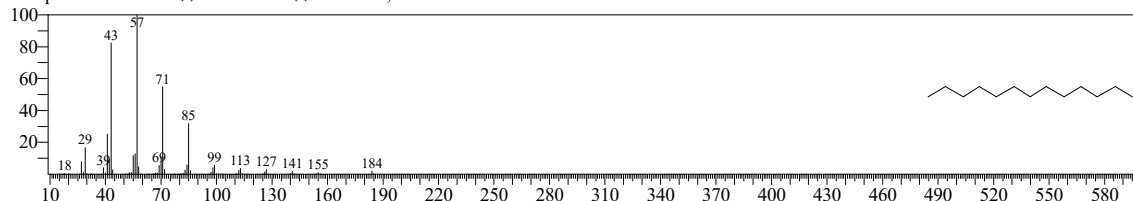SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:3 Entry:19412 Library:NIST20R.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
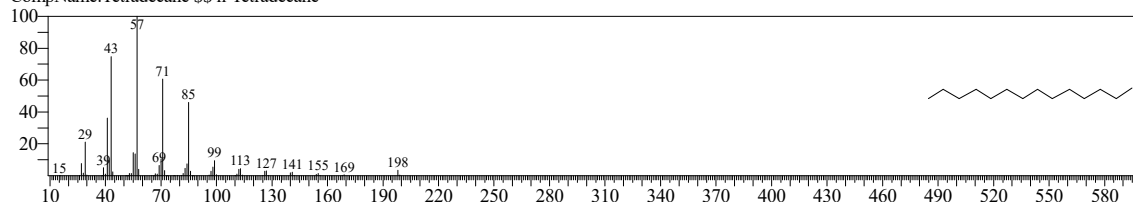CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

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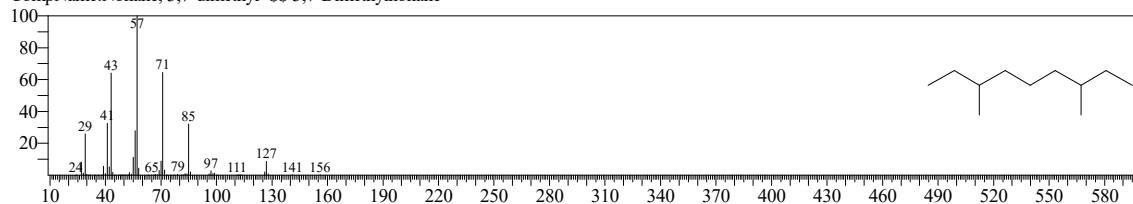SI:87 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

Hit#:5 Entry:21047 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:17302-32-8 MolWeight:156 RetIndex:986
CompName:Nonane, 3,7-dimethyl- $$ 3,7-Dimethylnonane
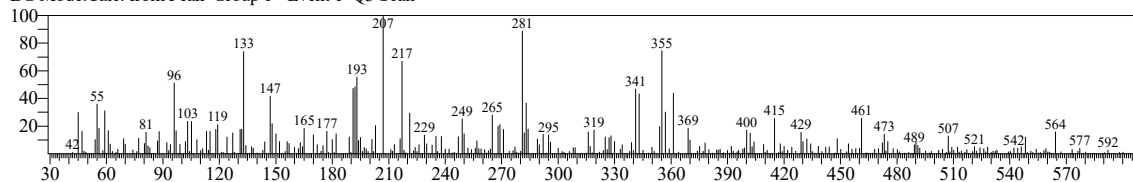
TNAU

