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Chromatogram T56-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-025.qgd

Peak Report TIC

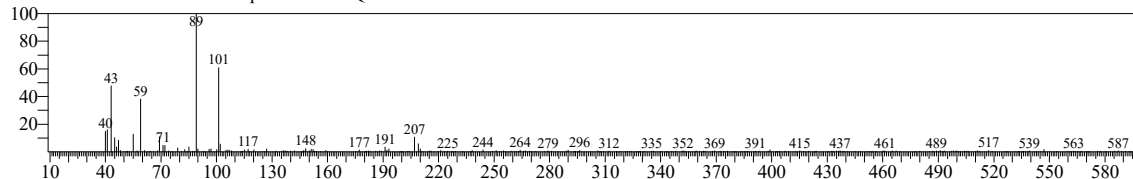| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.968	31241	5.28	11972	4.40	2.61	70	3,3-Dimethoxy-2-butanone
2	7.945	61151	10.33	27794	10.22	2.20	88	Decane
3	9.688	48897	8.26	30115	11.07	1.62	88	Undecane
4	15.467	56927	9.61	34223	12.58	1.66	91	2,4-Di-tert-butylphenol
5	19.948	16537	2.79	10342	3.80	1.60	41	Glycerol-3TMS
6	28.074	8019	1.35	8012	2.95	1.00	30	3,4-Dihydroxymandelic acid-4TMS
7	28.135	11539	1.95	7651	2.81	1.51	38	3-Hydroxyanthranilic acid-2TMS
8	28.185	12028	2.03	7604	2.80	1.58	33	3,4-Dihydroxymandelic acid-4TMS
9	28.594	53408	9.02	11902	4.38	4.49	34	Mannose-5TMS(1)
10	28.660	36590	6.18	7875	2.90	4.65	33	Hypoxanthine-2TMS
11	29.325	11493	1.94	10986	4.04	1.05	38	3-Hydroxyanthranilic acid-3TMS
12	29.406	41482	7.00	8006	2.94	5.18	41	3-Hydroxyphenylacetic acid-2TMS
13	29.539	13418	2.27	10475	3.85	1.28	32	Batyl alcohol-2TMS
14	29.732	32258	5.45	9091	3.34	3.55	35	3,4-Dihydroxymandelic acid-4TMS
15	31.165	6631	1.12	8045	2.96	0.82	36	3-Hydroxyanthranilic acid-2TMS
16	31.325	7611	1.29	6699	2.46	1.14	38	3,4-Dihydroxymandelic acid-4TMS
17	31.860	13677	2.31	7973	2.93	1.72	36	3,4-Dihydroxymandelic acid-4TMS
18	31.900	80074	13.52	30340	11.15	2.64	28	4-Hydroxybenzoic acid-2TMS
19	31.970	8131	1.37	7699	2.83	1.06	35	Anthranilic acid-2TMS
20	32.305	27041	4.57	6114	2.25	4.42	28	3,4-Dihydroxymandelic acid-4TMS
21	32.852	14031	2.37	9092	3.34	1.54	33	3,4-Dihydroxymandelic acid-4TMS
		592184	100.00	272010	100.00			

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Library

<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:254
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.05(3336)
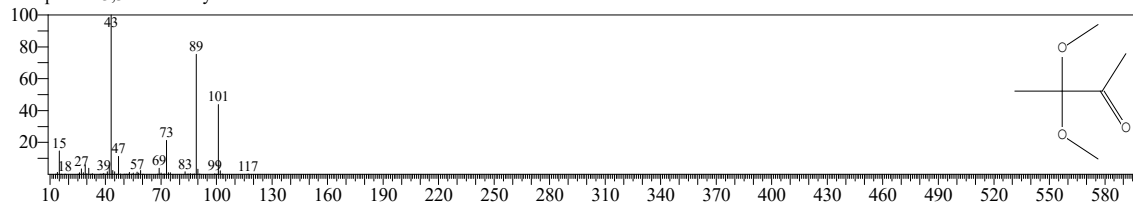BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:9263 Library:NIST20M1.lib
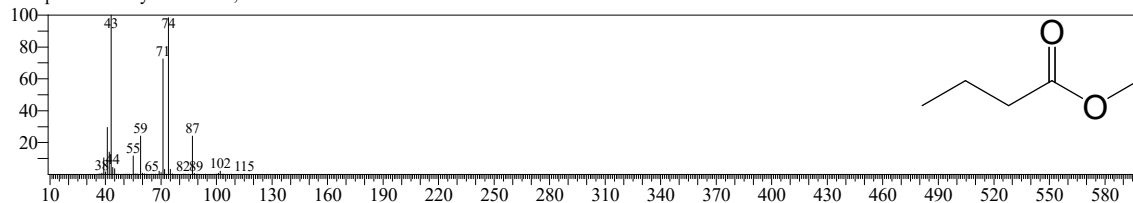SI:70 Formula:C6H12O3 CAS:21983-72-2 MolWeight:132 RetIndex:821
CompName:3,3-Dimethoxy-2-butanone

Hit#:2 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
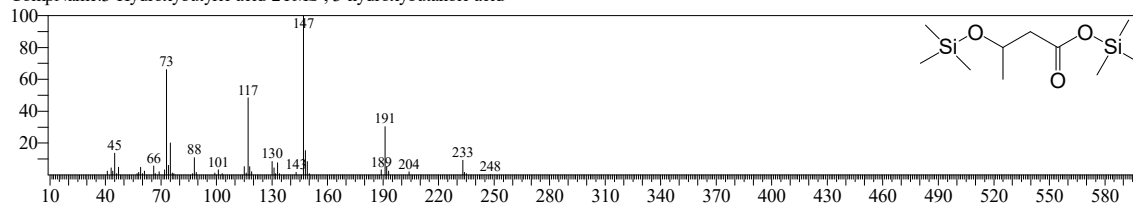SI:52 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid

Hit#:3 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
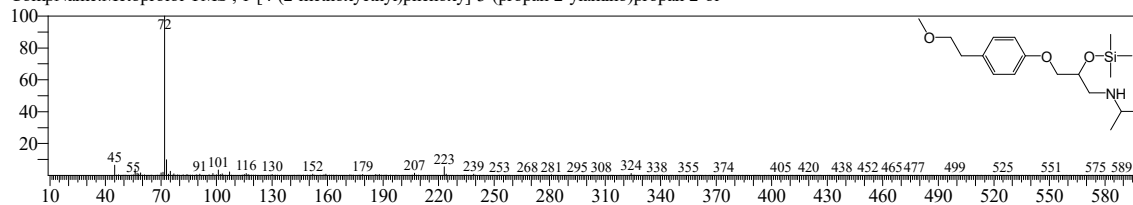CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid

Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H33NO3Si CAS:37350-58-6 MolWeight:339 RetIndex:2094
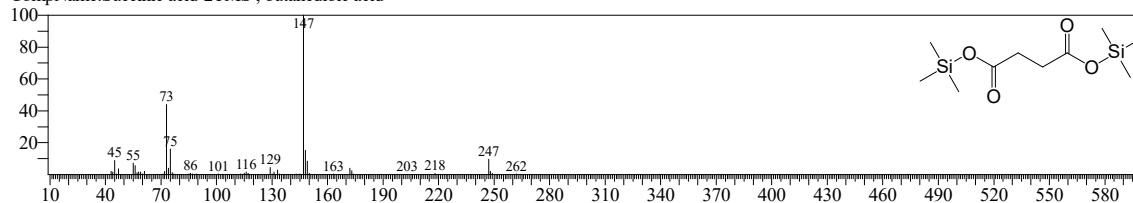CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol

Hit#:5 Entry:92 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C10H22O4Si2 CAS:110-15-6 MolWeight:262 RetIndex:1313
CompName:Succinic acid-2TMS ; butanedioic acid
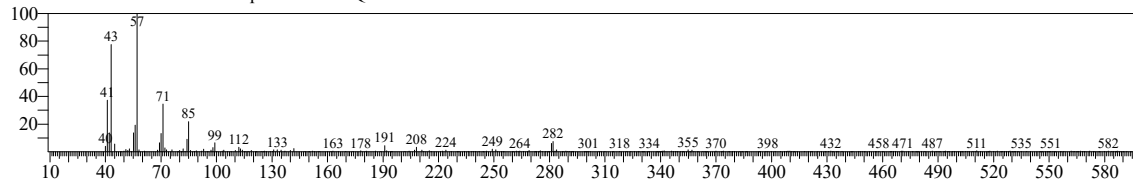
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<< Target >>
Line#:2 R.Time:7.945(Scan#:690) MassPeaks:303
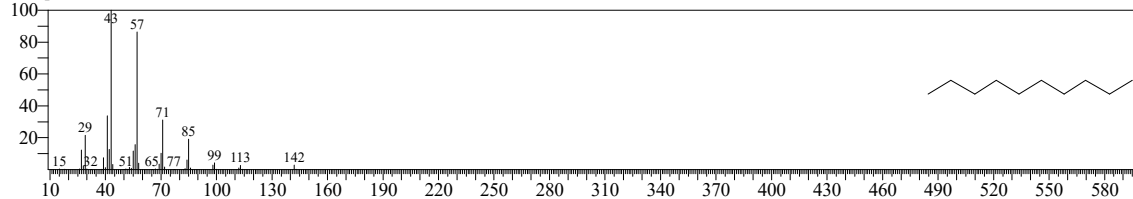RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(6400)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:9444 Library:NIST20R.lib
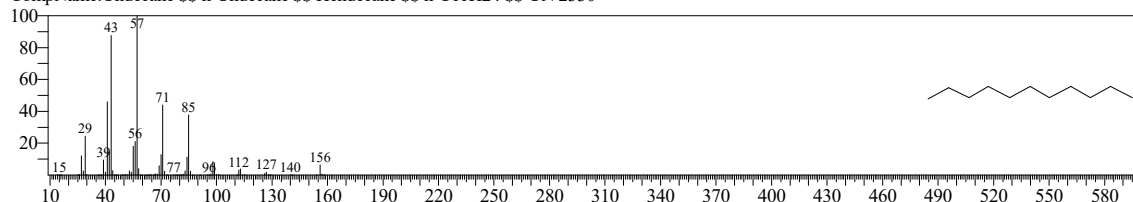SI:88 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

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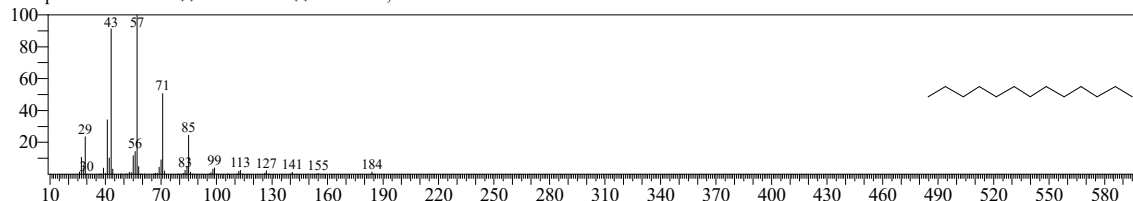SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

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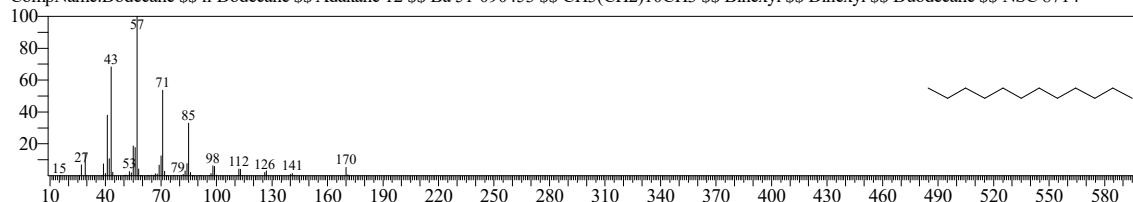SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:4 Entry:30057 Library:NIST20M1.lib
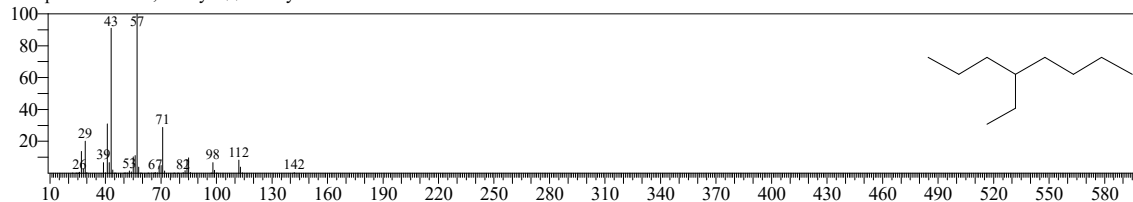SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

Hit#:5 Entry:9458 Library:NIST20R.lib
SI:87 Formula:C10H22 CAS:15869-86-0 MolWeight:142 RetIndex:951
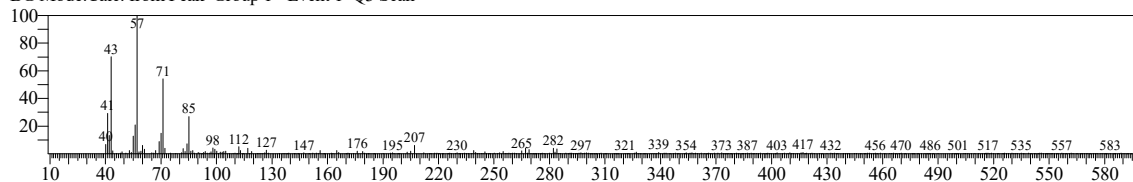CompName:Octane, 4-ethyl- $$ 4-Ethyloctane

