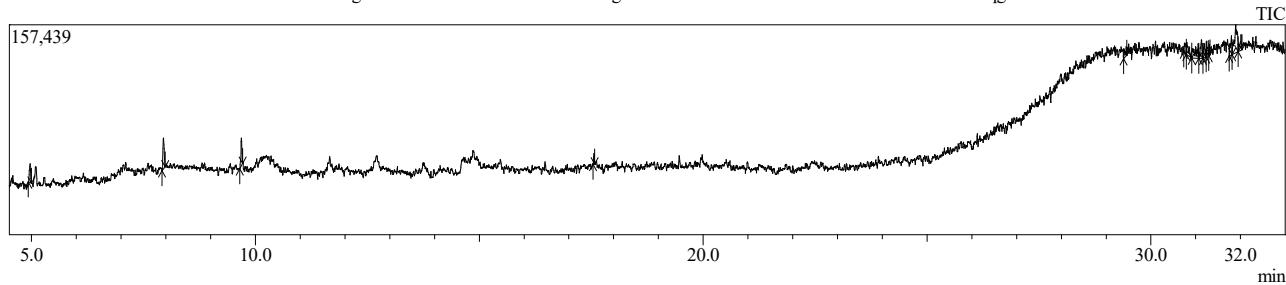


# TNAU

## Sample Information

Analyzed by : Admin  
 Analyzed : 05-Aug-22 9:47:33 AM  
 Sample Type : Unknown  
 Level # : 1  
 Sample Name : T56-3  
 Sample ID : T56-3  
 IS Amount : [1]=1  
 Sample Amount : 1  
 Dilution Factor : 1  
 Vial # : 26  
 Injection Volume : 1.00  
 Data File : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-027.qgd  
 Org Data File : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-027.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 4:44:49 PM

Chromatogram T56-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-027.qgd



Peak Report TIC

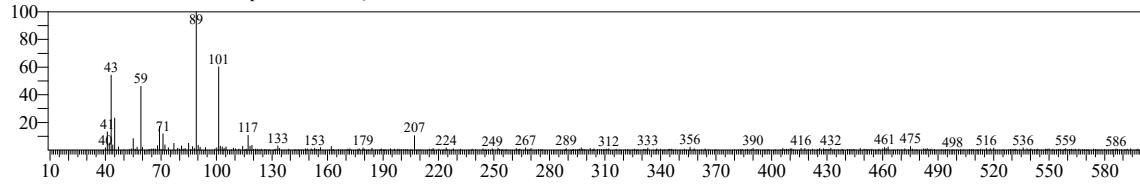
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.965	25670	5.60	14243	7.52	1.80	72	2-Propanol, 1,1'-oxybis-
2	7.944	44203	9.64	23221	12.27	1.90	89	Undecane
3	9.685	34032	7.42	20815	11.00	1.63	89	Tridecane
4	17.560	7545	1.65	7990	4.22	0.94	34	Hypoxanthine-2TMS
5	29.449	16671	3.64	7035	3.72	2.37	33	3,4-Dihydroxymandelic acid-4TMS
6	30.745	16494	3.60	5324	2.81	3.10	37	Fendiline-TMS
7	30.800	26834	5.85	8467	4.47	3.17	34	Epinephrine-3TMS
8	31.055	50135	10.94	11024	5.82	4.55	35	4-Aminobenzoic acid-2TMS
9	31.130	32610	7.11	13857	7.32	2.35	39	4-Aminobenzoic acid-2TMS
10	31.180	25671	5.60	10623	5.61	2.42	36	3,4-Dihydroxymandelic acid-4TMS
11	31.245	21843	4.77	11471	6.06	1.90	29	Protocatechuic acid-3TMS
12	31.302	7951	1.73	8300	4.38	0.96	44	Protocatechuic acid-3TMS
13	31.795	31192	6.81	14493	7.66	2.15	41	Pyridoxine-3TMS
14	31.893	90884	19.83	20998	11.09	4.33	27	Antranilic acid-2TMS
15	32.015	26631	5.81	11437	6.04	2.33	36	4-Hydroxyphenyllactic acid-3TMS
		458366	100.00	189298	100.00			

Library

# TNAU

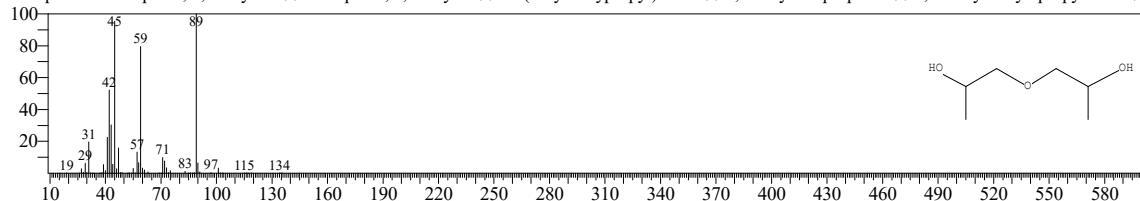
<<Target >>

Line#:1 R.Time:4.965(Scan#:94) MassPeaks:321  
 RawMode:Averaged 4.960-4.970(93-95) BasePeak:89.05(2918)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



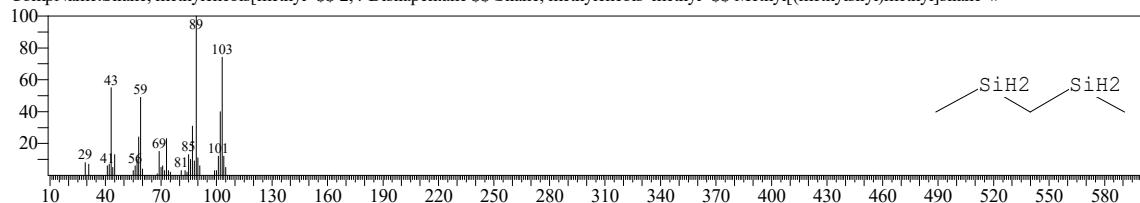
Hit#:1 Entry:7425 Library:NIST20R.lib

SI:72 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 \$\$



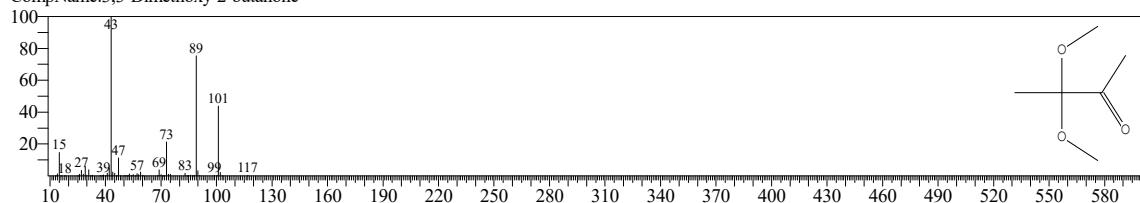
Hit#:2 Entry:2591 Library:NIST20M1.lib

SI:71 Formula:C3H12Si2 CAS:5654-05-7 MolWeight:104 RetIndex:0  
 CompName:Silane, methylenabis[methyl- \$\$ 2,4-Disilapentane \$\$ Silane, methylenabis\*methyl- \$\$ Methyl[(methylsilyl)methyl]silane #



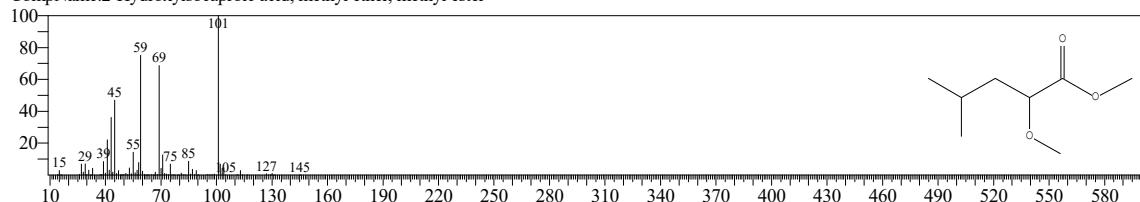
Hit#:3 Entry:9263 Library:NIST20M1.lib

SI:70 Formula:C6H12O3 CAS:21983-72-2 MolWeight:132 RetIndex:821  
 CompName:3,3-Dimethoxy-2-butanone



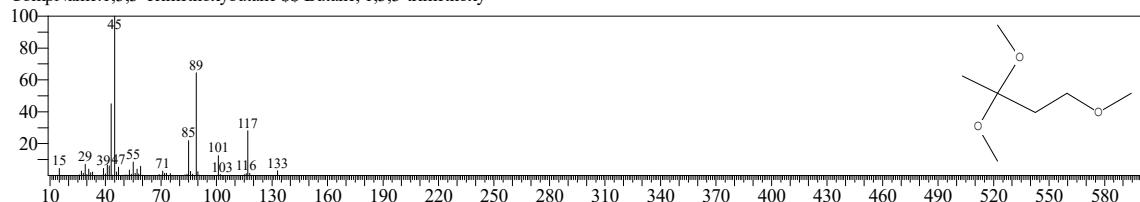
Hit#:4 Entry:22897 Library:NIST20M1.lib

SI:70 Formula:C8H16O3 CAS:0-00-0 MolWeight:160 RetIndex:931  
 CompName:2-Hydroxyisocaproic acid, methyl ester,



Hit#:5 Entry:16032 Library:NIST20M1.lib

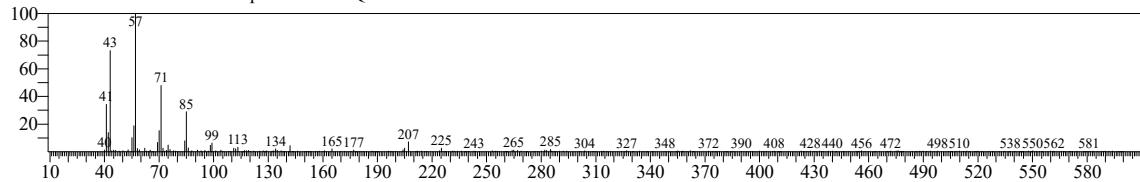
SI:70 Formula:C7H16O3 CAS:6607-66-5 MolWeight:148 RetIndex:860  
 CompName:1,3,3-Trimethoxybutane \$\$ Butane, 1,3,3-trimethoxy-



# TNAU

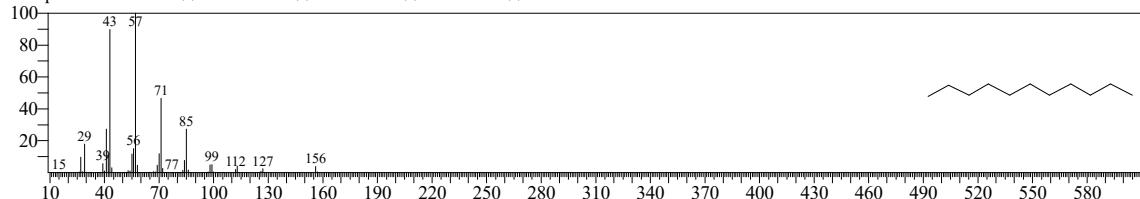
<<Target >>

Line#2 R.Time:7.945(Scan#:690) MassPeaks:286  
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5600)  
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



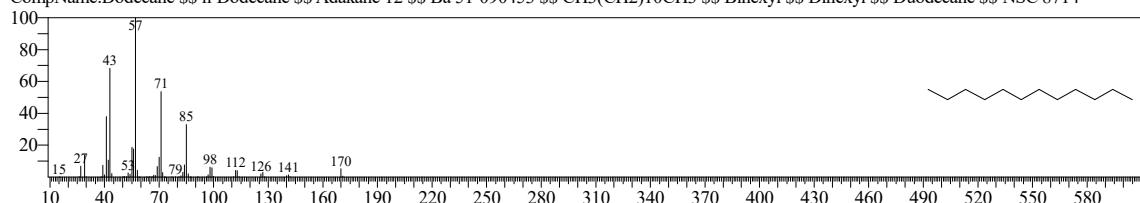
Hit#1 Entry:21042 Library:NIST20M1.lib

SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100  
CompName:Undecane \$\$ n-Undecane \$\$ Hendecane \$\$ n-C11H24 \$\$ UN 2330



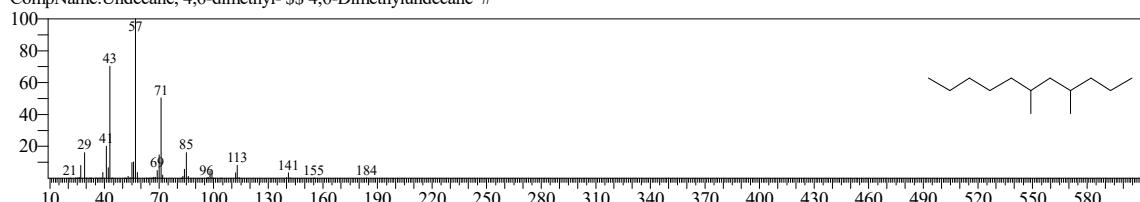
Hit#2 Entry:30057 Library:NIST20M1.lib

SI:88 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200  
CompName:Dodecane \$\$ n-Dodecane \$\$ Adakane 12 \$\$ Ba 51-090453 \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl \$\$ Dihexyl \$\$ Duodecane \$\$ NSC 8714



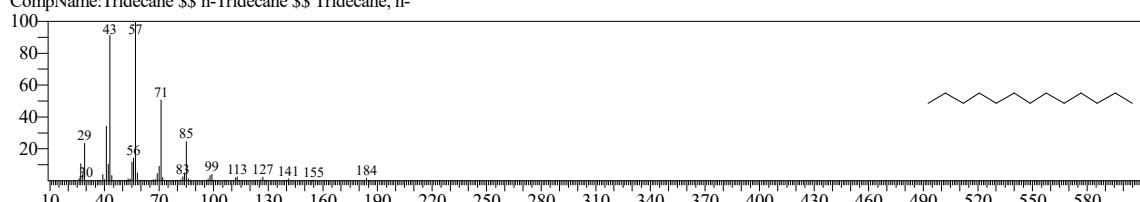
Hit#3 Entry:40271 Library:NIST20M1.lib

SI:88 Formula:C13H28 CAS:17312-82-2 MolWeight:184 RetIndex:1185  
CompName:Undecane, 4,6-dimethyl- \$\$ 4,6-Dimethylundecane #



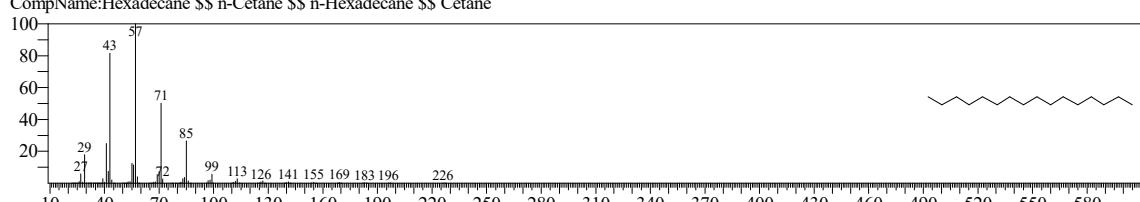
Hit#4 Entry:40226 Library:NIST20M1.lib

SI:88 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300  
CompName:Tridecane \$\$ n-Tridecane \$\$ Tridecane, n-



Hit#5 Entry:27737 Library:NIST20R.lib

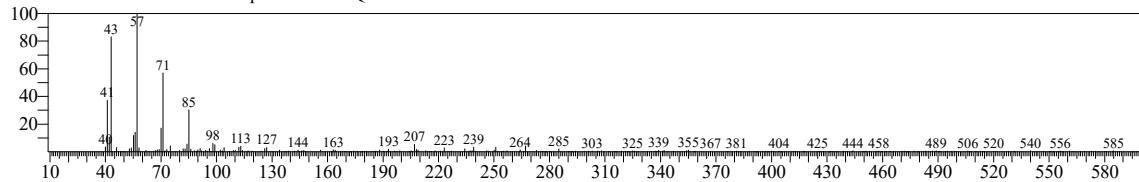
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600  
CompName:Hexadecane \$\$ n-Cetane \$\$ n-Hexadecane \$\$ Cetane



# TNAU

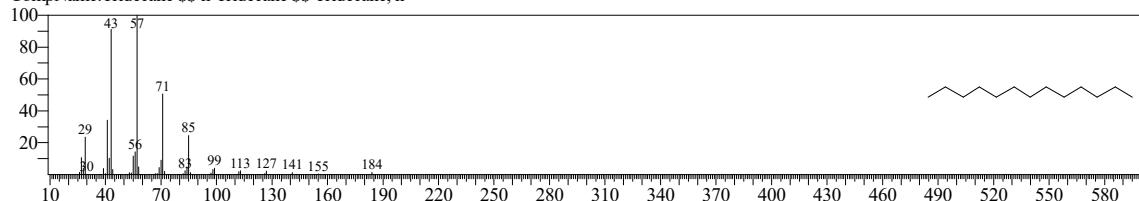
<<Target >>

Line#3 R.Time:9.685(Scan#:1038) MassPeaks:250  
 RawMode:Averaged 9.680-9.690(1037-1039) BasePeak:57.10(4746)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



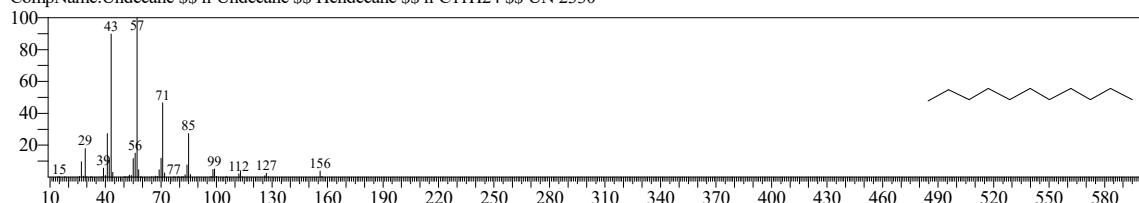
Hit#1 Entry:40226 Library:NIST20M1.lib

SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300  
 CompName:Tridecane \$\$ n-Tridecane \$\$ Tridecane, n-



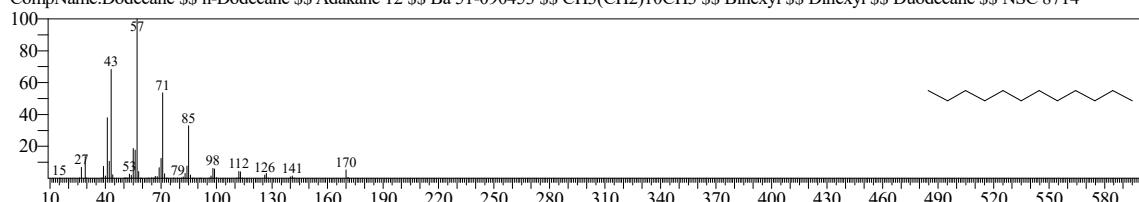
Hit#2 Entry:21042 Library:NIST20M1.lib

SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100  
 CompName:Undecane \$\$ n-Undecane \$\$ Hendecane \$\$ n-C11H24 \$\$ UN 2330



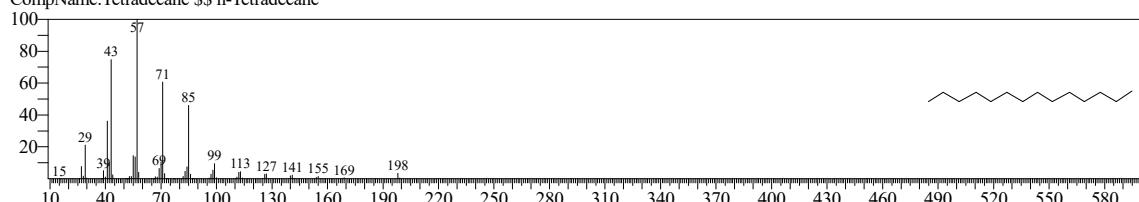
Hit#3 Entry:30057 Library:NIST20M1.lib

SI:89 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200  
 CompName:Dodecane \$\$ n-Dodecane \$\$ Adakane 12 \$\$ Ba 51-090453 \$\$ CH<sub>3</sub>(CH<sub>2</sub>)<sub>10</sub>CH<sub>3</sub> \$\$ Bihexyl \$\$ Dihexyl \$\$ Duodecane \$\$ NSC 8714



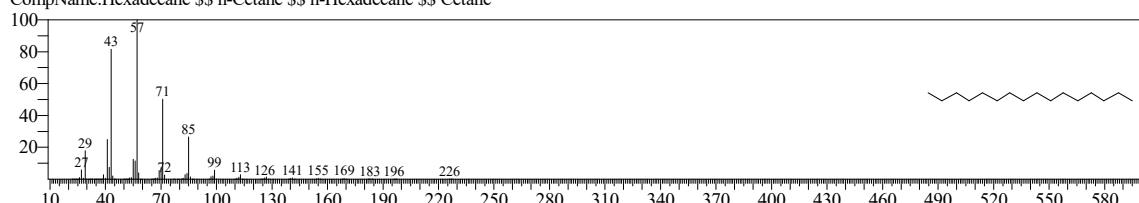
Hit#4 Entry:22497 Library:NIST20R.lib

SI:88 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400  
 CompName:Tetradecane \$\$ n-Tetradecane