<< Target >>
Line#:4 R.Time:28.110(Scan#:4723) MassPeaks:315
RawMode:Averaged 28.105-28.115(4722-4724) BasePeak:207.05(720)
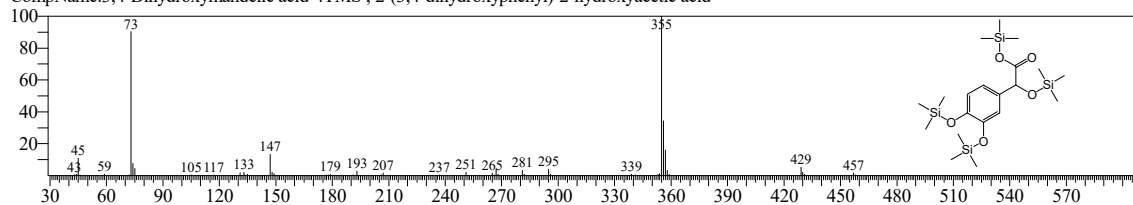BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
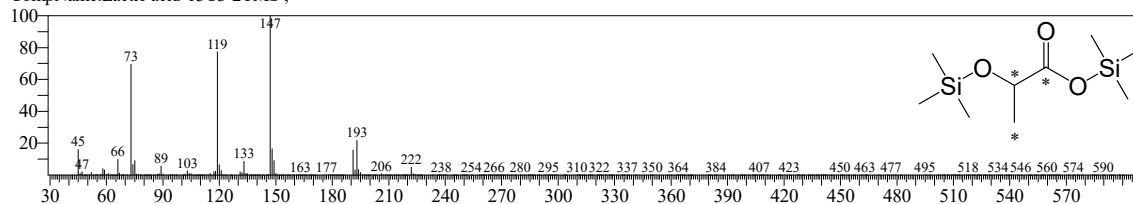SI:31 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
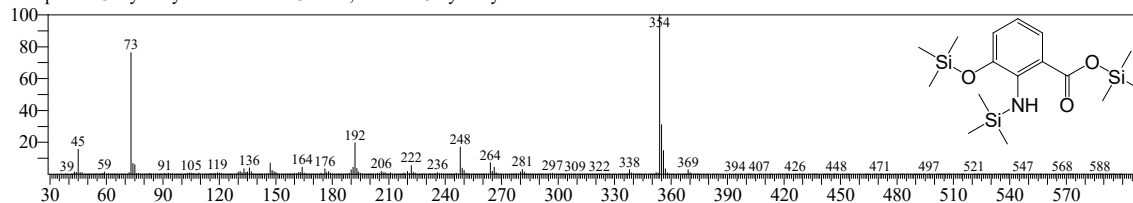SI:29 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;

Hit#:3 Entry:354 Library:OA_TMS_DB5_67min_V3.lib
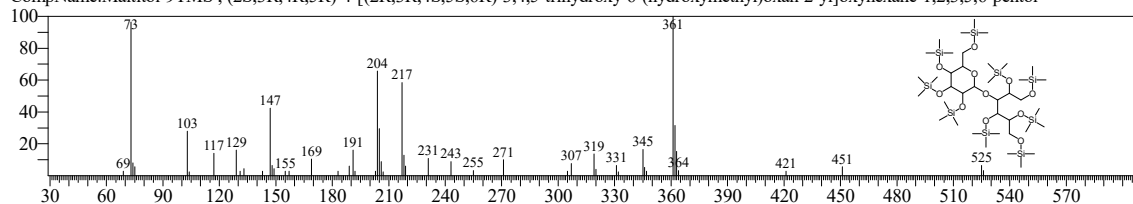SI:29 Formula:C16H31NO3Si3 CAS:548-93-6 MolWeight:369 RetIndex:1886
CompName:3-Hydroxyanthranilic acid-3TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:4 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
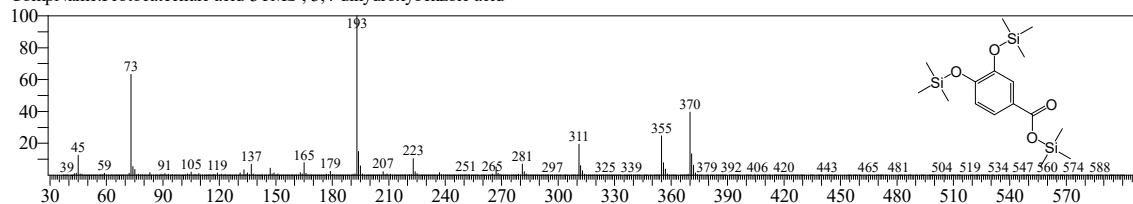CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
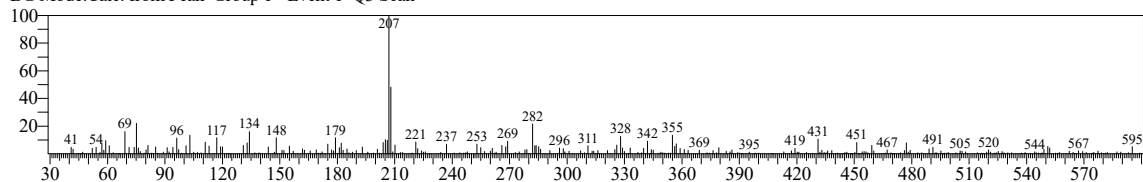CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