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<< Target >>
Line#:3 R.Time:9.685(Scan#:1038) MassPeaks:382
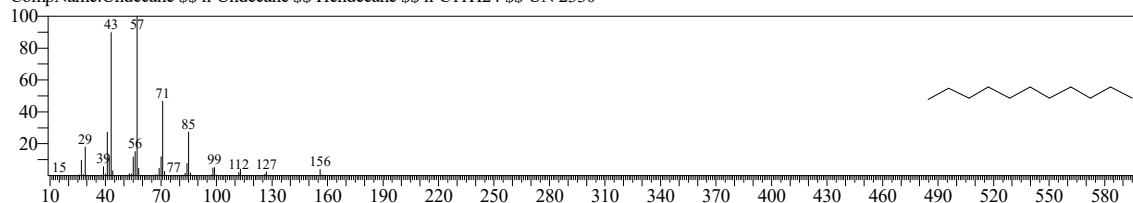RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.05(5553)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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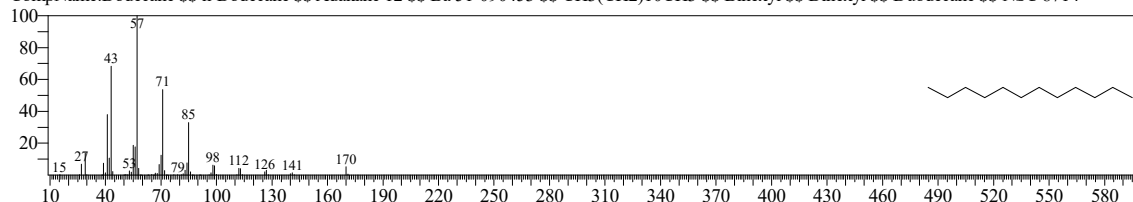SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330

Hit#:2 Entry:30057 Library:NIST20M1.lib
SI:88 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
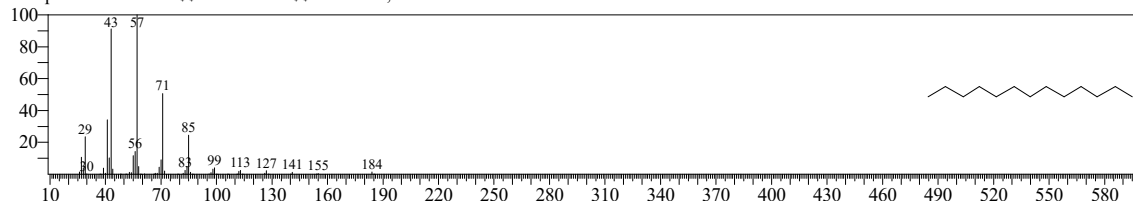CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

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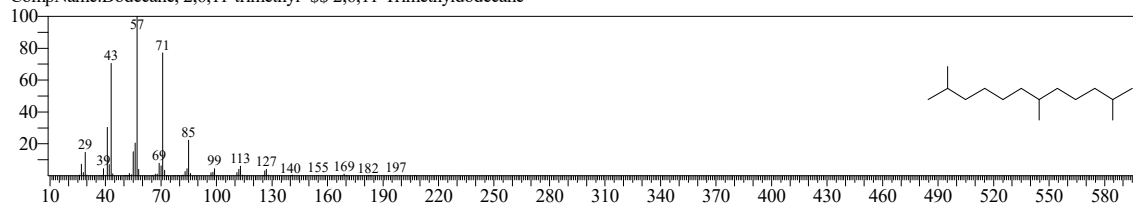CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

Hit#:4 Entry:25291 Library:NIST20R.lib
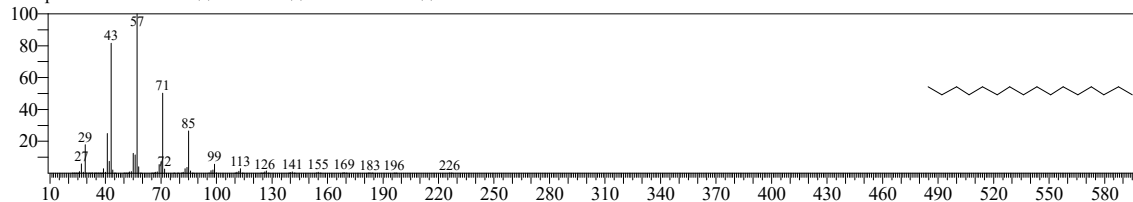SI:87 Formula:C15H32 CAS:31295-56-4 MolWeight:212 RetIndex:1320
CompName:Dodecane, 2,6,11-trimethyl- $$ 2,6,11-Trimethyldodecane

Hit#:5 Entry:27737 Library:NIST20R.lib
SI:87 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
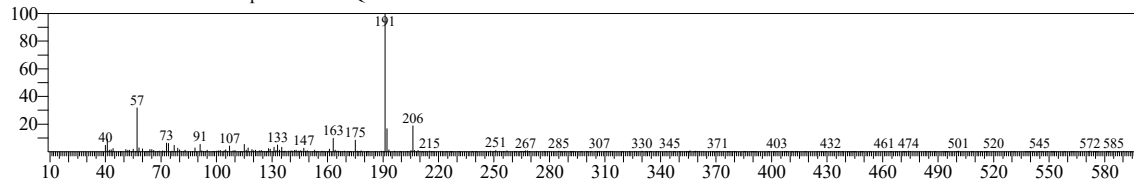CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

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<< Target >>
Line#:4 R.Time:15.465(Scan#:2194) MassPeaks:286
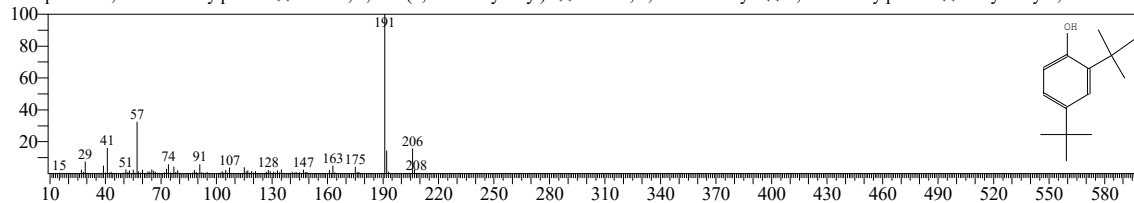RawMode:Averaged 15.460-15.470(2193-2195) BasePeak:191.10(10416)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:59048 Library:NIST20M1.lib
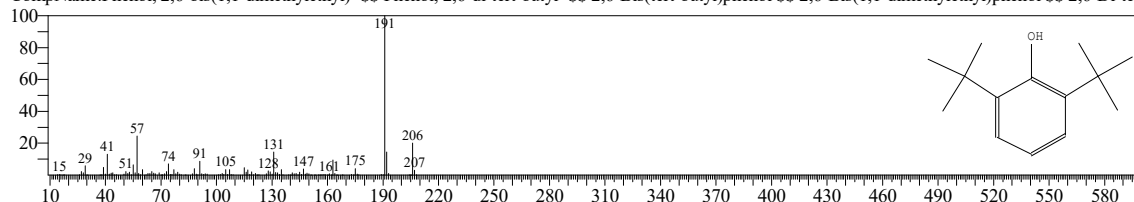SI:91 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu

Hit#:2 Entry:59031 Library:NIST20M1.lib
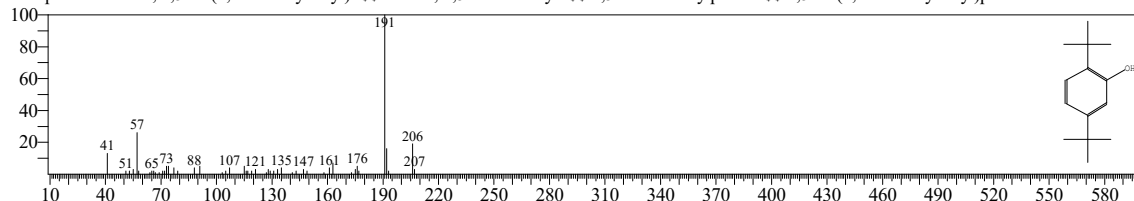SI:90 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

Hit#:3 Entry:24098 Library:NIST20R.lib
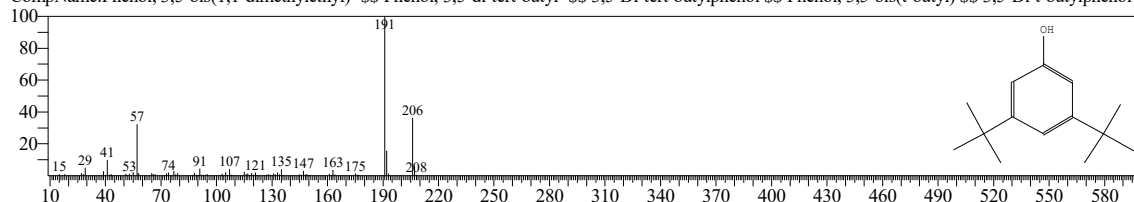SI:88 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol

Hit#:4 Entry:24110 Library:NIST20R.lib
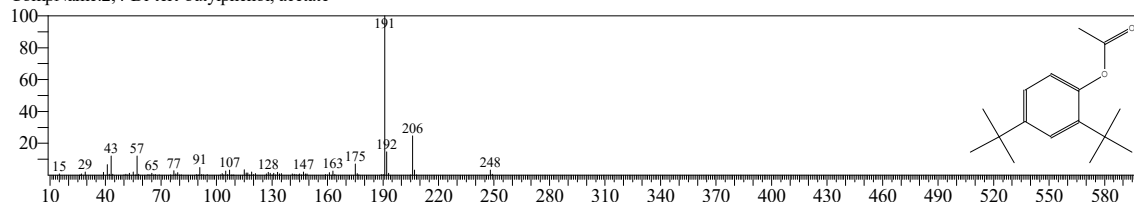SI:88 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:84 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
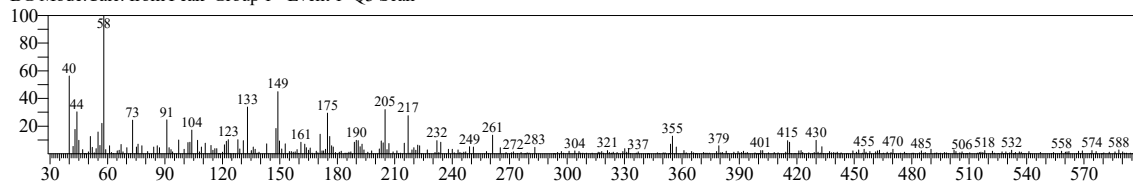CompName:2,4-Di-tert-butylphenol, acetate

<< Target >>
Line#:5 R.Time:19.950(Scan#:3091) MassPeaks:336
RawMode:Averaged 19.945-19.955(3090-3092) BasePeak:58.05(1049)
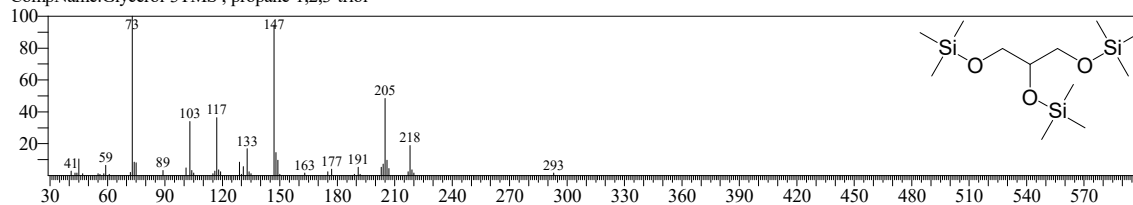BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
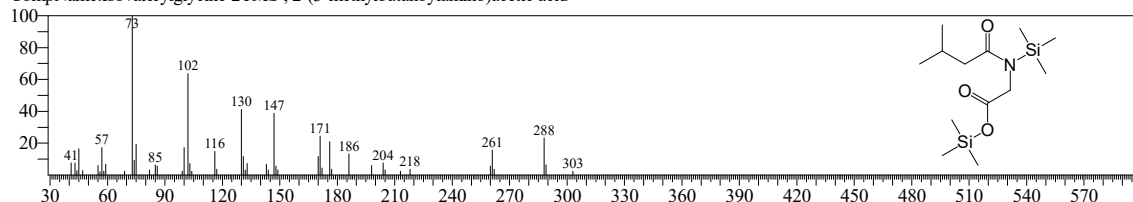SI:41 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol

Hit#:2 Entry:152 Library:OA_TMS_DB5_67min_V3.lib
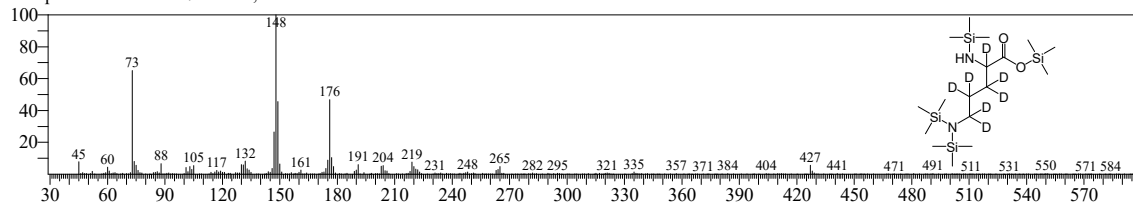SI:39 Formula:C13H29NO3Si2 CAS:16284-60-9 MolWeight:303 RetIndex:1518
CompName:Isovalerylglycine-2TMS ; 2-(3-methylbutanoylamino)acetic acid

Hit#:3 Entry:313 Library:OA_TMS_DB5_67min_V3.lib
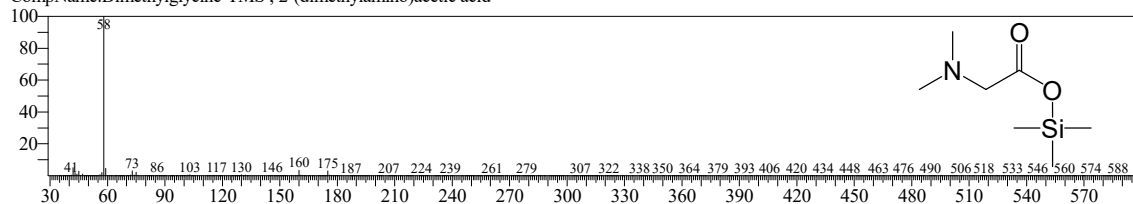SI:38 Formula: CAS:0-00-0 MolWeight:427 RetIndex:1831
CompName:Ornithine-d7-4TMS ;

Hit#:4 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
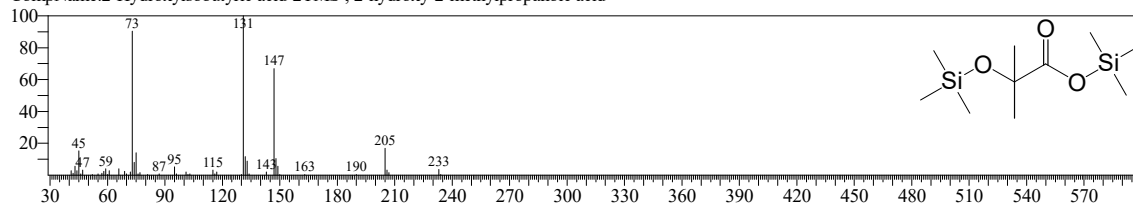SI:38 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid

Hit#:5 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid
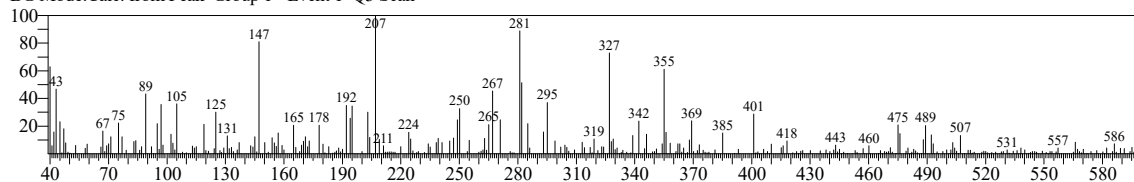
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<< Target >>
Line#:6 R.Time:28.075(Scan#:4716) MassPeaks:303
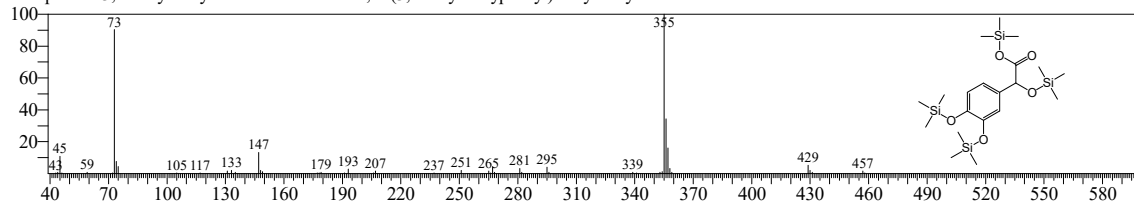RawMode:Averaged 28.070-28.080(4715-4717) BasePeak:207.00(663)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
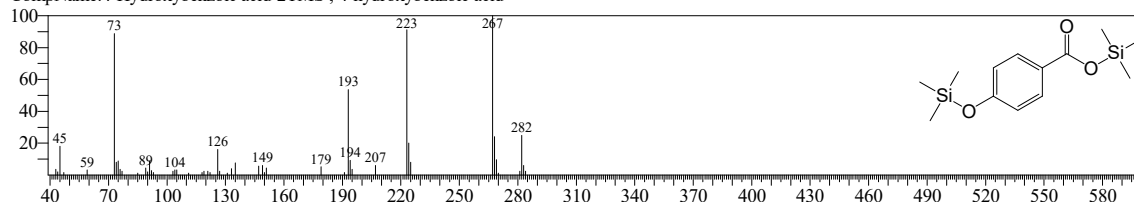SI:30 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
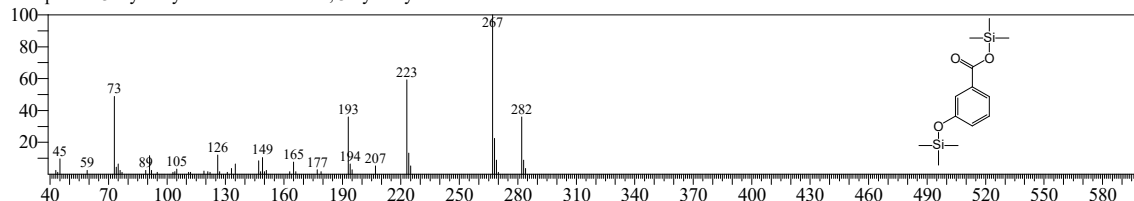CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
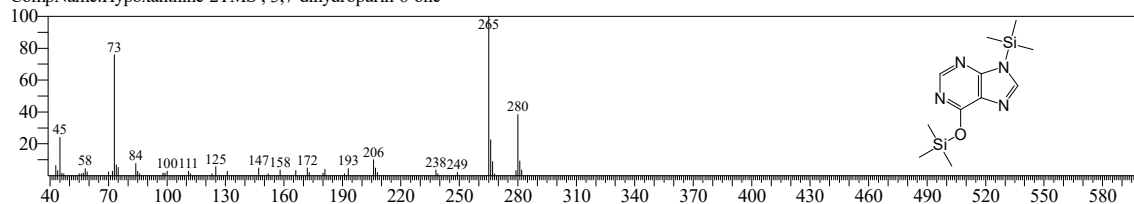CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
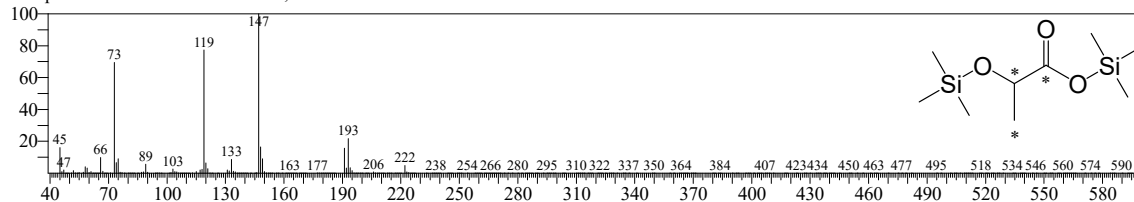CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:5 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;
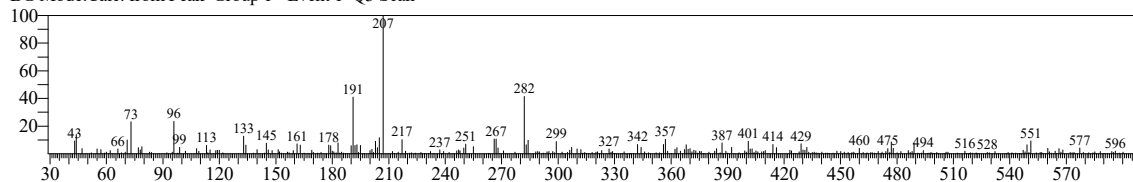
TNAU

<< Target >>
Line#:7 R.Time:28.135(Scan#:4728) MassPeaks:299
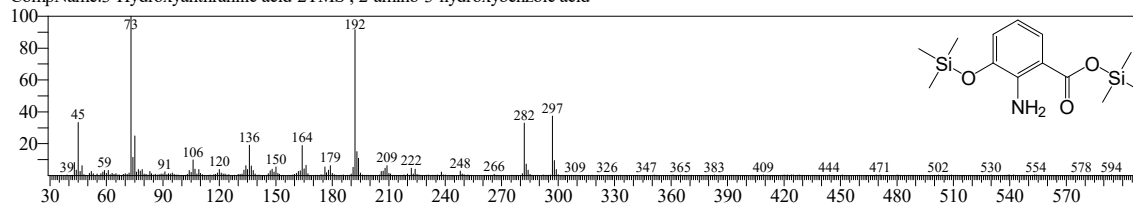RawMode:Averaged 28.130-28.140(4727-4729) BasePeak:207.05(1646)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
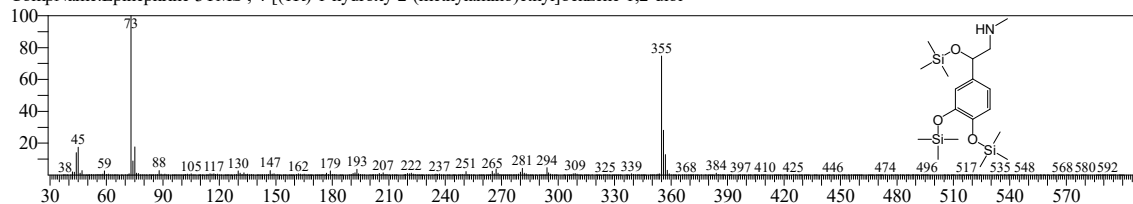SI:38 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
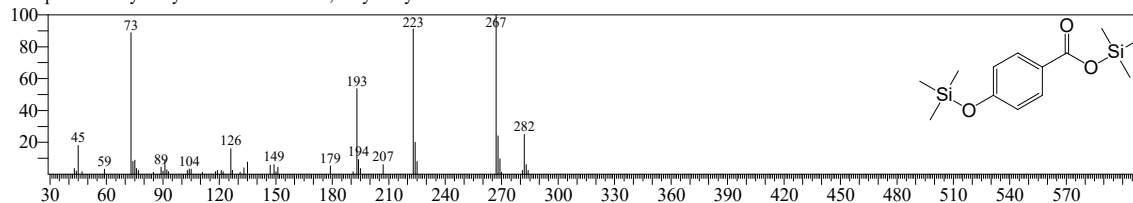SI:35 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
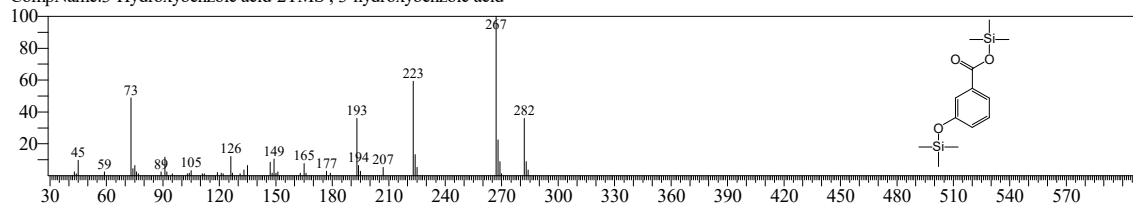CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
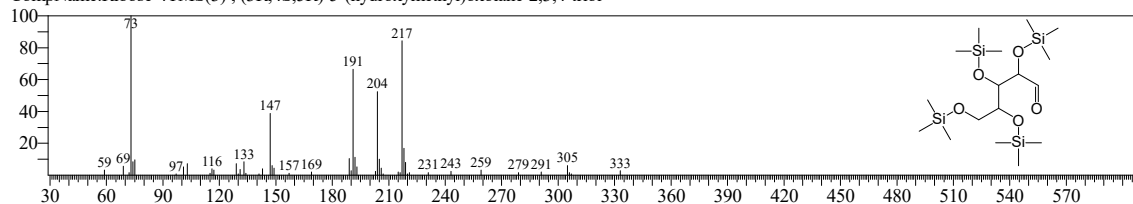SI:34 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:5 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
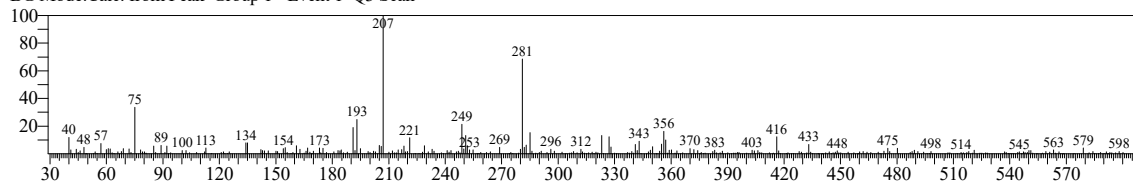
TNAU

<< Target >>
Line#:8   R.Time:28.185(Scan#:4738) MassPeaks:307
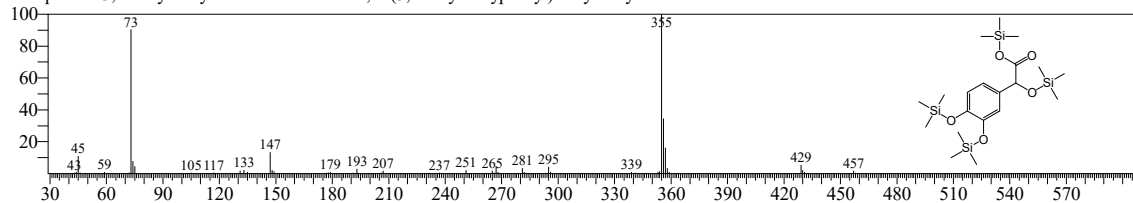RawMode:Averaged 28.180-28.190(4737-4739) BasePeak:207.05(2023)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
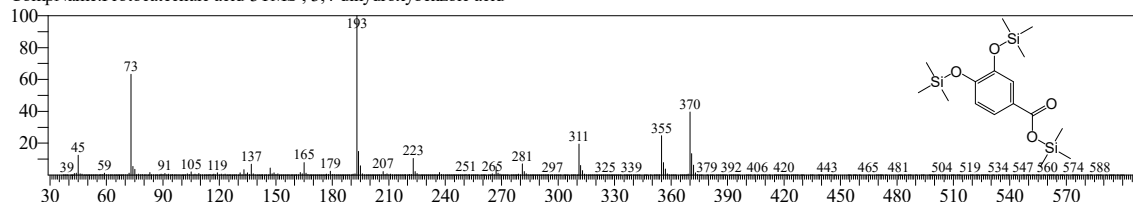SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
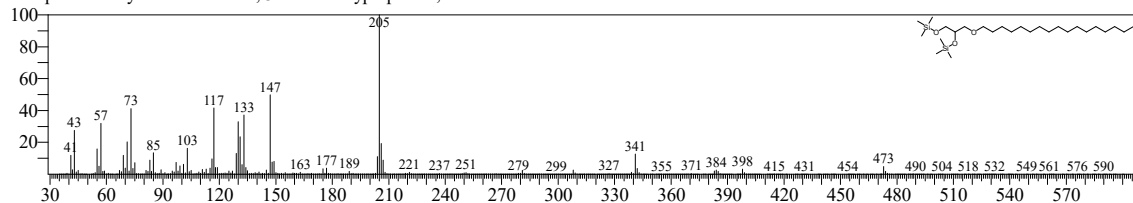CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

Hit#:3 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
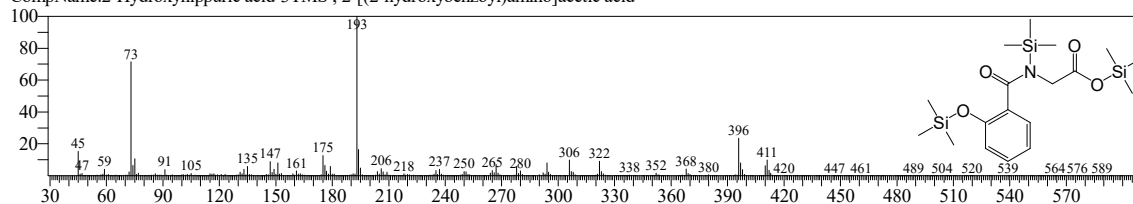CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

Hit#:4 Entry:420 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973
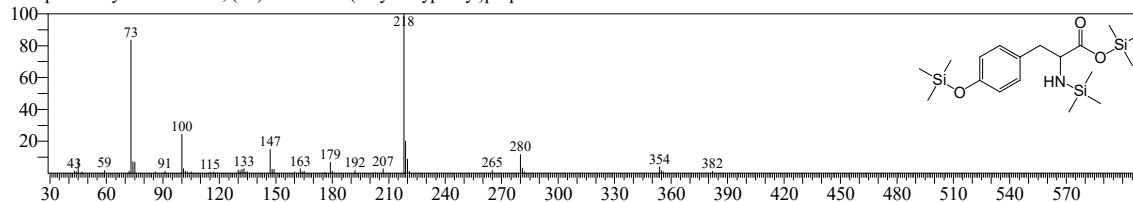CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid

Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
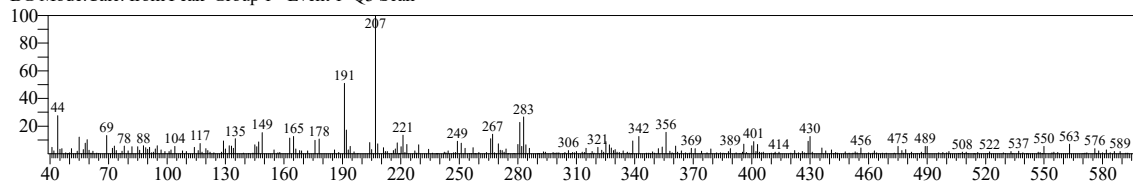CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

TNAU

<< Target >>
Line#:9 R.Time:28.595(Scan#:4820) MassPeaks:304
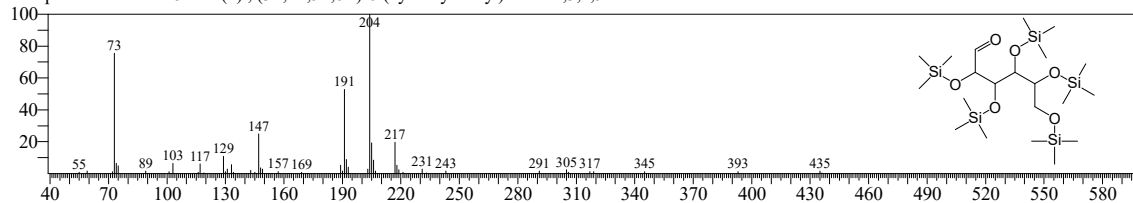RawMode:Averaged 28.590-28.600(4819-4821) BasePeak:207.00(1523)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:288 Library:OA_TMS_DB5_67min_V3.lib
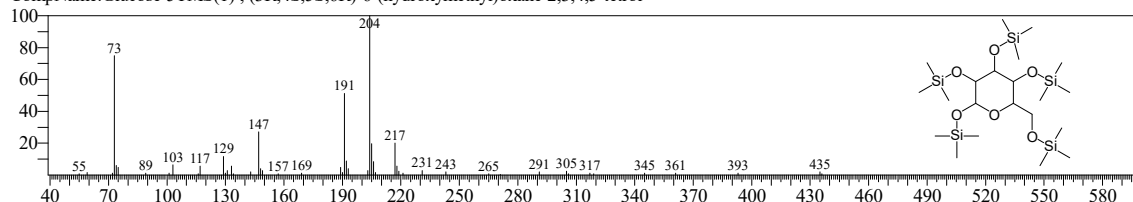SI:34 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1771
CompName:Mannose-5TMS(1) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:2 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
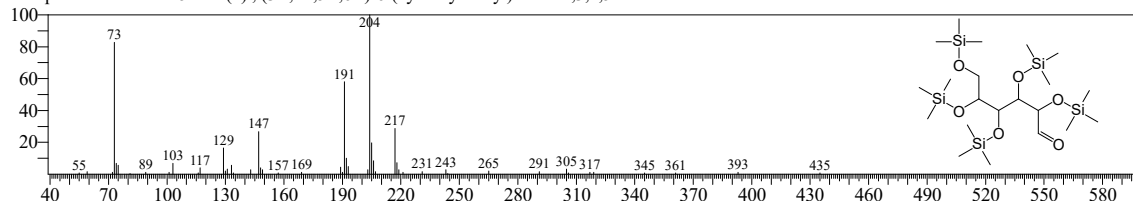SI:34 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:3 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
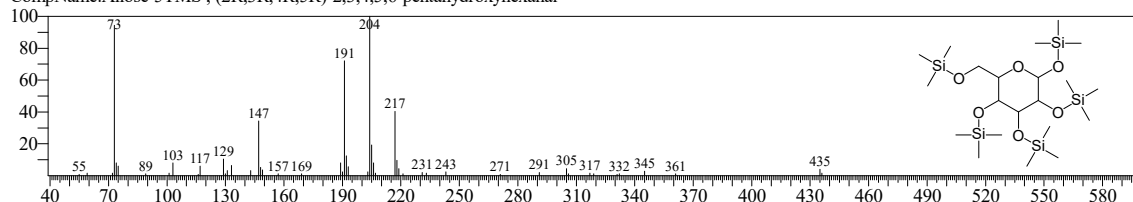SI:34 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1824
CompName:Galactose-5TMS(1) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

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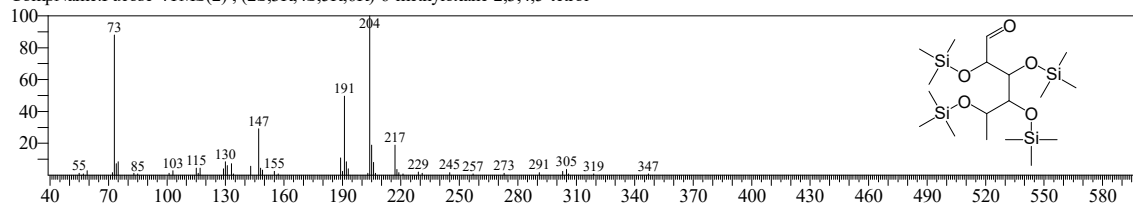CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

Hit#:5 Entry:271 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1738
CompName:Fucose-4TMS(2) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol
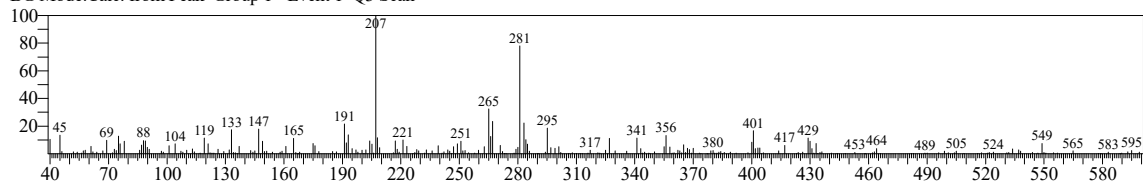
TNAU

<< Target >>
Line#:10 R.Time:28.660(Scan#:4833) MassPeaks:247
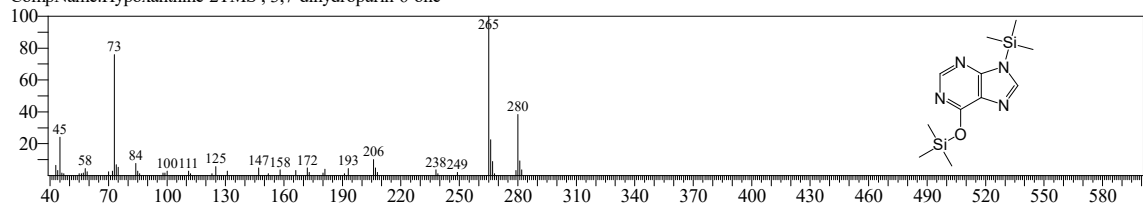RawMode:Averaged 28.655-28.665(4832-4834) BasePeak:207.05(1726)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
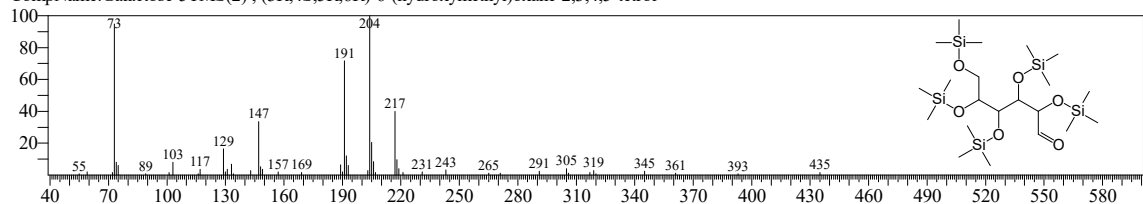SI:33 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:2 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
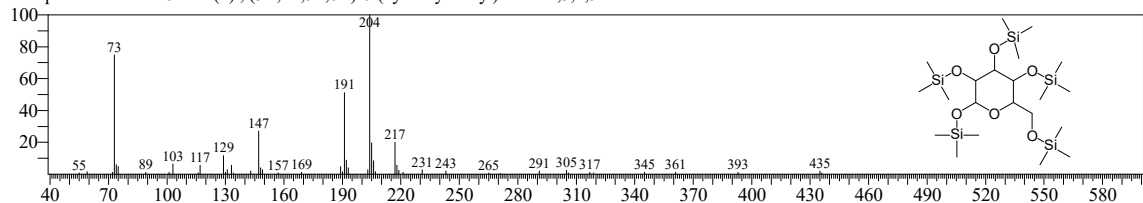CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:3 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
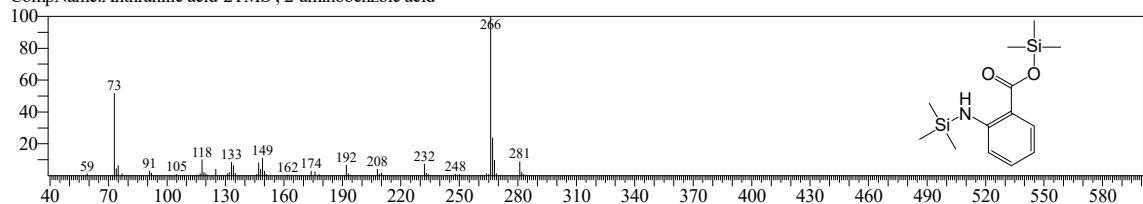SI:32 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
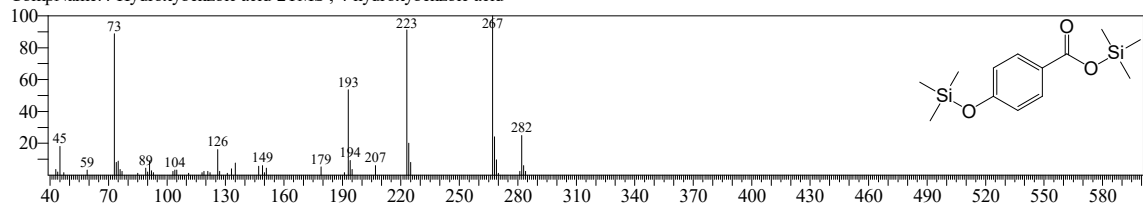SI:32 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
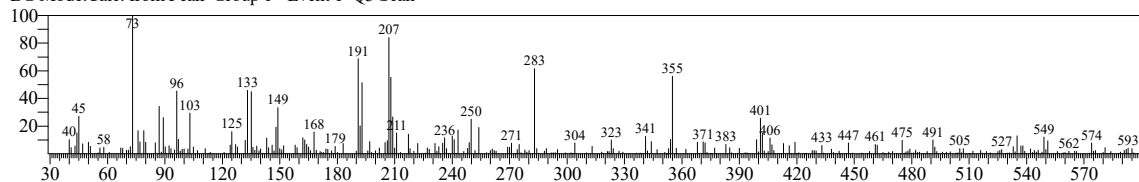CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

TNAU

<< Target >>
Line#:11 R.Time:29.325(Scan#:4966) MassPeaks:300
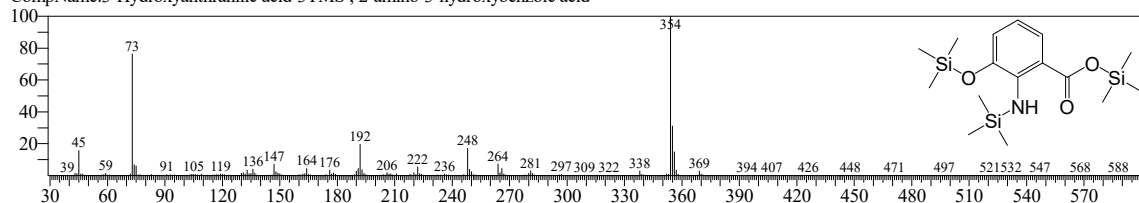RawMode:Averaged 29.320-29.330(4965-4967) BasePeak:73.10(996)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:354 Library:OA_TMS_DB5_67min_V3.lib
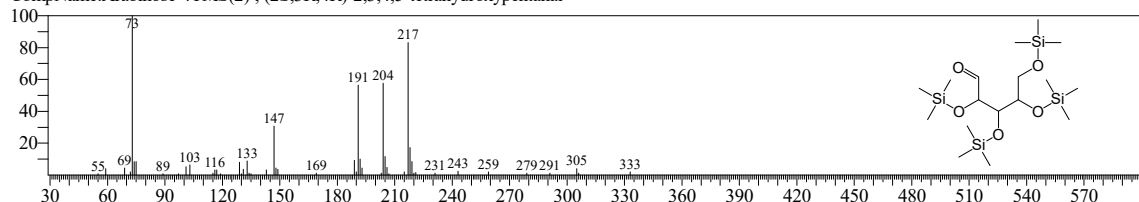SI:38 Formula:C16H31NO3Si3 CAS:548-93-6 MolWeight:369 RetIndex:1886
CompName:3-Hydroxyanthranilic acid-3TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:2 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
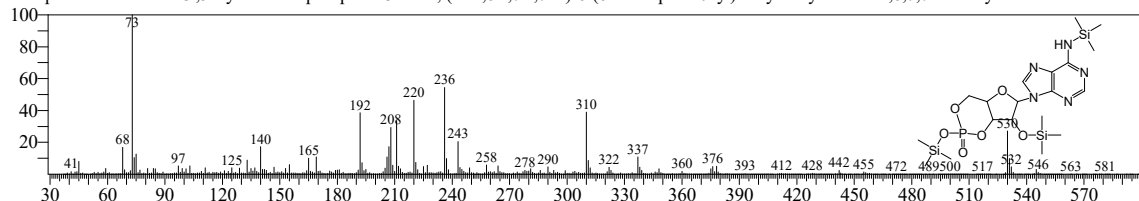SI:38 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

Hit#:3 Entry:566 Library:OA_TMS_DB5_67min_V3.lib
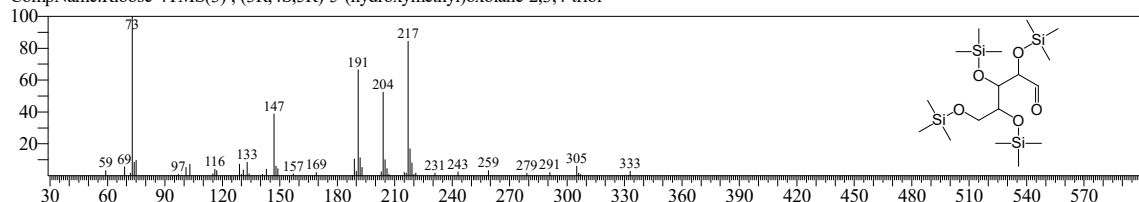SI:36 Formula:C19H36N5O6PSi3 CAS:60-92-4 MolWeight:545 RetIndex:3138
CompName:Adenosine 3',5'-cyclic monophosphate-3TMS ; (4aR,6R,7R,7aS)-6-(6-aminopurin-9-yl)-2-hydroxy-2-oxo-4a,6,7,7a-tetrahydro-4H-fur

Hit#:4 Entry:236 Library:OA_TMS_DB5_67min_V3.lib
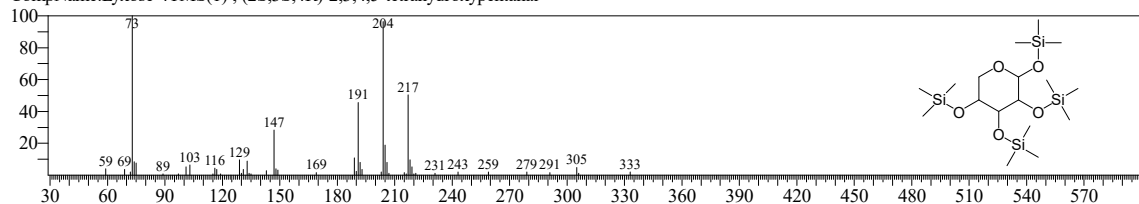SI:36 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1673
CompName:Ribose-4TMS(3) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

Hit#:5 Entry:205 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1624
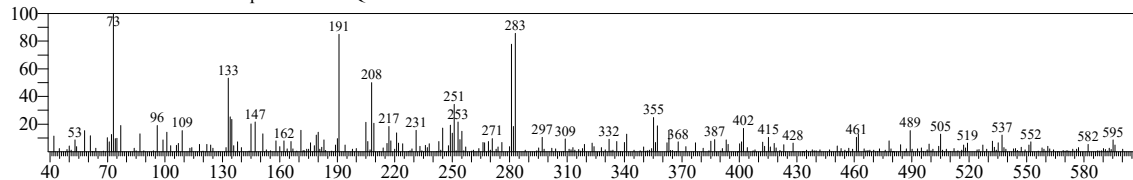CompName:Lyxose-4TMS(1) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal

TNAU

<< Target >>
Line#:12   R.Time:29.405(Scan#:4982) MassPeaks:297
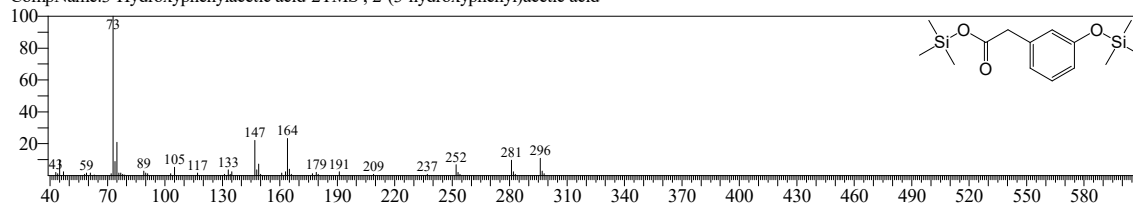RawMode:Averaged 29.400-29.410(4981-4983) BasePeak:73.05(878)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
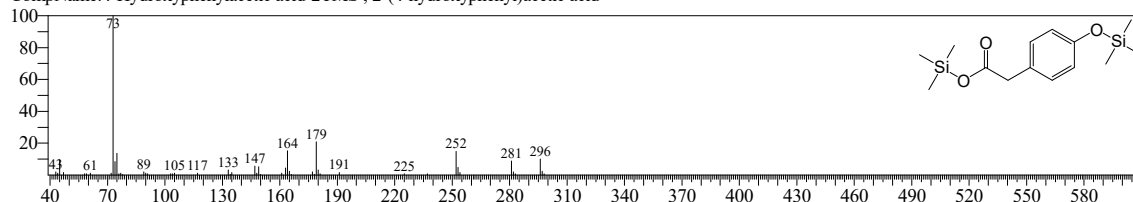SI:41 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

Hit#:2 Entry:220 Library:OA_TMS_DB5_67min_V3.lib
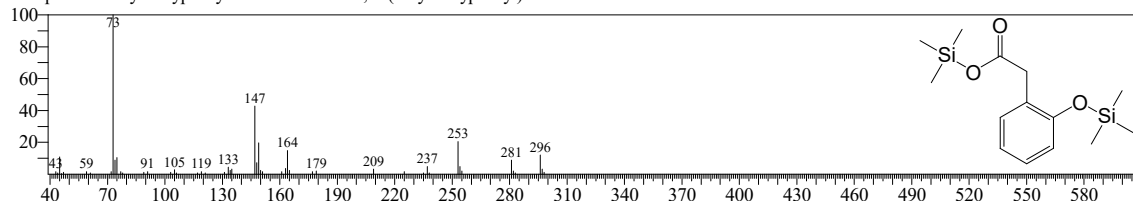SI:40 Formula:C14H24O3Si2 CAS:156-38-7 MolWeight:296 RetIndex:1647
CompName:4-Hydroxyphenylacetic acid-2TMS ; 2-(4-hydroxyphenyl)acetic acid

Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
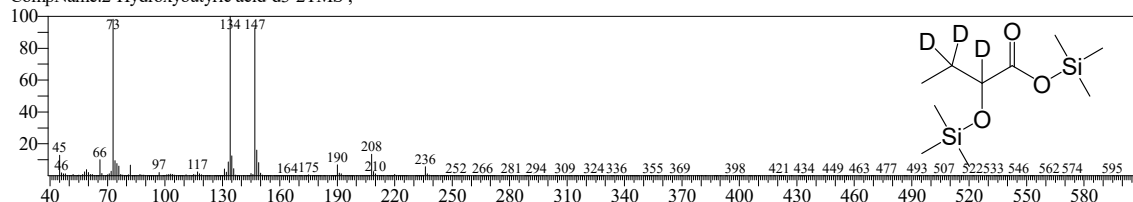SI:40 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

Hit#:4 Entry:25 Library:OA_TMS_DB5_67min_V3.lib
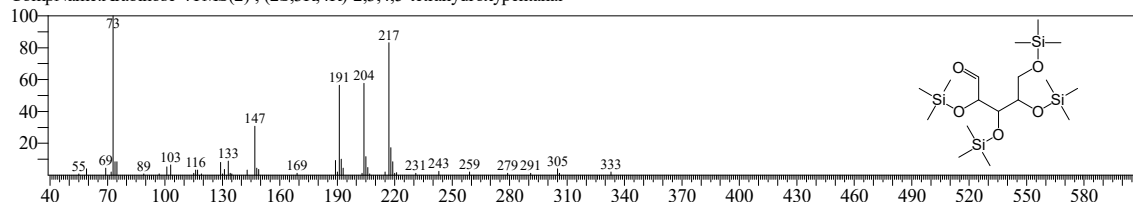SI:39 Formula: CAS:0-00-0 MolWeight:251 RetIndex:1130
CompName:2-Hydroxybutyric acid-d3-2TMS ;

Hit#:5 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal
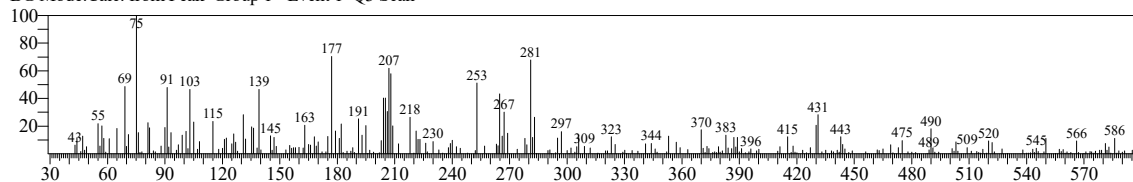
TNAU

<< Target >>
Line#:13 R.Time:29.540(Scan#:5009) MassPeaks:287
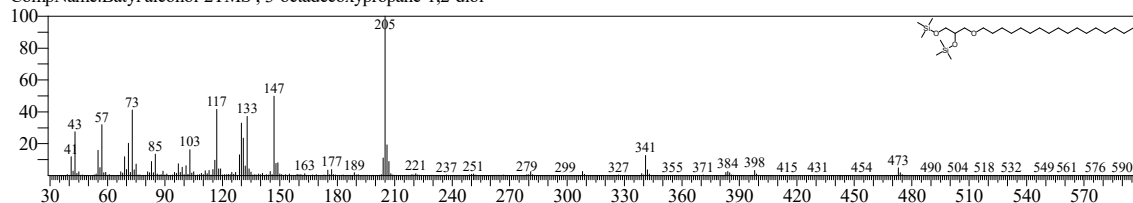RawMode:Averaged 29.535-29.545(5008-5010) BasePeak:75.05(798)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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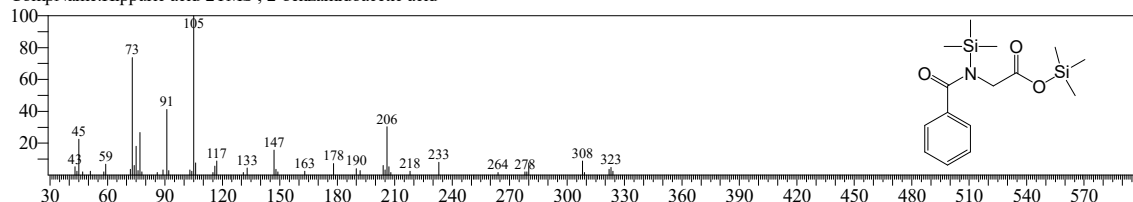SI:32 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

Hit#:2 Entry:307 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C15H25NO3Si2 CAS:66407-11-2 MolWeight:323 RetIndex:1819
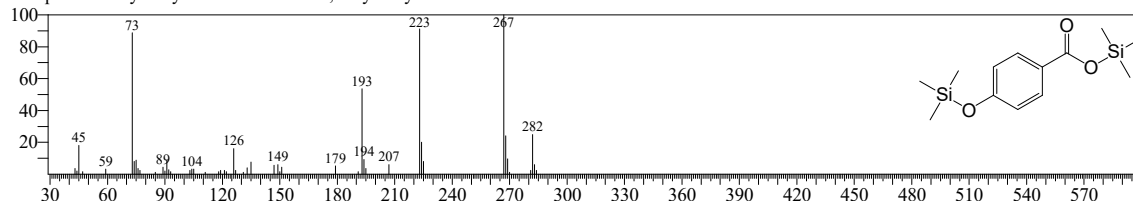CompName:Hippuric acid-2TMS ; 2-benzamidoacetic acid

Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
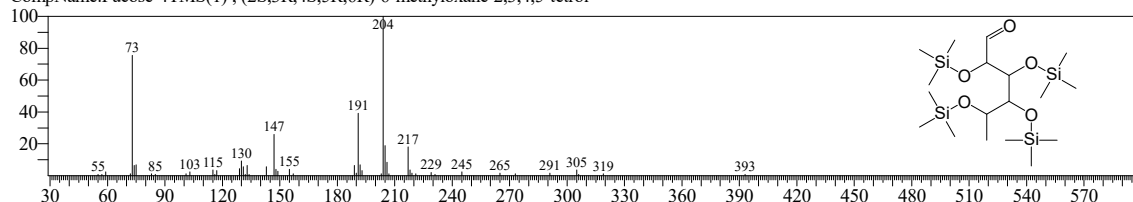CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:4 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
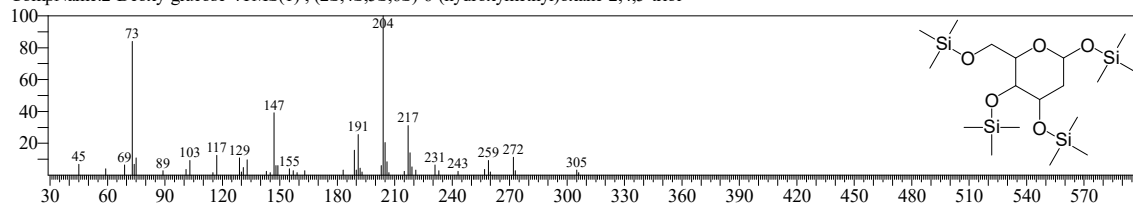CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

Hit#:5 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:27 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
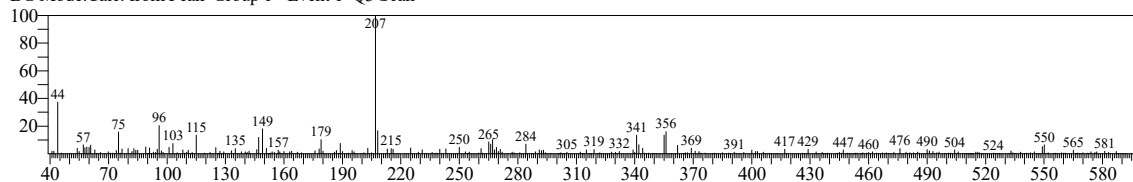
TNAU

<< Target >>
Line#:14 R.Time:29.730(Scan#:5047) MassPeaks:295
RawMode:Averaged 29.725-29.735(5046-5048) BasePeak:207.00(2884)
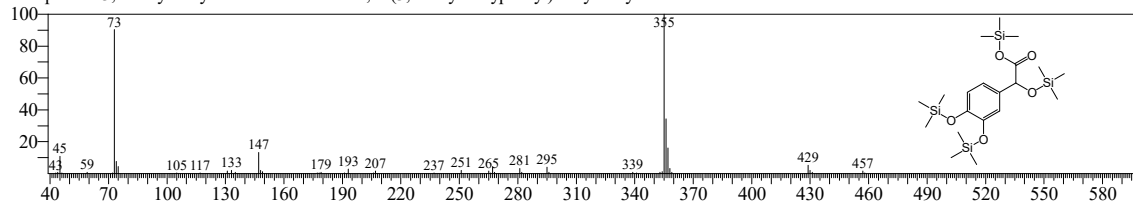BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
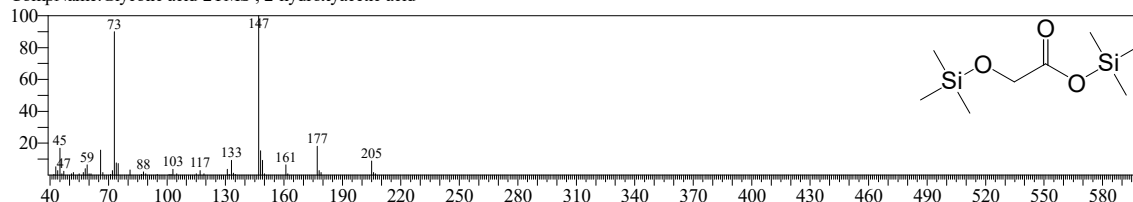SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
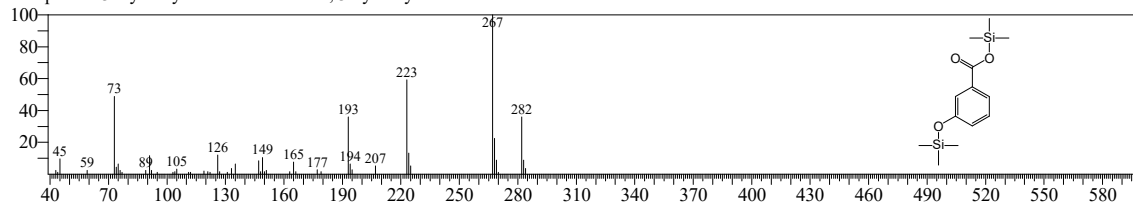CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
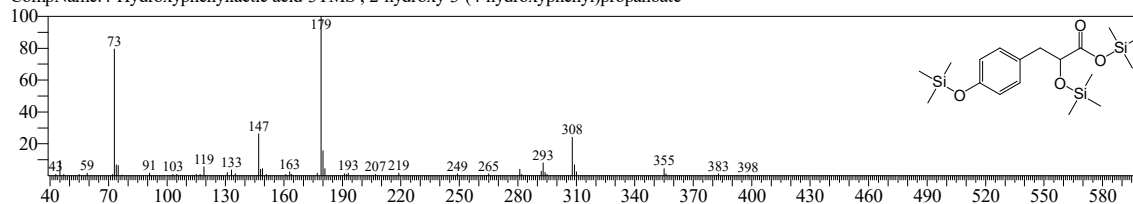SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
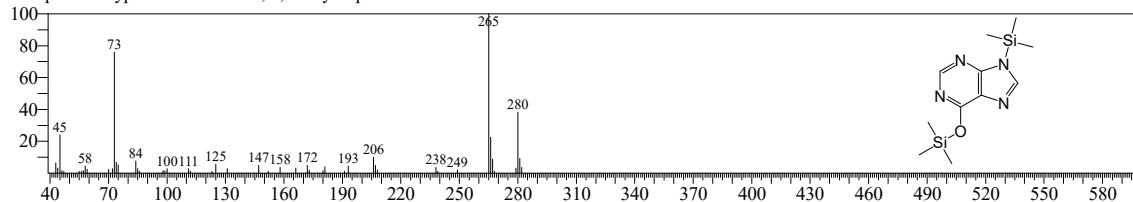SI:29 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

Hit#:5 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
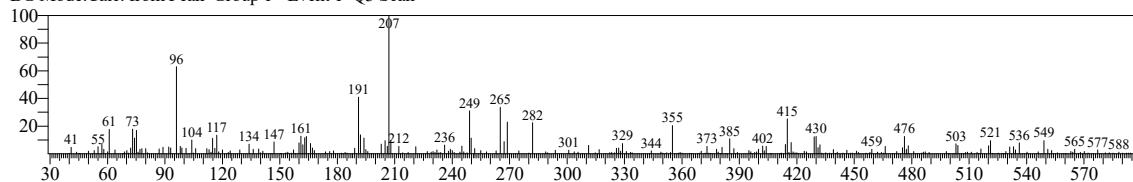CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

TNAU

<< Target >>
Line#:15 R.Time:31.165(Scan#:5334) MassPeaks:270
RawMode:Averaged 31.160-31.170(5333-5335) BasePeak:207.05(1343)
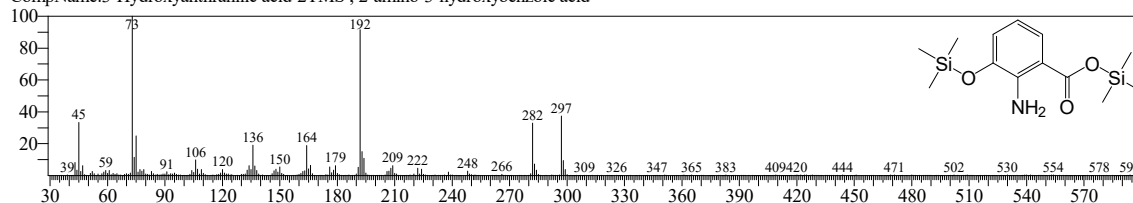BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
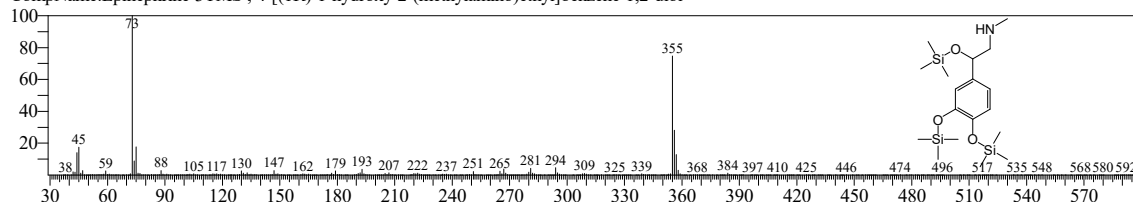SI:36 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
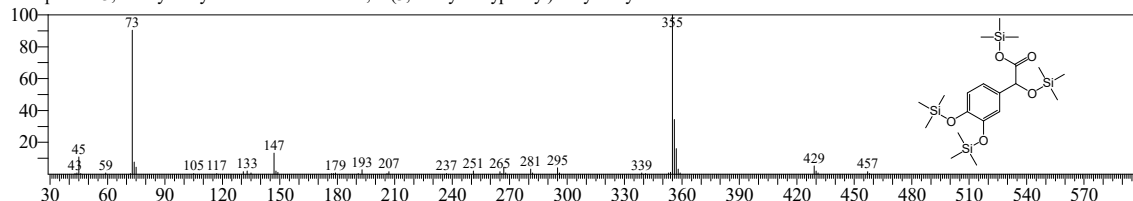SI:33 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
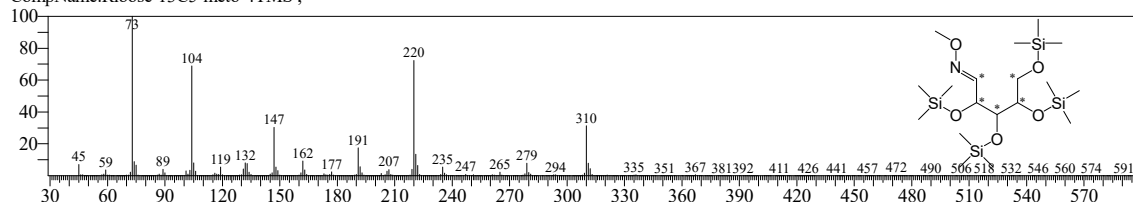SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:4 Entry:256 Library:OA_TMS_DB5_67min_V3.lib
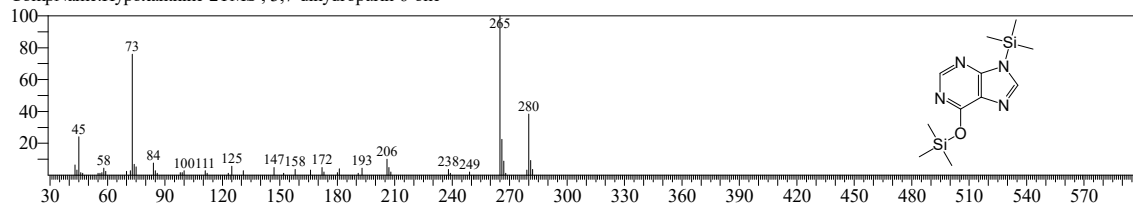SI:32 Formula: CAS:0-00-0 MolWeight:472 RetIndex:1698
CompName:Ribose-13C5-meto-4TMS ;

Hit#:5 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one
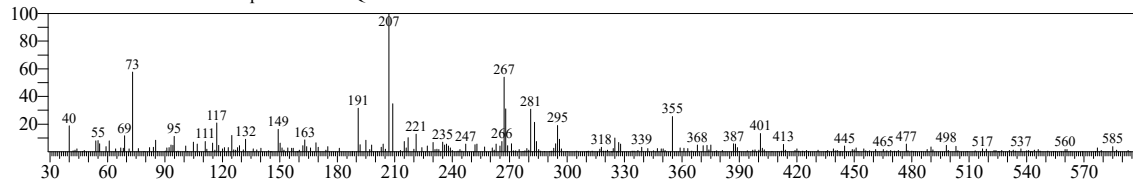
TNAU

<< Target >>
Line#:16 R.Time:31.325(Scan#:5366) MassPeaks:270
RawMode:Averaged 31.320-31.330(5365-5367) BasePeak:207.00(1452)
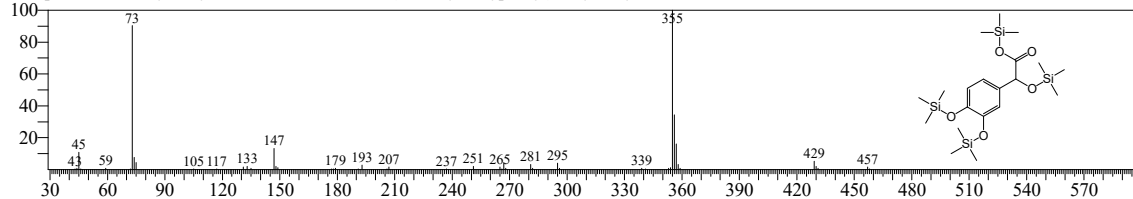BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
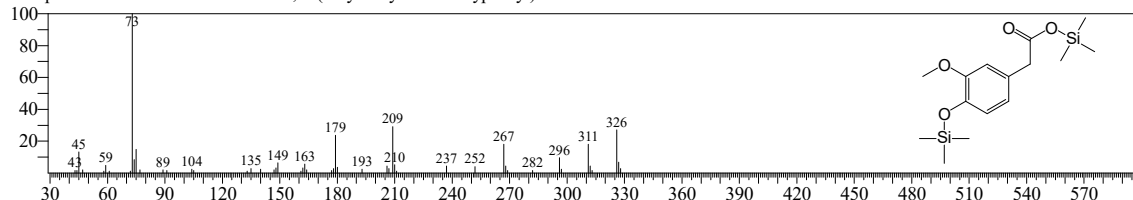SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
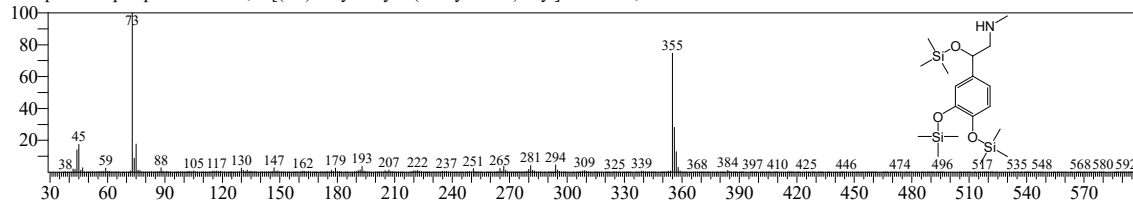CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
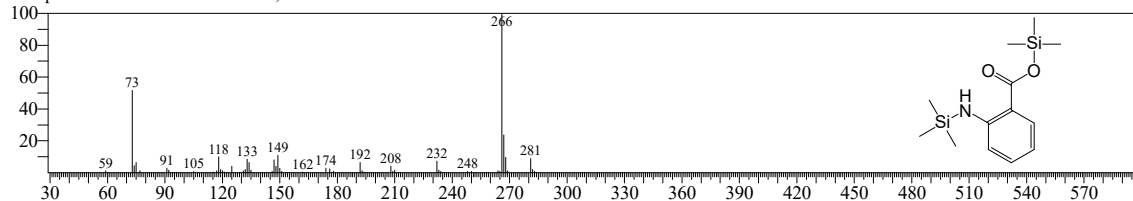SI:37 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
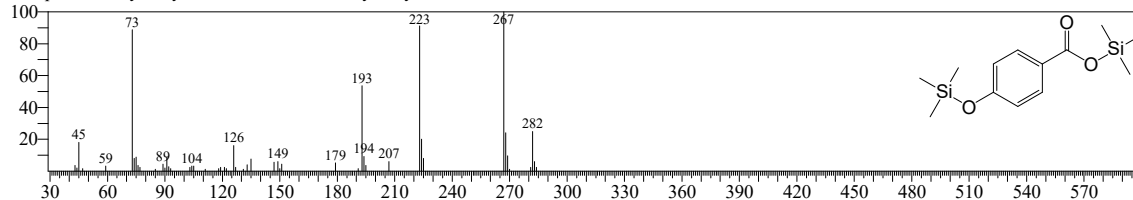SI:37 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
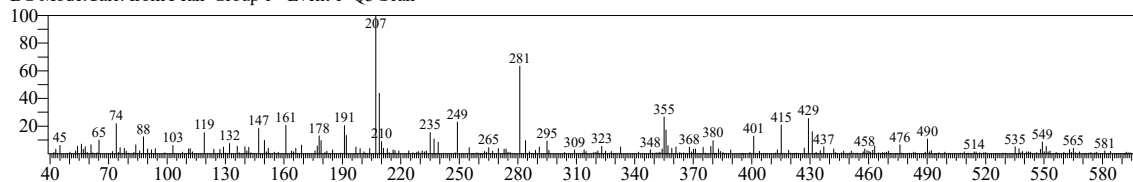CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

TNAU

<< Target >>
Line#:17 R.Time:31.860(Scan#:5473) MassPeaks:273
RawMode:Averaged 31.855-31.865(5472-5474) BasePeak:207.05(1534)
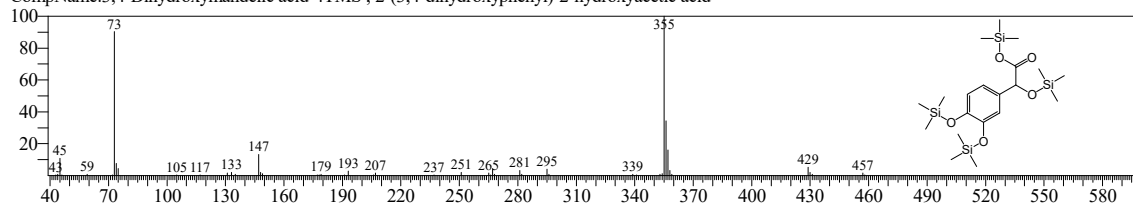BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
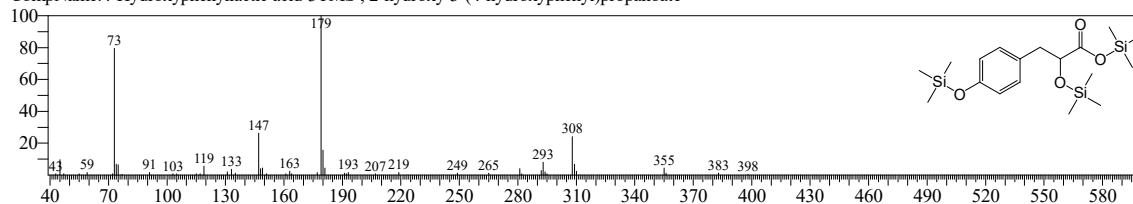SI:36 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
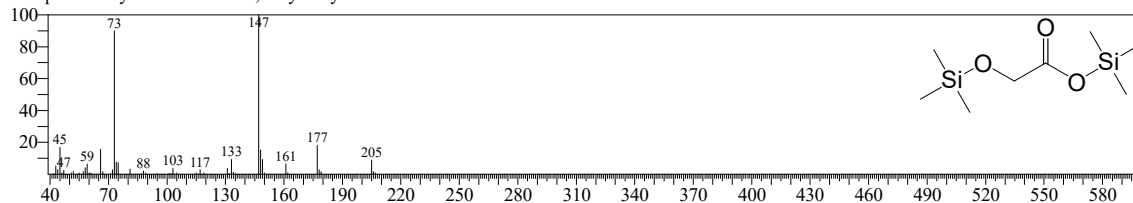CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

Hit#:3 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
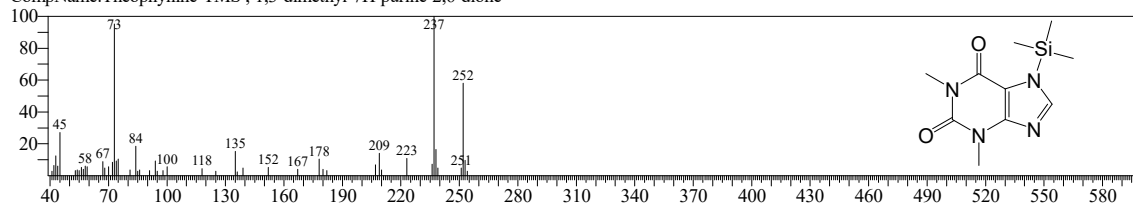SI:25 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid

Hit#:4 Entry:395 Library:OA_TMS_DB5_67min_V3.lib
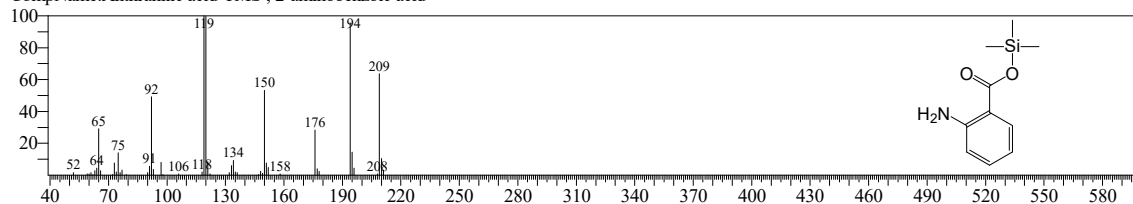SI:25 Formula:C10H16N4O2Si CAS:58-55-9 MolWeight:252 RetIndex:1936
CompName:Theophylline-TMS ; 1,3-dimethyl-7H-purine-2,6-dione

Hit#:5 Entry:142 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C10H15NO2Si CAS:118-92-3 MolWeight:209 RetIndex:1495
CompName:Anthranilic acid-TMS ; 2-aminobenzoic acid
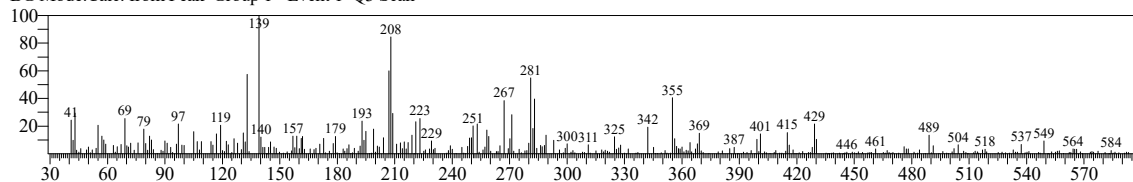
TNAU

<< Target >>
Line#:18 R.Time:31.900(Scan#:5481) MassPeaks:351
RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.20(1427)
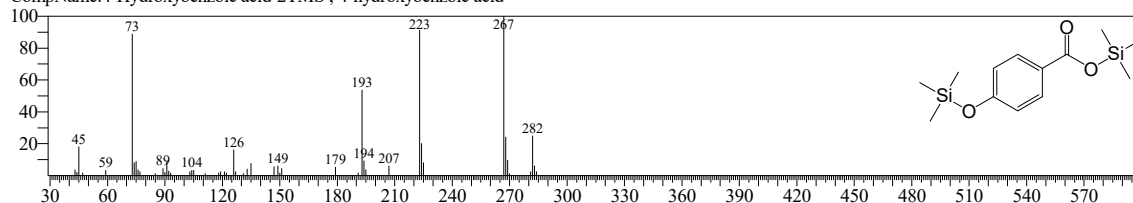BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
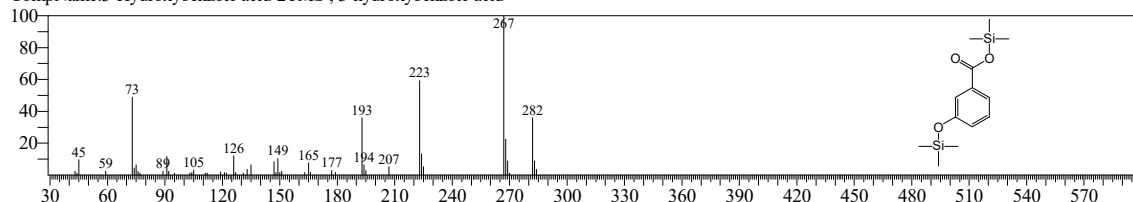SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

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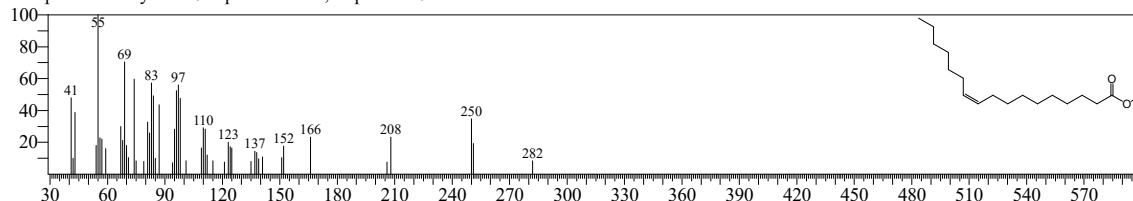CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

Hit#:3 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:27 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
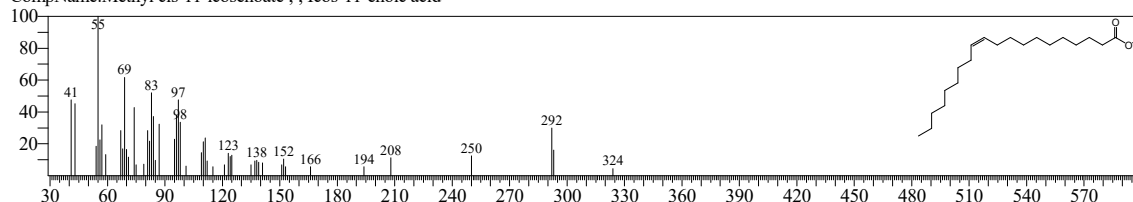CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

Hit#:4 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:25 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
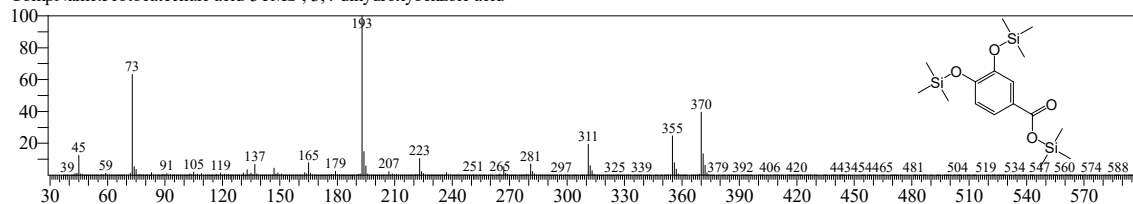CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid

Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
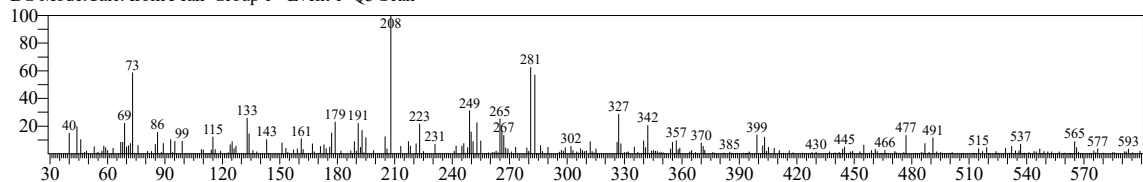CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

TNAU

<< Target >>
Line#:19 R.Time:31.970(Scan#:5495) MassPeaks:268
RawMode:Averaged 31.965-31.975(5494-5496) BasePeak:208.05(1068)
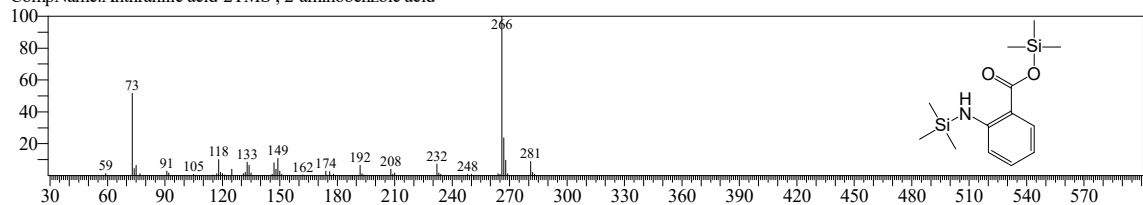BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
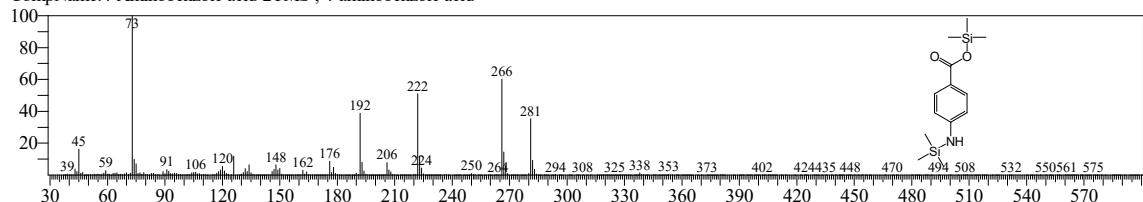CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

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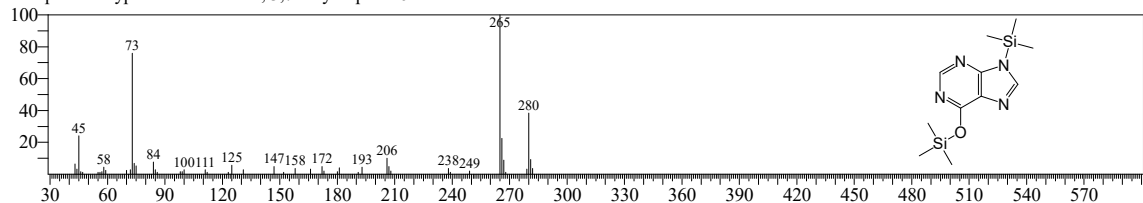CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

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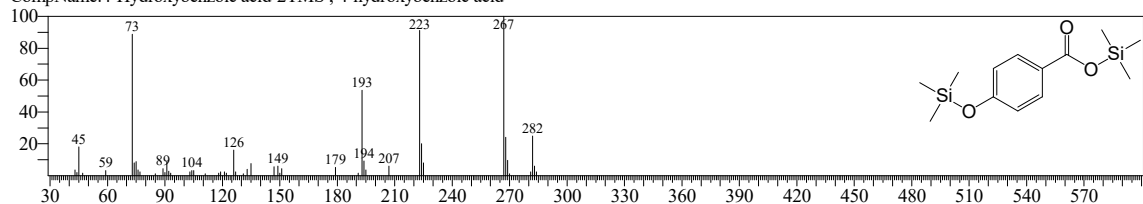CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

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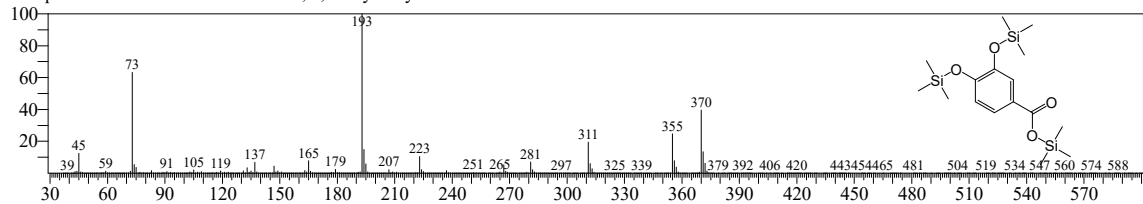SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
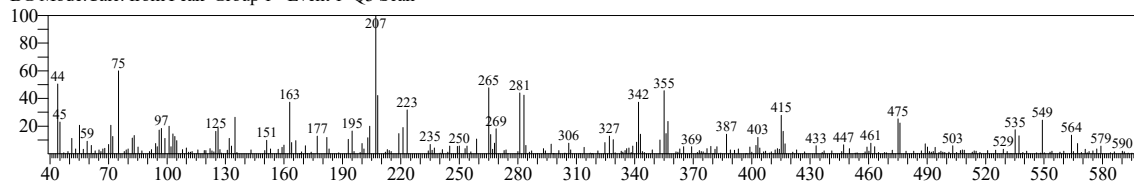CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

TNAU

<< Target >>
Line#:20 R.Time:32.305(Scan#:5562) MassPeaks:277
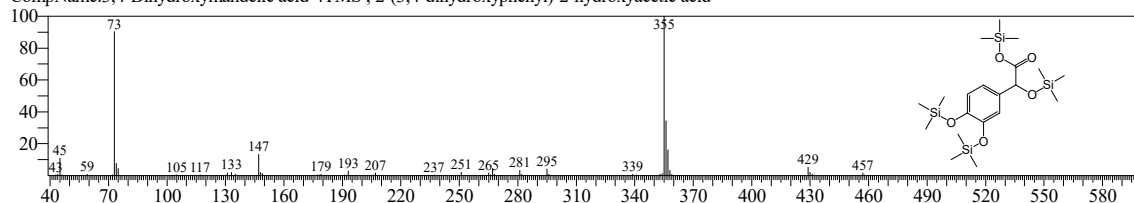RawMode:Averaged 32.300-32.310(5561-5563) BasePeak:207.05(891)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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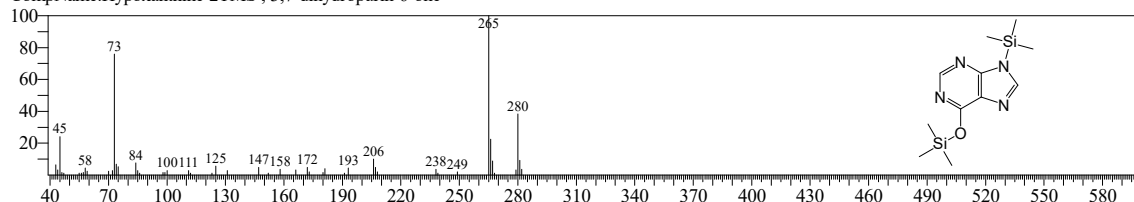SI:28 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
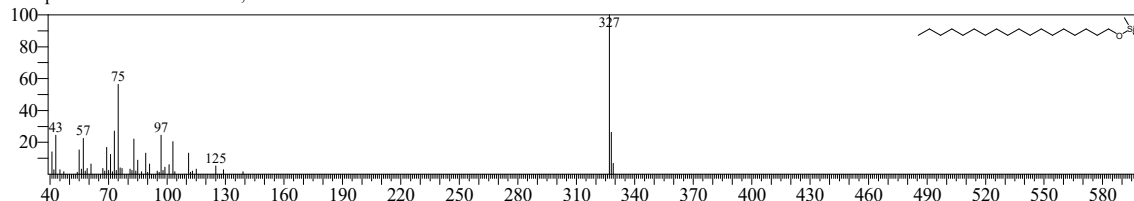SI:27 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:3 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
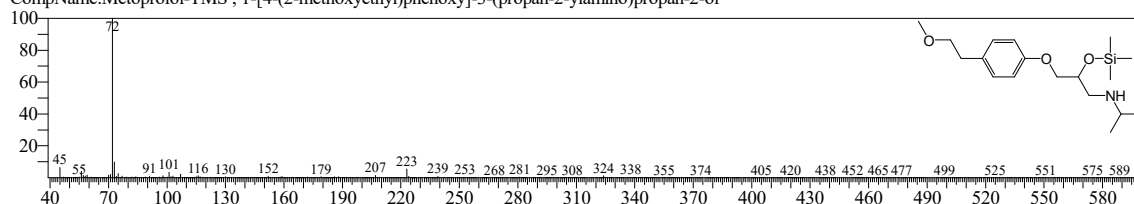SI:27 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol

Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C18H33NO3Si CAS:37350-58-6 MolWeight:339 RetIndex:2094
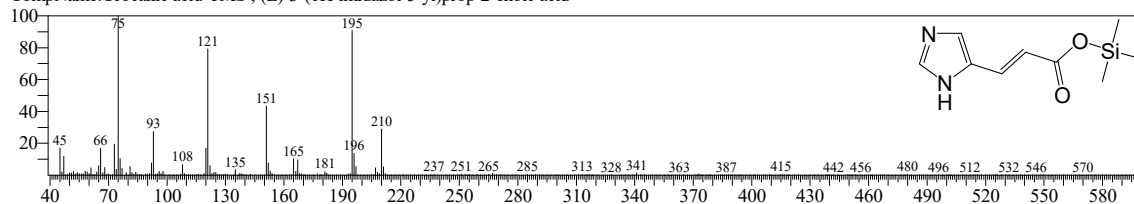CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol

Hit#:5 Entry:361 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C9H14N2O2Si CAS:104-98-3 MolWeight:210 RetIndex:1896
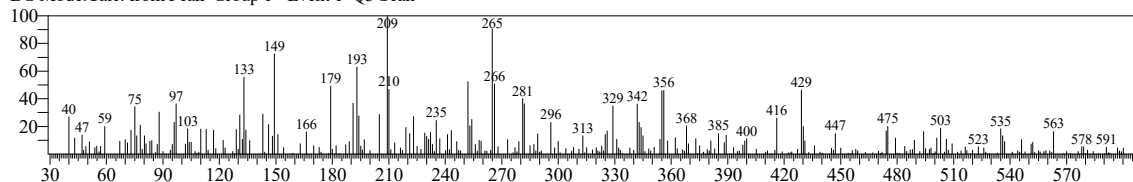CompName:Urocanic acid-TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

TNAU

<< Target >>
Line#:21 R.Time:32.850(Scan#:5671) MassPeaks:301
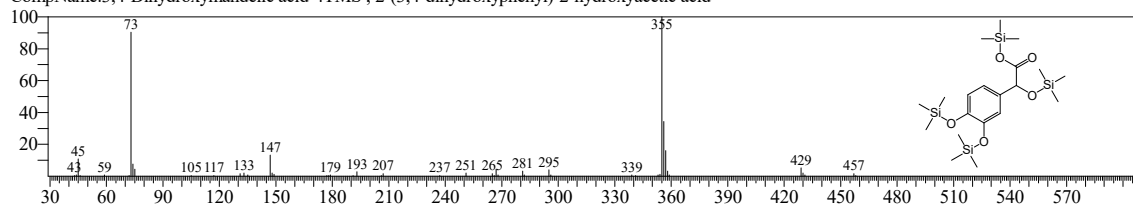RawMode:Averaged 32.845-32.855(5670-5672) BasePeak:209.10(626)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
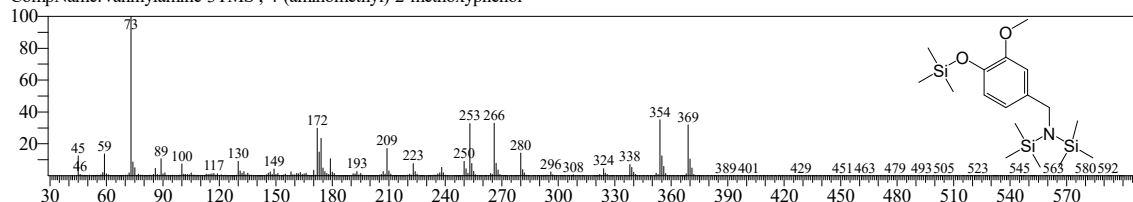SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

Hit#:2 Entry:368 Library:OA_TMS_DB5_67min_V3.lib
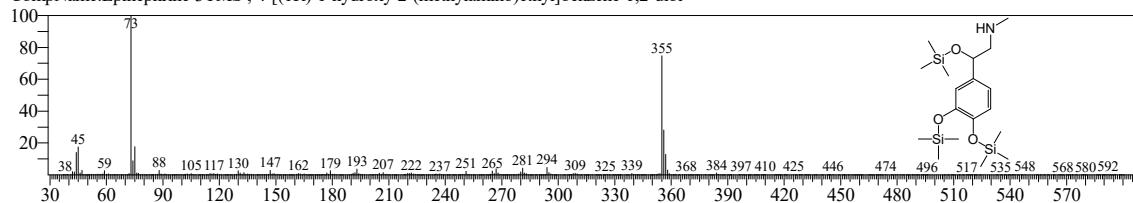SI:31 Formula:C17H35NO2Si3 CAS:1196-92-5 MolWeight:369 RetIndex:1899
CompName:Vanillylamine-3TMS ; 4-(aminomethyl)-2-methoxyphenol

Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
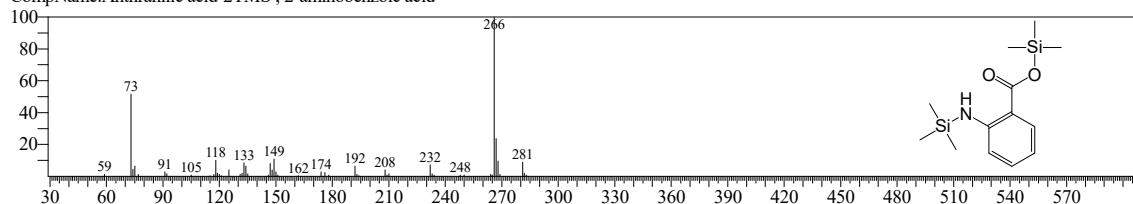SI:31 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

Hit#:4 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#:5 Entry:420 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973
CompName:2-Hydroxyhippuric acid-3TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid