TNAU

Chromatogram C87-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-009.qgd

Peak Report TIC

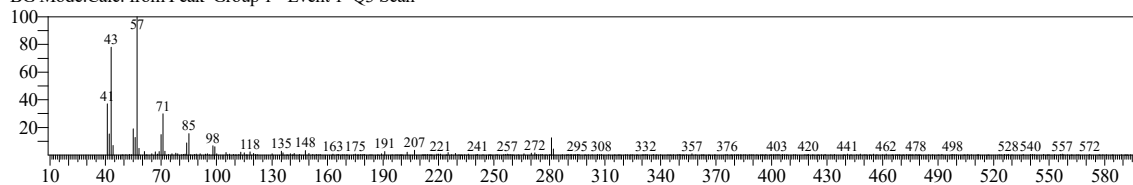| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.945	39250	30.92	20034	29.28	1.96	86	Decane
2	9.687	37455	29.50	24019	35.10	1.56	87	Dodecane
3	31.907	20924	16.48	13458	19.67	1.55	33	Inosine-4TMS
4	32.510	29324	23.10	10914	15.95	2.69	28	Lactitol-9TMS
		126953	100.00	68425	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:284
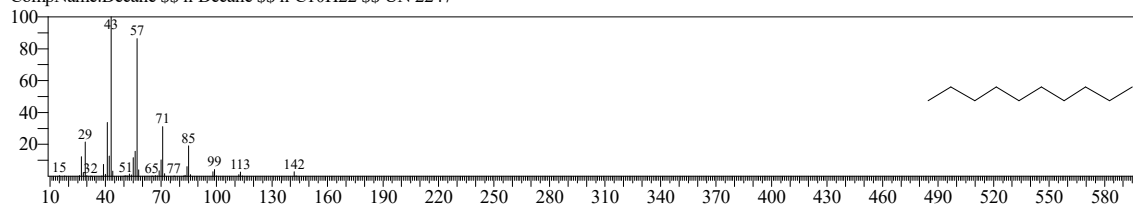RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5390)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:9444 Library:NIST20R.lib
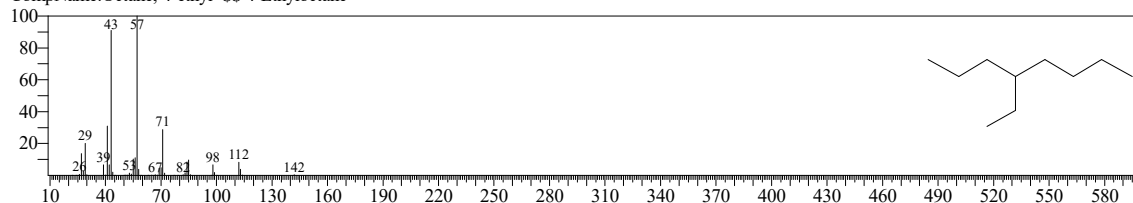SI:86 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

Hit#:2 Entry:9458 Library:NIST20R.lib
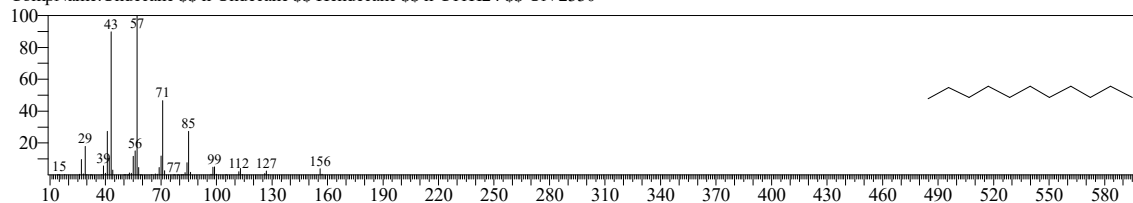SI:86 Formula:C10H22 CAS:15869-86-0 MolWeight:142 RetIndex:951
CompName:Octane, 4-ethyl- $$ 4-Ethyloctane

Hit#:3 Entry:21042 Library:NIST20M1.lib
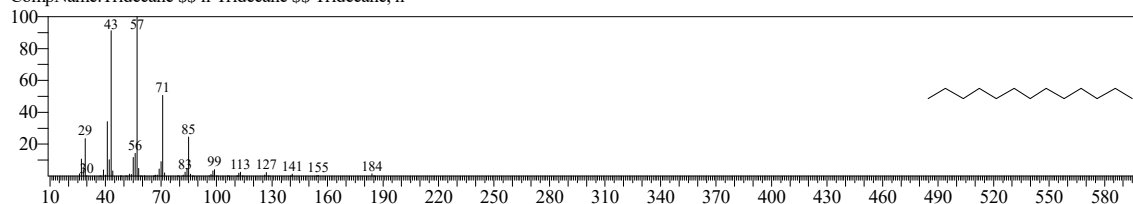SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:4 Entry:40226 Library:NIST20M1.lib
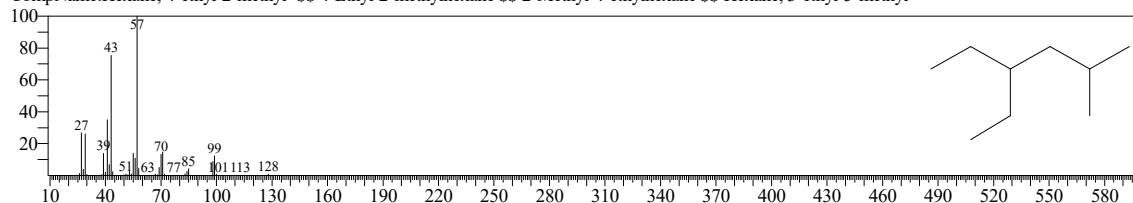SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:5 Entry:8094 Library:NIST20M1.lib
SI:86 Formula:C9H20 CAS:3074-75-7 MolWeight:128 RetIndex:788
CompName:Hexane, 4-ethyl-2-methyl- $$ 4-Ethyl-2-methylhexane $$ 2-Methyl-4-ethylhexane $$ Hexane, 3-ethyl-5-methyl
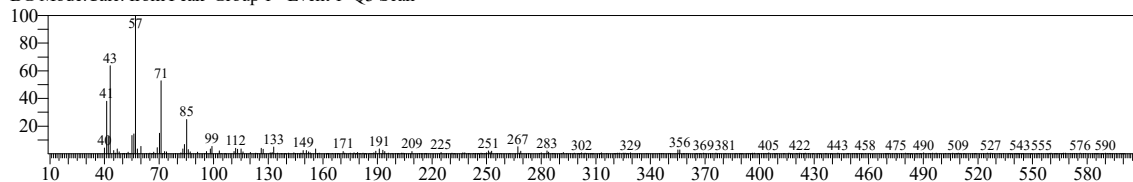
TNAU

<< Target >>
Line#:2   R.Time:9.685(Scan#:1038) MassPeaks:294
RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.10(5329)
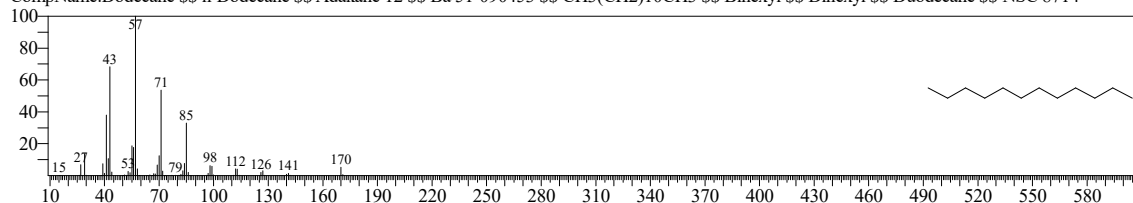BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
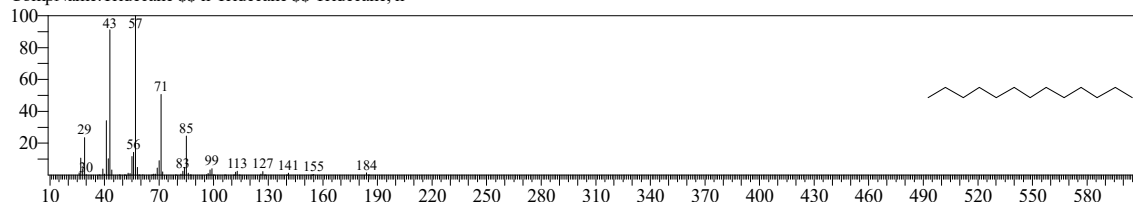CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:2 Entry:40226 Library:NIST20M1.lib
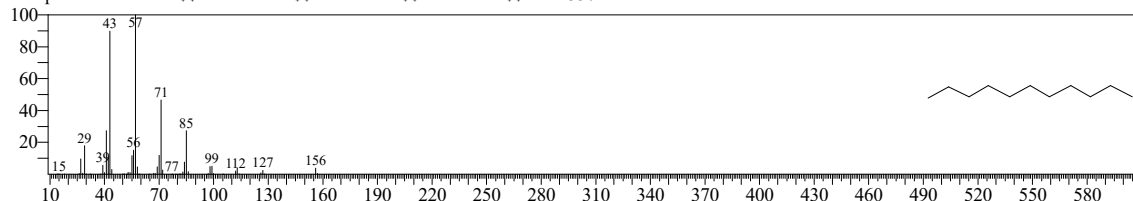SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:3 Entry:21042 Library:NIST20M1.lib
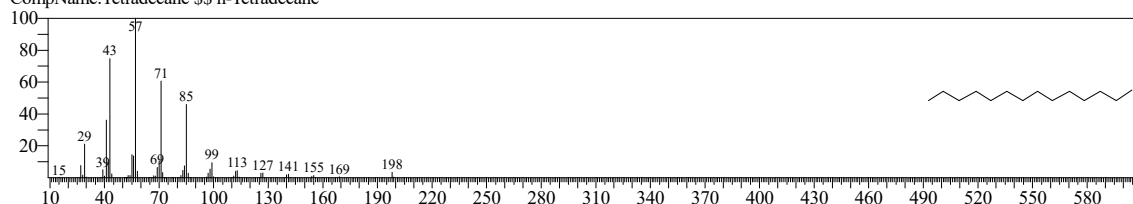SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:4 Entry:22497 Library:NIST20R.lib
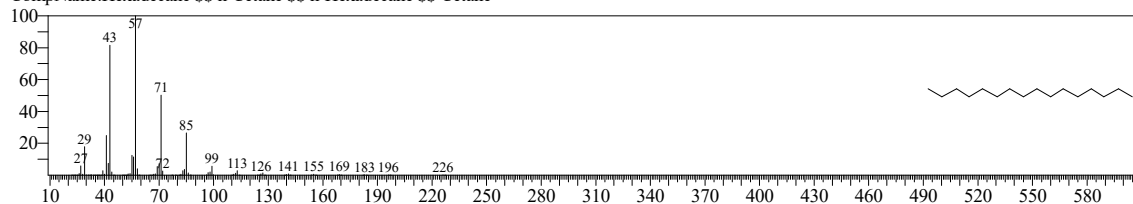SI:86 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

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
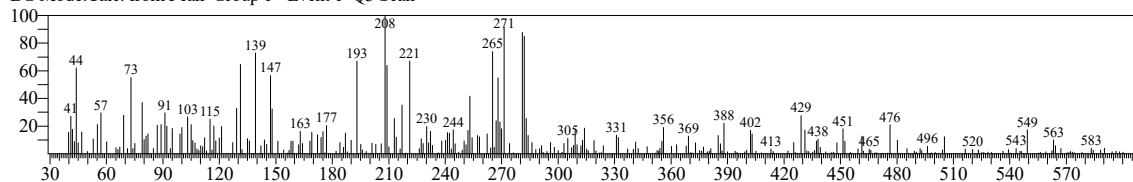
TNAU