Hit#5 Entry:27737 Library:NIST20R.lib

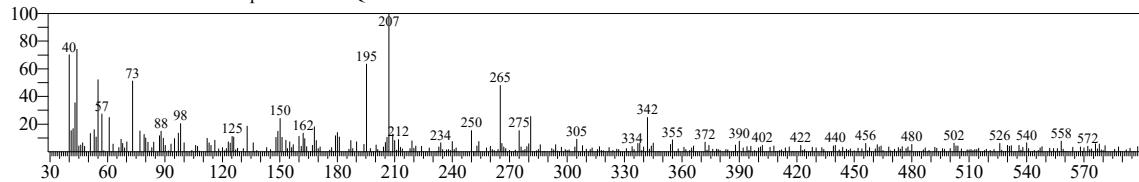
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600  
 CompName:Hexadecane \$\$ n-Cetane \$\$ n-Hexadecane \$\$ Cetane



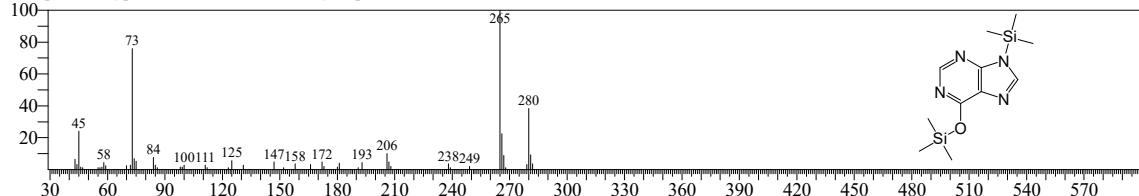
# TNAU

<<Target >>

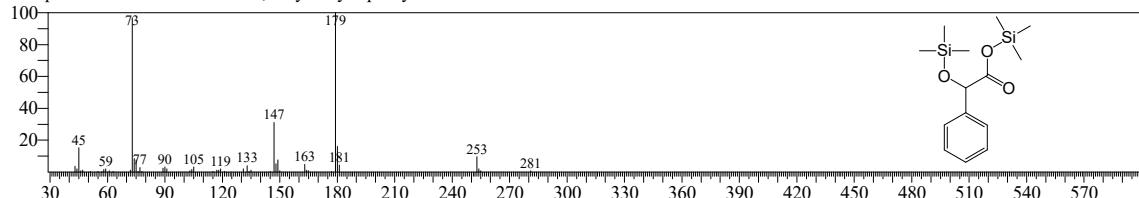
Line#4 R.Time:17.560(Scan#:2613) MassPeaks:330  
 RawMode:Averaged 17.555-17.565(2612-2614) BasePeak:207.05(591)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



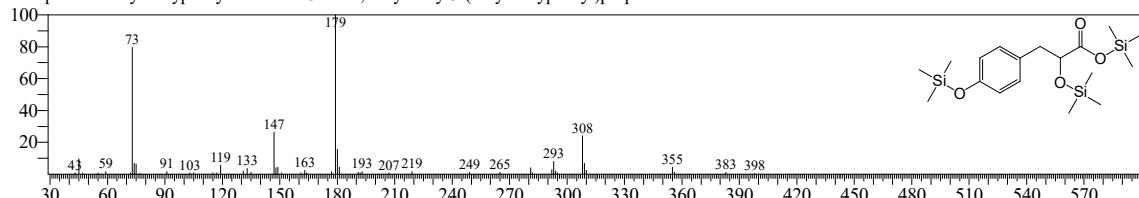
Hit#1 Entry:310 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:34 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822  
 CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



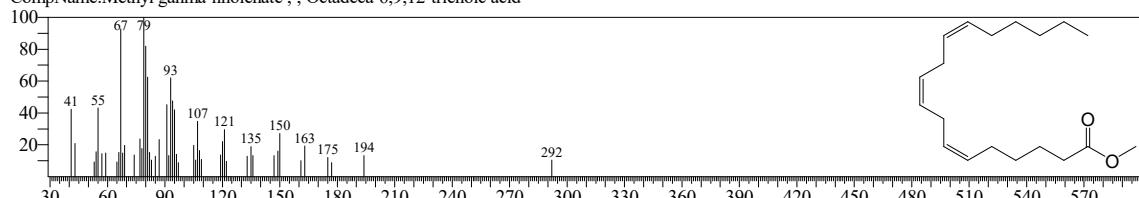
Hit#2 Entry:138 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:32 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486  
 CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



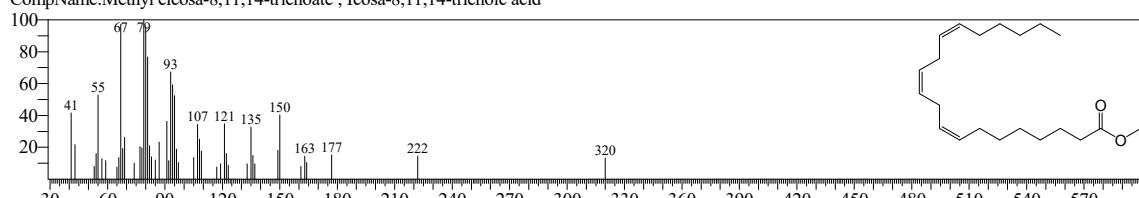
Hit#3 Entry:382 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:31 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918  
 CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#4 Entry:23 Library:FA\_ME\_SP2560\_EI\_V3.lib  
 SI:30 Formula:C19H32O2 CAS:506-26-3 MolWeight:292 RetIndex:2852  
 CompName:Methyl gamma-linolenate ; Octadeca-6,9,12-trienoic acid



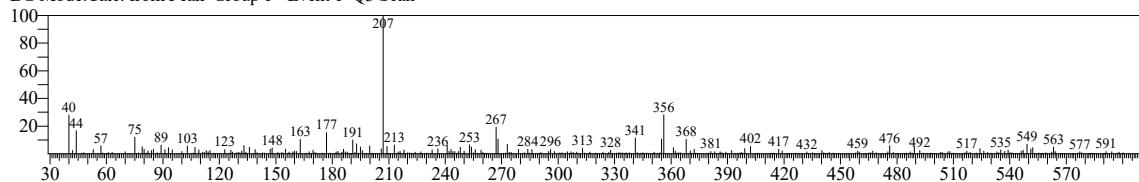
Hit#5 Entry:29 Library:FA\_ME\_SP2560\_EI\_V3.lib  
 SI:30 Formula:C21H36O2 CAS:1783-84-2 MolWeight:320 RetIndex:3049  
 CompName:Methyl eicosa-8,11,14-trienoate ; Icosa-8,11,14-trienoic acid



# TNAU

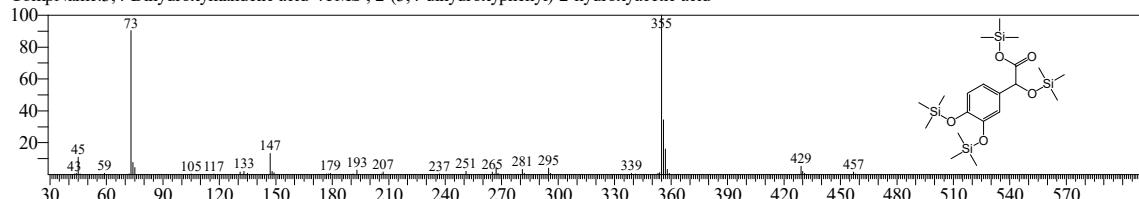
<<Target >>

Line#5 R.Time:29.450(Scan#:4991) MassPeaks:303  
 RawMode:Averaged 29.445-29.455(4990-4992) BasePeak:207.05(2228)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



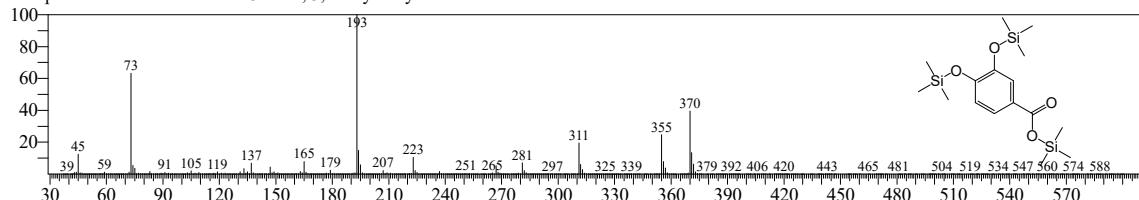
Hit#1 Entry:402 Library:OA\_TMS\_DB5\_67min\_V3.lib

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



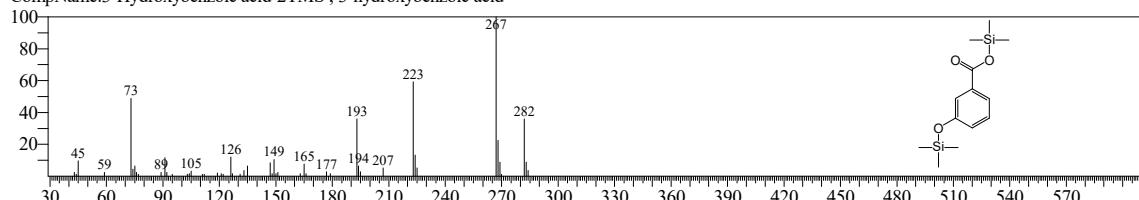
Hit#2 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:30 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833  
 CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



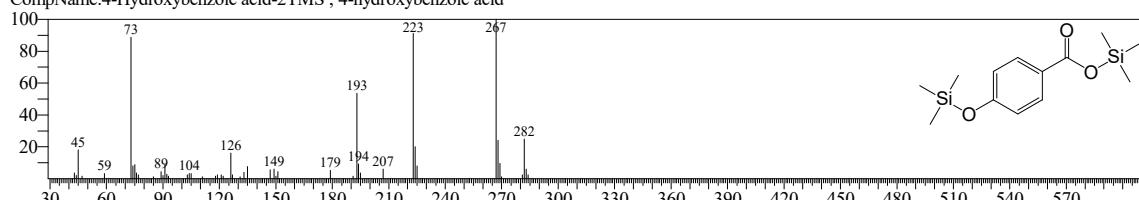
Hit#3 Entry:179 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:28 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572  
 CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



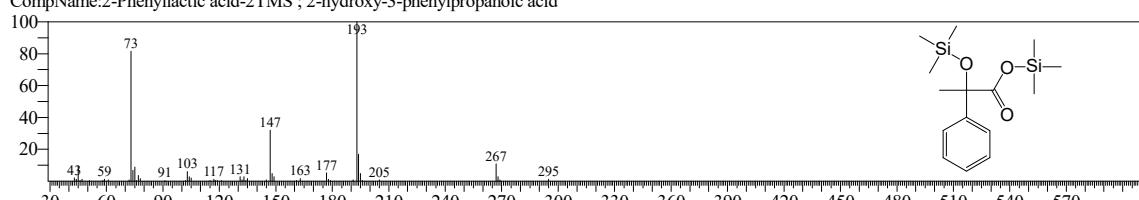
Hit#4 Entry:211 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:27 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636  
 CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#5 Entry:150 Library:OA\_TMS\_DB5\_67min\_V3.lib

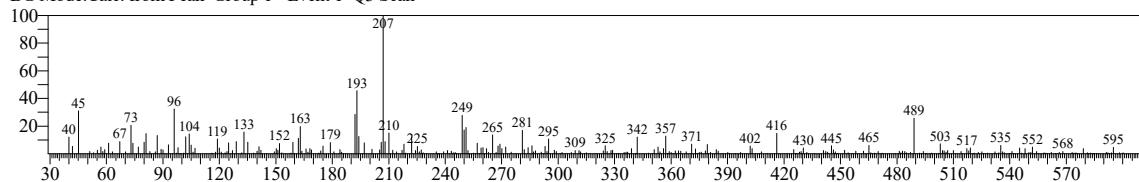
SI:24 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517  
 CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



# TNAU

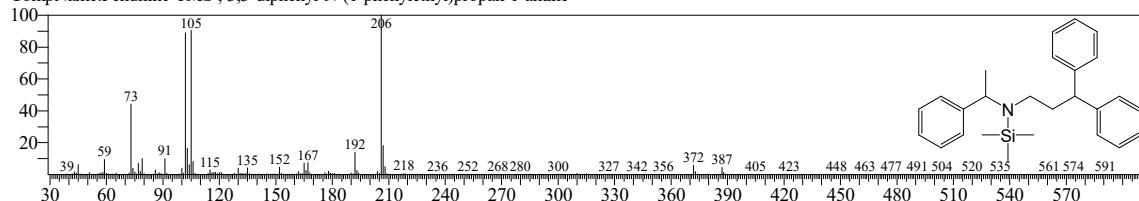
<<Target >>

Line#:6 R.Time:30.745(Scan#:5250) MassPeaks:282  
 RawMode:Averaged 30.740-30.750(5249-5251) BasePeak:207.00(1446)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



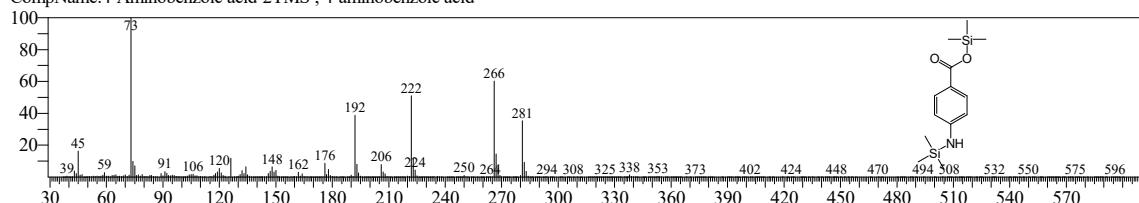
Hit#:1 Entry:537 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:37 Formula:C26H33NSi CAS:13042-18-7 MolWeight:387 RetIndex:2646  
 CompName:Fendiline-TMS ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine



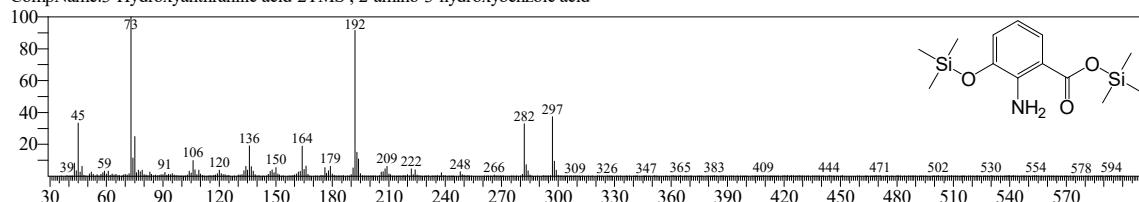
Hit#:2 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



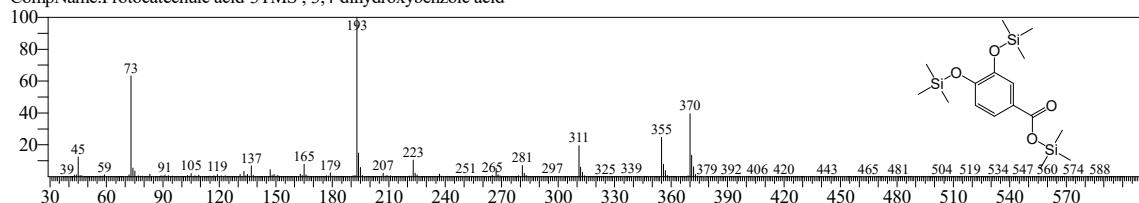
Hit#:3 Entry:290 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:35 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773  
 CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



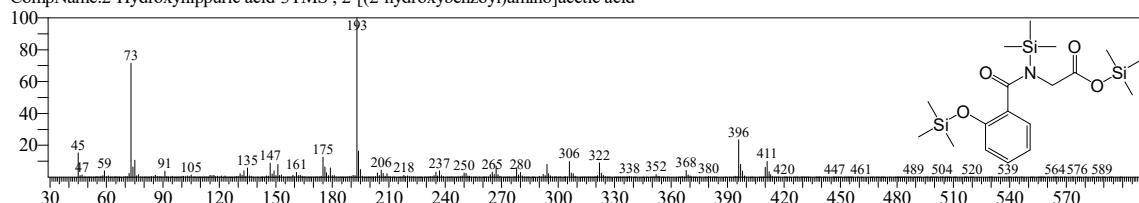
Hit#:4 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833  
 CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:5 Entry:420 Library:OA\_TMS\_DB5\_67min\_V3.lib

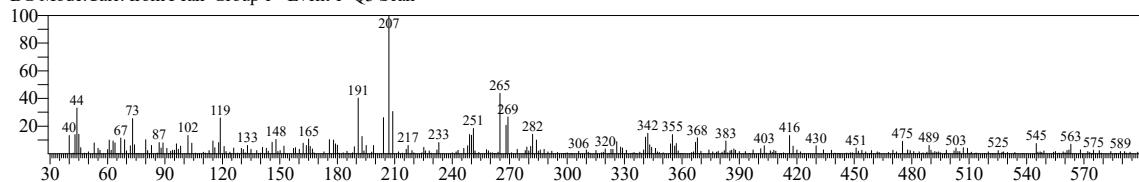
SI:34 Formula:C18H33NO4Si3 CAS:487-54-7 MolWeight:411 RetIndex:1973  
 CompName:2-Hydroxyhippuric acid-3TMS ; 2-[2-hydroxybenzoyl]aminoacetic acid



# TNAU

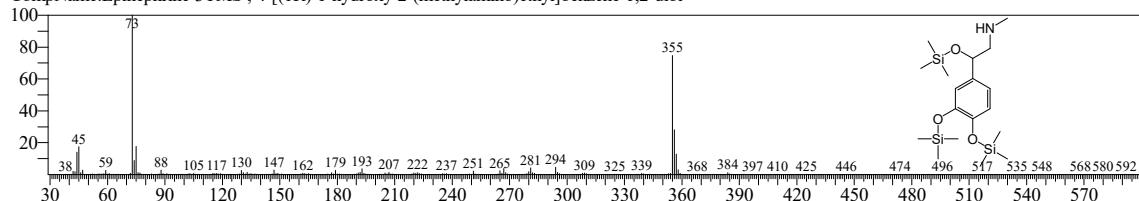
<<Target >>

Line#:7 R.Time:30.800(Scan#:5261) MassPeaks:309  
 RawMode:Averaged 30.795-30.805(5260-5262) BasePeak:207.00(1248)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



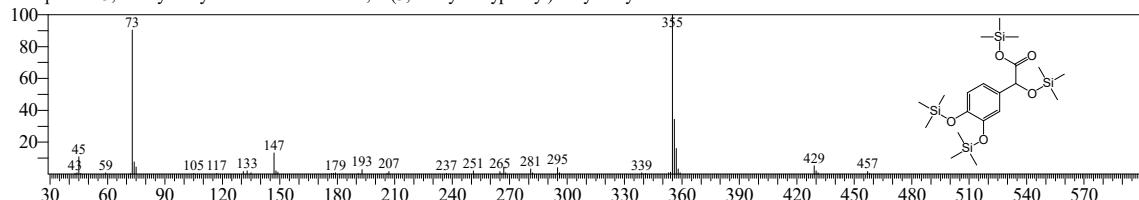
Hit#:1 Entry:343 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:34 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868  
 CompName:Epinephrine-3TMS ; 4-[{(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



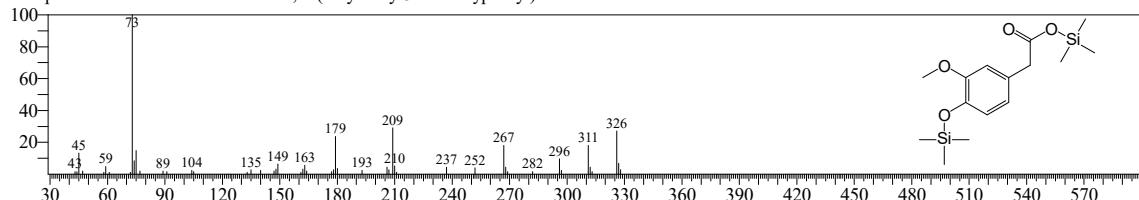
Hit#:2 Entry:402 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:34 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942  
 CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



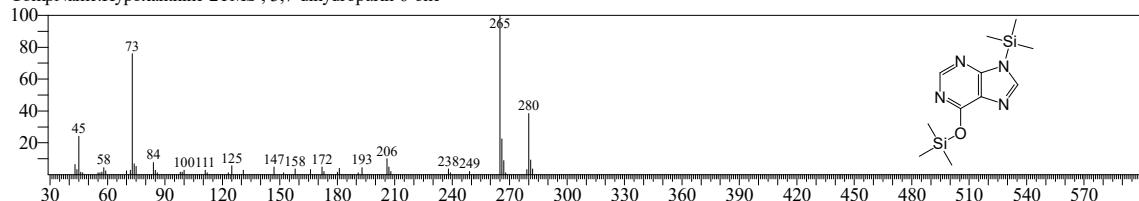
Hit#:3 Entry:294 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:33 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782  
 CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



