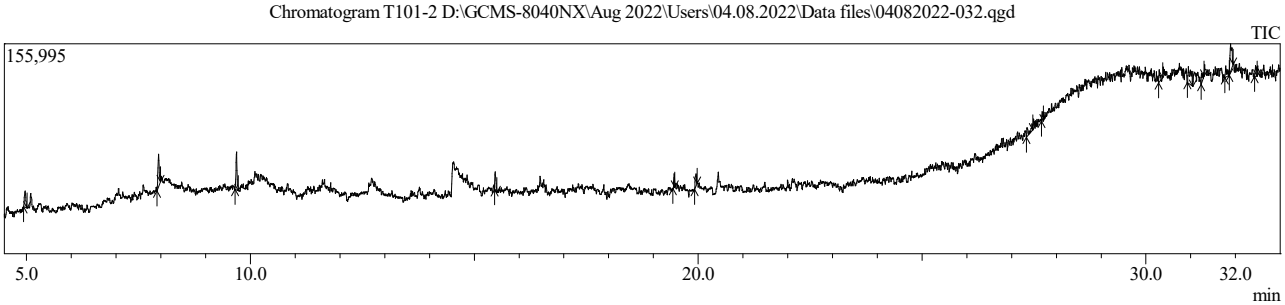
# TNAU

Sample Information

| | |
|---|---|
| Analyzed by | : Admin |
| Analyzed | : 05-Aug-22 1:02:35 PM |
| Sample Type | : Unknown |
| Level # | : 1 |
| Sample Name | : T101-2 |
| Sample ID | : T101-2 |
| IS Amount | : [1]=1 |
| Sample Amount | : 1 |
| Dilution Factor | : 1 |
| Vial # | : 31 |
| Injection Volume | : 1.00 |
| Data File | : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-032.qgd |
| Org Data File | : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-032.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 4:47:44 PM |

Chromatogram T101-2 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-032.qgd



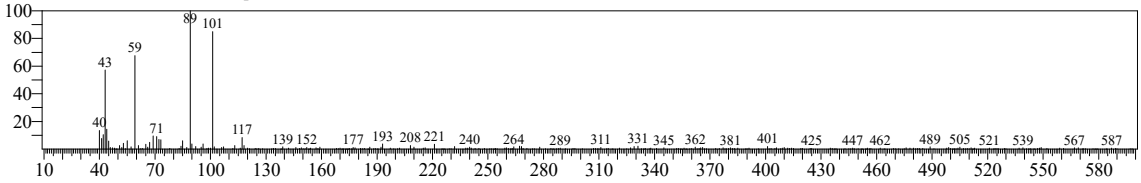

Peak Report TIC

| Peak# | R.Time | Area | Area% | Height | Height% | A/H | Similarity | Name |
|---|---|---|---|---|---|---|---|---|
| 1 | 4.966 | 25192 | 6.70 | 11914 | 6.78 | 2.11 | 71 | 2-Propanol, 1,1'-oxybis- |
| 2 | 7.947 | 47496 | 12.63 | 24326 | 13.85 | 1.95 | 90 | Undecane |
| 3 | 9.689 | 48560 | 12.91 | 28424 | 16.18 | 1.71 | 88 | Undecane |
| 4 | 15.465 | 22472 | 5.97 | 13824 | 7.87 | 1.63 | 76 | 2,4-Di-tert-butylphenol |
| 5 | 19.465 | 13467 | 3.58 | 10432 | 5.94 | 1.29 | 72 | 1,2-Benzenedicarboxylic acid, bis(2-methylpro |
| 6 | 19.952 | 17467 | 4.64 | 8636 | 4.92 | 2.02 | 62 | Dimethylglycine-TMS |
| 7 | 27.340 | 23420 | 6.23 | 6315 | 3.59 | 3.71 | 39 | 4-Hydroxyphenyllactic acid-3TMS |
| 8 | 27.680 | 8998 | 2.39 | 7013 | 3.99 | 1.28 | 37 | Anthranilic acid-2TMS |
| 9 | 30.295 | 13083 | 3.48 | 9031 | 5.14 | 1.45 | 36 | Epinephrine-3TMS |
| 10 | 30.948 | 51203 | 13.61 | 12364 | 7.04 | 4.14 | 33 | 3-(3-Hydroxyphenyl)-3-hydroxypropionic acid |
| 11 | 31.240 | 14164 | 3.77 | 7494 | 4.27 | 1.89 | 40 | Galactose-5TMS(2) |
| 12 | 31.780 | 17021 | 4.52 | 7462 | 4.25 | 2.28 | 34 | Anthranilic acid-2TMS |
| 13 | 31.890 | 59585 | 15.84 | 20527 | 11.68 | 2.90 | 28 | Methyl arachidonate |
| 14 | 32.447 | 14031 | 3.73 | 7912 | 4.50 | 1.77 | 32 | Hypoxanthine-2TMS |
| | | 376159 | 100.00 | 175674 | 100.00 | | | |

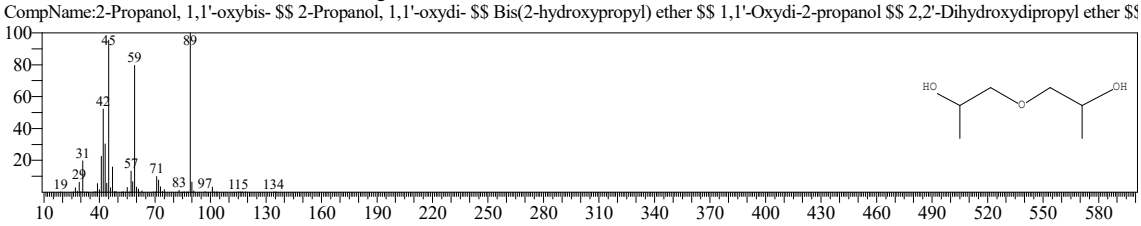
Library

# TNAU

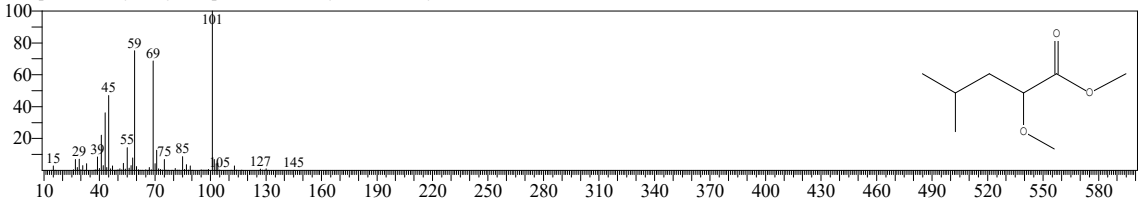
<< Target >>
Line#:1 R.Time:4.965(Scan#:94) MassPeaks:284
RawMode:Averaged 4.960-4.970(93-95) BasePeak:89.00(2620)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



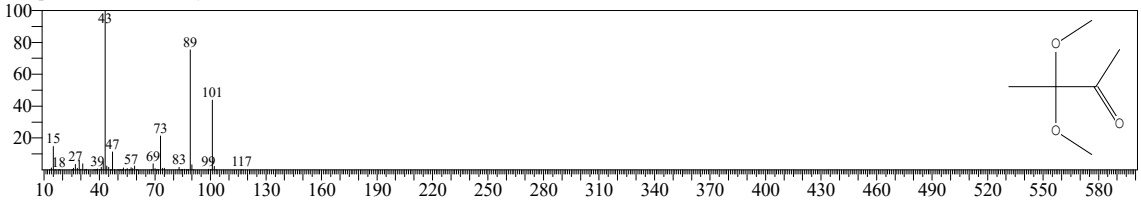
Hit#:1 Entry:7425 Library:NIST20R.lib
SI:71 Formula:C6H14O3 CAS:110-98-5 MolWeight:134 RetIndex:1018
CompName:2-Propanol, 1,1'-oxybis- $$ 2-Propanol, 1,1'-oxydi- $$ Bis(2-hydroxypropyl) ether $$ 1,1'-Oxydi-2-propanol $$ 2,2'-Dihydroxydipropyl ether $$



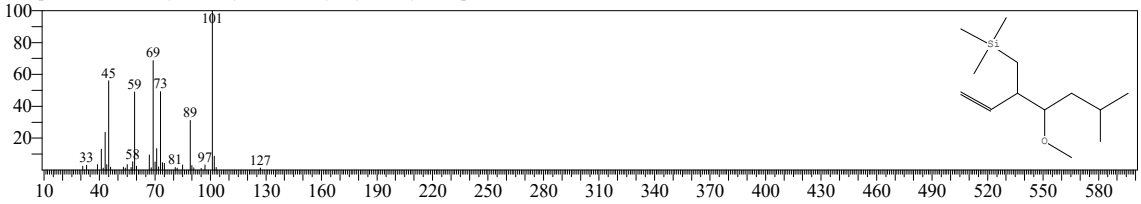
Hit#:2 Entry:22897 Library:NIST20M1.lib
SI:71 Formula:C8H16O3 CAS:0-00-0 MolWeight:160 RetIndex:931
CompName:2-Hydroxyisocaproic acid, methyl ether, methyl ester



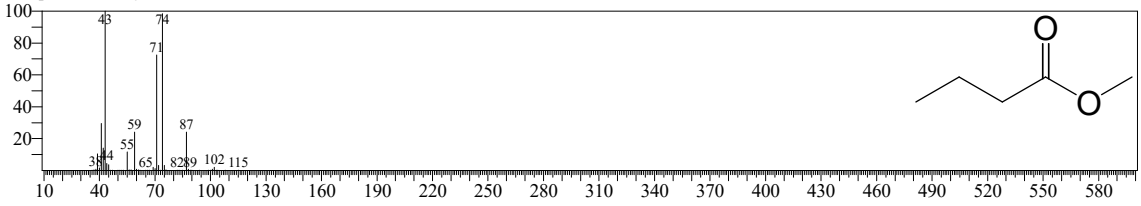
Hit#:3 Entry:9263 Library:NIST20M1.lib
SI:71 Formula:C6H12O3 CAS:21983-72-2 MolWeight:132 RetIndex:821
CompName:3,3-Dimethoxy-2-butanone