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<< Target >>
Line#:5 R.Time:29.110(Scan#:4923) MassPeaks:285
RawMode:Averaged 29.105-29.115(4922-4924) BasePeak:207.00(1828)
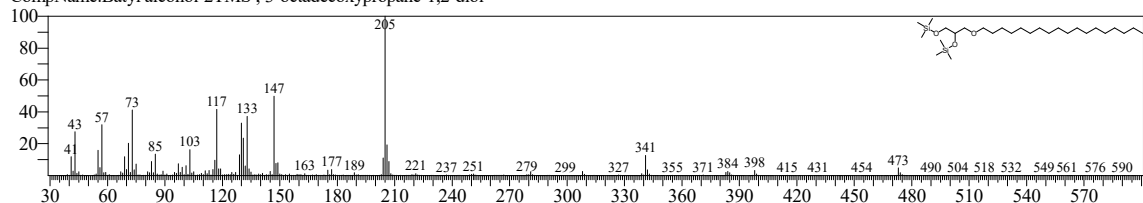BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
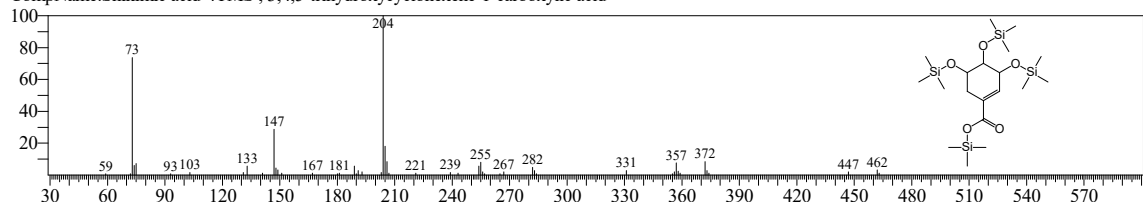SI:38 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

Hit#:2 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
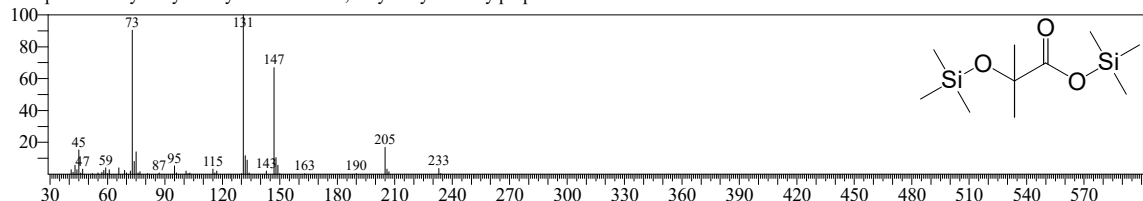SI:31 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid

Hit#:3 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
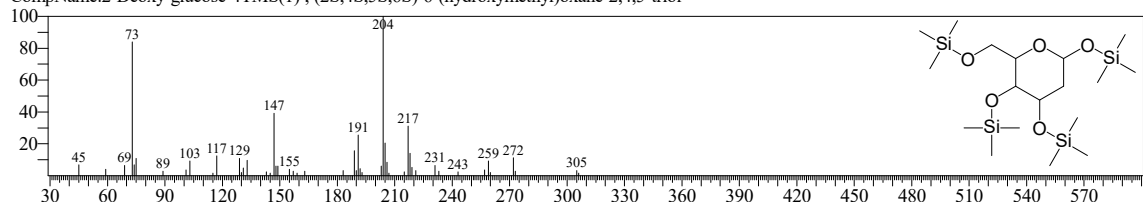SI:31 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

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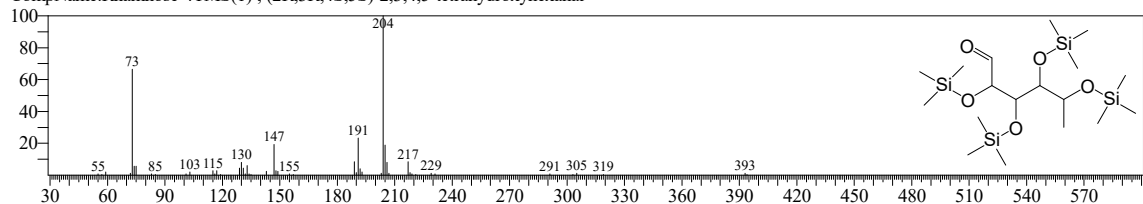CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

Hit#:5 Entry:219 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1646
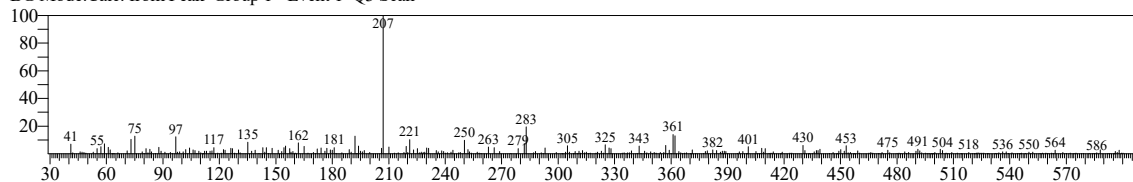CompName:Rhamnose-4TMS(1) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

TNAU

<< Target >>
Line#:6 R.Time:29.555(Scan#:5012) MassPeaks:321
RawMode:Averaged 29.550-29.560(5011-5013) BasePeak:207.05(3164)
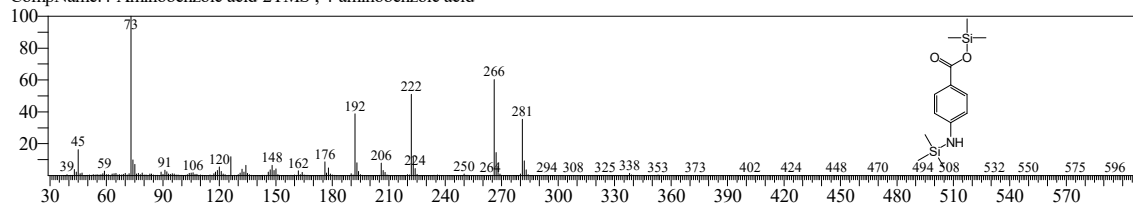BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
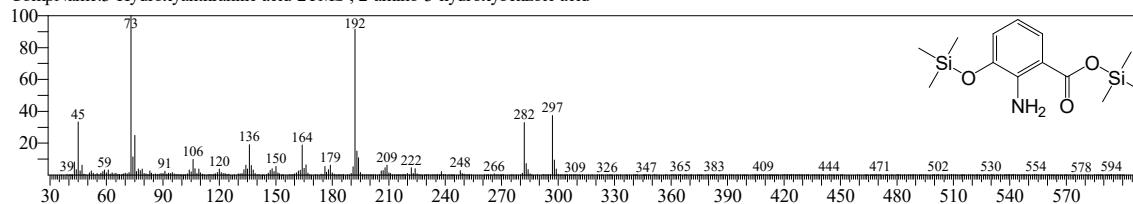SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