<< Target >>
Line#:3 R.Time:31.905(Scan#:5482) MassPeaks:292
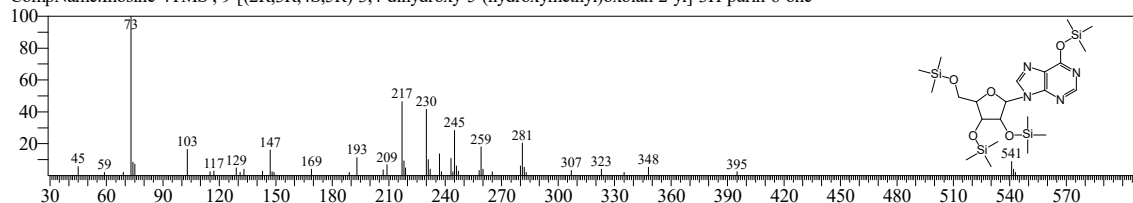RawMode:Averaged 31.900-31.910(5481-5483) BasePeak:208.10(848)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
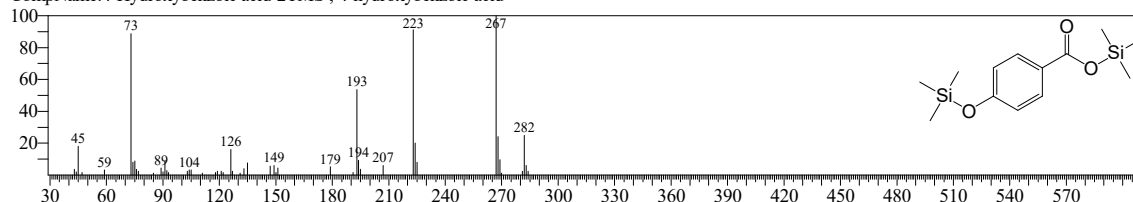SI:33 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

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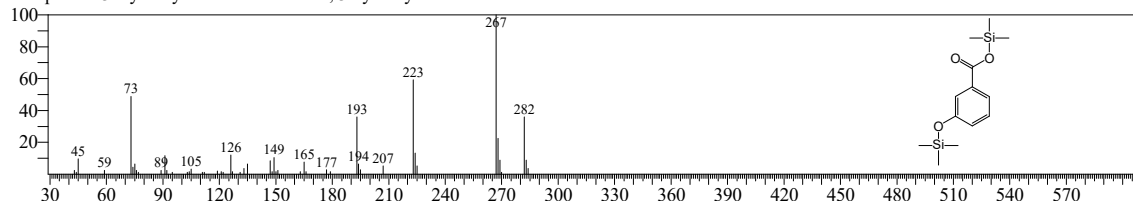SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
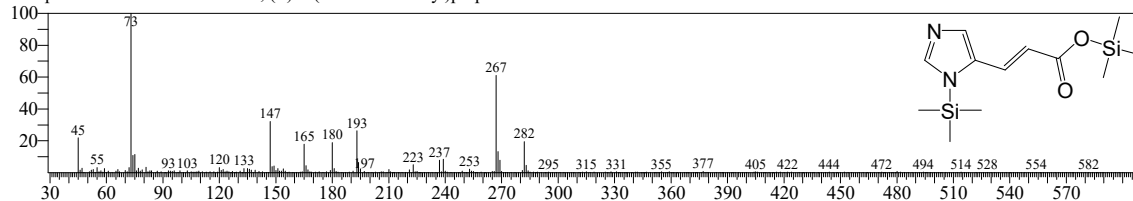CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:4 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
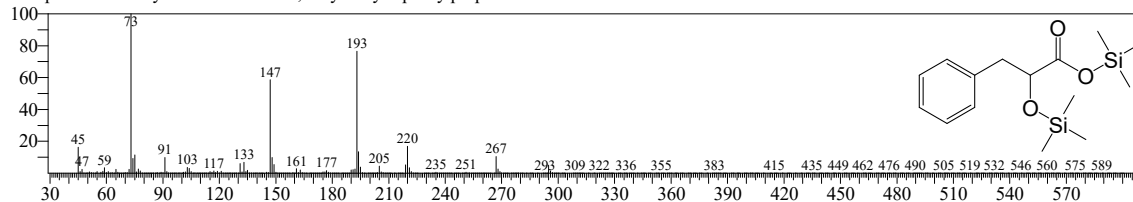CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

Hit#:5 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
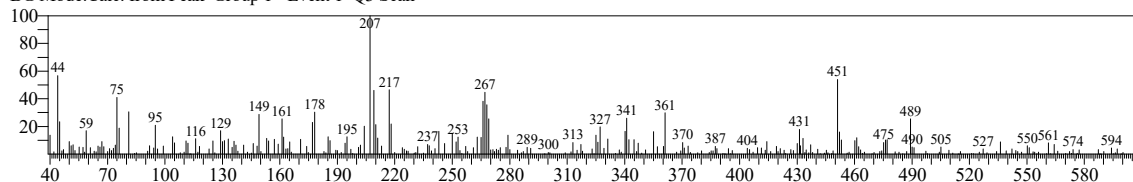CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