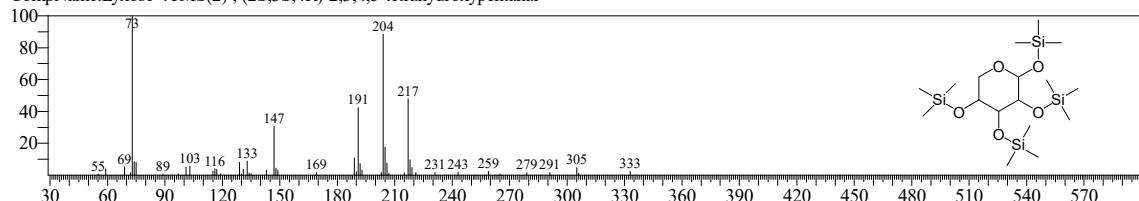
Hit#:4 Entry:310 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:32 Formula:C11H20N4O5Si2 CAS:68-94-0 MolWeight:280 RetIndex:1822  
 CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:5 Entry:238 Library:OA\_TMS\_DB5\_67min\_V3.lib

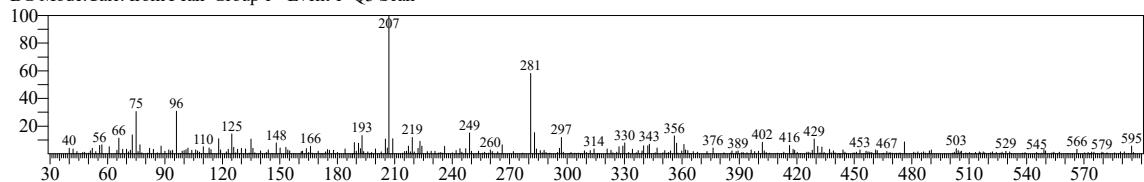
SI:31 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675  
 CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



# TNAU

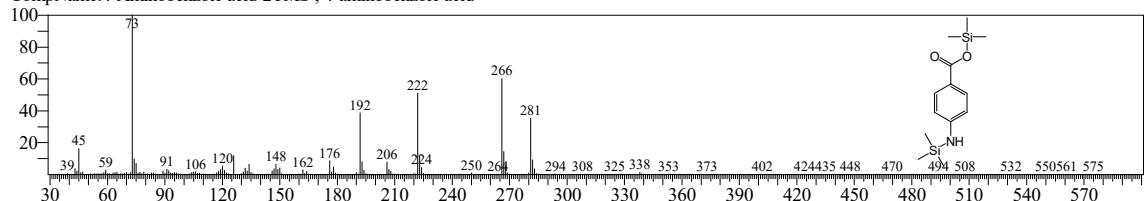
<<Target >>

Line#:8 R.Time:31.055(Scan#:5312) MassPeaks:315  
 RawMode:Averaged 31.050-31.060(5311-5313) BasePeak:207.05(1942)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



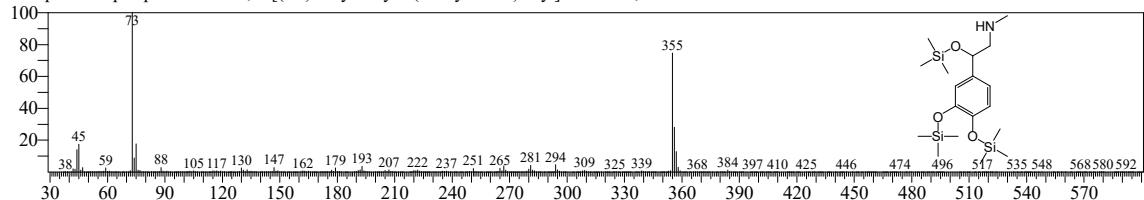
Hit#1 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:35 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



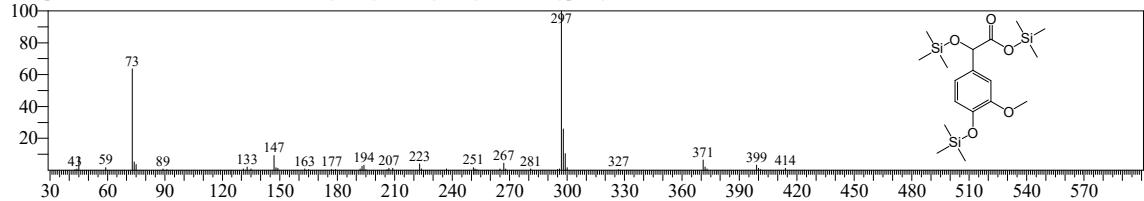
Hit#2 Entry:343 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:32 Formula:C18H37NO3Si CAS:51-43-4 MolWeight:399 RetIndex:1868  
 CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



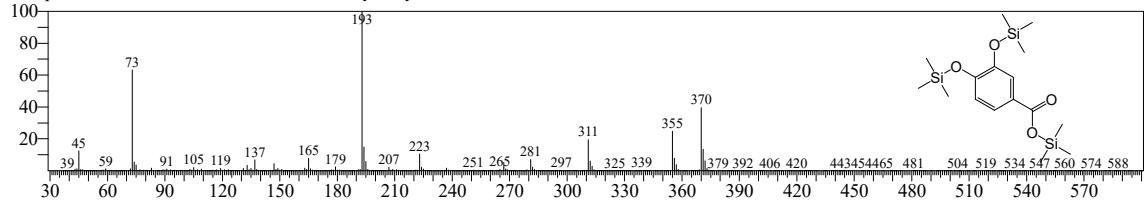
Hit#3 Entry:359 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:31 Formula:C18H34O5Si3 CAS:55-10-7 MolWeight:414 RetIndex:1894  
 CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid



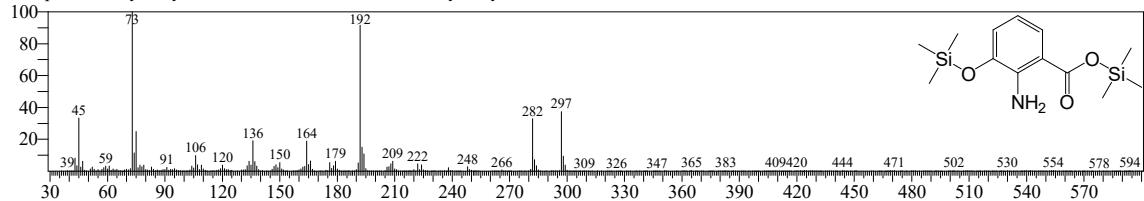
Hit#4 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:31 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833  
 CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#5 Entry:290 Library:OA\_TMS\_DB5\_67min\_V3.lib

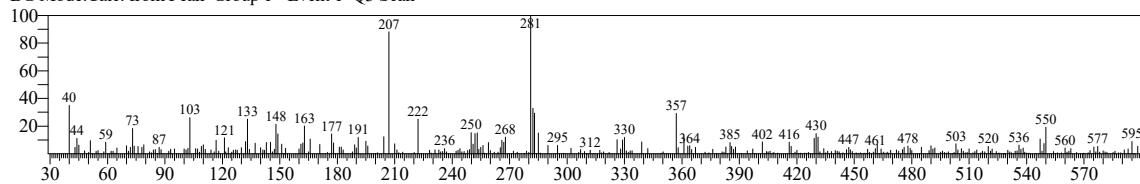
SI:31 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773  
 CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



# TNAU

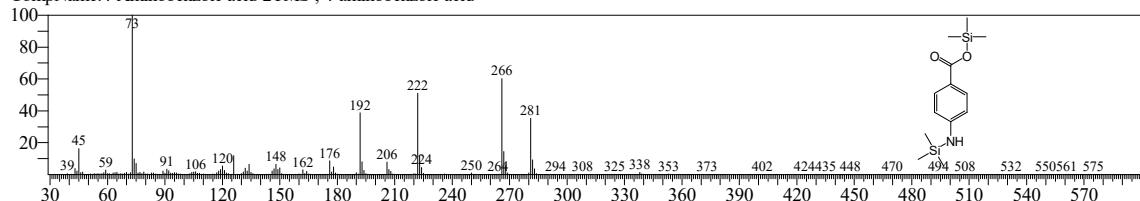
<<Target >>

Line#9 R.Time:31.130(Scan#:5327) MassPeaks:331  
 RawMode:Averaged 31.125-31.135(5326-5328) BasePeak:281.05(1431)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



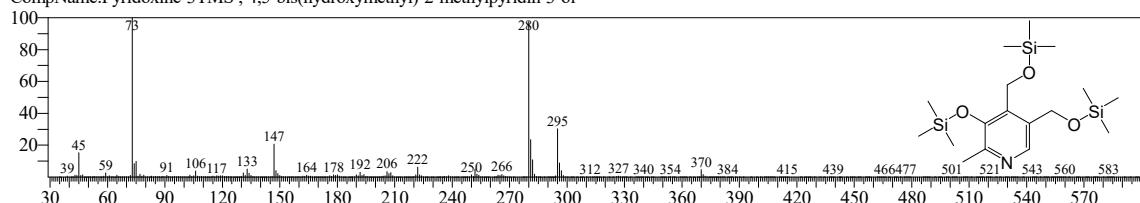
Hit#1 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:39 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



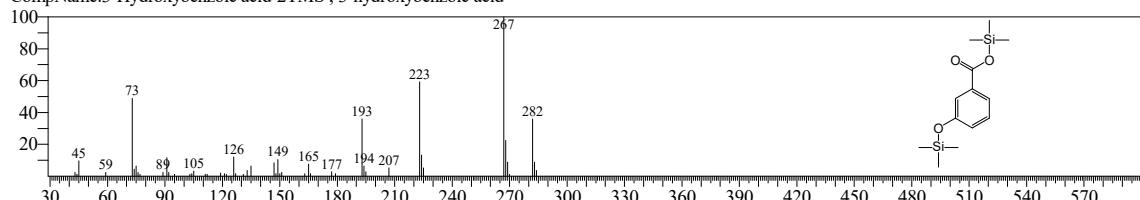
Hit#2 Entry:384 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:32 Formula:C17H35NO3Si2 CAS:65-23-6 MolWeight:385 RetIndex:1919  
 CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



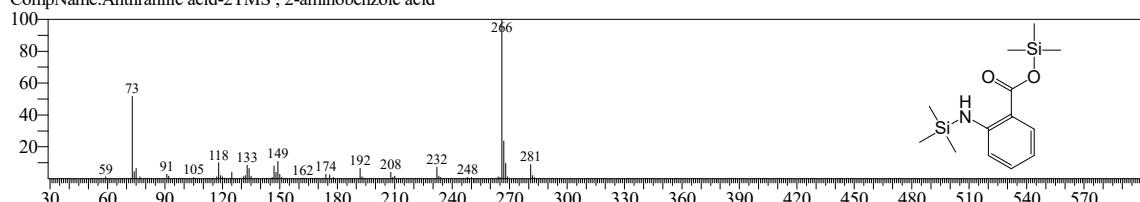
Hit#3 Entry:179 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572  
 CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



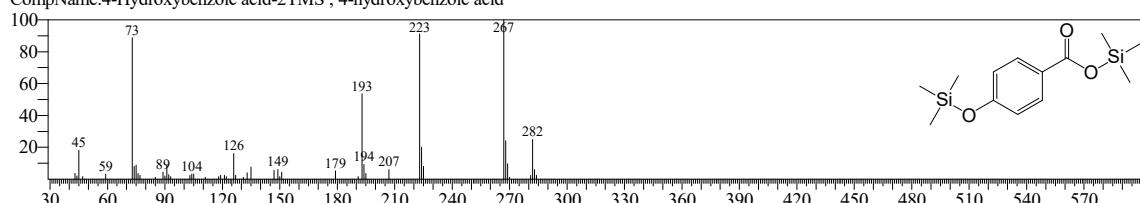
Hit#4 Entry:203 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:31 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

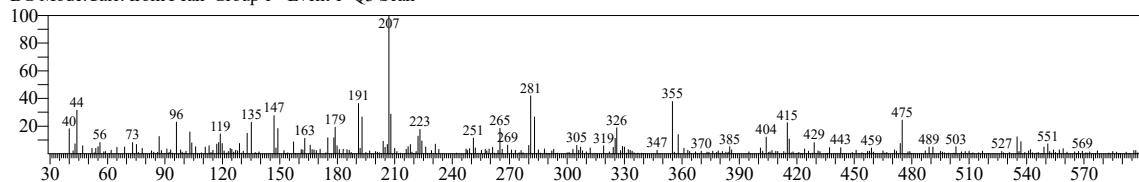
SI:30 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636  
 CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



# TNAU

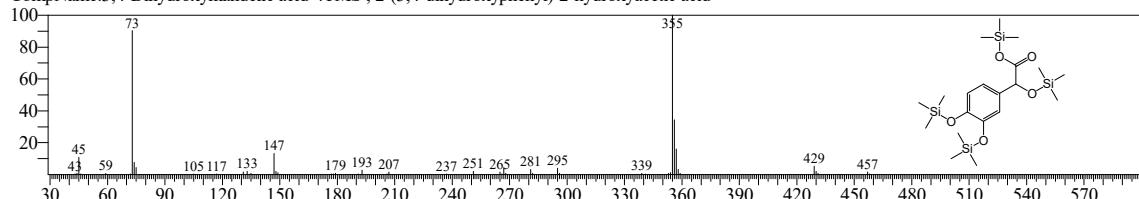
<<Target >>

Line#:10 R.Time:31.180(Scan#:5337) MassPeaks:307  
 RawMode:Averaged 31.175-31.185(5336-5338) BasePeak:207.05(1390)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



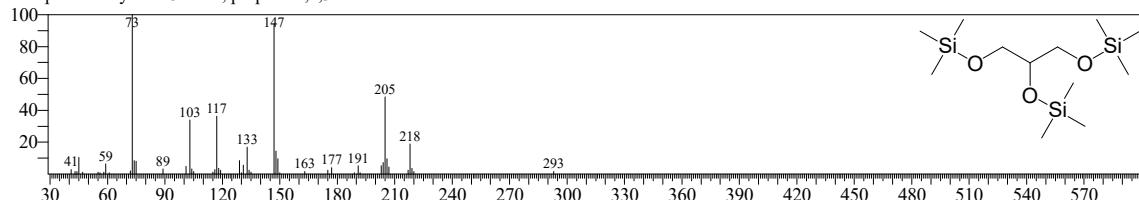
Hit#:1 Entry:402 Library:OA\_TMS\_DB5\_67min\_V3.lib

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



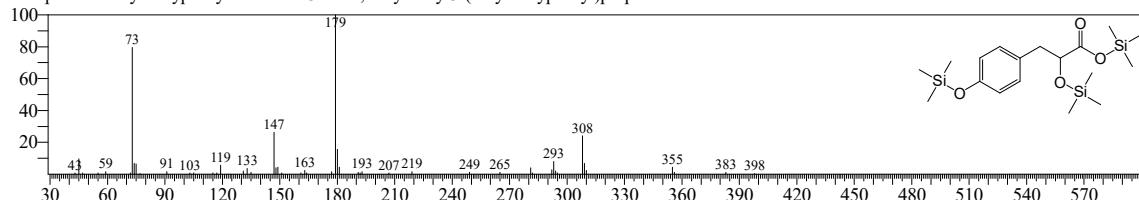
Hit#:2 Entry:77 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:36 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279  
 CompName:Glycerol-3TMS ; propane-1,2,3-triol



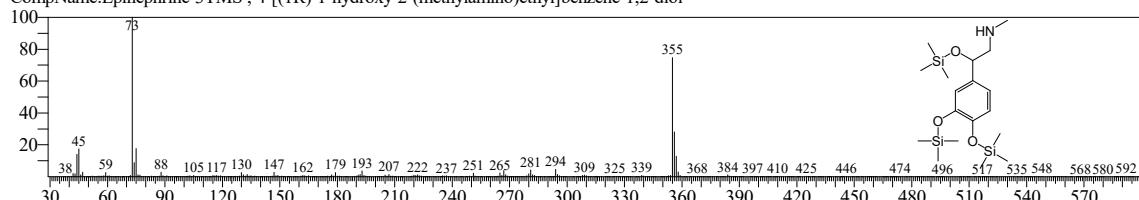
Hit#:3 Entry:382 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:34 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918  
 CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



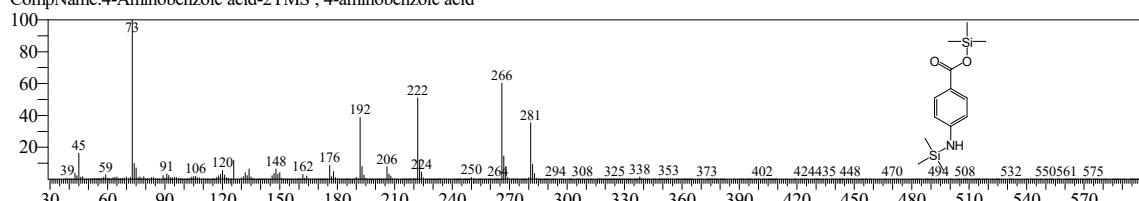
Hit#:4 Entry:343 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:34 Formula:C18H37NO2Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868  
 CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:5 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

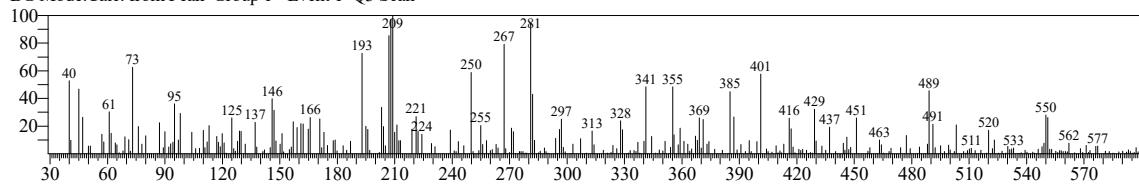
SI:34 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



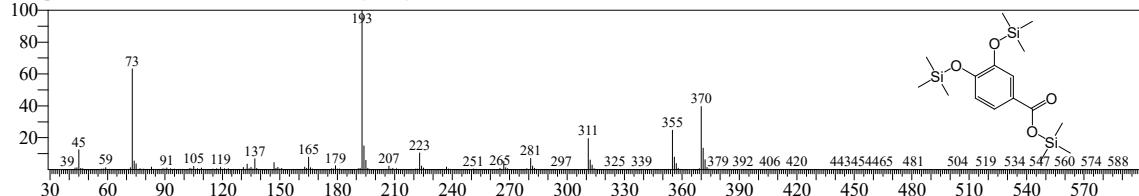
# TNAU

<<Target >>

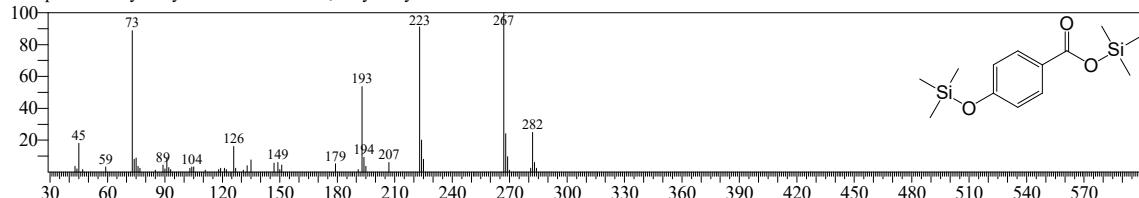
Line#:11 R.Time:31.245(Scan#5350) MassPeaks:305  
 RawMode:Averaged 31.240-31.250(5349-5351) BasePeak:209.05(526)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



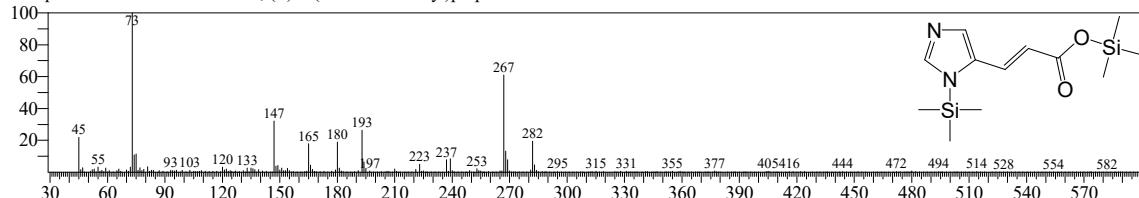
Hit#:1 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:29 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833  
 CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



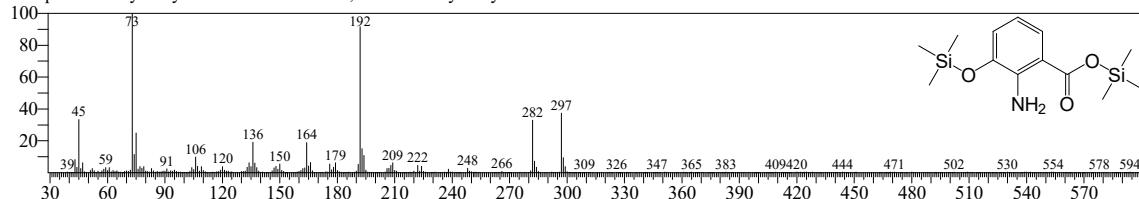
Hit#:2 Entry:211 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636  
 CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



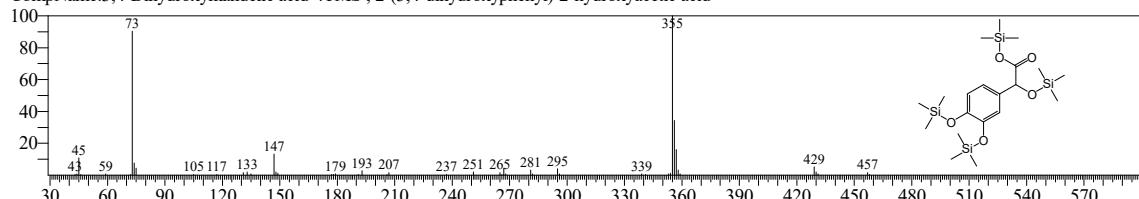
Hit#:3 Entry:438 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:28 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014  
 CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:4 Entry:290 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:27 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773  
 CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



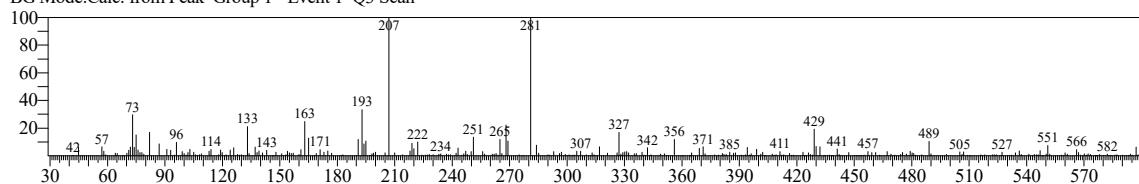
Hit#:5 Entry:402 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942  
 CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



# TNAU

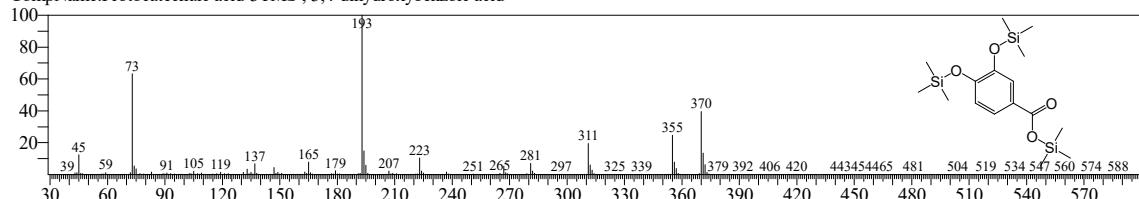
<<Target >>

Line#:12 R.Time:31.300(Scan#:5361) MassPeaks:287  
 RawMode:Averaged 31.295-31.305(5360-5362) BasePeak:207.00(1701)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



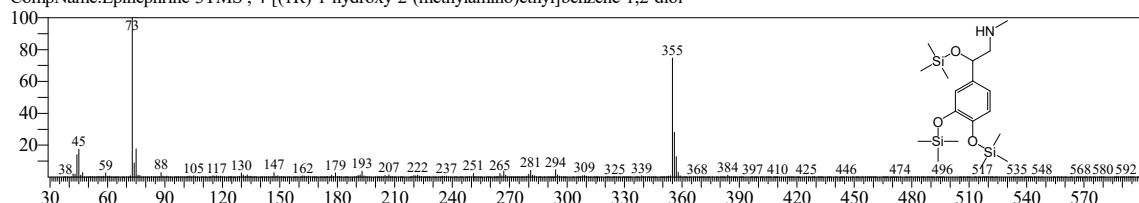
Hit#:1 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:44 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833  
 CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



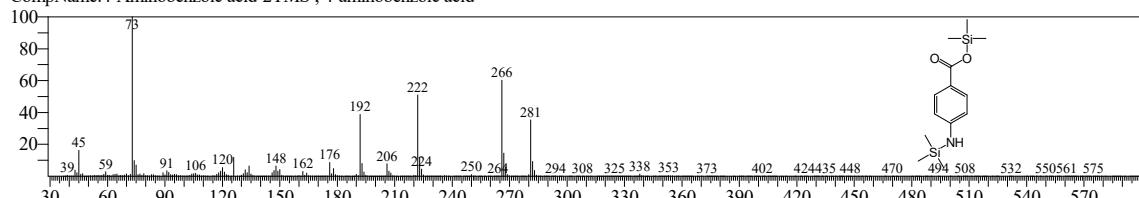
Hit#:2 Entry:343 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868  
 CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



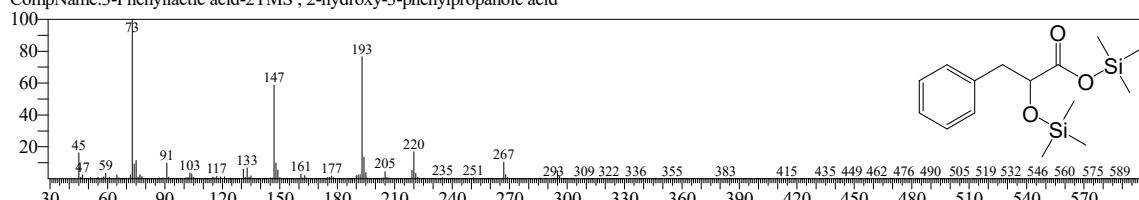
Hit#:3 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



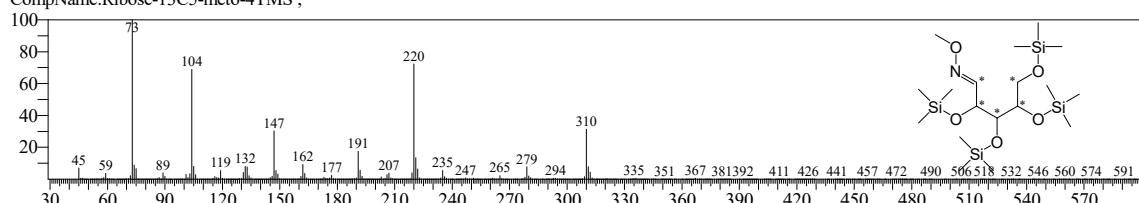
Hit#:4 Entry:194 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:36 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599  
 CompName:3-Phenylactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:5 Entry:256 Library:OA\_TMS\_DB5\_67min\_V3.lib

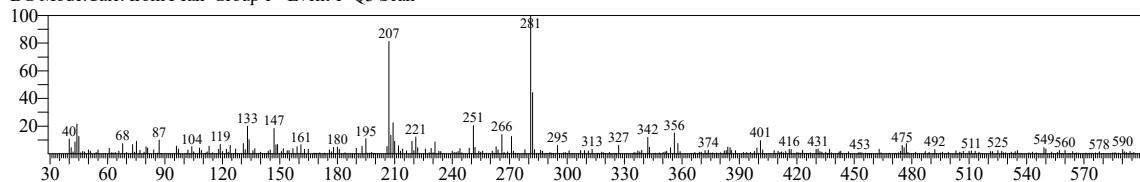
SI:36 Formula: CAS:0-00-0 MolWeight:472 RetIndex:1698  
 CompName:Ribose-13C5-meto-4TMS ;



# TNAU

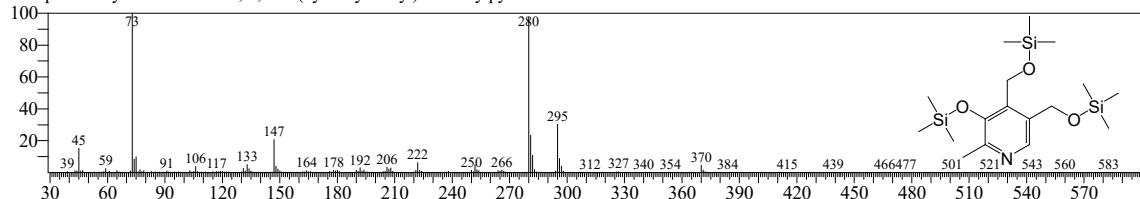
<<Target >>

Line#:13 R.Time:31.795(Scan#:5460) MassPeaks:311  
 RawMode:Averaged 31.790-31.800(5459-5461) BasePeak:281.05(1884)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



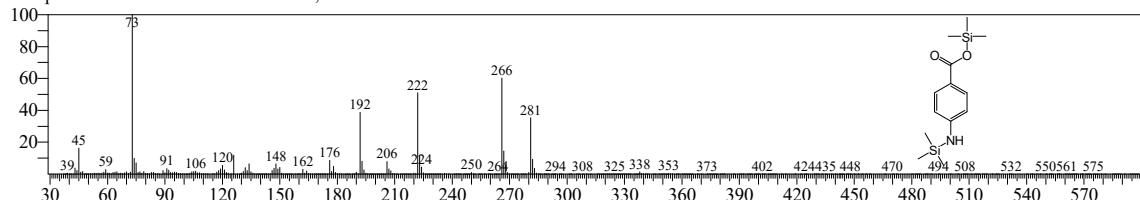
Hit#:1 Entry:384 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:41 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919  
 CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



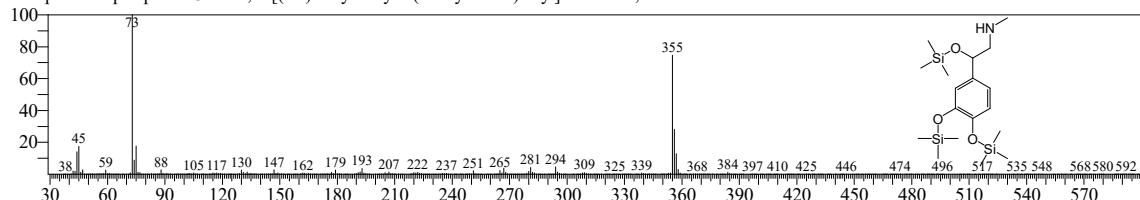
Hit#:2 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845  
 CompName:4 Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



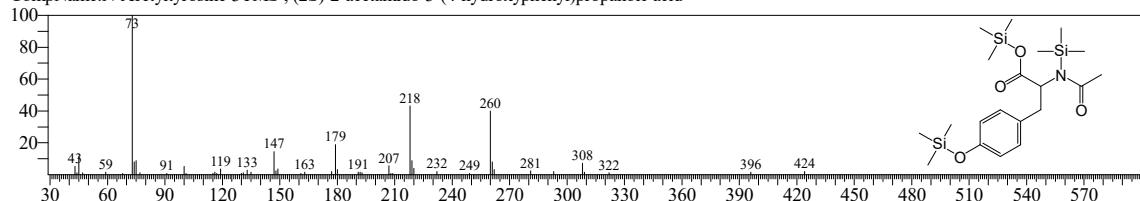
Hit#:3 Entry:343 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868  
 CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



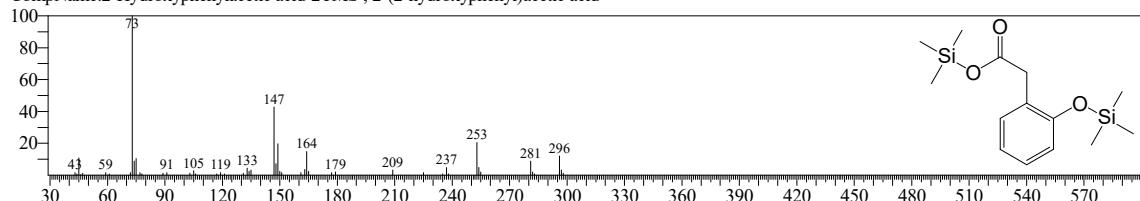
Hit#:4 Entry:461 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:36 Formula:C20H37NO4Si3 CAS:537-55-3 MolWeight:439 RetIndex:2119  
 CompName:N-Acetyltyrosine-3TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid



Hit#:5 Entry:184 Library:OA\_TMS\_DB5\_67min\_V3.lib

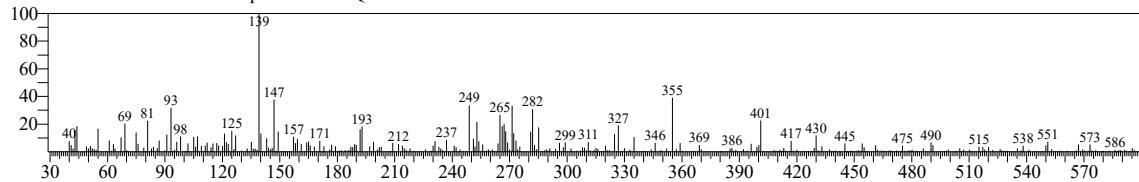
SI:35 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579  
 CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



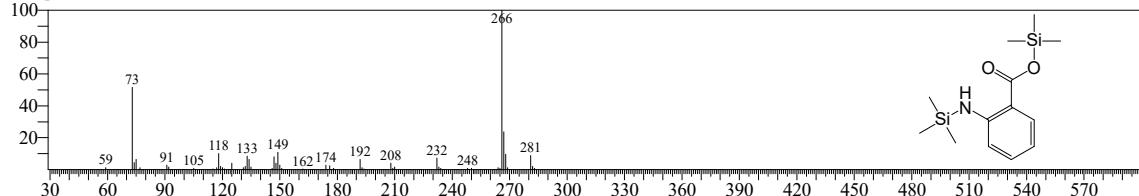
# TNAU

<<Target >>

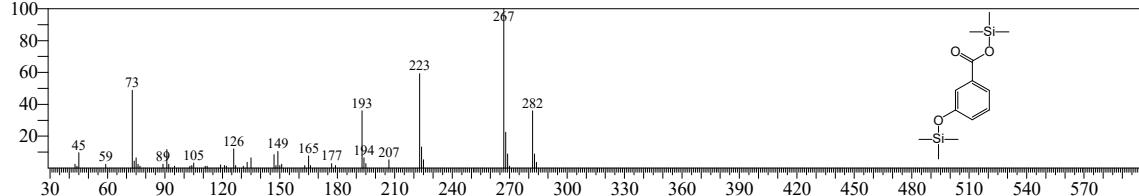
Line#:14 R.Time:31.895(Scan#:5480) MassPeaks:303  
 RawMode:Averaged 31.890-31.900(5479-5481) BasePeak:139.10(1752)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



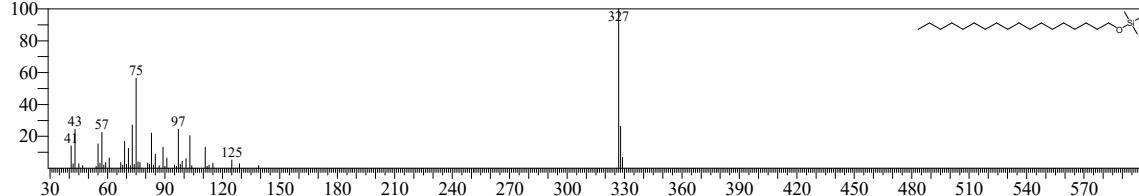
Hit#:1 Entry:203 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:27 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623  
 CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



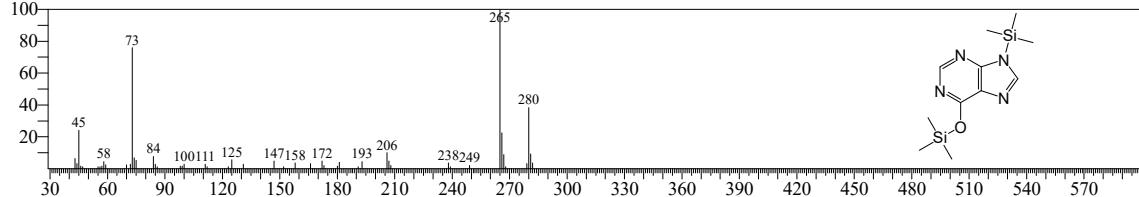
Hit#:2 Entry:179 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:27 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572  
 CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



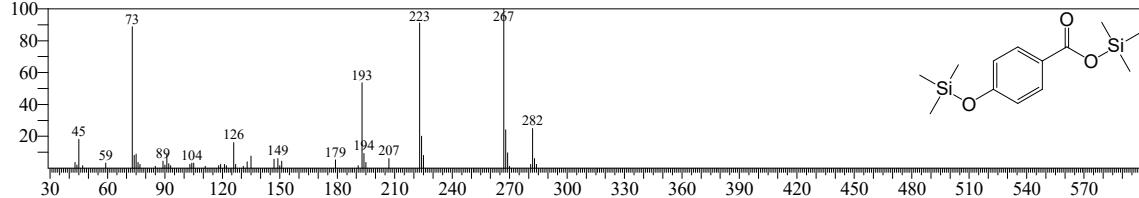
Hit#:3 Entry:477 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:27 Formula:C21H46OSi1 CAS:112-92-5 MolWeight:342 RetIndex:2156  
 CompName:Octadecanol-TMS ; octadecan-1-ol



Hit#:4 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



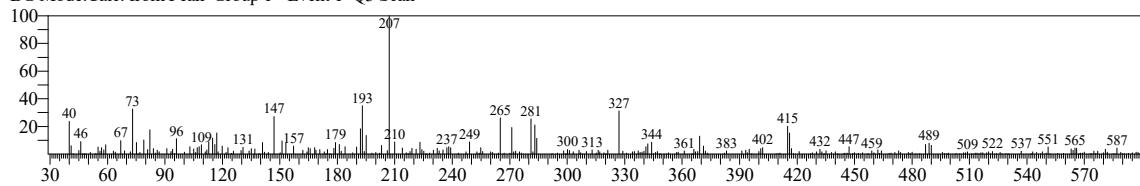
Hit#:5 Entry:211 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:26 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636  
 CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



# TNAU

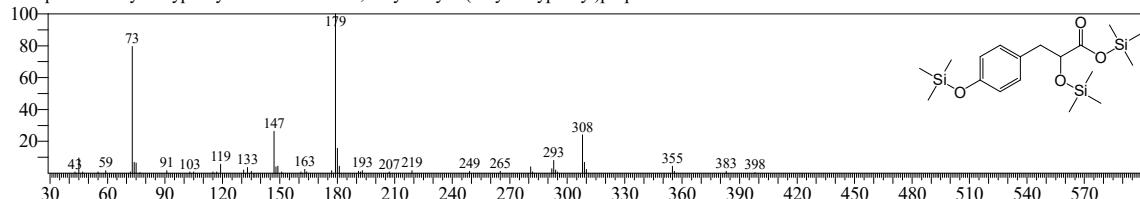
<<Target >>

Line#:15 R.Time:32.015(Scan#:5504) MassPeaks:302  
 RawMode:Averaged 32.010-32.020(5503-5505) BasePeak:207.05(1794)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



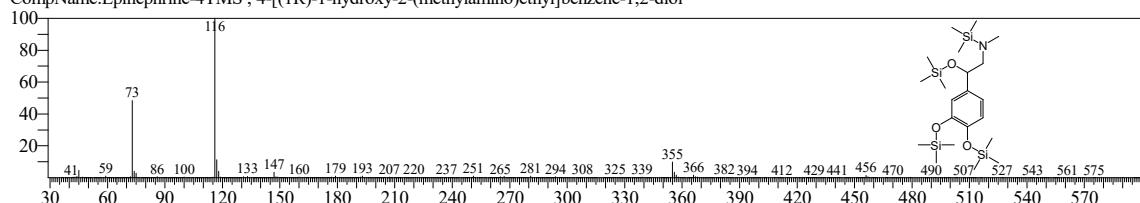
Hit#:1 Entry:382 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:36 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918  
 CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:2 Entry:431 Library:OA\_TMS\_DB5\_67min\_V3.lib

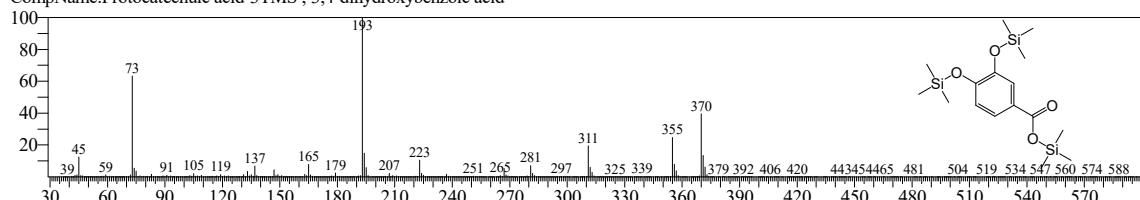
SI:34 Formula:C21H45NO3Si4 CAS:51-43-4 MolWeight:471 RetIndex:1989  
 CompName:Epinephrine-4TMS ; 4-[{(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:3 Entry:315 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:32 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833

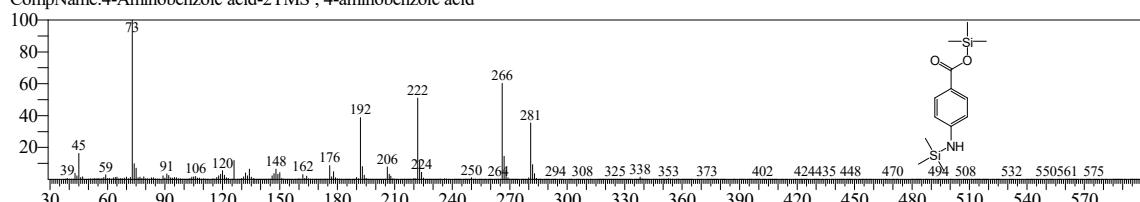
CompName:Protocatechic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:328 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845

CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:5 Entry:310 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:31 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822

CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

