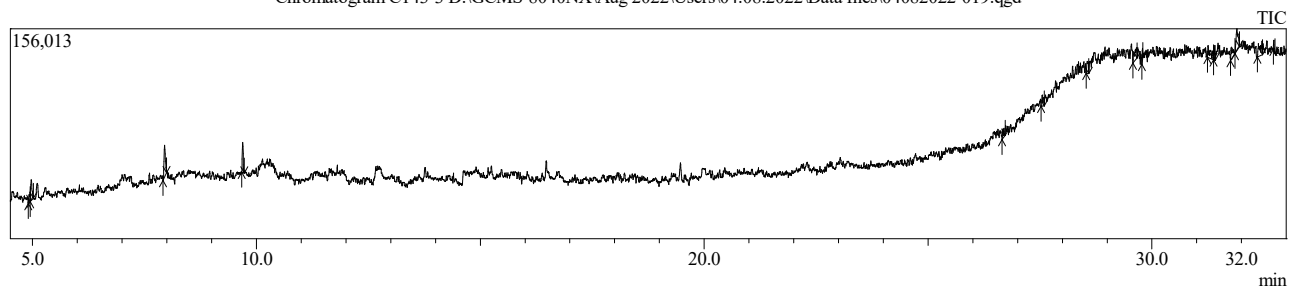# TNAU

Analyzed by     : Admin
Analyzed         : 05-Aug-22 4:36:32 AM
Sample Type     : Unknown
Level #          : 1
Sample Name    : C143-3
Sample ID       : C143-3
IS Amount      : [1]=1
Sample Amount  : 1
Dilution Factor   : 1
Vial #           : 19
Injection Volume : 1.00
Data File       : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-019.qgd
Org Data File   : D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-019.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 4:34:21 PM

Chromatogram C143-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-019.qgd



Peak Report TIC

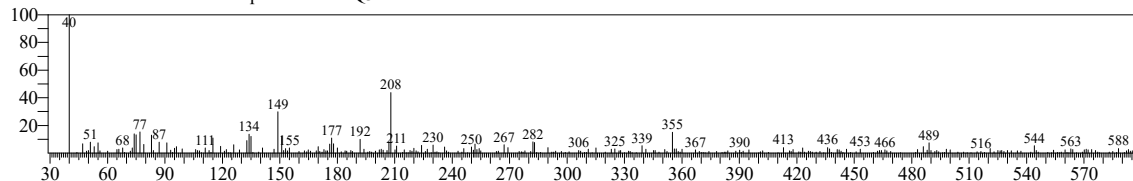| Peak# | R.Time | Area | Area% | Height | Height% | A/H | Similarity | Name |
|---|---|---|---|---|---|---|---|---|
| 1 | 4.915 | 14131 | 3.60 | 4774 | 2.84 | 2.96 | 29 | 3-Hydroxybenzoic acid-2TMS |
| 2 | 4.970 | 32901 | 8.38 | 15426 | 9.17 | 2.13 | 48 | Methyl butanoate |
| 3 | 7.948 | 49389 | 12.58 | 23593 | 14.02 | 2.09 | 86 | Tridecane |
| 4 | 9.692 | 34637 | 8.82 | 22330 | 13.27 | 1.55 | 88 | Undecane |
| 5 | 26.665 | 13505 | 3.44 | 6514 | 3.87 | 2.07 | 32 | 3,4-Dihydroxymandelic acid-4TMS |
| 6 | 27.545 | 15738 | 4.01 | 7854 | 4.67 | 2.00 | 34 | 3,4-Dihydroxymandelic acid-4TMS |
| 7 | 28.553 | 21652 | 5.51 | 8956 | 5.32 | 2.42 | 29 | 3,4-Dihydroxymandelic acid-4TMS |
| 8 | 29.655 | 29702 | 7.56 | 8190 | 4.87 | 3.63 | 38 | 3,4-Dihydroxymandelic acid-4TMS |
| 9 | 29.789 | 8238 | 2.10 | 8884 | 5.28 | 0.93 | 40 | 3,4-Dihydroxymandelic acid-4TMS |
| 10 | 31.250 | 37290 | 9.49 | 8064 | 4.79 | 4.62 | 40 | Hypoxanthine-2TMS |
| 11 | 31.389 | 12066 | 3.07 | 10761 | 6.39 | 1.12 | 36 | Galactose-5TMS(2) |
| 12 | 31.770 | 23284 | 5.93 | 8729 | 5.19 | 2.67 | 34 | Homogentisic acid-3TMS |
| 13 | 31.898 | 51086 | 13.01 | 16088 | 9.56 | 3.18 | 37 | Urocanic acid-2TMS |
| 14 | 32.458 | 40512 | 10.31 | 10306 | 6.12 | 3.93 | 35 | Epinephrine-3TMS |
| 15 | 32.722 | 8624 | 2.20 | 7813 | 4.64 | 1.10 | 36 | 3,4-Dihydroxymandelic acid-4TMS |
|  |  | 392755 | 100.00 | 168282 | 100.00 |  |  |  |

Library

# TNAU

<< Target >>
Line#:1 R.Time:4.915(Scan#:84) MassPeaks:291
RawMode:Averaged 4.910-4.920(83-85) BasePeak:40.00(768)
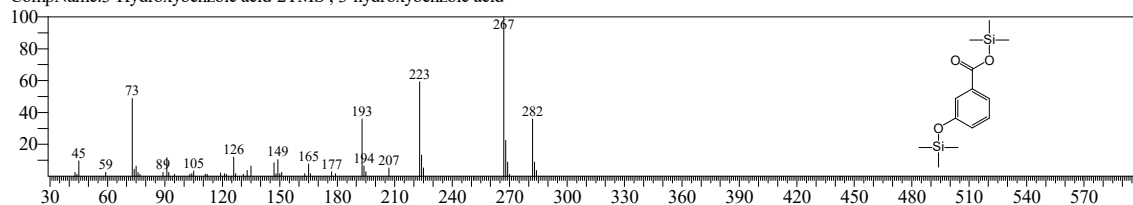BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
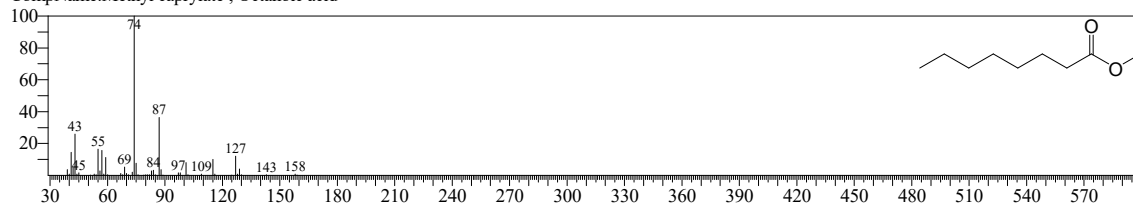SI:29 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:2 Entry:3 Library:FA_ME_SP2560_EI_V3.lib
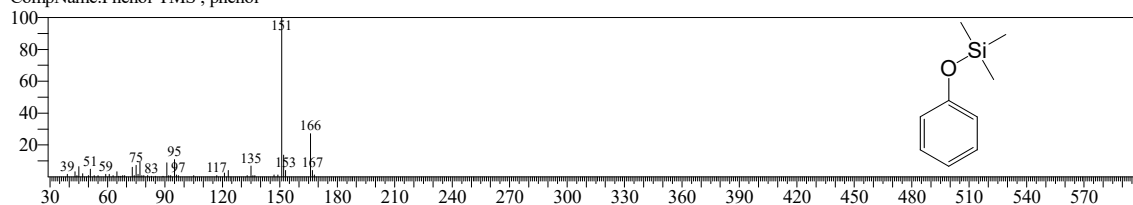SI:28 Formula:C9H18O2 CAS:124-07-2 MolWeight:158 RetIndex:1550
CompName:Methyl caprylate ; Octanoic acid



Hit#:3 Entry:7 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C9H14OSi CAS:108-95-2 MolWeight:166 RetIndex:1060
CompName:Phenol-TMS ; phenol



Hit#:4 Entry:4 Library:FA_ME_SP2560_EI_V3.lib
SI:28 Formula:C11H22O2 CAS:334-48-5 MolWeight:186 RetIndex:1767
CompName:Methyl caprate ; Decanoic acid



Hit#:5 Entry:5 Library:FA_ME_SP2560_EI_V3.lib
SI:28 Formula:C12H24O2 CAS:112-37-8 MolWeight:200 RetIndex:1875
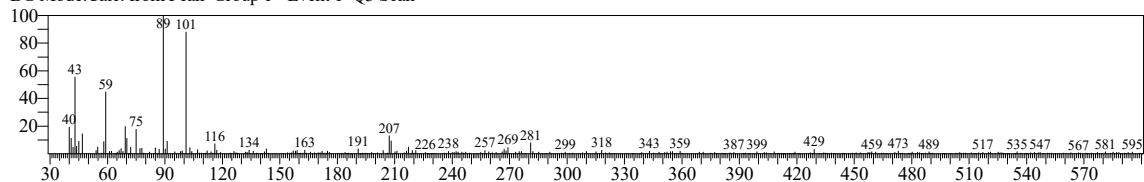CompName:Methyl undecanoate ; Undecanoic acid

# TNAU

<< Target >>
Line#:2   R.Time:4.970(Scan#:95)  MassPeaks:297
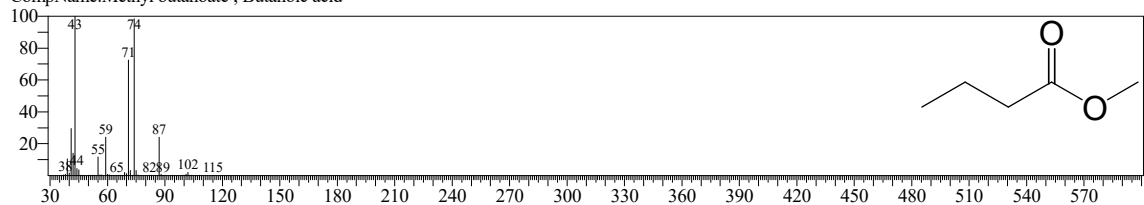RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.10(2098)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:1  Library:FA_ME_SP2560_EI_V3.lib
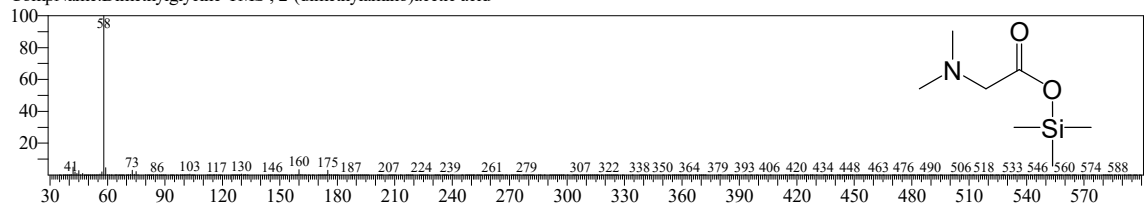SI:48  Formula:C5H10O2  CAS:107-92-6  MolWeight:102  RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



Hit#:2  Entry:1  Library:OA_TMS_DB5_67min_V3.lib
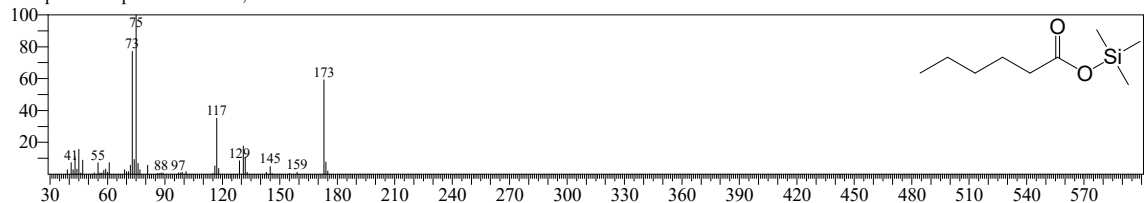SI:43  Formula:C7H17NO2Si  CAS:1118-68-9  MolWeight:175  RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



Hit#:3  Entry:11  Library:OA_TMS_DB5_67min_V3.lib
SI:42  Formula:C9H20O2Si  CAS:142-62-1  MolWeight:188  RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid



Hit#:4  Entry:456  Library:OA_TMS_DB5_67min_V3.lib
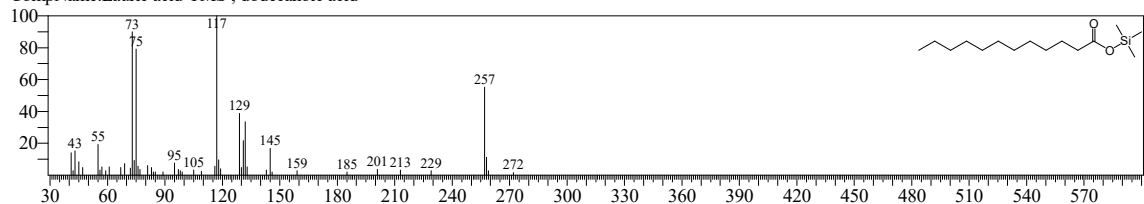SI:38  Formula:C18H33NO3Si  CAS:37350-58-6  MolWeight:339  RetIndex:2094
CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol



Hit#:5  Entry:223  Library:OA_TMS_DB5_67min_V3.lib
SI:36  Formula:C15H32O2Si  CAS:143-07-7  MolWeight:272  RetIndex:1653
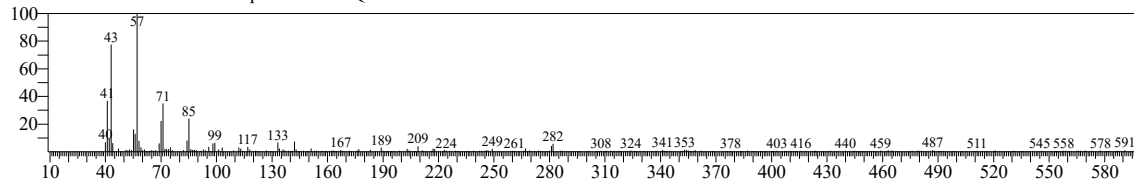CompName:Lauric acid-TMS ; dodecanoic acid

# TNAU

<< Target >>
Line#:3   R.Time:7.945(Scan#:690)  MassPeaks:301
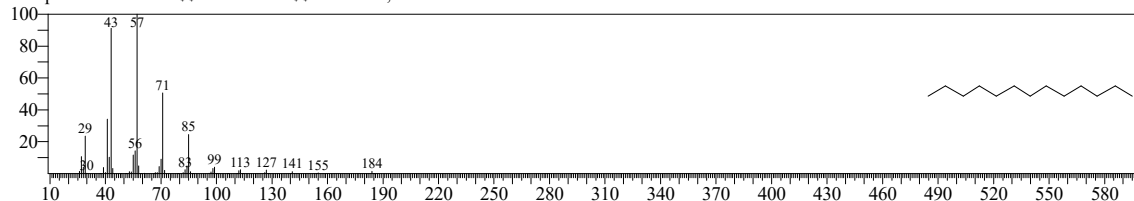RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.05(5027)
BG Mode:Calc. from Peak Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:40226  Library:NIST20M1.lib
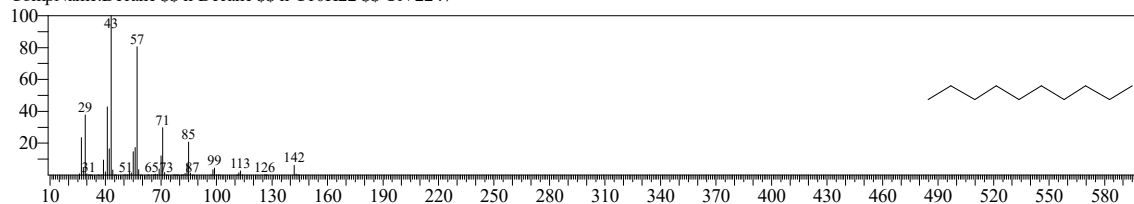SI:86  Formula:C13H28  CAS:629-50-5  MolWeight:184  RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:2  Entry:9443  Library:NIST20R.lib
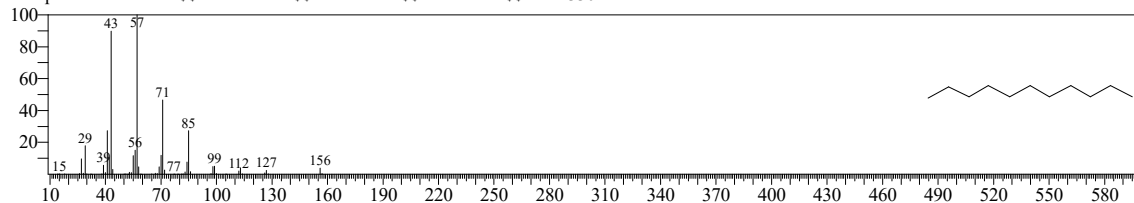SI:86  Formula:C10H22  CAS:124-18-5  MolWeight:142  RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



Hit#:3  Entry:21042  Library:NIST20M1.lib
SI:86  Formula:C11H24  CAS:1120-21-4  MolWeight:156  RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



Hit#:4  Entry:13607  Library:NIST20M1.lib
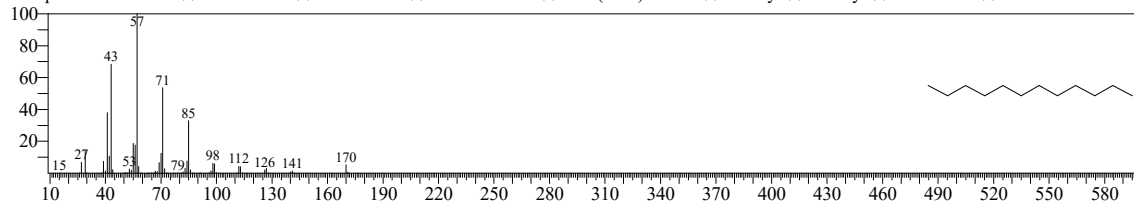SI:86  Formula:C10H22  CAS:15869-89-3  MolWeight:142  RetIndex:887
CompName:Octane, 2,5-dimethyl- $$ 2,5-Dimethyloctane



Hit#:5  Entry:30057  Library:NIST20M1.lib
SI:85  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
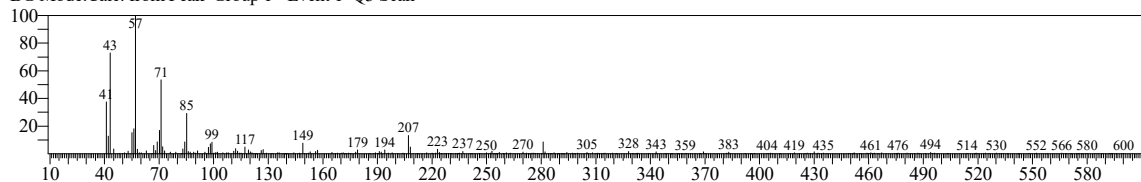
# TNAU

<< Target >>
Line#:4  R.Time:9.690(Scan#:1039)  MassPeaks:256
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.10(4608)
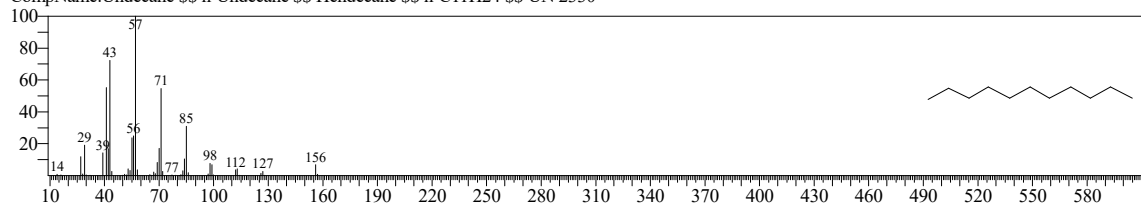BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:12898  Library:NIST20R.lib
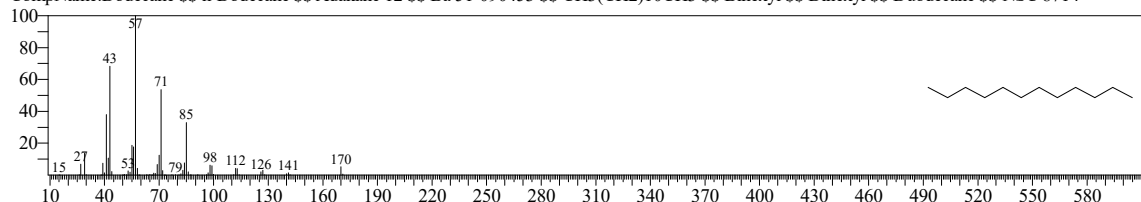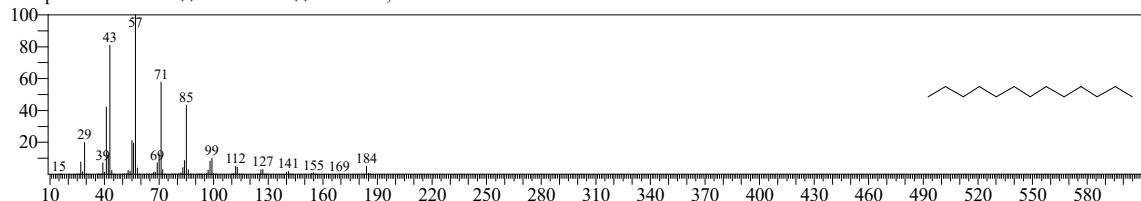SI:88  Formula:C11H24  CAS:1120-21-4  MolWeight:156  RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



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



Hit#:3  Entry:19410  Library:NIST20R.lib
SI:87  Formula:C13H28  CAS:629-50-5  MolWeight:184  RetIndex:1300
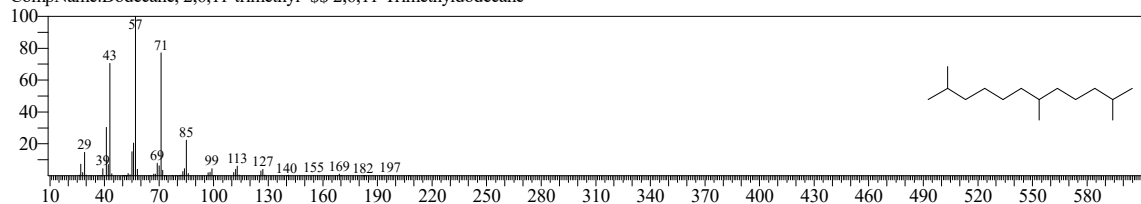CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



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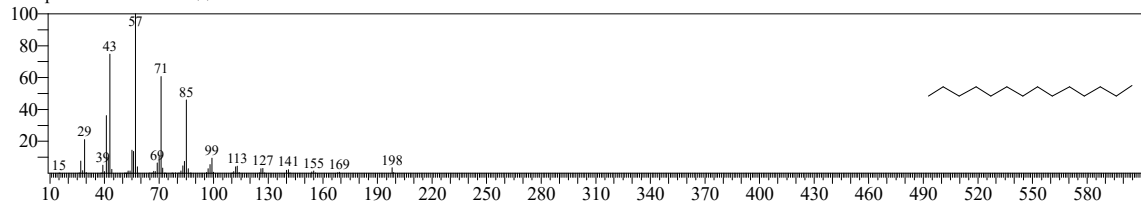SI:87  Formula:C15H32  CAS:31295-56-4  MolWeight:212  RetIndex:1320
CompName:Dodecane, 2,6,11-trimethyl- $$ 2,6,11-Trimethyldodecane



Hit#:5  Entry:22497  Library:NIST20R.lib
SI:87  Formula:C14H30  CAS:629-59-4  MolWeight:198  RetIndex:1400
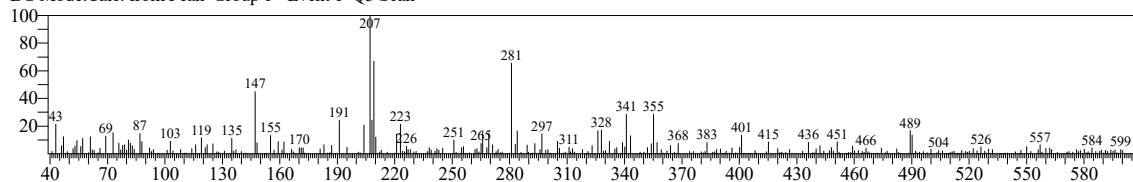CompName:Tetradecane $$ n-Tetradecane

# TNAU

<< Target >>
Line#:5  R.Time:26.665(Scan#:4434)  MassPeaks:314
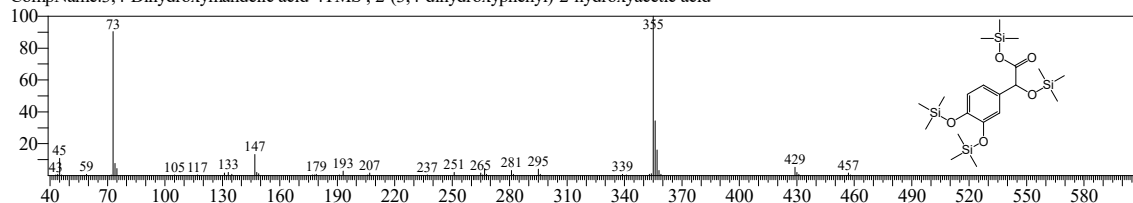RawMode:Averaged 26.660-26.670(4433-4435) BasePeak:207.05(871)
BG Mode:Calc. from Peak Group 1 - Event 1  Q3 Scan



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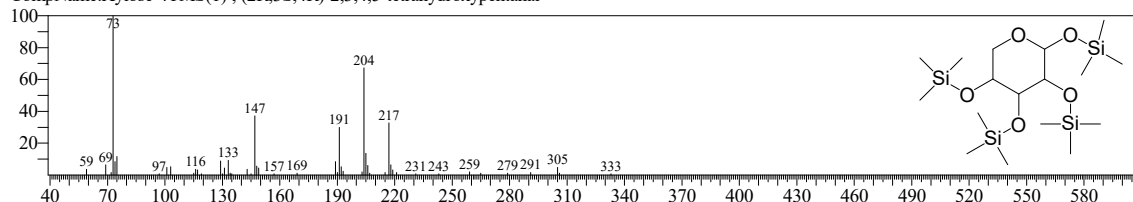SI:32  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:2  Entry:267  Library:OA_TMS_DB5_67min_V3.lib
SI:30  Formula:C17H42O5Si4  CAS:58-86-6  MolWeight:438  RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:3  Entry:528  Library:OA_TMS_DB5_67min_V3.lib
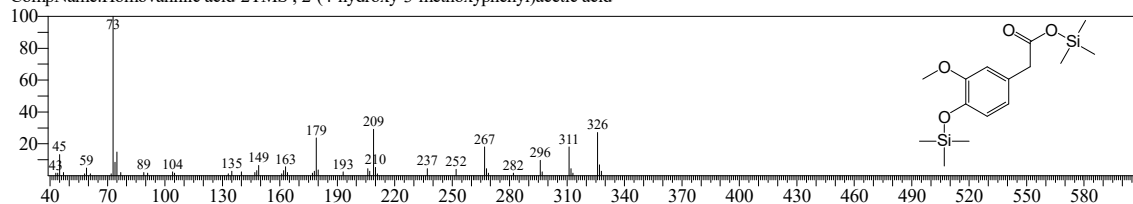SI:30  Formula:C17H28Cl2N2O5Si2  CAS:56-75-7  MolWeight:466  RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



Hit#:4  Entry:294  Library:OA_TMS_DB5_67min_V3.lib
SI:30  Formula:C15H26O4Si2  CAS:306-08-1  MolWeight:326  RetIndex:1782
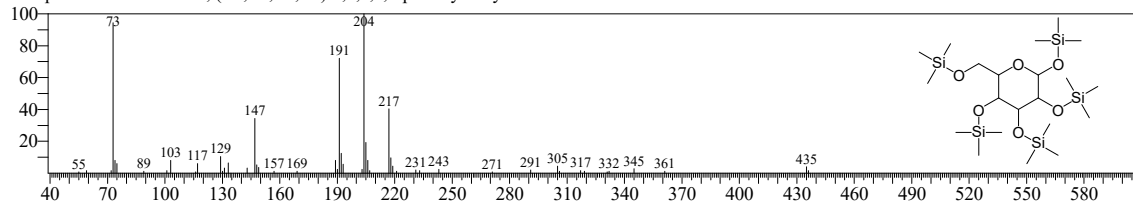CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



Hit#:5  Entry:349  Library:OA_TMS_DB5_67min_V3.lib
SI:29  Formula:C21H52O6Si5  CAS:2595-97-3  MolWeight:540  RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal
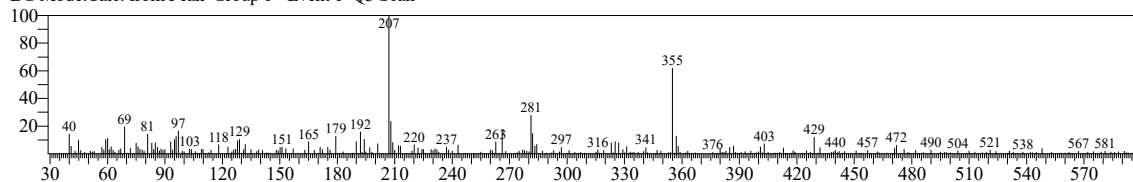
# TNAU

<< Target >>
Line#:6  R.Time:27.545(Scan#:4610)  MassPeaks:284
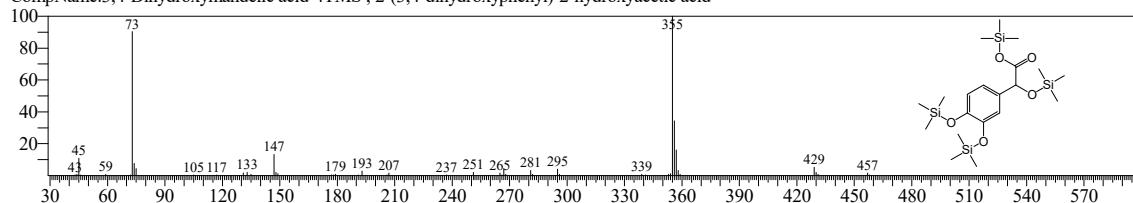RawMode:Averaged 27.540-27.550(4609-4611) BasePeak:207.05(1676)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:402  Library:OA_TMS_DB5_67min_V3.lib
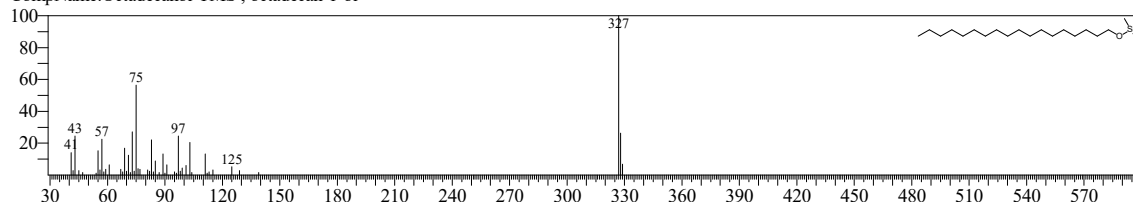SI:34  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:2  Entry:477  Library:OA_TMS_DB5_67min_V3.lib
SI:25  Formula:C21H46OSi  CAS:112-92-5  MolWeight:342  RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol



Hit#:3  Entry:558  Library:OA_TMS_DB5_67min_V3.lib
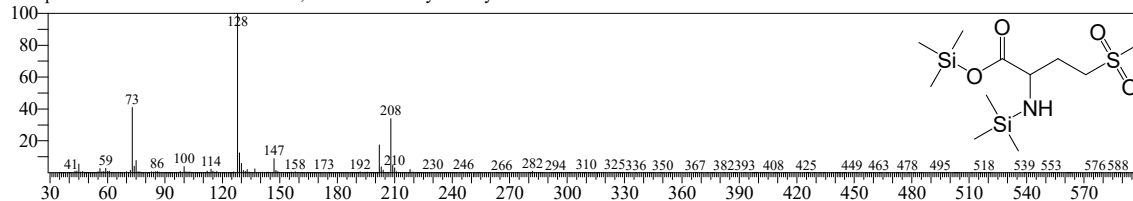SI:25  Formula:C19H39N2O8PSi3  CAS:365-07-1  MolWeight:538  RetIndex:2905
CompName:Thymidine monophosphate-3TMS ; [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxopyrimidin-1-yl)oxolan-2-yl]methyl dihydrogen phosph



Hit#:4  Entry:329  Library:OA_TMS_DB5_67min_V3.lib
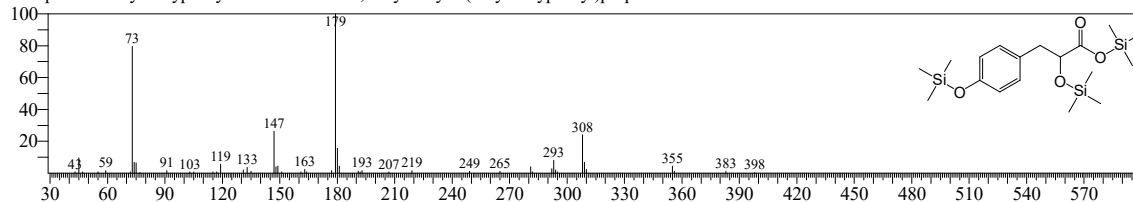SI:25  Formula:C11H27NO4SSi2  CAS:820-10-0  MolWeight:325  RetIndex:1848
CompName:Methionine sulfone-2TMS ; 2-amino-4-methylsulfonylbutanoic acid



Hit#:5  Entry:382  Library:OA_TMS_DB5_67min_V3.lib
SI:24  Formula:C18H34O4Si3  CAS:6482-98-0  MolWeight:398  RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate
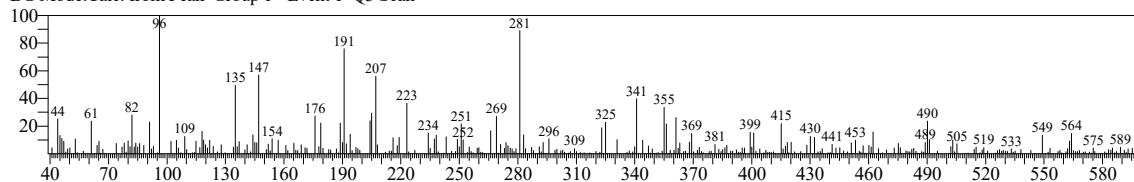
# TNAU

<< Target >>
Line#:7  R.Time:28.555(Scan#:4812)  MassPeaks:333
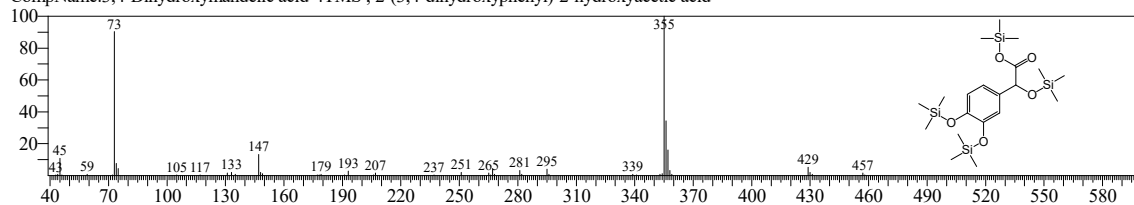RawMode:Averaged 28.550-28.560(4811-4813) BasePeak:96.10(829)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



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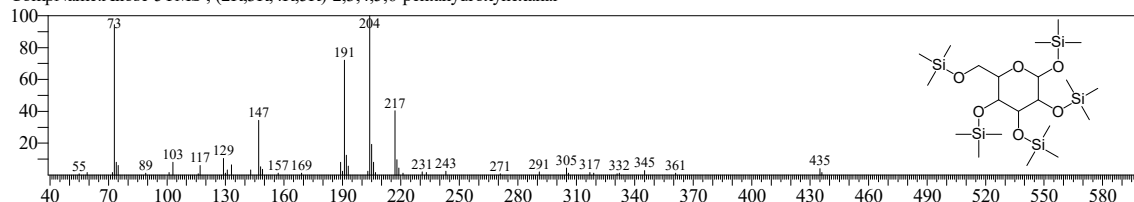SI:29  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:2  Entry:349  Library:OA_TMS_DB5_67min_V3.lib
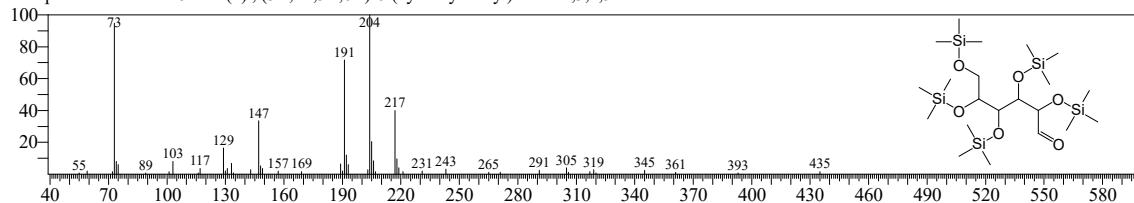SI:25  Formula:C21H52O6Si5  CAS:2595-97-3  MolWeight:540  RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal



Hit#:3  Entry:345  Library:OA_TMS_DB5_67min_V3.lib
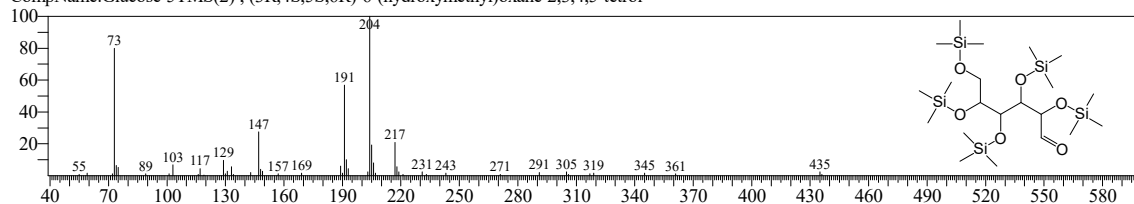SI:25  Formula:C21H52O6Si5  CAS:59-23-4  MolWeight:540  RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4  Entry:437  Library:OA_TMS_DB5_67min_V3.lib
SI:24  Formula:C21H52O6Si5  CAS:50-99-7  MolWeight:540  RetIndex:2002
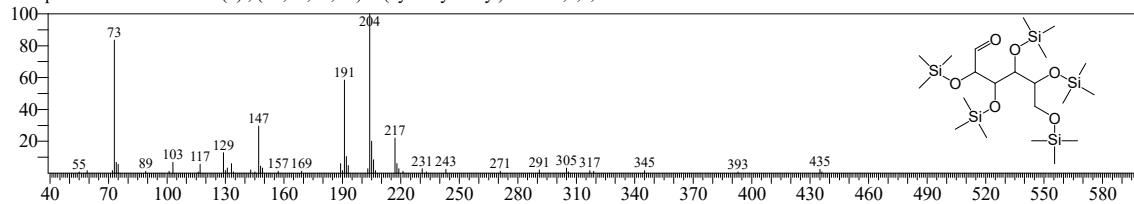CompName:Glucose-5TMS(2) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:5  Entry:348  Library:OA_TMS_DB5_67min_V3.lib
SI:23  Formula:C21H52O6Si5  CAS:3458-28-4  MolWeight:540  RetIndex:1872
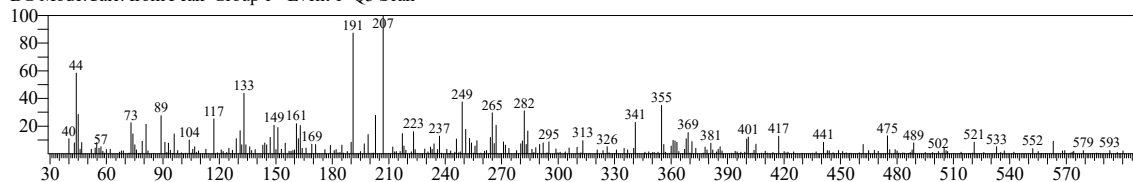CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

# TNAU

<< Target >>
Line#:8  R.Time:29.655(Scan#:5032)  MassPeaks:283
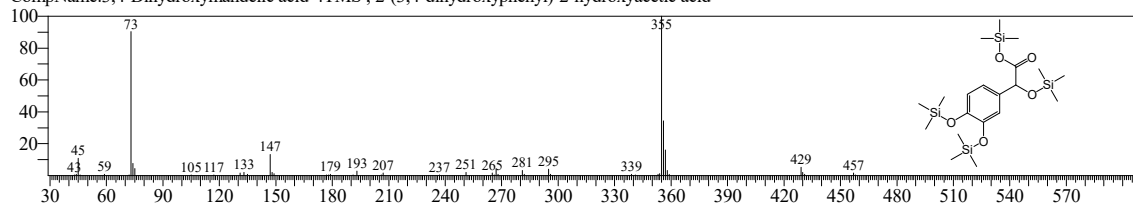RawMode:Averaged 29.650-29.660(5031-5033) BasePeak:207.05(1043)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



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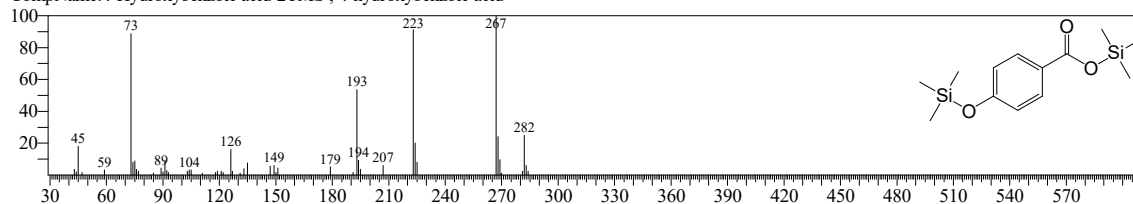SI:38  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:2  Entry:211  Library:OA_TMS_DB5_67min_V3.lib
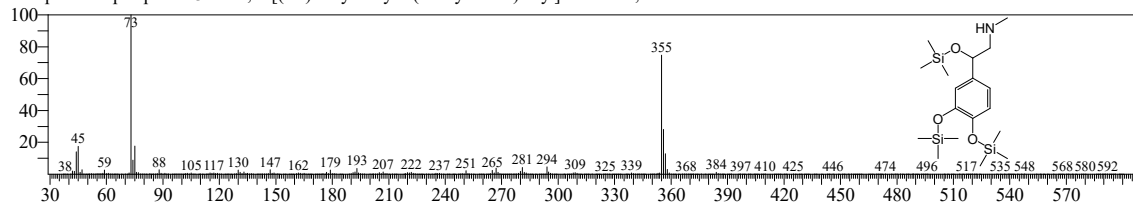SI:37  Formula:C13H22O3Si2  CAS:99-96-7  MolWeight:282  RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



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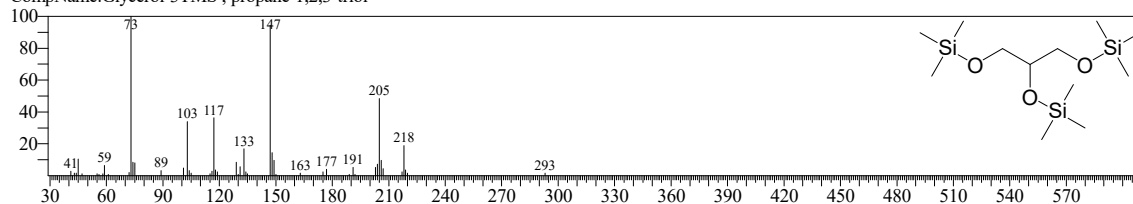SI:37  Formula:C18H37NO3Si3  CAS:51-43-4  MolWeight:399  RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4  Entry:77  Library:OA_TMS_DB5_67min_V3.lib
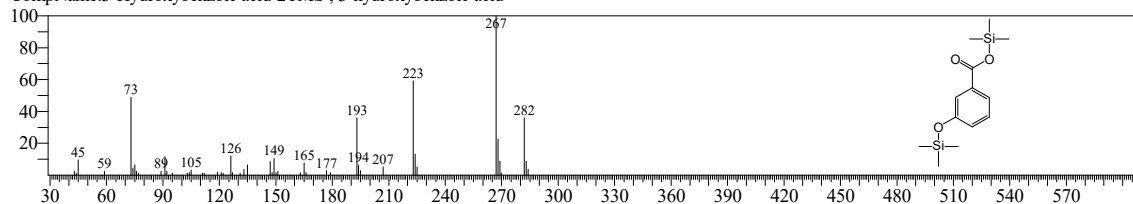SI:36  Formula:C12H32O3Si3  CAS:56-81-5  MolWeight:308  RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



Hit#:5  Entry:179  Library:OA_TMS_DB5_67min_V3.lib
SI:35  Formula:C13H22O3Si2  CAS:99-06-9  MolWeight:282  RetIndex:1572
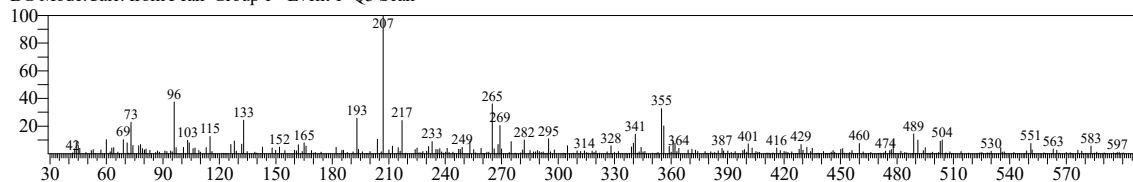CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

# TNAU

<< Target >>
Line#:9  R.Time:29.790(Scan#:5059)  MassPeaks:314
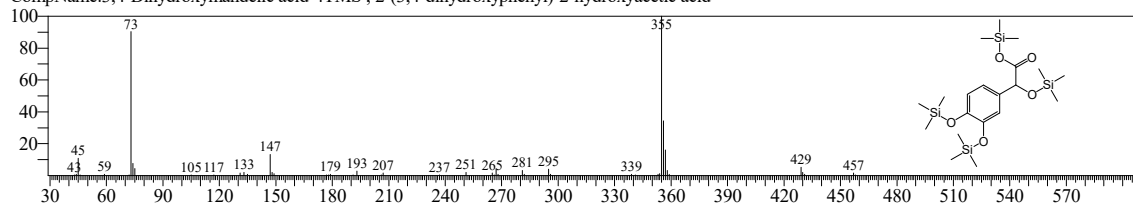RawMode:Averaged 29.785-29.795(5058-5060) BasePeak:207.05(1353)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1  Entry:402  Library:OA_TMS_DB5_67min_V3.lib
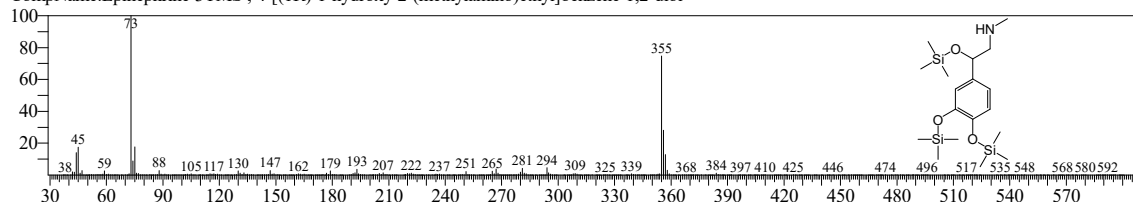SI:40  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



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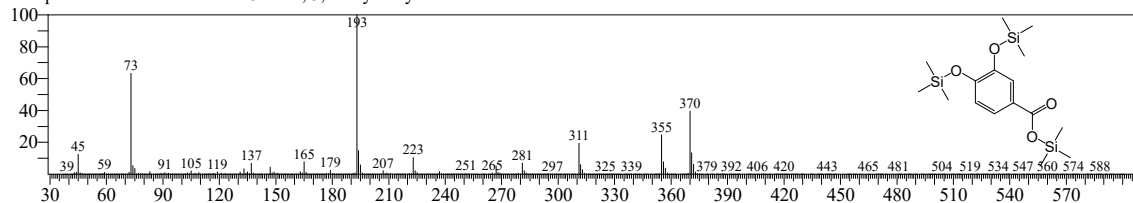SI:40  Formula:C18H37NO3Si3  CAS:51-43-4  MolWeight:399  RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:3  Entry:315  Library:OA_TMS_DB5_67min_V3.lib
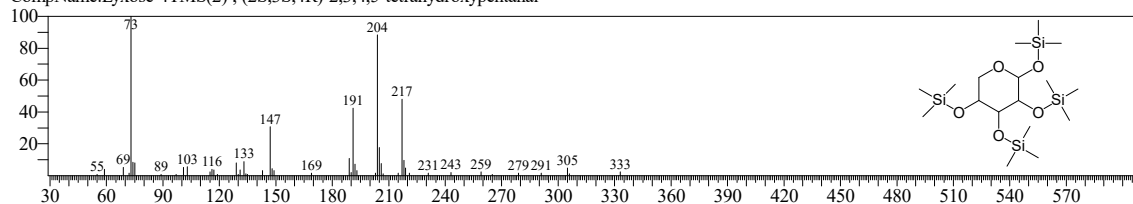SI:34  Formula:C16H30O4Si3  CAS:99-50-3  MolWeight:370  RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4  Entry:238  Library:OA_TMS_DB5_67min_V3.lib
SI:33  Formula:C17H42O5Si4  CAS:1114-34-7  MolWeight:438  RetIndex:1675
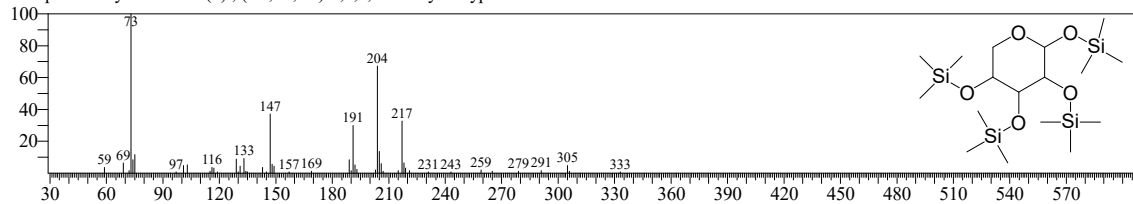CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:5  Entry:267  Library:OA_TMS_DB5_67min_V3.lib
SI:33  Formula:C17H42O5Si4  CAS:58-86-6  MolWeight:438  RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal
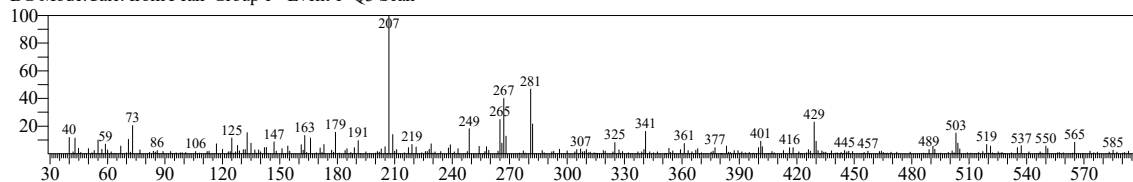
# TNAU

<< Target >>
Line#:10  R.Time:31.250(Scan#:5351)  MassPeaks:283
RawMode:Averaged 31.245-31.255(5350-5352) BasePeak:207.05(1706)
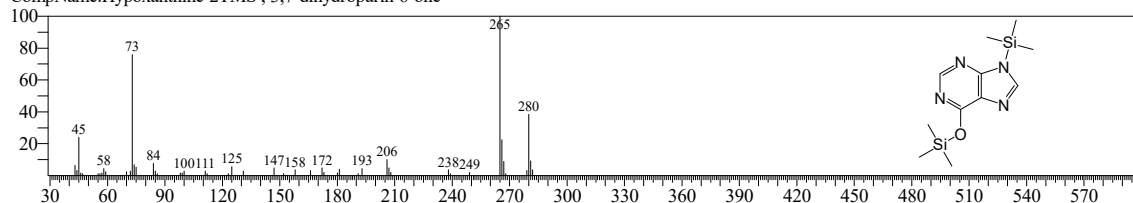BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:310  Library:OA_TMS_DB5_67min_V3.lib
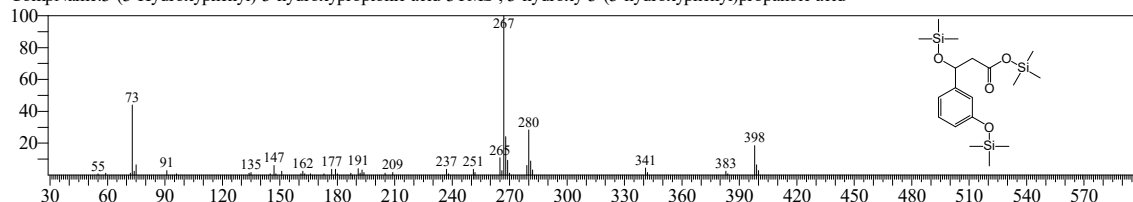SI:40  Formula:C11H20N4OSi2  CAS:68-94-0  MolWeight:280  RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:2  Entry:341  Library:OA_TMS_DB5_67min_V3.lib
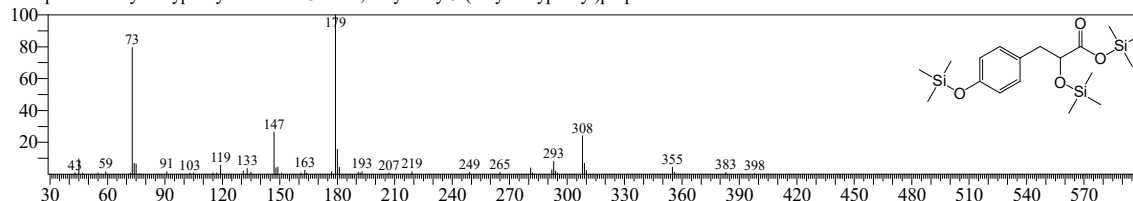SI:39  Formula:C18H34O4Si3  CAS:3247-75-4  MolWeight:398  RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:3  Entry:382  Library:OA_TMS_DB5_67min_V3.lib
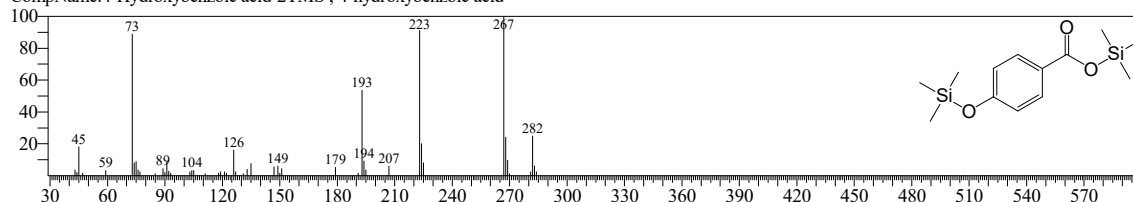SI:36  Formula:C18H34O4Si3  CAS:6482-98-0  MolWeight:398  RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



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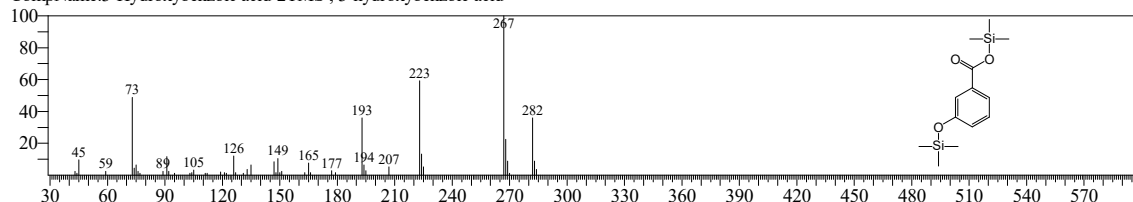SI:34  Formula:C13H22O3Si2  CAS:99-96-7  MolWeight:282  RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:5  Entry:179  Library:OA_TMS_DB5_67min_V3.lib
SI:34  Formula:C13H22O3Si2  CAS:99-06-9  MolWeight:282  RetIndex:1572
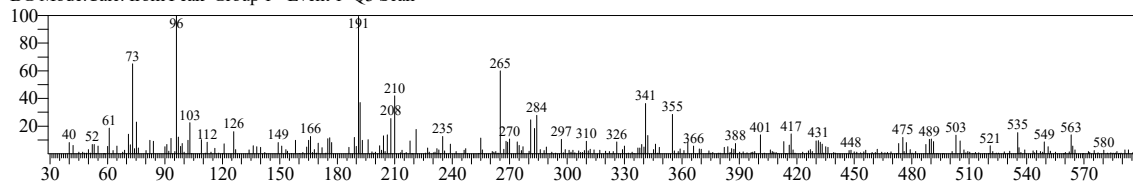CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

# TNAU

<< Target >>
Line#:11  R.Time:31.390(Scan#:5379)  MassPeaks:313
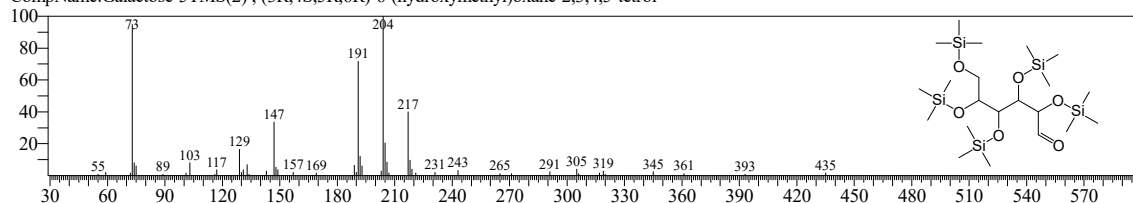RawMode:Averaged 31.385-31.395(5378-5380) BasePeak:96.05(1039)
BG Mode:Calc. from Peak  Group 1 - Event 1 Q3 Scan



Hit#:1  Entry:345  Library:OA_TMS_DB5_67min_V3.lib
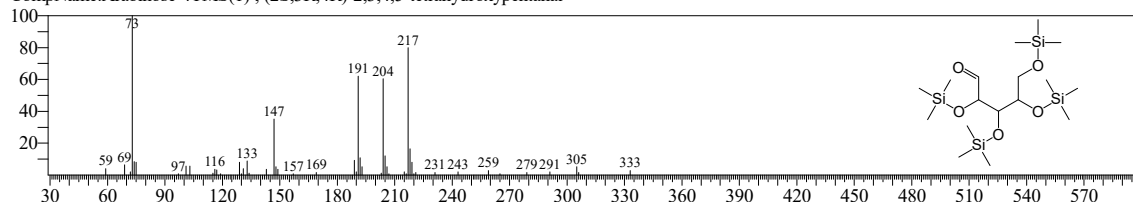SI:36  Formula:C21H52O6Si5  CAS:59-23-4  MolWeight:540  RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:2  Entry:210  Library:OA_TMS_DB5_67min_V3.lib
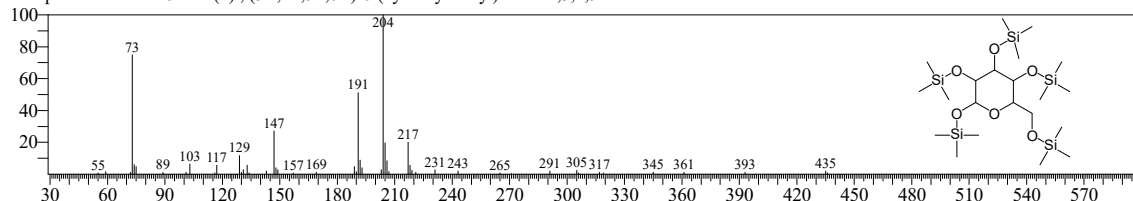SI:35  Formula:C17H42O5Si4  CAS:10323-20-3  MolWeight:438  RetIndex:1634
CompName:Arabinose-4TMS(1) ; (2S,3R,4R)-2,3,4,5-tetrahydroxypentanal



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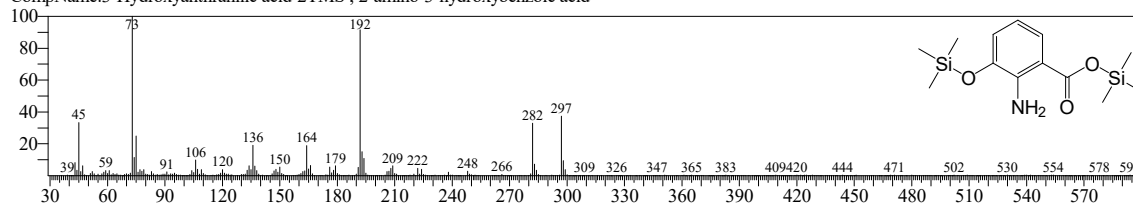CompName:Glucose-5TMS(1) ; (3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol



Hit#:4  Entry:290  Library:OA_TMS_DB5_67min_V3.lib
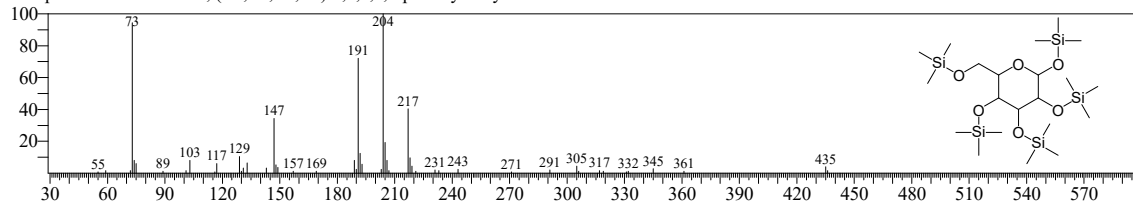SI:34  Formula:C13H23NO3Si2  CAS:548-93-6  MolWeight:297  RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



Hit#:5  Entry:349  Library:OA_TMS_DB5_67min_V3.lib
SI:34  Formula:C21H52O6Si5  CAS:2595-97-3  MolWeight:540  RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal
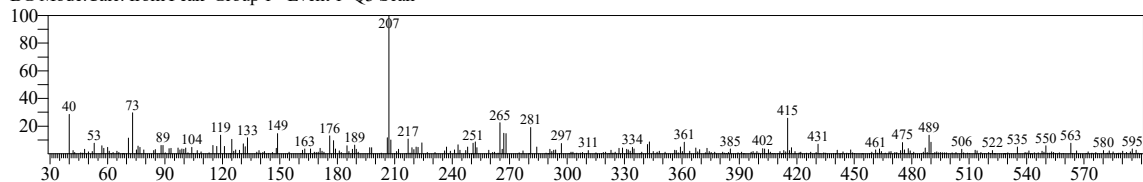
# TNAU

<< Target >>
Line#:12  R.Time:31.770(Scan#:5455)  MassPeaks:320
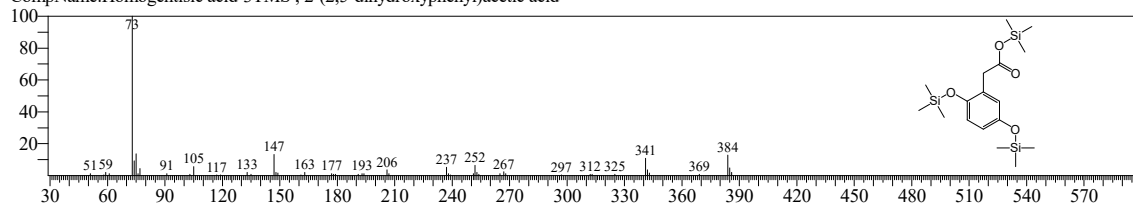RawMode:Averaged 31.765-31.775(5454-5456) BasePeak:207.05(1968)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



Hit#:1  Entry:332  Library:OA_TMS_DB5_67min_V3.lib
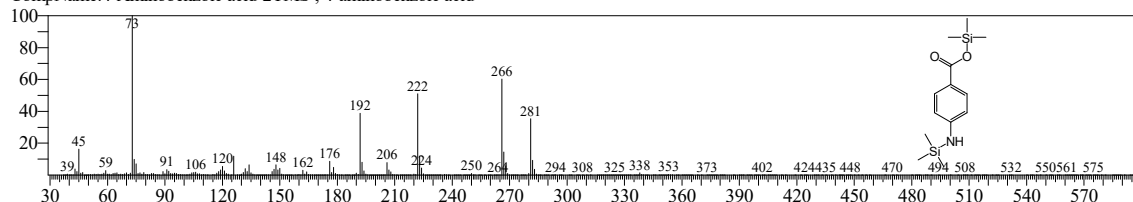SI:34  Formula:C17H32O4Si3  CAS:451-13-8  MolWeight:384  RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid



Hit#:2  Entry:328  Library:OA_TMS_DB5_67min_V3.lib
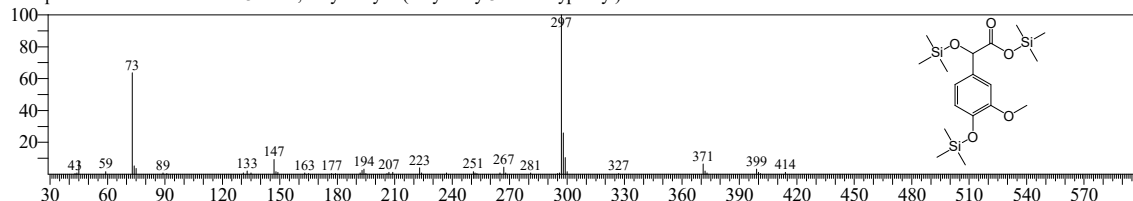SI:34  Formula:C13H23NO2Si2  CAS:150-13-0  MolWeight:281  RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:3  Entry:359  Library:OA_TMS_DB5_67min_V3.lib
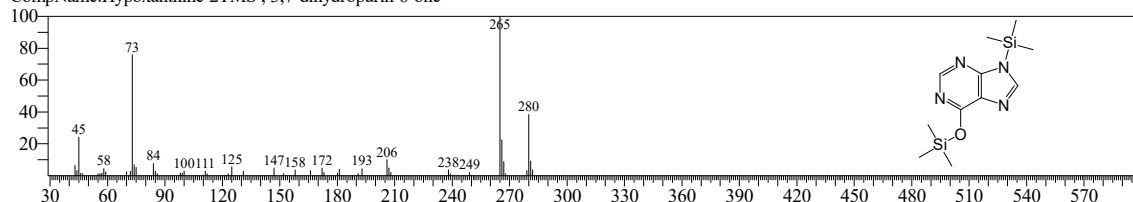SI:33  Formula:C18H34O5Si3  CAS:55-10-7  MolWeight:414  RetIndex:1894
CompName:Vanilmandelic acid-3TMS ; 2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetic acid



Hit#:4  Entry:310  Library:OA_TMS_DB5_67min_V3.lib
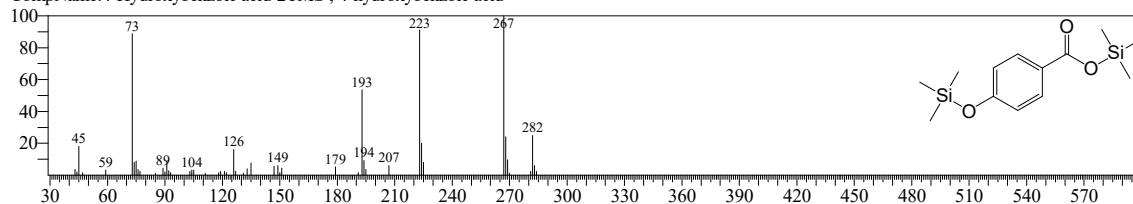SI:33  Formula:C11H20N4OSi2  CAS:68-94-0  MolWeight:280  RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:5  Entry:211  Library:OA_TMS_DB5_67min_V3.lib
SI:31  Formula:C13H22O3Si2  CAS:99-96-7  MolWeight:282  RetIndex:1636
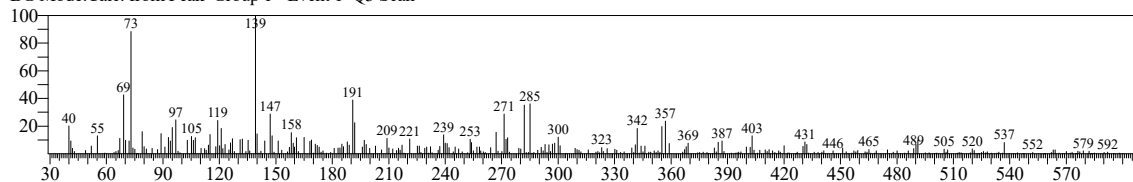CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

# TNAU

<< Target >>
Line#:13 R.Time:31.900(Scan#:5481) MassPeaks:316
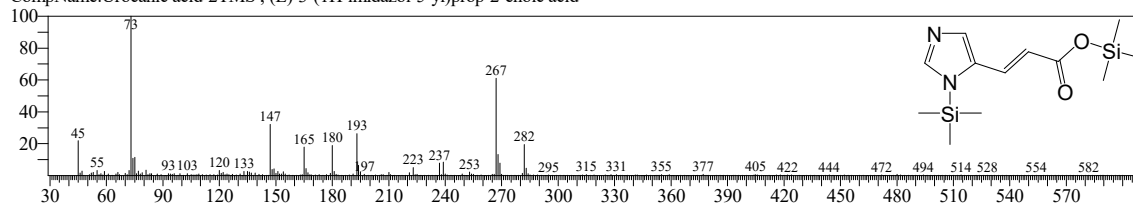RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:139.15(1561)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
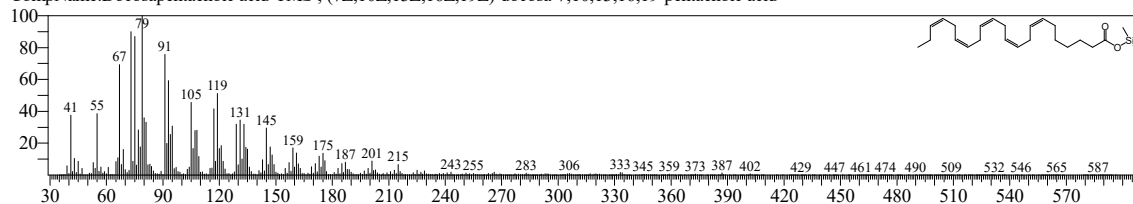SI:37 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



Hit#:2 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
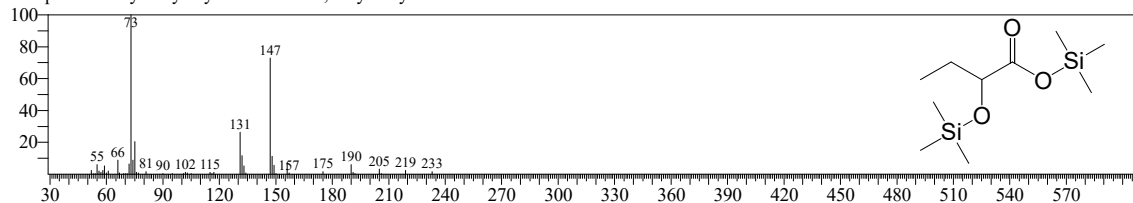CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



Hit#:3 Entry:23 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C10H24O3Si2 CAS:600-15-7 MolWeight:248 RetIndex:1129
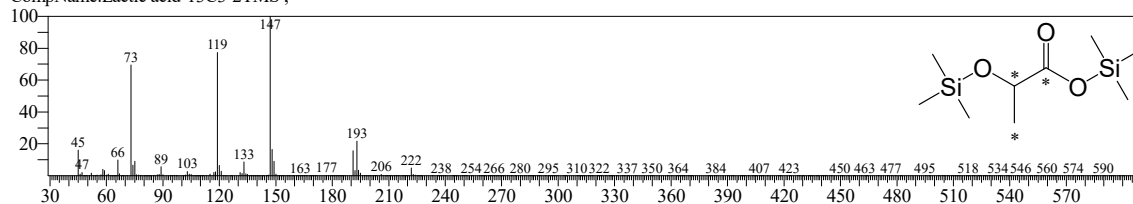CompName:2-Hydroxybutyric acid-2TMS ; 2-hydroxybutanoic acid



Hit#:4 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
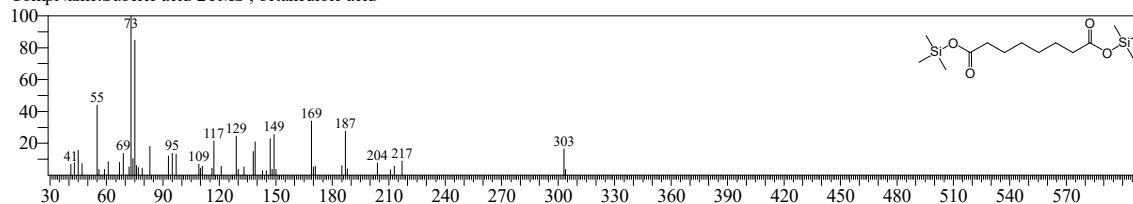SI:35 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;



Hit#:5 Entry:258 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C14H30O4Si2 CAS:505-48-6 MolWeight:318 RetIndex:1700
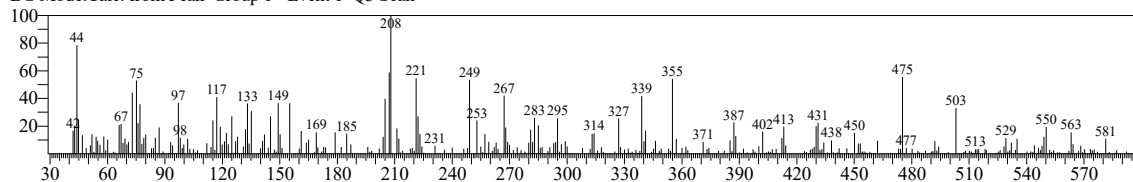CompName:Suberic acid-2TMS ; octanedioic acid

# TNAU

<< Target >>
Line#:14  R.Time:32.460(Scan#:5593)  MassPeaks:312
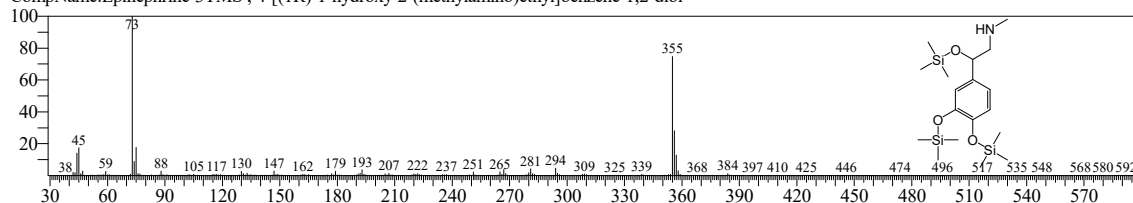RawMode:Averaged 32.455-32.465(5592-5594) BasePeak:208.00(679)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



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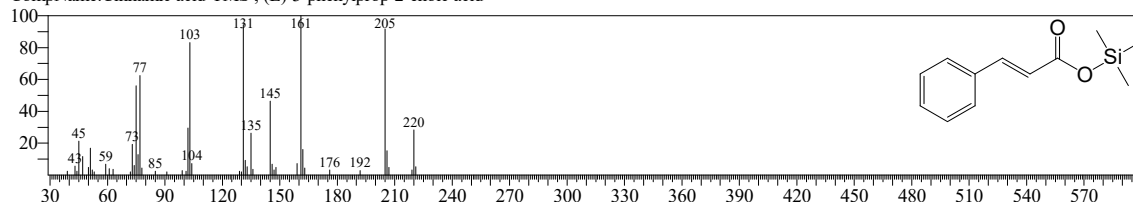SI:35  Formula:C18H37NO3Si3  CAS:51-43-4  MolWeight:399  RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:2  Entry:171  Library:OA_TMS_DB5_67min_V3.lib
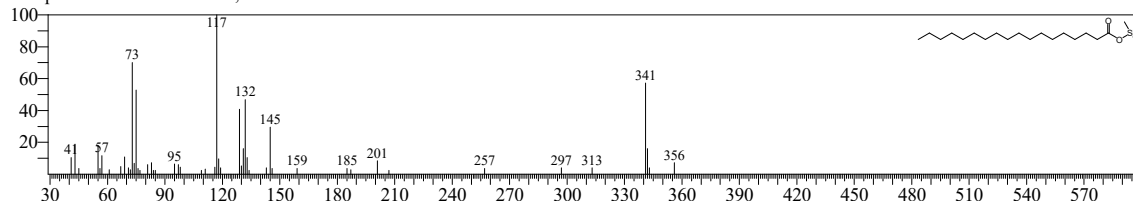SI:33  Formula:C12H16O2Si  CAS:140-10-3  MolWeight:220  RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid



Hit#:3  Entry:491  Library:OA_TMS_DB5_67min_V3.lib
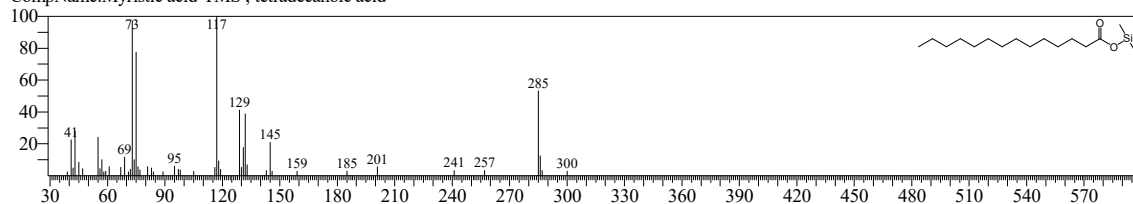SI:31  Formula:C21H44O2Si  CAS:57-11-4  MolWeight:356  RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



Hit#:4  Entry:331  Library:OA_TMS_DB5_67min_V3.lib
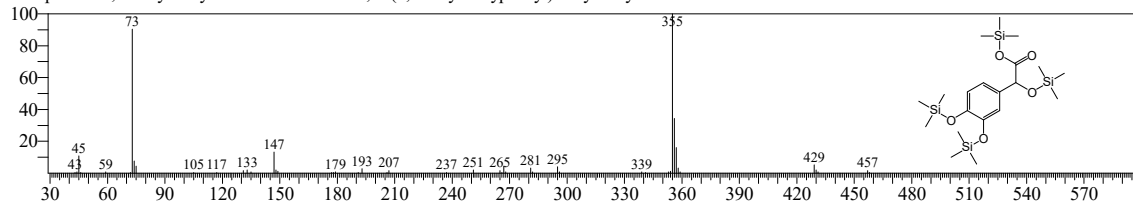SI:31  Formula:C17H36O2Si  CAS:544-63-8  MolWeight:300  RetIndex:1850
CompName:Myristic acid-TMS ; tetradecanoic acid



Hit#:5  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
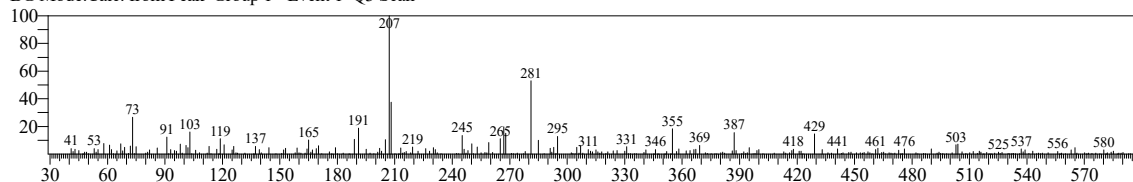
# TNAU

<< Target >>
Line#:15  R.Time:32.720(Scan#:5645)  MassPeaks:307
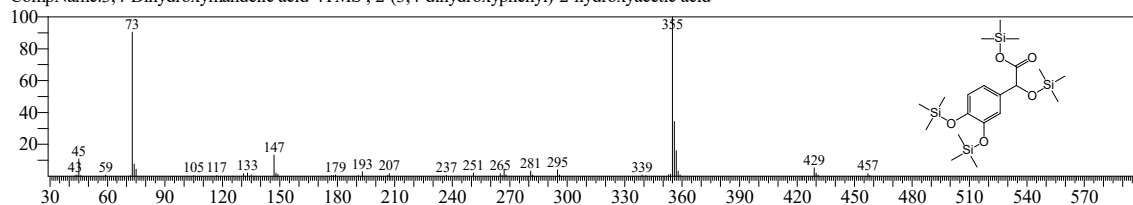RawMode:Averaged 32.715-32.725(5644-5646) BasePeak:207.05(1732)
BG Mode:Calc. from Peak  Group 1 - Event 1  Q3 Scan



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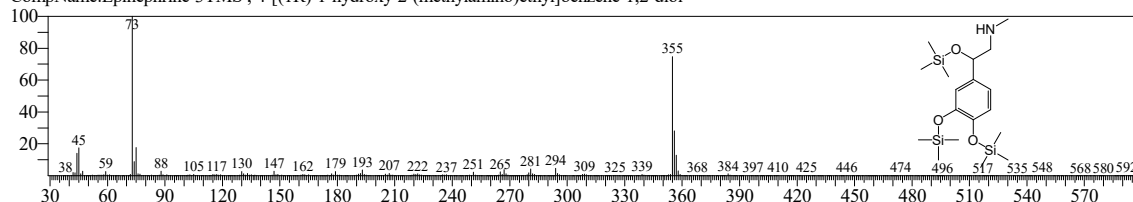SI:36  Formula:C20H42O4Si4  CAS:775-01-9  MolWeight:458  RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



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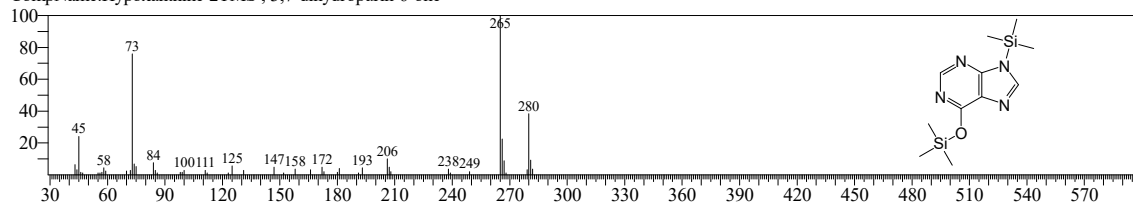CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



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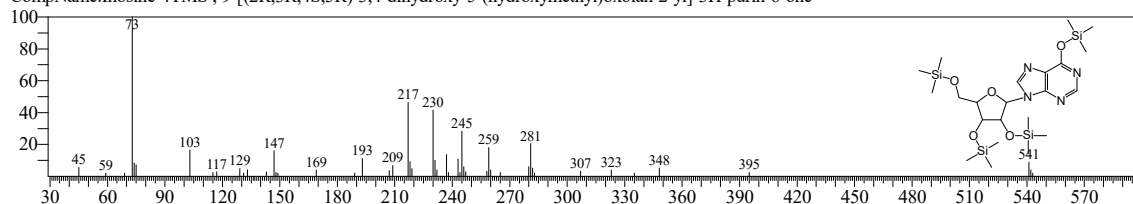CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4  Entry:535  Library:OA_TMS_DB5_67min_V3.lib
SI:35  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: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