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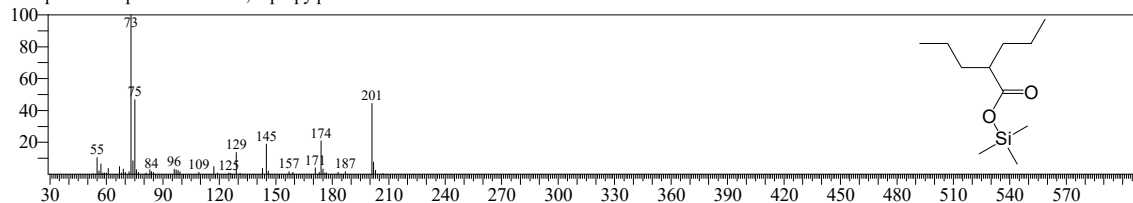SI:33 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:3 Entry:32 Library:OA_TMS_DB5_67min_V3.lib
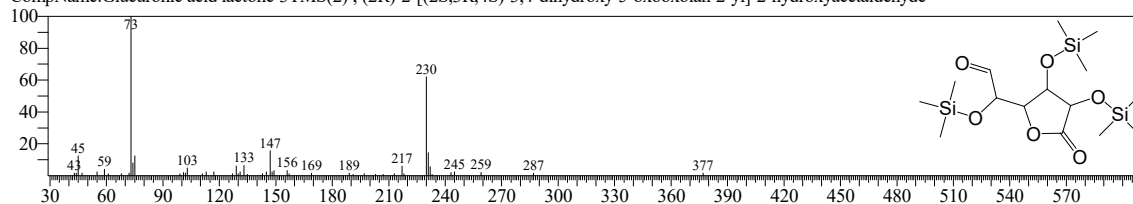SI:33 Formula:C11H24O2Si CAS:99-66-1 MolWeight:216 RetIndex:1152
CompName:Valproic acid-TMS ; 2-propylpentanoic acid

Hit#:4 Entry:336 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C15H32O6Si3 CAS:32449-92-6 MolWeight:392 RetIndex:1854
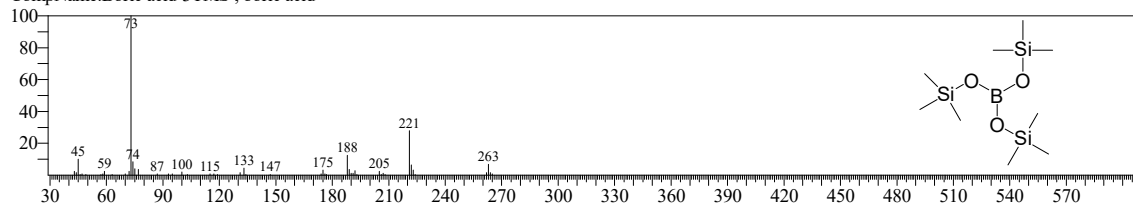CompName:Glucuronic acid lactone-3TMS(2) ; (2R)-2-[(2S,3R,4S)-3,4-dihydroxy-5-oxooxolan-2-yl]-2-hydroxyacetaldehyde

Hit#:5 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
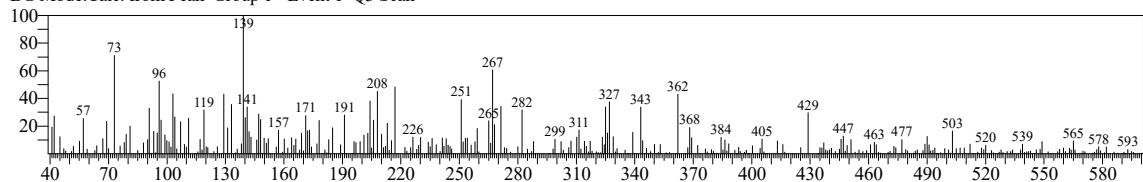CompName:Boric acid-3TMS ; boric acid

