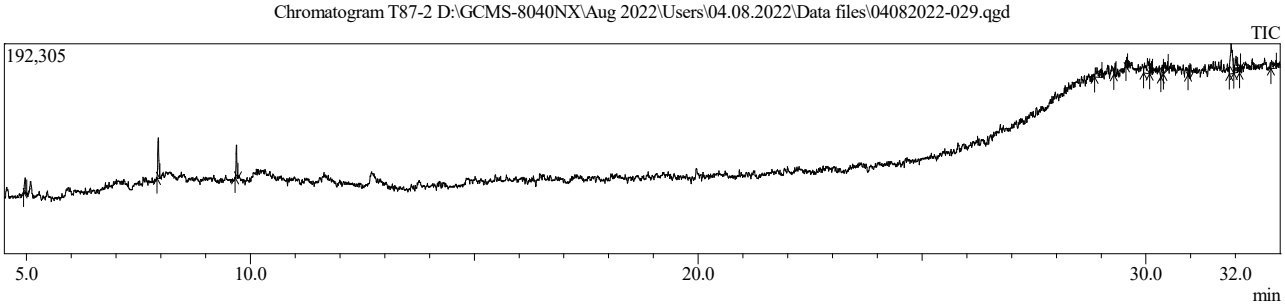
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 11:05:27 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T87-2
Sample ID	: T87-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 28
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-029.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-029.qgd
Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Org Method File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Method file\27072022_methodfile.qgm
Report File	:
Tuning File	: D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 04082022.qgt
[Comment]	
Jerry samples	
Modified by	: Admin
Modified	: 05-Aug-22 4:45:51 PM

Chromatogram T87-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-029.qgd



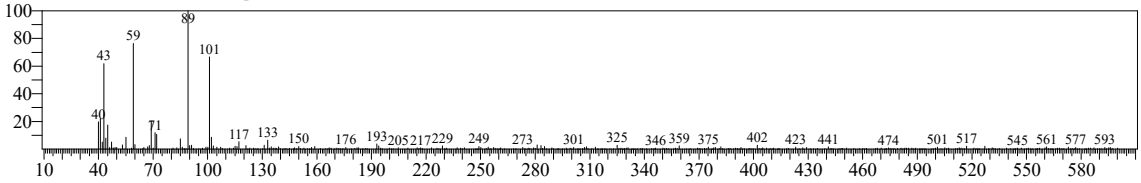
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.969	23743	4.72	14114	6.46	1.68	74	2-Propanol, 1,1'-oxybis-
2	7.940	62547	12.43	37011	16.95	1.69	91	Undecane
3	9.688	42271	8.40	29843	13.67	1.42	89	Undecane
4	28.907	41795	8.31	8484	3.89	4.93	23	3,4-Dihydroxymandelic acid-4TMS
5	29.313	15624	3.11	11400	5.22	1.37	33	3,4-Dihydroxymandelic acid-4TMS
6	29.573	9603	1.91	9129	4.18	1.05	37	Lyxose-4TMS(2)
7	30.035	58294	11.59	13708	6.28	4.25	26	Hippuric acid-TMS
8	30.127	21860	4.35	11470	5.25	1.91	26	Hypoxanthine-2TMS
9	30.360	20246	4.02	9535	4.37	2.12	40	Ribose-4TMS(4)
10	30.480	30074	5.98	7760	3.55	3.88	25	2-Deoxy-glucose-4TMS(1)
11	30.964	12153	2.42	10778	4.94	1.13	30	4-Hydroxybenzoic acid-2TMS
12	31.902	90756	18.04	27345	12.52	3.32	32	Urocanic acid-2TMS
13	32.015	40892	8.13	14982	6.86	2.73	33	Hypoxanthine-2TMS
14	32.100	3762	0.75	5277	2.42	0.71	32	3,4-Dihydroxymandelic acid-4TMS
15	32.805	29406	5.85	7509	3.44	3.92	47	4-Hydroxybenzoic acid-2TMS
		503026	100.00	218345	100.00			

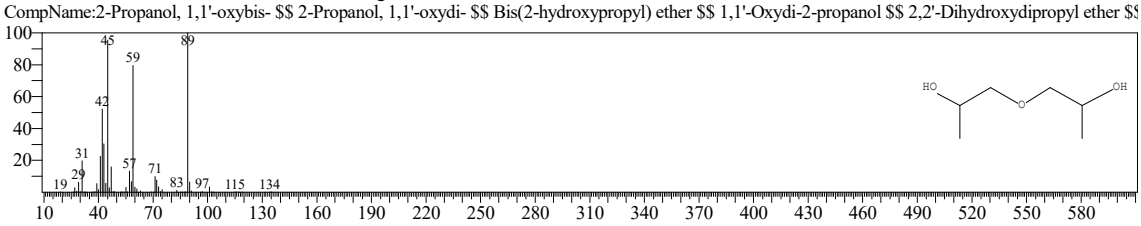
Library

TNAU

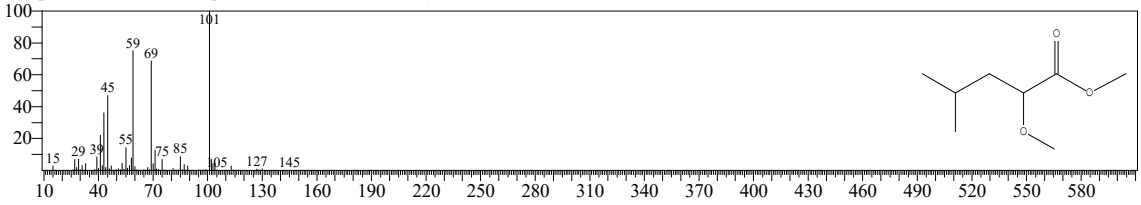
<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:344
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.15(2593)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



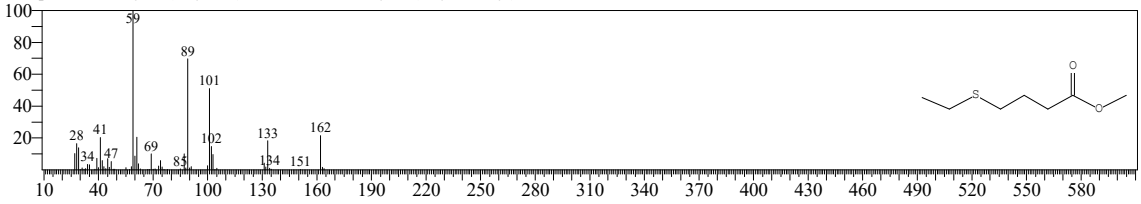
Hit#:1 Entry:7425 Library:NIST20R.lib
SI:74 Formula:C6H14O3 CAS:110-98-5 MolWeight:134 RetIndex:1018
CompName:2-Propanol, 1,1'-oxybis- $$ 2-Propanol, 1,1'-oxydi- $$ Bis(2-hydroxypropyl) ether $$ 1,1'-Oxydi-2-propanol $$ 2,2'-Dihydroxydipropyl ether $$



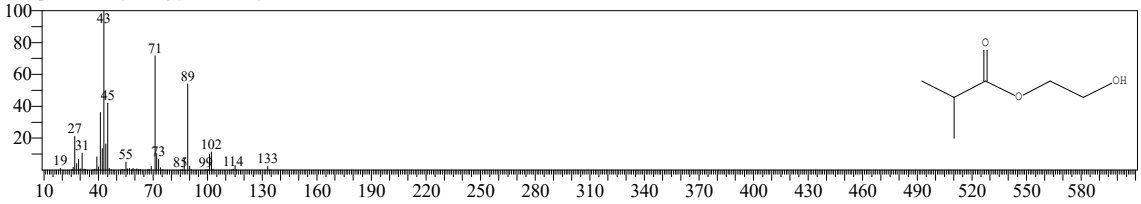
Hit#:2 Entry:22897 Library:NIST20M1.lib
SI:74 Formula:C8H16O3 CAS:0-00-0 MolWeight:160 RetIndex:931
CompName:2-Hydroxyisocaproic acid, methyl ether, methyl ester



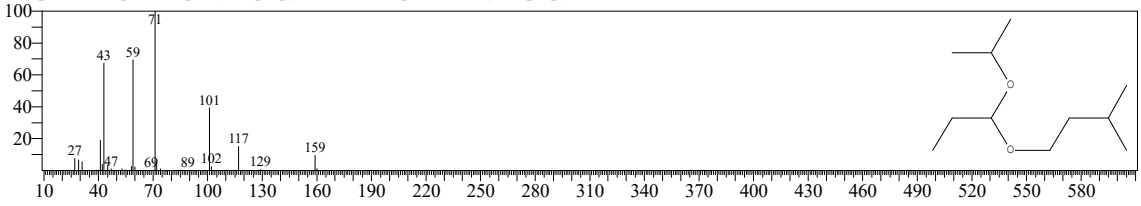
Hit#:3 Entry:23889 Library:NIST20M1.lib
SI:71 Formula:C7H14O2S CAS:0-00-0 MolWeight:162 RetIndex:1135
CompName:Methyl 4-(ethylthio)butanoate $$ Methyl 4-(ethylsulfanyl)butanoate #



Hit#:4 Entry:9217 Library:NIST20M1.lib
SI:70 Formula:C6H12O3 CAS:0-00-0 MolWeight:132 RetIndex:964
CompName:Ethylene glycol isobutyrate

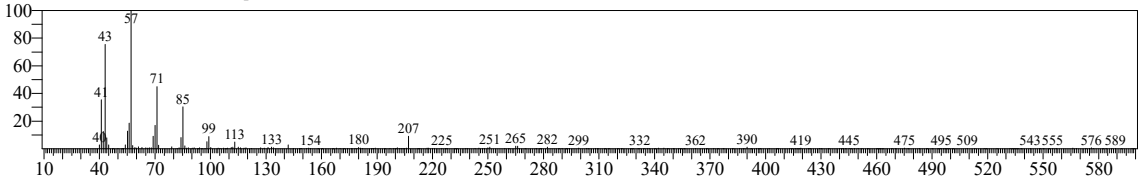


Hit#:5 Entry:43056 Library:NIST20M1.lib
SI:70 Formula:C11H24O2 CAS:0-00-0 MolWeight:188 RetIndex:1074
CompName:Propanal isopentyl isopropyl acetal $$ Propanal isoamyl isopropyl acetal

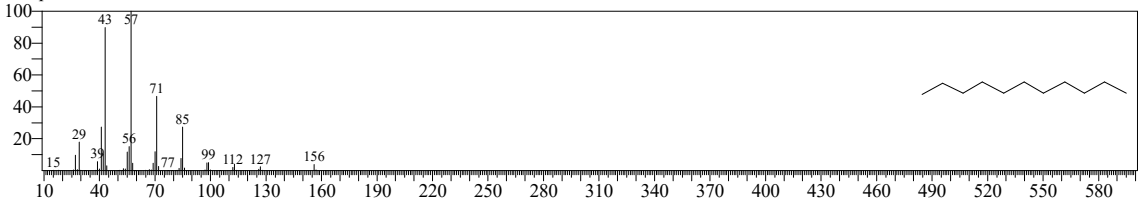


TNAU

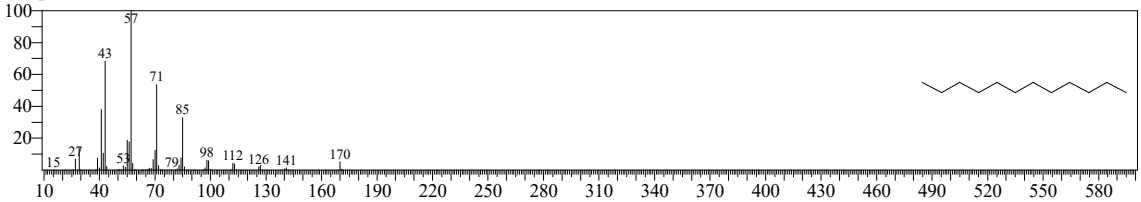
<< Target >>
Line#:2 R.Time:7.940(Scan#:689) MassPeaks:240
RawMode:Averaged 7.935-7.945(688-690) BasePeak:57.10(8801)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



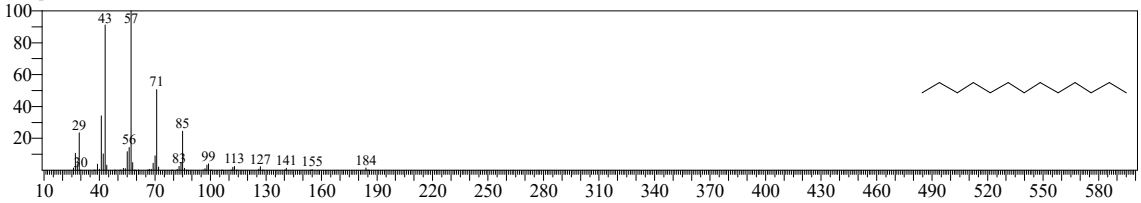
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:91 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



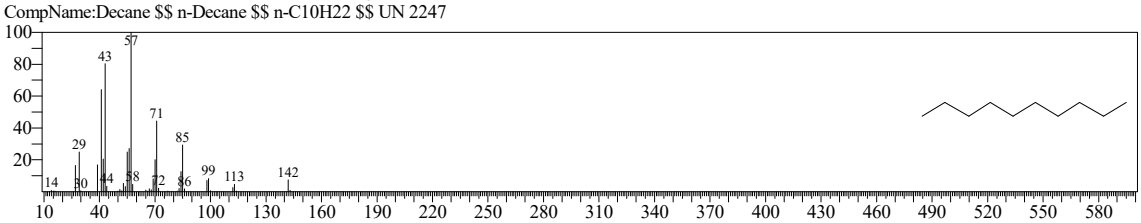
Hit#:2 Entry:30057 Library:NIST20M1.lib
SI:91 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



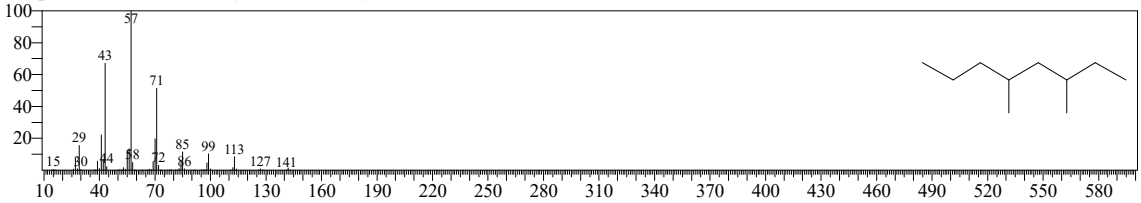
Hit#:3 Entry:40226 Library:NIST20M1.lib
SI:90 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:13604 Library:NIST20M1.lib
SI:90 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

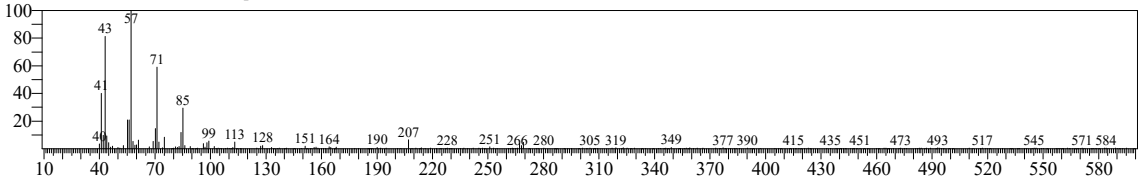


Hit#:5 Entry:13631 Library:NIST20M1.lib
SI:90 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

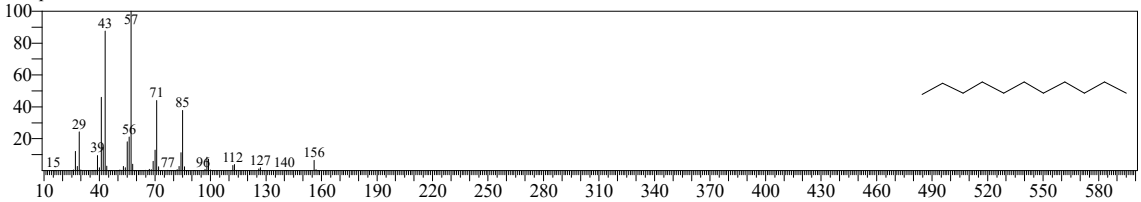


TNAU

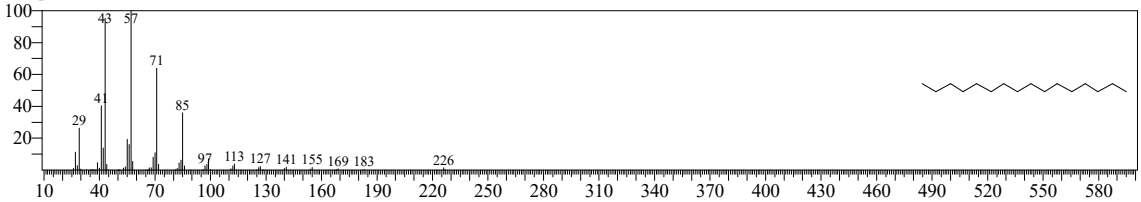
<< Target >>
Line#:3 R.Time:9.690(Scan#:1039) MassPeaks:274
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(5753)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



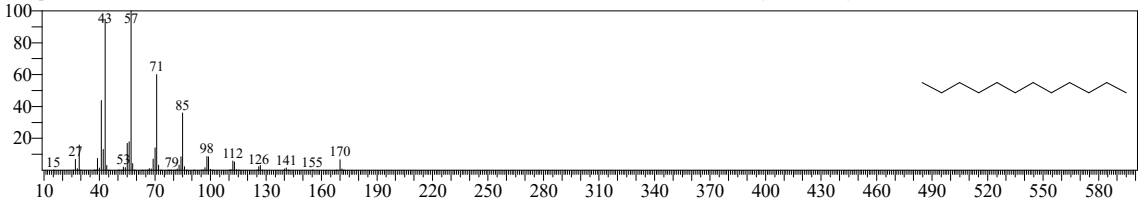
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



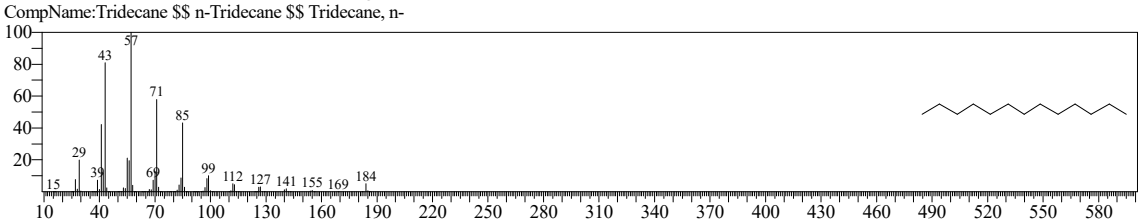
Hit#:2 Entry:27736 Library:NIST20R.lib
SI:89 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane



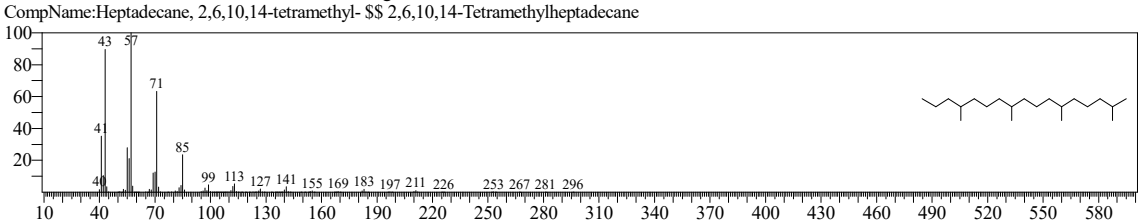
Hit#:3 Entry:16191 Library:NIST20R.lib
SI:89 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:19410 Library:NIST20R.lib
SI:88 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

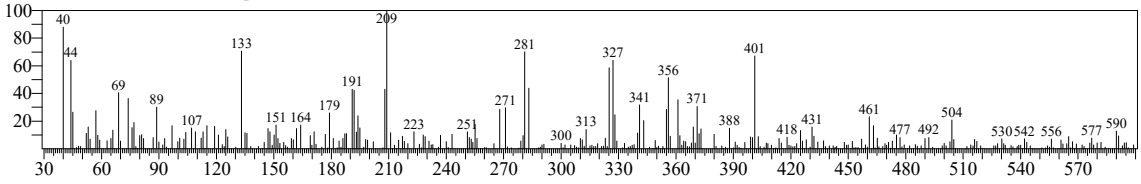


Hit#:5 Entry:159057 Library:NIST20M1.lib
SI:88 Formula:C21H44 CAS:18344-37-1 MolWeight:296 RetIndex:1852
CompName:Heptadecane, 2,6,10,14-tetramethyl- $$ 2,6,10,14-Tetramethylheptadecane

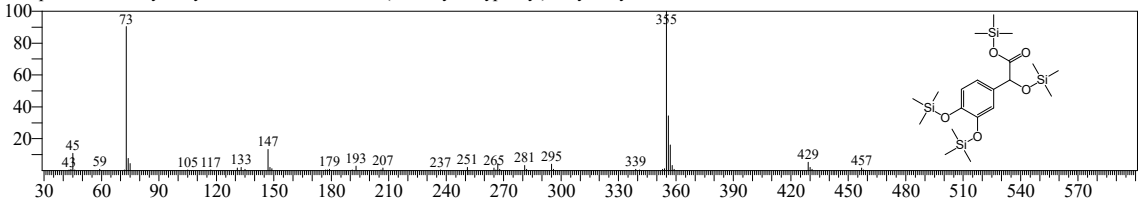


TNAU

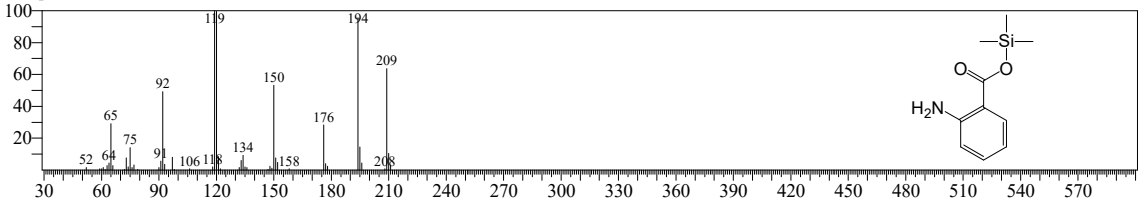
<< Target >>
Line#:4 R.Time:28.905(Scan#:4882) MassPeaks:330
RawMode:Averaged 28.900-28.910(4881-4883) BasePeak:209.00(658)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



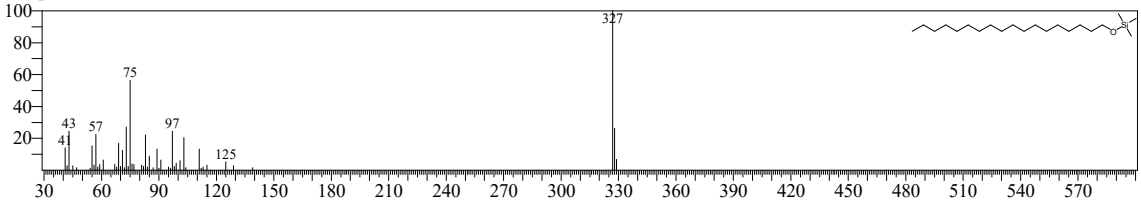
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



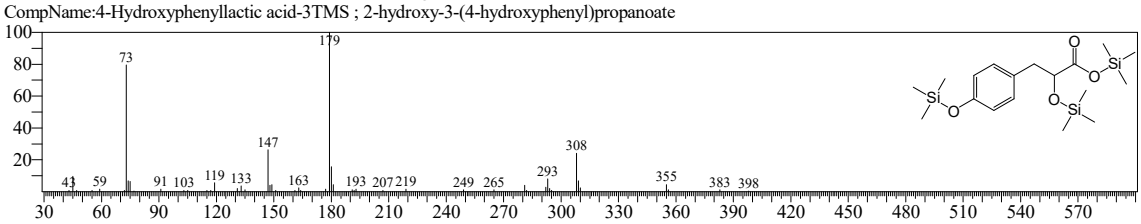
Hit#:2 Entry:142 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C10H15NO2Si CAS:118-92-3 MolWeight:209 RetIndex:1495
CompName:Anthranilic acid-TMS ; 2-aminobenzoic acid



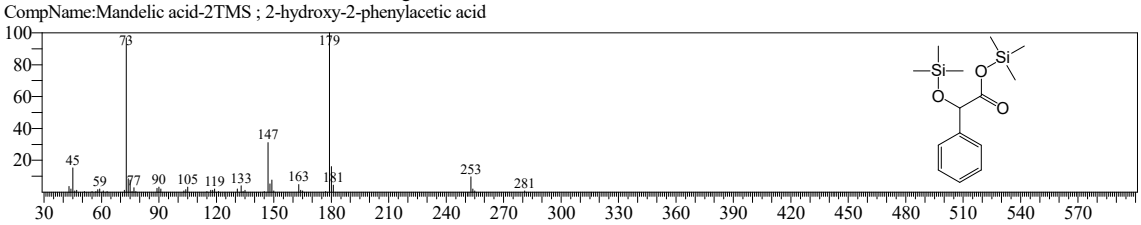
Hit#:3 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol



Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

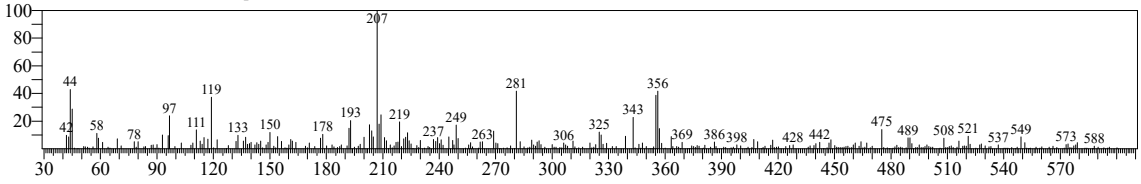


Hit#:5 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid

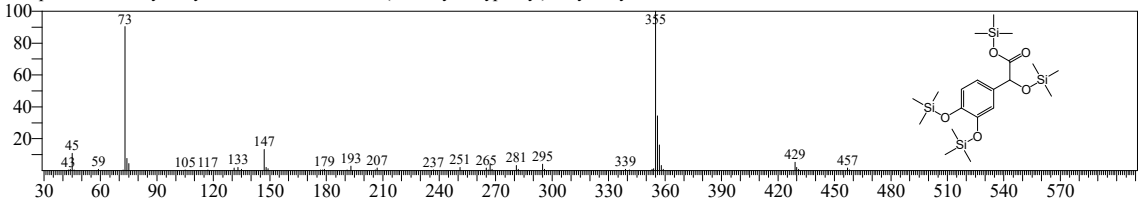


TNAU

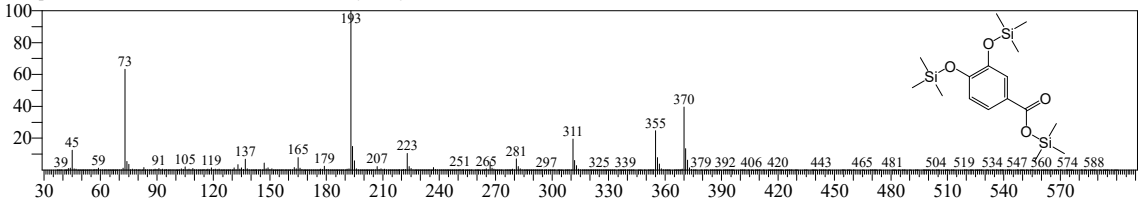
<< Target >>
Line#:5 R.Time:29.315(Scan#:4964) MassPeaks:342
RawMode:Averaged 29.310-29.320(4963-4965) BasePeak:207.05(1341)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



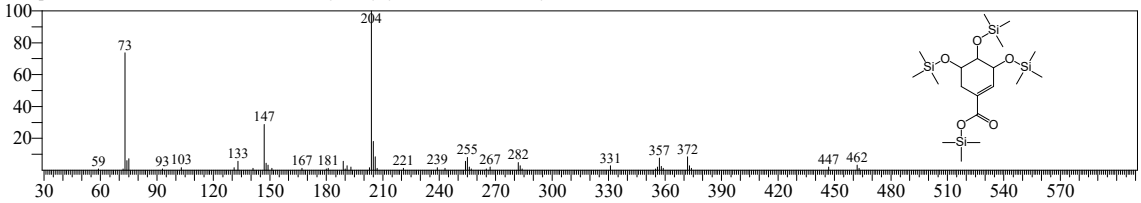
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



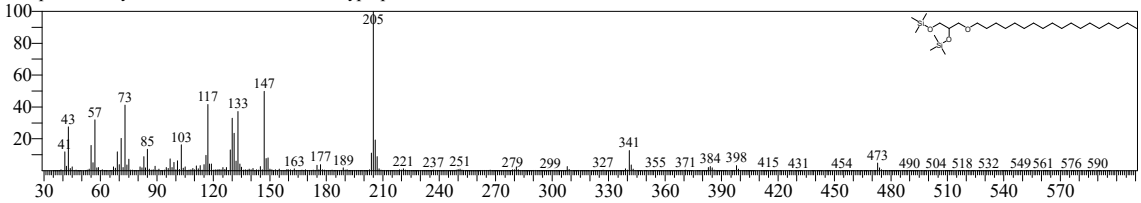
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



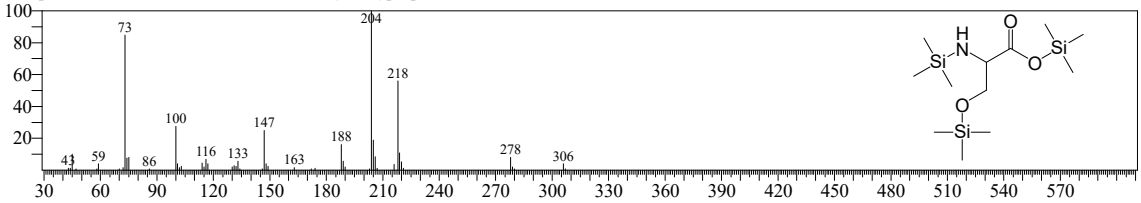
Hit#:3 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

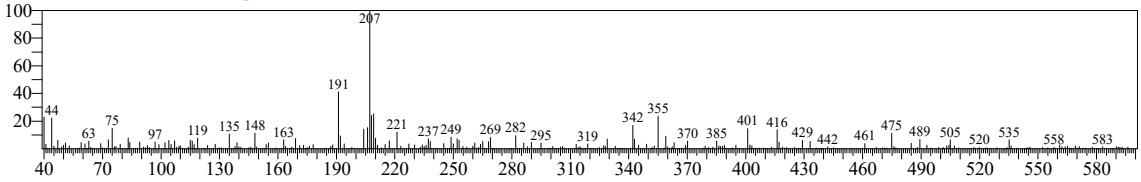


Hit#:5 Entry:104 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C12H31NO3Si3 CAS:56-45-1 MolWeight:321 RetIndex:1367
CompName:Serine-3TMS ; (2S)-2-amino-3-hydroxypropanoic acid

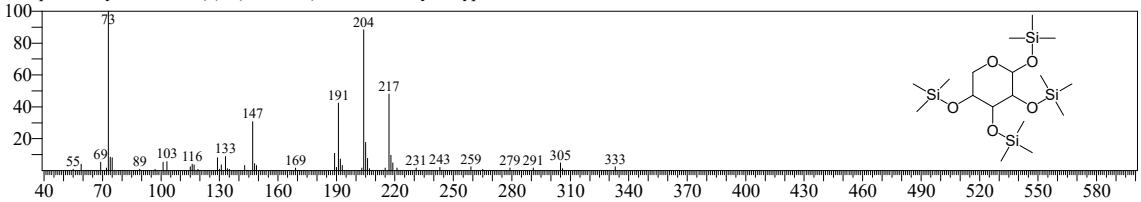


TNAU

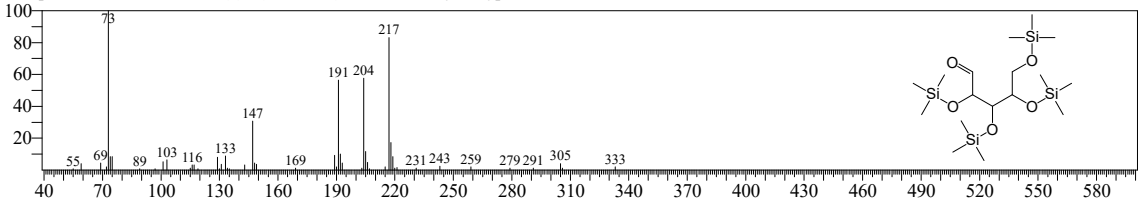
<< Target >>
Line#:6 R.Time:29.575(Scan#:5016) MassPeaks:268
RawMode:Averaged 29.570-29.580(5015-5017) BasePeak:207.05(2087)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



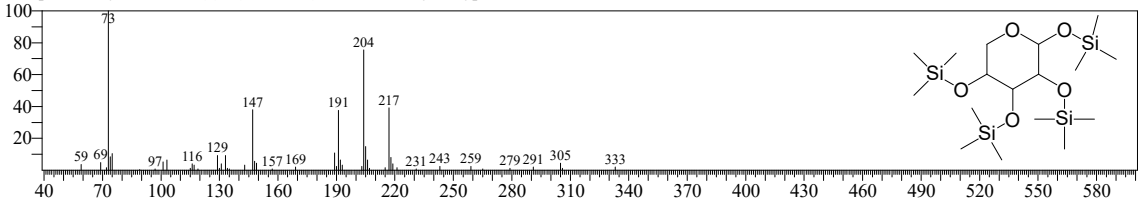
Hit#:1 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



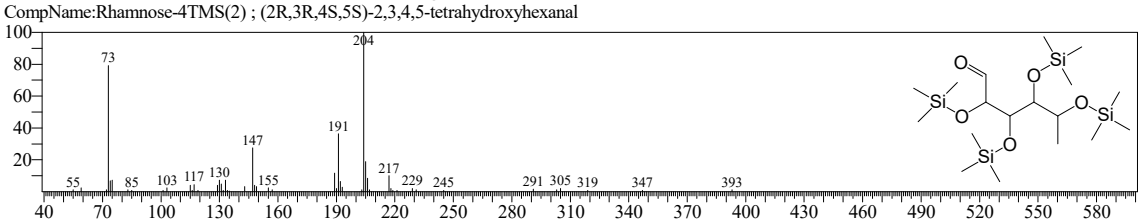
Hit#:2 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



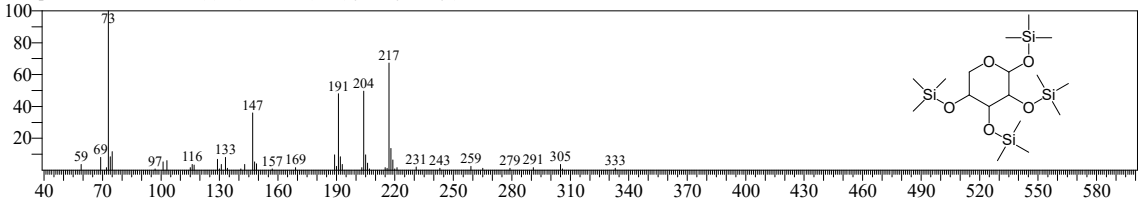
Hit#:3 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:261 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1719
CompName:Rhamnose-4TMS(2) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

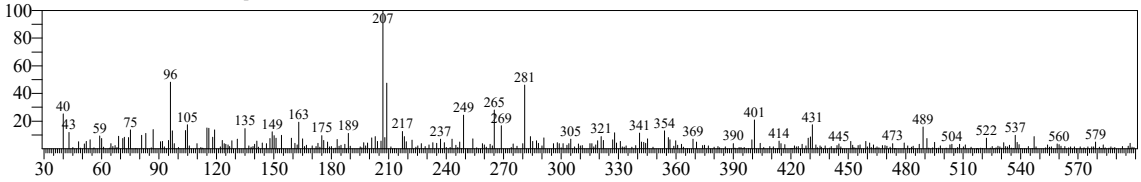


Hit#:5 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

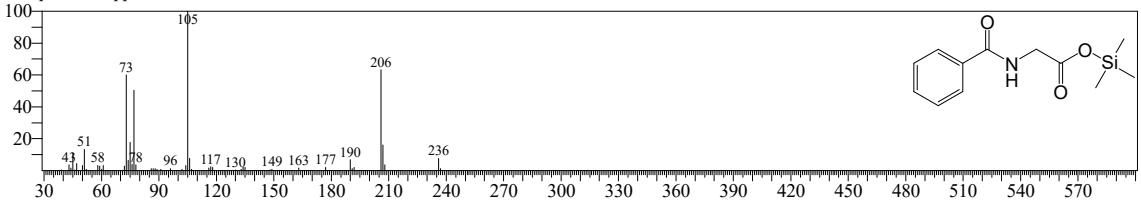


TNAU

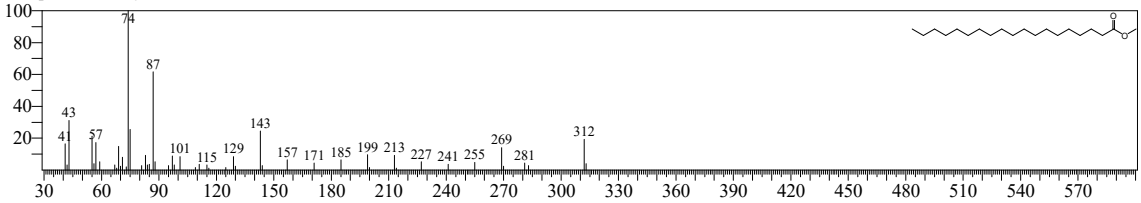
<< Target >>
Line#:7 R.Time:30.035(Scan#:5108) MassPeaks:332
RawMode:Averaged 30.030-30.040(5107-5109) BasePeak:207.00(1294)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



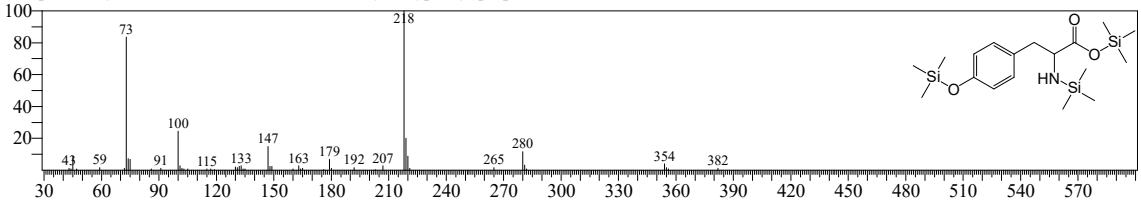
Hit#:1 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



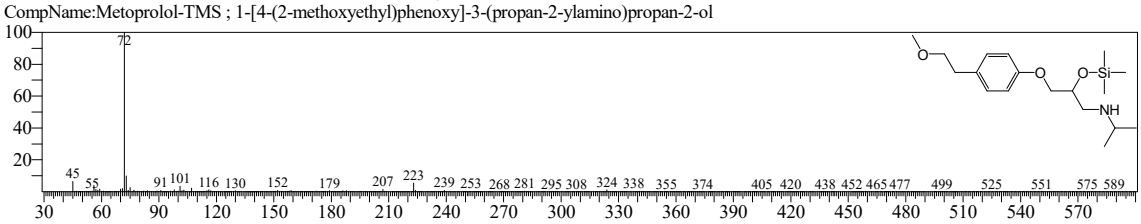
Hit#:2 Entry:19 Library:FA_ME_SP2560_EI_V3.lib
SI:26 Formula:C20H40O2 CAS:646-30-0 MolWeight:312 RetIndex:2699
CompName:Methyl nonadecanoate ; Nonadecanoic acid



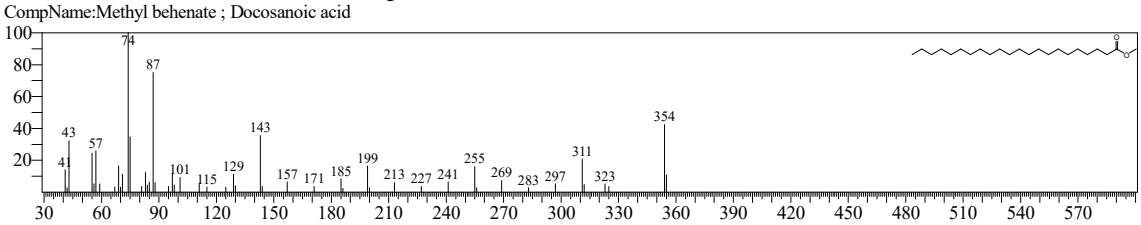
Hit#:3 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid



Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:24 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

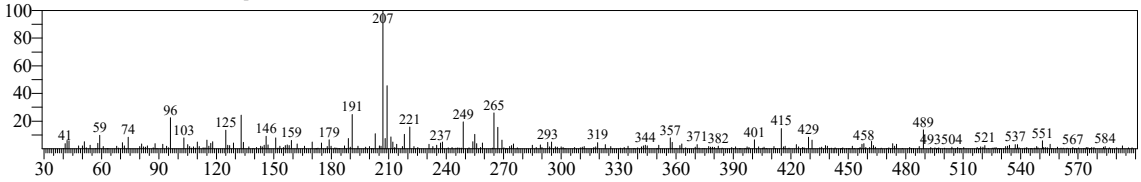


Hit#:5 Entry:28 Library:FA_ME_SP2560_EI_V3.lib
SI:24 Formula:C23H46O2 CAS:112-85-6 MolWeight:354 RetIndex:3005
CompName:Methyl behenate ; Docosanoic acid

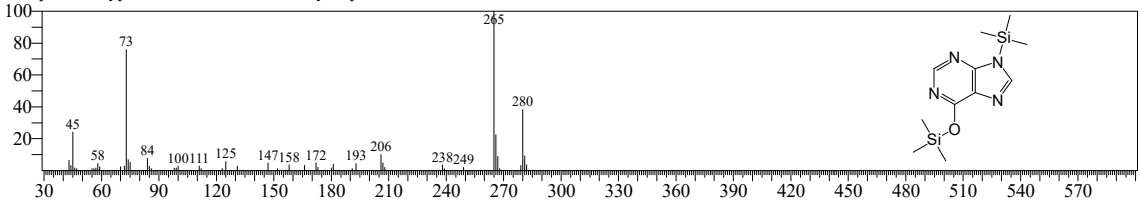


TNAU

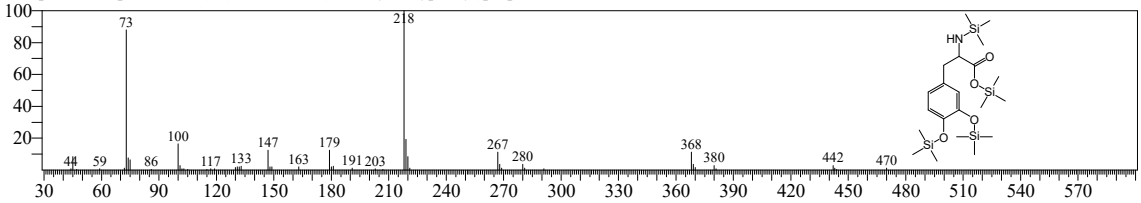
<< Target >>
Line#:8 R.Time:30.125(Scan#:5126) MassPeaks:297
RawMode:Averaged 30.120-30.130(5125-5127) BasePeak:207.05(2220)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



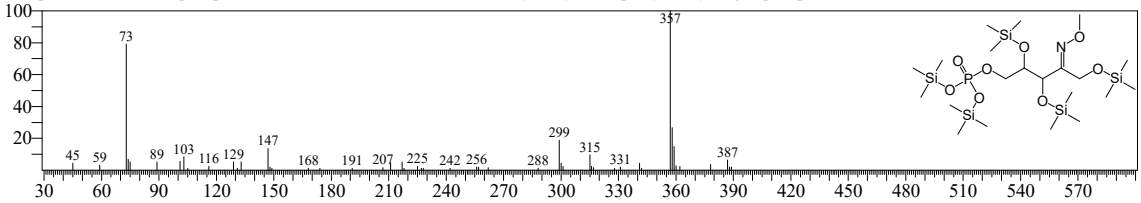
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



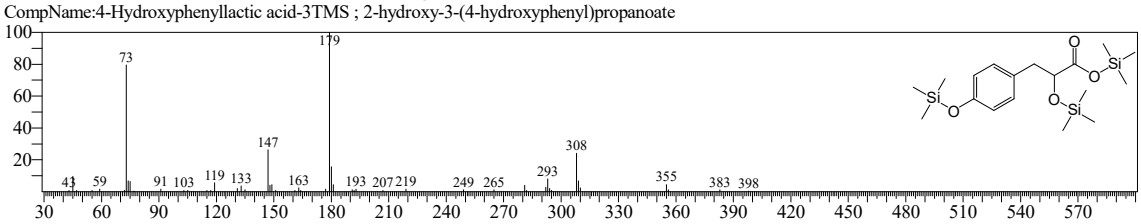
Hit#:2 Entry:463 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C21H43NO4Si4 CAS:59-92-7 MolWeight:485 RetIndex:2123
CompName:Dopa-4TMS ; (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid



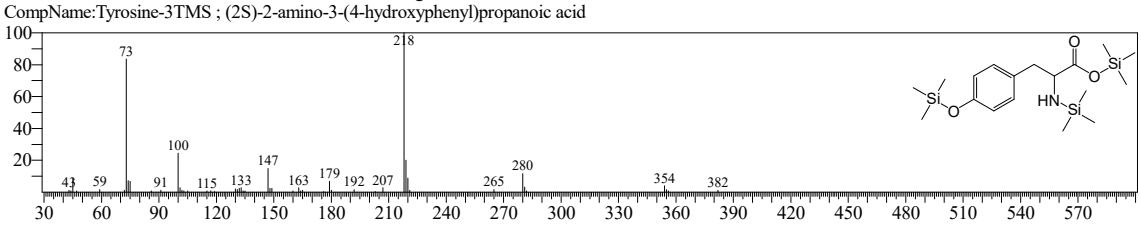
Hit#:3 Entry:476 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C21H54NO8PSi5 CAS:4151-19-3 MolWeight:619 RetIndex:2152
CompName:Ribulose 5-phosphate-meto-5TMS(2) ; [(2R,3R)-2,3,5-trihydroxy-4-oxopentyl] dihydrogen phosphate



Hit#:4 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

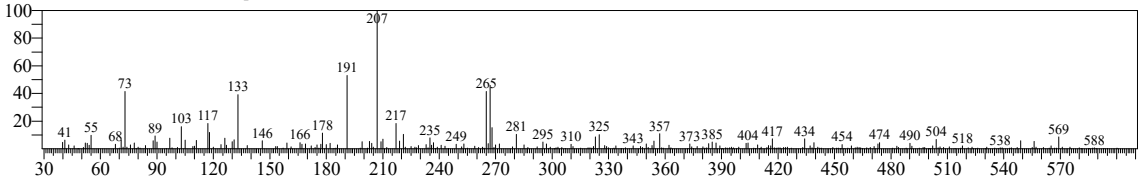


Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

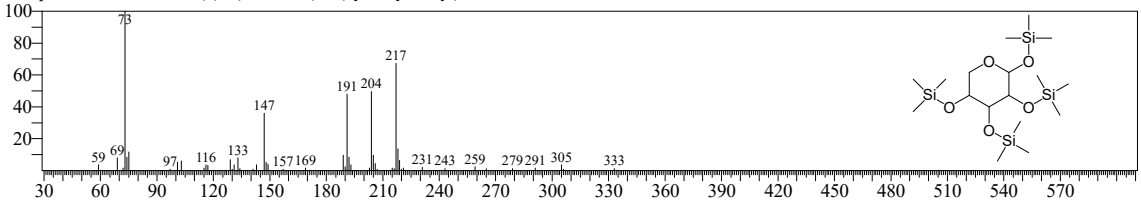


TNAU

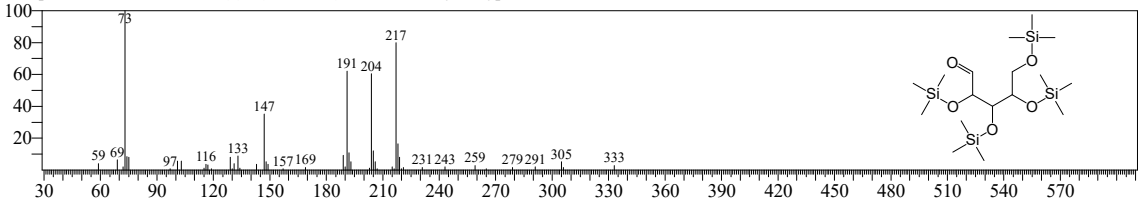
<< Target >>
Line#:9 R.Time:30.360(Scan#:5173) MassPeaks:271
RawMode:Averaged 30.355-30.365(5172-5174) BasePeak:207.05(1974)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



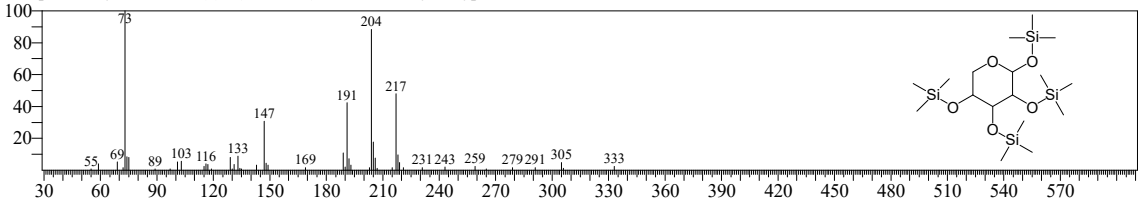
Hit#:1 Entry:250 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1691
CompName:Ribose-4TMS(4) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol



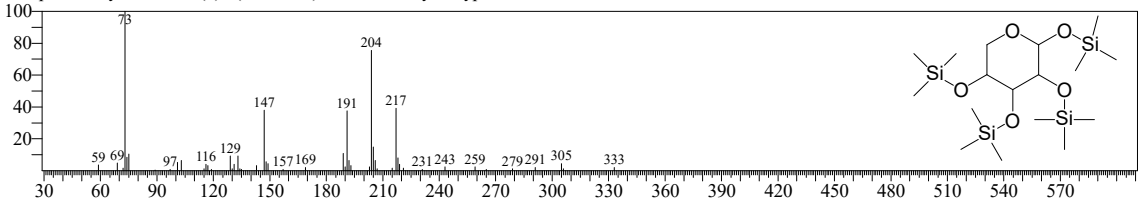
Hit#:2 Entry:210 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



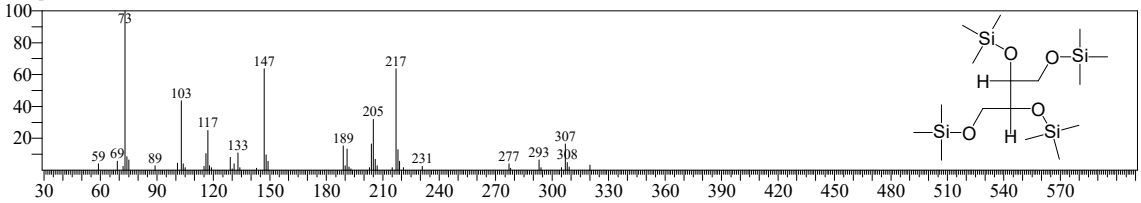
Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

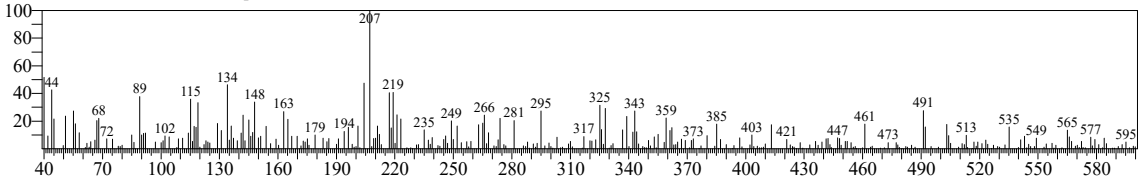


Hit#:5 Entry:148 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C16H42O4Si4 CAS:2418-52-2 MolWeight:410 RetIndex:1512
CompName:Threitol-4TMS ; (2R,3R)-butane-1,2,3,4-tetrol

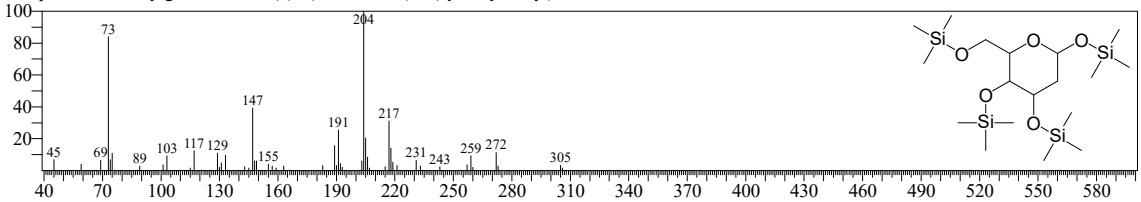


TNAU

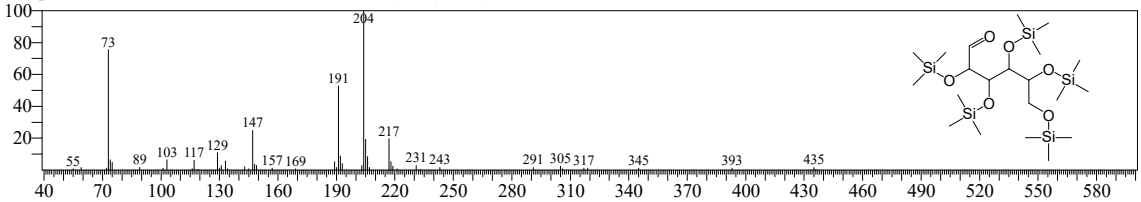
<< Target >>
Line#:10 R.Time:30.480(Scan#:5197) MassPeaks:316
RawMode:Averaged 30.475-30.485(5196-5198) BasePeak:207.05(647)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



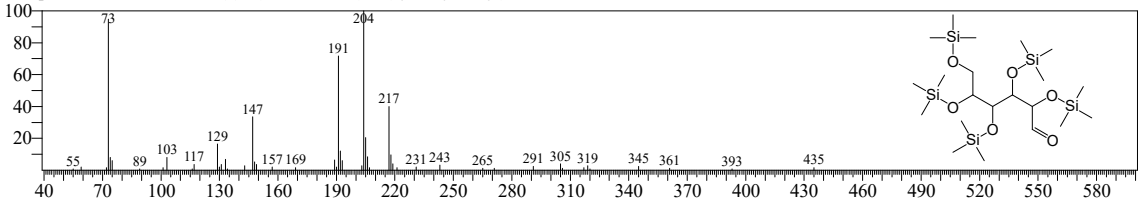
Hit#:1 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



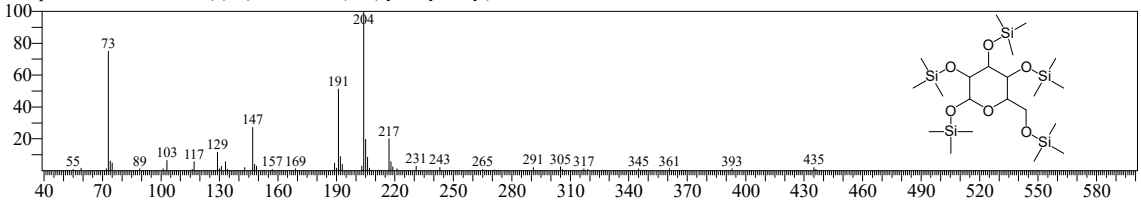
Hit#:2 Entry:288 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1771
CompName:Mannose-5TMS(1) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



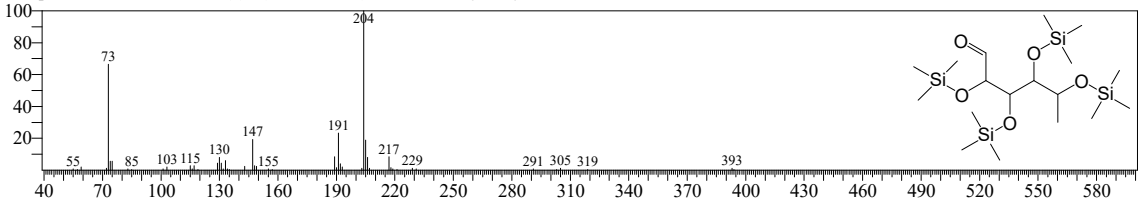
Hit#:3 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:23 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

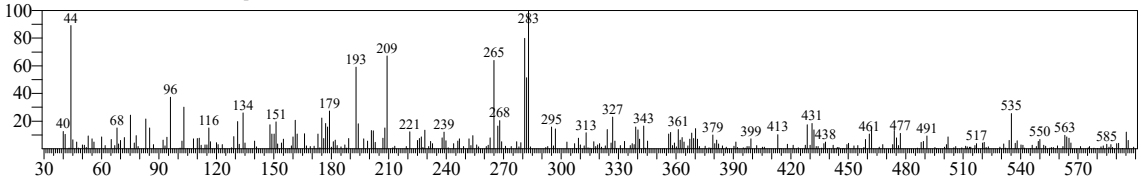


Hit#:5 Entry:219 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1646
CompName:Rhamnose-4TMS(1) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

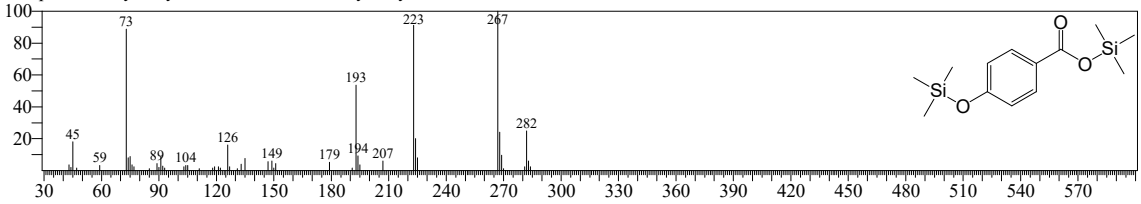


TNAU

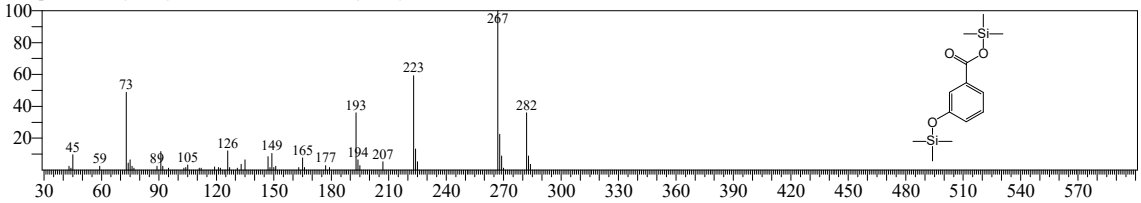
<< Target >>
Line#:11 R.Time:30.965(Scan#:5294) MassPeaks:312
RawMode:Averaged 30.960-30.970(5293-5295) BasePeak:283.05(833)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



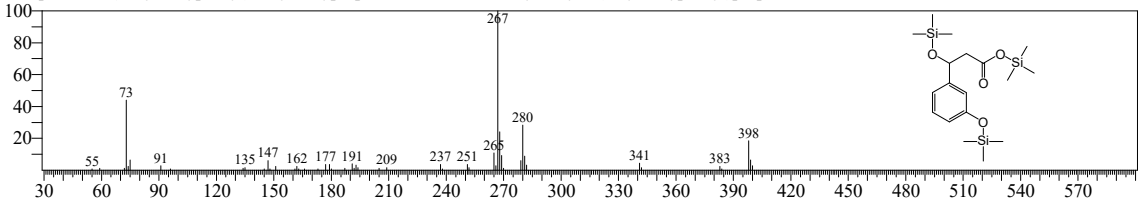
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



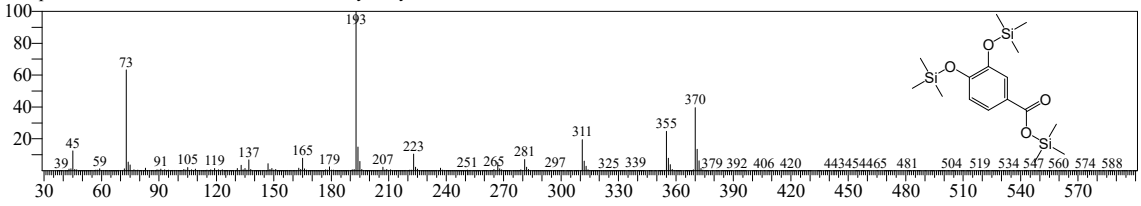
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



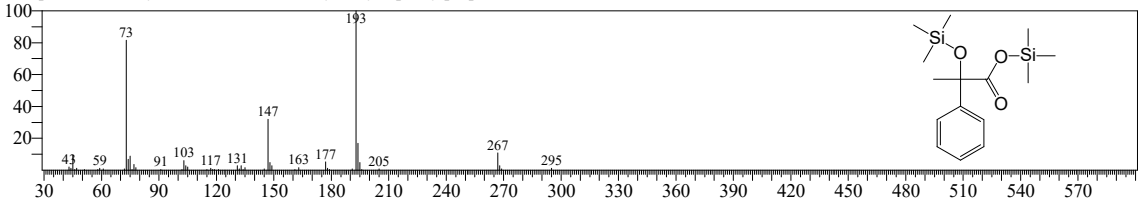
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry: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

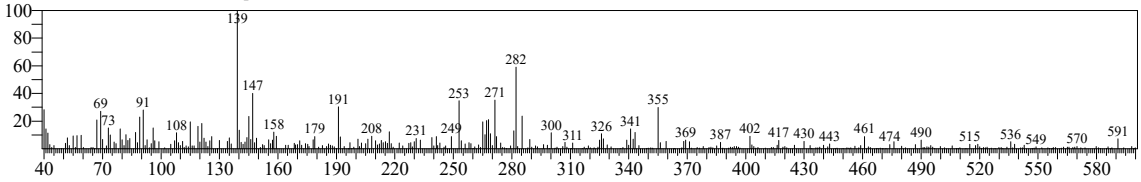


Hit#:5 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

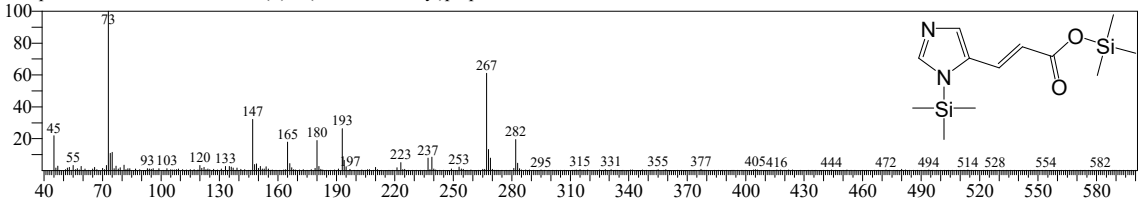


TNAU

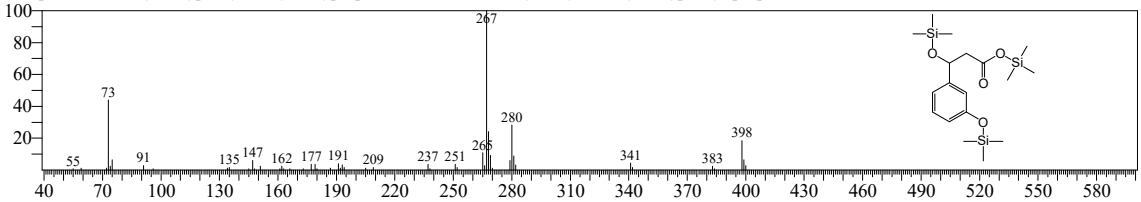
<< Target >>
Line#:12 R.Time:31.900(Scan#:5481) MassPeaks:348
RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.10(1967)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



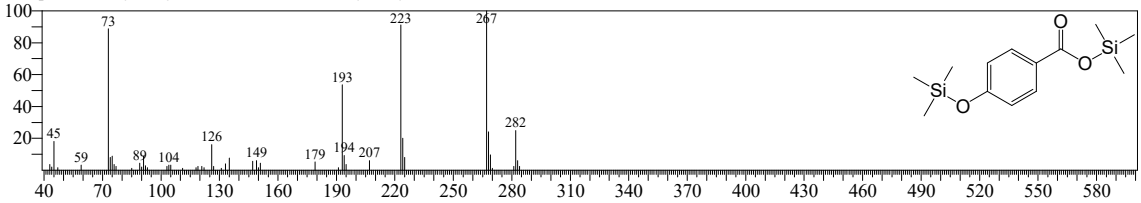
Hit#:1 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



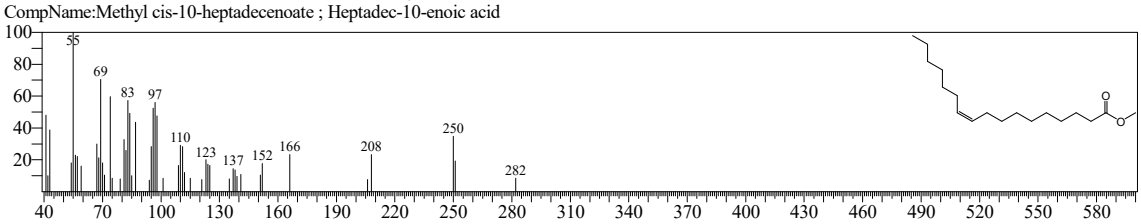
Hit#:2 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



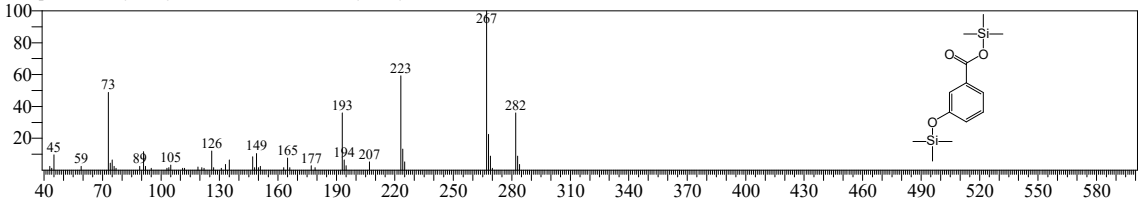
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:29 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

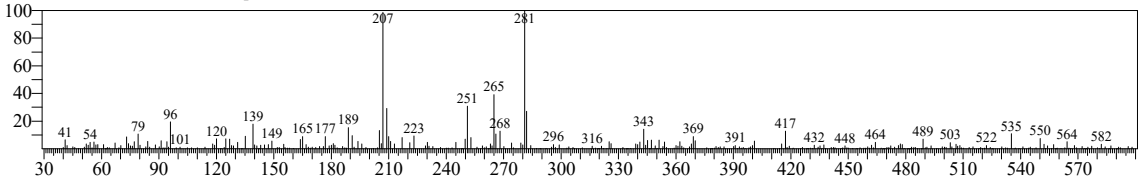


Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

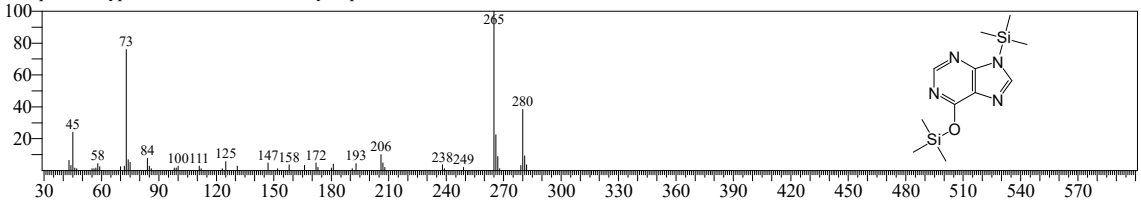


TNAU

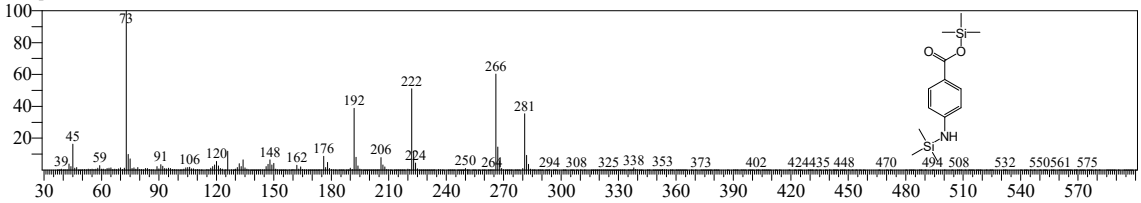
<< Target >>
Line#:13 R.Time:32.015(Scan#:5504) MassPeaks:329
RawMode:Averaged 32.010-32.020(5503-5505) BasePeak:281.00(2130)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



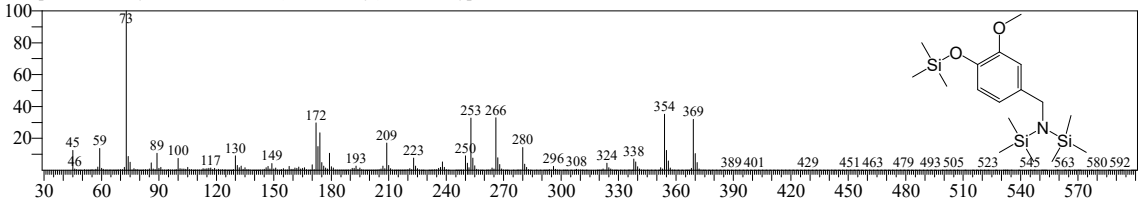
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



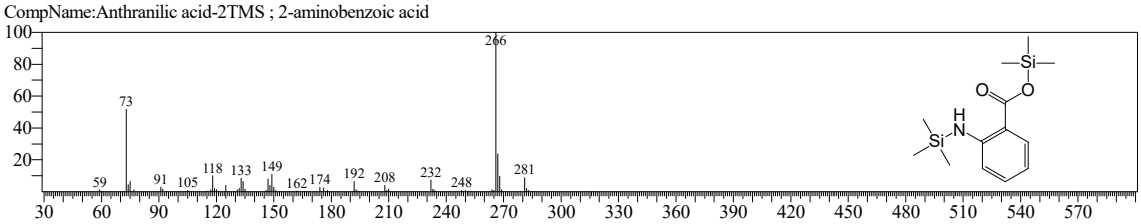
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



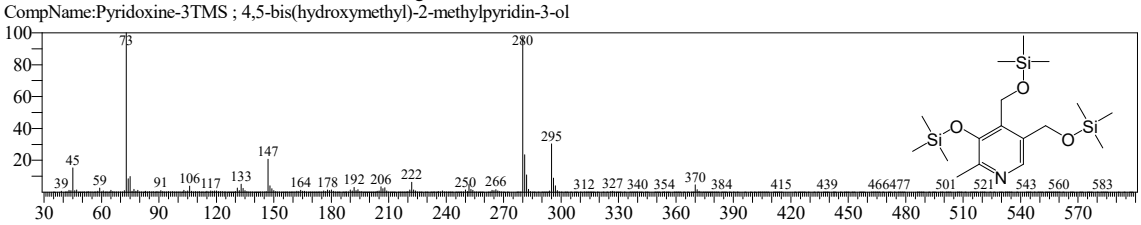
Hit#:3 Entry:368 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H35NO2Si3 CAS:1196-92-5 MolWeight:369 RetIndex:1899
CompName:Vanillylamine-3TMS ; 4-(aminomethyl)-2-methoxyphenol



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

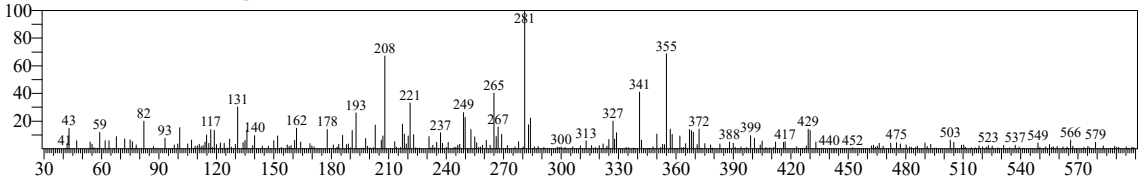


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

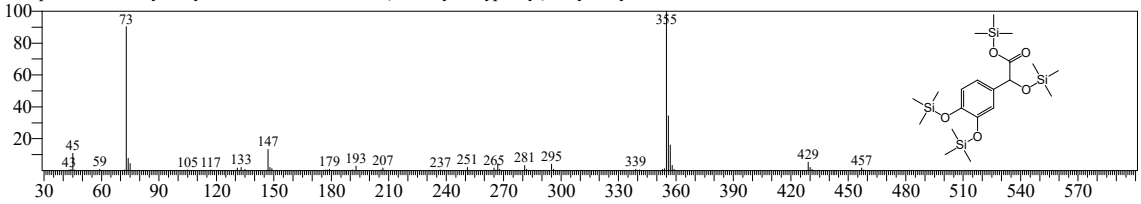


TNAU

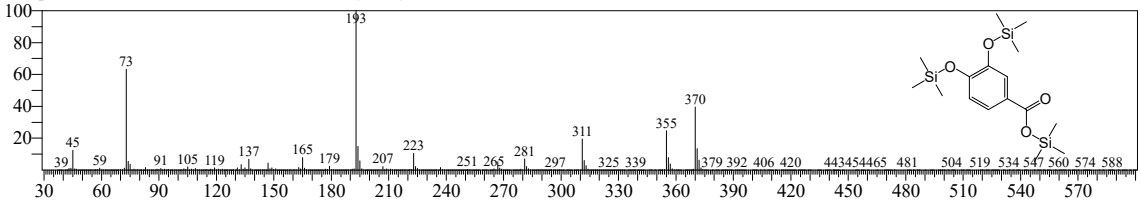
<< Target >>
Line#:14 R.Time:32.100(Scan#:5521) MassPeaks:267
RawMode:Averaged 32.095-32.105(5520-5522) BasePeak:281.05(815)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



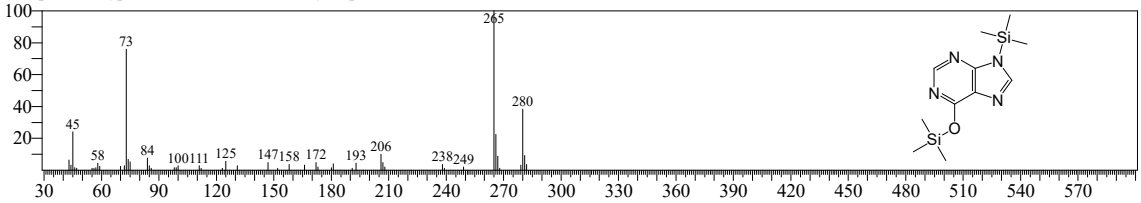
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



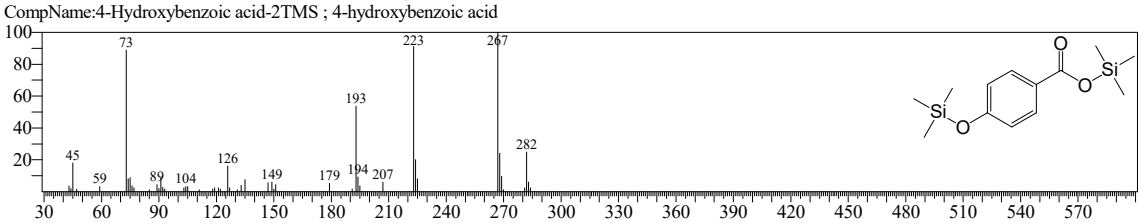
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



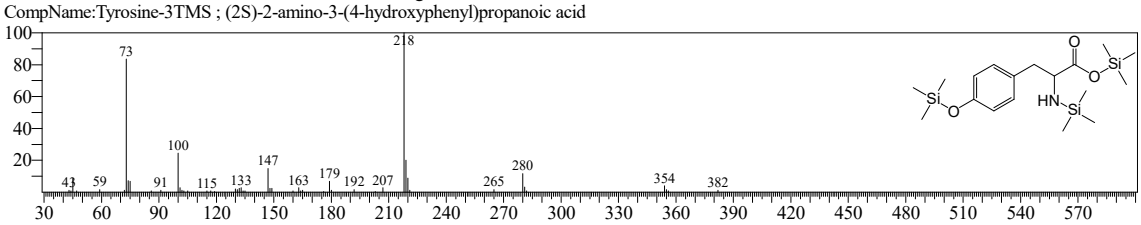
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

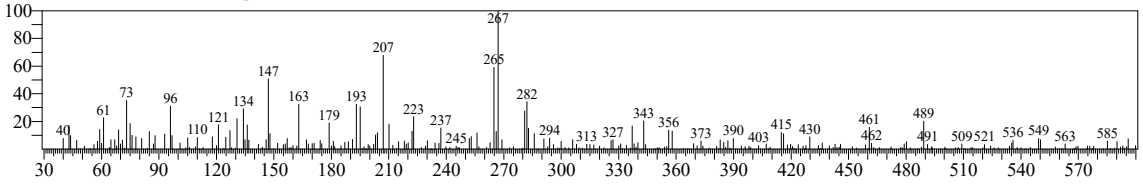


Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

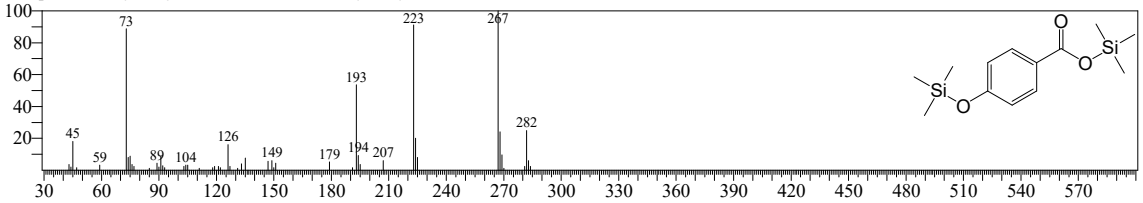


TNAU

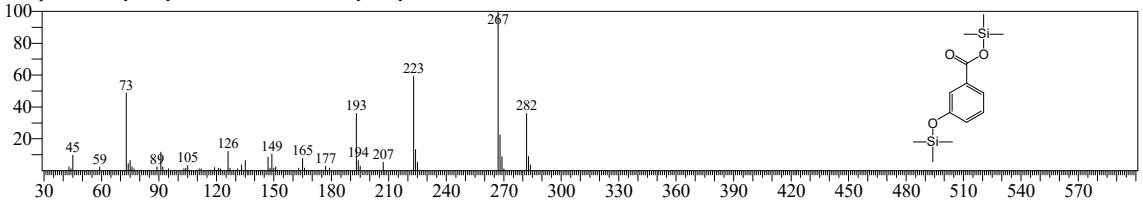
<< Target >>
Line#:15 R.Time:32.805(Scan#:5662) MassPeaks:285
RawMode:Averaged 32.800-32.810(5661-5663) BasePeak:267.00(1103)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



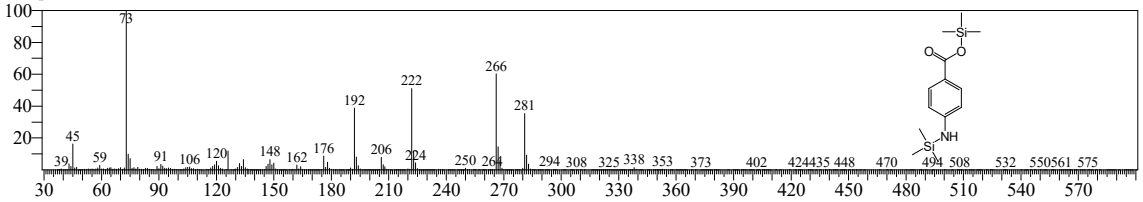
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



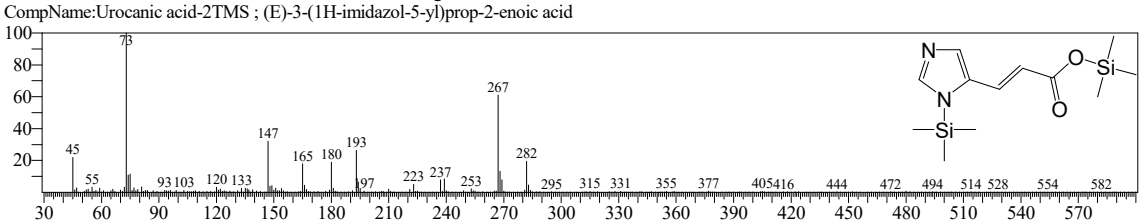
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:39 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:341 Library:OA_TMS_DB5_67min_V3.lib
SI:39 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