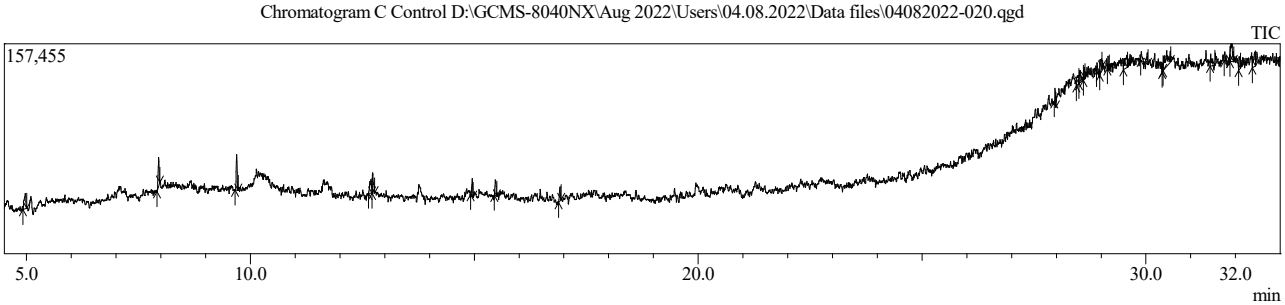
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 05-Aug-22 5:15:33 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: C Control
Sample ID	: C Control
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 20
Injection Volume	: 1.00
Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-020.qgd
Org Data File	: D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-020.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 4:50:50 PM

Chromatogram C Control D:\GCMS-8040NX\Aug 2022\Users\04.08.2022\Data files\04082022-020.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	4.971	29976	5.48	11560	4.42	2.59	72	2-Propanol, 1,1'-oxybis-
2	7.950	33568	6.13	21505	8.22	1.56	87	Decane
3	9.693	41751	7.63	26905	10.29	1.55	89	Undecane
4	12.665	29319	5.36	8789	3.36	3.34	47	4-Hydroxybenzoic acid-2TMS
5	12.731	27061	4.94	15170	5.80	1.78	47	3,4-Dihydroxymandelic acid-4TMS
6	14.954	16503	3.01	13222	5.05	1.25	78	Cycloheptasiloxane, tetradecamethyl-
7	15.470	19023	3.48	11861	4.53	1.60	79	2,4-Di-tert-butylphenol
8	16.913	16544	3.02	10635	4.07	1.56	64	3,4-Dihydroxymandelic acid-4TMS
9	27.971	11474	2.10	12523	4.79	0.92	40	3,4-Dihydroxymandelic acid-4TMS
10	28.455	19289	3.52	5960	2.28	3.24	28	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
11	28.515	22275	4.07	9121	3.49	2.44	32	3-(3-Hydroxyphenyl)-3-hydroxypropionic acid
12	28.623	11833	2.16	8857	3.39	1.34	41	3,4-Dihydroxymandelic acid-4TMS
13	28.905	11175	2.04	6871	2.63	1.63	37	3-Hydroxyanthranilic acid-2TMS
14	29.009	20774	3.80	7484	2.86	2.78	31	Shikimic acid-4TMS
15	29.152	9652	1.76	9621	3.68	1.00	31	3-Hydroxybenzoic acid-2TMS
16	29.568	34282	6.26	9478	3.62	3.62	33	3,4-Dihydroxymandelic acid-4TMS
17	29.897	19265	3.52	6874	2.63	2.80	37	4-Aminobenzoic acid-2TMS
18	30.370	6349	1.16	5171	1.98	1.23	25	Protocatechuic acid-3TMS
19	30.462	59518	10.87	11765	4.50	5.06	37	Homovanillic acid-2TMS
20	31.445	12750	2.33	9105	3.48	1.40	38	3-Hydroxybenzoic acid-2TMS
21	31.755	9505	1.74	5589	2.14	1.70	30	Hypoxanthine-2TMS
22	31.908	43503	7.95	13114	5.01	3.32	36	3-Hydroxybenzoic acid-2TMS

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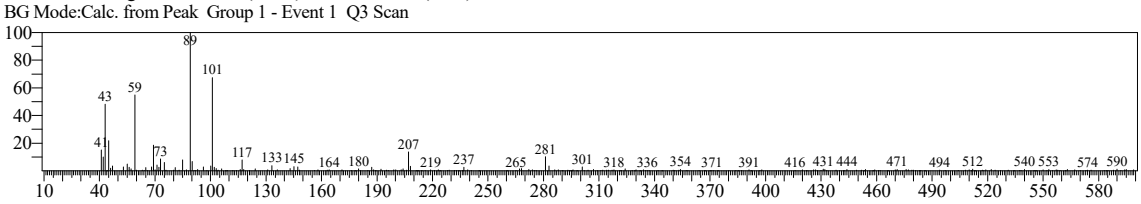
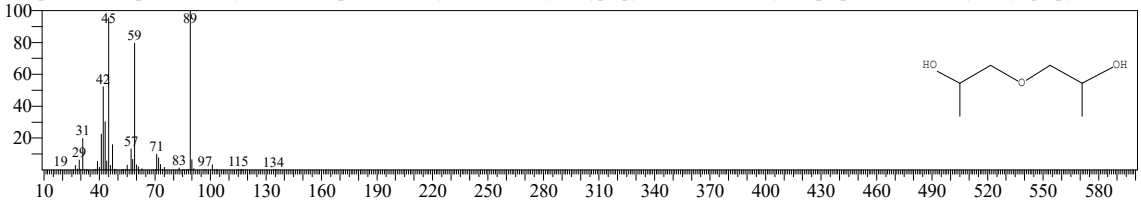
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
23	32.083	14756	2.70	9715	3.71	1.52	42	Glycerol-3TMS
24	32.428	27248	4.98	10686	4.09	2.55	38	3-Phenyllactic acid-2TMS
		547393	100.00	261581	100.00			

Library

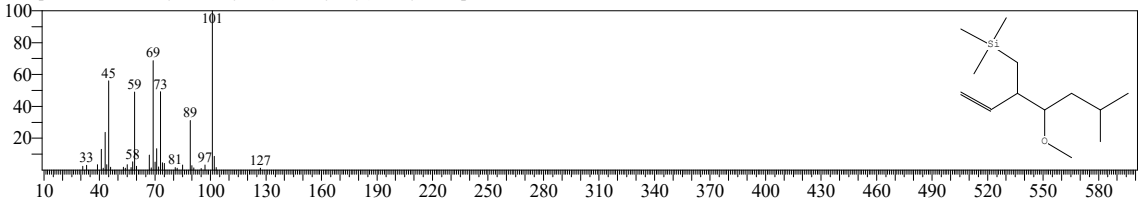
<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:239
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.10(3084)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



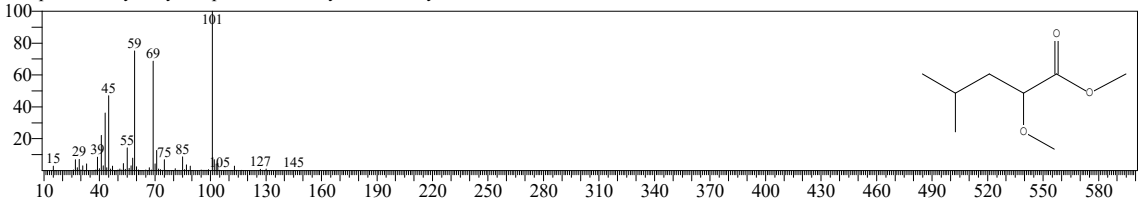
Hit#:1 Entry:7425 Library:NIST20R.lib
SI:72 Formula:C6H14O3 CAS:110-98-5 MolWeight:134 RetIndex:1018
CompName:2-Propanol, 1,1'-oxybis- $$ 2-Propanol, 1,1'-oxydi- $$ Bis(2-hydroxypropyl) ether $$ 1,1'-Oxydi-2-propanol $$ 2,2'-Dihydroxydipropyl ether $$



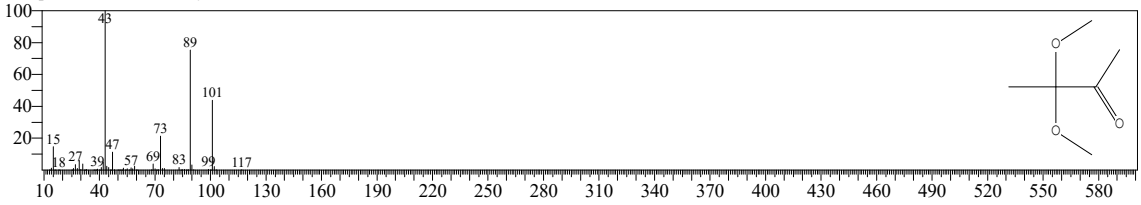
Hit#:2 Entry:81501 Library:NIST20M1.lib
SI:71 Formula:C13H28OSi CAS:0-00-0 MolWeight:228 RetIndex:1097
CompName:4-Methoxy-6-methyl-3-(trimethylsilyl)methyl-1-heptene



Hit#:3 Entry:22897 Library:NIST20M1.lib
SI:71 Formula:C8H16O3 CAS:0-00-0 MolWeight:160 RetIndex:931
CompName:2-Hydroxyisocaproic acid, methyl ether, methyl ester

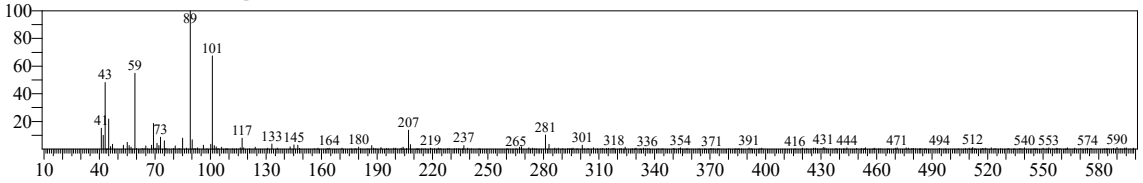


Hit#:4 Entry:9263 Library:NIST20M1.lib
SI:71 Formula:C6H12O3 CAS:21983-72-2 MolWeight:132 RetIndex:821
CompName:3,3-Dimethoxy-2-butanone

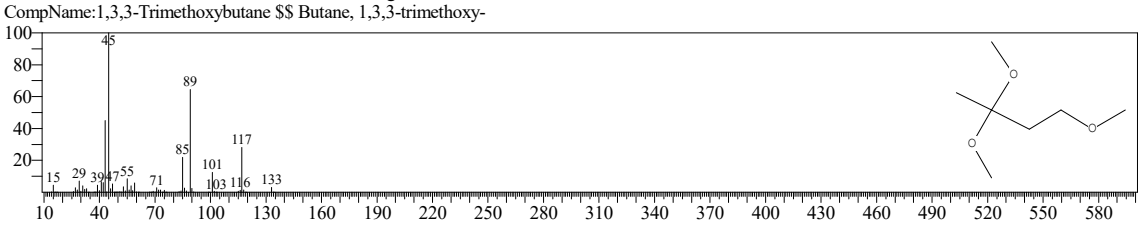


TNAU

<< Target >>
Line#:1 R.Time:4.970(Scan#:95) MassPeaks:239
RawMode:Averaged 4.965-4.975(94-96) BasePeak:89.10(3084)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

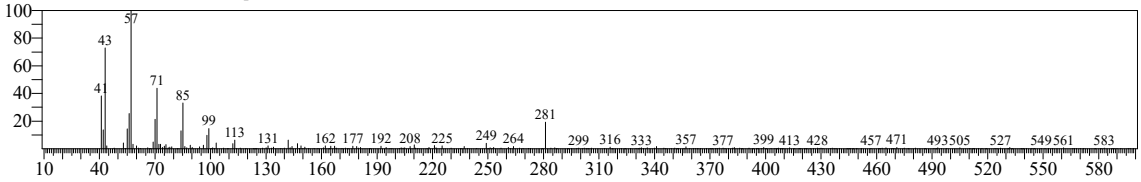


Hit#:5 Entry:16032 Library:NIST20M1.lib
SI:70 Formula:C7H16O3 CAS:6607-66-5 MolWeight:148 RetIndex:860
CompName:1,3,3-Trimethoxybutane $$ Butane, 1,3,3-trimethoxy-

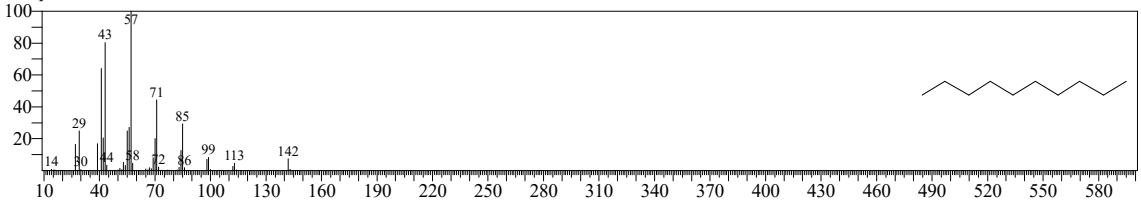


TNAU

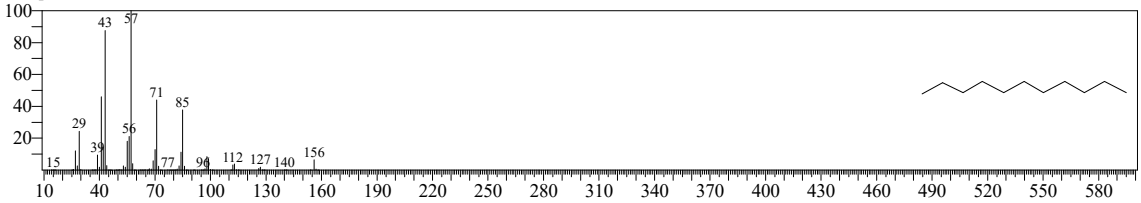
<< Target >>
Line#:2 R.Time:7.950(Scan#:691) MassPeaks:264
RawMode:Averaged 7.945-7.955(690-692) BasePeak:57.05(4332)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



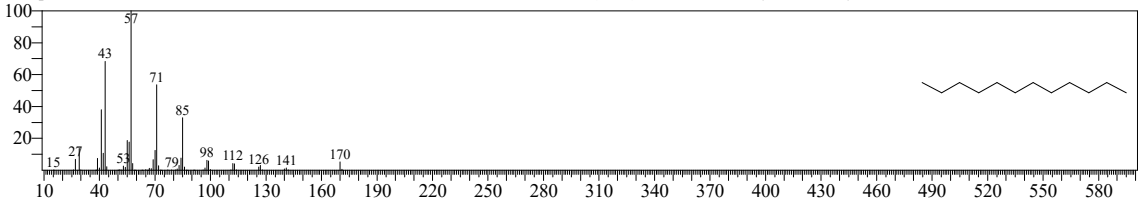
Hit#:1 Entry:13604 Library:NIST20M1.lib
SI:87 Formula:C10H22 CAS:124-18-5 MolWeight:142 RetIndex:1000
CompName:Decane $$ n-Decane $$ n-C10H22 $$ UN 2247



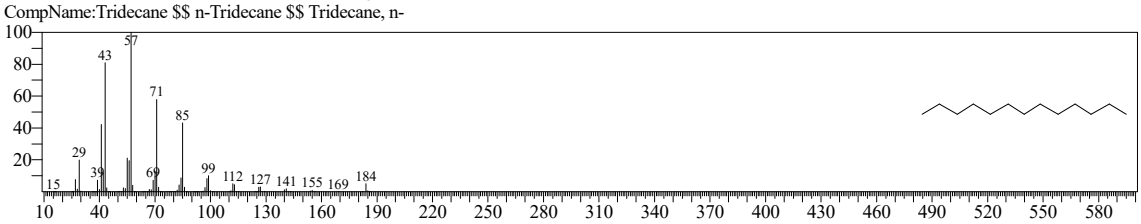
Hit#:2 Entry:12897 Library:NIST20R.lib
SI:86 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



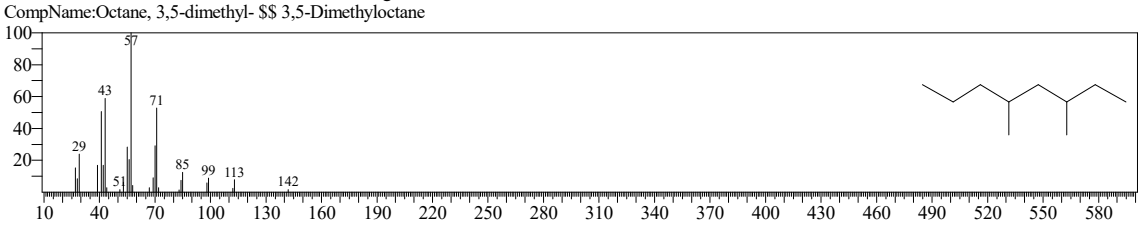
Hit#:3 Entry:30057 Library:NIST20M1.lib
SI:85 Formula:C12H26 CAS:112-40-3 MolWeight:170 RetIndex:1200
CompName:Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ Duodecane $$ NSC 8714



Hit#:4 Entry:19410 Library:NIST20R.lib
SI:85 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-

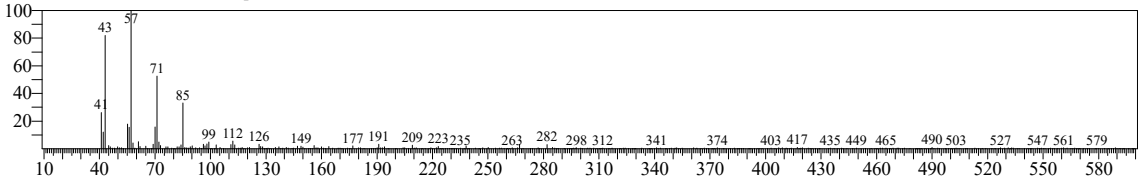


Hit#:5 Entry:9465 Library:NIST20R.lib
SI:85 Formula:C10H22 CAS:15869-93-9 MolWeight:142 RetIndex:887
CompName:Octane, 3,5-dimethyl- $$ 3,5-Dimethyloctane

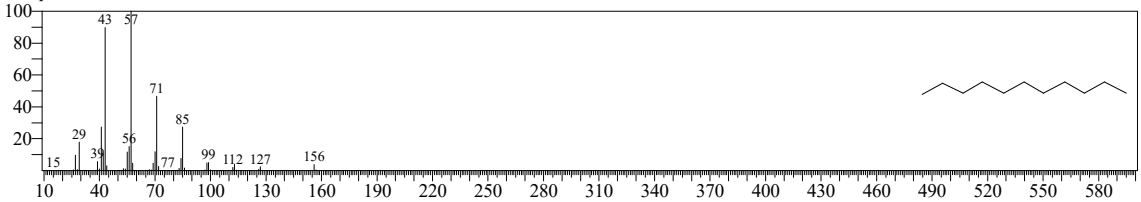


TNAU

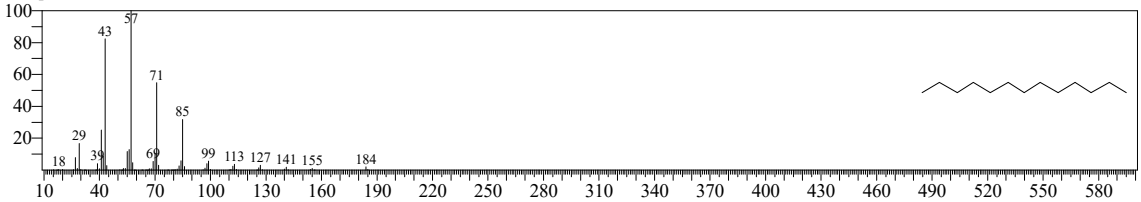
<< Target >>
Line#:3 R.Time:9.695(Scan#:1040) MassPeaks:340
RawMode:Averaged 9.690-9.700(1039-1041) BasePeak:57.10(5253)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



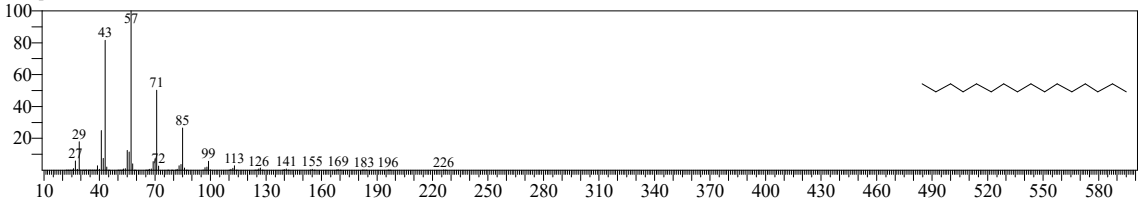
Hit#:1 Entry:21042 Library:NIST20M1.lib
SI:89 Formula:C11H24 CAS:1120-21-4 MolWeight:156 RetIndex:1100
CompName:Undecane $$ n-Undecane $$ Hendecane $$ n-C11H24 $$ UN 2330



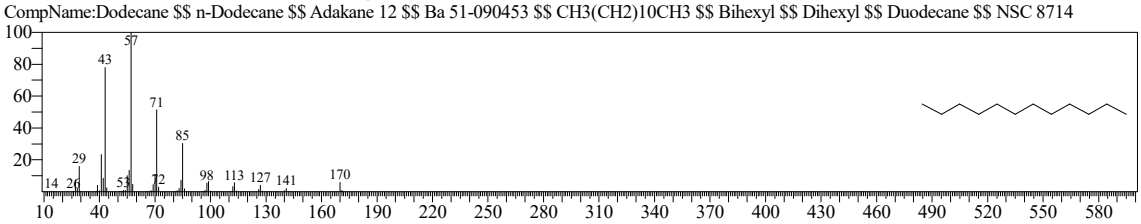
Hit#:2 Entry:19412 Library:NIST20R.lib
SI:89 Formula:C13H28 CAS:629-50-5 MolWeight:184 RetIndex:1300
CompName:Tridecane $$ n-Tridecane $$ Tridecane, n-



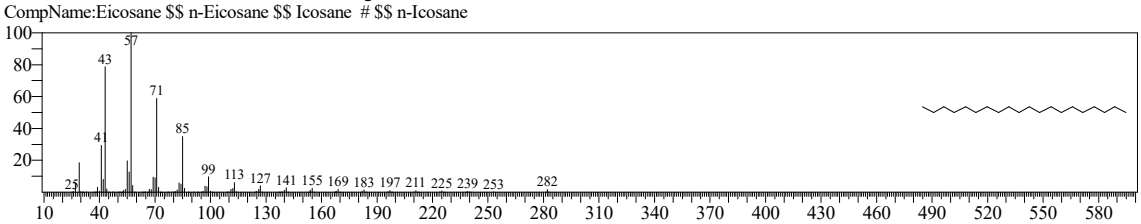
Hit#:3 Entry:27737 Library:NIST20R.lib
SI:89 Formula:C16H34 CAS:544-76-3 MolWeight:226 RetIndex:1600
CompName:Hexadecane $$ n-Cetane $$ n-Hexadecane $$ Cetane



Hit#:4 Entry:16192 Library:NIST20R.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

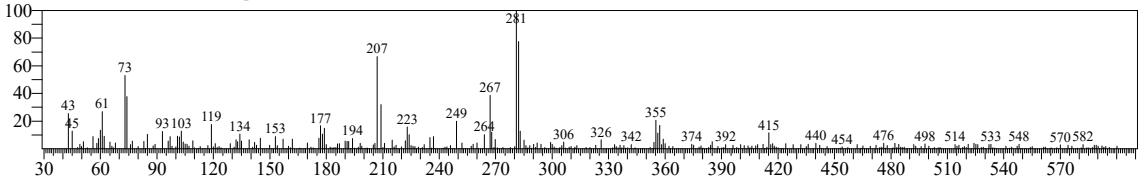


Hit#:5 Entry:34259 Library:NIST20R.lib
SI:87 Formula:C20H42 CAS:112-95-8 MolWeight:282 RetIndex:2000
CompName:Eicosane $$ n-Eicosane $$ Icosane # $$ n-Icosane

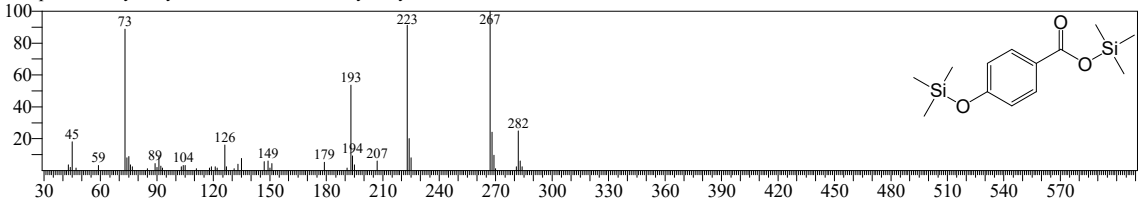


TNAU

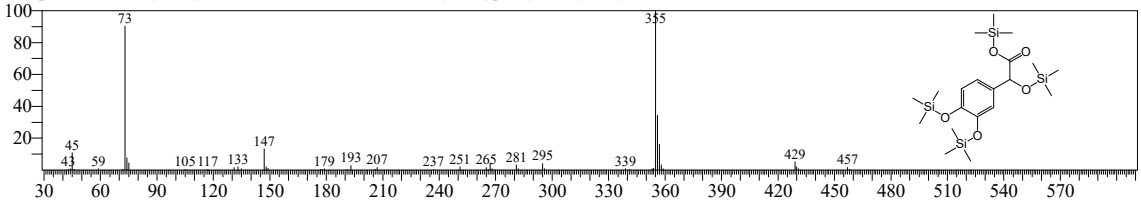
<< Target >>
Line#:4 R.Time:12.665(Scan#:1634) MassPeaks:309
RawMode:Averaged 12.660-12.670(1633-1635) BasePeak:281.05(794)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



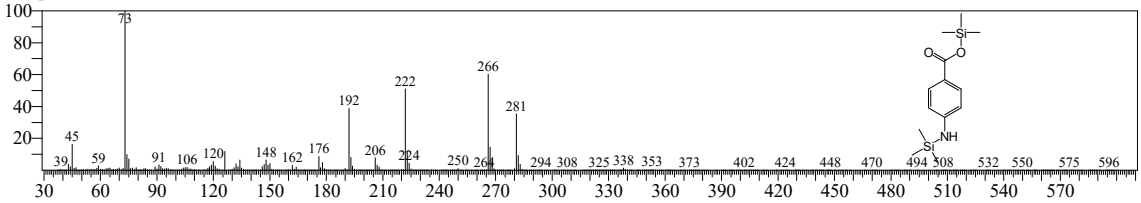
Hit#:1 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



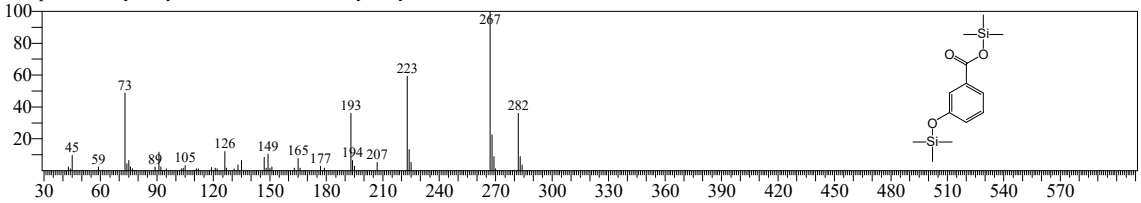
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



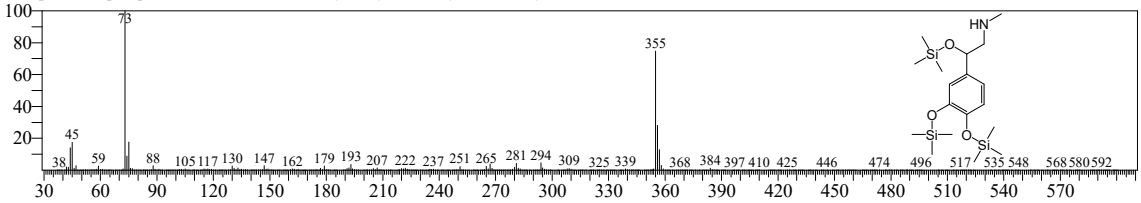
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid

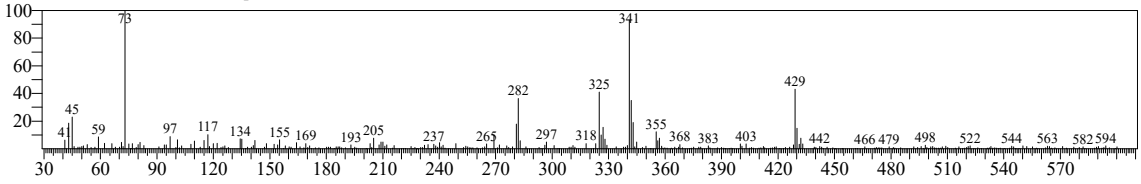


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

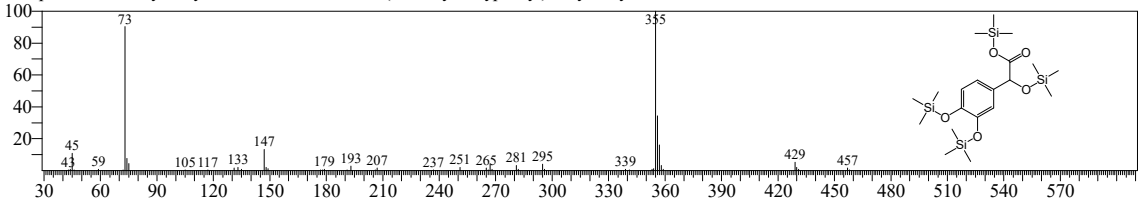


TNAU

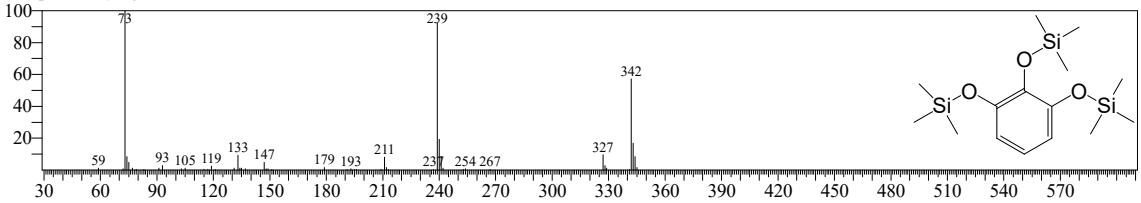
<< Target >>
Line#:5 R.Time:12.730(Scan#:1647) MassPeaks:302
RawMode:Averaged 12.725-12.735(1646-1648) BasePeak:73.10(1519)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



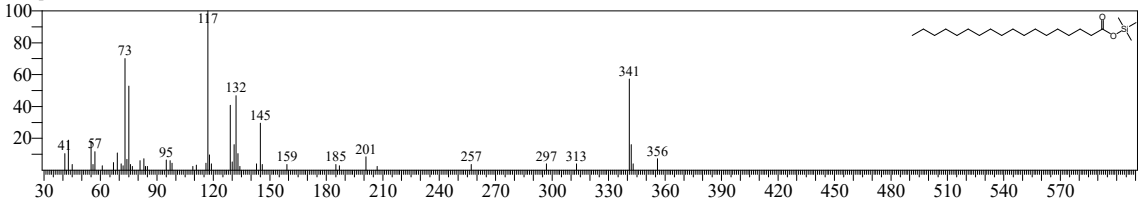
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



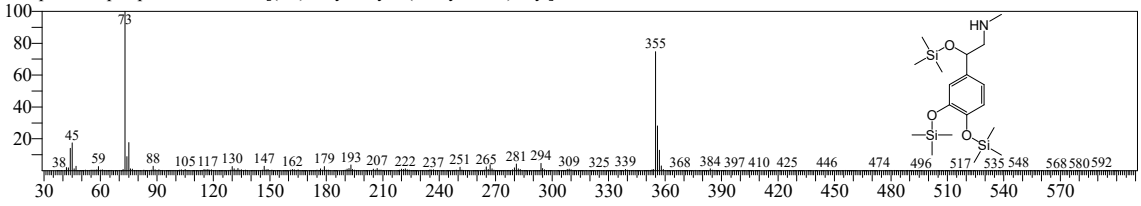
Hit#:2 Entry:173 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C15H30O3Si3 CAS:87-66-1 MolWeight:342 RetIndex:1559
CompName:Pyrogallol-3TMS ; benzene-1,2,3-triol



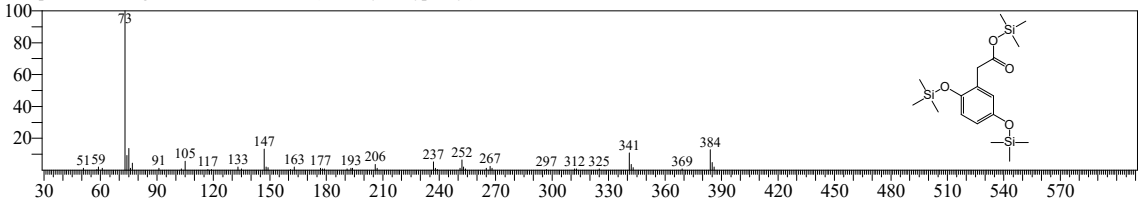
Hit#:3 Entry:491 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244
CompName:Stearic acid-TMS ; octadecanoic acid



Hit#:4 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

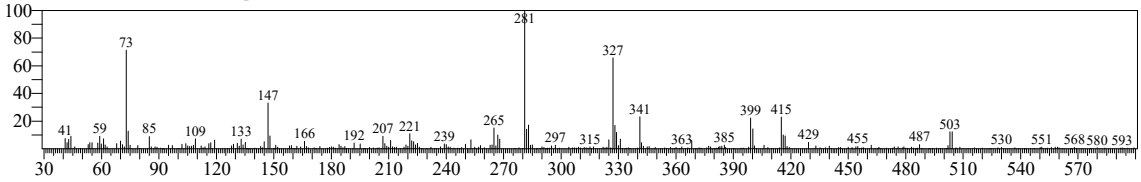


Hit#:5 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid

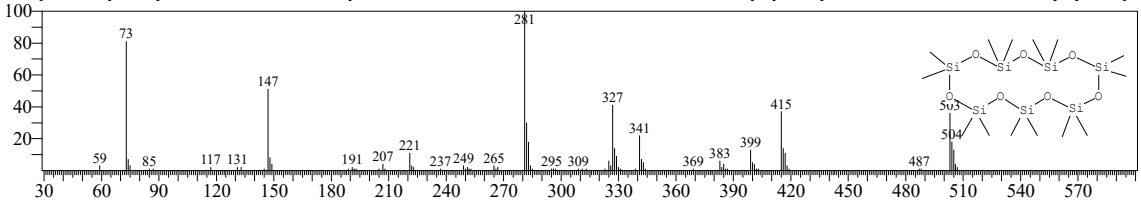


TNAU

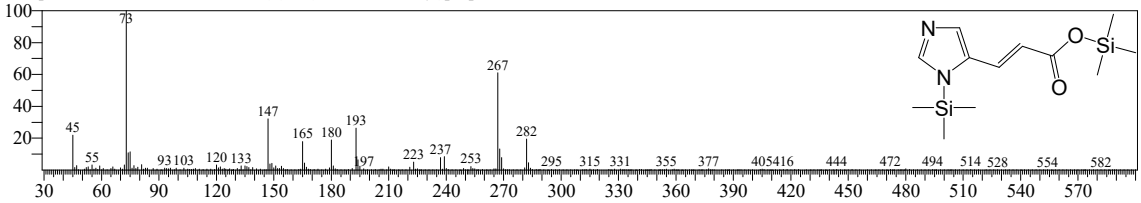
<< Target >>
Line#:6 R.Time:14.955(Scan#:2092) MassPeaks:306
RawMode:Averaged 14.950-14.960(2091-2093) BasePeak:281.00(1703)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



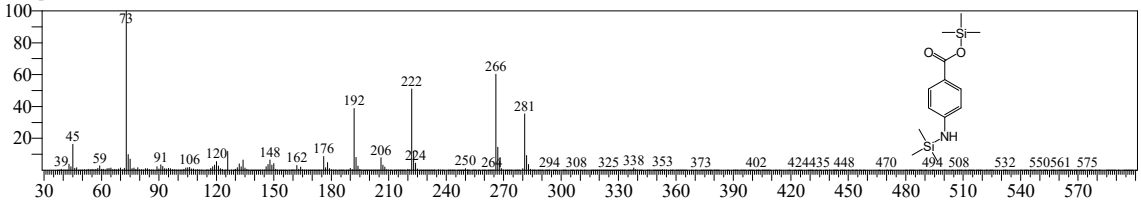
Hit#:1 Entry:43264 Library:NIST20R.lib
SI:78 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohept



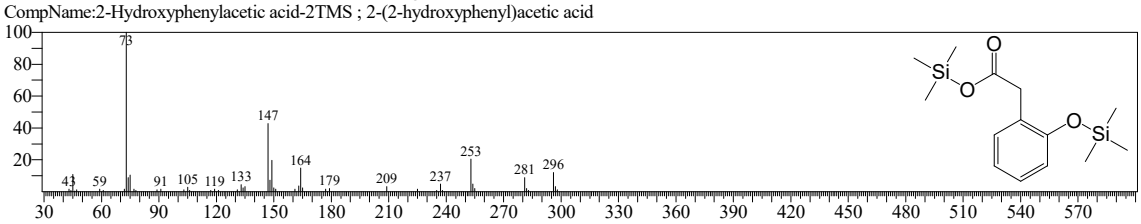
Hit#:2 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



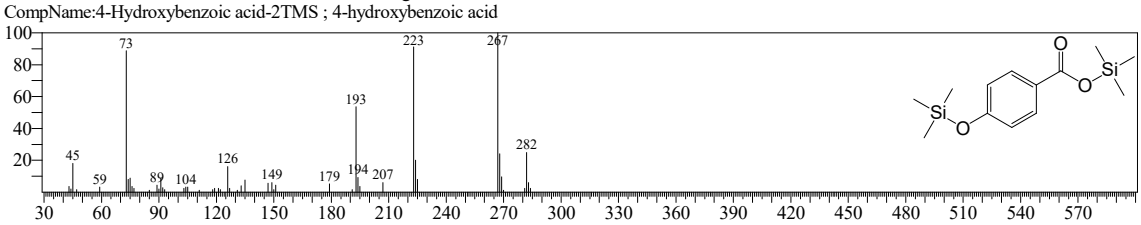
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

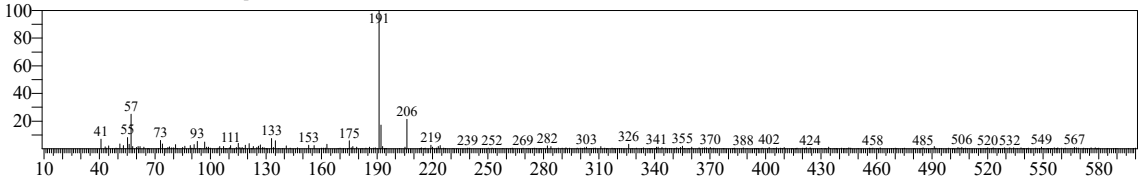


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

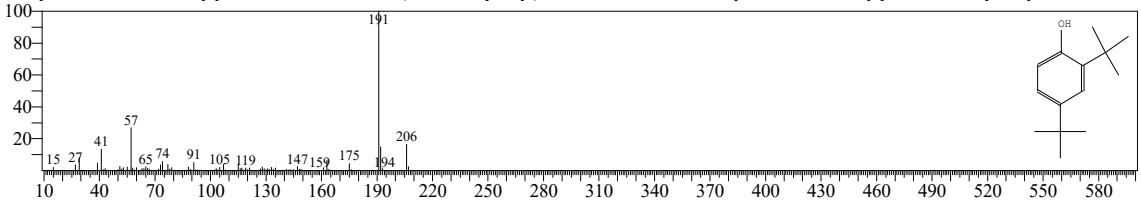


TNAU

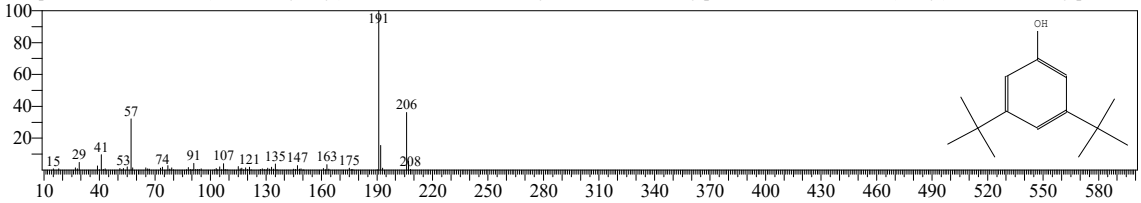
<< Target >>
Line#:7 R.Time:15.470(Scan#:2195) MassPeaks:287
RawMode:Averaged 15.465-15.475(2194-2196) BasePeak:191.10(4177)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



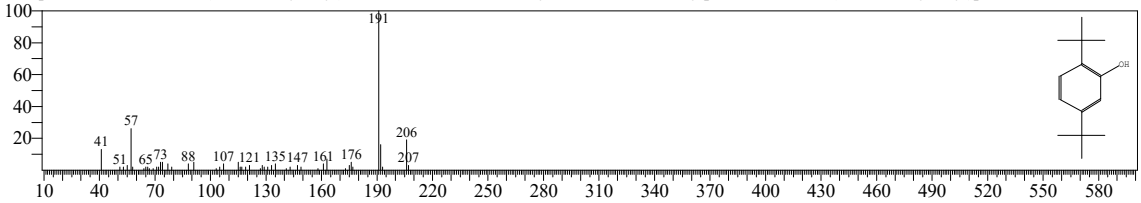
Hit#:1 Entry:24086 Library:NIST20R.lib
SI:79 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



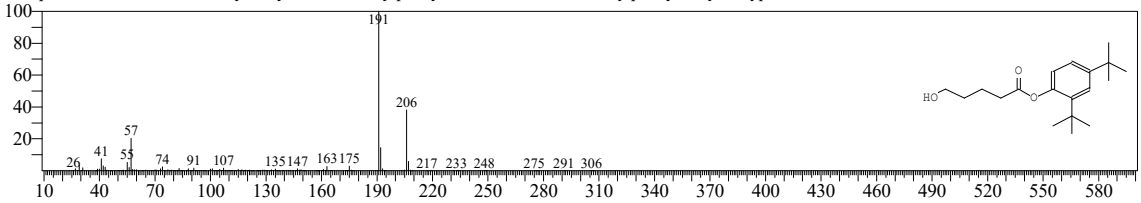
Hit#:2 Entry:24110 Library:NIST20R.lib
SI:78 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



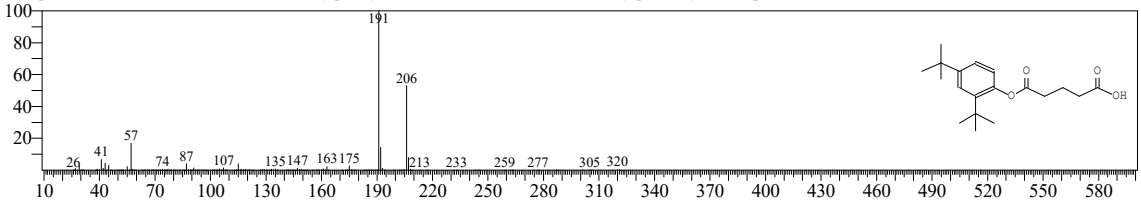
Hit#:3 Entry:24098 Library:NIST20R.lib
SI:77 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol



Hit#:4 Entry:170993 Library:NIST20M1.lib
SI:77 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #

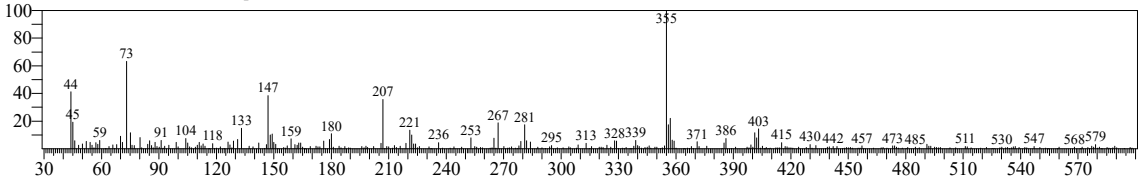


Hit#:5 Entry:187279 Library:NIST20M1.lib
SI:77 Formula:C19H28O4 CAS:0-00-0 MolWeight:320 RetIndex:2369
CompName:Pentanedioic acid, (2,4-di-t-butylphenyl) mono-ester $$ 5-(2,4-Ditert-butylphenoxy)-5-oxopentanoic acid #

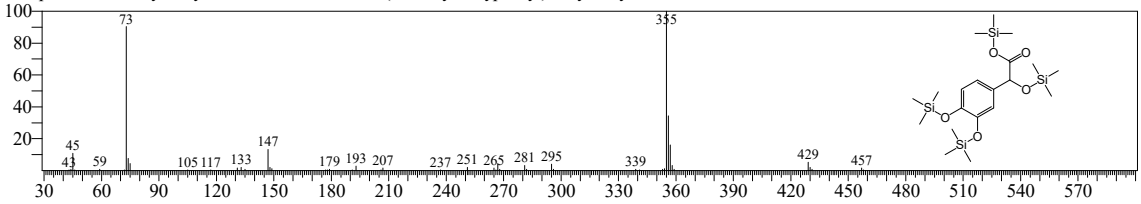


TNAU

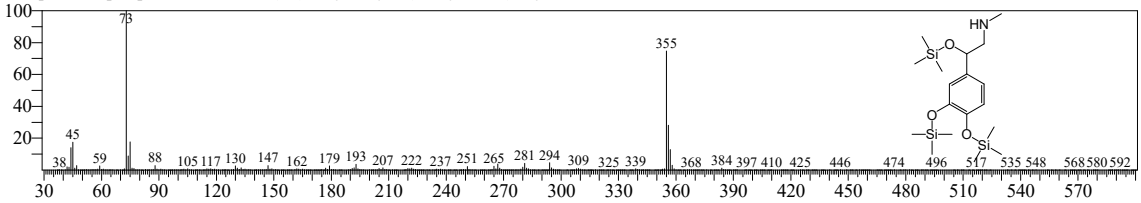
<< Target >>
Line#:8 R.Time:16.915(Scan#:2484) MassPeaks:312
RawMode:Averaged 16.910-16.920(2483-2485) BasePeak:355.05(1425)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



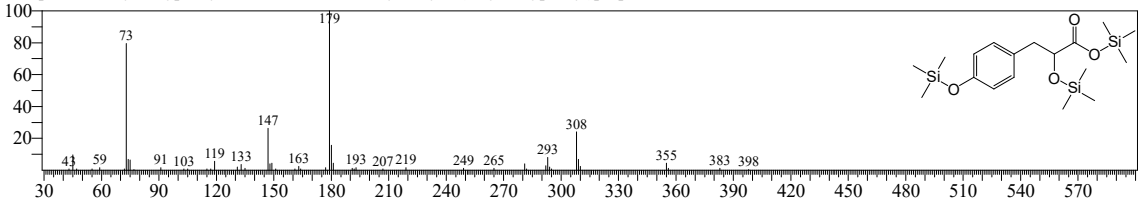
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:64 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



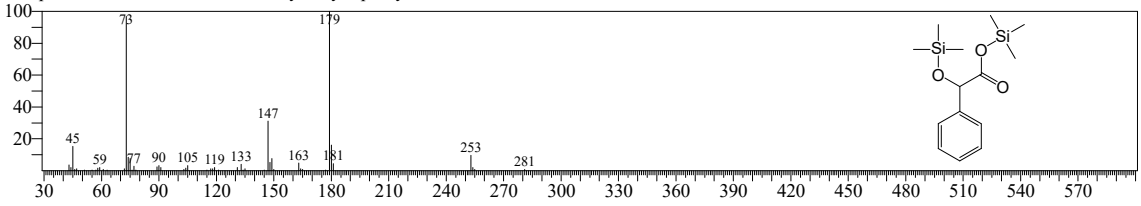
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:63 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



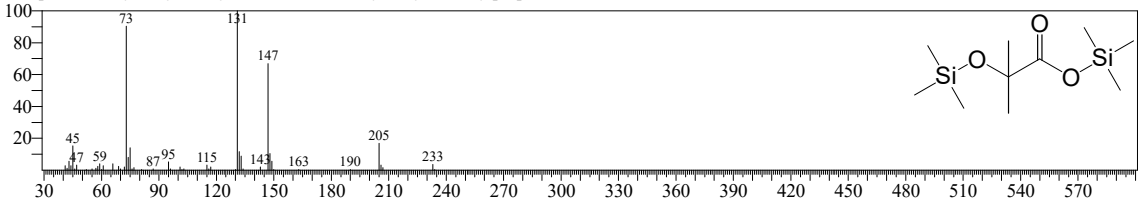
Hit#:3 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:4 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid

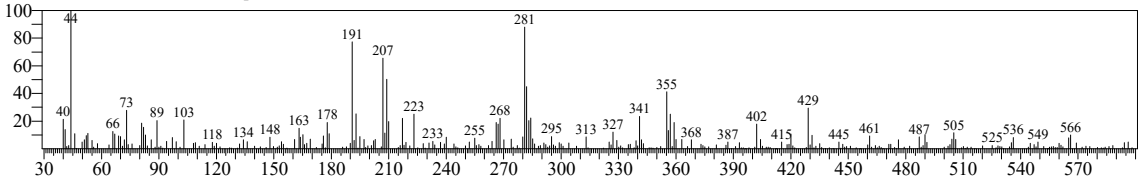


Hit#:5 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

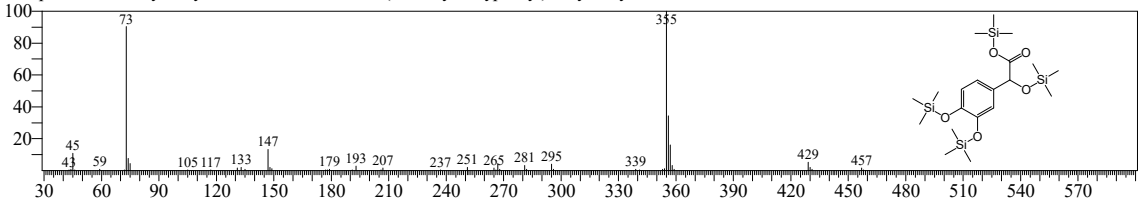


TNAU

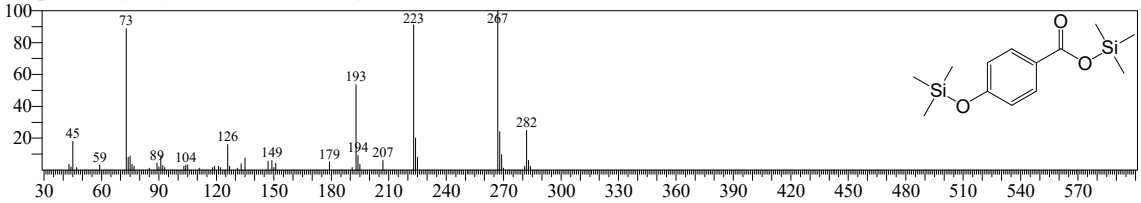
<< Target >>
Line#:9 R.Time:27.970(Scan#:4695) MassPeaks:305
RawMode:Averaged 27.965-27.975(4694-4696) BasePeak:44.00(1030)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



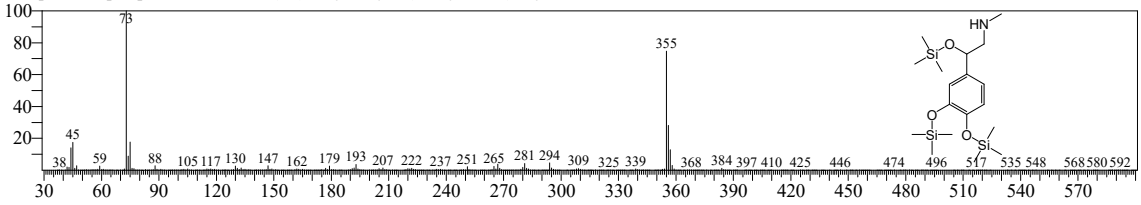
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



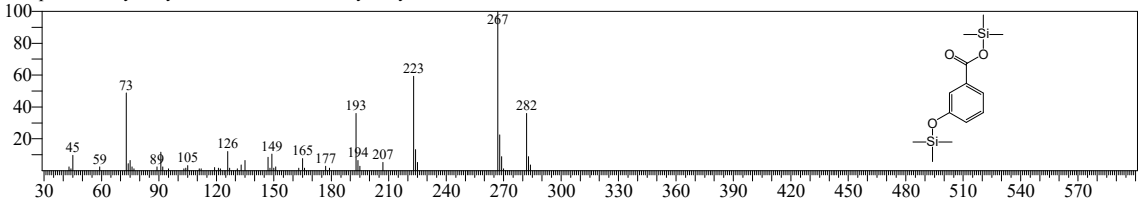
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



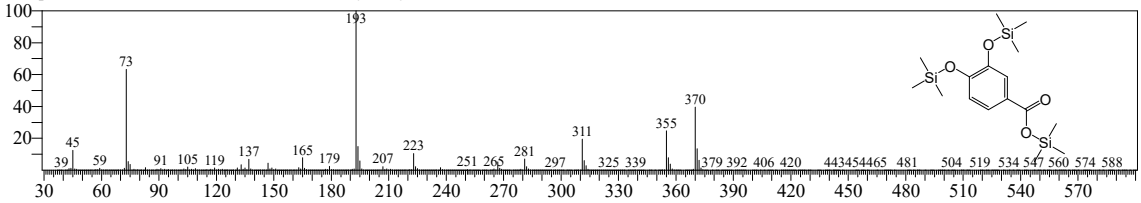
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry: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

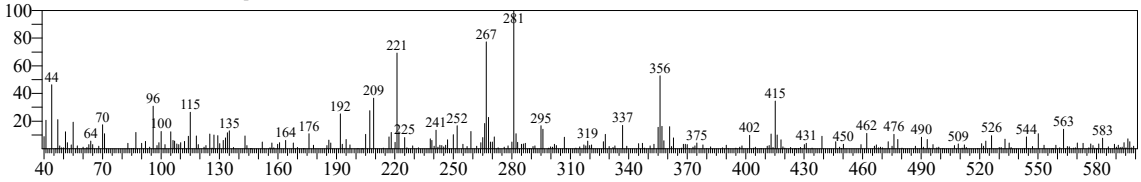


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

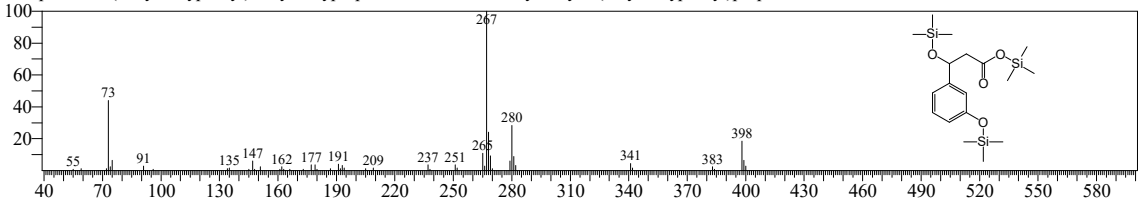


TNAU

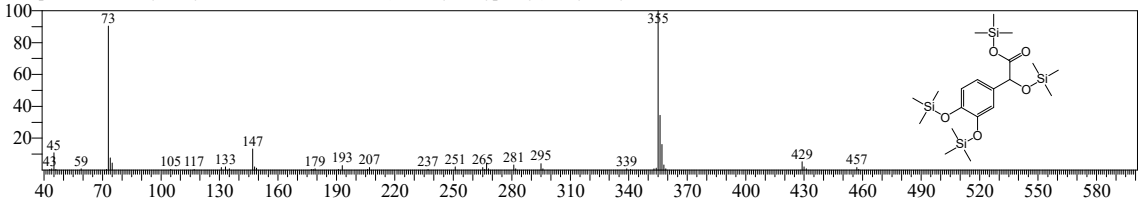
<< Target >>
Line#:10 R.Time:28.455(Scan#:4792) MassPeaks:279
RawMode:Averaged 28.450-28.460(4791-4793) BasePeak:281.00(894)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



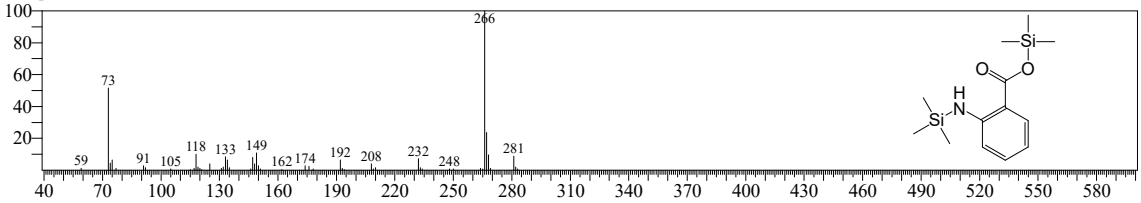
Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



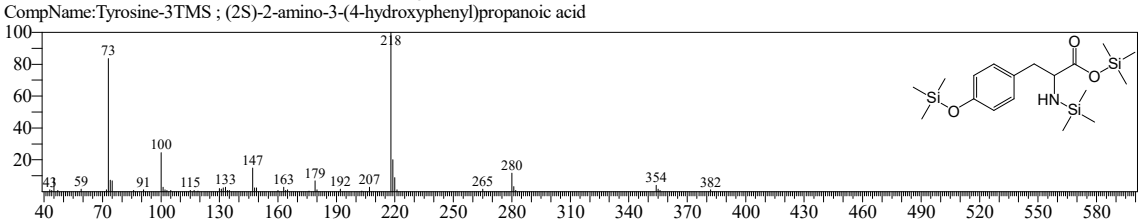
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



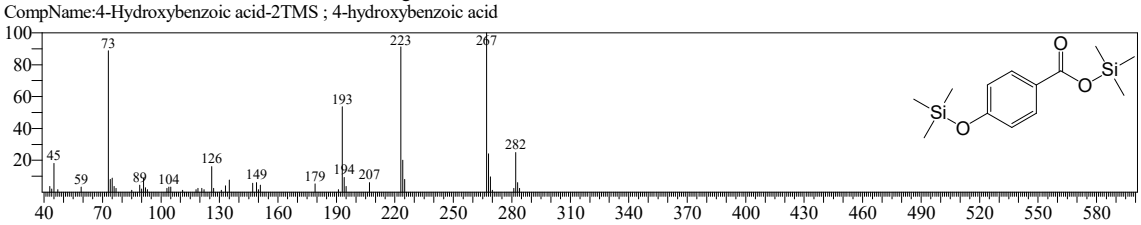
Hit#:3 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



Hit#:4 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

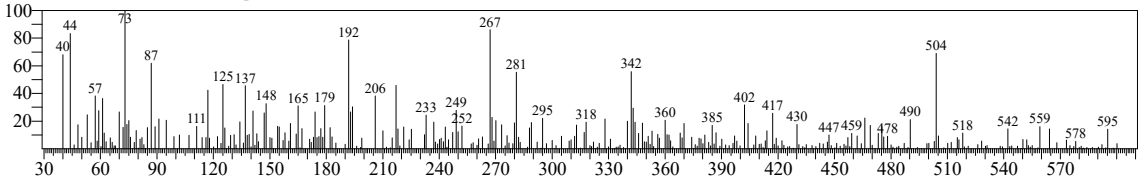


Hit#:5 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

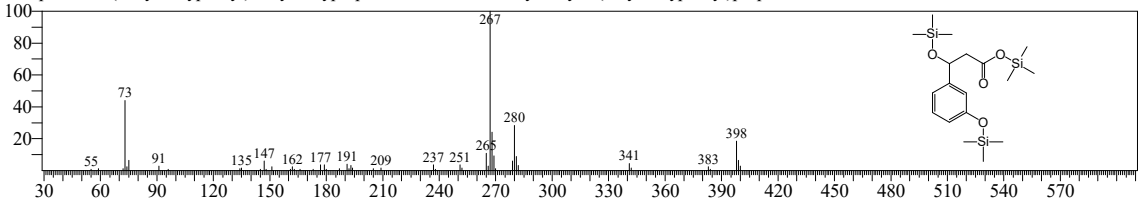


TNAU

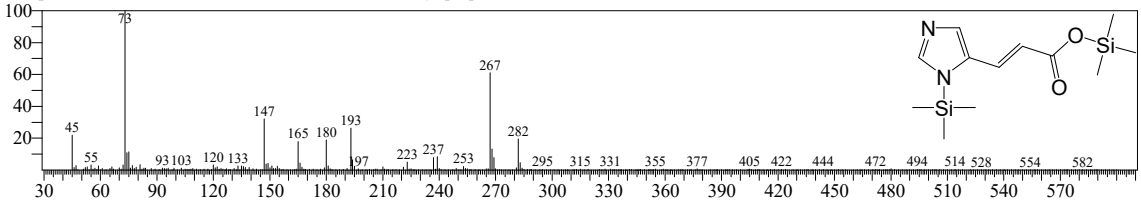
<< Target >>
Line#:11 R.Time:28.515(Scan#:4804) MassPeaks:320
RawMode:Averaged 28.510-28.520(4803-4805) BasePeak:73.05(428)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



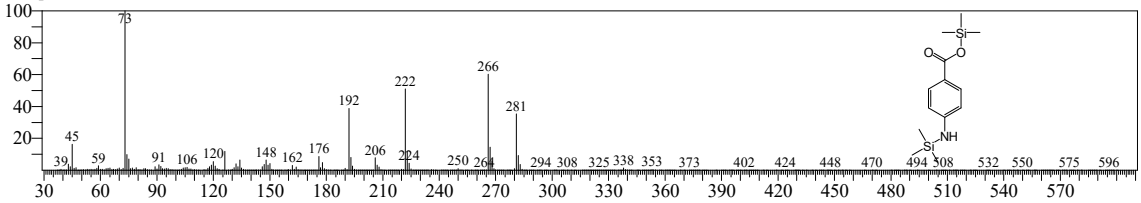
Hit#:1 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid



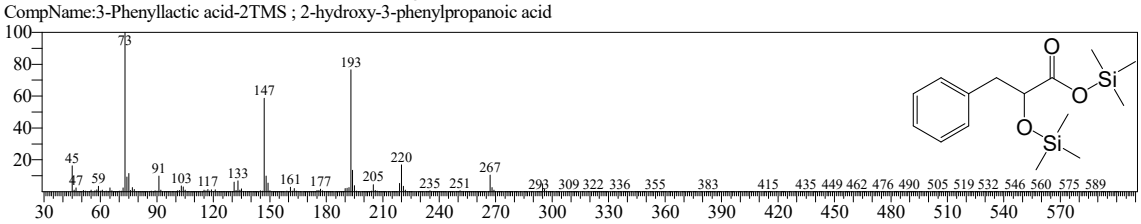
Hit#:2 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid



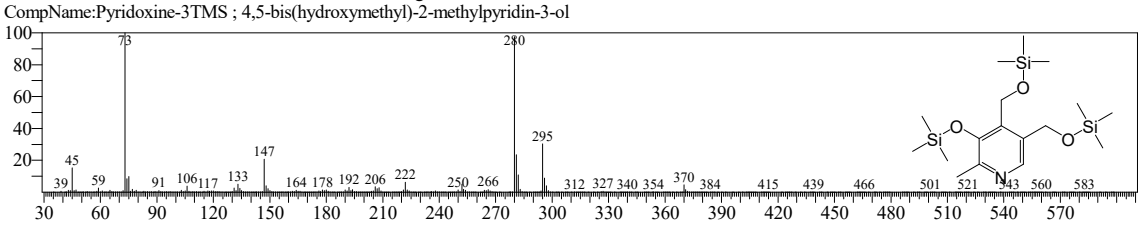
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

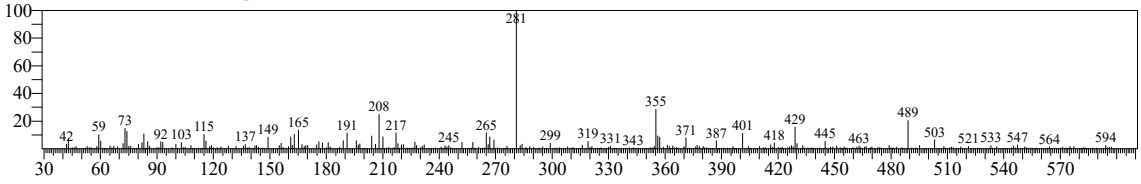


Hit#:5 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol

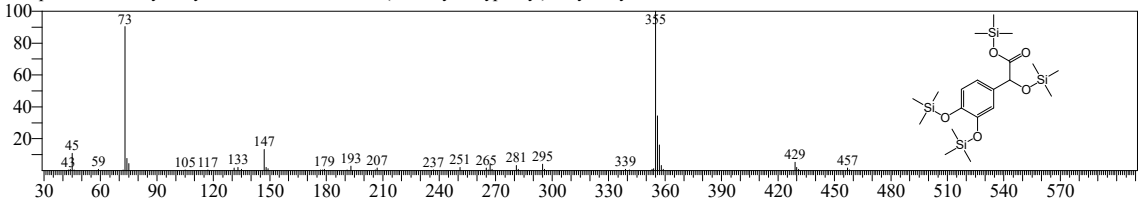


TNAU

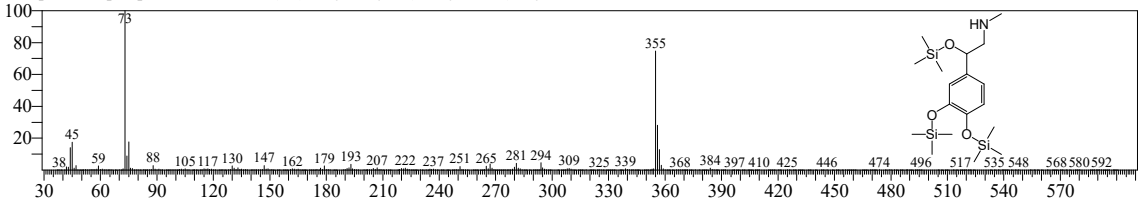
<< Target >>
Line#:12 R.Time:28.625(Scan#:4826) MassPeaks:315
RawMode:Averaged 28.620-28.630(4825-4827) BasePeak:281.05(2242)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



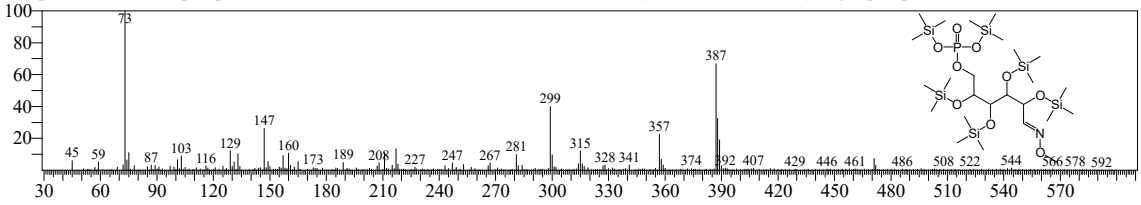
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



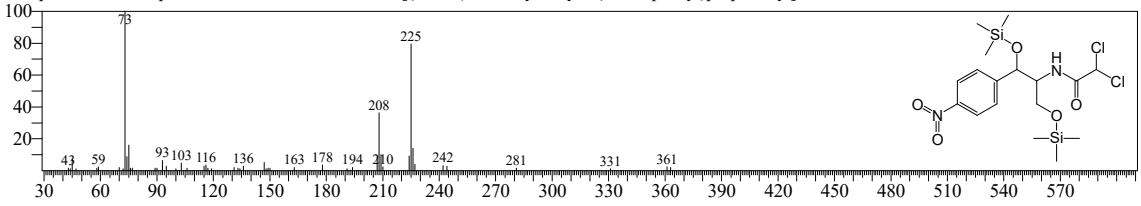
Hit#:2 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



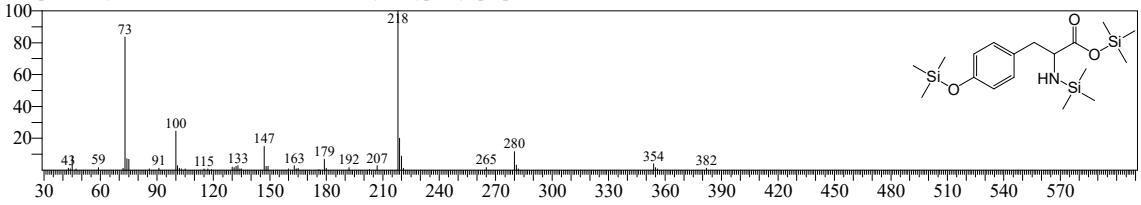
Hit#:3 Entry:507 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C25H64NO9PSi6 CAS:3672-15-9 MolWeight:721 RetIndex:2377
CompName:Mannose 6-phosphate-meto-6TMS(2) ; [(2R,3S,4S,5S)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl dihydrogen phosphate



Hit#:4 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

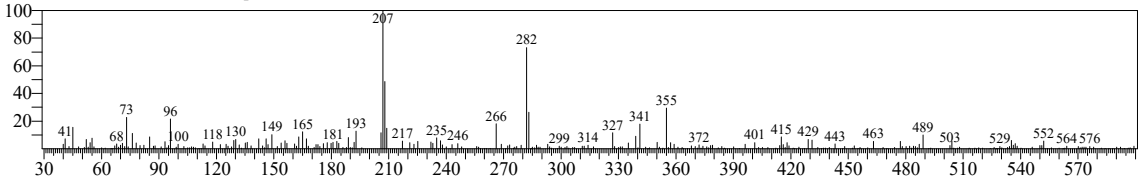


Hit#:5 Entry:413 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C18H35NO3Si3 CAS:60-18-4 MolWeight:397 RetIndex:1958
CompName:Tyrosine-3TMS ; (2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid

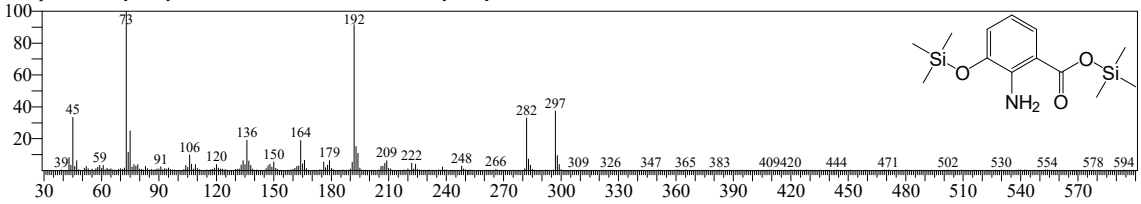


TNAU

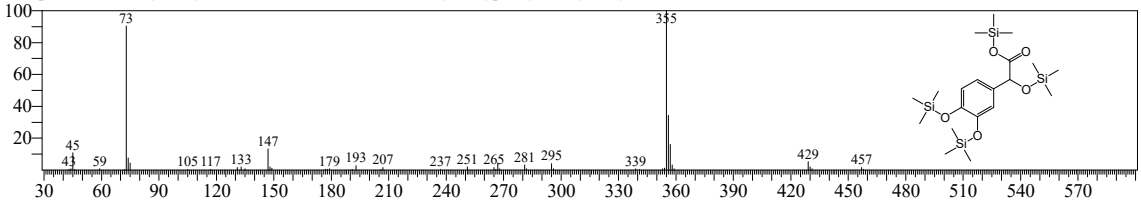
<< Target >>
Line#:13 R.Time:28.905(Scan#:4882) MassPeaks:285
RawMode:Averaged 28.900-28.910(4881-4883) BasePeak:207.05(1582)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



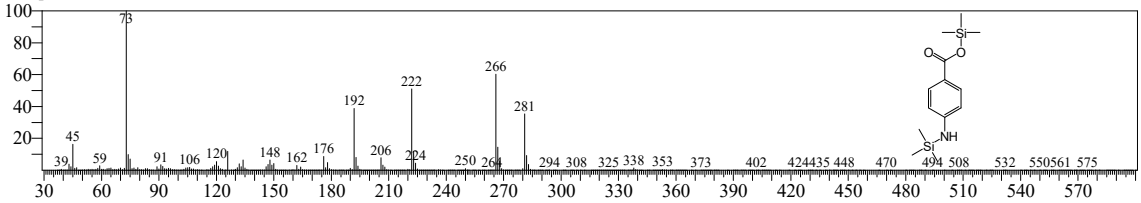
Hit#:1 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



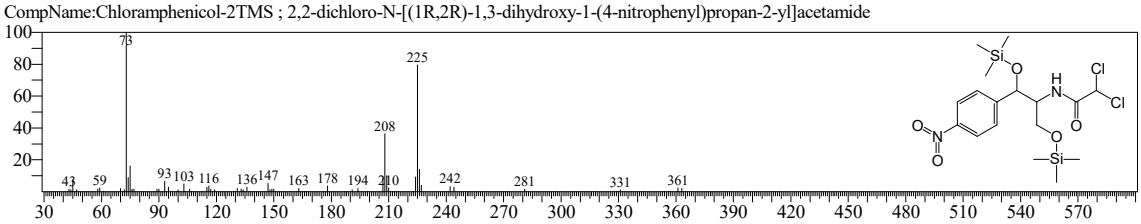
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



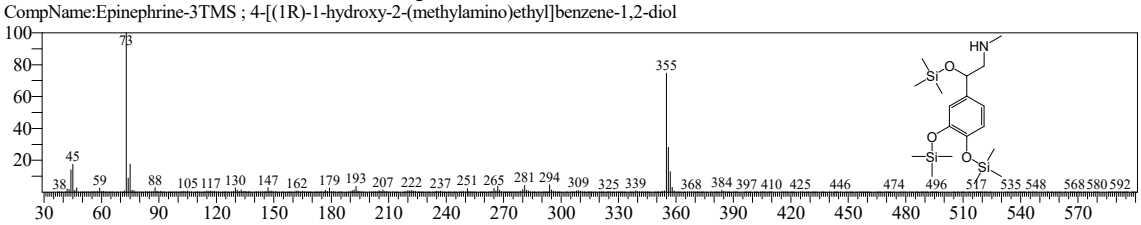
Hit#:3 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



Hit#:4 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:34 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

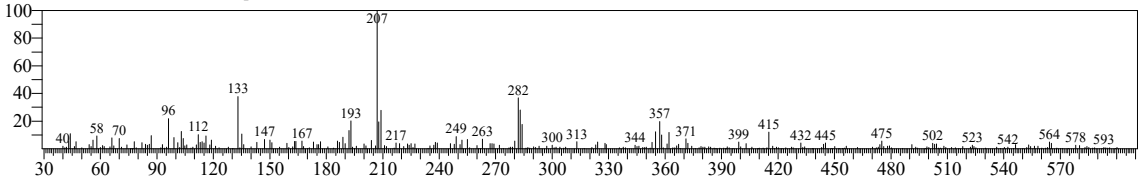


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

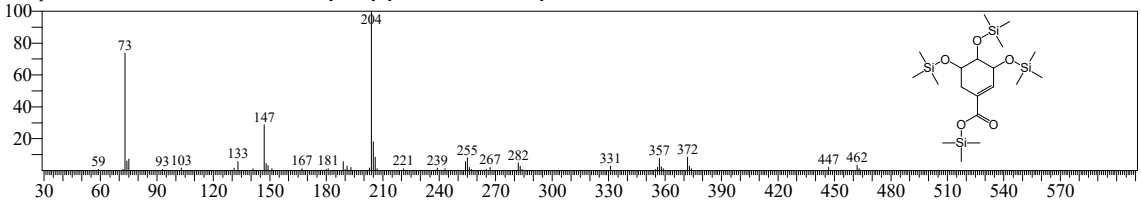


TNAU

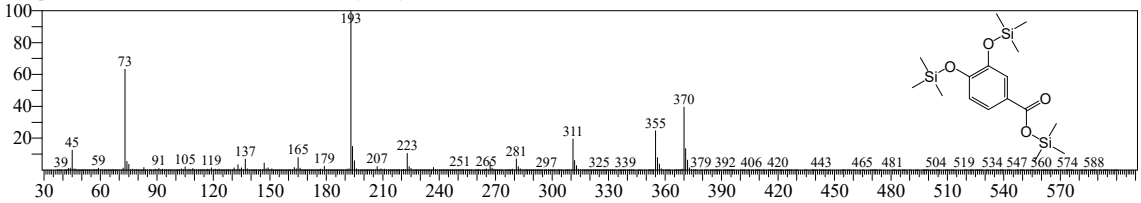
<< Target >>
Line#:14 R.Time:29.010(Scan#:4903) MassPeaks:295
RawMode:Averaged 29.005-29.015(4902-4904) BasePeak:207.05(1681)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



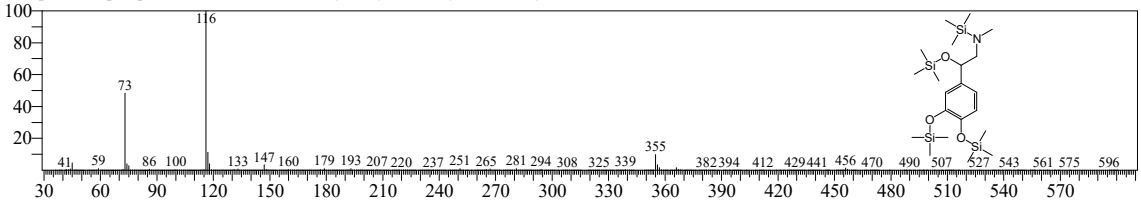
Hit#:1 Entry:308 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C19H42O5Si4 CAS:138-59-0 MolWeight:462 RetIndex:1819
CompName:Shikimic acid-4TMS ; 3,4,5-trihydroxycyclohexene-1-carboxylic acid



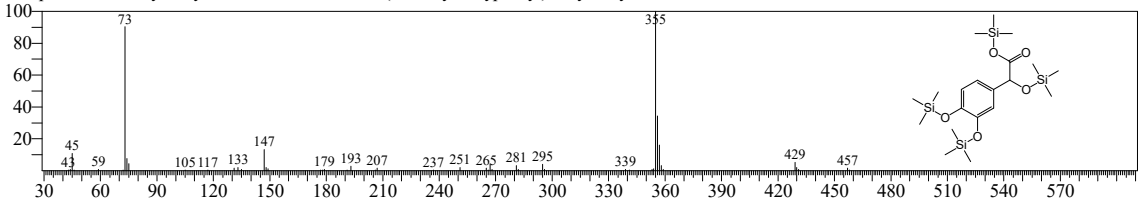
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



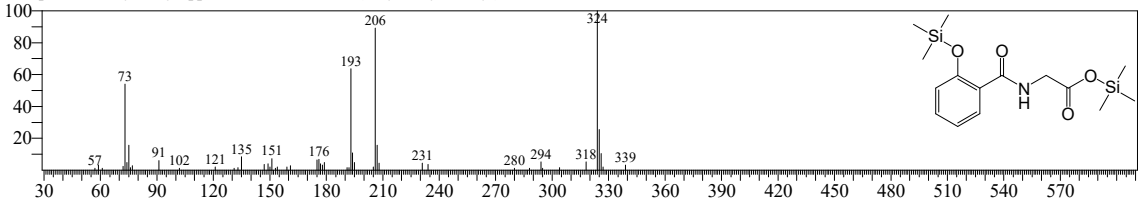
Hit#:3 Entry:431 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C21H45NO3Si4 CAS:51-43-4 MolWeight:471 RetIndex:1989
CompName:Epinephrine-4TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

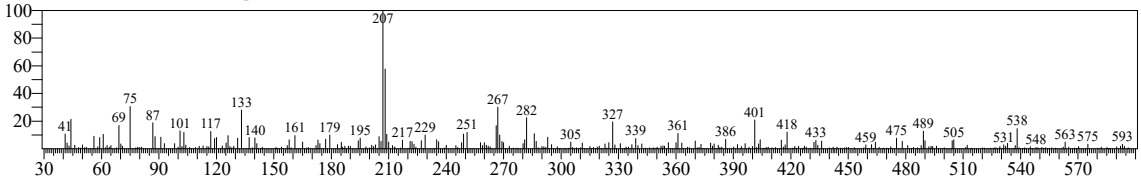


Hit#:5 Entry:452 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C15H25NO4Si2 CAS:487-54-7 MolWeight:339 RetIndex:2086
CompName:2-Hydroxyhippuric acid-2TMS ; 2-[(2-hydroxybenzoyl)amino]acetic acid

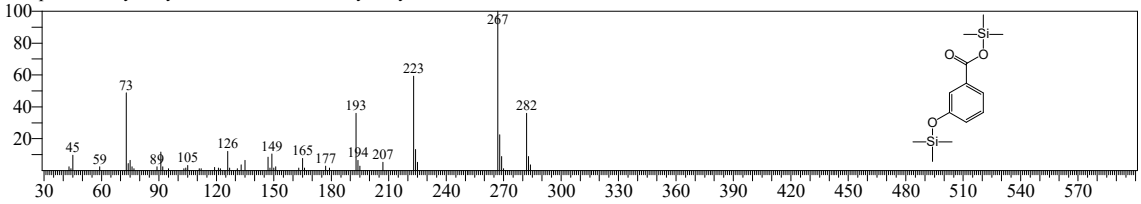


TNAU

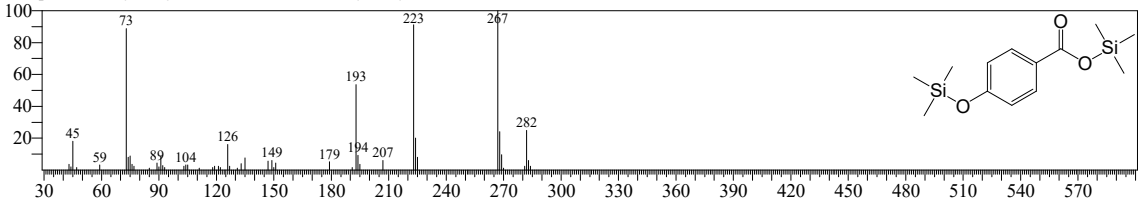
<< Target >>
Line#:15 R.Time:29.150(Scan#:4931) MassPeaks:312
RawMode:Averaged 29.145-29.155(4930-4932) BasePeak:207.05(1376)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



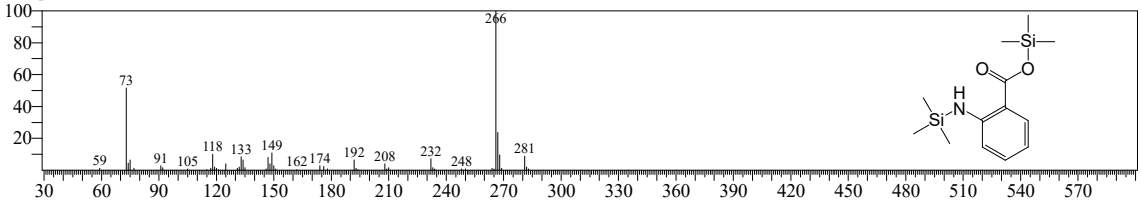
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



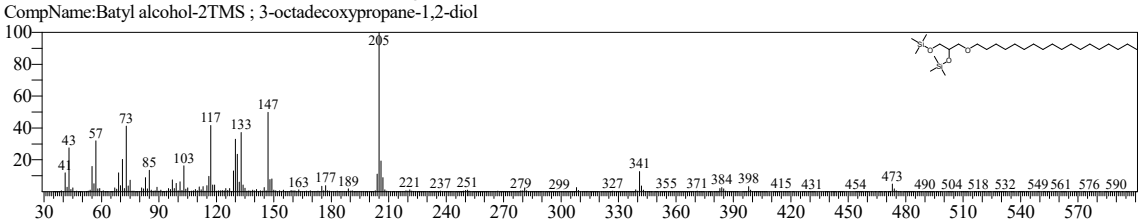
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



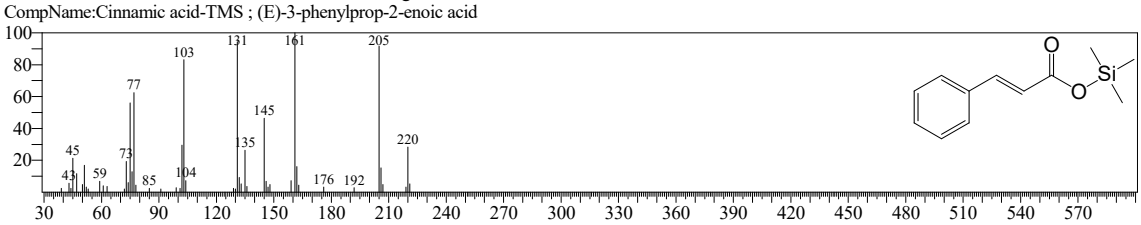
Hit#:3 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid



Hit#:4 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:29 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol

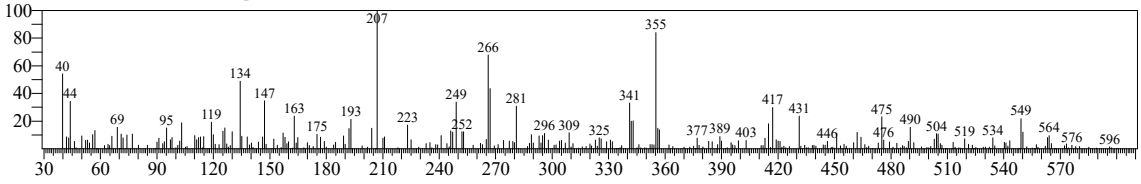


Hit#:5 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid

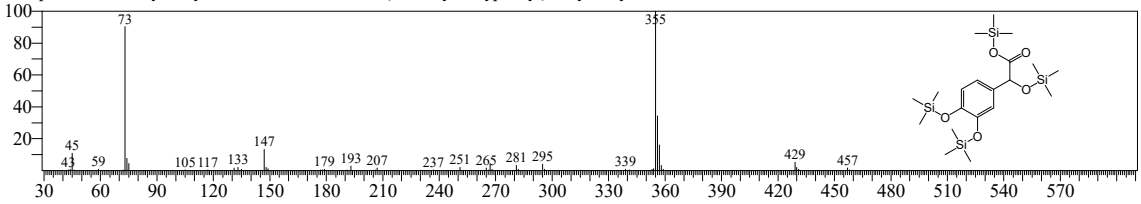


TNAU

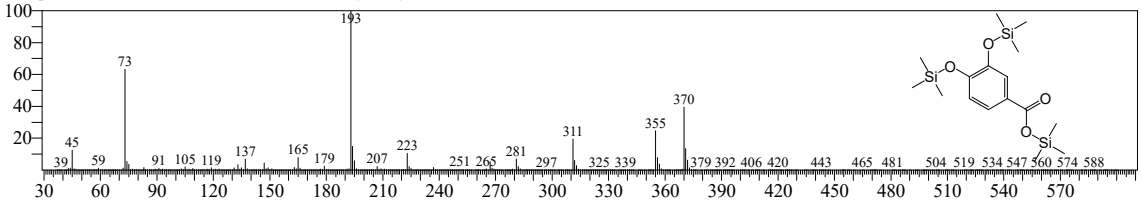
<< Target >>
Line#:16 R.Time:29.570(Scan#:5015) MassPeaks:308
RawMode:Averaged 29.565-29.575(5014-5016) BasePeak:207.05(991)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



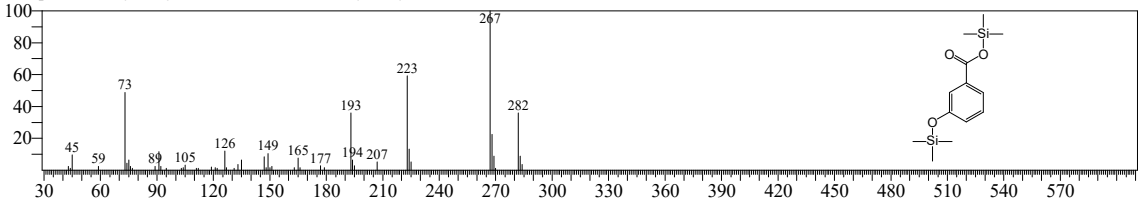
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



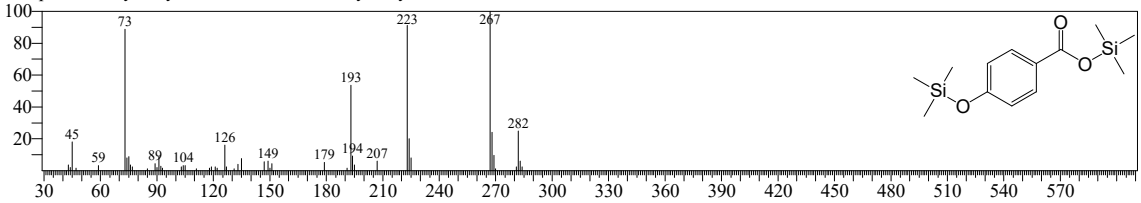
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



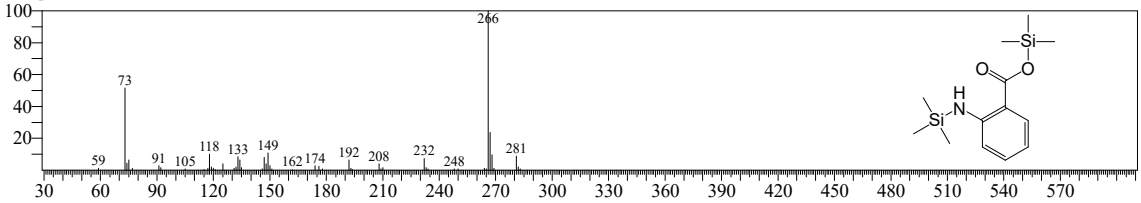
Hit#:3 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



Hit#:4 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid

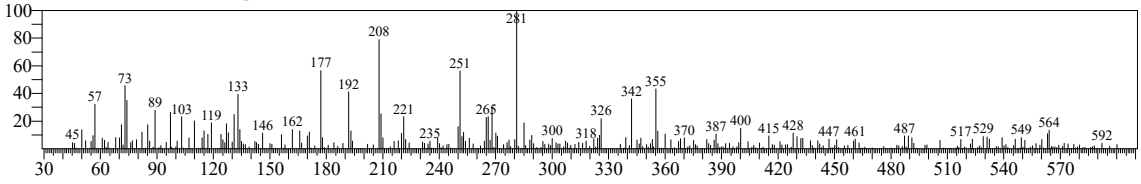


Hit#:5 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

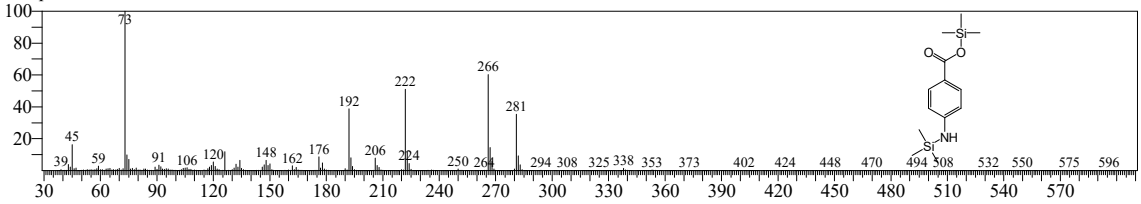


TNAU

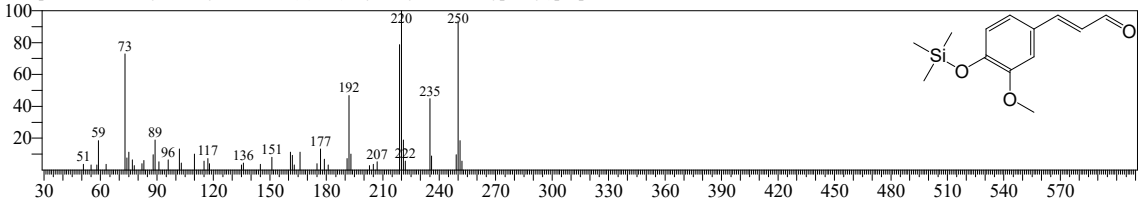
<< Target >>
Line#:17 R.Time:29.895(Scan#:5080) MassPeaks:323
RawMode:Averaged 29.890-29.900(5079-5081) BasePeak:281.10(822)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



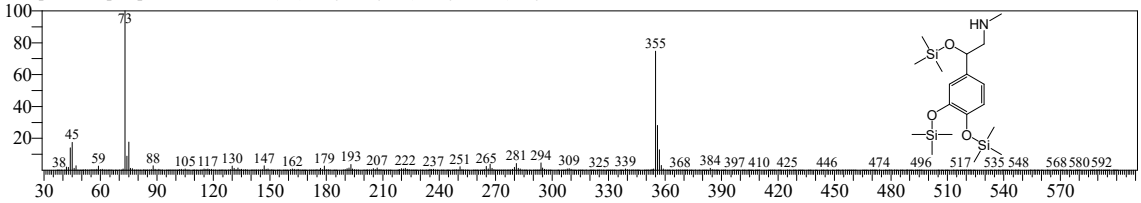
Hit#:1 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid



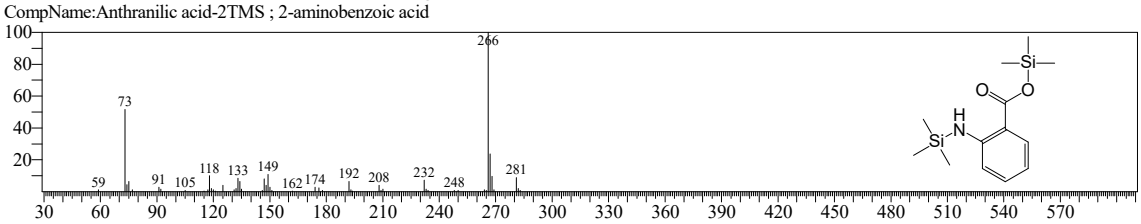
Hit#:2 Entry:339 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H18O3Si CAS:458-36-6 MolWeight:250 RetIndex:1859
CompName:Coniferyl aldehyde-TMS ; (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal



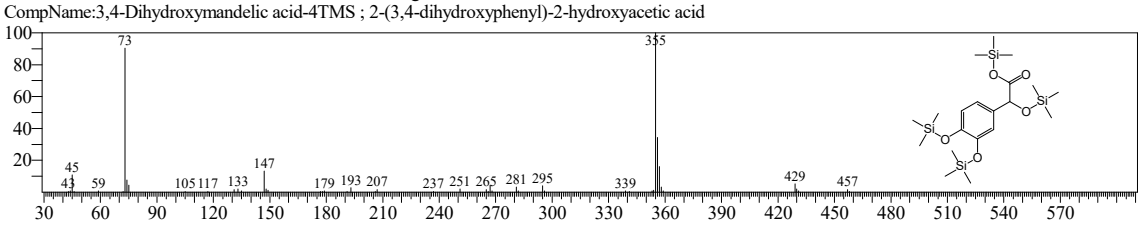
Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

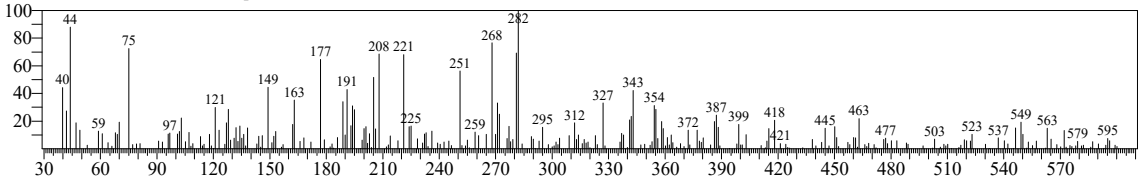


Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

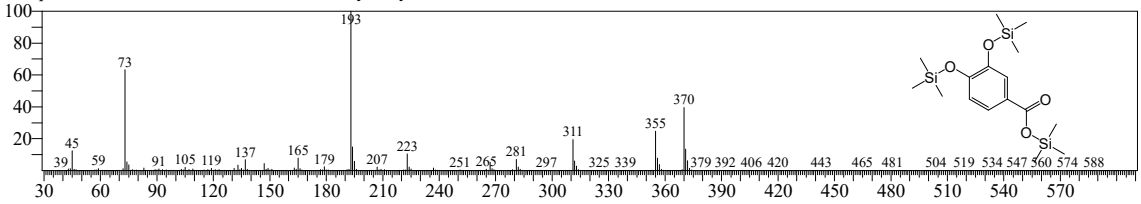


TNAU

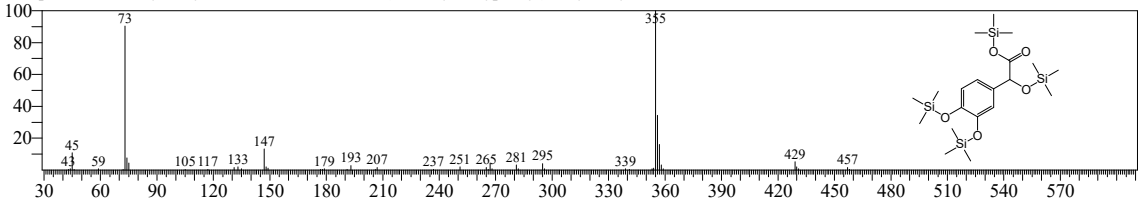
<< Target >>
Line#:18 R.Time:30.370(Scan#:5175) MassPeaks:275
RawMode:Averaged 30.365-30.375(5174-5176) BasePeak:282.05(456)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



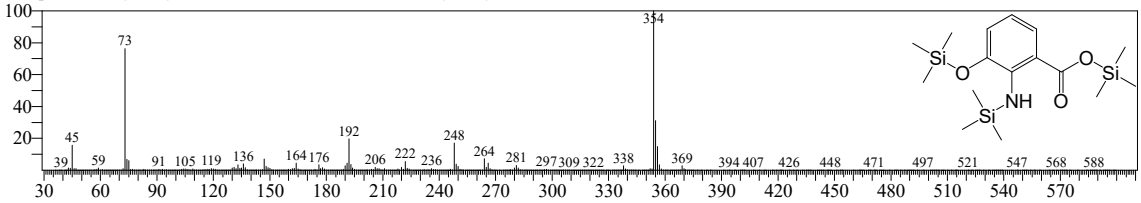
Hit#:1 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



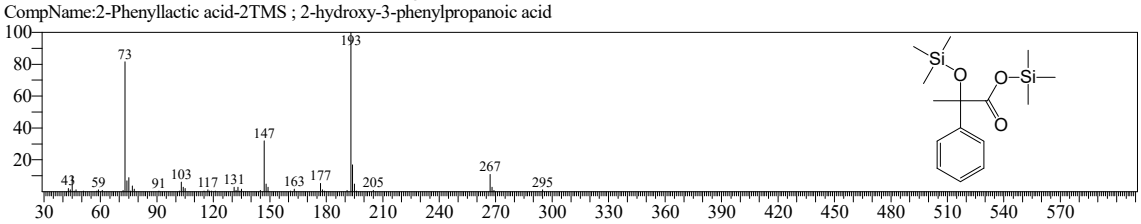
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



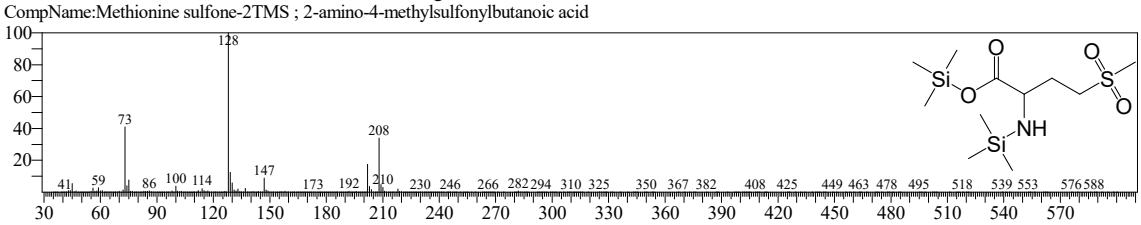
Hit#:3 Entry:354 Library:OA_TMS_DB5_67min_V3.lib
SI:24 Formula:C16H31NO3Si3 CAS:548-93-6 MolWeight:369 RetIndex:1886
CompName:3-Hydroxyanthranilic acid-3TMS ; 2-amino-3-hydroxybenzoic acid



Hit#:4 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:23 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid

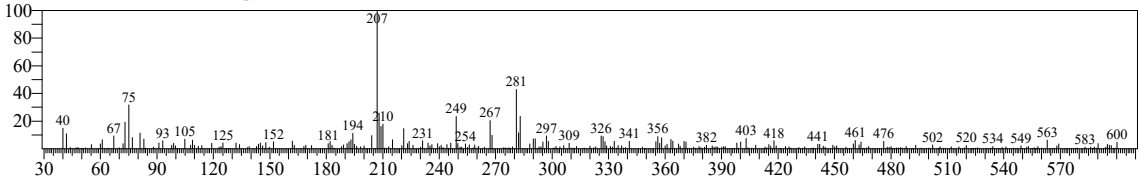


Hit#:5 Entry:329 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C11H27NO4SSi2 CAS:820-10-0 MolWeight:325 RetIndex:1848
CompName:Methionine sulfone-2TMS ; 2-amino-4-methylsulfonylbutanoic acid

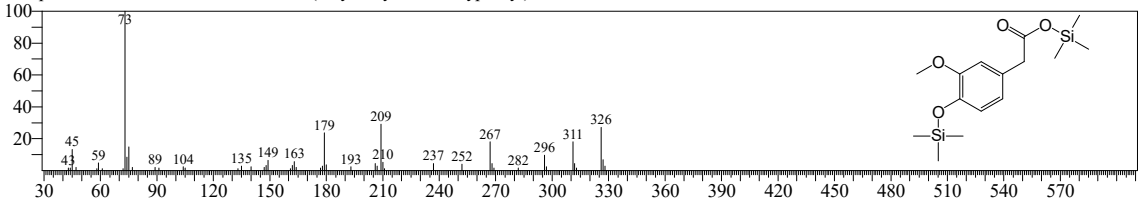


TNAU

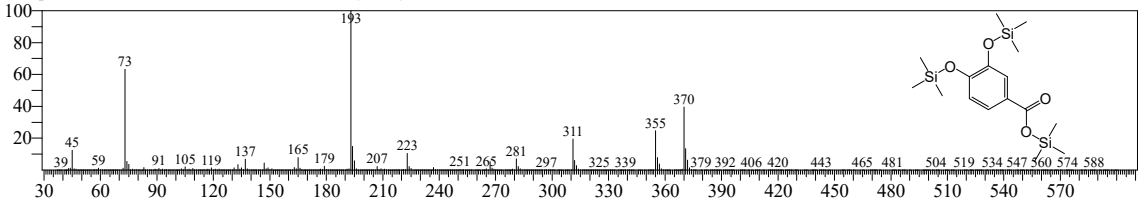
<< Target >>
Line#:19 R.Time:30.460(Scan#:5193) MassPeaks:293
RawMode:Averaged 30.455-30.465(5192-5194) BasePeak:207.00(1917)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



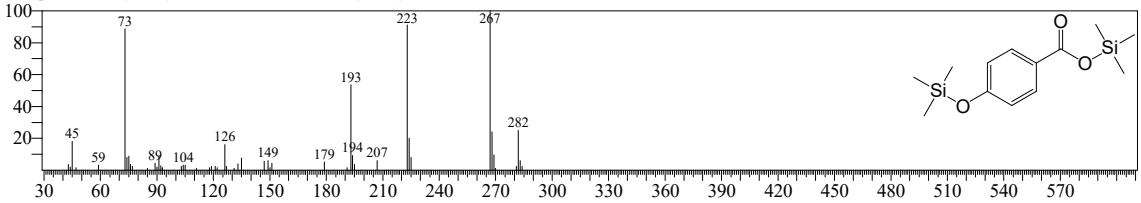
Hit#:1 Entry:294 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O4Si2 CAS:306-08-1 MolWeight:326 RetIndex:1782
CompName:Homovanillic acid-2TMS ; 2-(4-hydroxy-3-methoxyphenyl)acetic acid



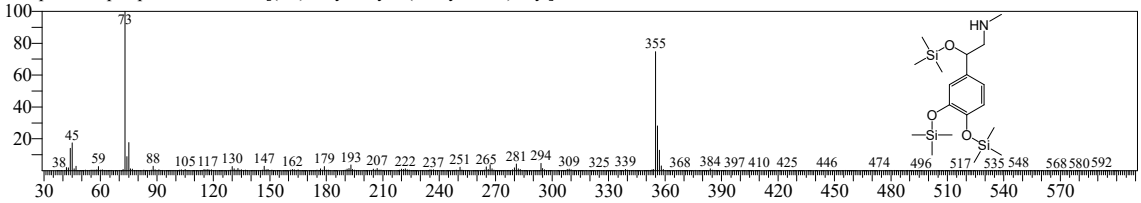
Hit#:2 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



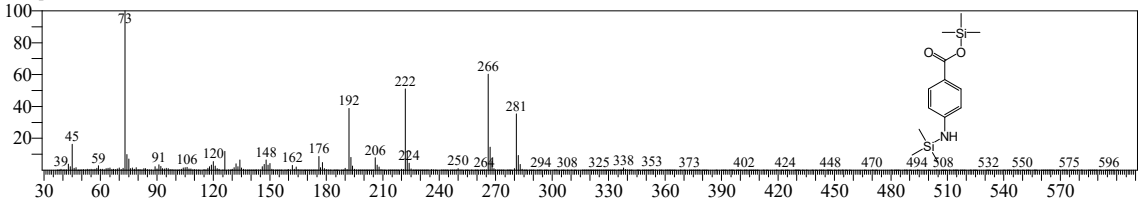
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 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

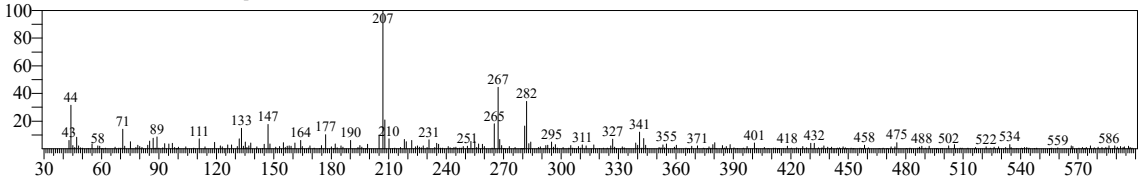


Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid

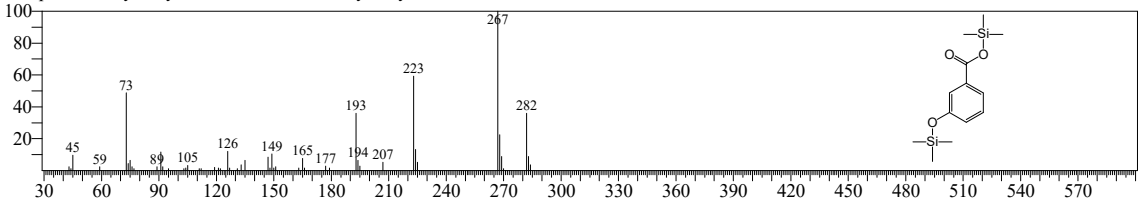


TNAU

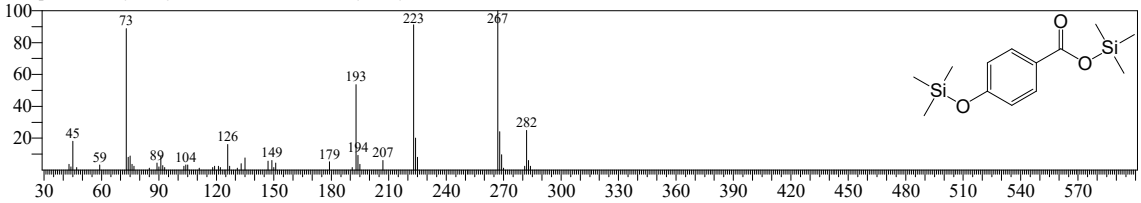
<< Target >>
Line#:20 R.Time:31.445(Scan#:5390) MassPeaks:301
RawMode:Averaged 31.440-31.450(5389-5391) BasePeak:207.00(2262)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



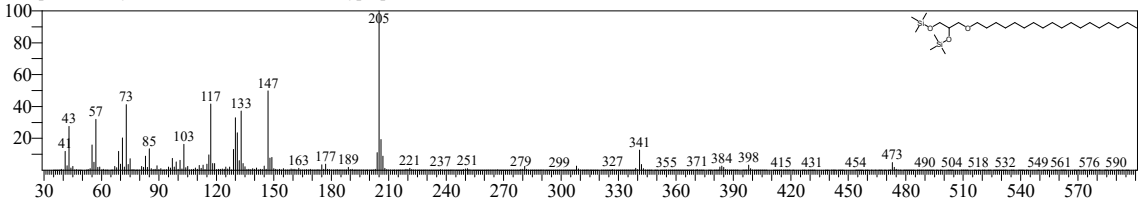
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



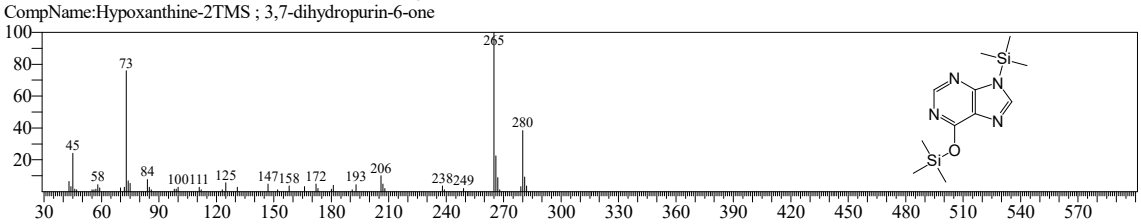
Hit#:2 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



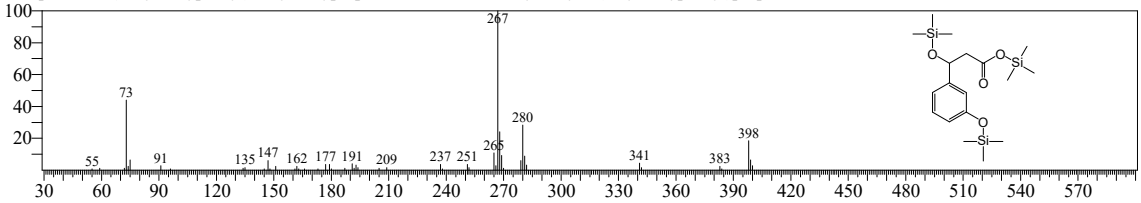
Hit#:3 Entry:539 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684
CompName:Batyl alcohol-2TMS ; 3-octadecoxypropane-1,2-diol



Hit#: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

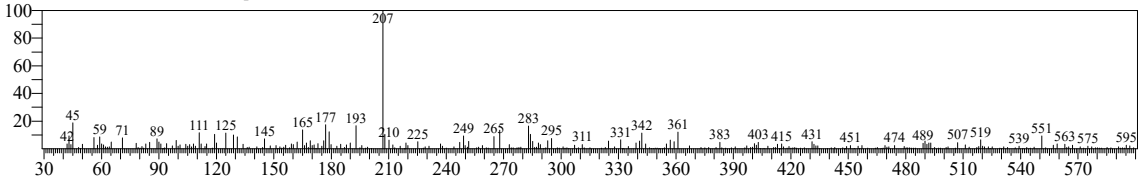


Hit#:5 Entry:341 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C18H34O4Si3 CAS:3247-75-4 MolWeight:398 RetIndex:1864
CompName:3-(3-Hydroxyphenyl)-3-hydroxypropionic acid-3TMS ; 3-hydroxy-3-(3-hydroxyphenyl)propanoic acid

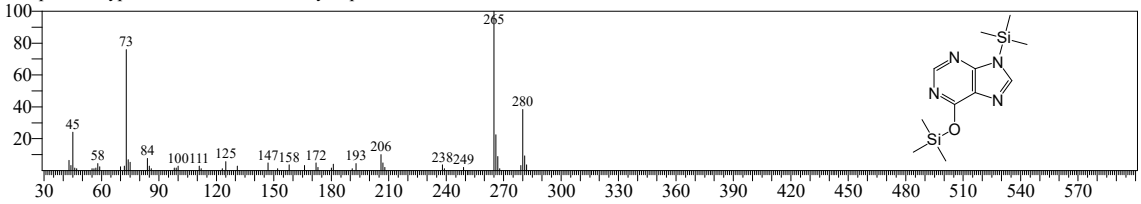


TNAU

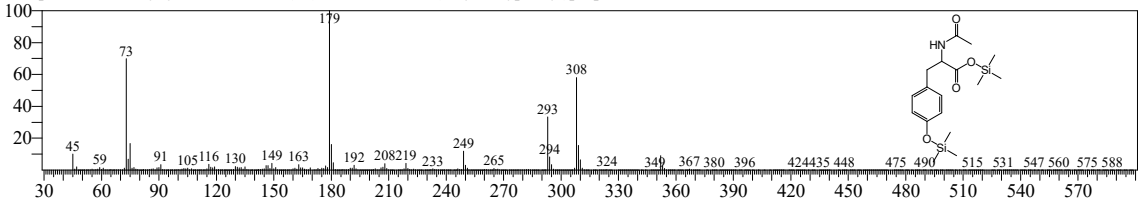
<< Target >>
Line#:21 R.Time:31.755(Scan#:5452) MassPeaks:296
RawMode:Averaged 31.750-31.760(5451-5453) BasePeak:207.05(1869)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



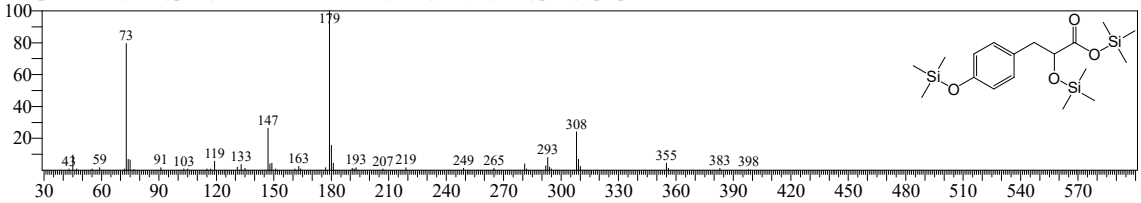
Hit#:1 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



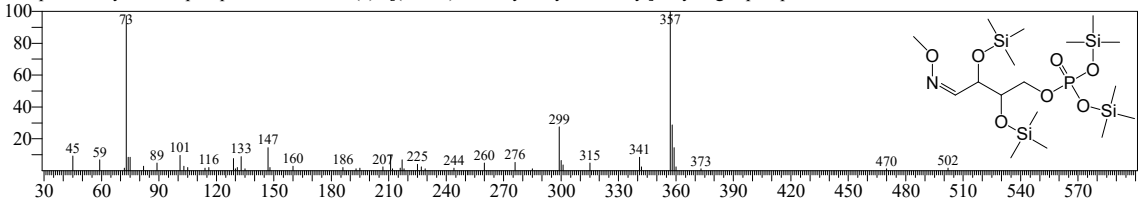
Hit#:2 Entry:474 Library:OA_TMS_DB5_67min_V3.lib
SI:28 Formula:C17H29NO4Si2 CAS:537-55-3 MolWeight:367 RetIndex:2148
CompName:N-Acetyltyrosine-2TMS ; (2S)-2-acetamido-3-(4-hydroxyphenyl)propanoic acid



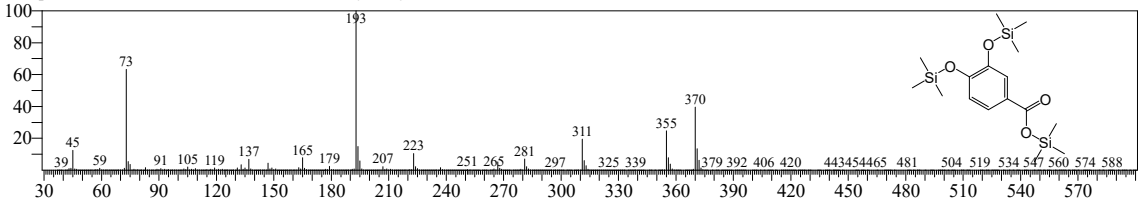
Hit#:3 Entry:382 Library:OA_TMS_DB5_67min_V3.lib
SI:27 Formula:C18H34O4Si3 CAS:6482-98-0 MolWeight:398 RetIndex:1918
CompName:4-Hydroxyphenyllactic acid-3TMS ; 2-hydroxy-3-(4-hydroxyphenyl)propanoate



Hit#:4 Entry:394 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1935
CompName:Erythrose 4-phosphate-meto-4TMS(2) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate

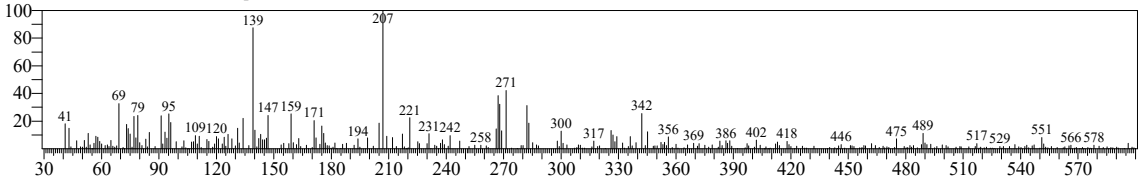


Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:25 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid

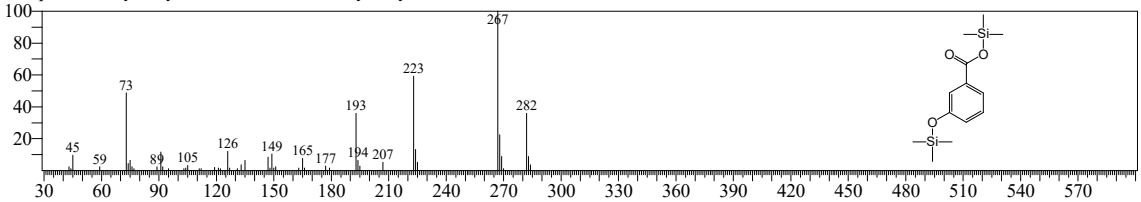


TNAU

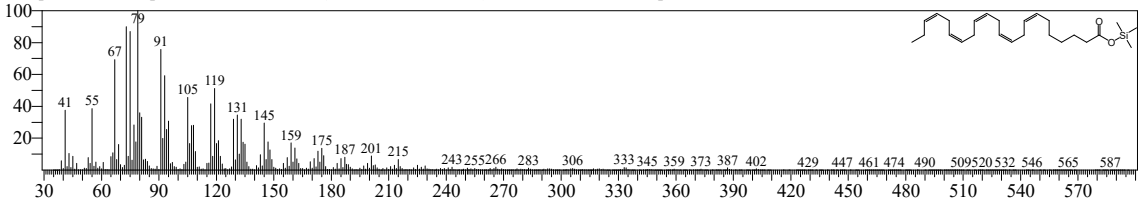
<< Target >>
Line#:22 R.Time:31.910(Scan#:5483) MassPeaks:332
RawMode:Averaged 31.905-31.915(5482-5484) BasePeak:207.05(1294)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



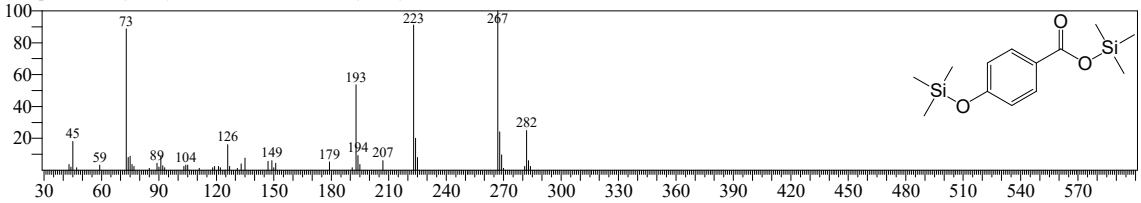
Hit#:1 Entry:179 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H22O3Si2 CAS:99-06-9 MolWeight:282 RetIndex:1572
CompName:3-Hydroxybenzoic acid-2TMS ; 3-hydroxybenzoic acid



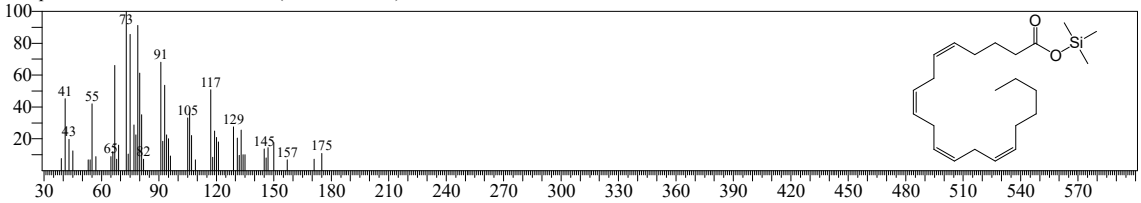
Hit#:2 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



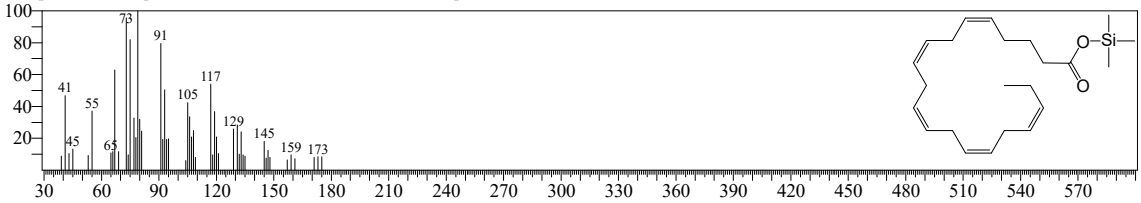
Hit#:3 Entry:211 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C13H22O3Si2 CAS:99-96-7 MolWeight:282 RetIndex:1636
CompName:4-Hydroxybenzoic acid-2TMS ; 4-hydroxybenzoic acid



Hit#:4 Entry:508 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C23H40O2Si CAS:506-32-1 MolWeight:376 RetIndex:2381
CompName:Arachidonic acid-TMS ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid

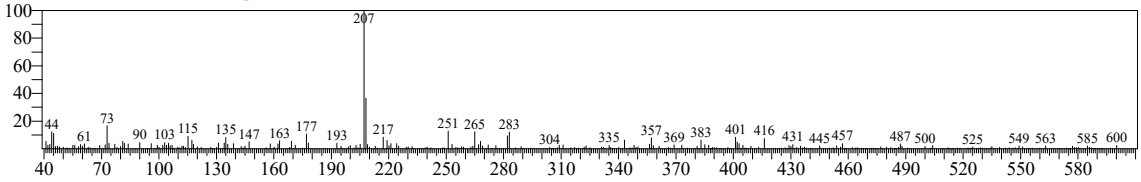


Hit#:5 Entry:509 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C23H38O2Si CAS:10417-94-4 MolWeight:374 RetIndex:2389
CompName:Eicosapentaenoic acid-TMS ; icosa-5,8,11,14,17-pentaenoic acid

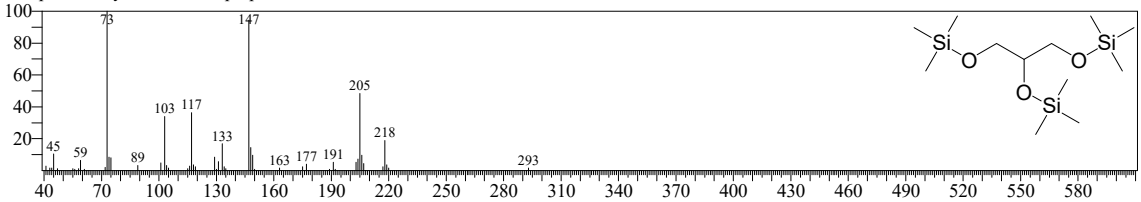


TNAU

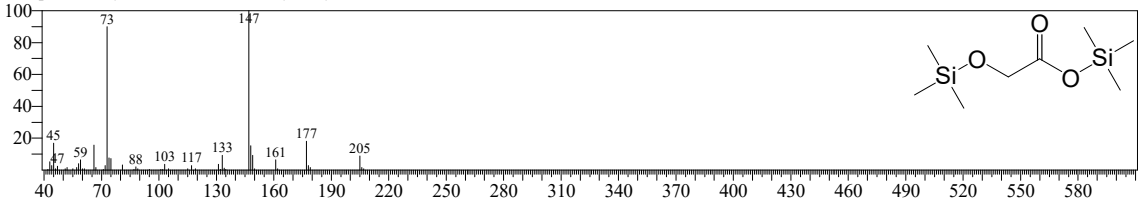
<< Target >>
Line#:23 R.Time:32.085(Scan#:5518) MassPeaks:282
RawMode:Averaged 32.080-32.090(5517-5519) BasePeak:207.05(3070)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



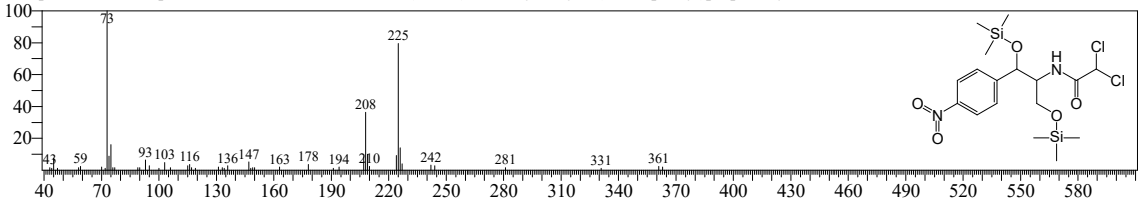
Hit#:1 Entry:77 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C12H32O3Si3 CAS:56-81-5 MolWeight:308 RetIndex:1279
CompName:Glycerol-3TMS ; propane-1,2,3-triol



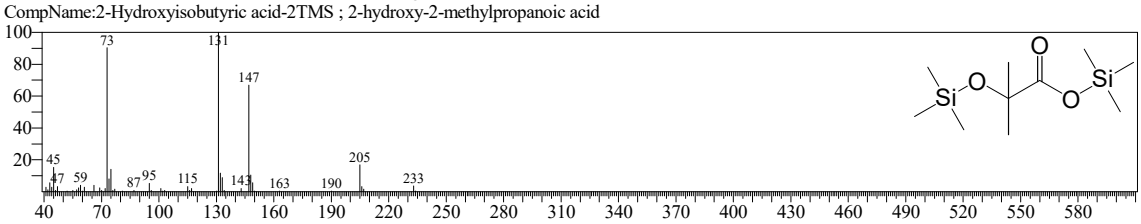
Hit#:2 Entry:13 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C8H20O3Si2 CAS:79-14-1 MolWeight:220 RetIndex:1074
CompName:Glycolic acid-2TMS ; 2-hydroxyacetic acid



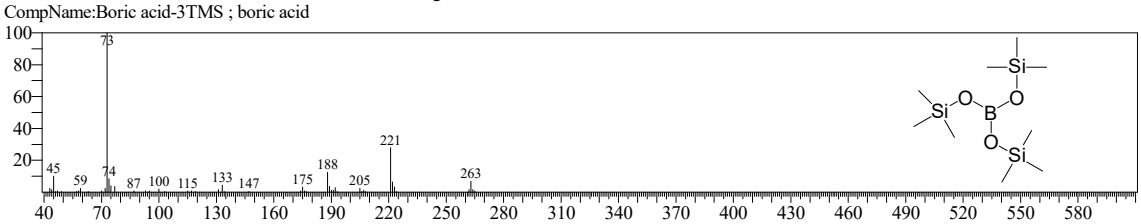
Hit#:3 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide



Hit#:4 Entry:10 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C10H24O3Si2 CAS:594-61-6 MolWeight:248 RetIndex:1067
CompName:2-Hydroxyisobutyric acid-2TMS ; 2-hydroxy-2-methylpropanoic acid

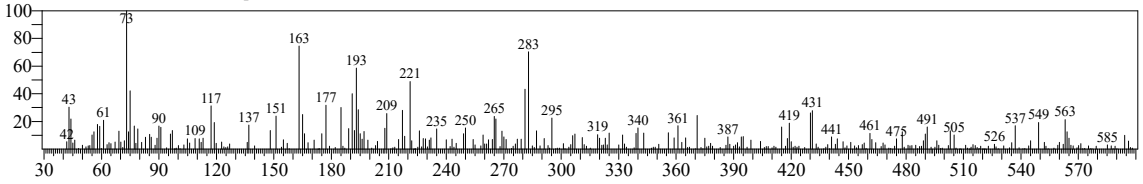


Hit#:5 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid

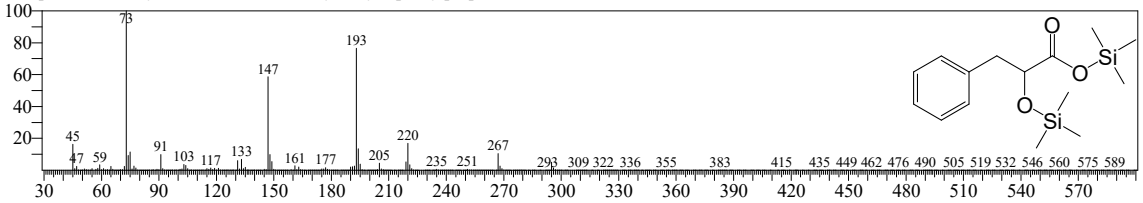


TNAU

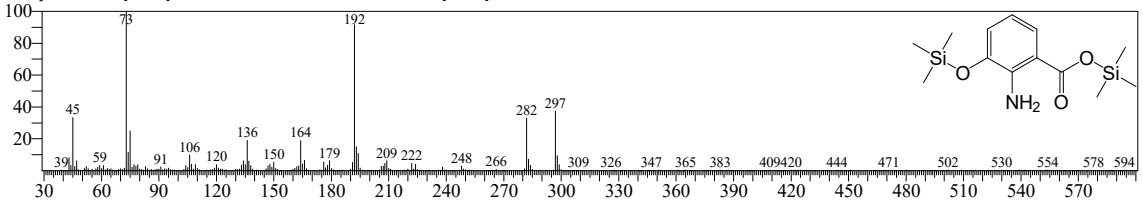
<< Target >>
Line#:24 R.Time:32.430(Scan#:5587) MassPeaks:338
RawMode:Averaged 32.425-32.435(5586-5588) BasePeak:73.10(898)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



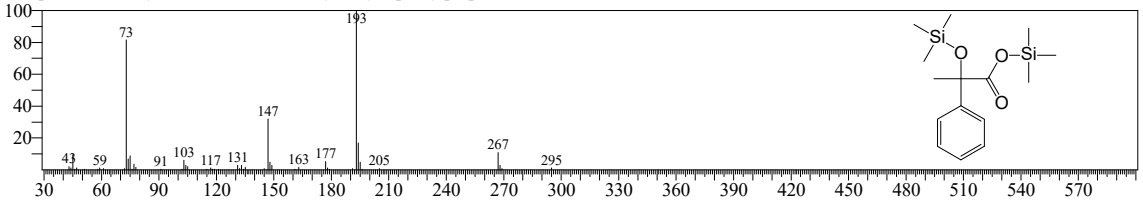
Hit#:1 Entry:194 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C15H26O3Si2 CAS:828-01-3 MolWeight:310 RetIndex:1599
CompName:3-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



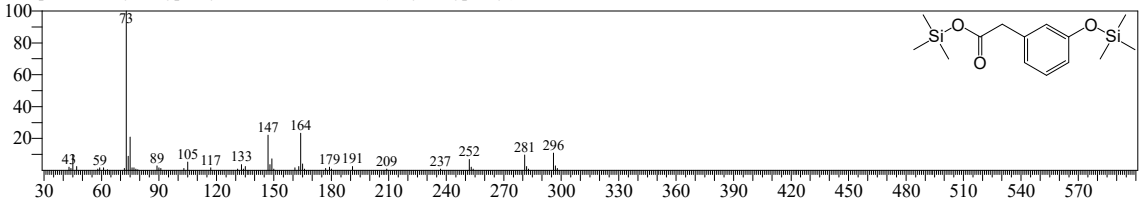
Hit#:2 Entry:290 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C13H23NO3Si2 CAS:548-93-6 MolWeight:297 RetIndex:1773
CompName:3-Hydroxyanthranilic acid-2TMS ; 2-amino-3-hydroxybenzoic acid



Hit#:3 Entry:150 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C15H26O3Si2 CAS:515-30-0 MolWeight:310 RetIndex:1517
CompName:2-Phenyllactic acid-2TMS ; 2-hydroxy-3-phenylpropanoic acid



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



Hit#:5 Entry:328 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C13H23NO2Si2 CAS:150-13-0 MolWeight:281 RetIndex:1845
CompName:4-Aminobenzoic acid-2TMS ; 4-aminobenzoic acid