Hit#:4 Entry:81501 Library:NIST20M1.lib
SI:70 Formula:C13H28OSi CAS:0-00-0 MolWeight:228 RetIndex:1097
CompName:4-Methoxy-6-methyl-3-(trimethylsilyl)methyl-1-heptene

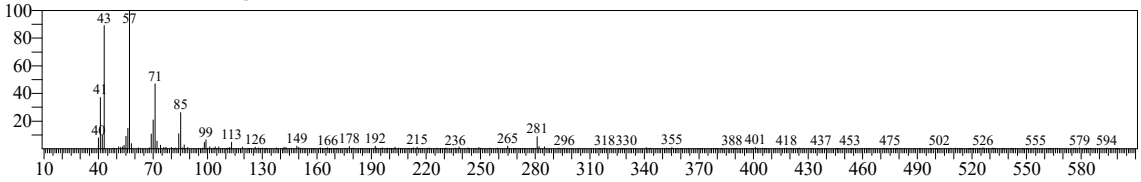


Hit#:5 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid

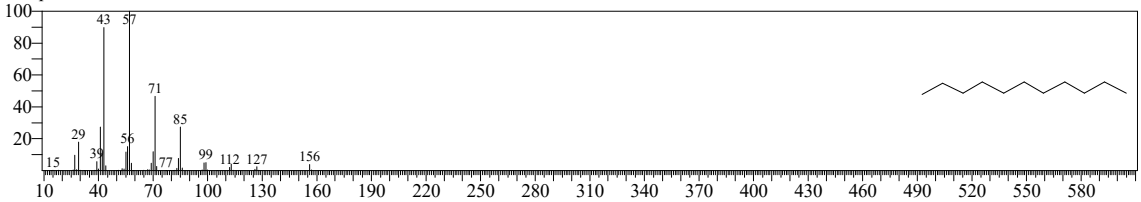


# TNAU

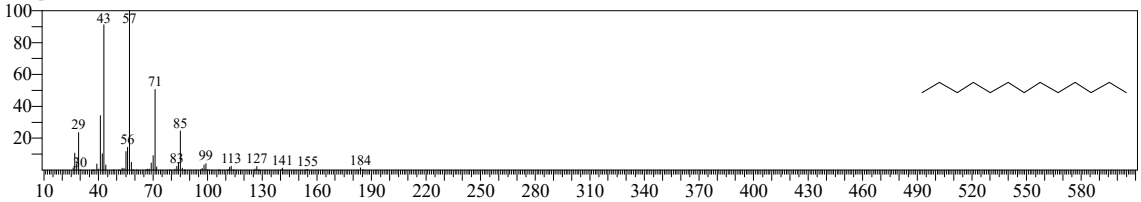
<< Target >>
Line#:2 R.Time:7.945(Scan#:690) MassPeaks:247
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(6028)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



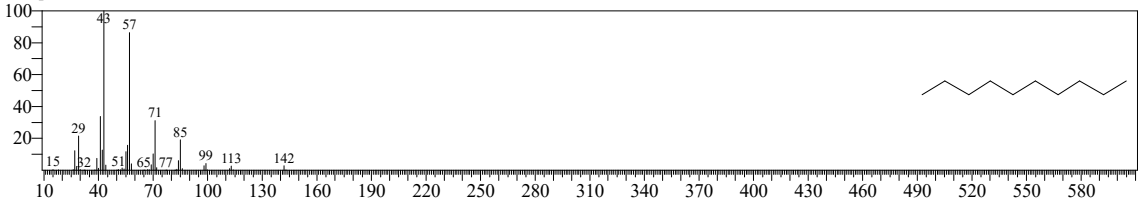
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:90 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



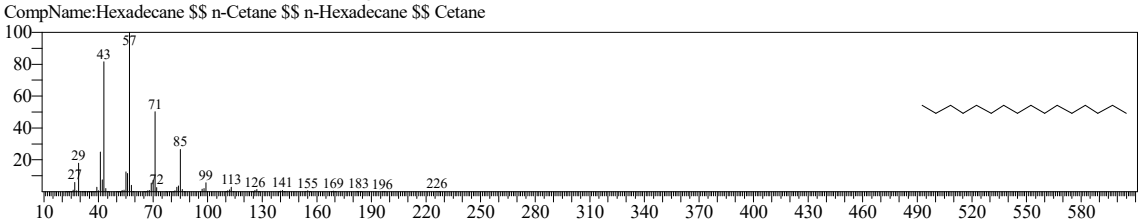
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



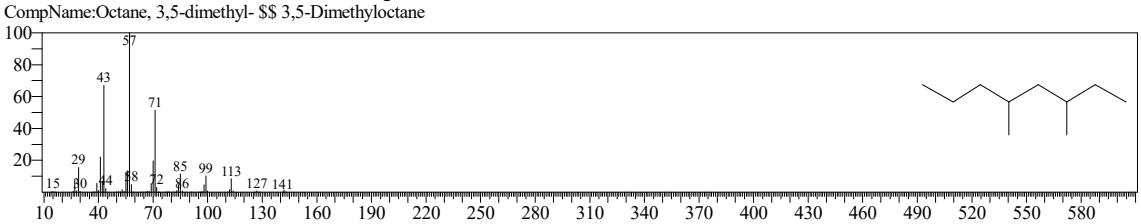
Hit#:3 Entry:9444 Library:NIST20R.lib
SI:88 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



Hit#:4 Entry:27737 Library:NIST20R.lib
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

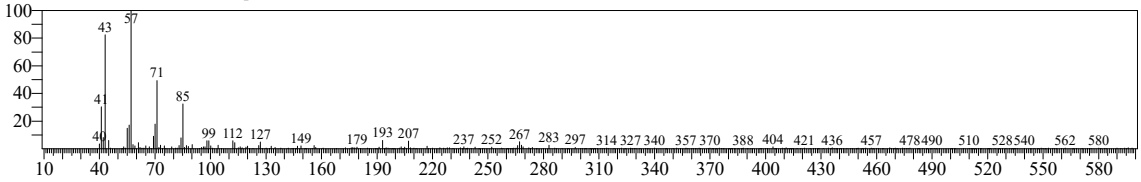


Hit#:5 Entry:13631 Library:NIST20M1.lib
SI:88 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

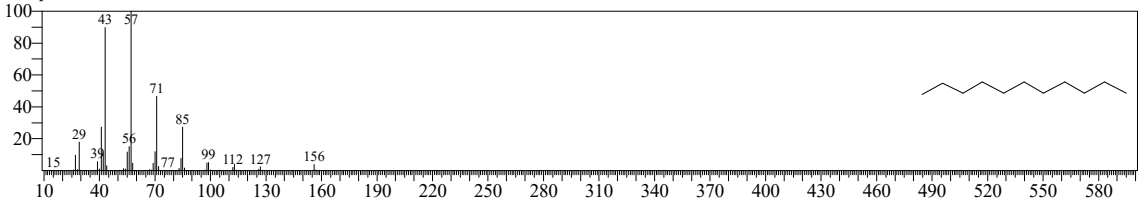


# TNAU

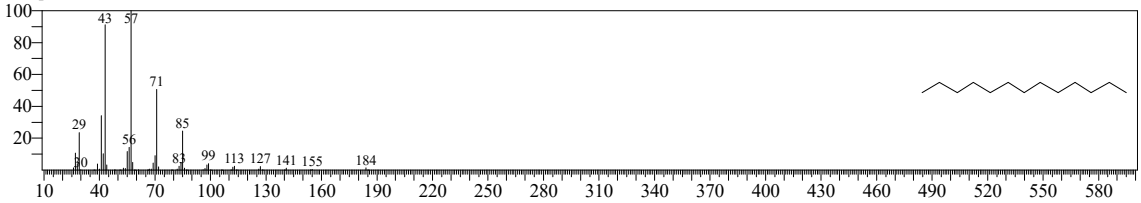
<< Target >>
Line#:3 R.Time:9.690(Scan#:1039) MassPeaks:316
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.05(5566)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



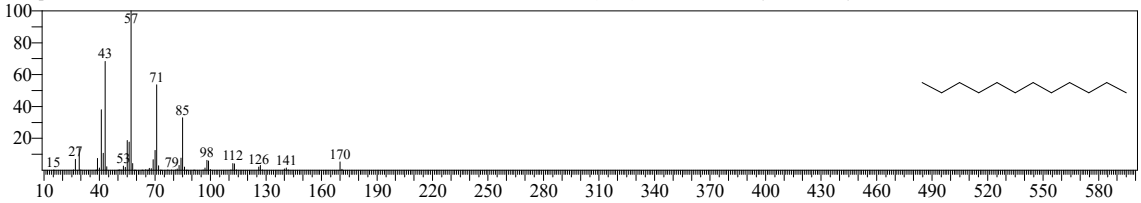
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:88 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



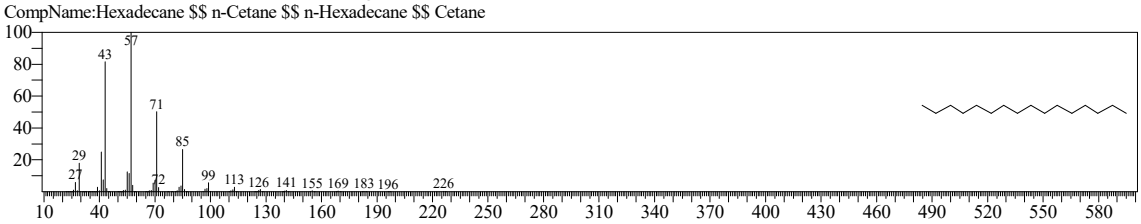
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:87 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