TNAU

<< Target >>
Line#:7 R.Time:31.915(Scan#:5484) MassPeaks:326
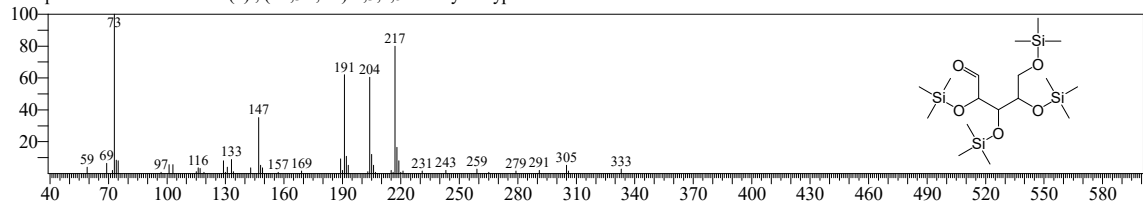RawMode:Averaged 31.910-31.920(5483-5485) BasePeak:139.15(887)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
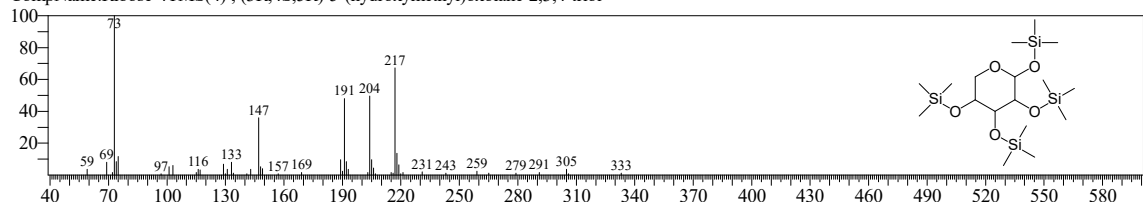SI:35 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:2 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
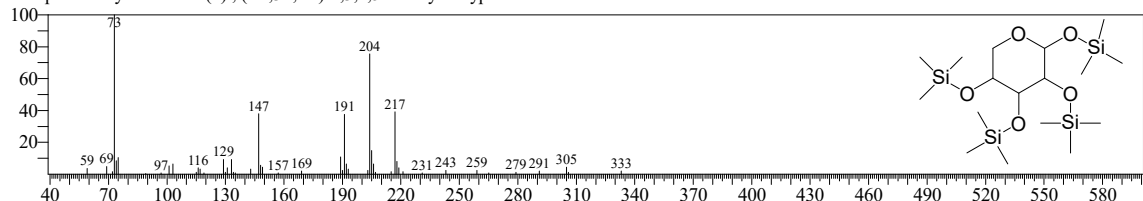SI:35 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

Hit#:3 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
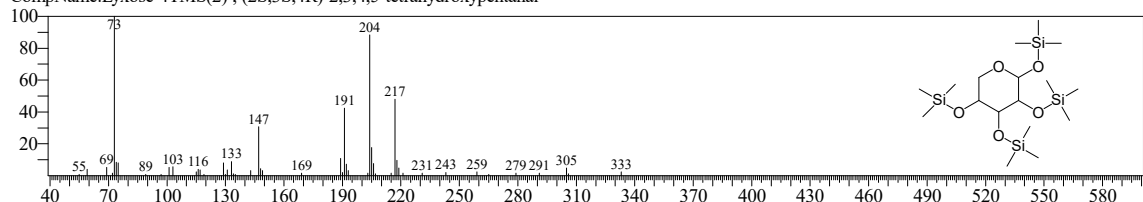CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:4 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
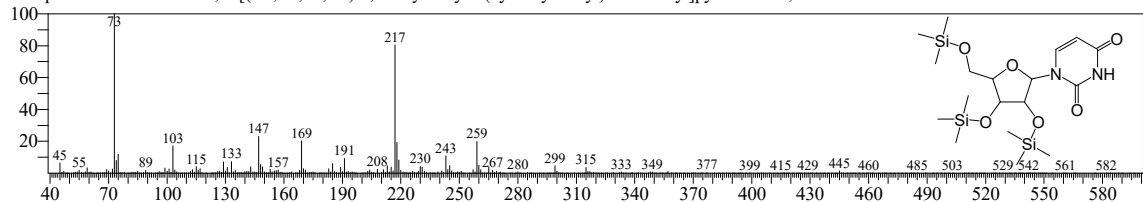SI:35 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:5 Entry:523 Library:OA_TMS_DB5_67min_V3.lib
SI:34 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
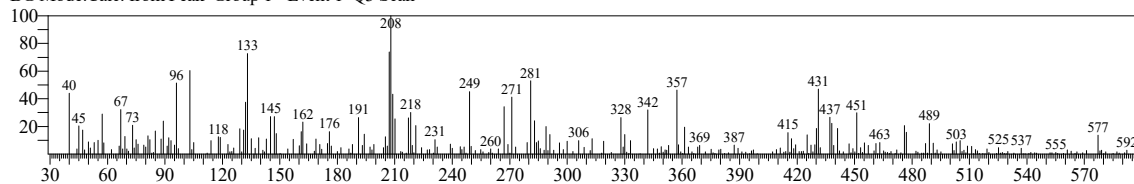
TNAU

<< Target >>
Line#:8 R.Time:32.480(Scan#:5597) MassPeaks:308
RawMode:Averaged 32.475-32.485(5596-5598) BasePeak:208.00(775)
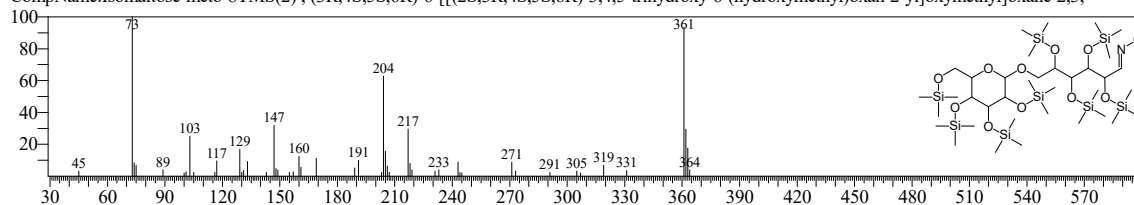BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:561 Library:OA_TMS_DB5_67min_V3.lib
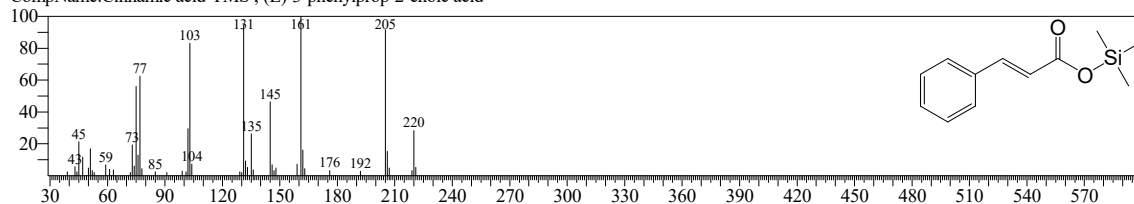SI:29 Formula:C37H89NO11Si8 CAS:499-40-1 MolWeight:947 RetIndex:2983
CompName:Isomaltose-meto-8TMS(2) ; (3R,4S,5S,6R)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxane-2,3,

Hit#:2 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
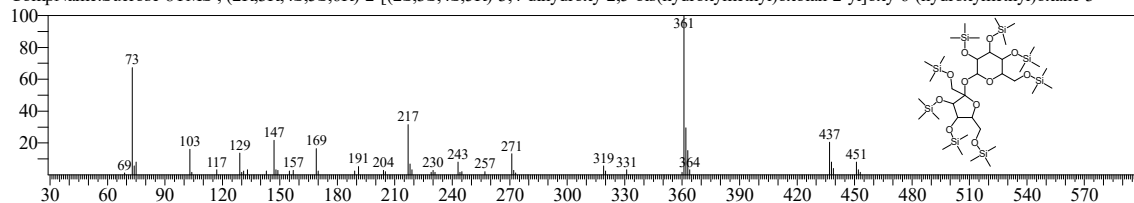SI:29 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid

Hit#:3 Entry:541 Library:OA_TMS_DB5_67min_V3.lib
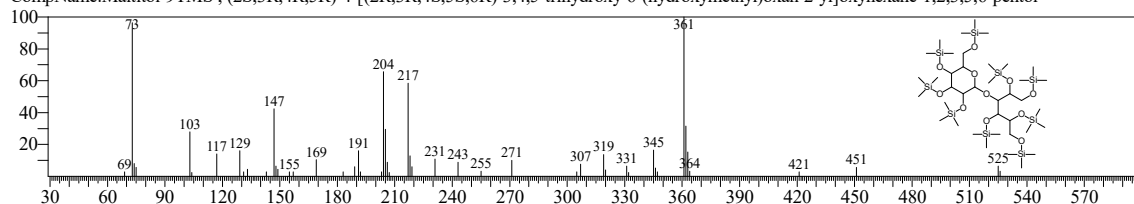SI:29 Formula:C36H86O11Si8 CAS:57-50-1 MolWeight:918 RetIndex:2705
CompName:Sucrose-8TMS ; (2R,3R,4S,5S,6R)-2-[(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy-6-(hydroxymethyl)oxane-3

Hit#:4 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
SI:28 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:268 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C20H52O5Si5 CAS:87-99-0 MolWeight:512 RetIndex:1732
CompName:Xylitol-5TMS ; (2S,4R)-pentane-1,2,3,4,5-pentol