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<< Target >>
Line#:4 R.Time:32.510(Scan#:5603) MassPeaks:295
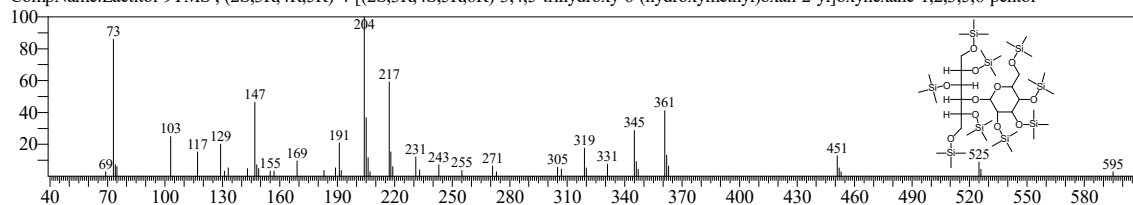RawMode:Averaged 32.505-32.515(5602-5604) BasePeak:207.05(1077)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:555 Library:OA_TMS_DB5_67min_V3.lib
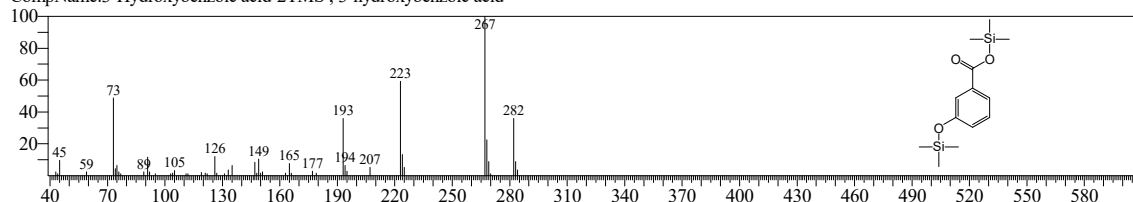SI:28 Formula:C39H96O11Si9 CAS:585-86-4 MolWeight:992 RetIndex:2845
CompName:Lactitol-9TMS ; (2S,3R,4R,5R)-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
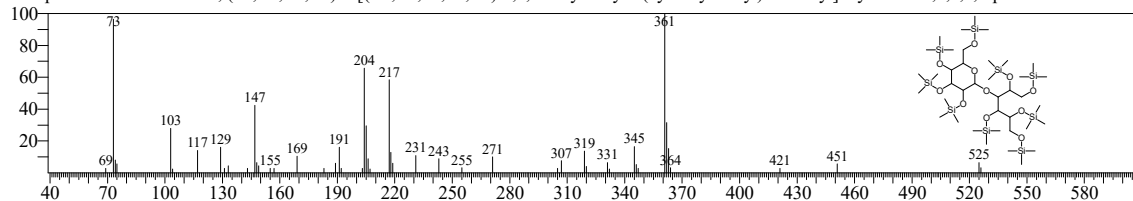SI:27 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:3 Entry:559 Library:OA_TMS_DB5_67min_V3.lib
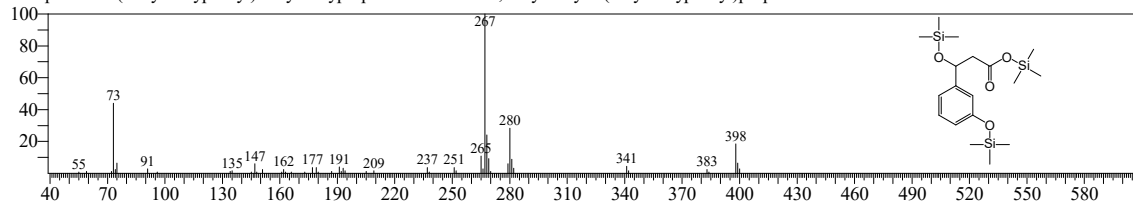SI:27 Formula:C39H96O11Si9 CAS:585-88-6 MolWeight:992 RetIndex:2923
CompName:Maltitol-9TMS ; (2S,3R,4R,5R)-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexane-1,2,3,5,6-pentol

Hit#:4 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:25 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:203 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid