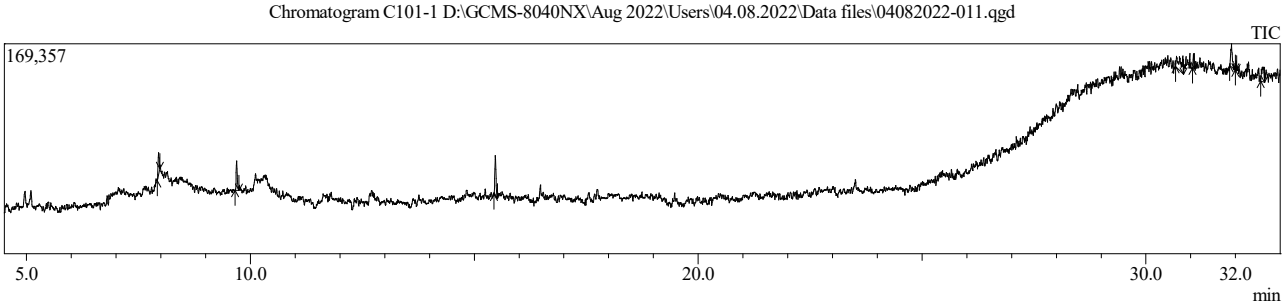
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 04-Aug-22 11:24:52 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C101-1
Sample ID	: C101-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 11
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-011.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-011.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 4:27:50 PM

Chromatogram C101-1 D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-011.qgd



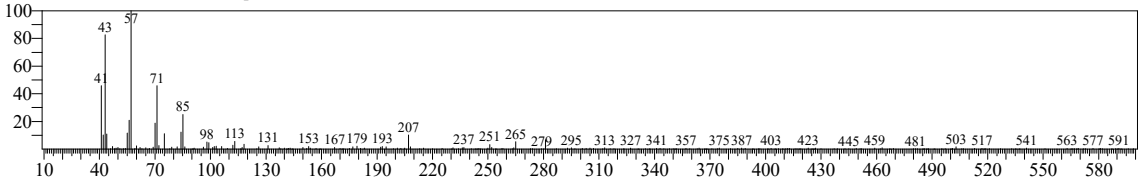
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	7.946	30490	10.09	18226	13.12	1.67	86	Undecane
2	9.692	42265	13.98	23710	17.07	1.78	91	Undecane
3	15.470	55758	18.45	32755	23.58	1.70	88	2,4-Di-tert-butylphenol
4	30.823	69780	23.09	14130	10.17	4.94	37	3-Hydroxybenzoic acid-2TMS
5	31.061	11705	3.87	11839	8.52	0.99	38	Epinephrine-3TMS
6	31.910	45720	15.13	18556	13.36	2.46	36	Suberic acid-2TMS
7	32.014	6449	2.13	7840	5.64	0.82	25	Anthranilic acid-2TMS
8	32.621	40090	13.26	11878	8.55	3.38	44	3,4-Dihydroxymandelic acid-4TMS
		302257	100.00	138934	100.00			

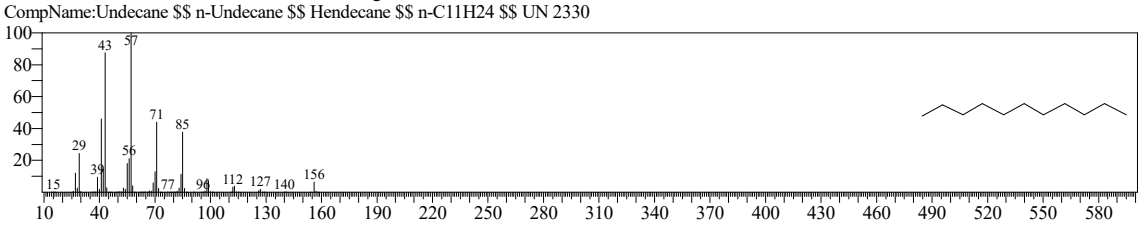
Library

TNAU

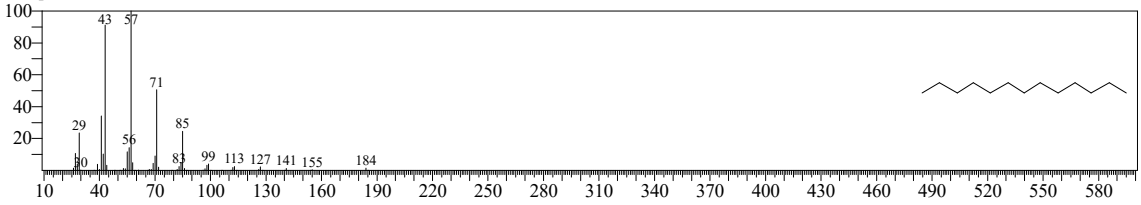
<< Target >>
Line#:1 R.Time:7.945(Scan#:690) MassPeaks:223
RawMode:Averaged 7.940-7.950(689-691) BasePeak:57.10(4453)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



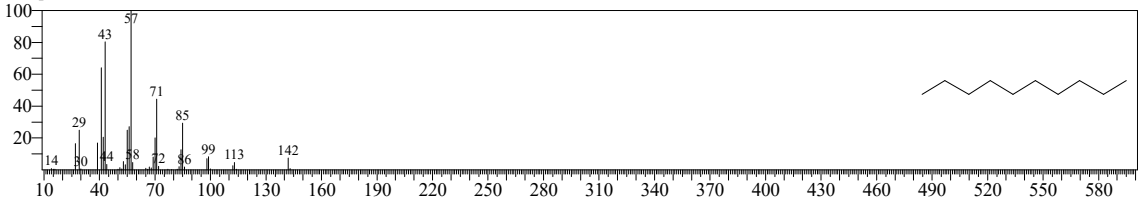
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



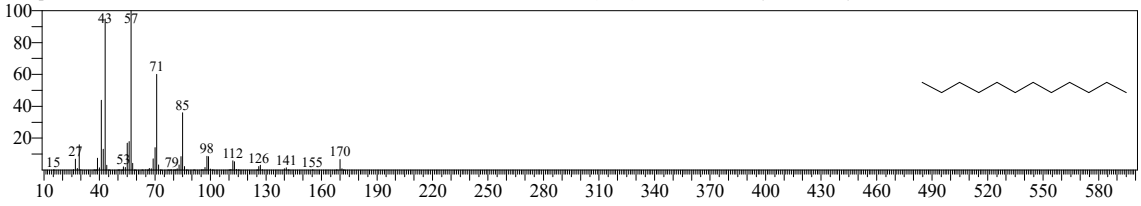
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:85 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



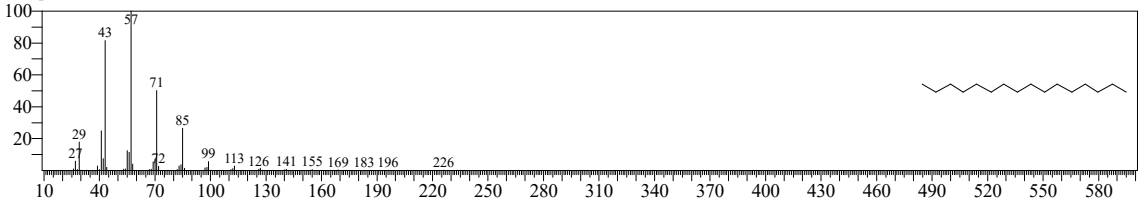
Hit#:3 Entry:13604 Library:NIST20M1.lib
SI:85 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



Hit#:4 Entry:16191 Library:NIST20R.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

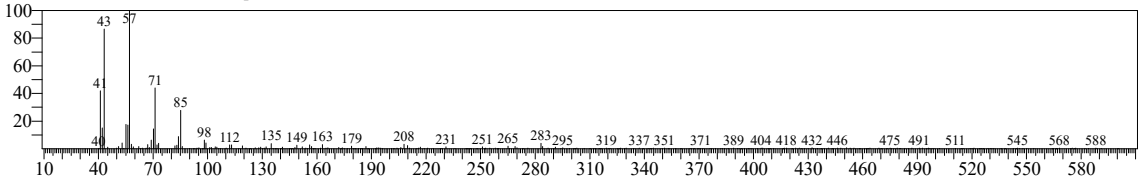


Hit#:5 Entry:27737 Library:NIST20R.lib
SI:84 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

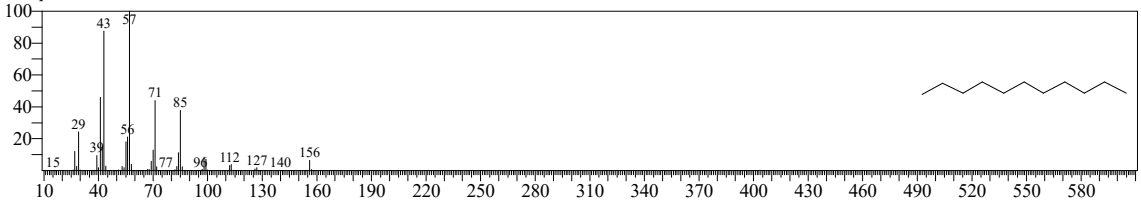


TNAU

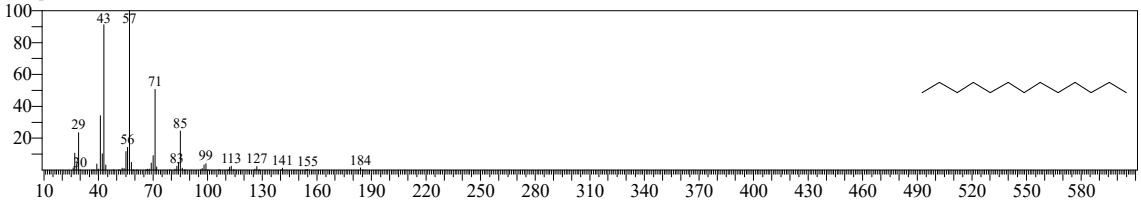
<< Target >>
Line#:2 R.Time:9.690(Scan#:1039) MassPeaks:279
RawMode:Averaged 9.685-9.695(1038-1040) BasePeak:57.05(5705)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



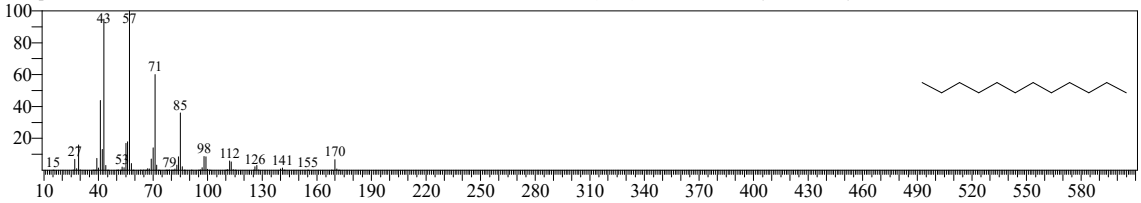
Hit#:1 Entry:12897 Library:NIST20R.lib
SI:91 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



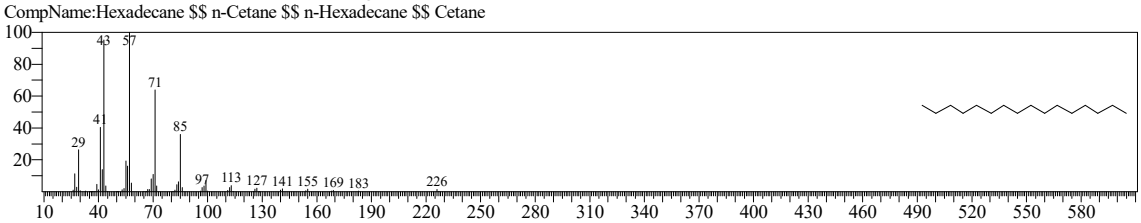
Hit#:2 Entry:40226 Library:NIST20M1.lib
SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



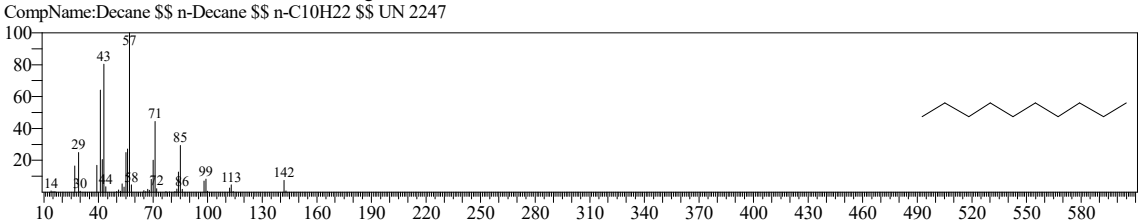
Hit#:3 Entry:16191 Library:NIST20R.lib
SI:89 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:27736 Library:NIST20R.lib
SI:88 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane

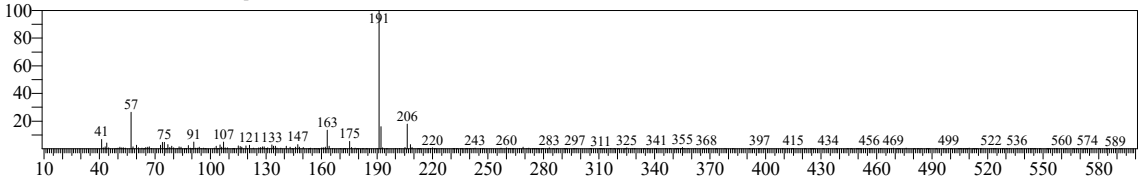


Hit#:5 Entry:13604 Library:NIST20M1.lib
SI:88 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247

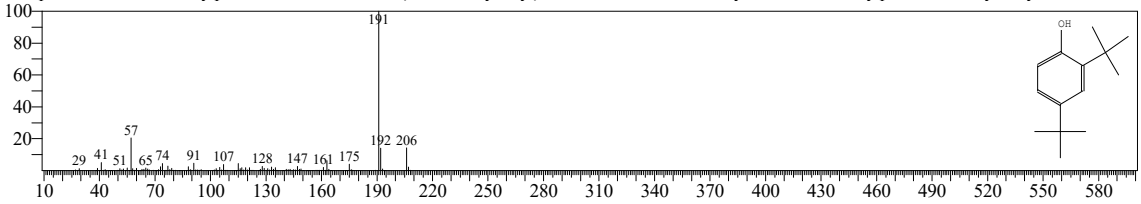


TNAU

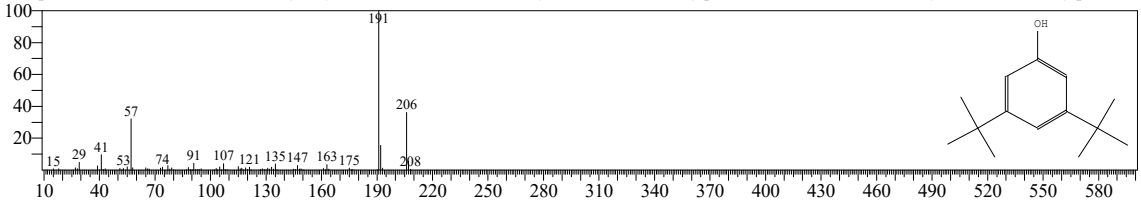
<< Target >>
Line#:3 R.Time:15.470(Scan#:2195) MassPeaks:271
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.15(11429)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



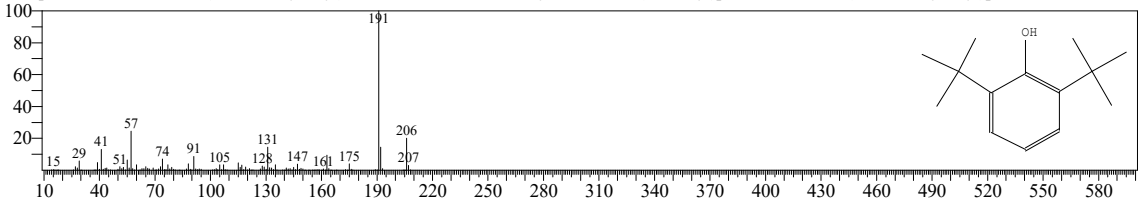
Hit#:1 Entry:24088 Library:NIST20R.lib
SI:88 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



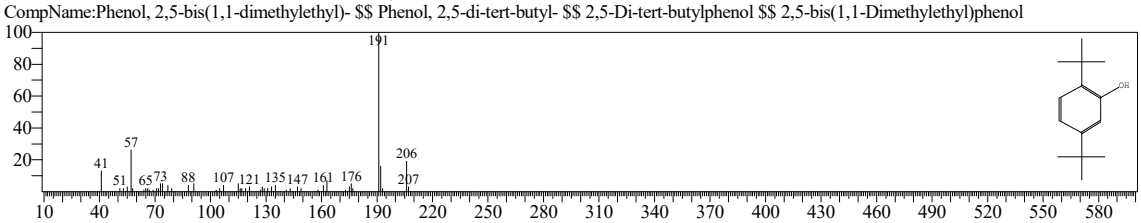
Hit#:2 Entry:24110 Library:NIST20R.lib
SI:85 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



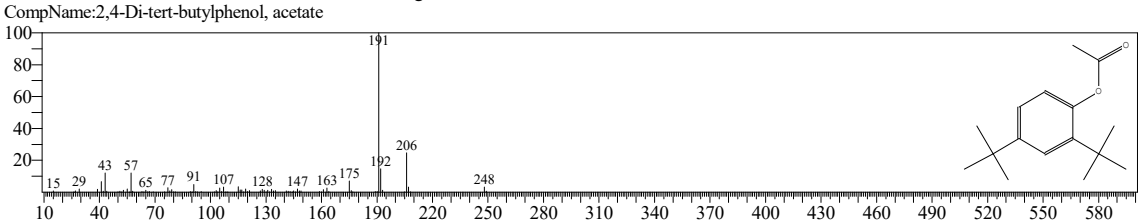
Hit#:3 Entry:59031 Library:NIST20M1.lib
SI:85 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert



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

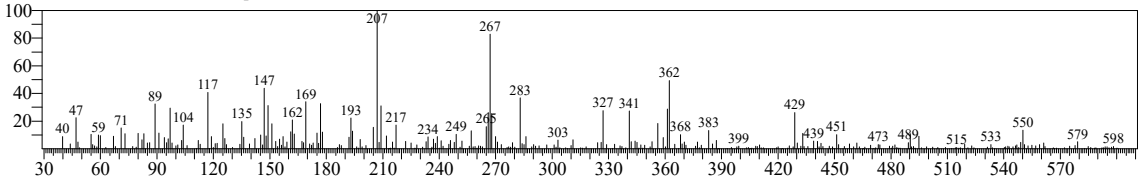


Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:83 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
CompName:2,4-Di-tert-butylphenol, acetate

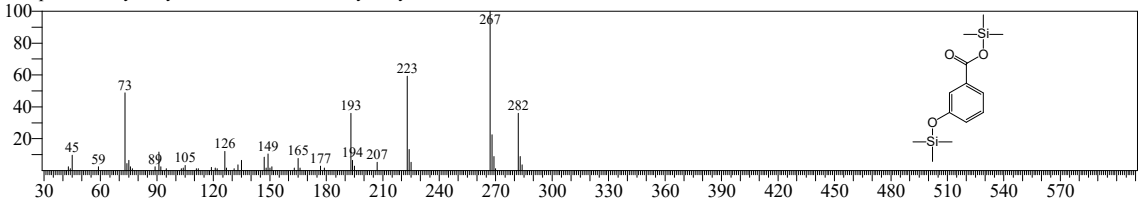


TNAU

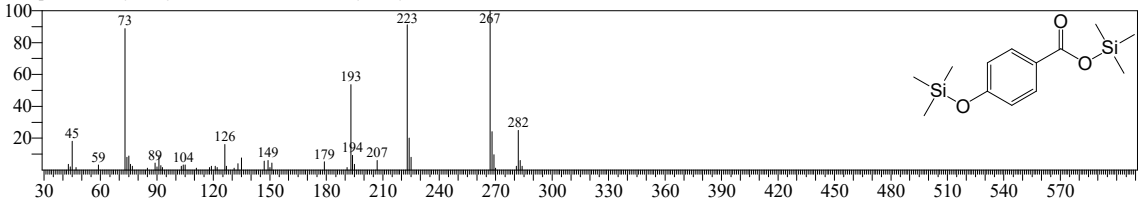
<< Target >>
Line#:4 R.Time:30.825(Scan#:5266) MassPeaks:314
RawMode:Averaged 30.820-30.830(5265-5267) BasePeak:207.05(1274)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



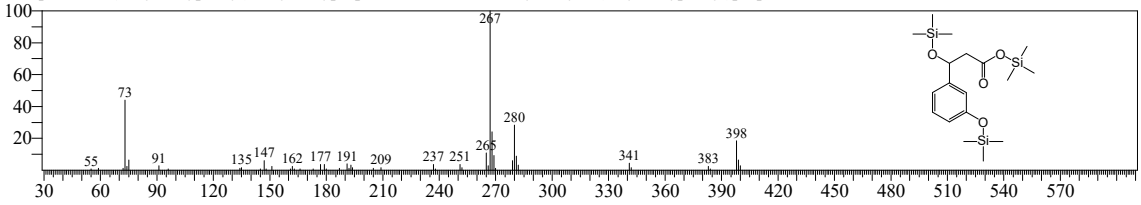
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



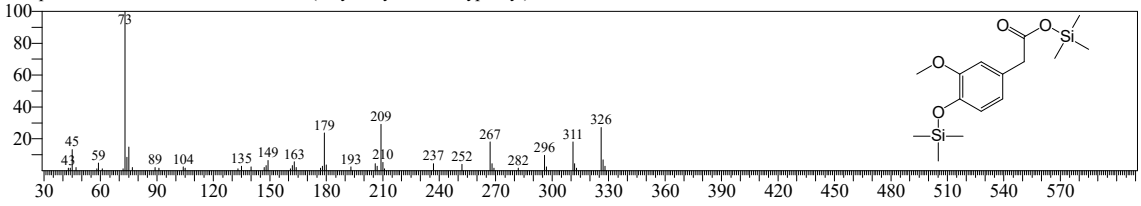
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



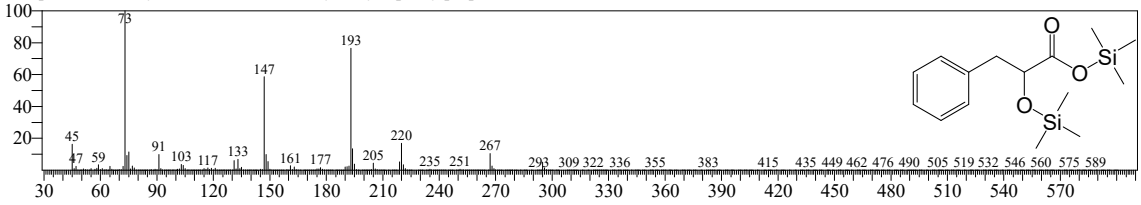
Hit#:3 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



Hit#:4 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid

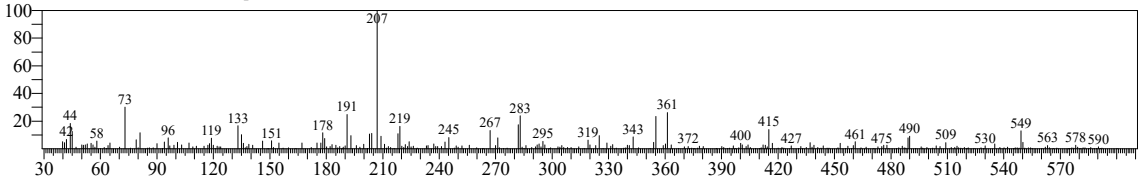


Hit#:5 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

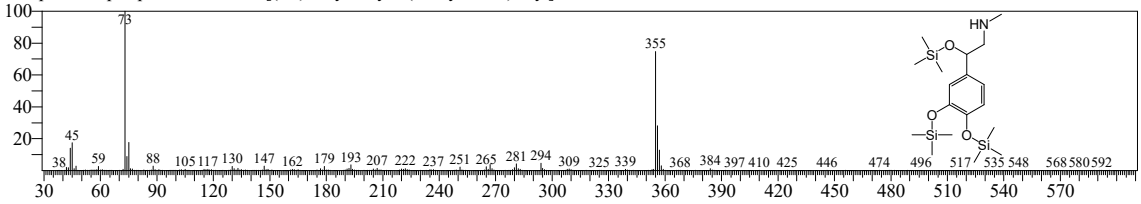


TNAU

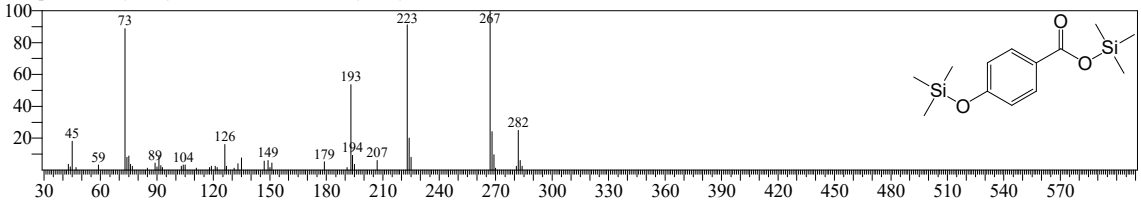
<< Target >>
Line#:5 R.Time:31.060(Scan#:5313) MassPeaks:293
RawMode:Averaged 31.055-31.065(5312-5314) BasePeak:207.05(2586)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



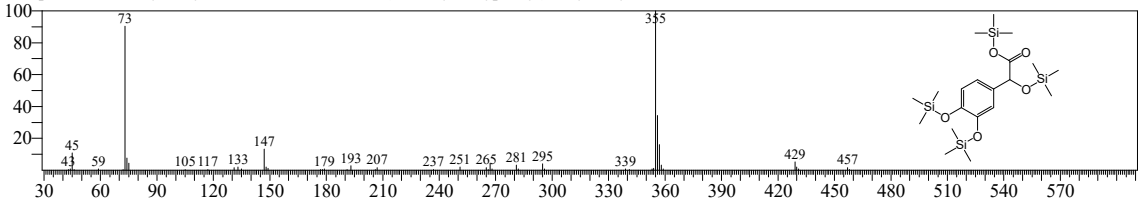
Hit#:1 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



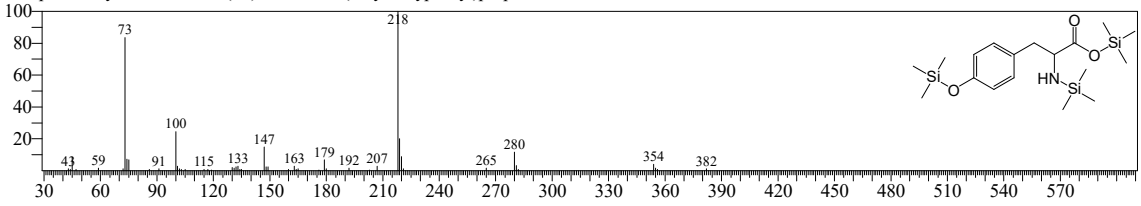
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



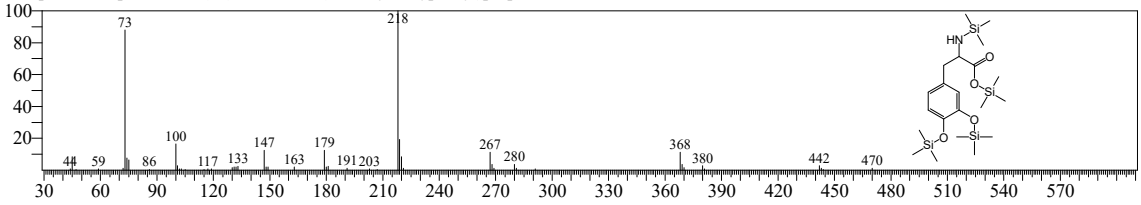
Hit#:3 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:4 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

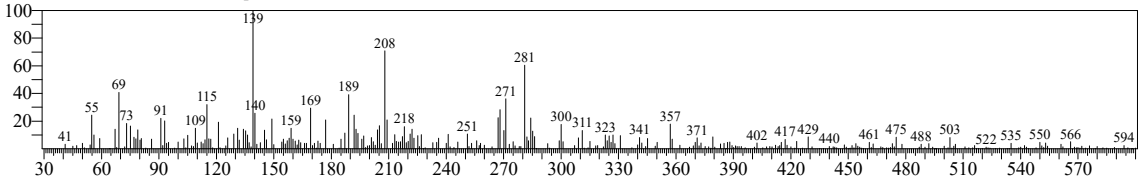


Hit#:5 Entry:463 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C21H43NO4Si4 CAS:59-92-7 MolWeight:485 RetIndex:2123
CompName:Dopa-4TMS ; (2S)-2-amino-3-(3,4-dihydroxyphenyl)propanoic acid

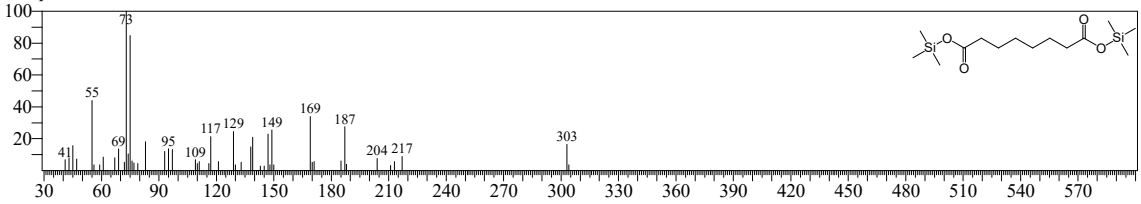


TNAU

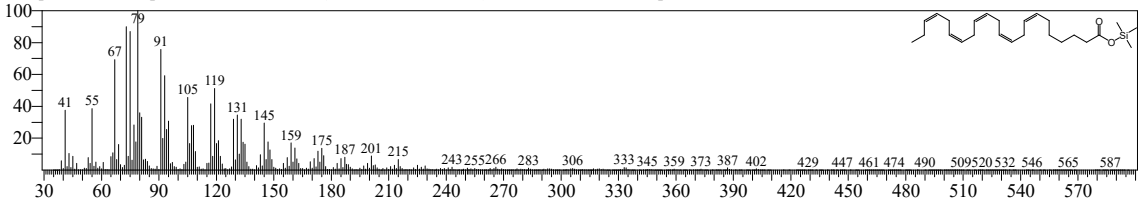
<< Target >>
Line#:6 R.Time:31.910(Scan#:5483) MassPeaks:315
RawMode:Averaged 31.905-31.915(5482-5484) BasePeak:139.15(1610)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



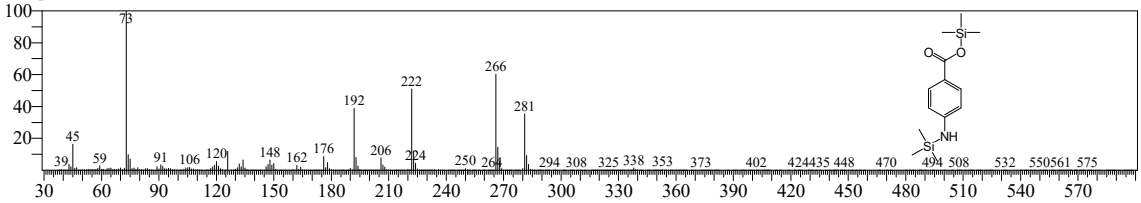
Hit#:1 Entry:258 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H30O4Si2 CAS:505-48-6 MolWeight:318 RetIndex:1700
CompName:Suberic acid-2TMS ; octanedioic acid



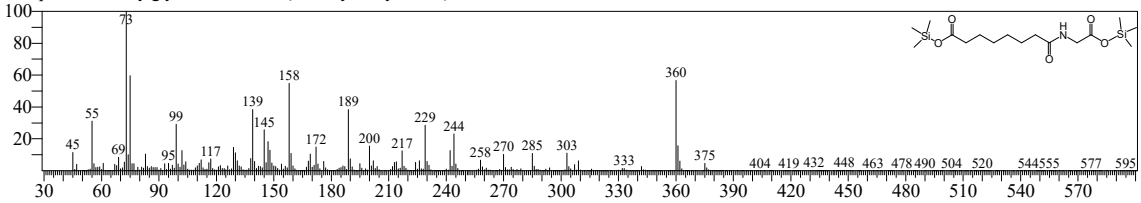
Hit#:2 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



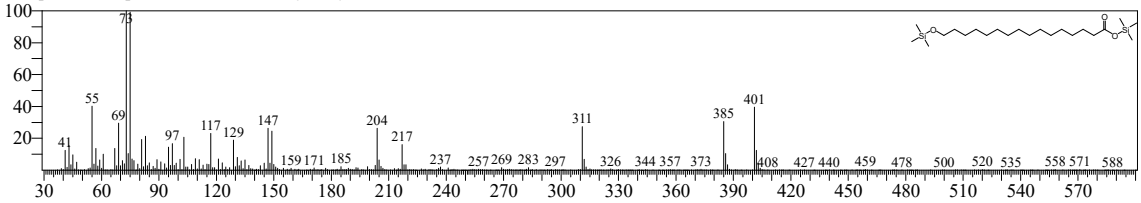
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:497 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C16H33NO5Si2 CAS:60317-54-6 MolWeight:375 RetIndex:2271
CompName:Suberylglycine-2TMS ; 8-(carboxymethylamino)-8-oxooctanoic acid

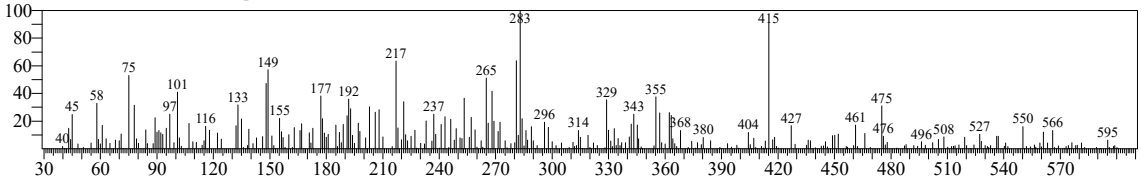


Hit#:5 Entry:511 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C22H48O3Si2 CAS:506-13-8 MolWeight:416 RetIndex:2396
CompName:Juniperic acid-2TMS ; 16-hydroxyhexadecanoic acid

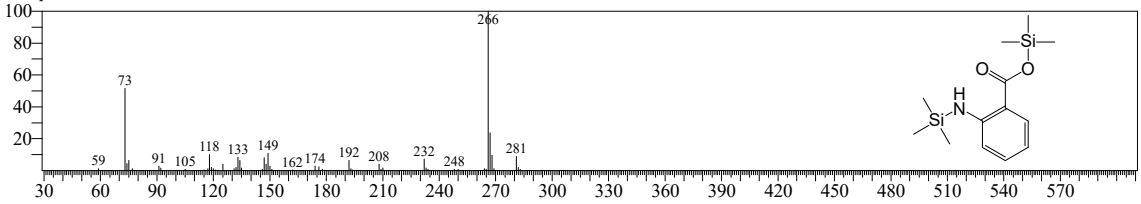


TNAU

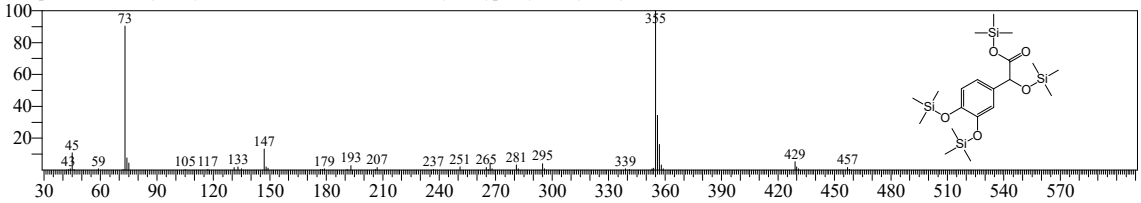
<< Target >>
Line#:7 R.Time:32.015(Scan#:5504) MassPeaks:304
RawMode:Averaged 32.010-32.020(5503-5505) BasePeak:283.00(580)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



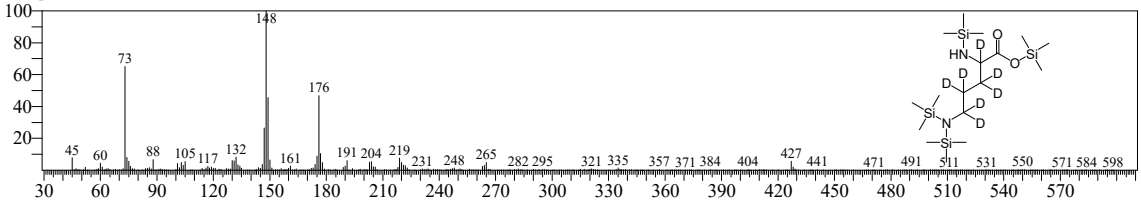
Hit#:1 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



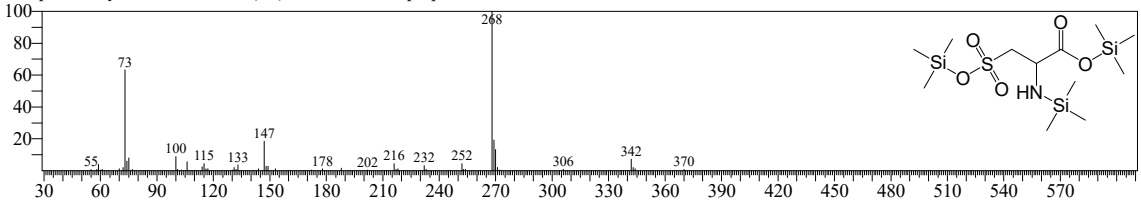
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



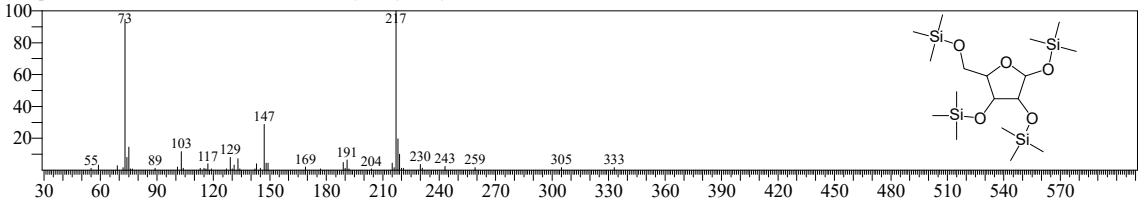
Hit#:3 Entry:313 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula: CAS:0-00-0 MolWeight:427 RetIndex:1831
CompName:Ornithine-d7-4TMS ;



Hit#:4 Entry:277 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C12H31NO5SSi3 CAS:498-40-8 MolWeight:385 RetIndex:1749
CompName:Cysteic acid-3TMS ; (2R)-2-amino-3-sulfopropanoic acid

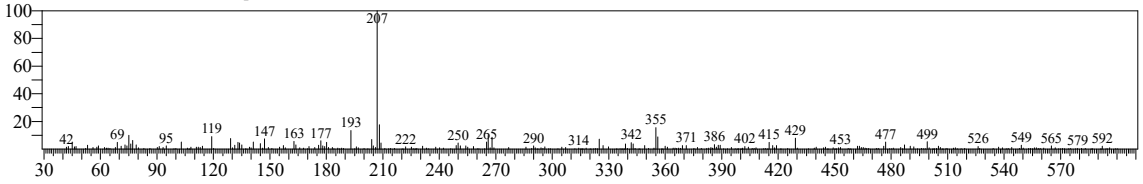


Hit#:5 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

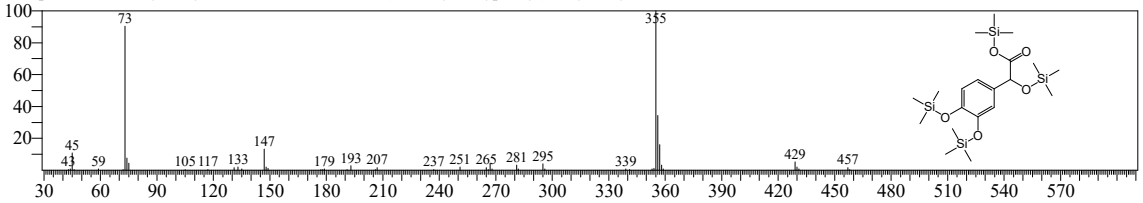


TNAU

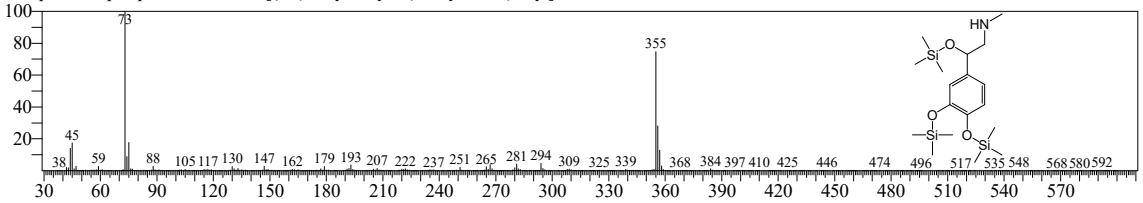
<< Target >>
Line#:8 R.Time:32.620(Scan#:5625) MassPeaks:299
RawMode:Averaged 32.615-32.625(5624-5626) BasePeak:207.05(4195)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



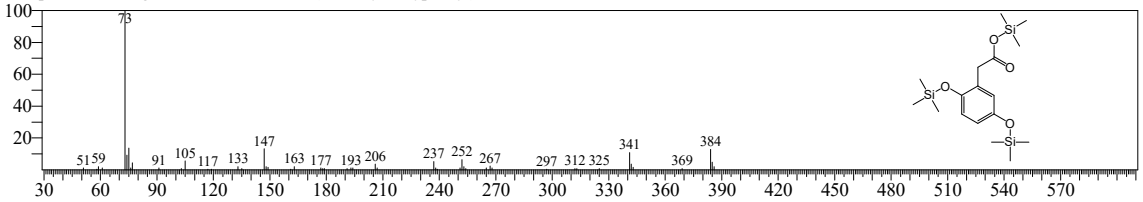
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



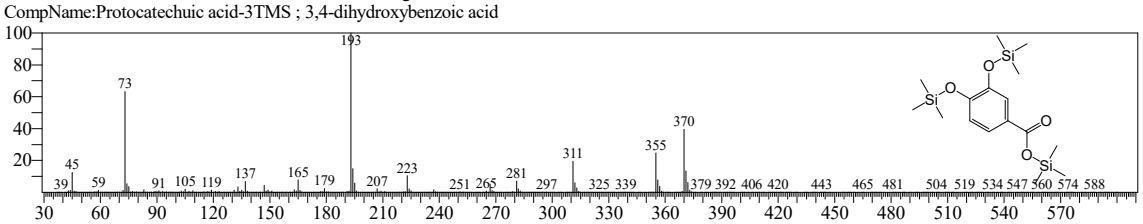
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:3 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid



Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



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