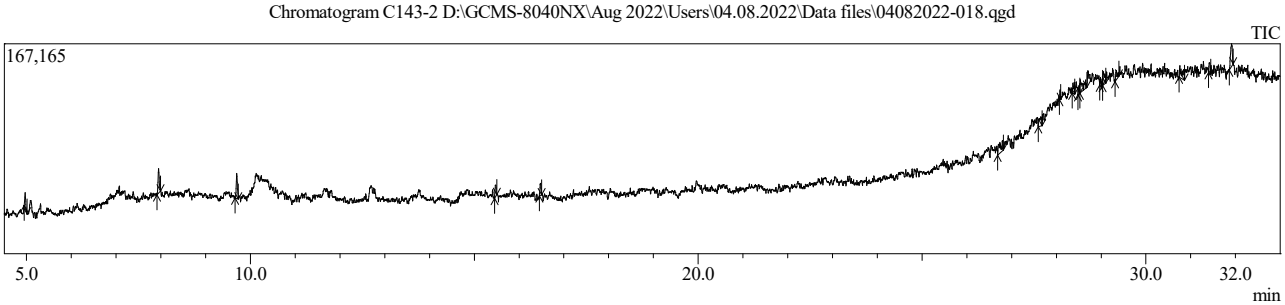
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 3:57:27 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C143-2
Sample ID	: C143-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 18
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-018.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-018.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 4:33:45 PM

Chromatogram C143-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-018.qgd



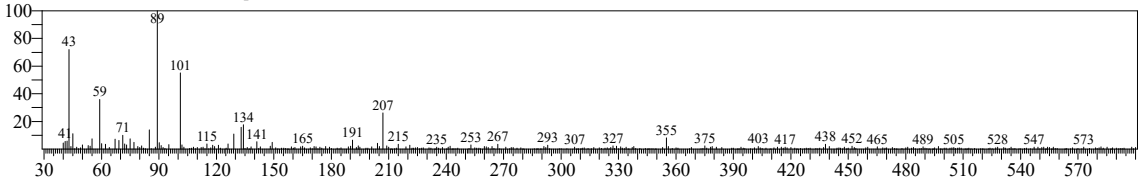
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.967	17503	4.13	12201	7.04	1.43	50	Methyl butanoate
2	7.947	37059	8.75	19594	11.31	1.89	87	Undecane
3	9.693	36125	8.52	19979	11.53	1.81	87	Tridecane
4	15.475	15769	3.72	9023	5.21	1.75	73	Phenol, 3,5-bis(1,1-dimethylethyl)-
5	16.479	16693	3.94	9466	5.46	1.76	75	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
6	26.794	38893	9.18	8500	4.91	4.58	46	Epinephrine-3TMS
7	27.605	27107	6.40	5505	3.18	4.92	32	4-Hydroxybenzoic acid-2TMS
8	28.081	5980	1.41	7699	4.44	0.78	30	Hypoxanthine-2TMS
9	28.397	17419	4.11	8927	5.15	1.95	37	3-Hydroxybenzoic acid-2TMS
10	28.495	11525	2.72	4983	2.88	2.31	29	3,4-Dihydroxymandelic acid-4TMS
11	28.535	43725	10.32	10296	5.94	4.25	33	Batyl alcohol-2TMS
12	28.980	9824	2.32	5729	3.31	1.71	36	Lyxose-4TMS(2)
13	29.045	27024	6.38	8910	5.14	3.03	41	3,4-Dihydroxymandelic acid-4TMS
14	29.330	16336	3.86	6790	3.92	2.41	35	Hypoxanthine-2TMS
15	30.758	37097	8.75	9238	5.33	4.02	34	Hippuric acid-TMS
16	31.420	14764	3.48	8558	4.94	1.73	33	Mandelic acid-2TMS
17	31.913	50918	12.02	17881	10.32	2.85	28	Methyl cis-4,7,10,13,16,19-Docosahexaenoate
		423761	100.00	173279	100.00			

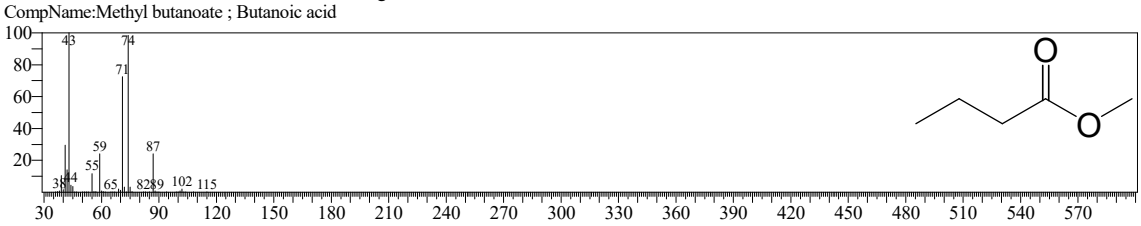
Library

TNAU

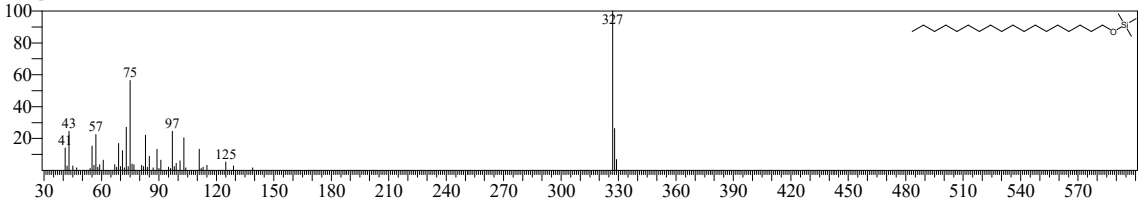
<< Target >>
Line#:1 R.Time:4.965(Scan#:94) MassPeaks:354
RawMode:Averaged 4.960-4.970(93-95) BasePeak:89.10(1804)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



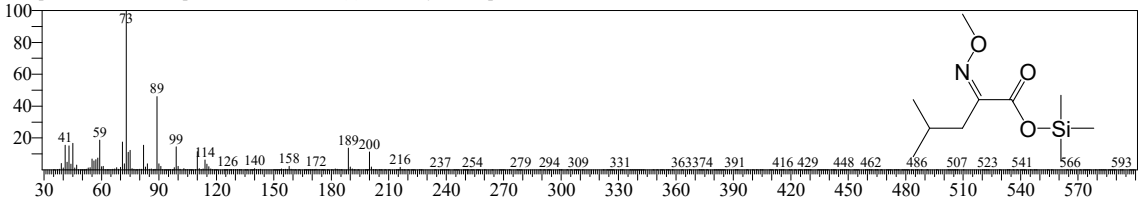
Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:50 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



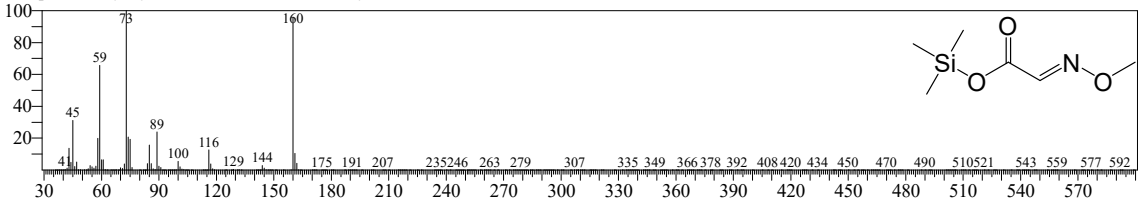
Hit#:2 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol



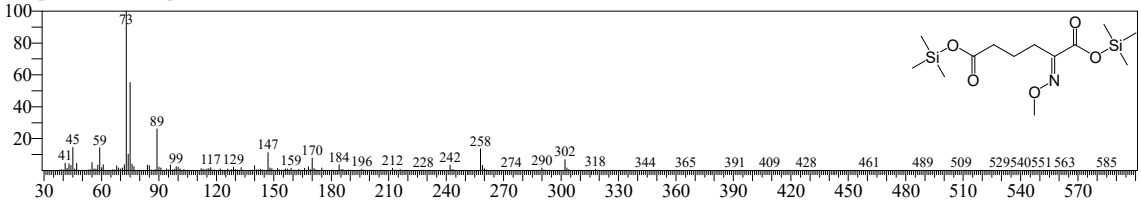
Hit#:3 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid



Hit#:4 Entry:2 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C6H13NO3Si CAS:298-12-4 MolWeight:175 RetIndex:990
CompName:Glyoxylic acid-meto-TMS ; oxaldehydic acid

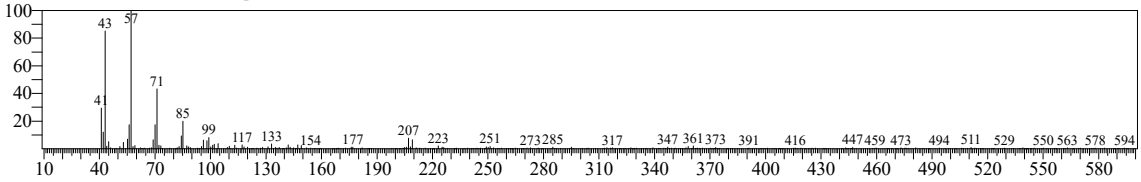


Hit#:5 Entry:215 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C13H27NO5Si2 CAS:3184-35-8 MolWeight:333 RetIndex:1640
CompName:2-Ketoadipic acid-meto-2TMS(1) ; 2-oxohexanedioic acid

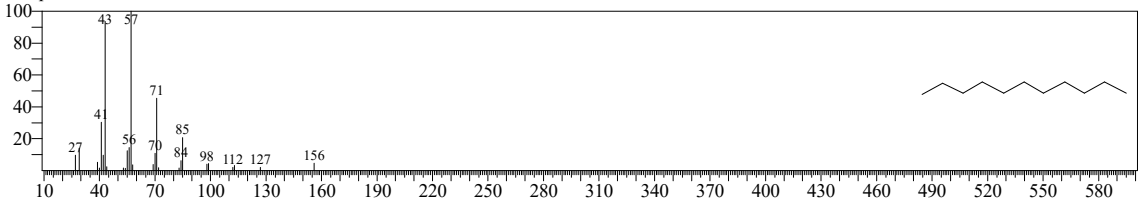


TNAU

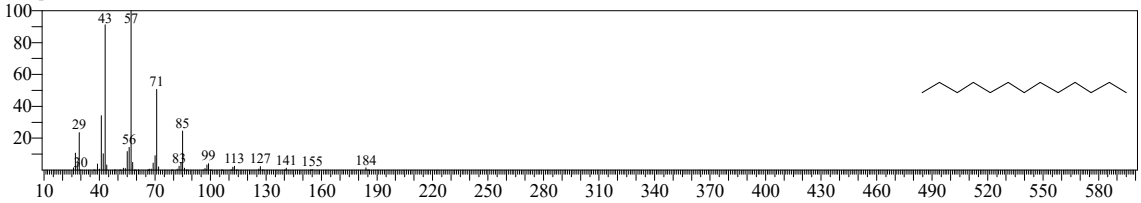
<< Target >>
Line#:2 R.Time:7.945(Scan#:690) MassPeaks:294
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(4395)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



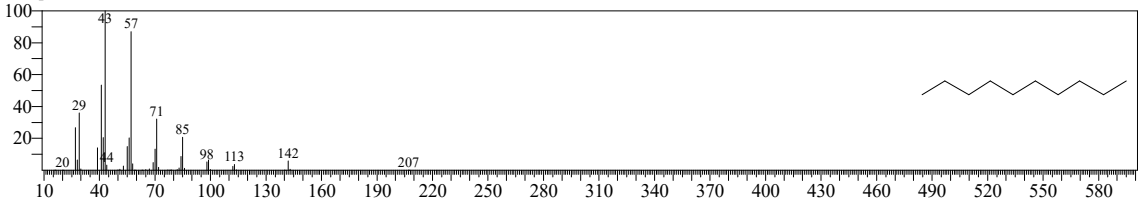
Hit#:1 Entry:12899 Library:NIST20R.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



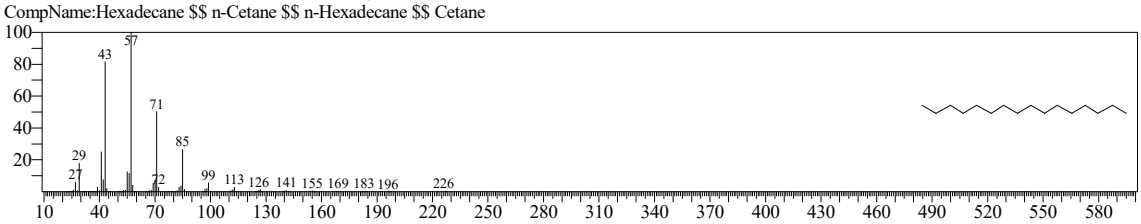
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



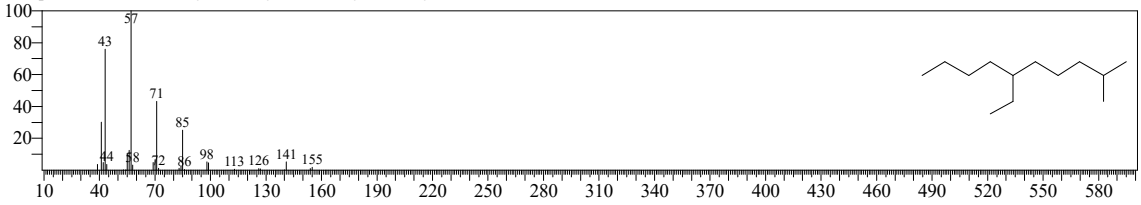
Hit#:3 Entry:9445 Library:NIST20R.lib
SI:85 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



Hit#:4 Entry:27737 Library:NIST20R.lib
SI:85 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

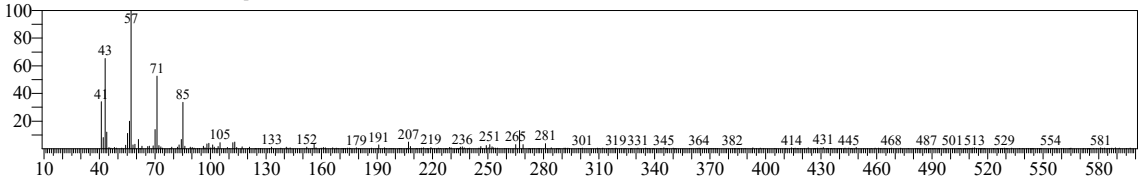


Hit#:5 Entry:40255 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:62108-21-8 MolWeight:184 RetIndex:1185
CompName:Decane, 6-ethyl-2-methyl- $$ 6-Ethyl-2-methyldecane #

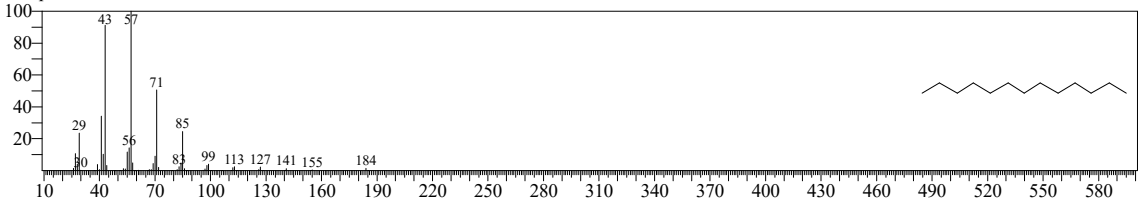


TNAU

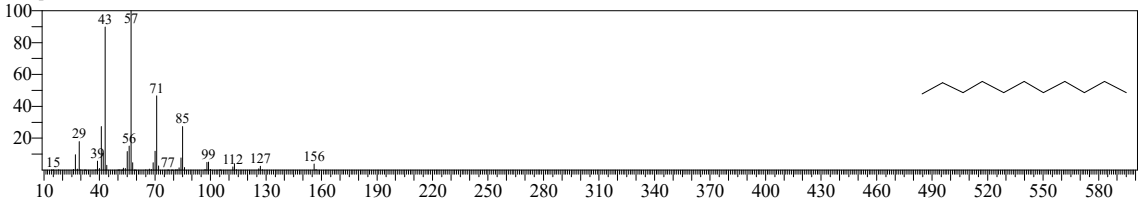
<< Target >>
Line#:3 R.Time:9.695(Scan#:1040) MassPeaks:291
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(4693)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



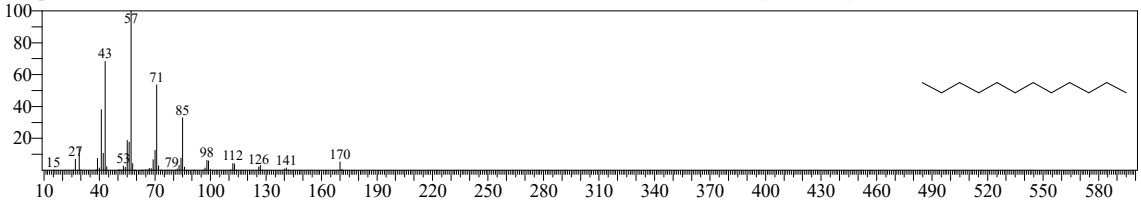
Hit#:1 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



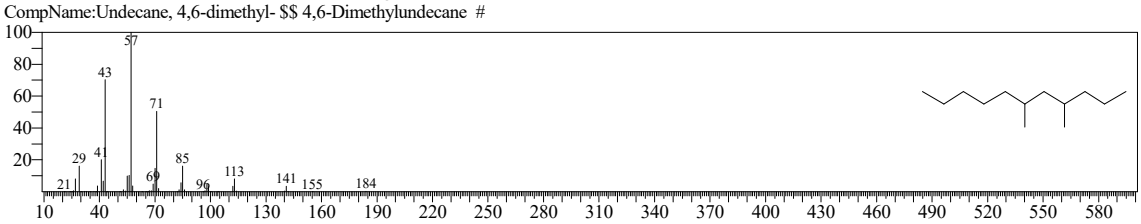
Hit#:2 Entry:21042 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



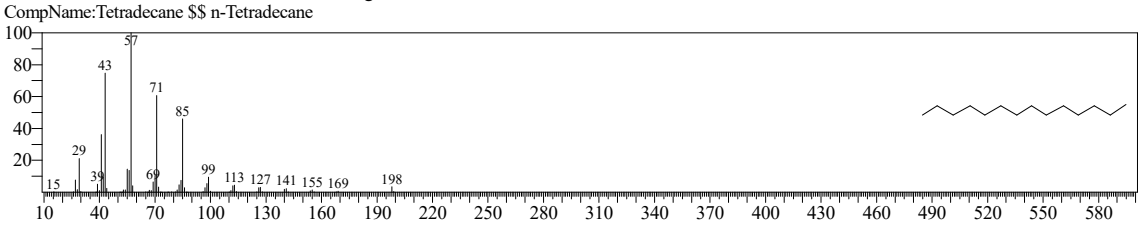
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:40271 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:17312-82-2 MolWeight:184 RetIndex:1185
CompName:Undecane, 4,6-dimethyl- $$ 4,6-Dimethylundecane #

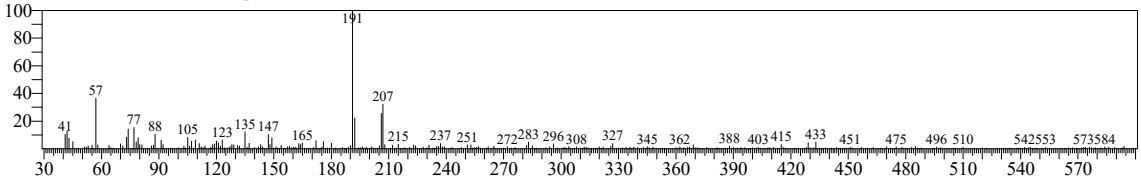


Hit#:5 Entry:22497 Library:NIST20R.lib
SI:85 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

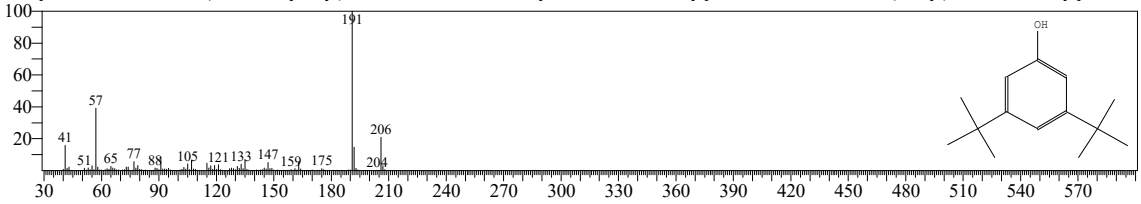


TNAU

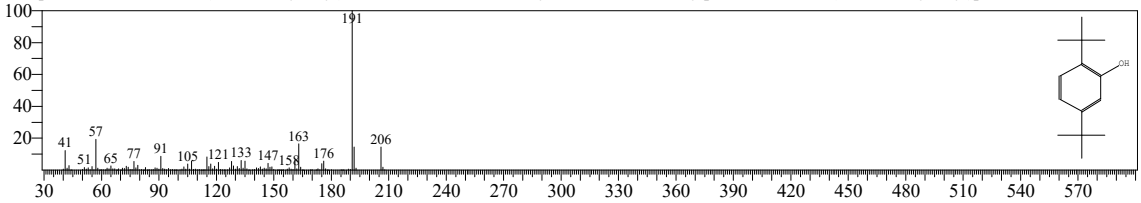
<< Target >>
Line#:4 R.Time:15.475(Scan#:2196) MassPeaks:302
RawMode:Averaged 15.470-15.480(2195-2197) BasePeak:191.05(1956)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



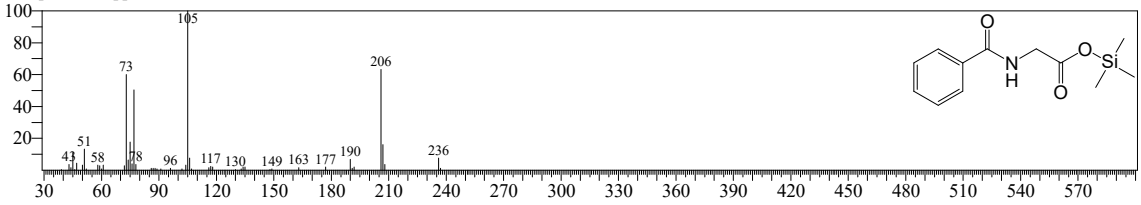
Hit#:1 Entry:24108 Library:NIST20R.lib
SI:73 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



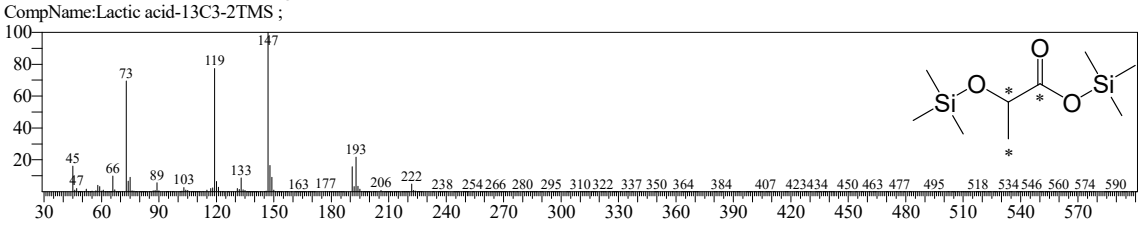
Hit#:2 Entry:24097 Library:NIST20R.lib
SI:70 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



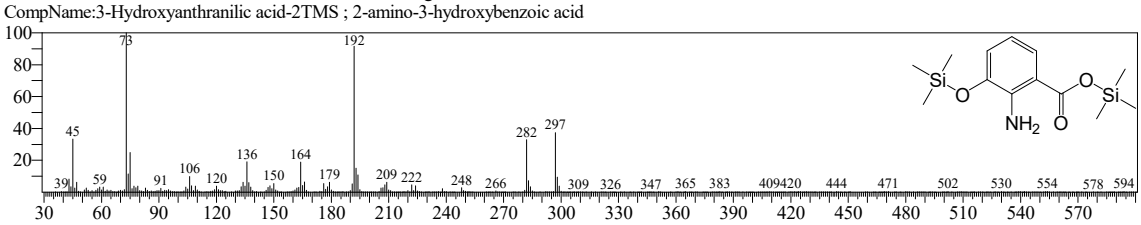
Hit#:3 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



Hit#:4 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;

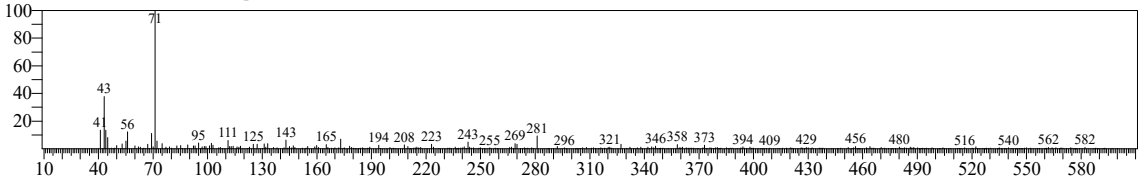


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

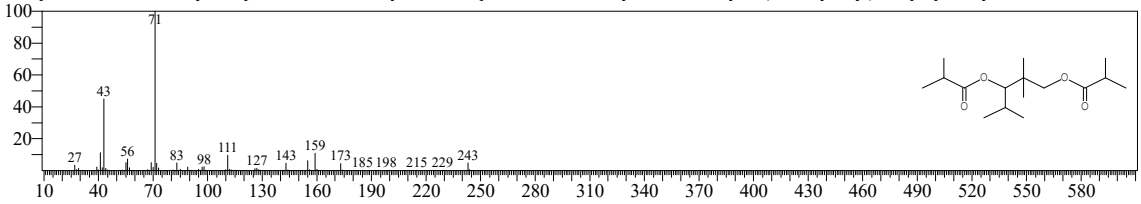


TNAU

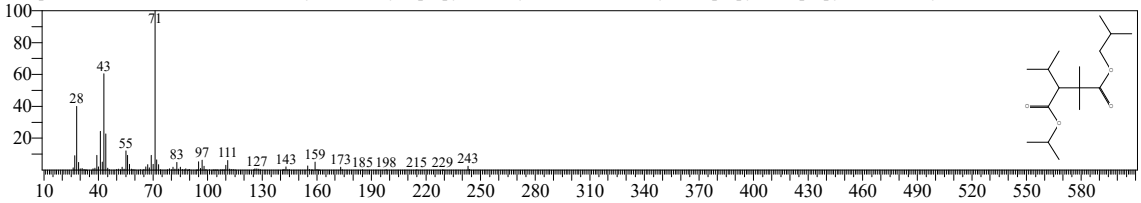
<< Target >>
Line#:5 R.Time:16.480(Scan#:2397) MassPeaks:314
RawMode:Averaged 16.475-16.485(2396-2398) BasePeak:71.05(3093)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



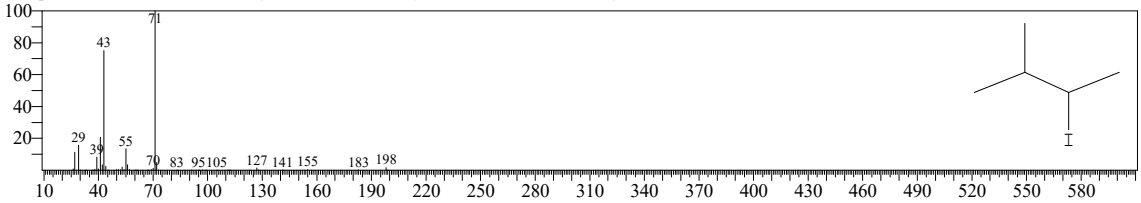
Hit#:1 Entry:34622 Library:NIST20R.lib
SI:75 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan



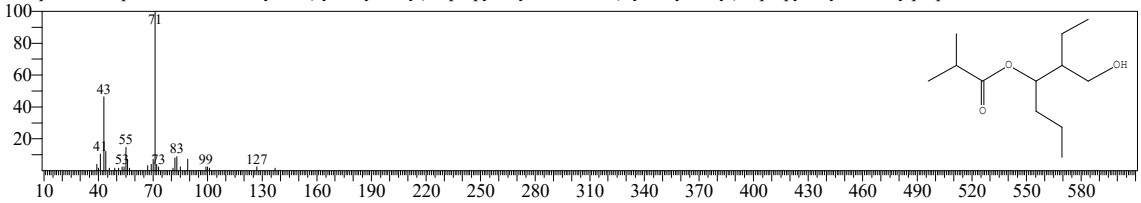
Hit#:2 Entry:146809 Library:NIST20M1.lib
SI:74 Formula:C16H30O4 CAS:0-00-0 MolWeight:286 RetIndex:1605
CompName:Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester $$ 1-Isobutyl 4-isopropyl 3-isopropyl-2,2-dimethylsuccinate #



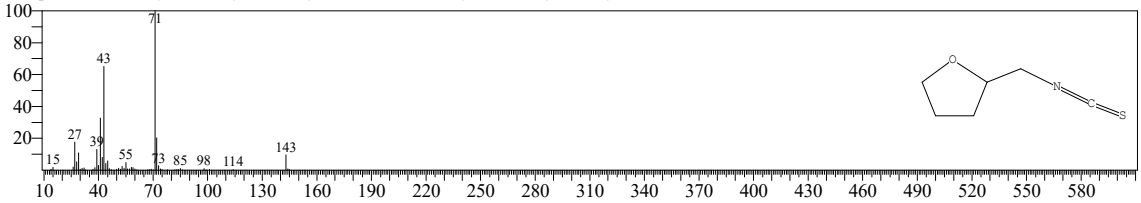
Hit#:3 Entry:50931 Library:NIST20M1.lib
SI:71 Formula:C5H11I CAS:18295-27-7 MolWeight:198 RetIndex:804
CompName:Butane, 2-iodo-3-methyl- $$ 2-Iodo-3-methylbutane $$ Butane, 3-methyl-2-iodo



Hit#:4 Entry:68586 Library:NIST20M1.lib
SI:70 Formula:C12H24O3 CAS:74367-32-1 MolWeight:216 RetIndex:1432
CompName:Propanoic acid, 2-methyl-, 2-(hydroxymethyl)-1-propylbutyl ester $$ 2-(Hydroxymethyl)-1-propylbutyl 2-methylpropanoate #

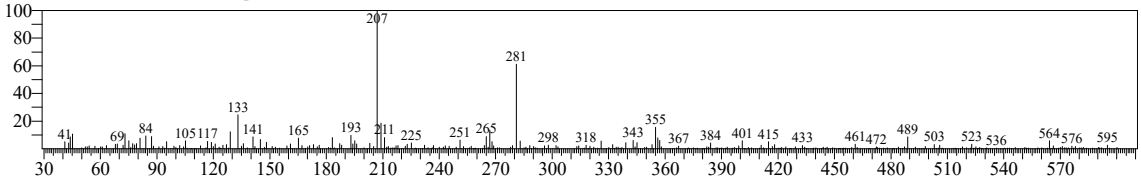


Hit#:5 Entry:13726 Library:NIST20M1.lib
SI:70 Formula:C6H9NOS CAS:36810-87-4 MolWeight:143 RetIndex:0
CompName:2-Tetrahydrofurfuryl isothiocyanate $$ 2-(Isothiocyanatomethyl)tetrahydrofuran #

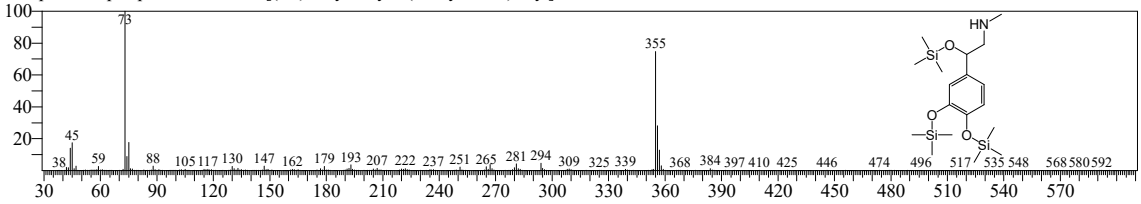


TNAU

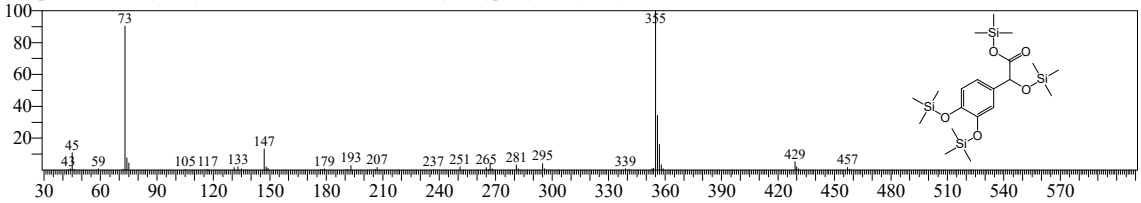
<< Target >>
Line#:6 R.Time:26.795(Scan#:4460) MassPeaks:301
RawMode:Averaged 26.790-26.800(4459-4461) BasePeak:207.05(1998)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



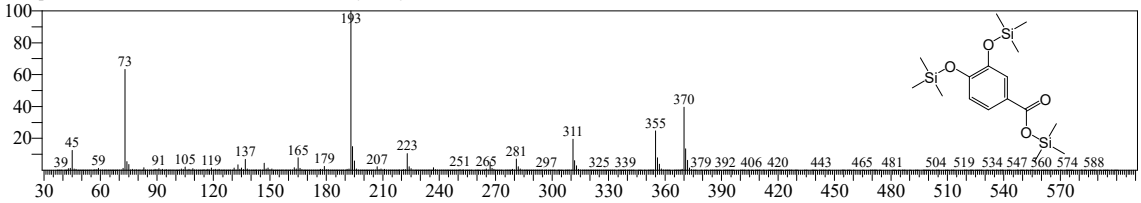
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



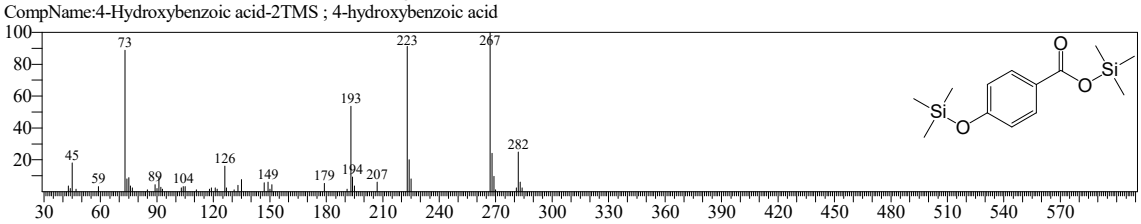
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



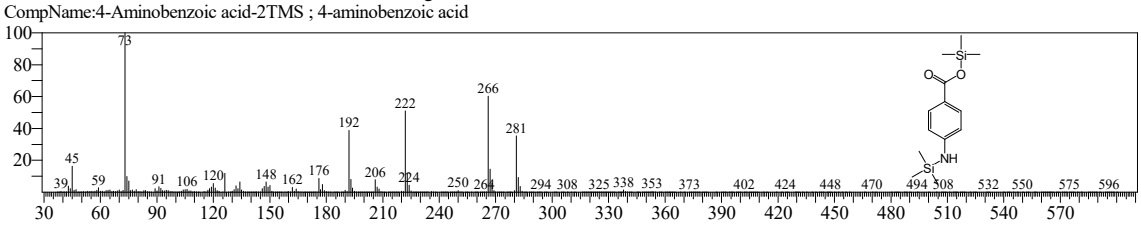
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

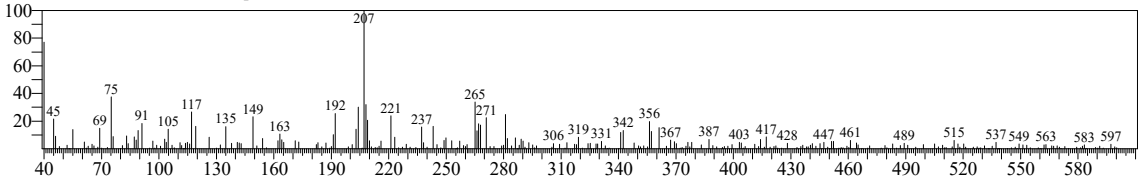


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

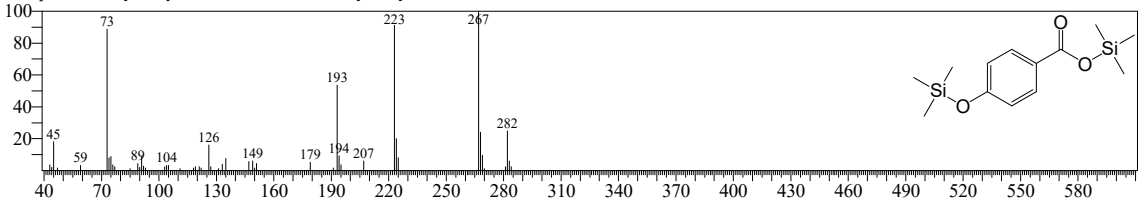


TNAU

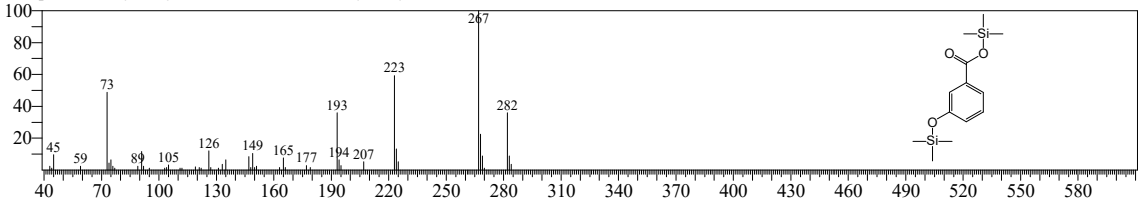
<< Target >>
Line#:7 R.Time:27.605(Scan#:4622) MassPeaks:278
RawMode:Averaged 27.600-27.610(4621-4623) BasePeak:207.05(1012)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



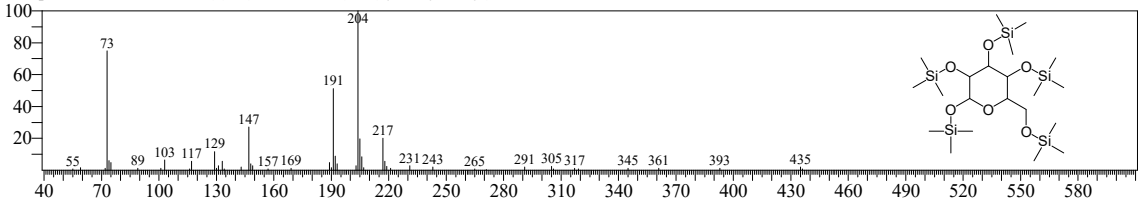
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



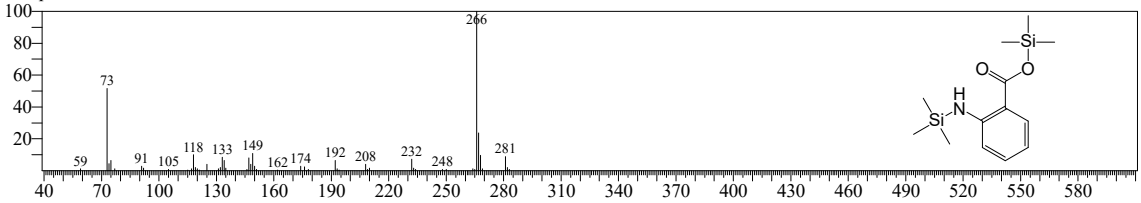
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



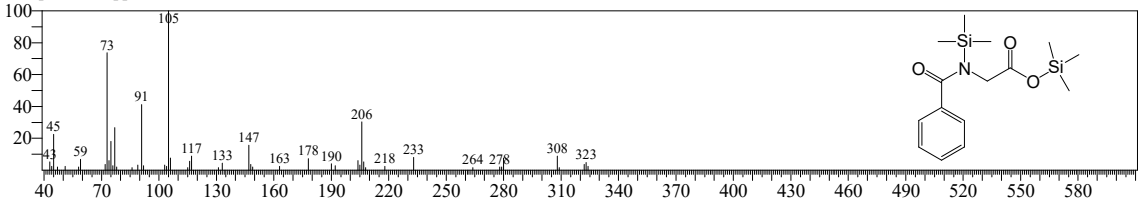
Hit#:3 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

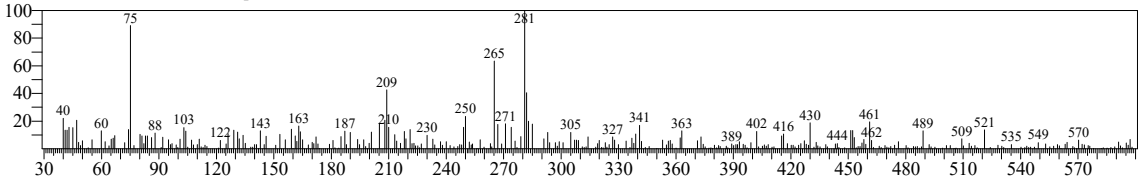


Hit#:5 Entry:307 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C15H25NO3Si2 CAS:66407-11-2 MolWeight:323 RetIndex:1819
CompName:Hippuric acid-2TMS ; 2-benzamidoacetic acid

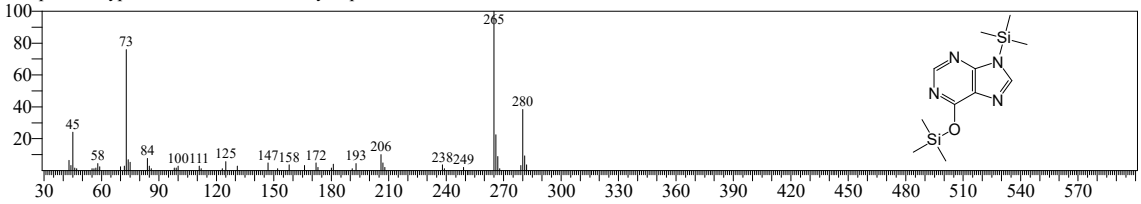


TNAU

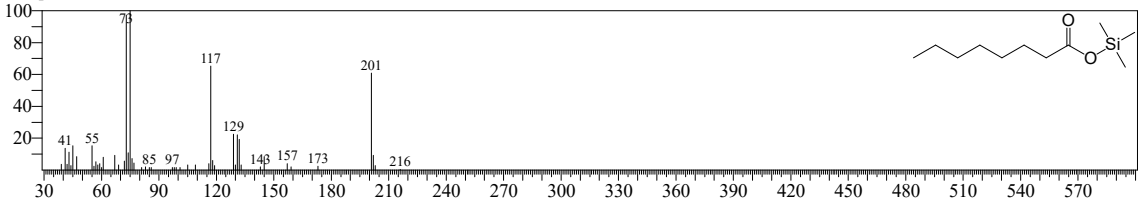
<< Target >>
Line#:8 R.Time:28.080(Scan#:4717) MassPeaks:326
RawMode:Averaged 28.075-28.085(4716-4718) BasePeak:281.00(860)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



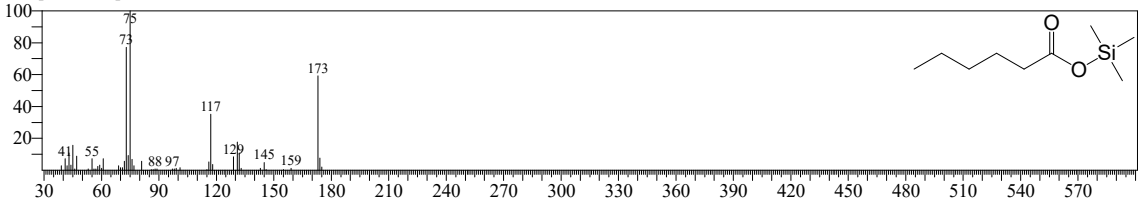
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



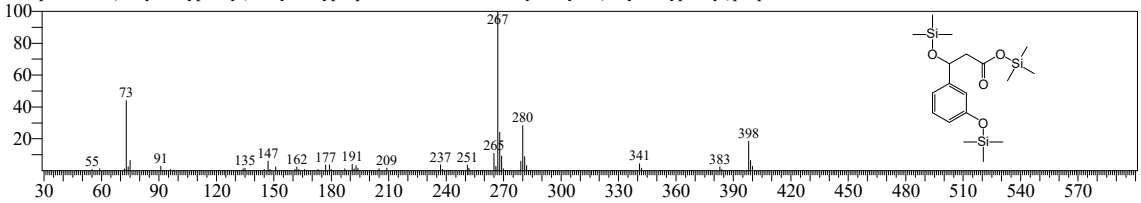
Hit#:2 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
CompName:Octanoic acid-TMS ; octanoic acid



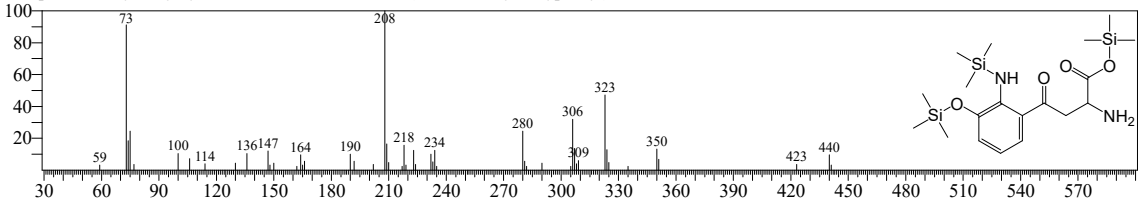
Hit#:3 Entry:11 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid



Hit#:4 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

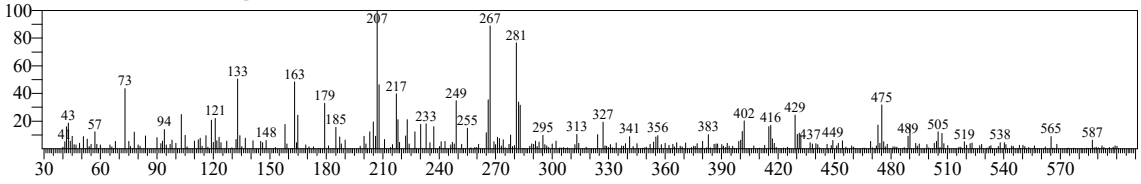


Hit#:5 Entry:506 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C19H36N2O4Si3 CAS:2147-61-7 MolWeight:440 RetIndex:2375
CompName:3-Hydroxy-kynurenine-3TMS ; 2-amino-4-(2-amino-3-hydroxyphenyl)-4-oxobutanoic acid

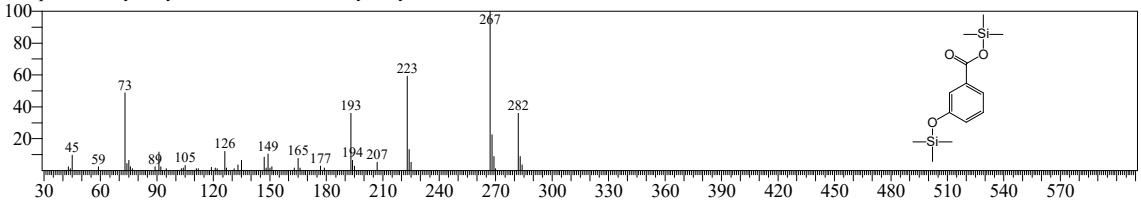


TNAU

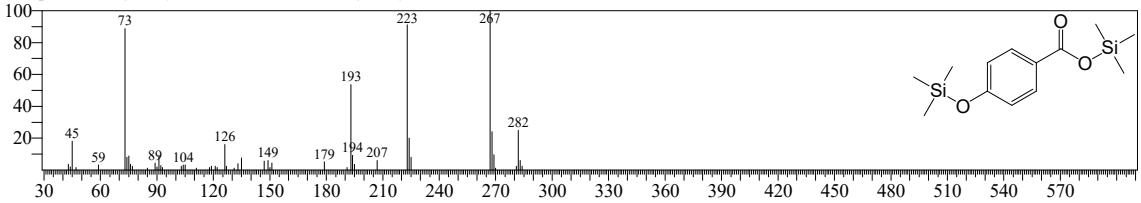
<< Target >>
Line#:9 R.Time:28.395(Scan#:4780) MassPeaks:304
RawMode:Averaged 28.390-28.400(4779-4781) BasePeak:207.05(860)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



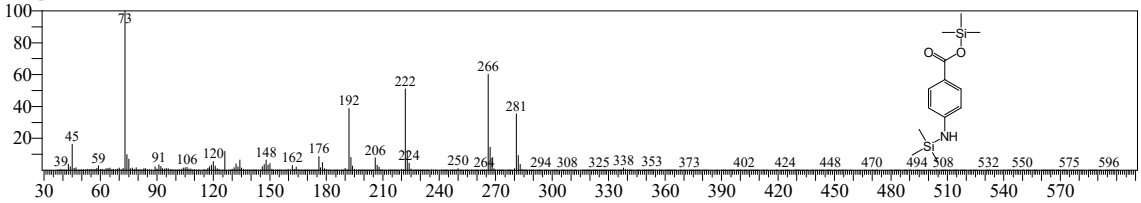
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



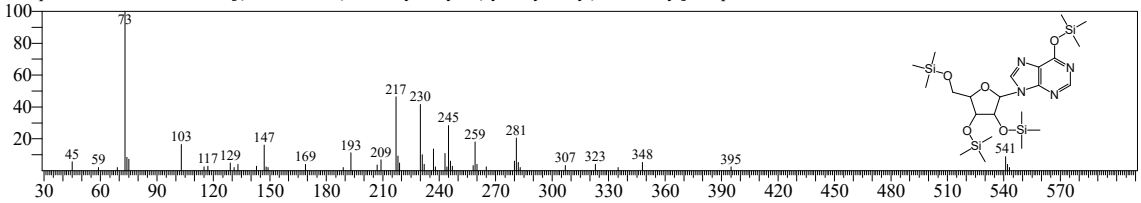
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



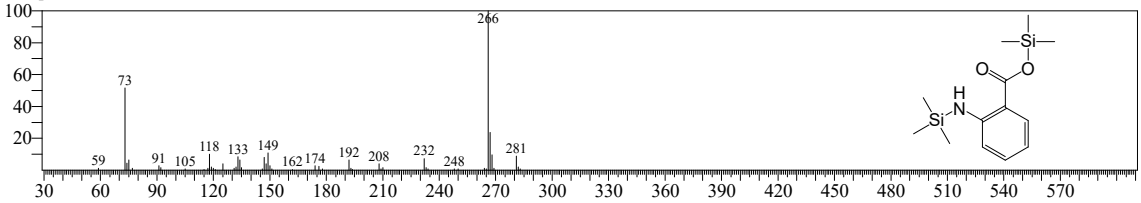
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

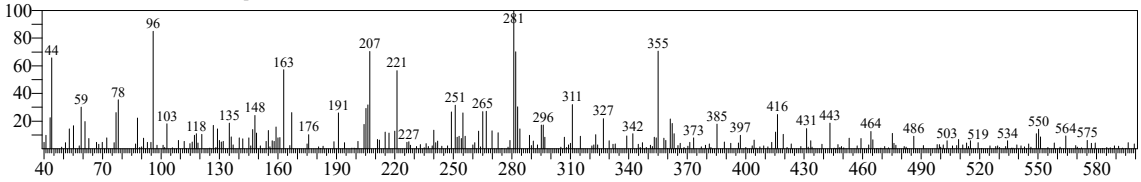


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

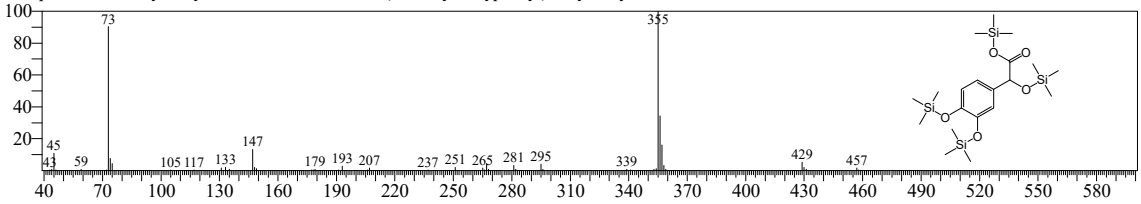


TNAU

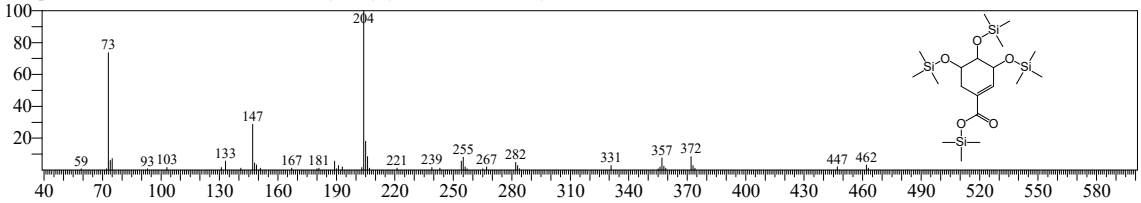
<< Target >>
Line#:10 R.Time:28.495(Scan#:4800) MassPeaks:279
RawMode:Averaged 28.490-28.500(4799-4801) BasePeak:281.05(592)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



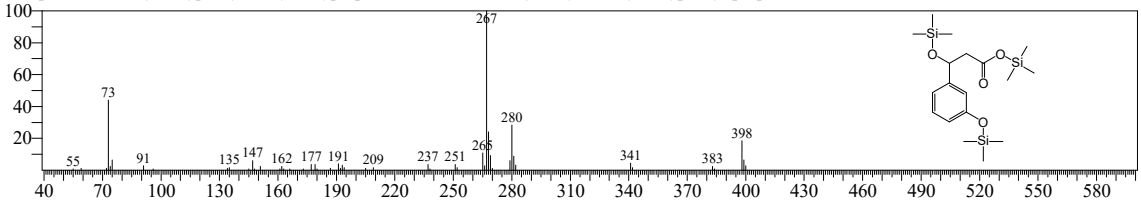
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



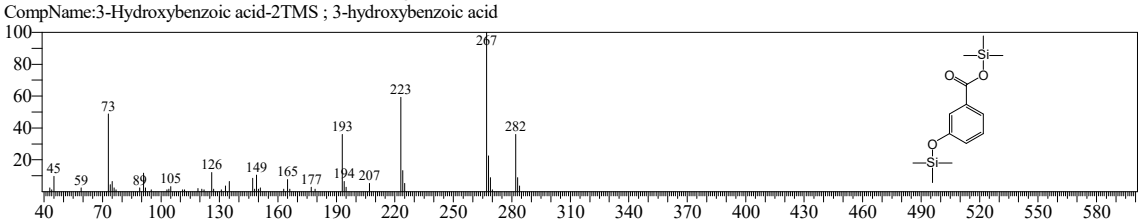
Hit#:2 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid



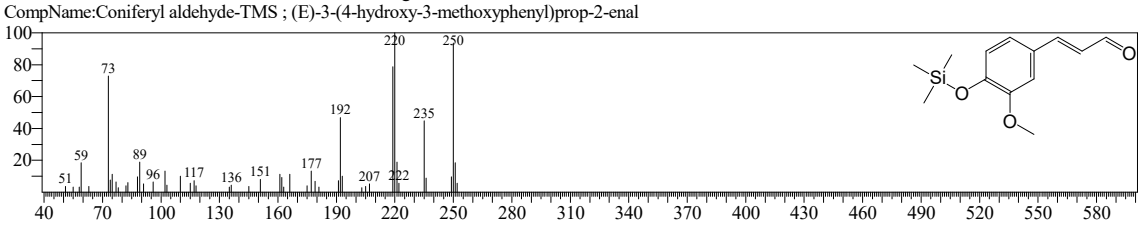
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

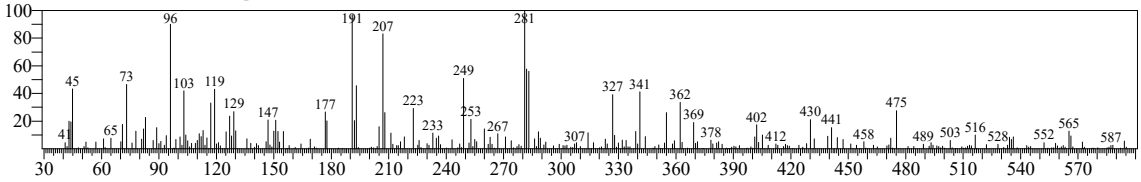


Hit#:5 Entry:339 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H18O3Si CAS:458-36-6 MolWeight:250 RetIndex:1859
CompName:Coniferyl aldehyde-TMS ; (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal

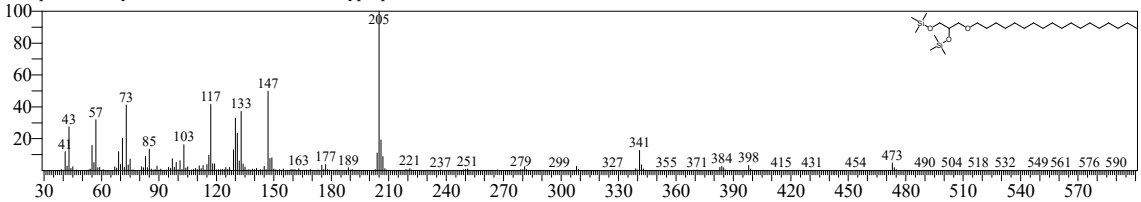


TNAU

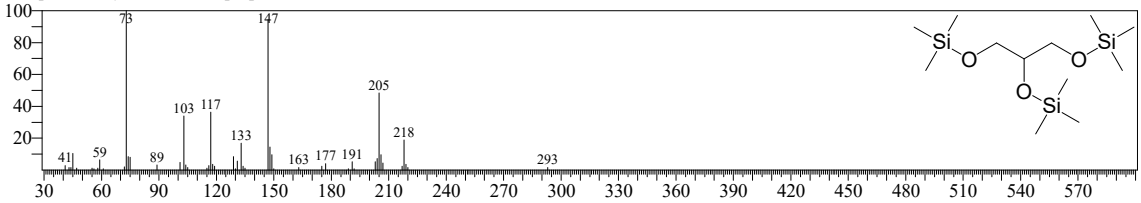
<< Target >>
Line#:11 R.Time:28.535(Scan#:4808) MassPeaks:292
RawMode:Averaged 28.530-28.540(4807-4809) BasePeak:281.05(756)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



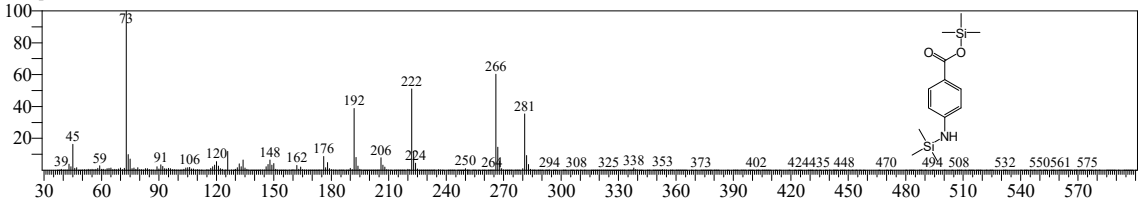
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



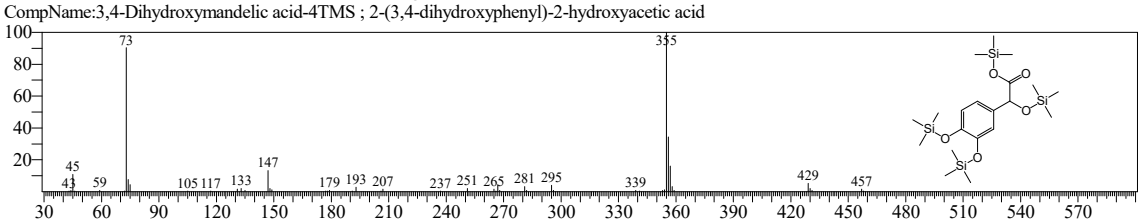
Hit#:2 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



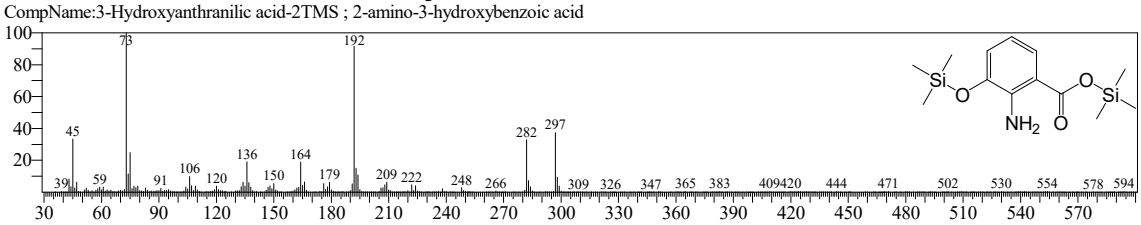
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



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

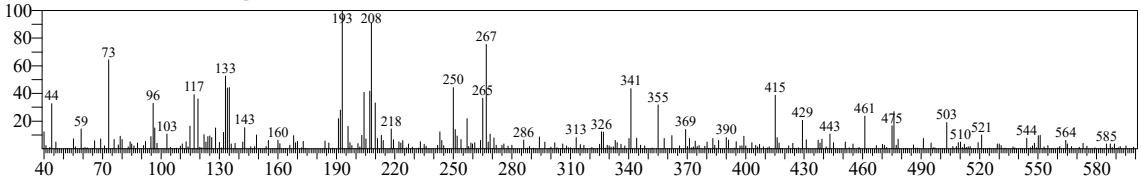


Hit#:5 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

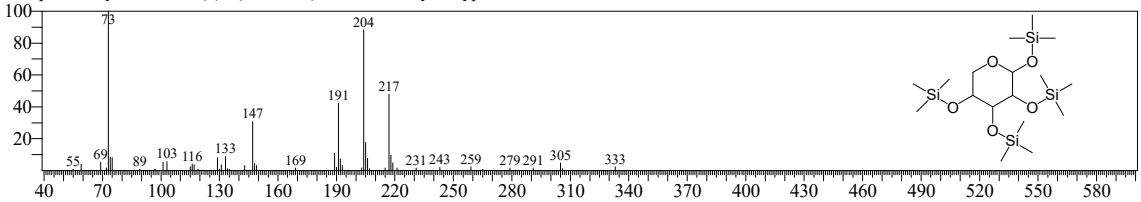


TNAU

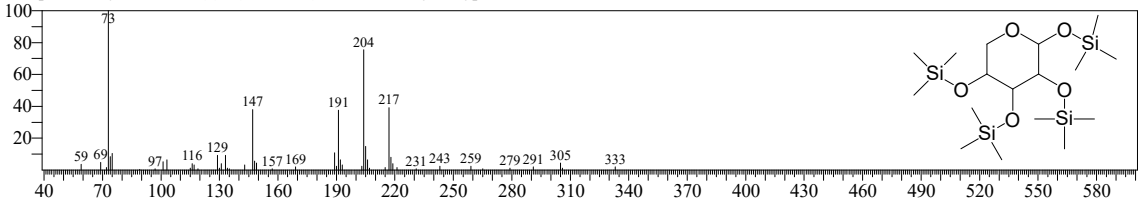
<< Target >>
Line#:12 R.Time:28.980(Scan#:4897) MassPeaks:292
RawMode:Averaged 28.975-28.985(4896-4898) BasePeak:193.00(755)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



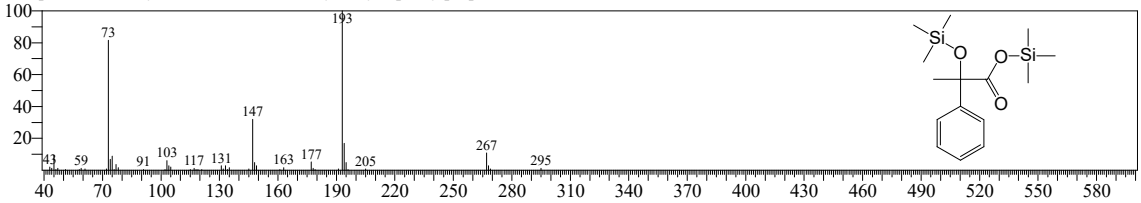
Hit#:1 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



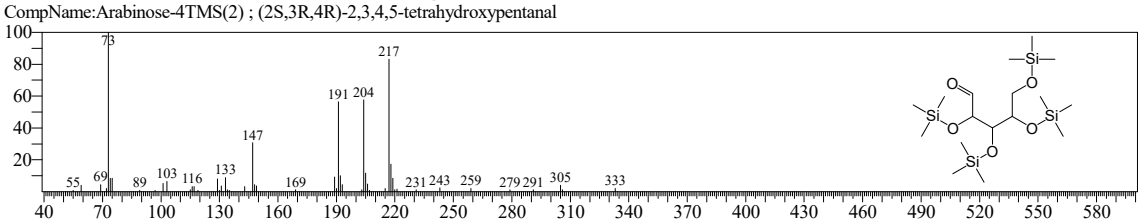
Hit#:2 Entry:295 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1784
CompName:Xylose-4TMS(2) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal



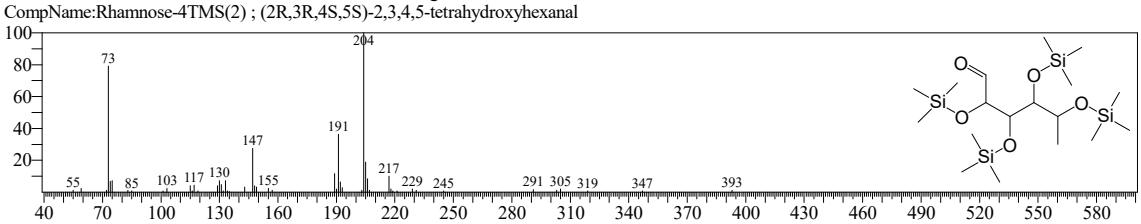
Hit#:3 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:4 Entry:232 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C17H42O5Si4 CAS:10323-20-3 MolWeight:438 RetIndex:1667
CompName:Arabinose-4TMS(2) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal

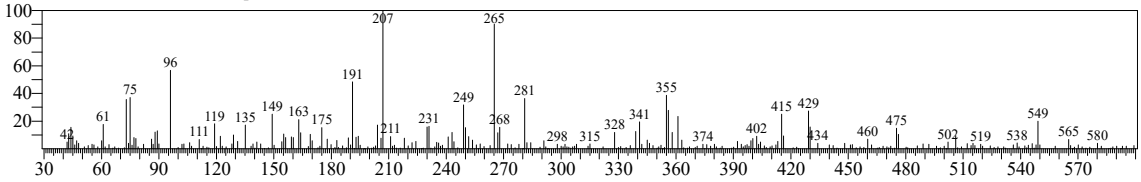


Hit#:5 Entry:261 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1719
CompName:Rhamnose-4TMS(2) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

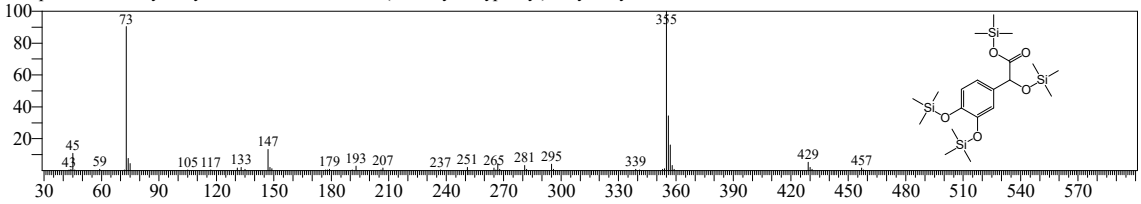


TNAU

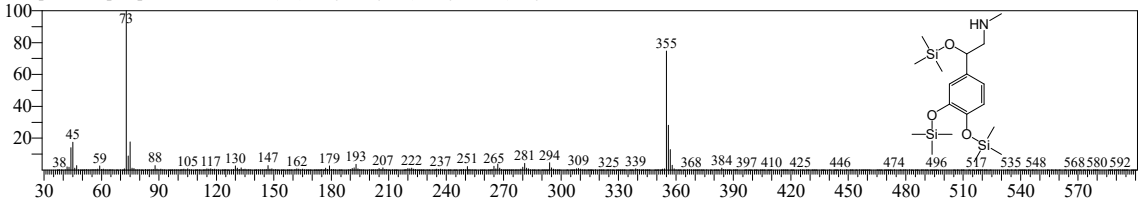
<< Target >>
Line#:13 R.Time:29.045(Scan#:4910) MassPeaks:294
RawMode:Averaged 29.040-29.050(4909-4911) BasePeak:207.05(1087)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



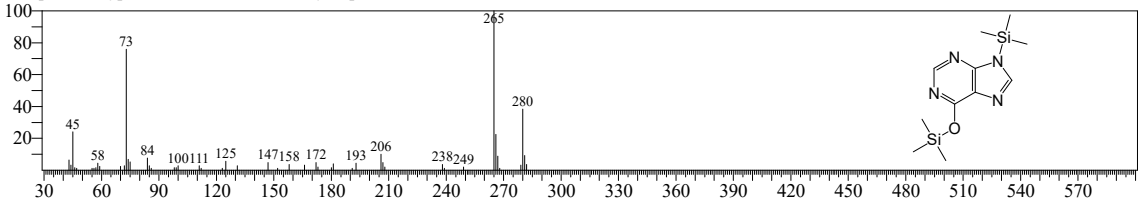
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



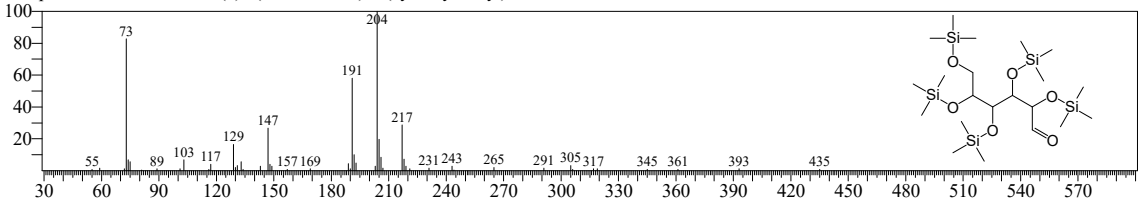
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



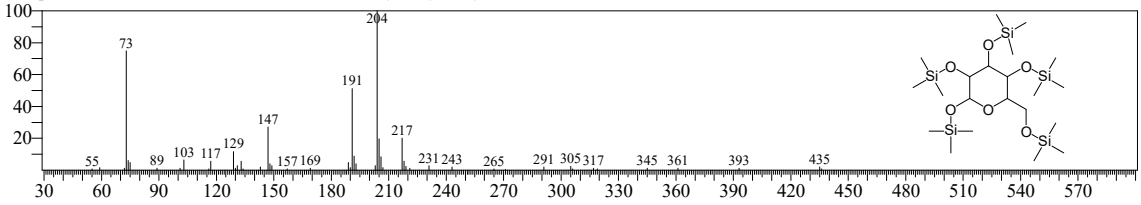
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
SI:32 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

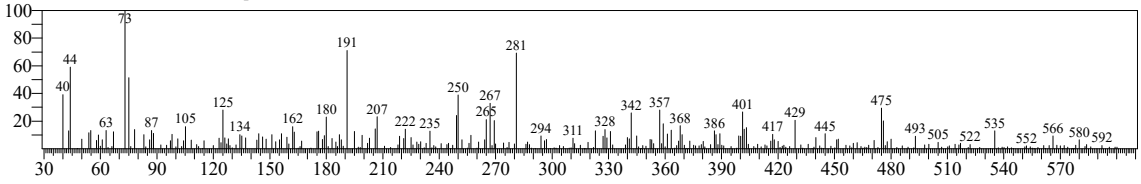


Hit#:5 Entry:386 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:1922
CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

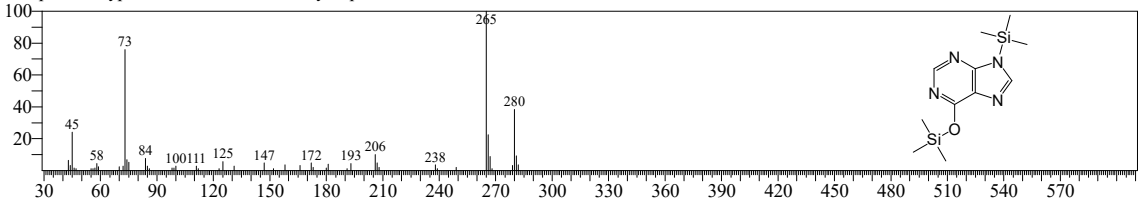


TNAU

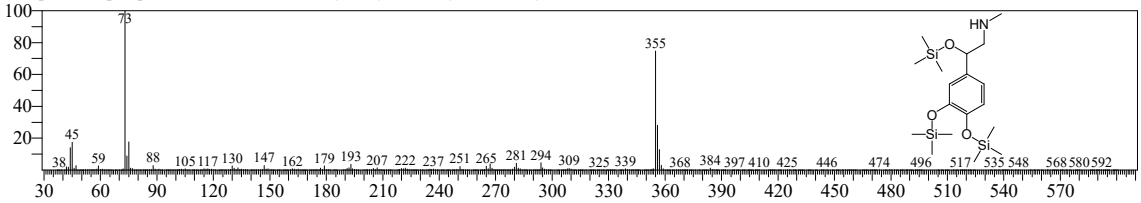
<< Target >>
Line#:14 R.Time:29.330(Scan#:4967) MassPeaks:303
RawMode:Averaged 29.325-29.335(4966-4968) BasePeak:73.10(895)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



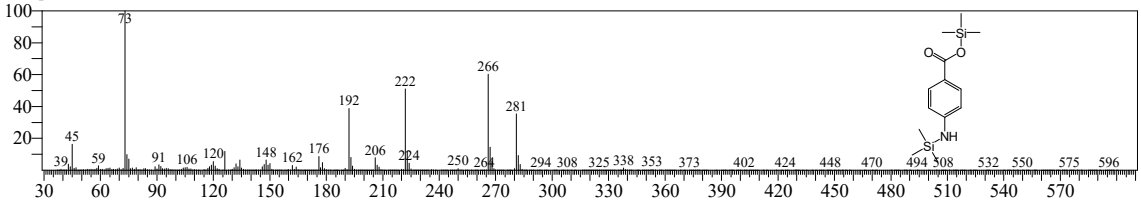
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



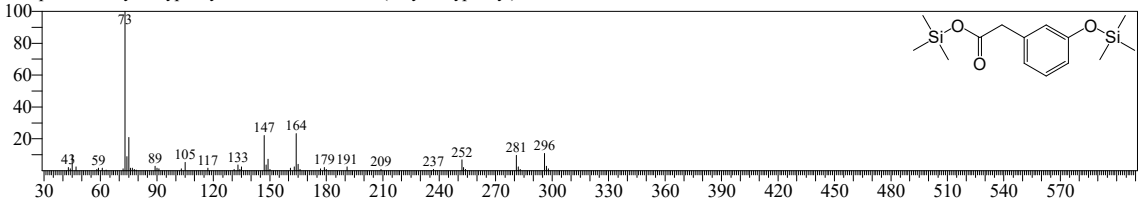
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



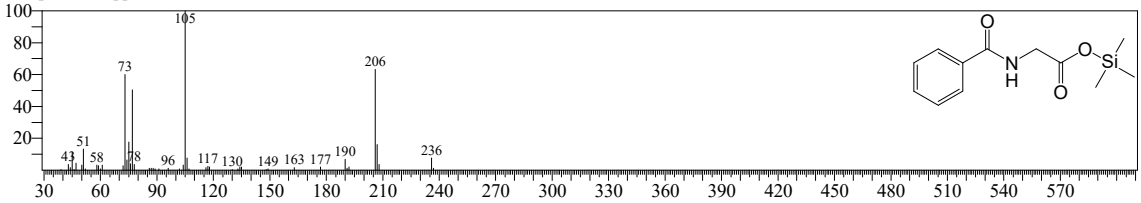
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

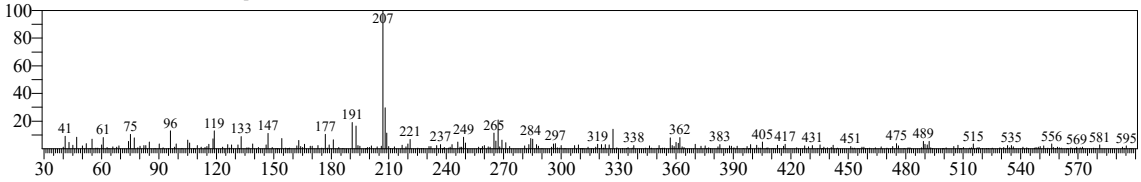


Hit#:5 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid

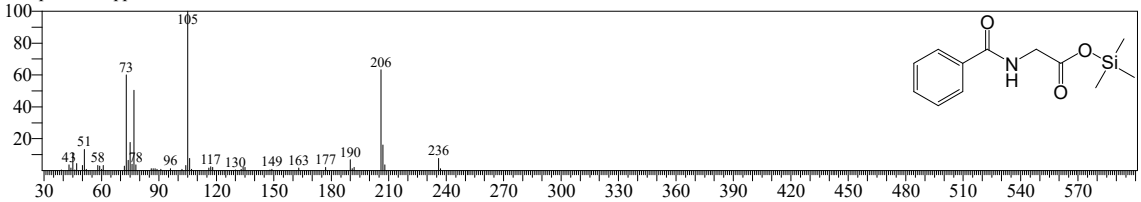


TNAU

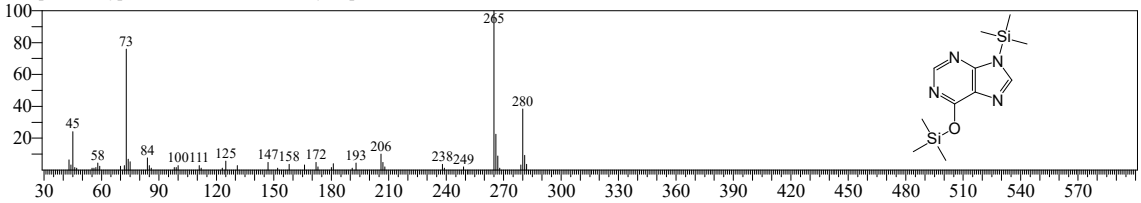
<< Target >>
Line#:15 R.Time:30.760(Scan#:5253) MassPeaks:296
RawMode:Averaged 30.755-30.765(5252-5254) BasePeak:207.05(2676)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



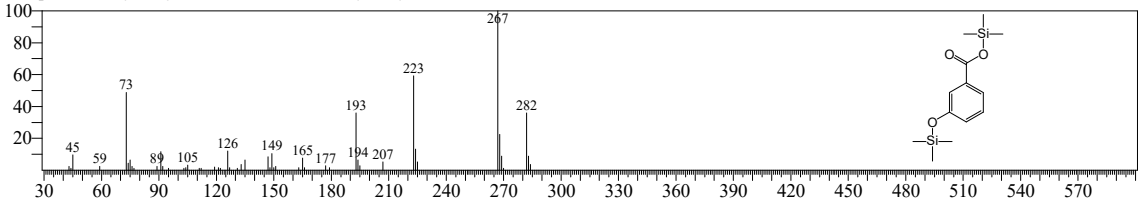
Hit#:1 Entry:330 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C12H17NO3Si CAS:66407-11-2 MolWeight:251 RetIndex:1849
CompName:Hippuric acid-TMS ; 2-benzamidoacetic acid



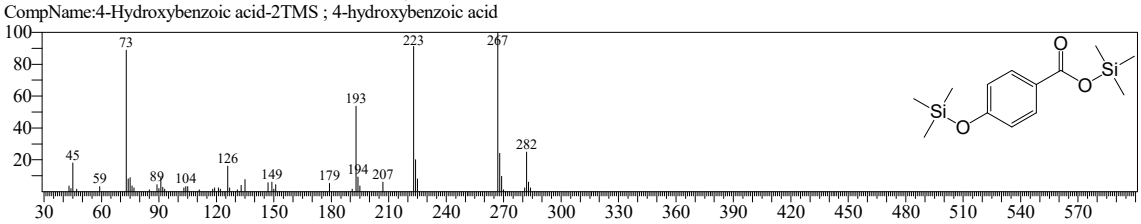
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



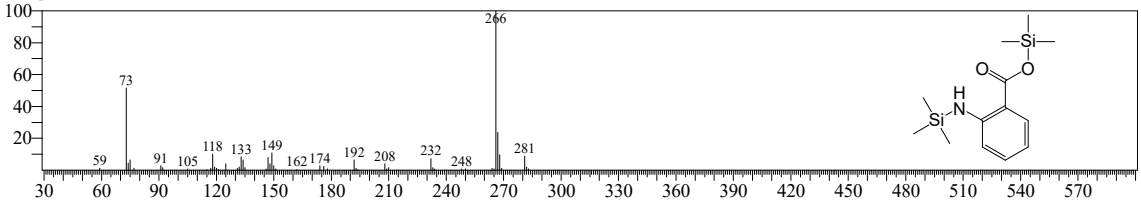
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

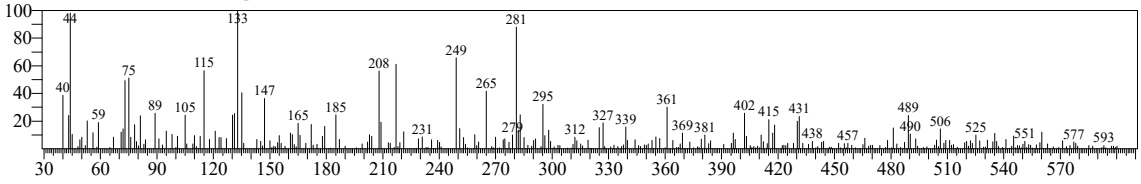


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

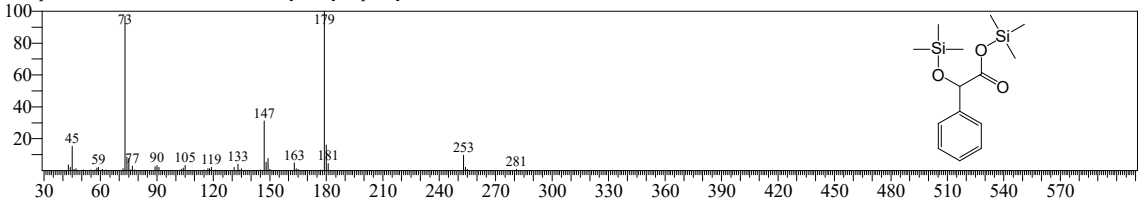


TNAU

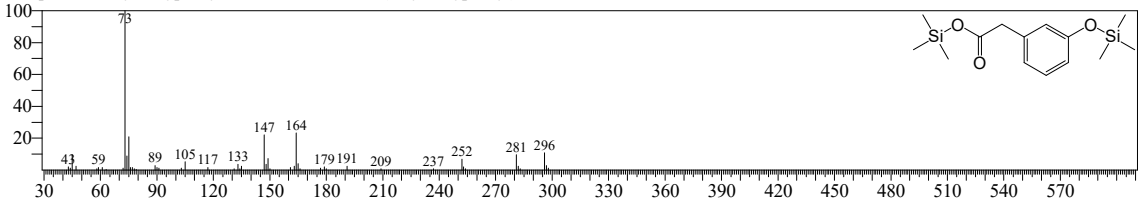
<< Target >>
Line#:16 R.Time:31.420(Scan#:5385) MassPeaks:306
RawMode:Averaged 31.415-31.425(5384-5386) BasePeak:132.95(792)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



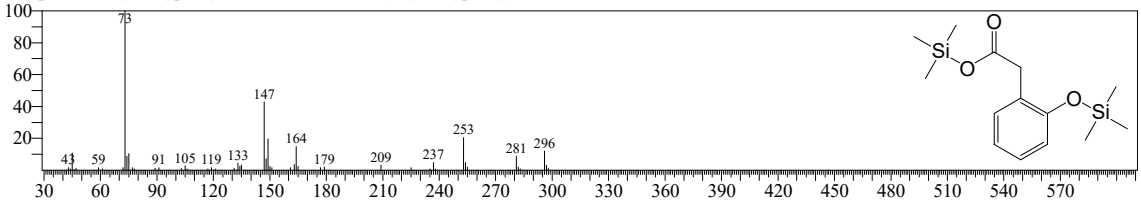
Hit#:1 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



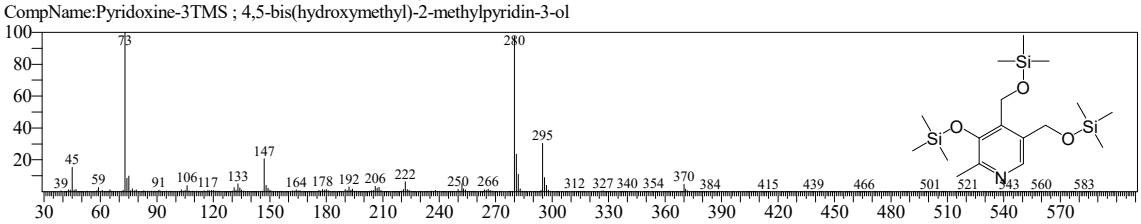
Hit#:2 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid



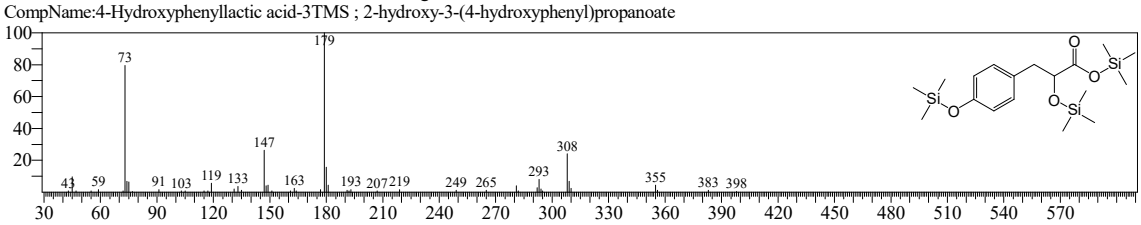
Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



Hit#:4 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

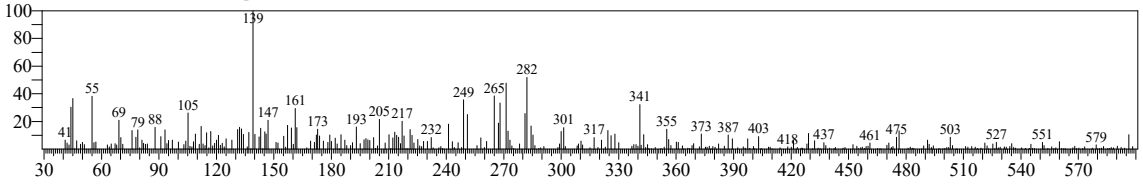


Hit#:5 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

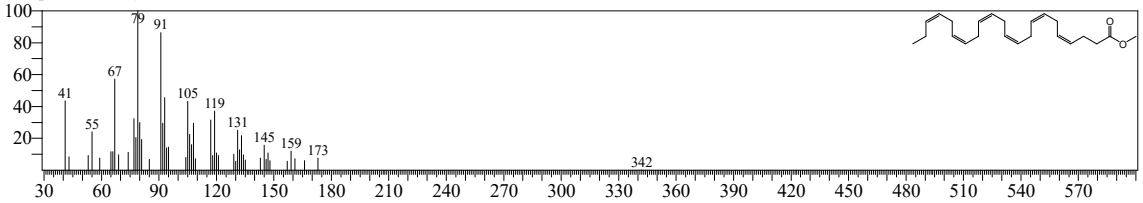


TNAU

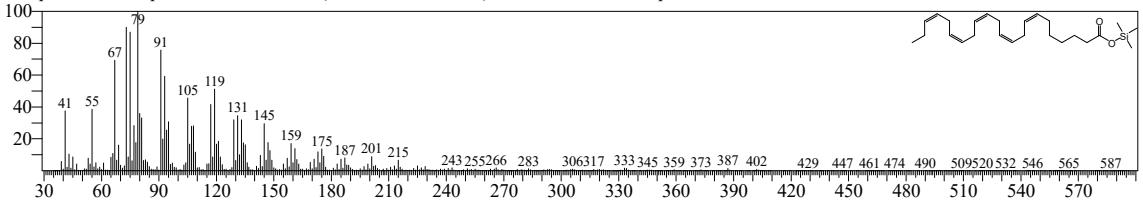
<< Target >>
Line#:17 R.Time:31.915(Scan#:5484) MassPeaks:343
RawMode:Averaged 31.910-31.920(5483-5485) BasePeak:139.10(1396)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



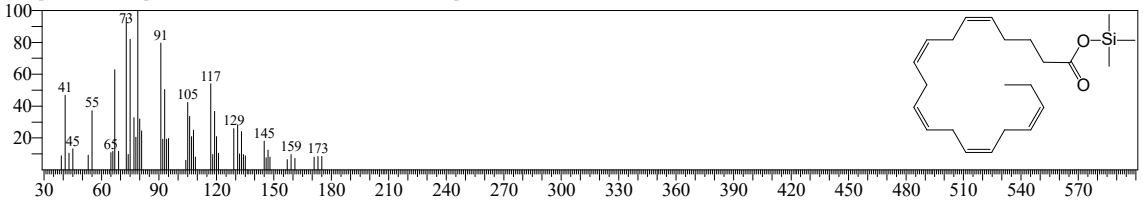
Hit#:1 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:28 Formula:C23H34O2 CAS:6217-54-5 MolWeight:342 RetIndex:3514
CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid



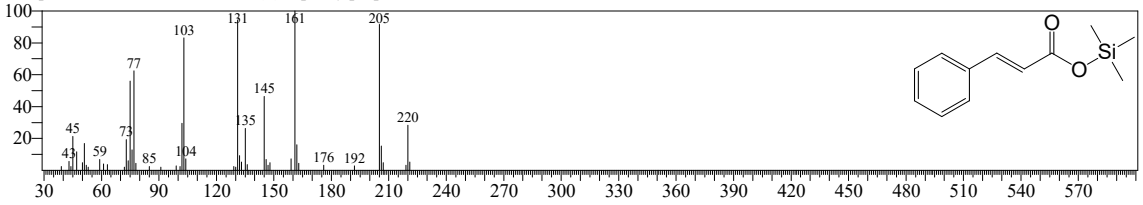
Hit#:2 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



Hit#:3 Entry:509 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C23H38O2Si CAS:10417-94-4 MolWeight:374 RetIndex:2389
CompName:Eicosapentaenoic acid-TMS ; icosa-5,8,11,14,17-pentaenoic acid



Hit#:4 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid



Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:26 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