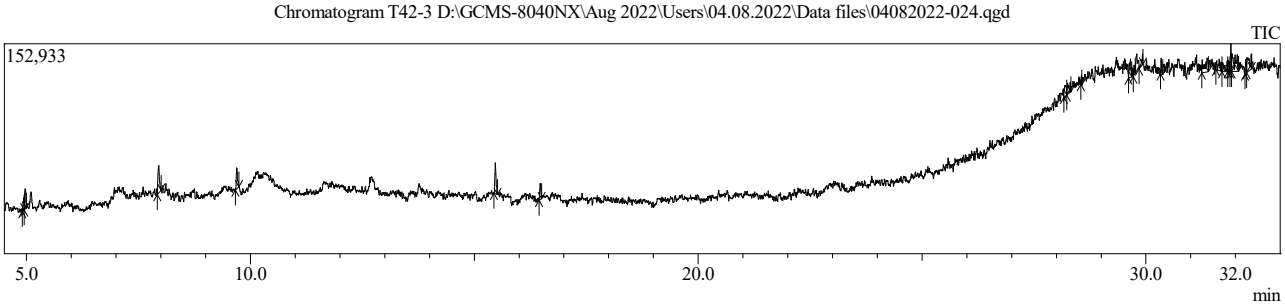
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 7:50:34 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: T42-3
Sample ID	: T42-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 23
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-024.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-024.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 4:43:07 PM

Chromatogram T42-3 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-024.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.935	18370	3.08	8576	3.64	2.14	32	4-Aminobenzoic acid-2TMS
2	4.968	26127	4.39	14903	6.33	1.75	54	Methyl butanoate
3	7.949	46990	7.89	20006	8.50	2.35	87	Decane
4	9.695	29974	5.03	15018	6.38	2.00	87	Undecane
5	15.470	39617	6.65	22675	9.64	1.75	86	Phenol, 3,5-bis(1,1-dimethylethyl)-
6	16.472	22214	3.73	11618	4.94	1.91	77	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
7	28.185	25638	4.30	8033	3.41	3.19	32	Batyl alcohol-2TMS
8	28.309	25832	4.34	7326	3.11	3.53	28	3-Hydroxyphenylacetic acid-2TMS
9	28.559	5503	0.92	6766	2.88	0.81	42	Glycerol-3TMS
10	29.656	30299	5.09	13045	5.54	2.32	39	3-Hydroxyanthranilic acid-2TMS
11	29.730	11870	1.99	7251	3.08	1.64	32	Anthranilic acid-2TMS
12	29.924	13854	2.33	7780	3.31	1.78	26	Glycerol-3TMS
13	30.340	14877	2.50	11586	4.92	1.28	33	Hypoxanthine-2TMS
14	31.255	48663	8.17	9508	4.04	5.12	34	3-Hydroxyanthranilic acid-2TMS
15	31.575	31053	5.21	5901	2.51	5.26	25	Protocatechuic acid-3TMS
16	31.705	26453	4.44	5748	2.44	4.60	37	Epinephrine-3TMS
17	31.835	20310	3.41	8325	3.54	2.44	34	4-Hydroxybenzoic acid-2TMS
18	31.898	26082	4.38	20067	8.53	1.30	40	4-Hydroxybenzoic acid-2TMS
19	32.040	70686	11.87	12218	5.19	5.79	45	Homovanillic acid-2TMS
20	32.225	13363	2.24	8285	3.52	1.61	33	Anthranilic acid-2TMS
21	32.350	47861	8.04	10694	4.54	4.48	34	3-Hydroxybutyric acid-2TMS
		595636	100.00	235329	100.00			

TNAU

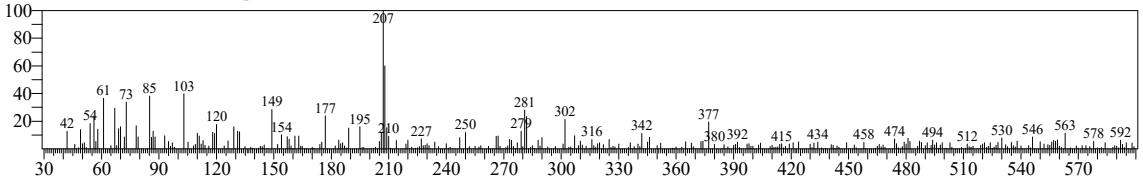
Library

<< Target >>

Line#:1 R.Time:4.935(Scan#:88) MassPeaks:307

RawMode:Averaged 4.930-4.940(87-89) BasePeak:207.05(419)

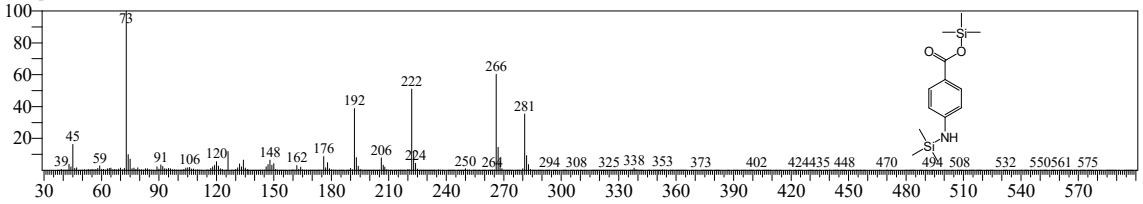
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib

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

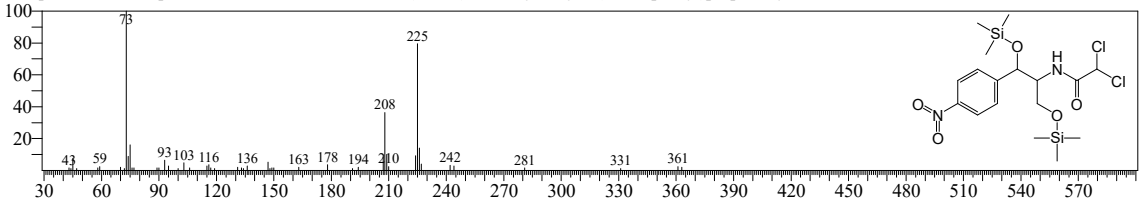
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:2 Entry:528 Library:OA_TMS_DB5_67min_V3.lib

SI:31 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508

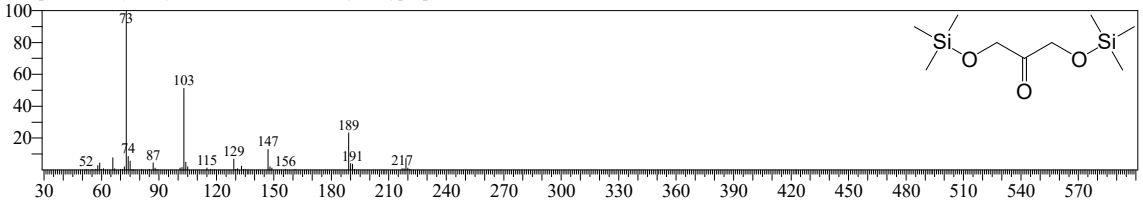
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



Hit#:3 Entry:57 Library:OA_TMS_DB5_67min_V3.lib

SI:30 Formula:C9H22O3Si2 CAS:96-26-4 MolWeight:234 RetIndex:1224

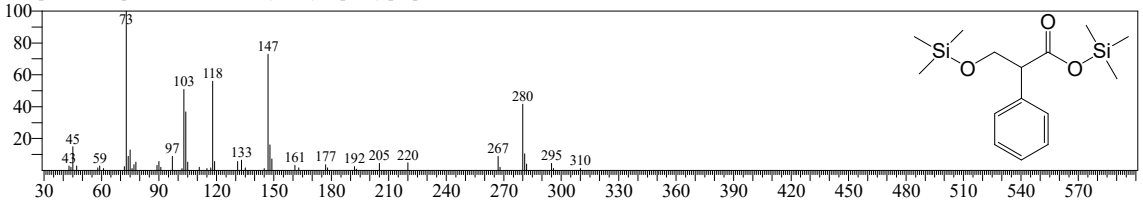
CompName:Dihydroxyacetone-2TMS ; 1,3-dihydroxypropan-2-one



Hit#:4 Entry:195 Library:OA_TMS_DB5_67min_V3.lib

SI:30 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600

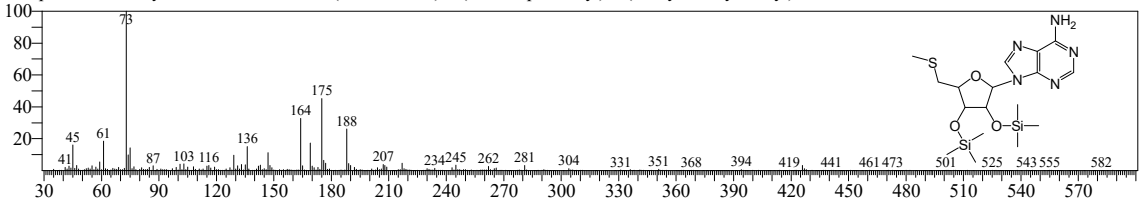
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid



Hit#:5 Entry:548 Library:OA_TMS_DB5_67min_V3.lib

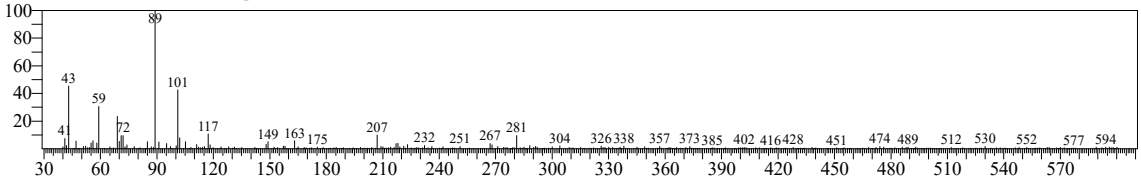
SI:30 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787

CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol

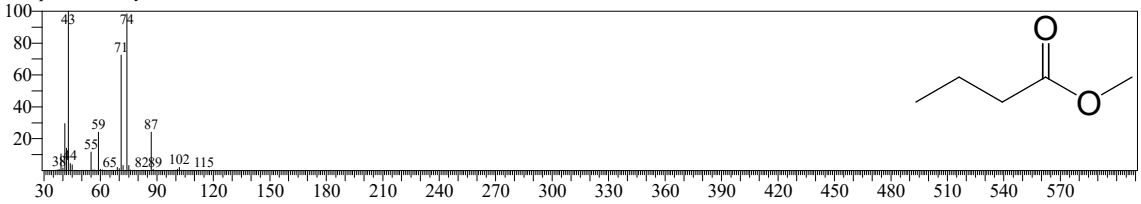


TNAU

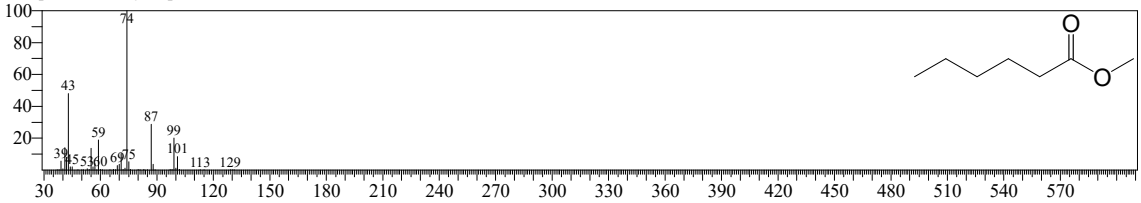
<< Target >>
Line#:2 R.Time:4.970(Scan#:95) MassPeaks:316
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.10(2325)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



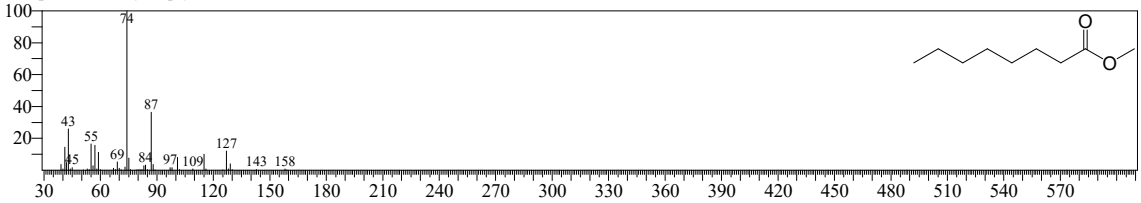
Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



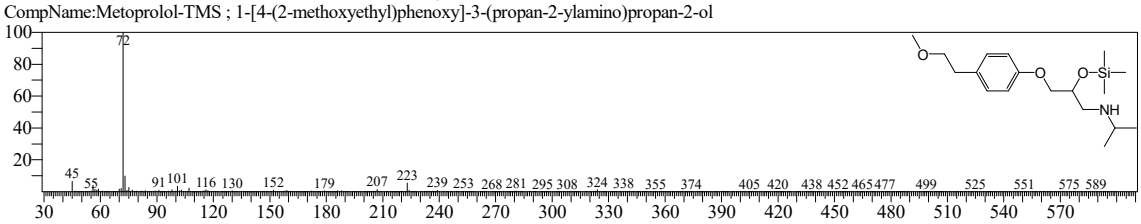
Hit#:2 Entry:2 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332
CompName:Methyl caproate ; Hexanoic acid



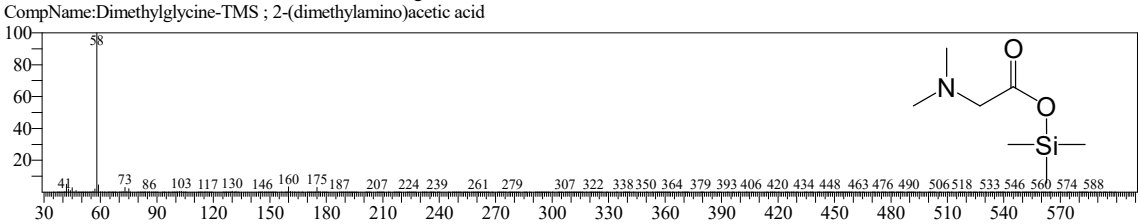
Hit#:3 Entry:3 Library:FA_ME_SP2560_EI_V3.lib
SI:44 Formula:C9H18O2 CAS:124-07-2 MolWeight:158 RetIndex:1550
CompName:Methyl caprylate ; Octanoic acid



Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:40 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

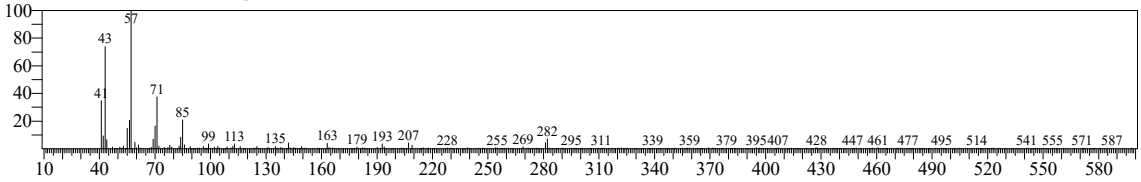


Hit#:5 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid

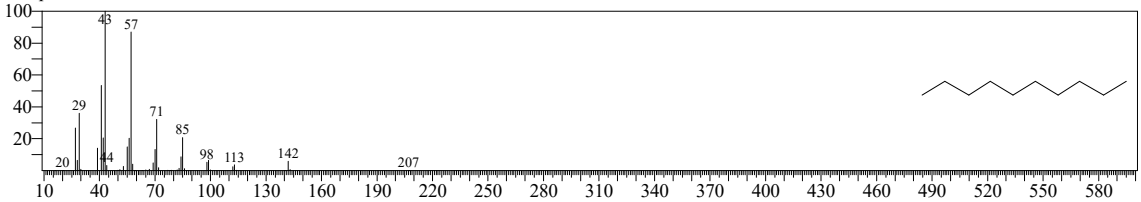


TNAU

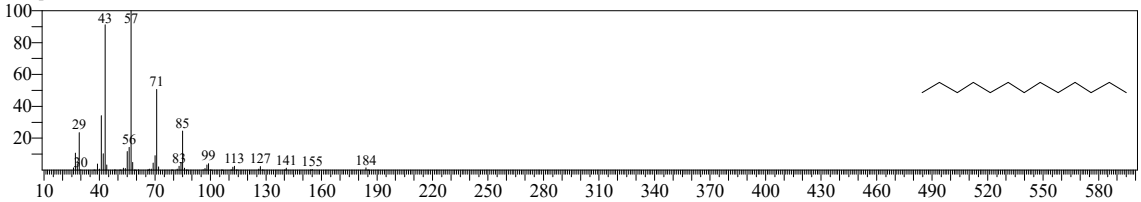
<< Target >>
Line#:3 R.Time:7.950(Scan#:691) MassPeaks:298
RawMode:Averaged 7.945-7.955(690-692) BasePeak:57.10(5014)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



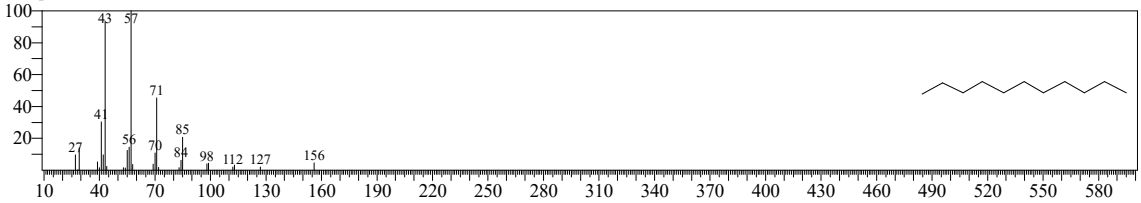
Hit#:1 Entry:9445 Library:NIST20R.lib
SI:87 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



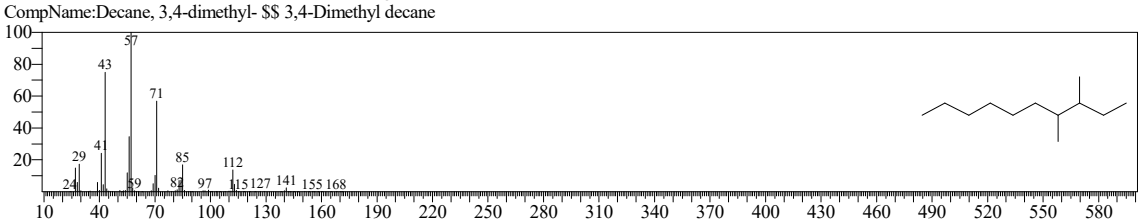
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



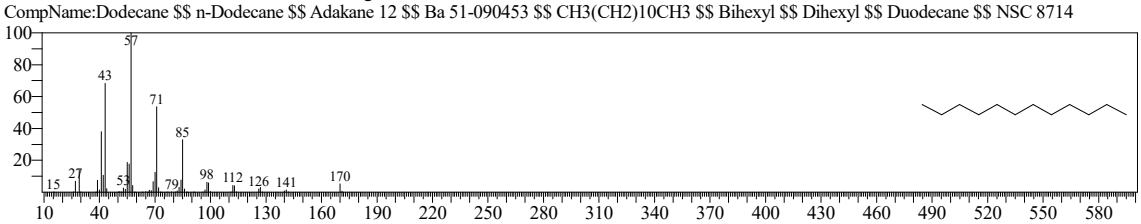
Hit#:3 Entry:12899 Library:NIST20R.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



Hit#:4 Entry:30052 Library:NIST20M1.lib
SI:86 Formula:C12H26 CAS:17312-45-7 MolWeight:170 RetIndex:1086
CompName:Decane, 3,4-dimethyl- $$ 3,4-Dimethyl decane

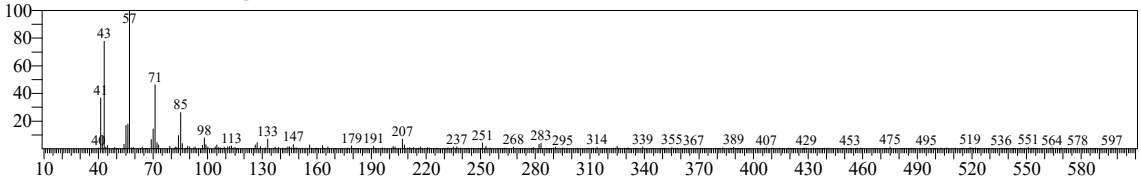


Hit#:5 Entry:30057 Library:NIST20M1.lib
SI:85 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714

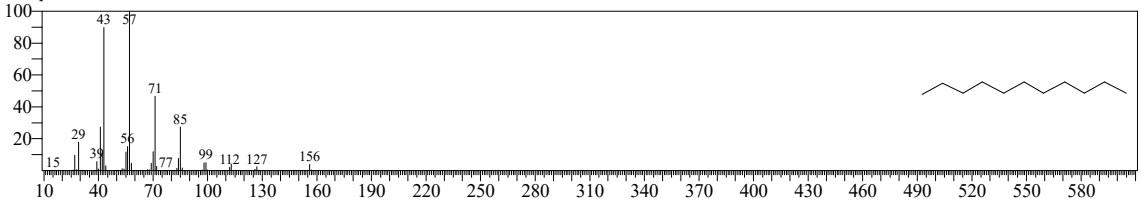


TNAU

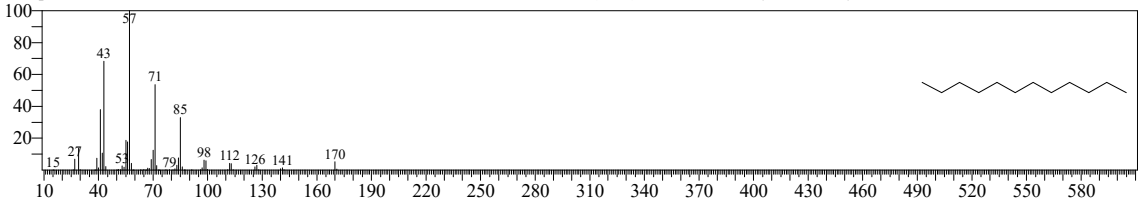
<< Target >>
Line#:4 R.Time:9.695(Scan#:1040) MassPeaks:291
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(3700)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



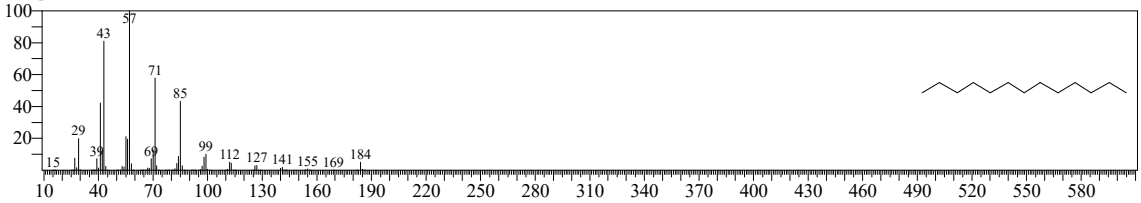
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:87 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



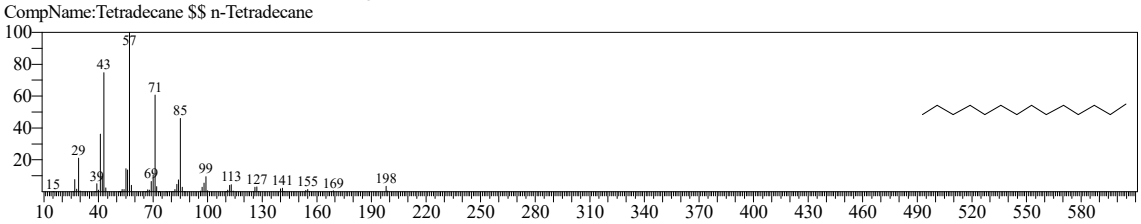
Hit#:2 Entry:30057 Library:NIST20M1.lib
SI:87 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



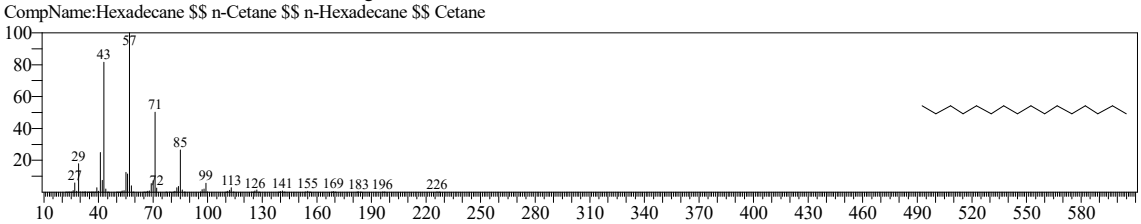
Hit#:3 Entry:19410 Library:NIST20R.lib
SI:86 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



Hit#:4 Entry:22497 Library:NIST20R.lib
SI:86 Formula:C14H30 CAS:629-59-4 MolWeight:198 RetIndex:1400
CompName:Tetradecane $$ n-Tetradecane

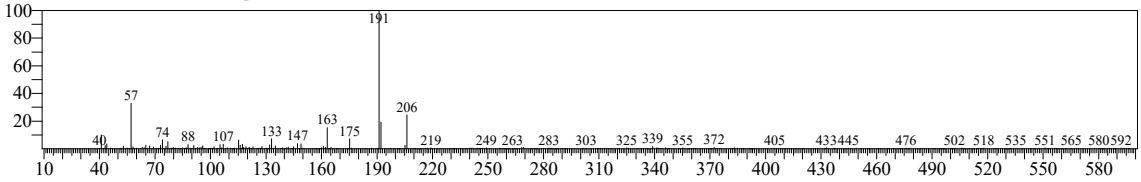


Hit#:5 Entry:27737 Library:NIST20R.lib
SI:86 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

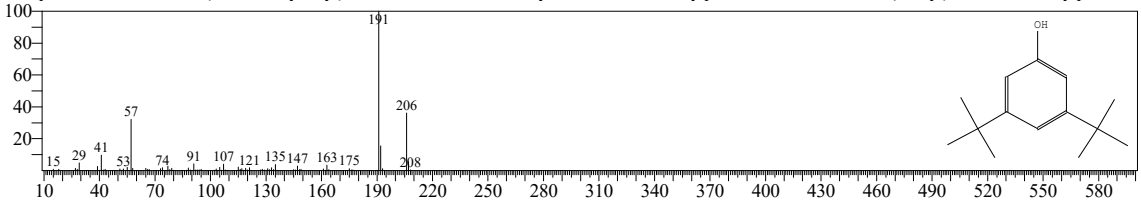


TNAU

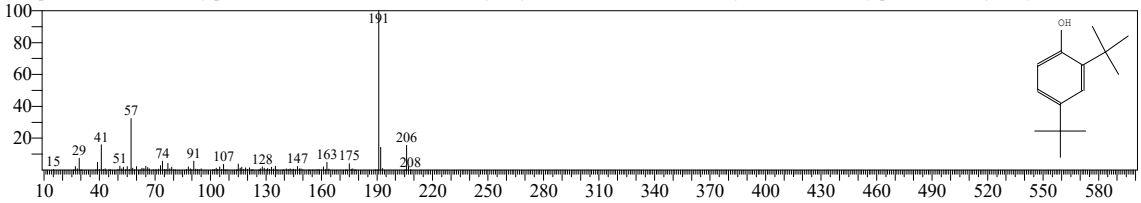
<< Target >>
Line#:5 R.Time:15.470(Scan#:2195) MassPeaks:273
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.10(7246)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



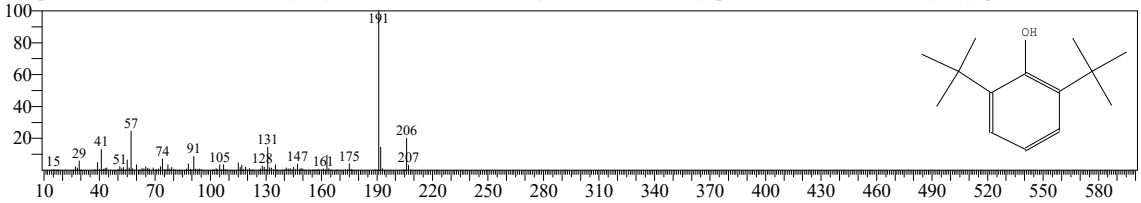
Hit#:1 Entry:24110 Library:NIST20R.lib
SI:86 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



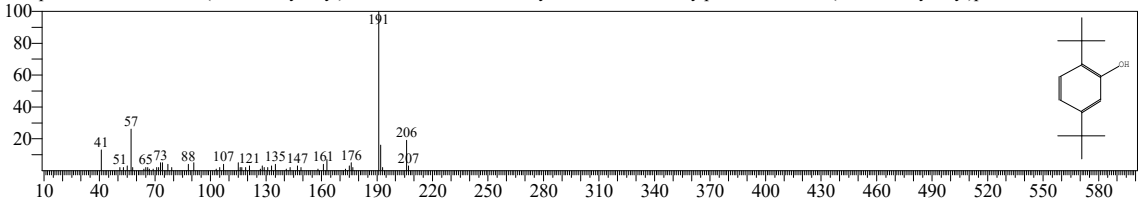
Hit#:2 Entry:59048 Library:NIST20M1.lib
SI:86 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



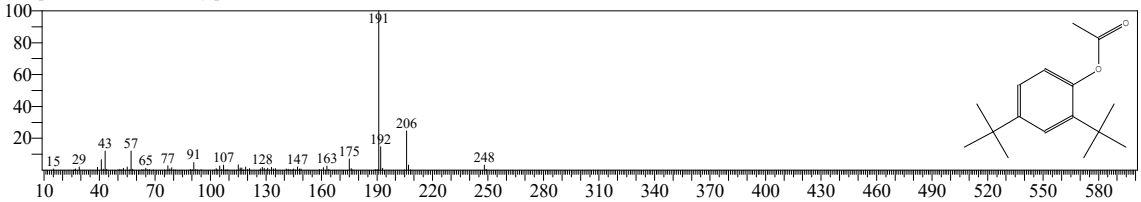
Hit#:3 Entry:59031 Library:NIST20M1.lib
SI:84 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert



Hit#:4 Entry:24098 Library:NIST20R.lib
SI:84 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

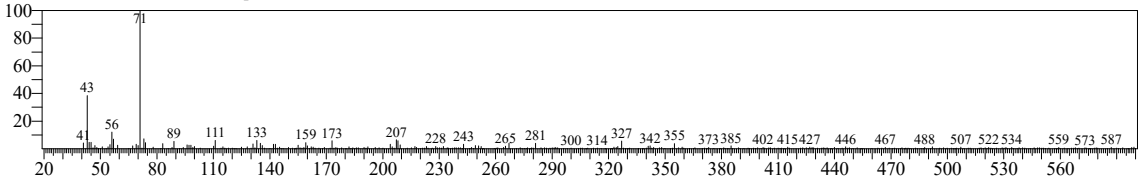


Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:82 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
CompName:2,4-Di-tert-butylphenol, acetate

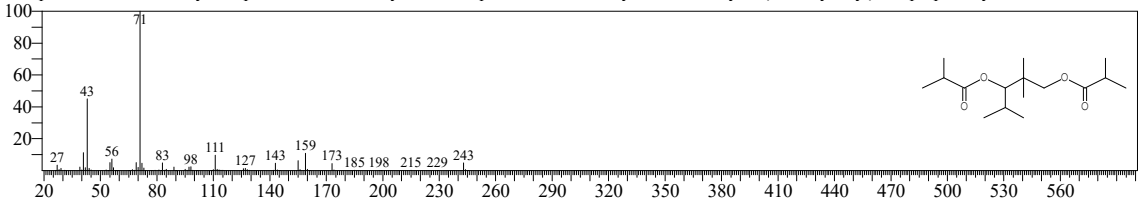


TNAU

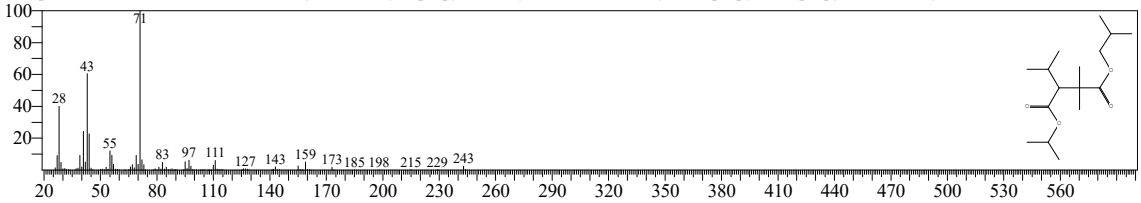
<< Target >>
Line#:6 R.Time:16.470(Scan#:2395) MassPeaks:342
RawMode:Averaged 16.465-16.475(2394-2396) BasePeak:71.00(3341)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



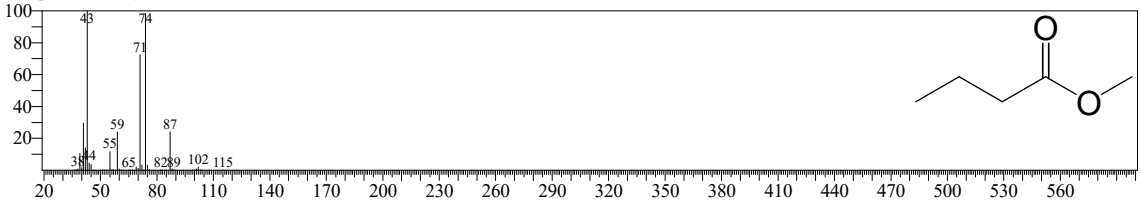
Hit#:1 Entry:34622 Library:NIST20R.lib
SI:77 Formula:C16H30O4 CAS:6846-50-0 MolWeight:286 RetIndex:1605
CompName:2,2,4-Trimethyl-1,3-pentanediol diisobutyrate $$ Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester $$ 1,3-Pentan



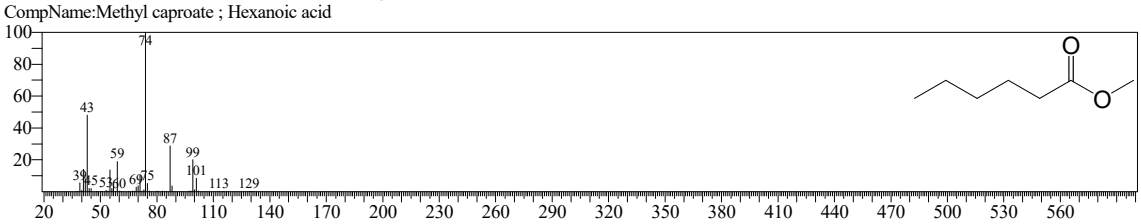
Hit#:2 Entry:146809 Library:NIST20M1.lib
SI:73 Formula:C16H30O4 CAS:0-00-0 MolWeight:286 RetIndex:1605
CompName:Pentanoic acid, 2,2,4-trimethyl-3-carboxyisopropyl, isobutyl ester $$ 1-Isobutyl 4-isopropyl 3-isopropyl-2,2-dimethylsuccinate #



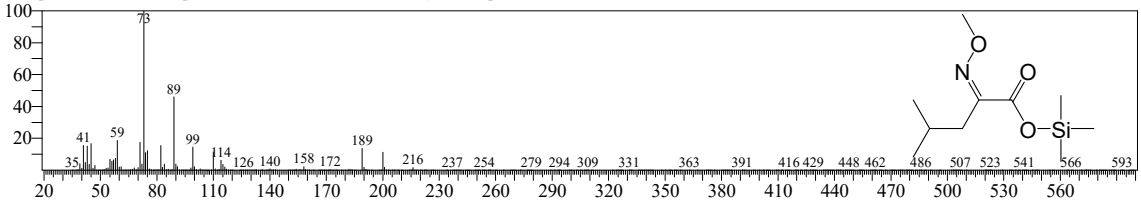
Hit#:3 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:58 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



Hit#:4 Entry:2 Library:FA_ME_SP2560_EI_V3.lib
SI:49 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332
CompName:Methyl caproate ; Hexanoic acid

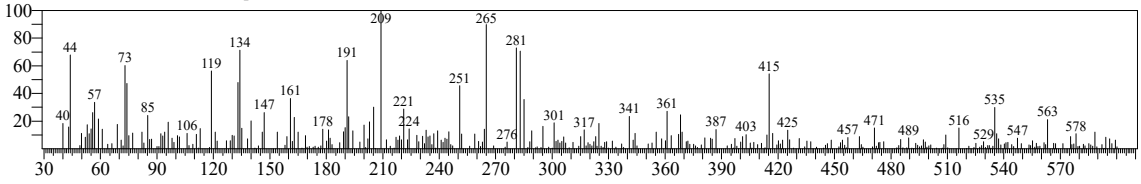


Hit#:5 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid

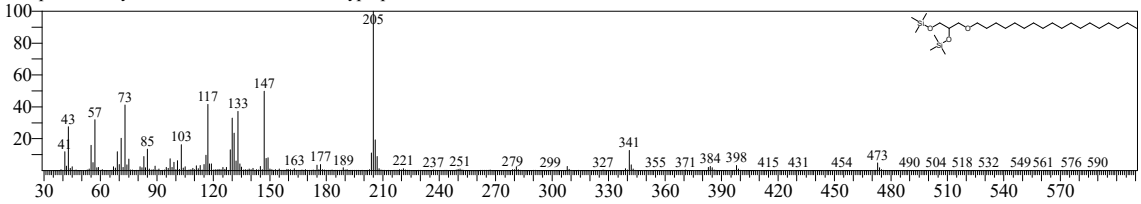


TNAU

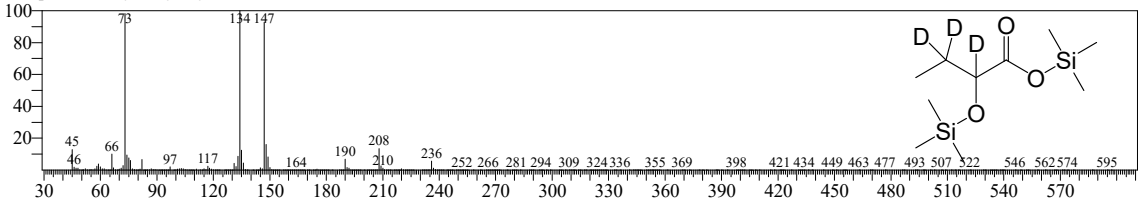
<< Target >>
Line#:7 R.Time:28.185(Scan#:4738) MassPeaks:328
RawMode:Averaged 28.180-28.190(4737-4739) BasePeak:209.00(552)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



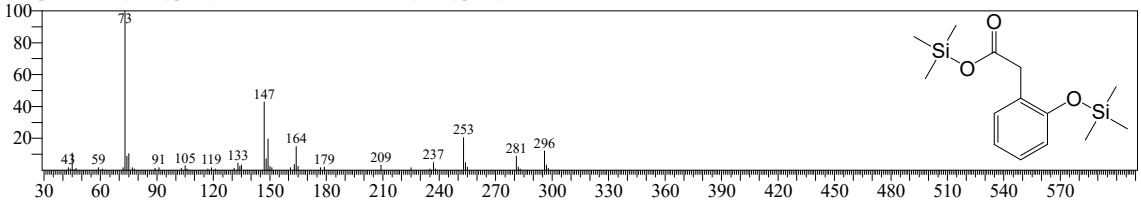
Hit#:1 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



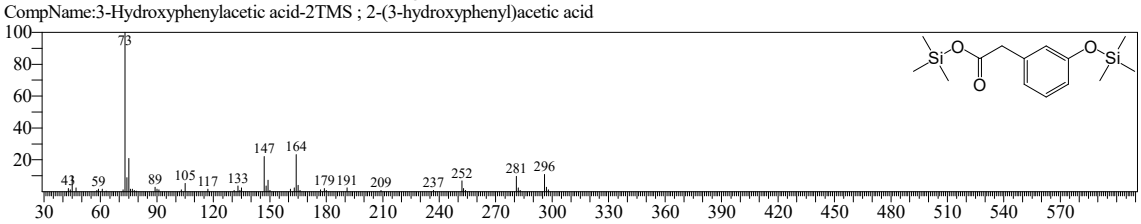
Hit#:2 Entry:25 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula: CAS:0-00-0 MolWeight:251 RetIndex:1130
CompName:2-Hydroxybutyric acid-d3-2TMS ;



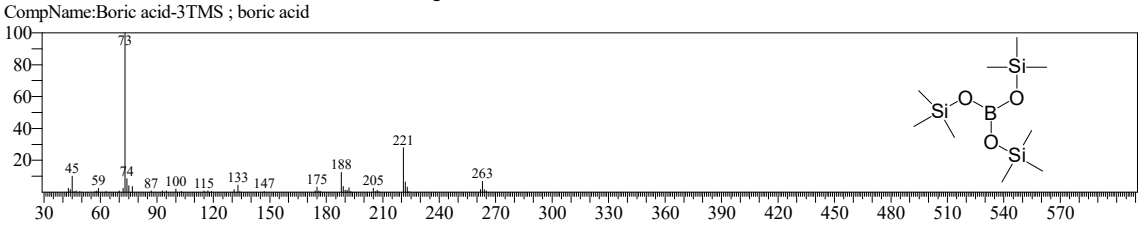
Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



Hit#:4 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

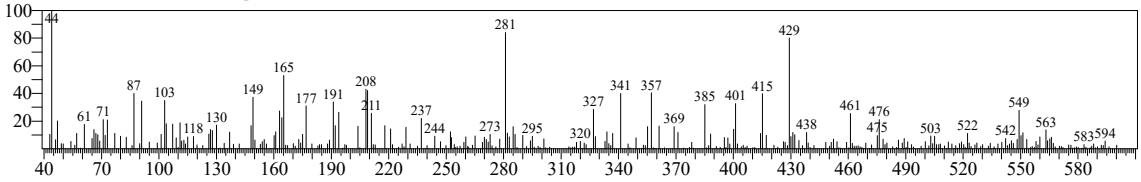


Hit#:5 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid

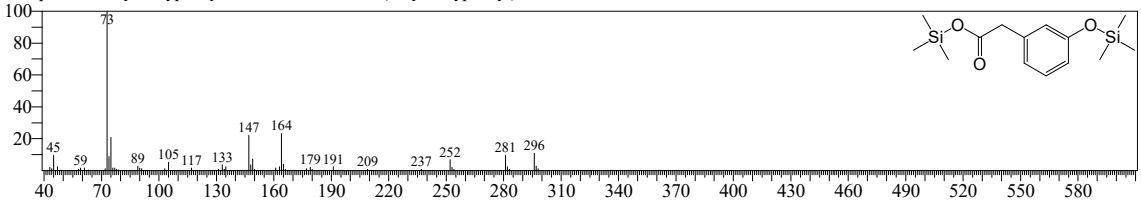


TNAU

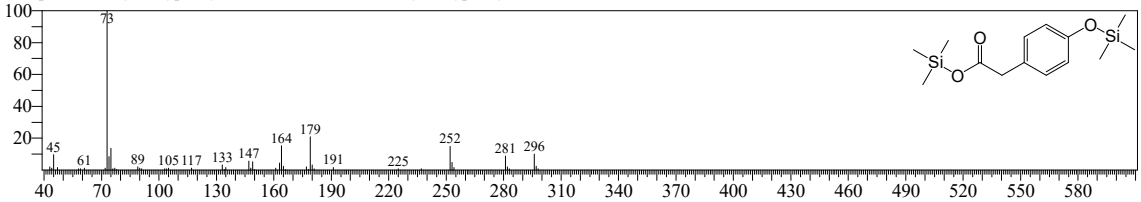
<< Target >>
Line#:8 R.Time:28.310(Scan#:4763) MassPeaks:326
RawMode:Averaged 28.305-28.315(4762-4764) BasePeak:44.00(680)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



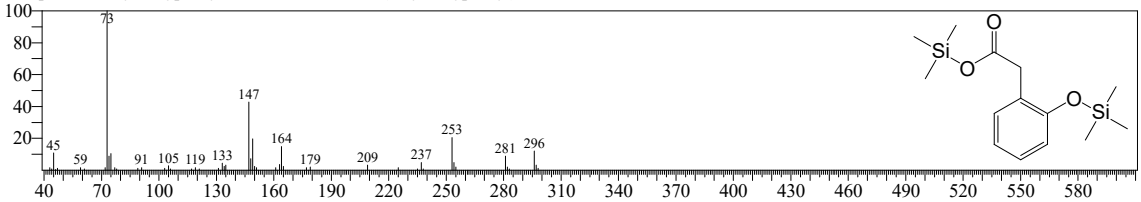
Hit#:1 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid



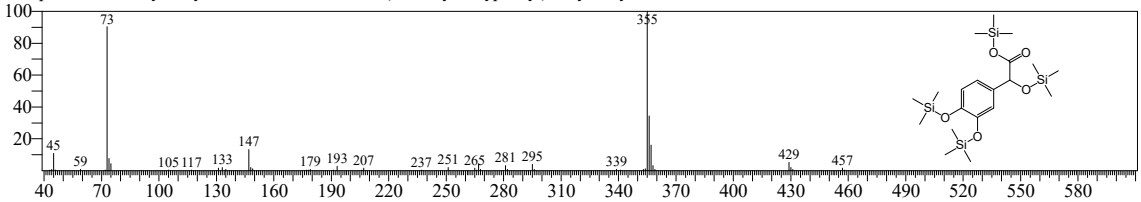
Hit#:2 Entry:220 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C14H24O3Si2 CAS:156-38-7 MolWeight:296 RetIndex:1647
CompName:4-Hydroxyphenylacetic acid-2TMS ; 2-(4-hydroxyphenyl)acetic acid



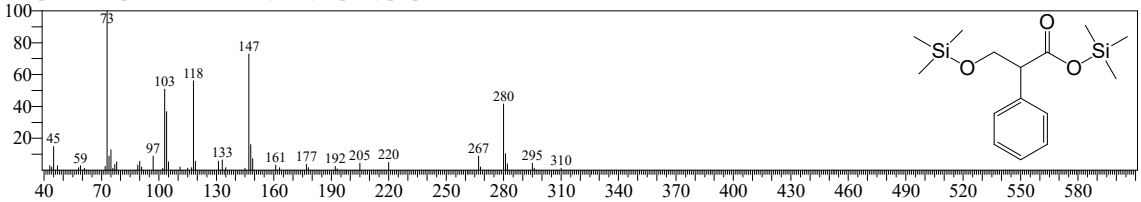
Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

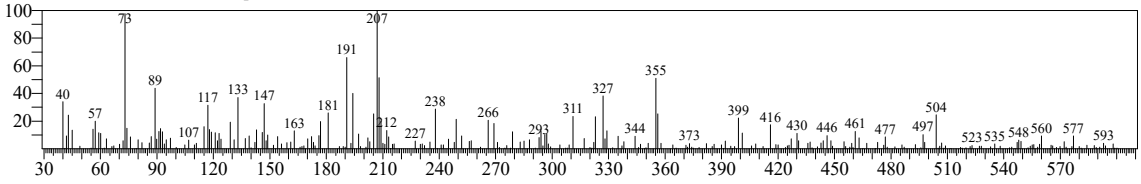


Hit#:5 Entry:195 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C15H26O3Si2 CAS:529-64-6 MolWeight:310 RetIndex:1600
CompName:Tropic acid-2TMS ; 3-hydroxy-2-phenylpropanoic acid

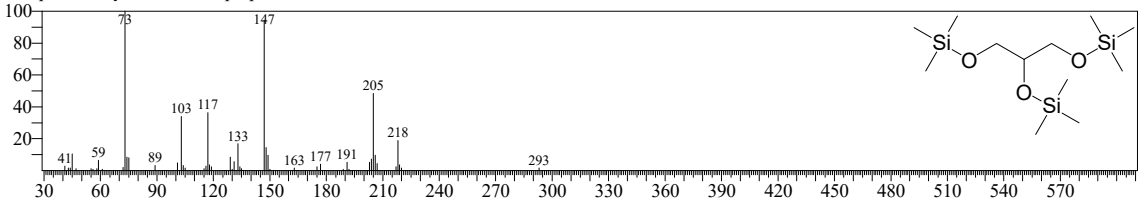


TNAU

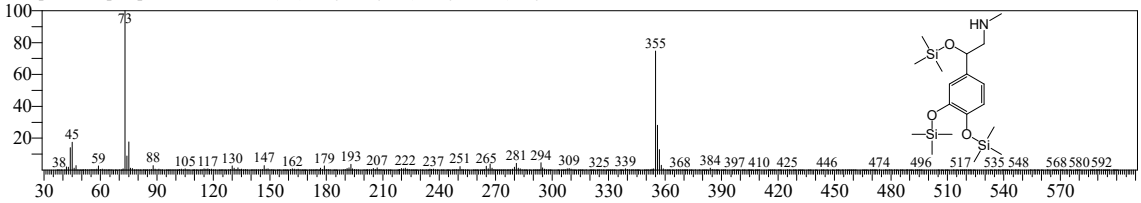
<< Target >>
Line#:9 R.Time:28.560(Scan#:4813) MassPeaks:268
RawMode:Averaged 28.555-28.565(4812-4814) BasePeak:207.00(731)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



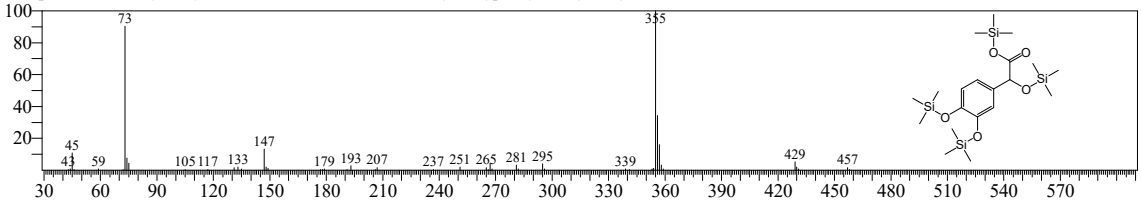
Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



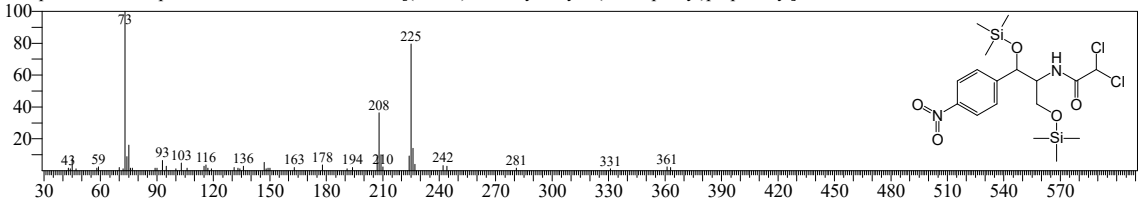
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



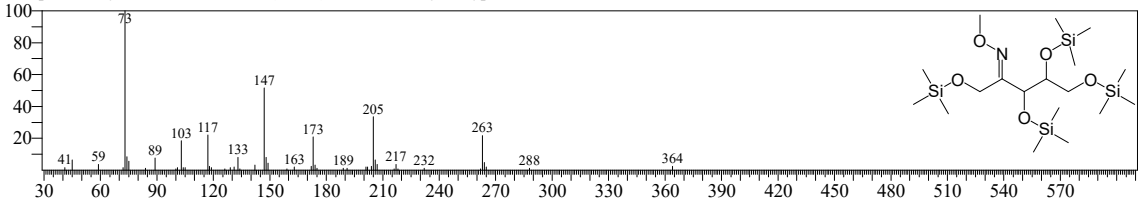
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:37 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

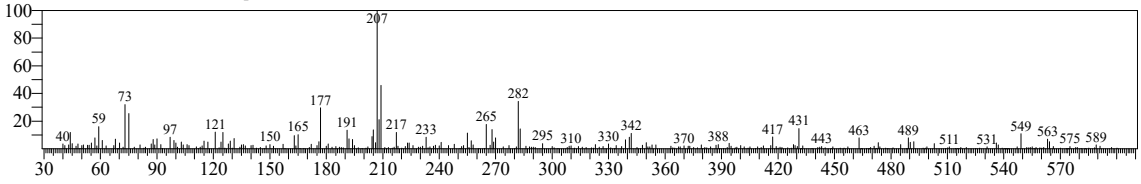


Hit#:5 Entry:255 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H45NO5Si4 CAS:551-84-8 MolWeight:467 RetIndex:1698
CompName:Xylulose-meto-4TMS ; (3S,4R)-1,3,4,5-tetrahydroxypentan-2-one

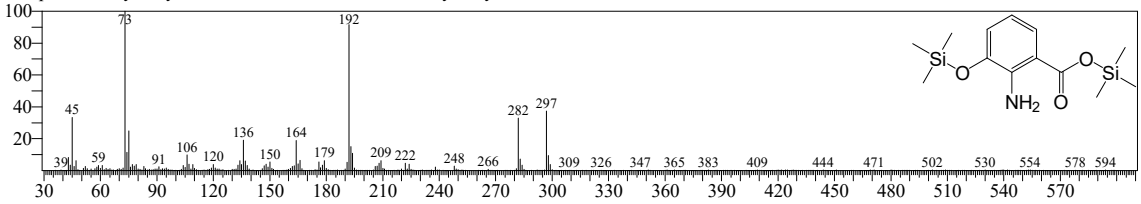


TNAU

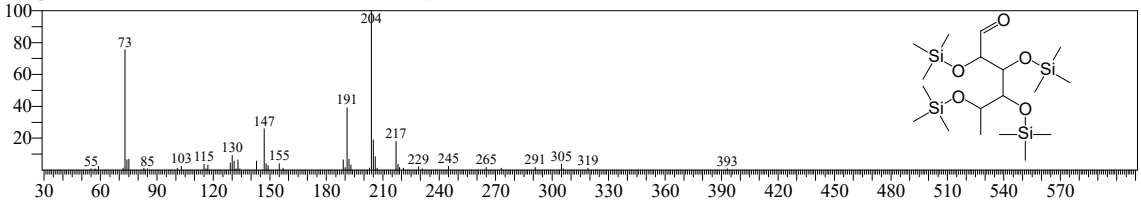
<< Target >>
Line#:10 R.Time:29.655(Scan#:5032) MassPeaks:307
RawMode:Averaged 29.650-29.660(5031-5033) BasePeak:207.05(1942)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



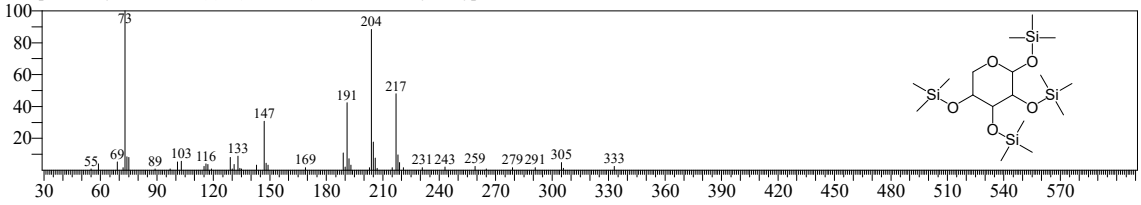
Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



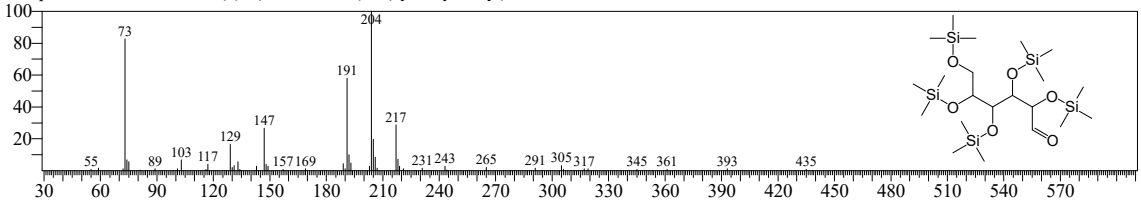
Hit#:2 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



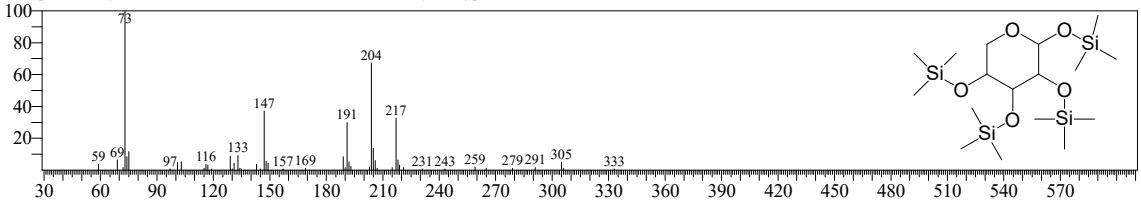
Hit#:3 Entry:238 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H42O5Si4 CAS:1114-34-7 MolWeight:438 RetIndex:1675
CompName:Lyxose-4TMS(2) ; (2S,3S,4R)-2,3,4,5-tetrahydroxypentanal



Hit#:4 Entry:311 Library:OA_TMS_DB5_67min_V3.lib
SI:36 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

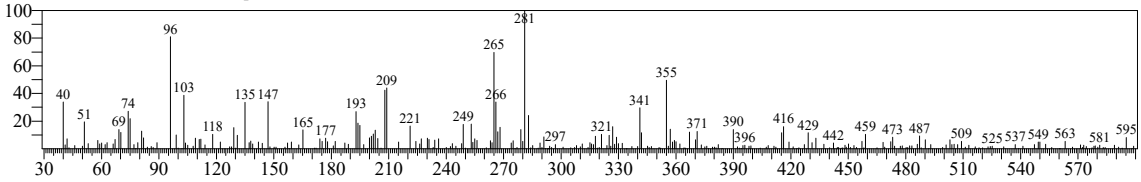


Hit#:5 Entry:267 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C17H42O5Si4 CAS:58-86-6 MolWeight:438 RetIndex:1732
CompName:Xylose-4TMS(1) ; (2R,3S,4R)-2,3,4,5-tetrahydroxypentanal

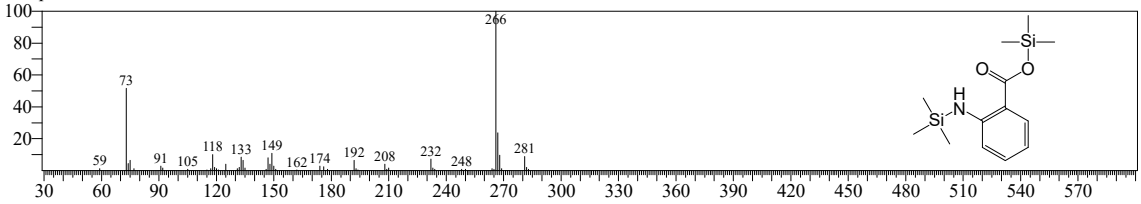


TNAU

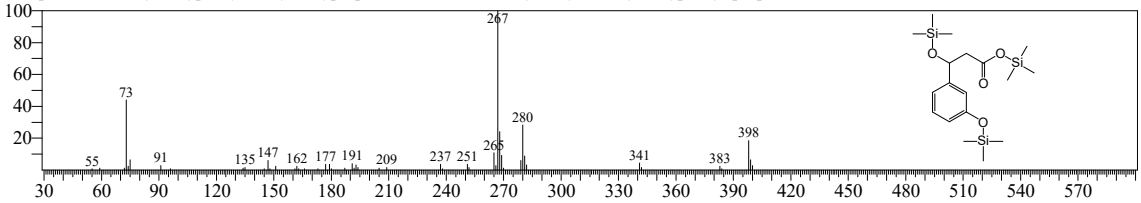
<< Target >>
Line#:11 R.Time:29.730(Scan#:5047) MassPeaks:286
RawMode:Averaged 29.725-29.735(5046-5048) BasePeak:281.00(975)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



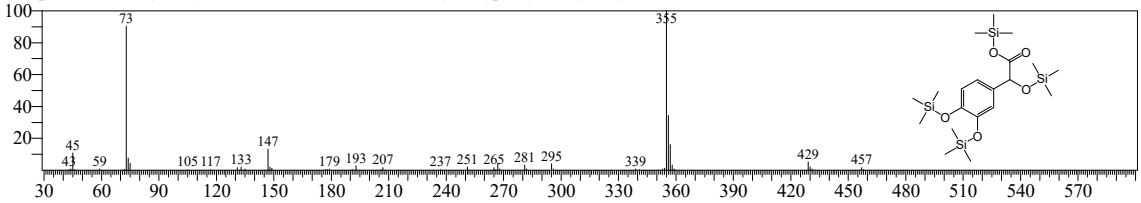
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



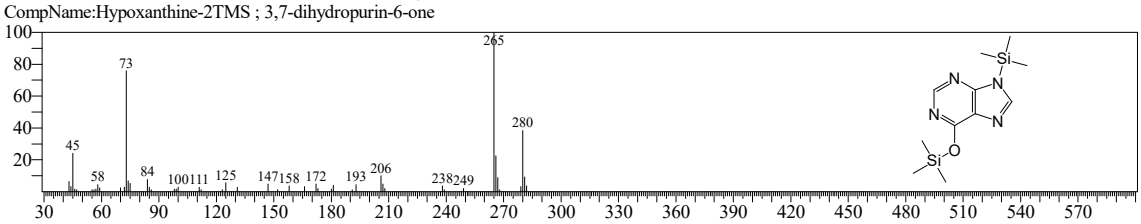
Hit#:2 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



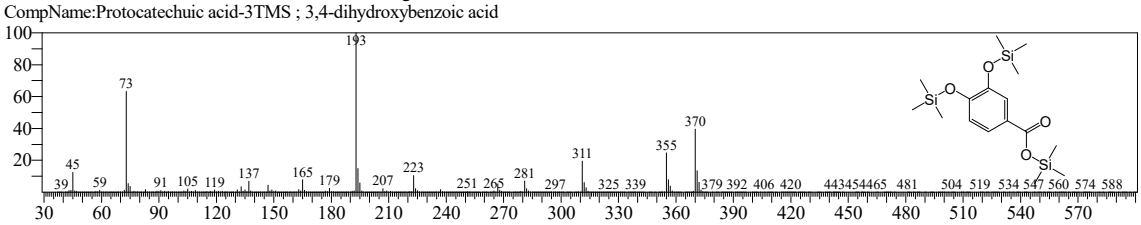
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 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

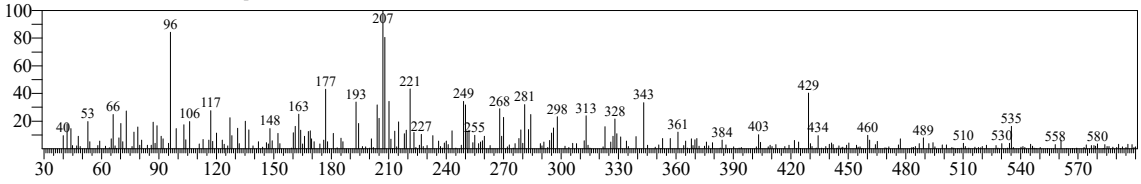


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

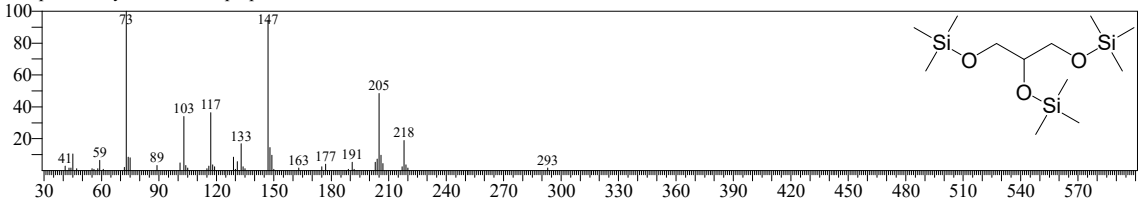


TNAU

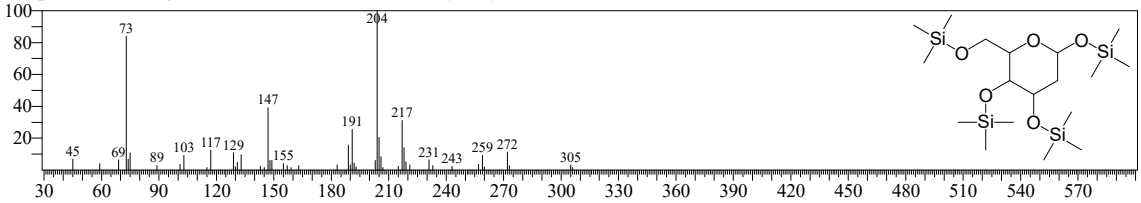
<< Target >>
Line#:12 R.Time:29.925(Scan#:5086) MassPeaks:301
RawMode:Averaged 29.920-29.930(5085-5087) BasePeak:207.05(693)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



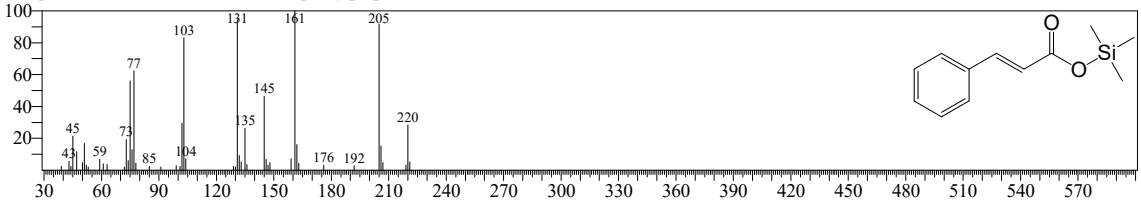
Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



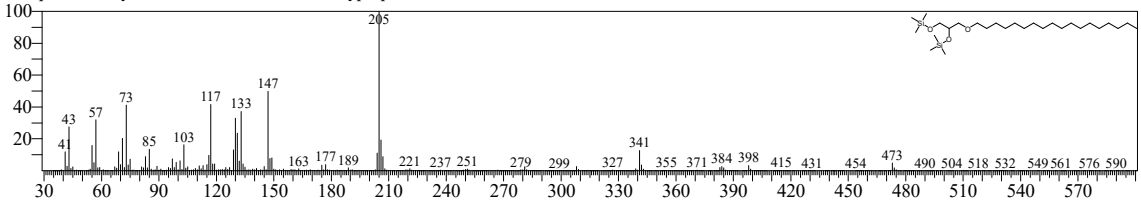
Hit#:2 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol



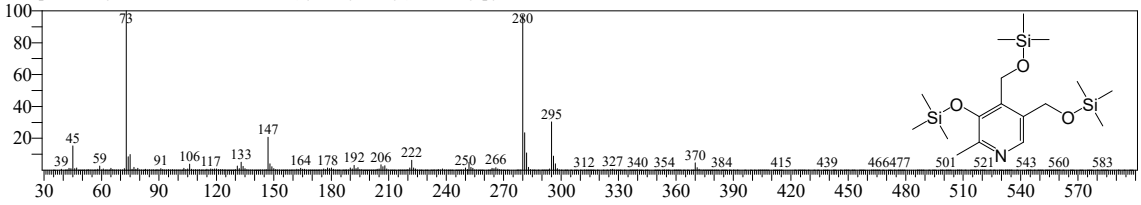
Hit#:3 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

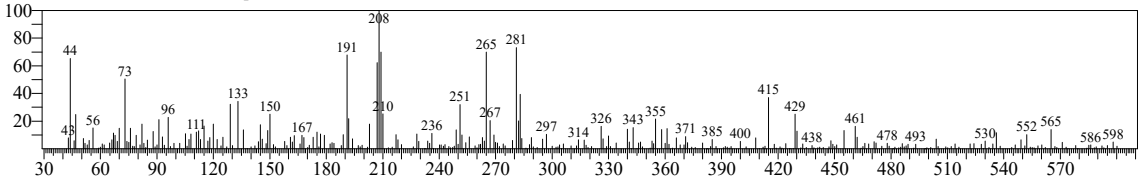


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

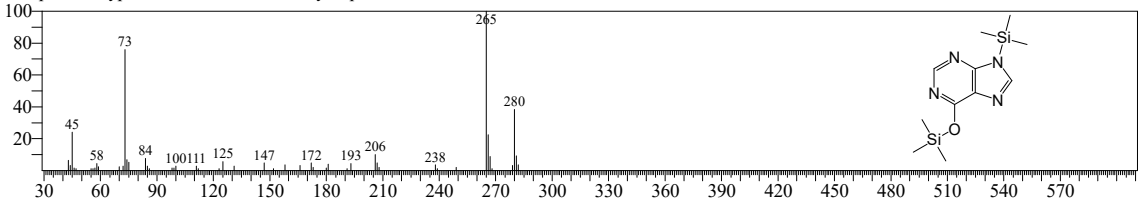


TNAU

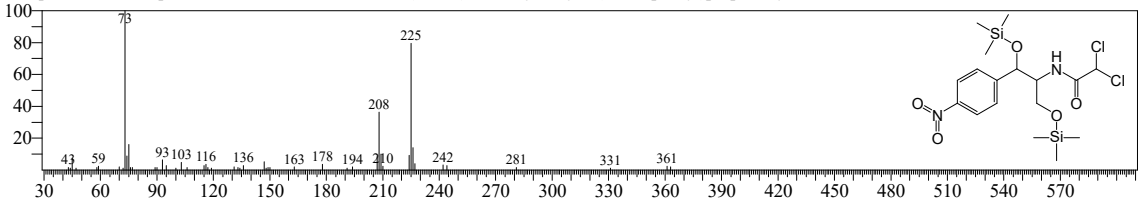
<< Target >>
Line#:13 R.Time:30.340(Scan#:5169) MassPeaks:311
RawMode:Averaged 30.335-30.345(5168-5170) BasePeak:208.05(935)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



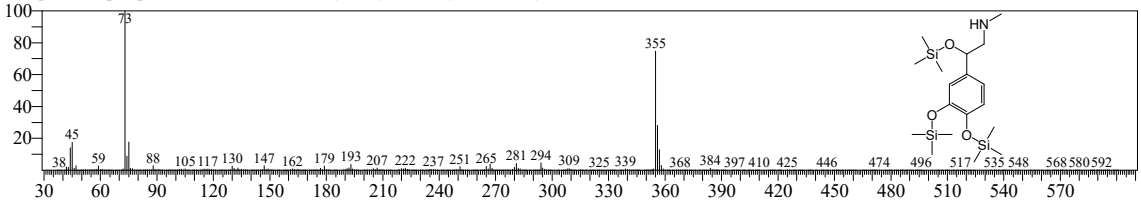
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



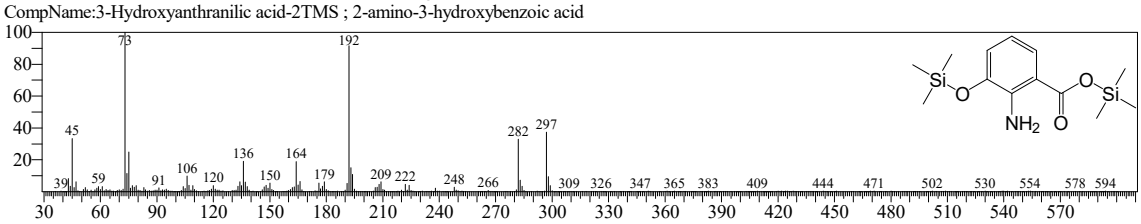
Hit#:2 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



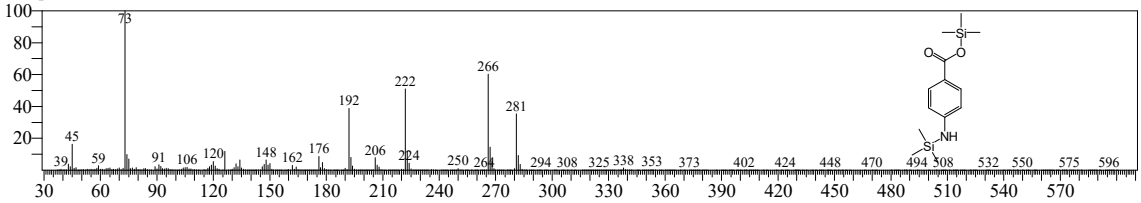
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid

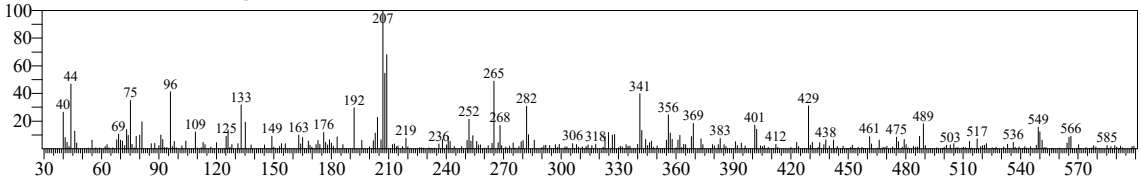


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

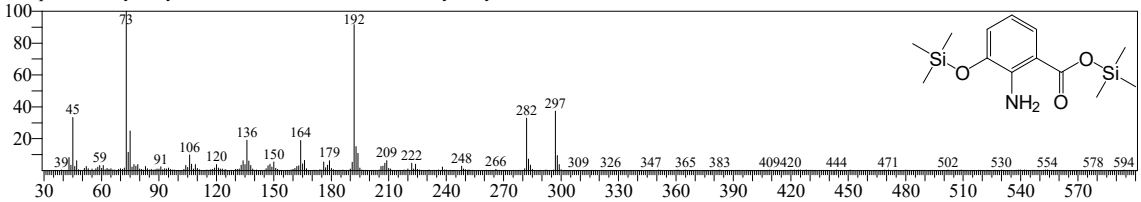


TNAU

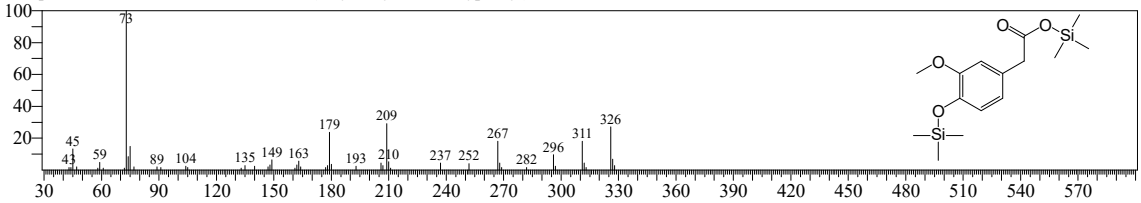
<< Target >>
Line#:14 R.Time:31.255(Scan#:5352) MassPeaks:305
RawMode:Averaged 31.250-31.260(5351-5353) BasePeak:207.05(996)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



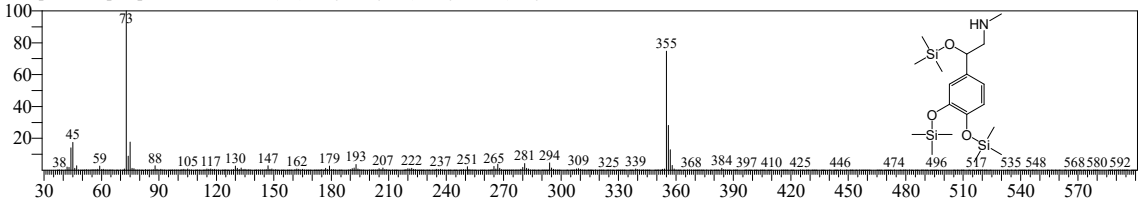
Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



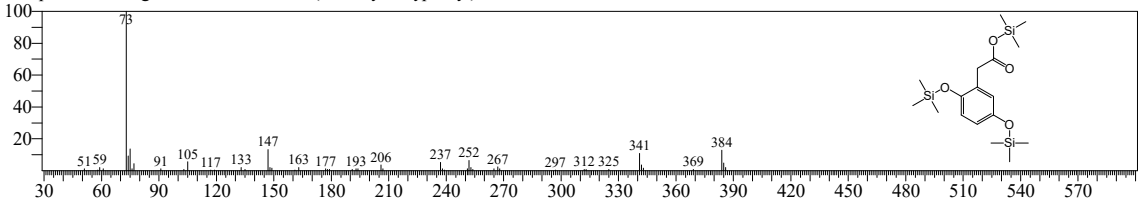
Hit#:2 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



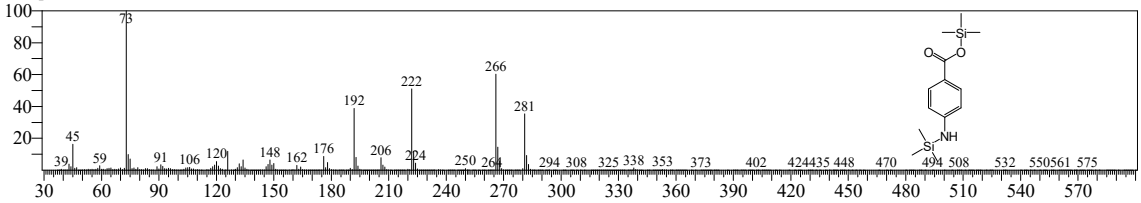
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid

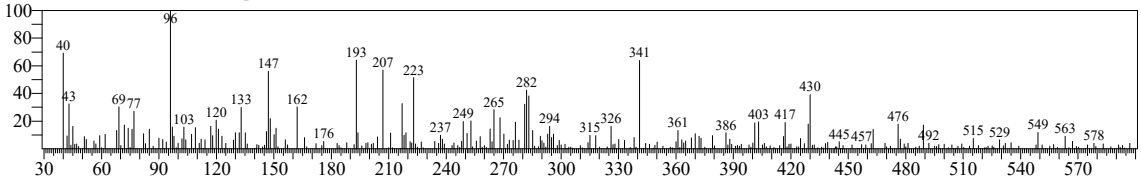


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

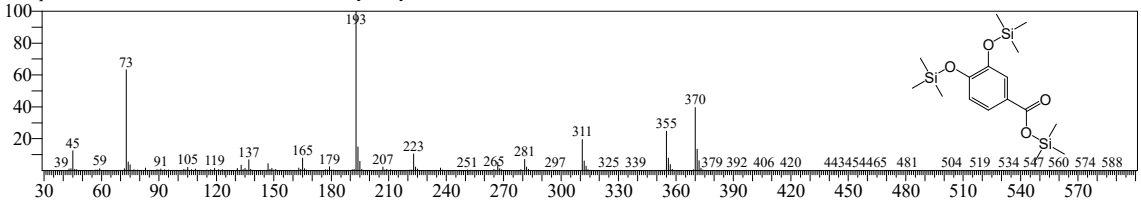


TNAU

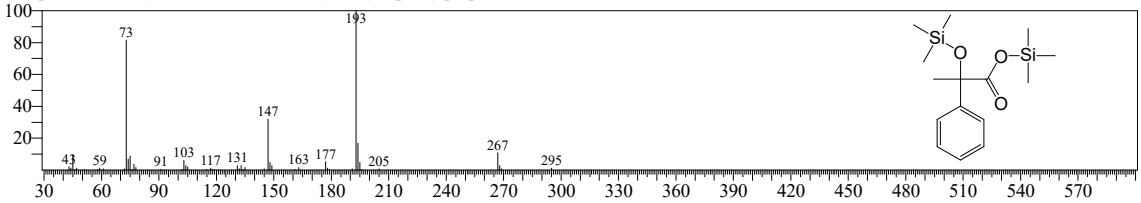
<< Target >>
Line#:15 R.Time:31.575(Scan#:5416) MassPeaks:305
RawMode:Averaged 31.570-31.580(5415-5417) BasePeak:96.00(671)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



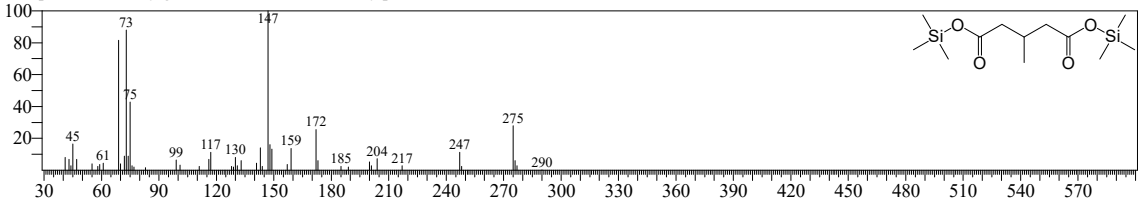
Hit#:1 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



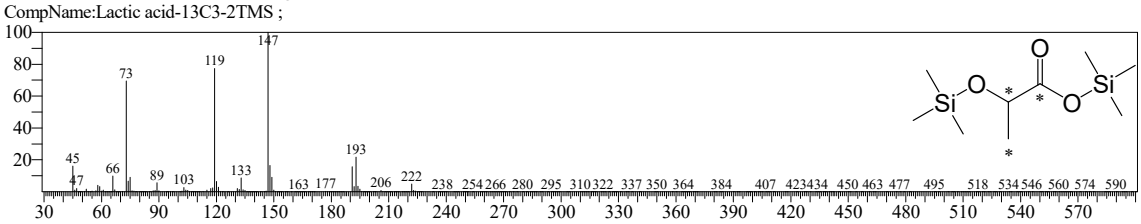
Hit#:2 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



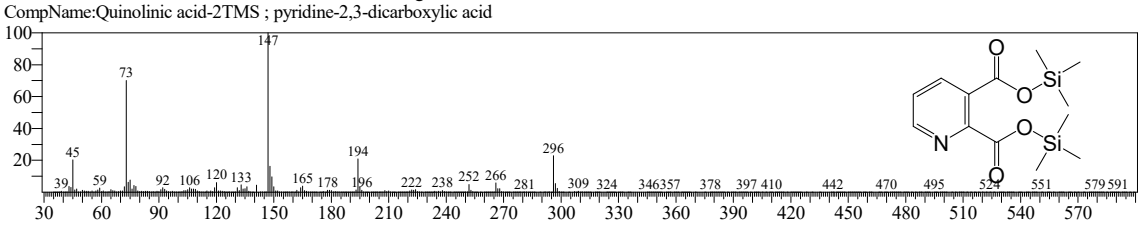
Hit#:3 Entry:119 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C12H26O4Si2 CAS:626-51-7 MolWeight:290 RetIndex:1426
CompName:3-Methylglutaric acid-2TMS ; 3-methylpentanedioic acid



Hit#:4 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;

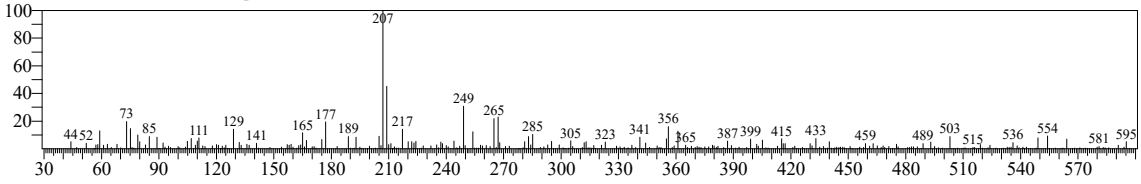


Hit#:5 Entry:272 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C13H21NO4Si2 CAS:89-00-9 MolWeight:311 RetIndex:1743
CompName:Quinolinic acid-2TMS ; pyridine-2,3-dicarboxylic acid

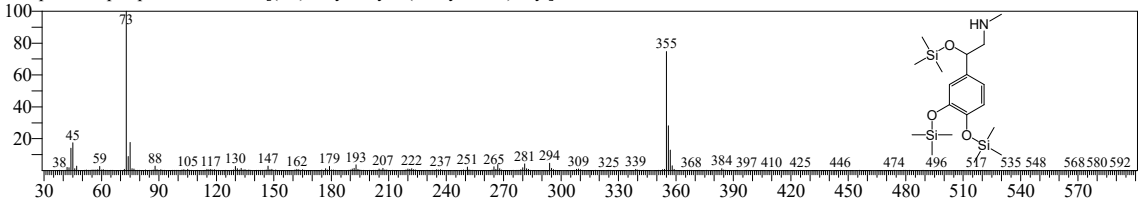


TNAU

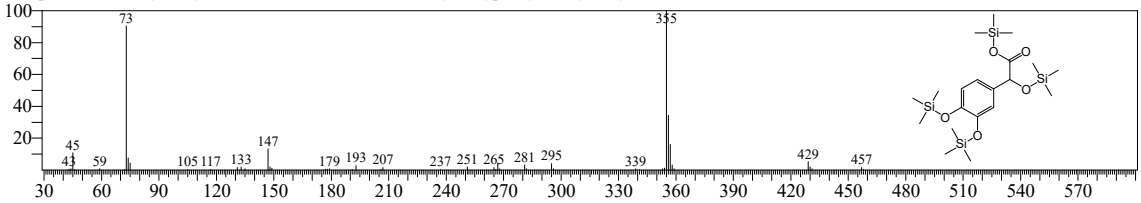
<< Target >>
Line#:16 R.Time:31.705(Scan#:5442) MassPeaks:294
RawMode:Averaged 31.700-31.710(5441-5443) BasePeak:207.05(1640)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



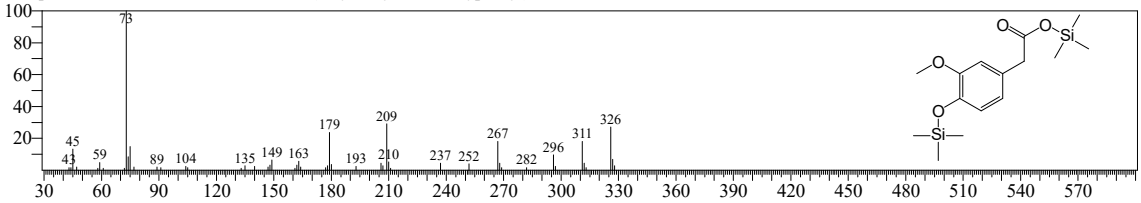
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



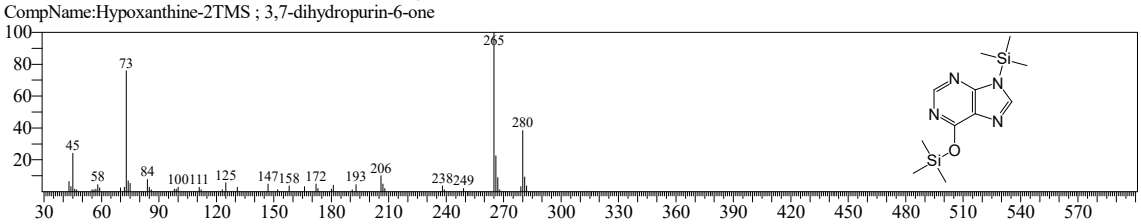
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



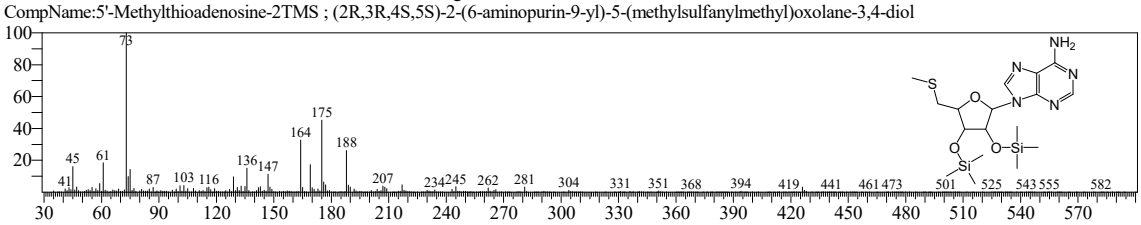
Hit#:3 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



Hit#:4 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

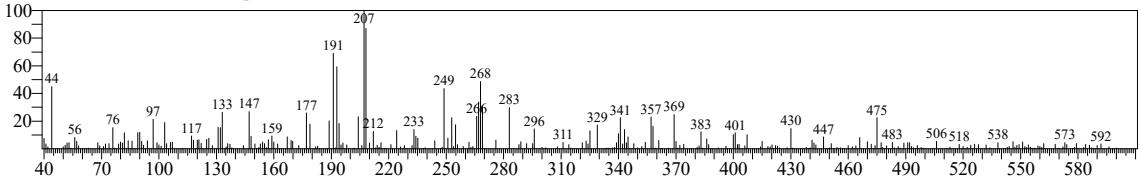


Hit#:5 Entry:548 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C17H31N5O3SSi2 CAS:2457-80-9 MolWeight:441 RetIndex:2787
CompName:5'-Methylthioadenosine-2TMS ; (2R,3R,4S,5S)-2-(6-aminopurin-9-yl)-5-(methylsulfanylmethyl)oxolane-3,4-diol

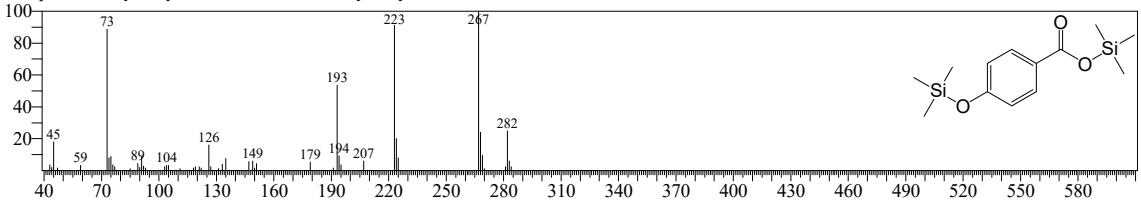


TNAU

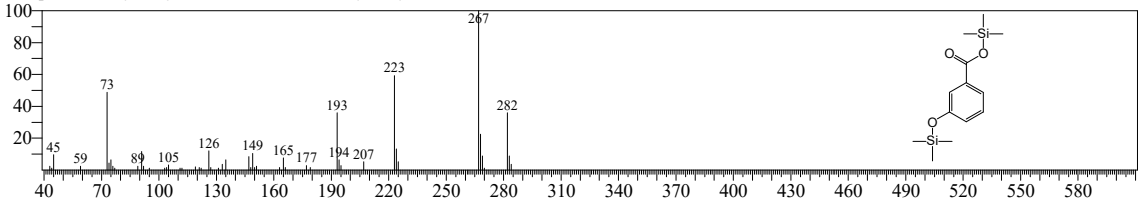
<< Target >>
Line#:17 R.Time:31.835(Scan#:5468) MassPeaks:278
RawMode:Averaged 31.830-31.840(5467-5469) BasePeak:207.05(813)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



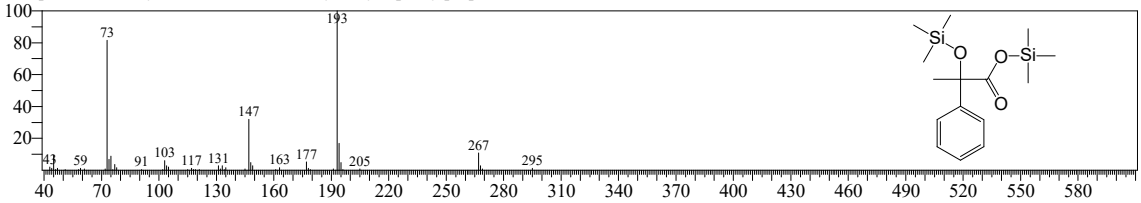
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



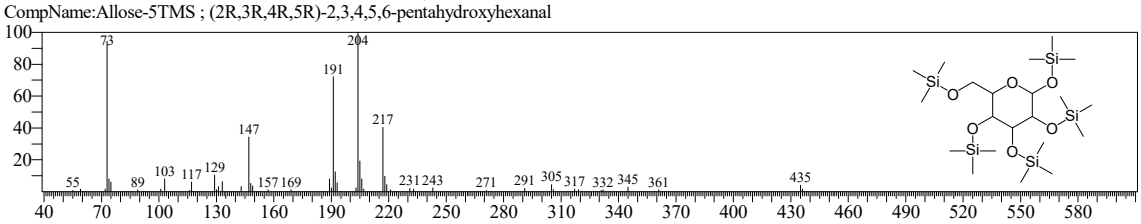
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



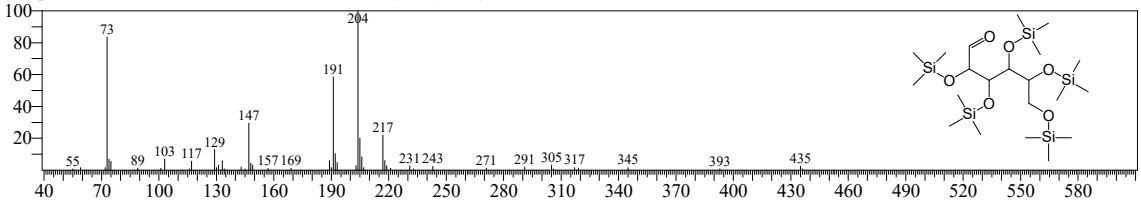
Hit#:3 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



Hit#:4 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

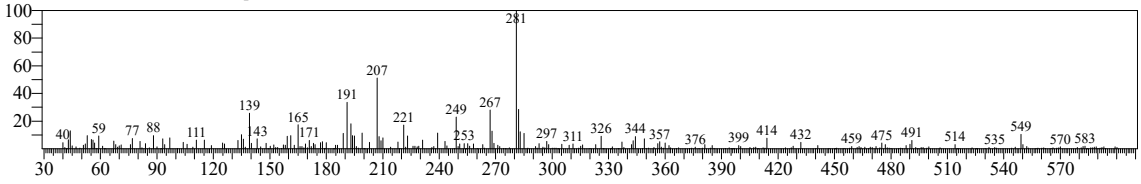


Hit#:5 Entry:348 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C21H52O6Si5 CAS:3458-28-4 MolWeight:540 RetIndex:1872
CompName:Mannose-5TMS(2) ; (3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

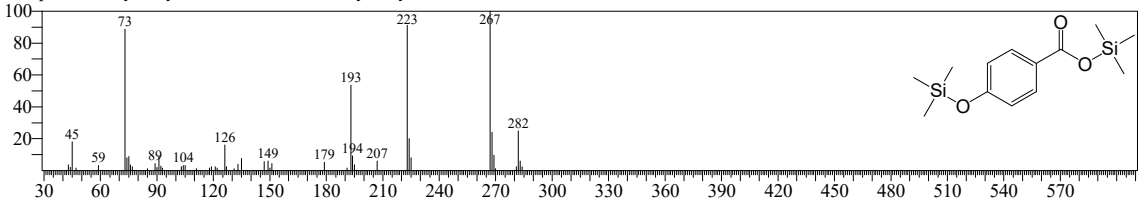


TNAU

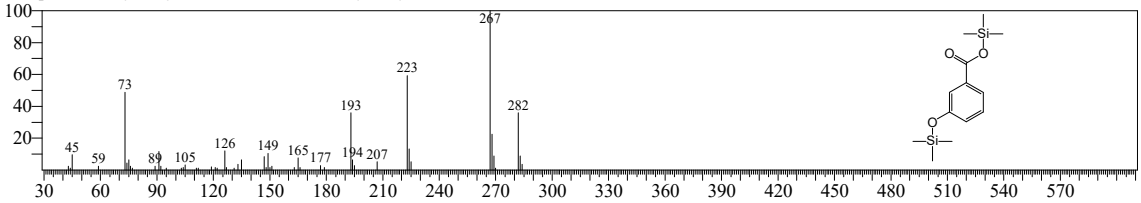
<< Target >>
Line#:18 R.Time:31.900(Scan#:5481) MassPeaks:283
RawMode:Averaged 31.895-31.905(5480-5482) BasePeak:281.05(1793)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



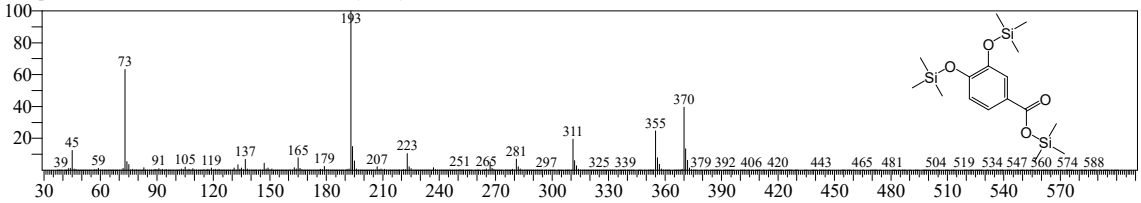
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



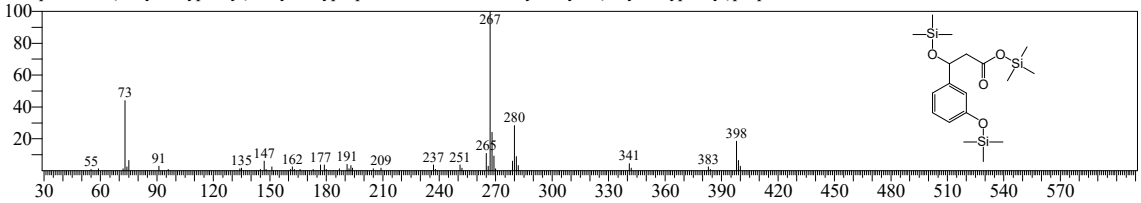
Hit#:2 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



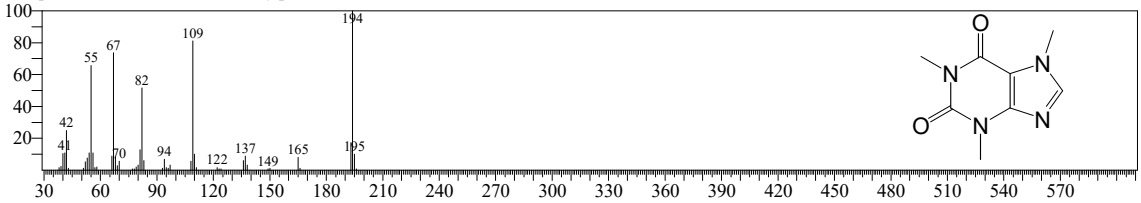
Hit#:3 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:4 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:27 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

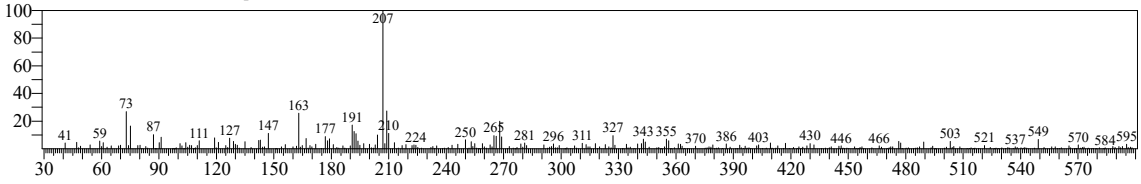


Hit#:5 Entry:342 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C8H10N4O2 CAS:58-08-2 MolWeight:194 RetIndex:1867
CompName:Caffeine ; 1,3,7-trimethylpurine-2,6-dione

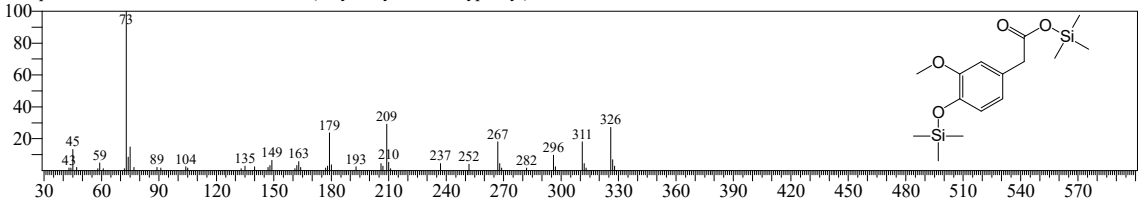


TNAU

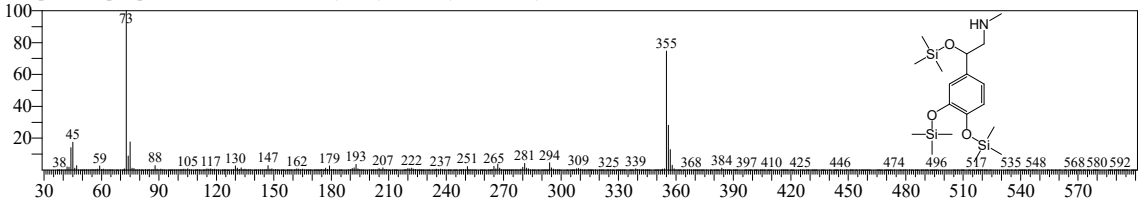
<< Target >>
Line#:19 R.Time:32.040(Scan#:5509) MassPeaks:321
RawMode:Averaged 32.035-32.045(5508-5510) BasePeak:207.05(2460)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



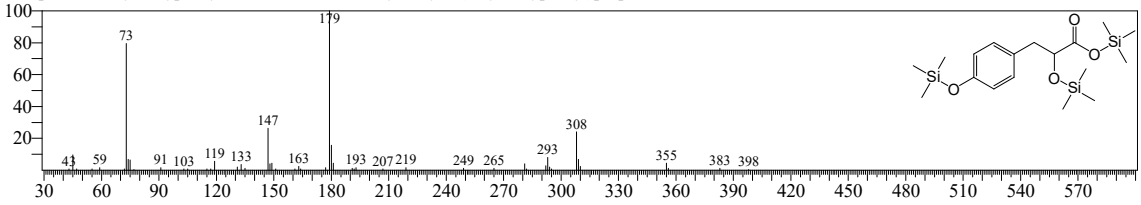
Hit#:1 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



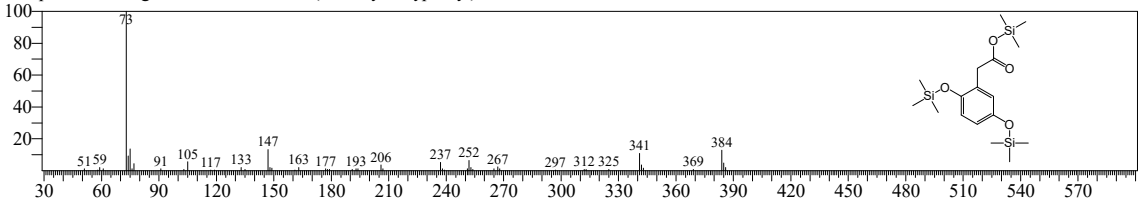
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



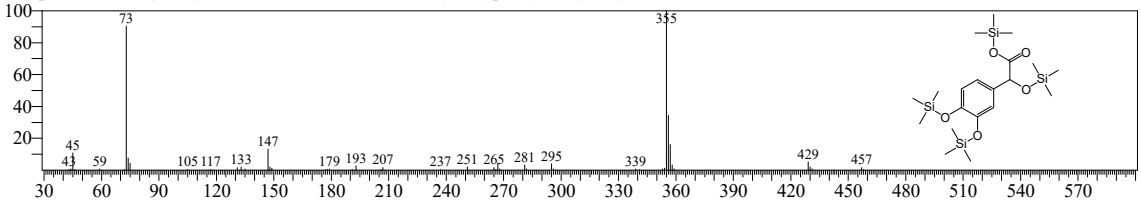
Hit#:3 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:4 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid

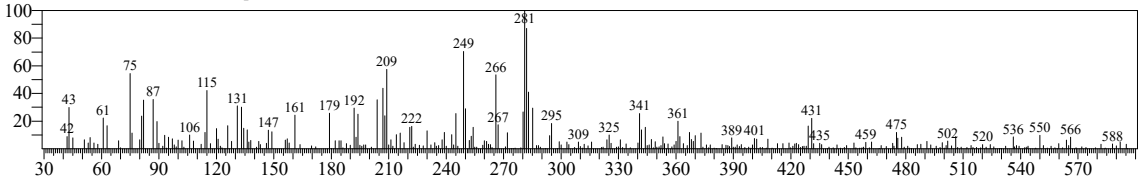


Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

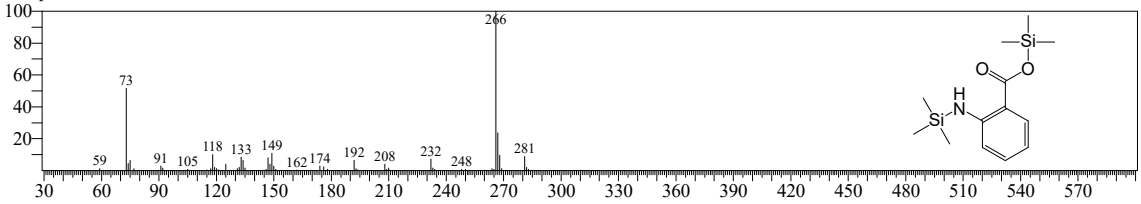


TNAU

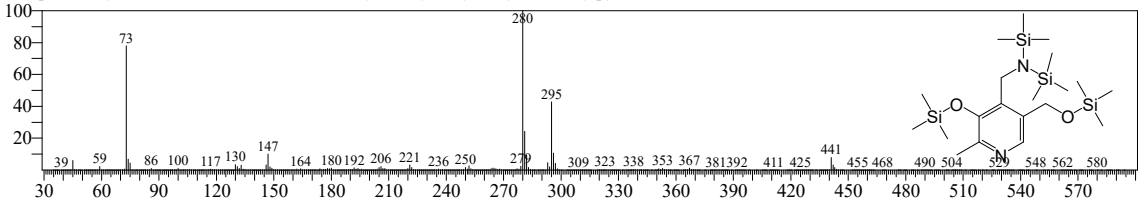
<< Target >>
Line#:20 R.Time:32.225(Scan#:5546) MassPeaks:315
RawMode:Averaged 32.220-32.230(5545-5547) BasePeak:281.05(668)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



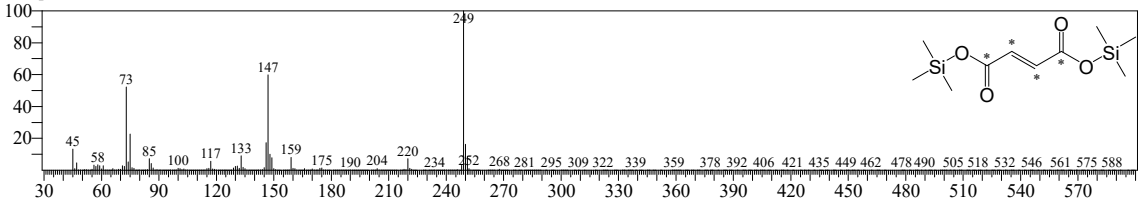
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



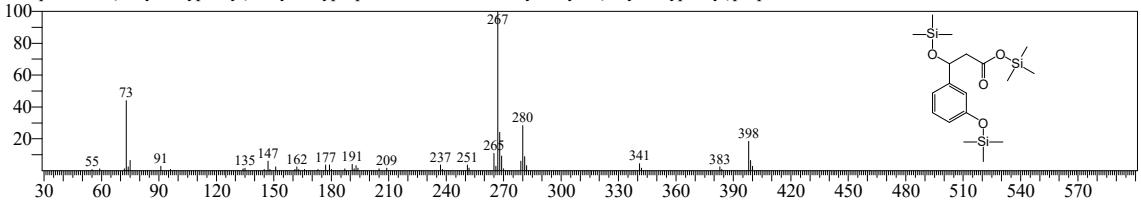
Hit#:2 Entry:469 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C20H44N2O2Si4 CAS:85-87-0 MolWeight:456 RetIndex:2139
CompName:Pyridoxamine-4TMS ; 4-(aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol



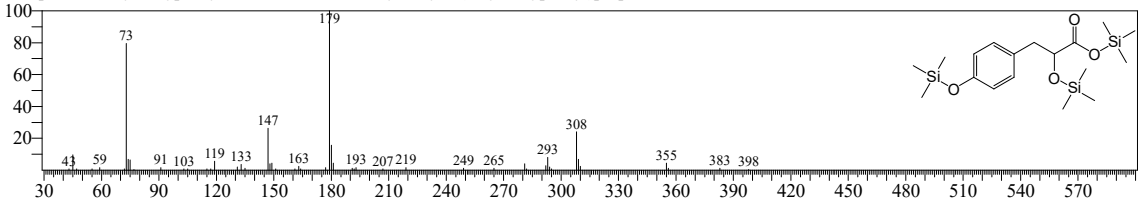
Hit#:3 Entry:100 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula: CAS:0-00-0 MolWeight:264 RetIndex:1346
CompName:Fumaric acid-13C4-2TMS ;



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

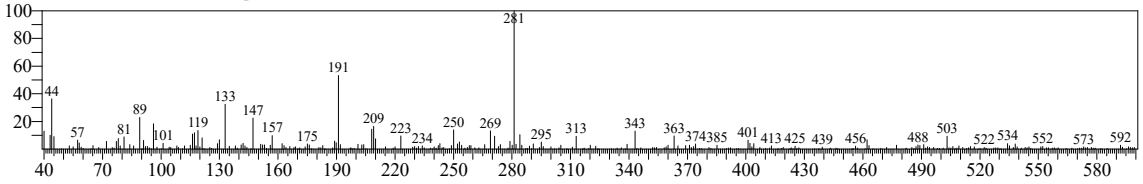


Hit#:5 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate

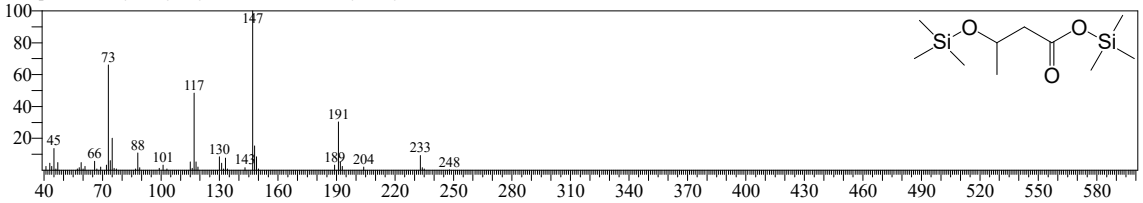


TNAU

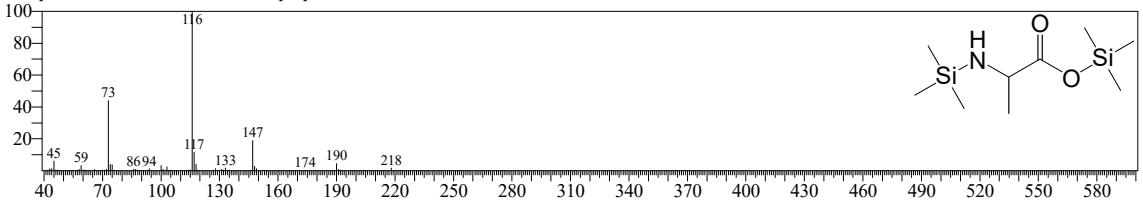
<< Target >>
Line#:21 R.Time:32.350(Scan#:5571) MassPeaks:299
RawMode:Averaged 32.345-32.355(5570-5572) BasePeak:281.05(2043)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



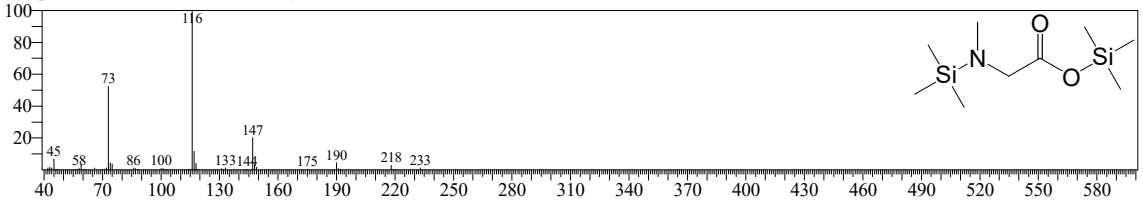
Hit#:1 Entry:35 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C10H24O3Si2 CAS:300-85-6 MolWeight:248 RetIndex:1161
CompName:3-Hydroxybutyric acid-2TMS ; 3-hydroxybutanoic acid



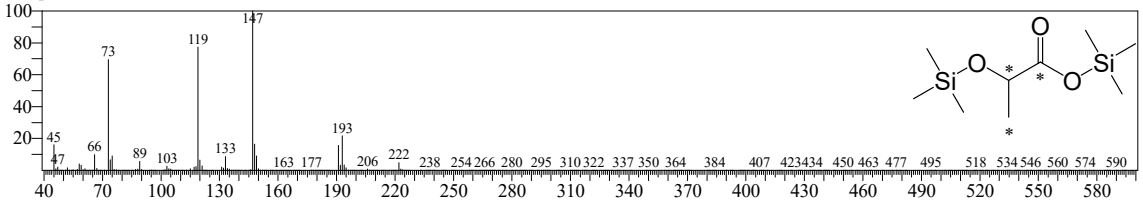
Hit#:2 Entry:16 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C9H23NO2Si2 CAS:302-72-7 MolWeight:233 RetIndex:1106
CompName:Alanine-2TMS ; 2-aminopropanoic acid



Hit#:3 Entry:29 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C9H23NO2Si2 CAS:107-97-1 MolWeight:233 RetIndex:1141
CompName:Sarcosine-2TMS ; 2-(methylamino)acetic acid



Hit#:4 Entry:9 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula: CAS:0-00-0 MolWeight:237 RetIndex:1062
CompName:Lactic acid-13C3-2TMS ;



Hit#:5 Entry:365 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H19NO3Si CAS:42013-20-7 MolWeight:265 RetIndex:1898
CompName:2-Methylhippuric acid-TMS ; 2-[(2-methylbenzoyl)amino]acetic acid