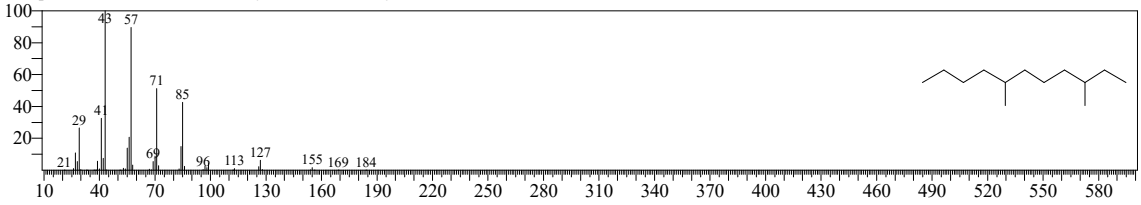
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:27737 Library:NIST20R.lib
SI:87 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

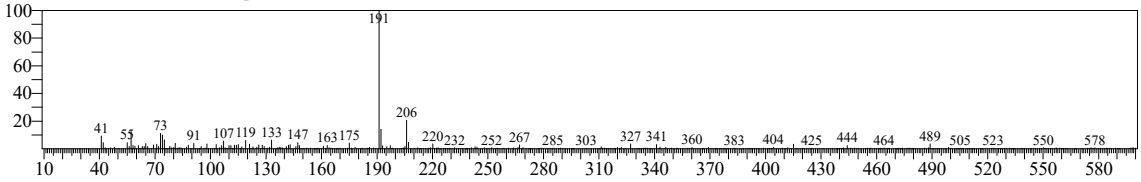


Hit#:5 Entry:40248 Library:NIST20M1.lib
SI:86 Formula:C13H28 CAS:17301-29-0 MolWeight:184 RetIndex:1185
CompName:Undecane, 3,7-dimethyl- $$ 3,7-Dimethylundecane #

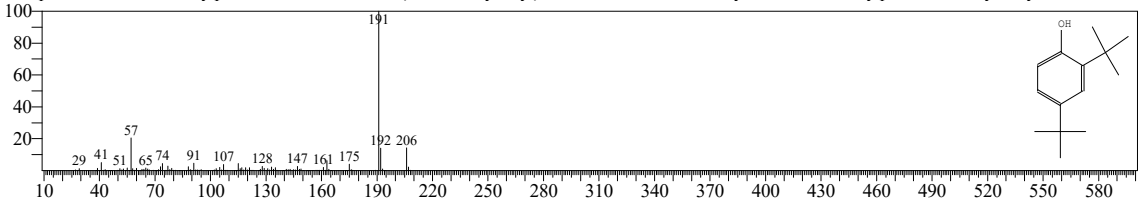


# TNAU

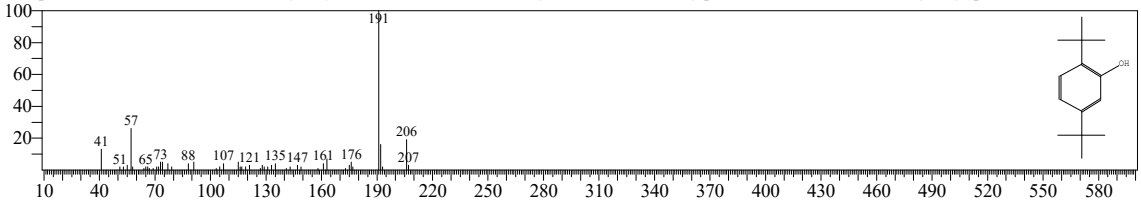
<< Target >>
Line#:4 R.Time:15.465(Scan#:2194) MassPeaks:312
RawMode:Averaged 15.460-15.470(2193-2195) BasePeak:191.10(4034)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



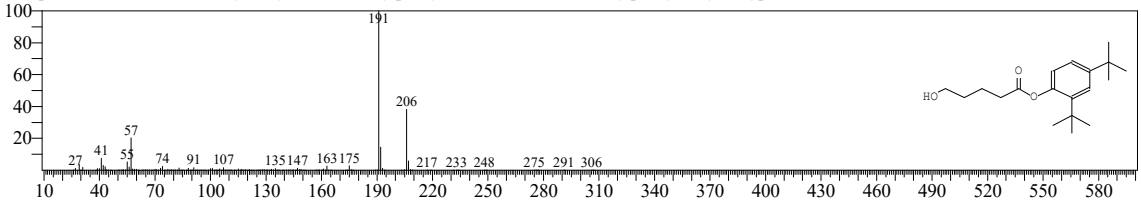

Hit#:1 Entry:24088 Library:NIST20R.lib
SI:76 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



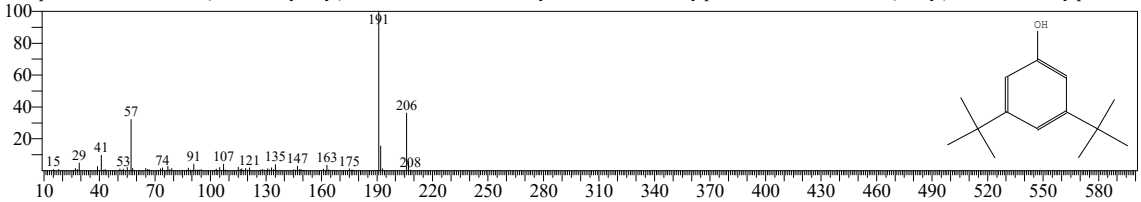

Hit#:2 Entry:24098 Library:NIST20R.lib
SI:76 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



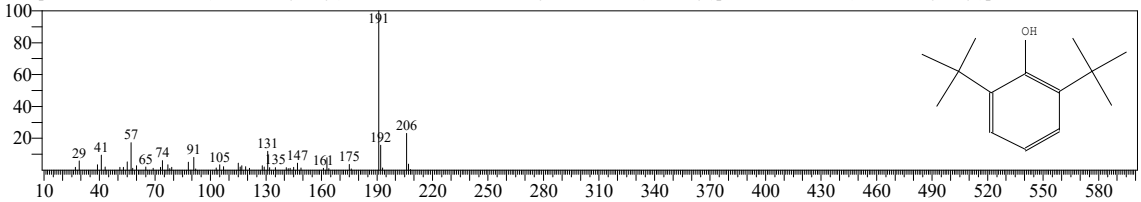

Hit#:3 Entry:170993 Library:NIST20M1.lib
SI:76 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #




Hit#:4 Entry:24110 Library:NIST20R.lib
SI:76 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

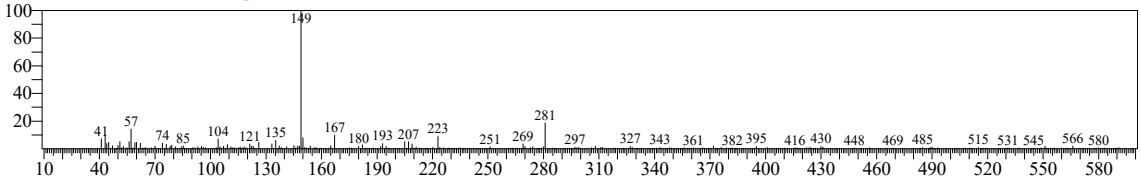



Hit#:5 Entry:24082 Library:NIST20R.lib
SI:75 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

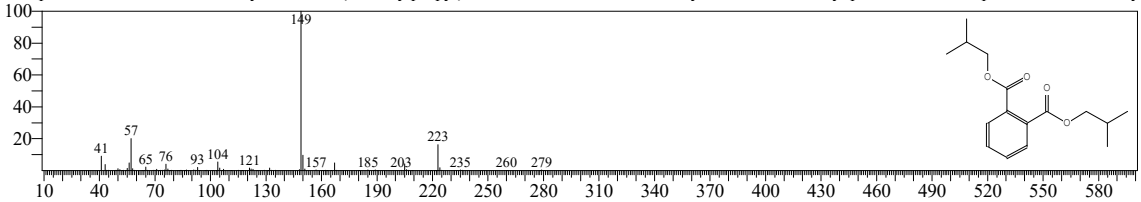


# TNAU

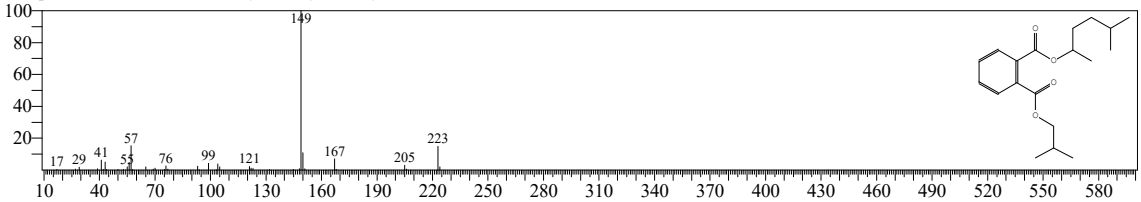
<< Target >>
Line#:5 R.Time:19.465(Scan#:2994) MassPeaks:285
RawMode:Averaged 19.460-19.470(2993-2995) BasePeak:149.00(3386)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



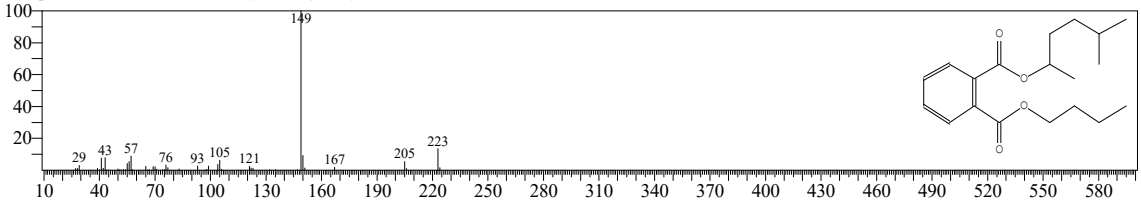

Hit#:1 Entry:33853 Library:NIST20R.lib
SI:72 Formula:C16H22O4 CAS:84-69-5 MolWeight:278 RetIndex:1908
CompName:1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester $$ Phthalic acid, diisobutyl ester $$ Diisobutyl phthalate $$ Hexaplas M/1B $$ Isobuty



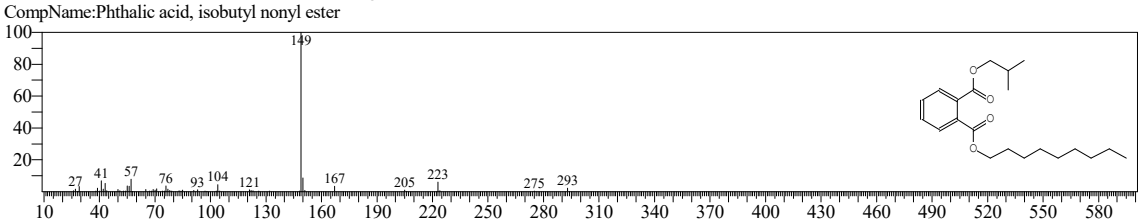

Hit#:2 Entry:187175 Library:NIST20M1.lib
SI:71 Formula:C19H28O4 CAS:0-00-0 MolWeight:320 RetIndex:2143
CompName:Phthalic acid, 5-methylhex-2-yl isobutyl ester



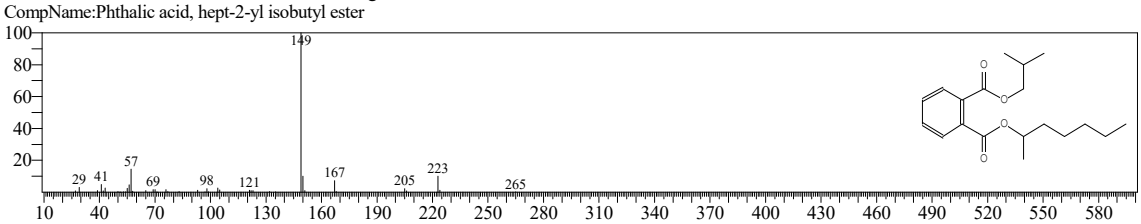

Hit#:3 Entry:187236 Library:NIST20M1.lib
SI:70 Formula:C19H28O4 CAS:0-00-0 MolWeight:320 RetIndex:2207
CompName:Phthalic acid, 5-methylhex-2-yl butyl ester




Hit#:4 Entry:218481 Library:NIST20M1.lib
SI:70 Formula:C21H32O4 CAS:0-00-0 MolWeight:348 RetIndex:2470
CompName:Phthalic acid, isobutyl nonyl ester

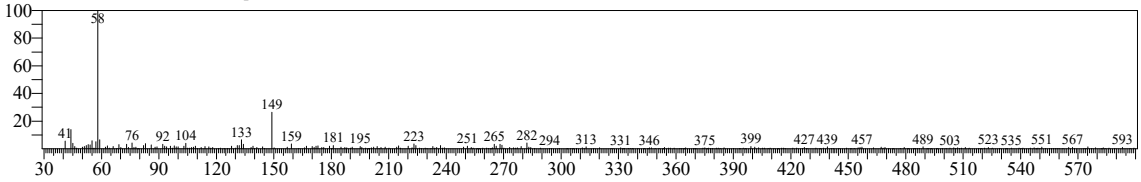



Hit#:5 Entry:187333 Library:NIST20M1.lib
SI:70 Formula:C19H28O4 CAS:0-00-0 MolWeight:320 RetIndex:2207
CompName:Phthalic acid, hept-2-yl isobutyl ester

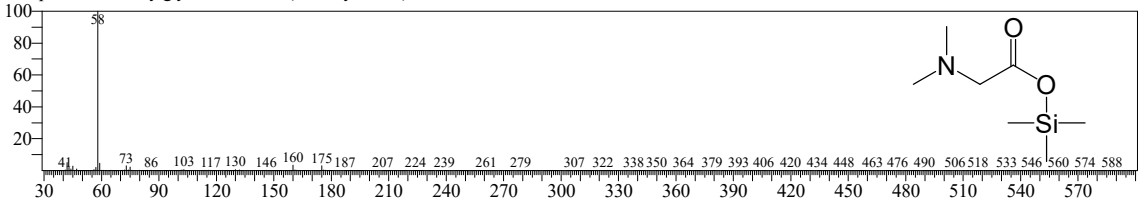


# TNAU

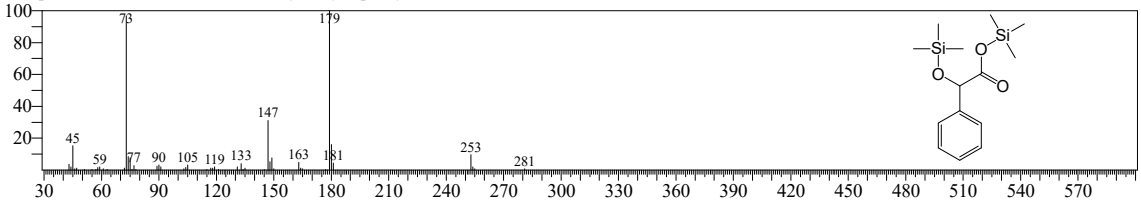
<< Target >>
Line#:6 R.Time:19.950(Scan#:3091) MassPeaks:299
RawMode:Averaged 19.945-19.955(3090-3092) BasePeak:58.10(3667)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



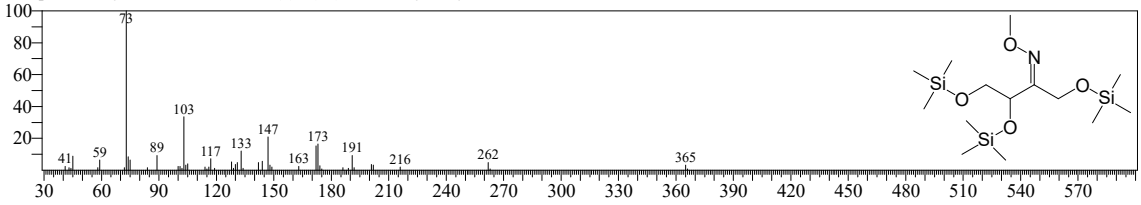
Hit#:1 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:62 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



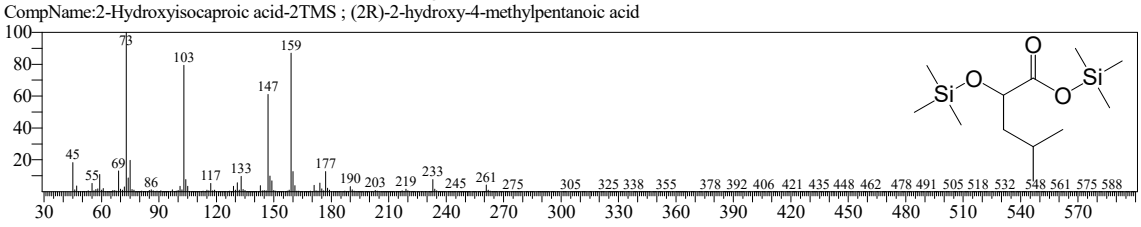
Hit#:2 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



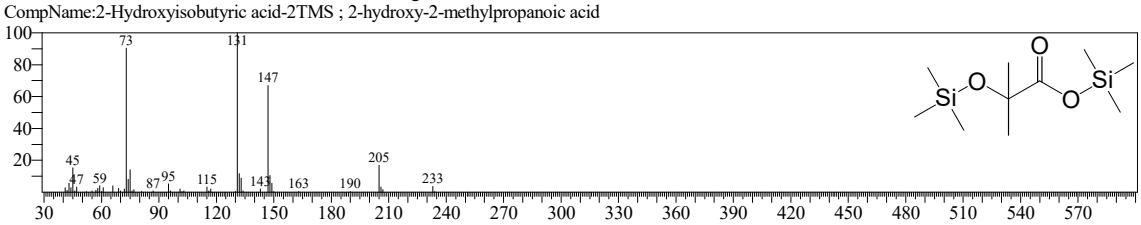
Hit#:3 Entry:133 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C14H35NO4Si3 CAS:533-50-6 MolWeight:365 RetIndex:1479
CompName:Erythrulose-meto-3TMS(1) ; (3S)-1,3,4-trihydroxybutan-2-one



Hit#:4 Entry:62 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C12H28O3Si2 CAS:20312-37-2 MolWeight:276 RetIndex:1244
CompName:2-Hydroxyisocaproic acid-2TMS ; (2R)-2-hydroxy-4-methylpentanoic acid

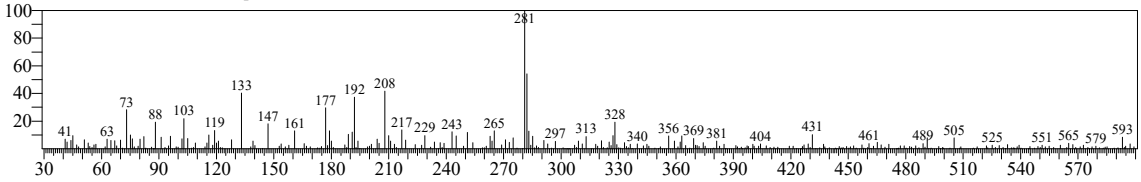


Hit#:5 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

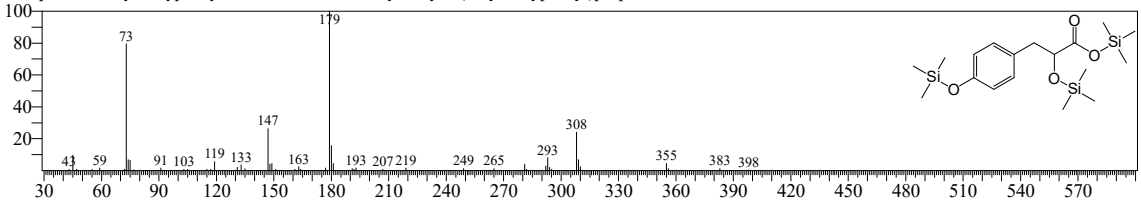


# TNAU

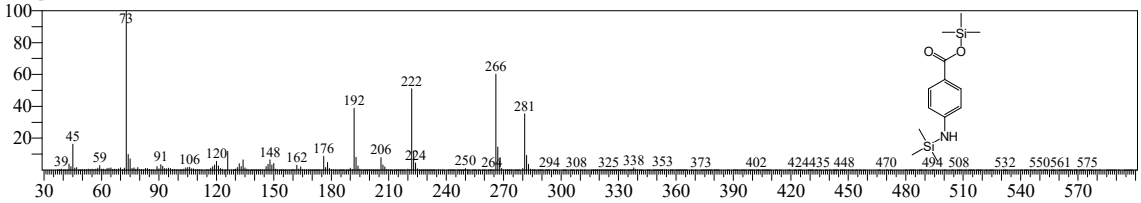
<< Target >>
Line#:7 R.Time:27.340(Scan#:4569) MassPeaks:304
RawMode:Averaged 27.335-27.345(4568-4570) BasePeak:281.00(1082)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



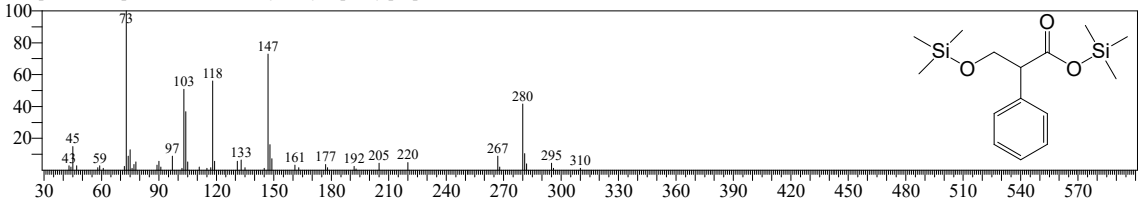
Hit#:1 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



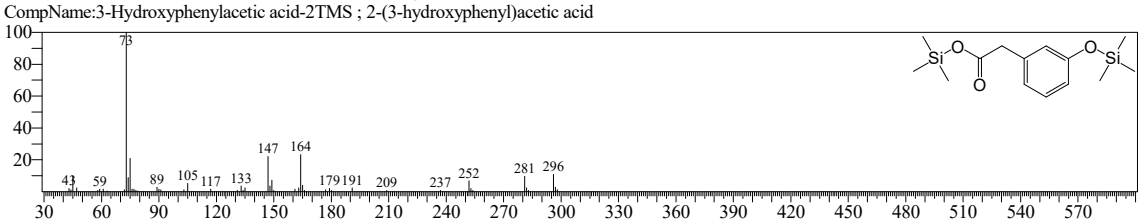
Hit#:2 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



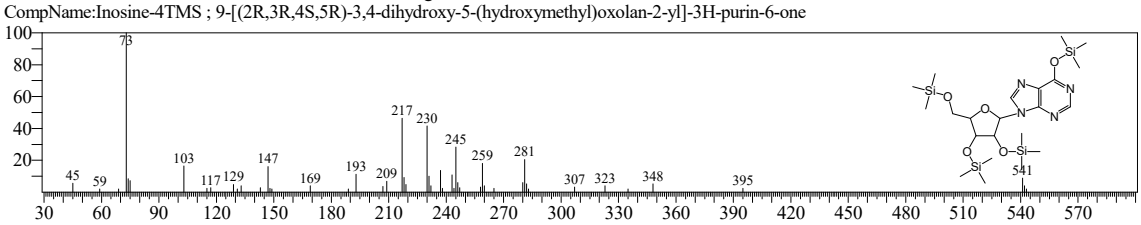
Hit#:3 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid



Hit#:4 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

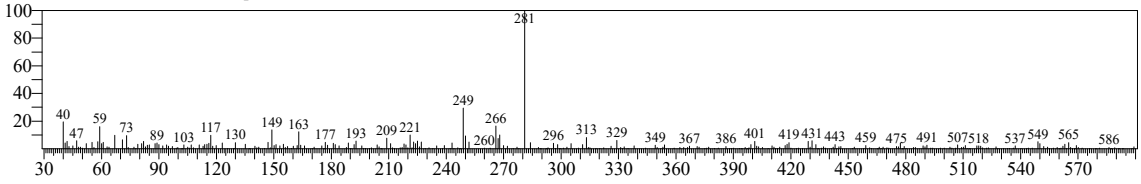


Hit#:5 Entry:535 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C22H44N4O5Si4 CAS:58-63-9 MolWeight:556 RetIndex:2605
CompName:Inosine-4TMS ; 9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-3H-purin-6-one

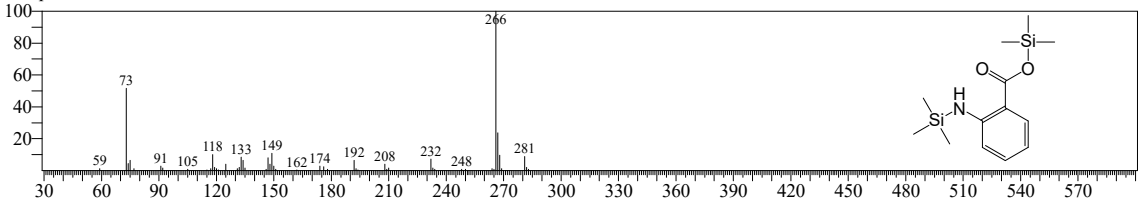


# TNAU

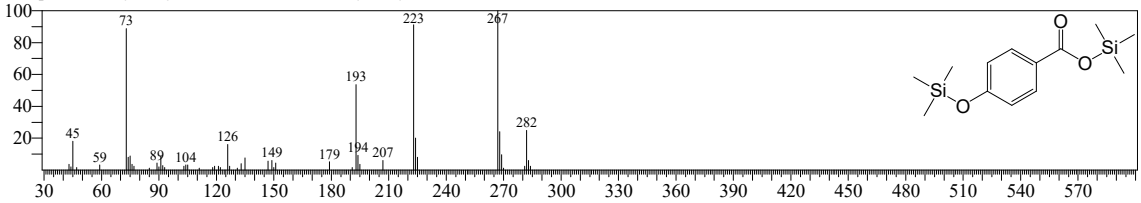
<< Target >>
Line#:8 R.Time:27.680(Scan#:4637) MassPeaks:309
RawMode:Averaged 27.675-27.685(4636-4638) BasePeak:281.00(2101)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



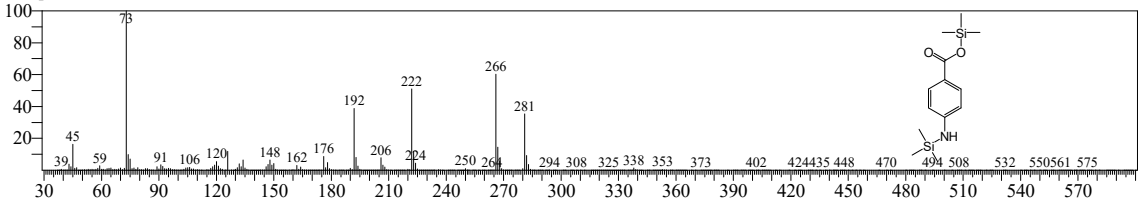
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



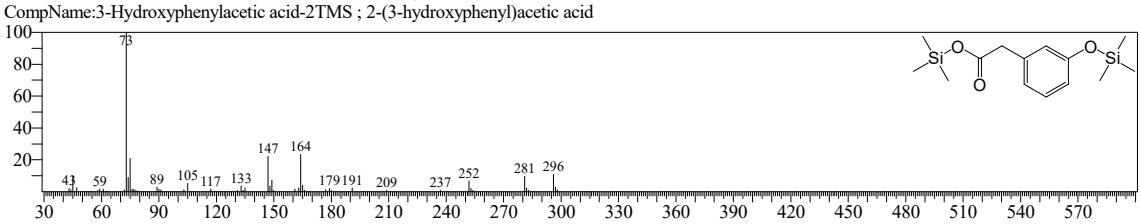
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



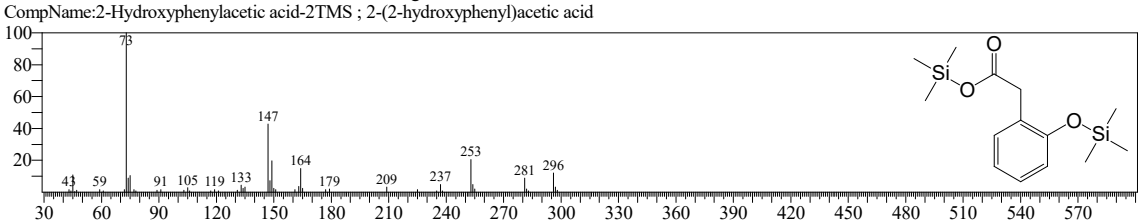
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



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

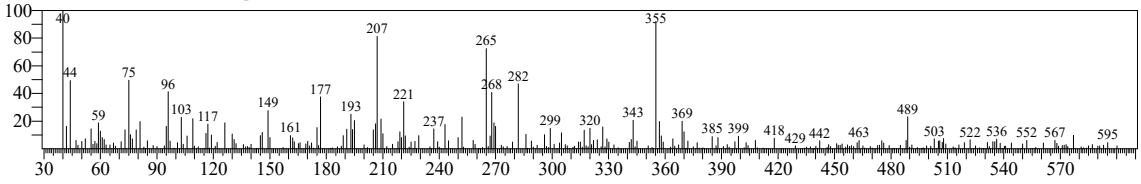


Hit#:5 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

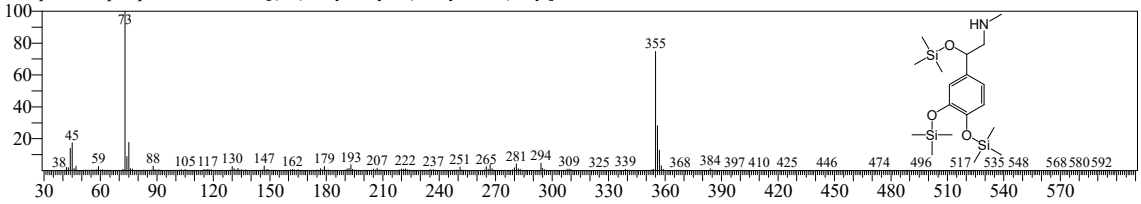


# TNAU

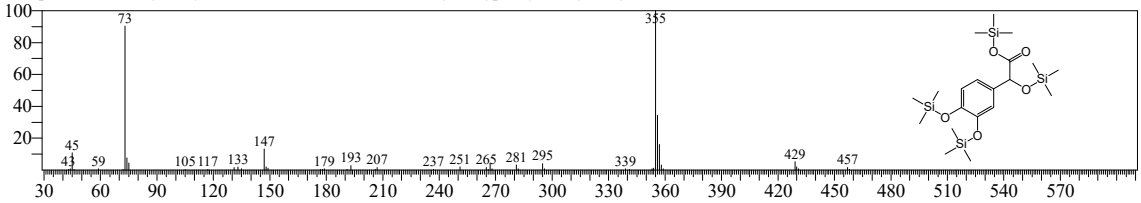
<< Target >>
Line#:9 R.Time:30.295(Scan#:5160) MassPeaks:302
RawMode:Averaged 30.290-30.300(5159-5161) BasePeak:40.00(913)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



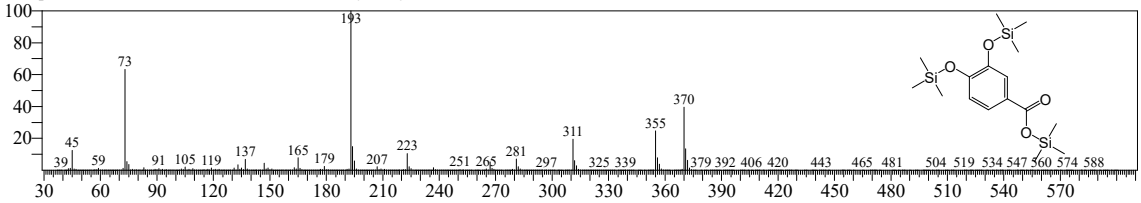
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



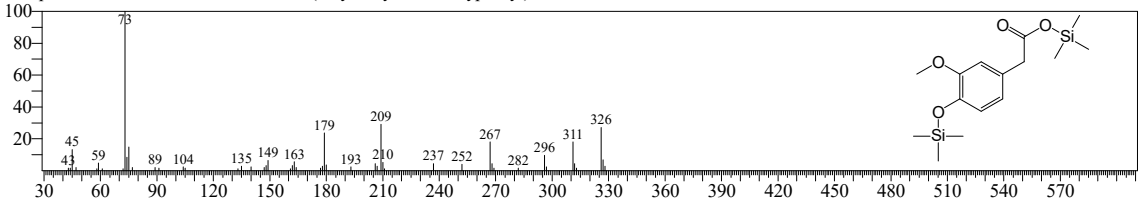
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



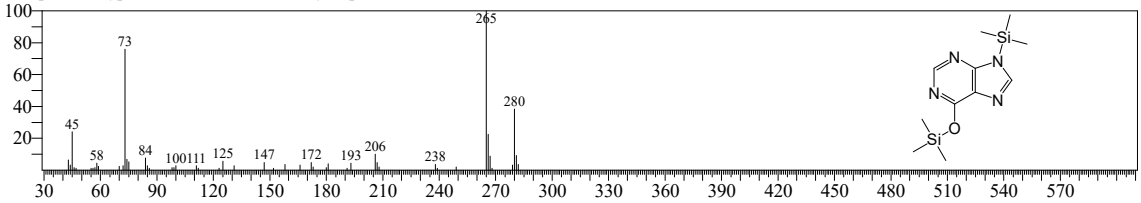
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

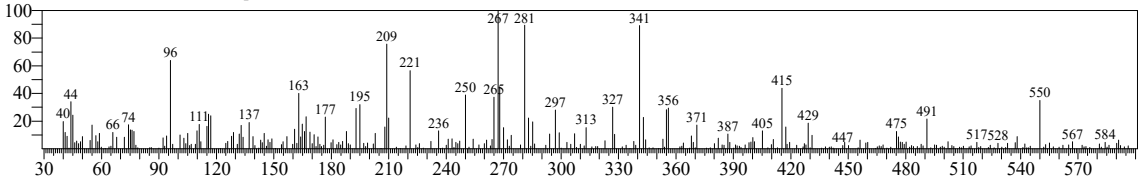


Hit#:5 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

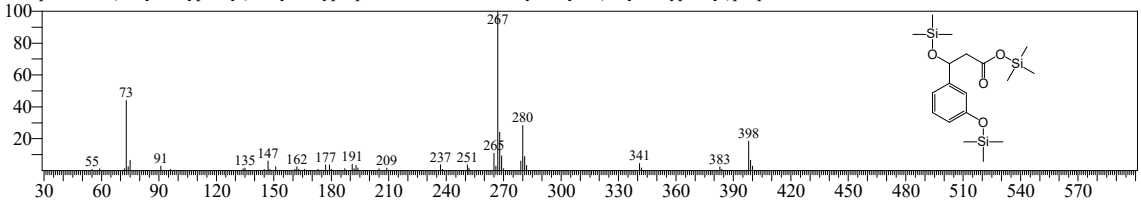


# TNAU

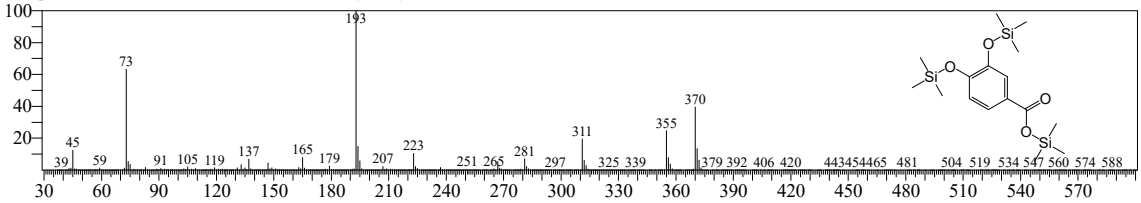
<< Target >>
Line#:10 R.Time:30.950(Scan#:5291) MassPeaks:314
RawMode:Averaged 30.945-30.955(5290-5292) BasePeak:267.05(815)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



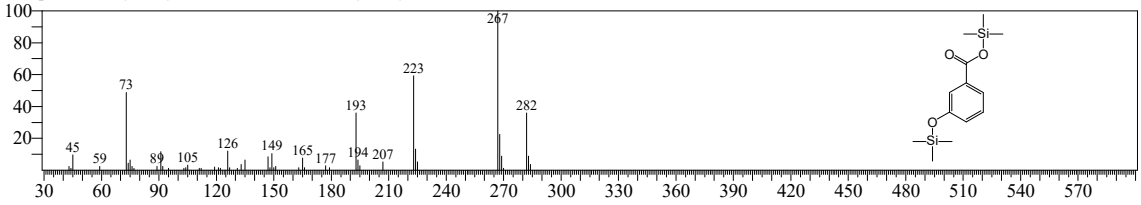
Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



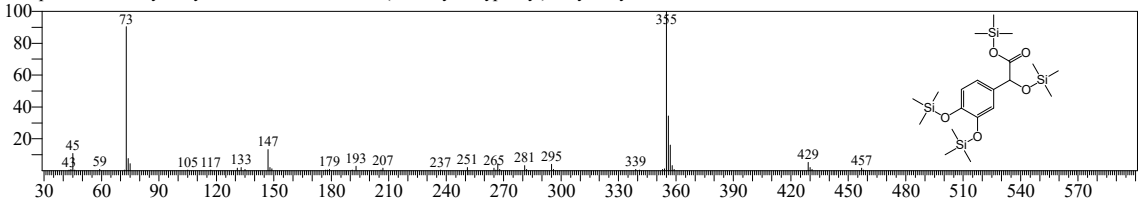
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



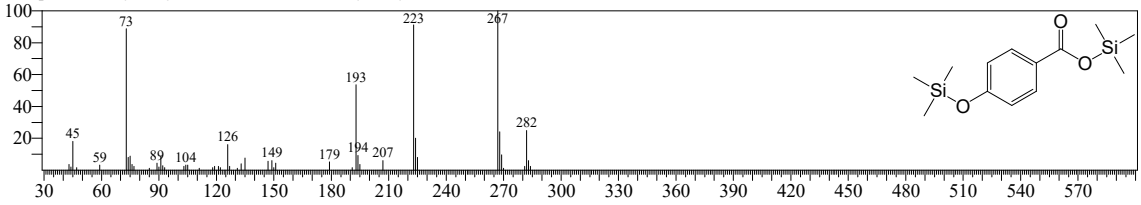
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



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

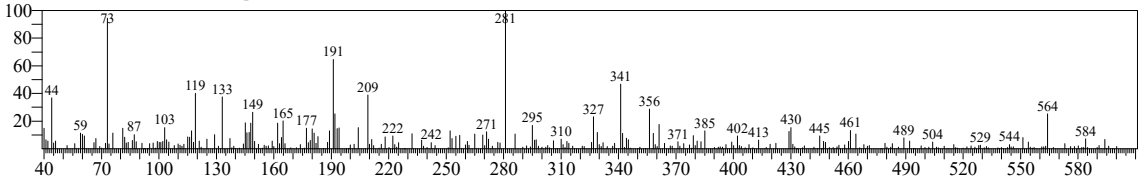


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

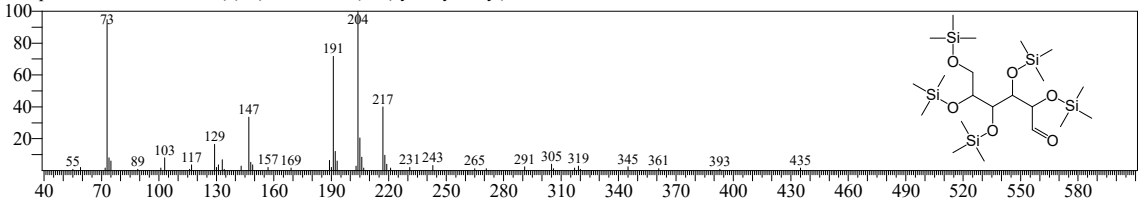


# TNAU

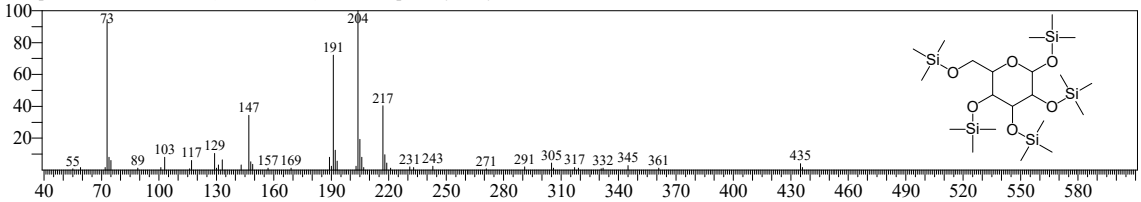
<< Target >>
Line#:11 R.Time:31.240(Scan#:5349) MassPeaks:302
RawMode:Averaged 31.235-31.245(5348-5350) BasePeak:281.05(873)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



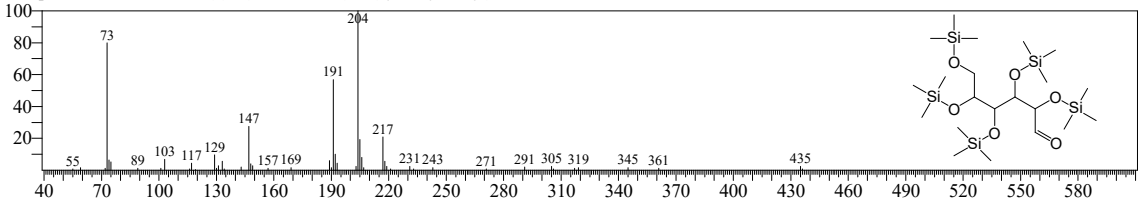
Hit#:1 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



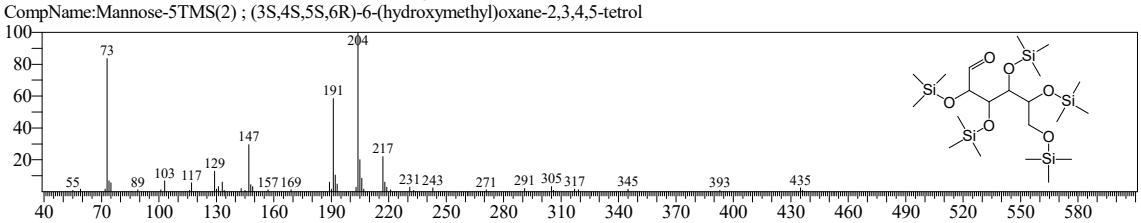
Hit#:2 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



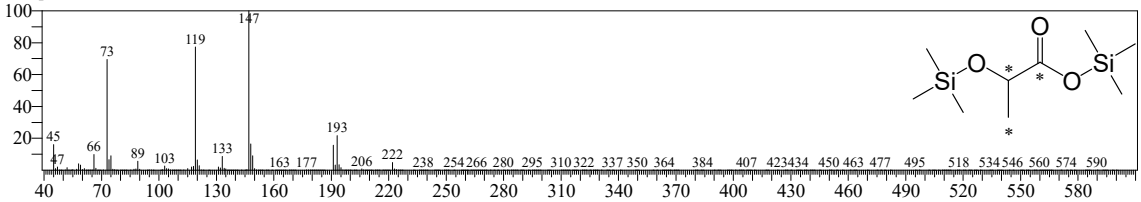
Hit#:3 Entry:437 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C21H52O6Si5 CAS:50-99-7 MolWeight:540 RetIndex:2002
CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

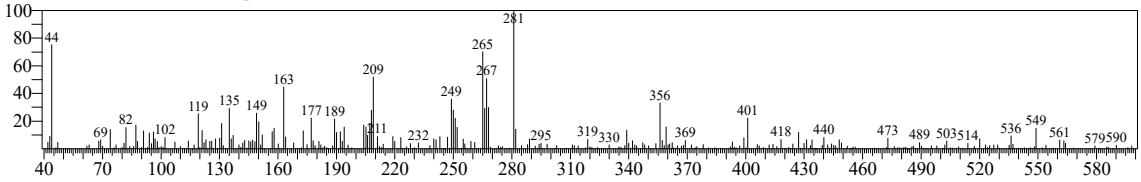


Hit#:5 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;

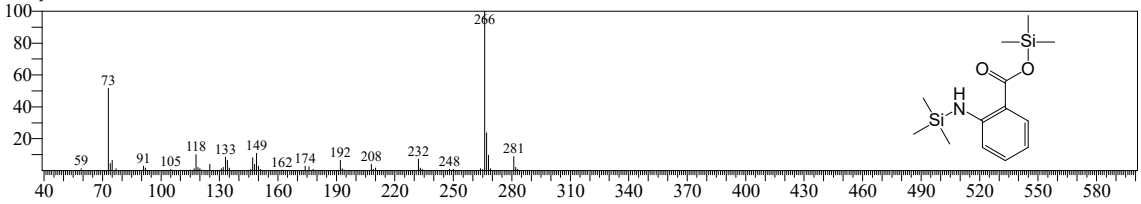


# TNAU

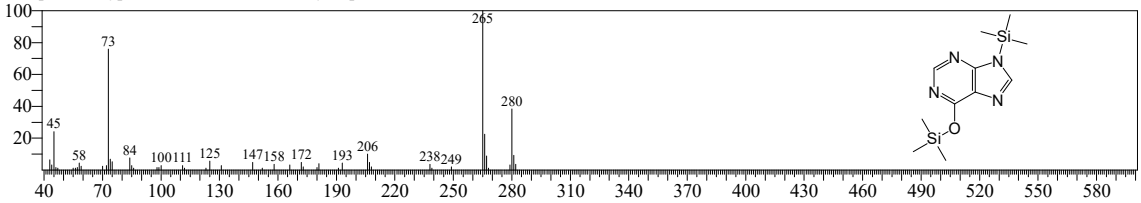
<< Target >>
Line#:12 R.Time:31.780(Scan#:5457) MassPeaks:282
RawMode:Averaged 31.775-31.785(5456-5458) BasePeak:281.00(1003)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



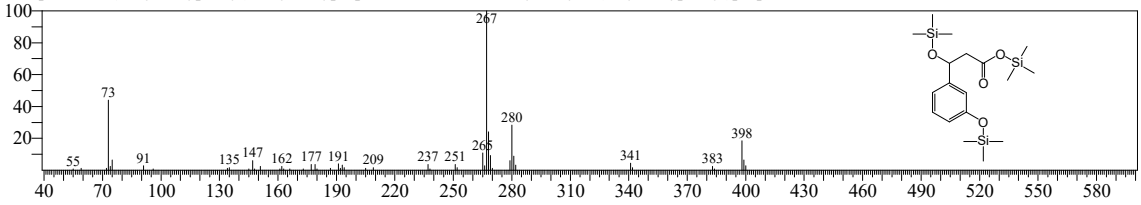
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



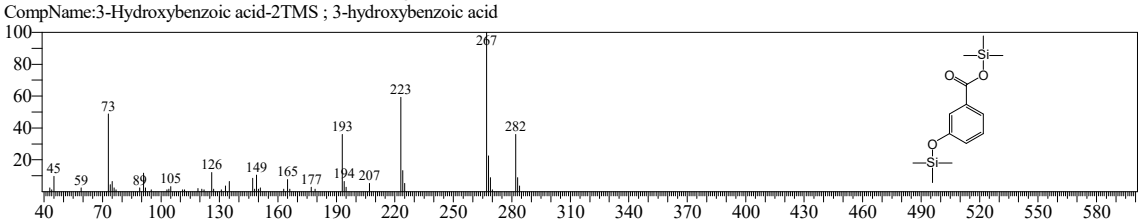
Hit#:2 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



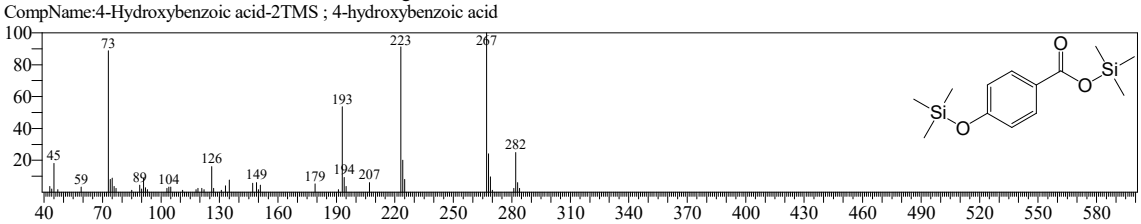
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

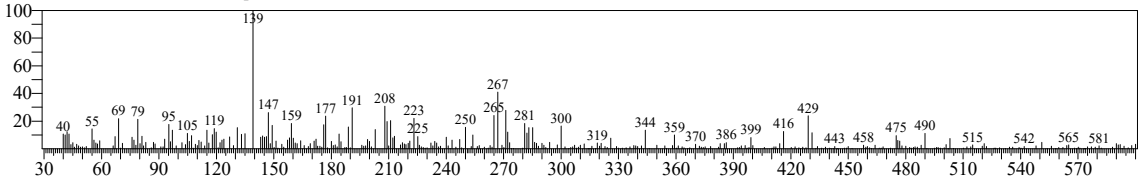


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

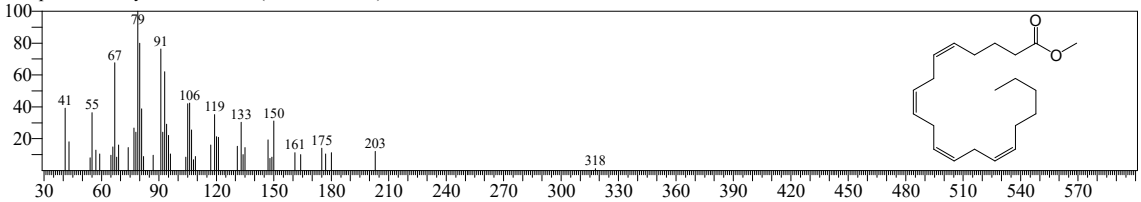


# TNAU

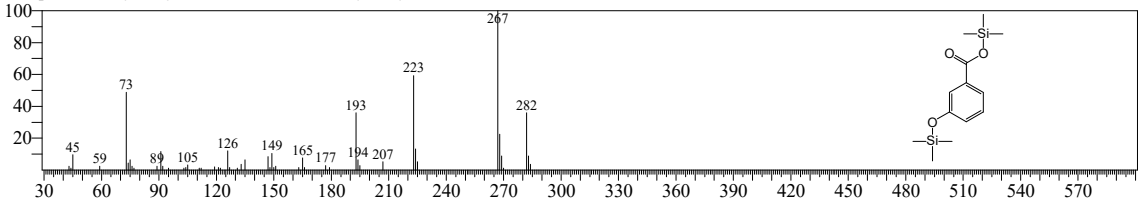
<< Target >>
Line#:13 R.Time:31.890(Scan#:5479) MassPeaks:343
RawMode:Averaged 31.885-31.895(5478-5480) BasePeak:139.15(1685)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



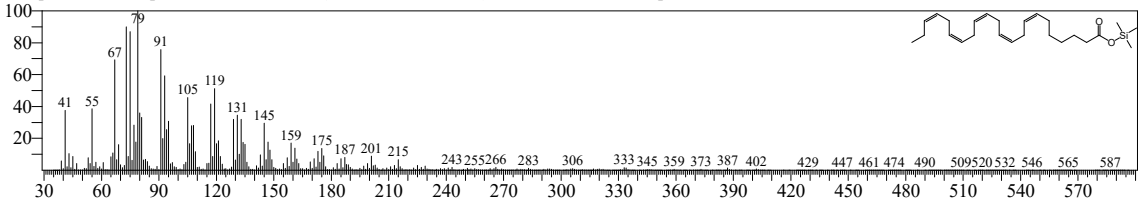

Hit#:1 Entry:33 Library:FA_ME_SP2560_EI_V3.lib
SI:28 Formula:C21H34O2 CAS:506-32-1 MolWeight:318 RetIndex:3109
CompName:Methyl arachidonate ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid



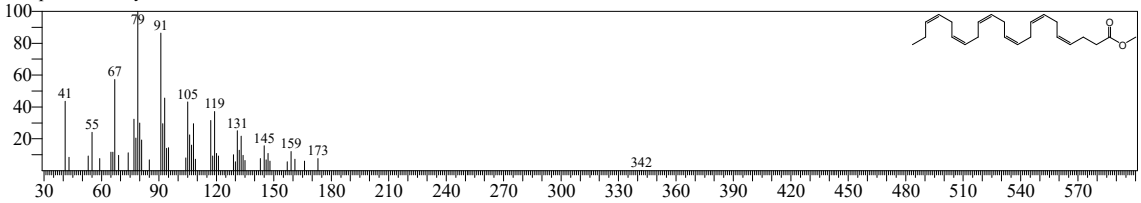

Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



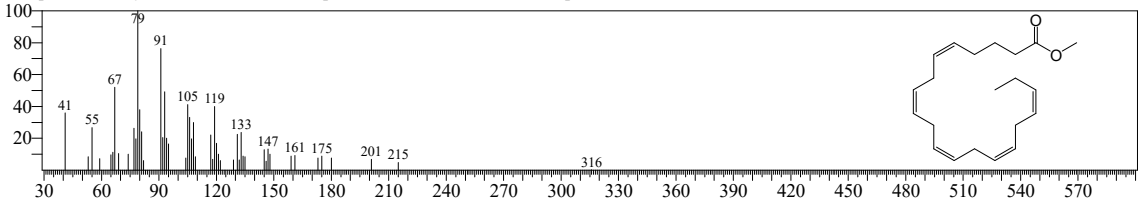

Hit#:3 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid




Hit#:4 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:26 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

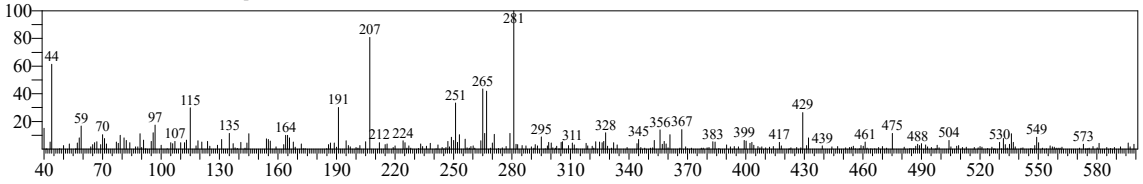



Hit#:5 Entry:36 Library:FA_ME_SP2560_EI_V3.lib
SI:26 Formula:C21H32O2 CAS:10417-94-4 MolWeight:316 RetIndex:3232
CompName:Methyl cis-5,8,11,14,17-Eicosapentaenoate ; Icosa-5,8,11,14,17-pentaenoic acid

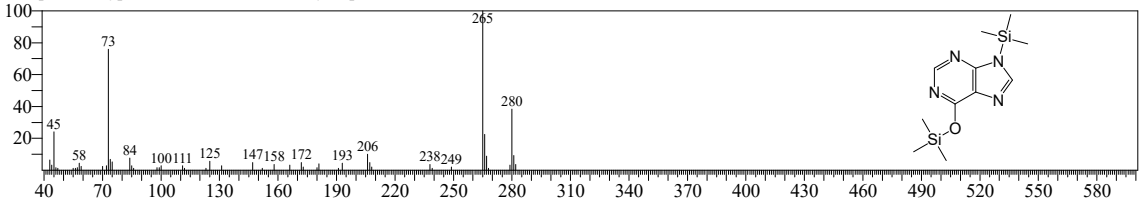


# TNAU

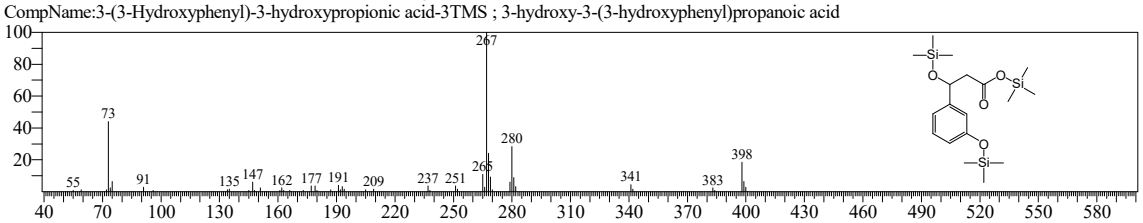
<< Target >>
Line#:14 R.Time:32.445(Scan#:5590) MassPeaks:301
RawMode:Averaged 32.440-32.450(5589-5591) BasePeak:281.00(1327)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



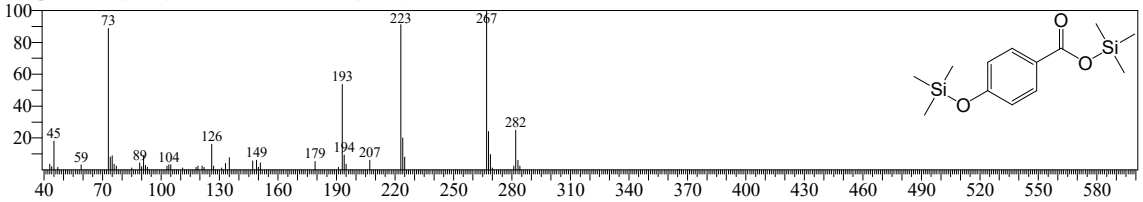
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



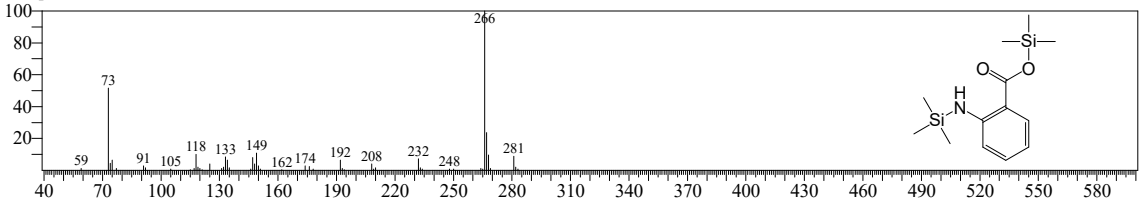
Hit#:2 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



Hit#:5 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid