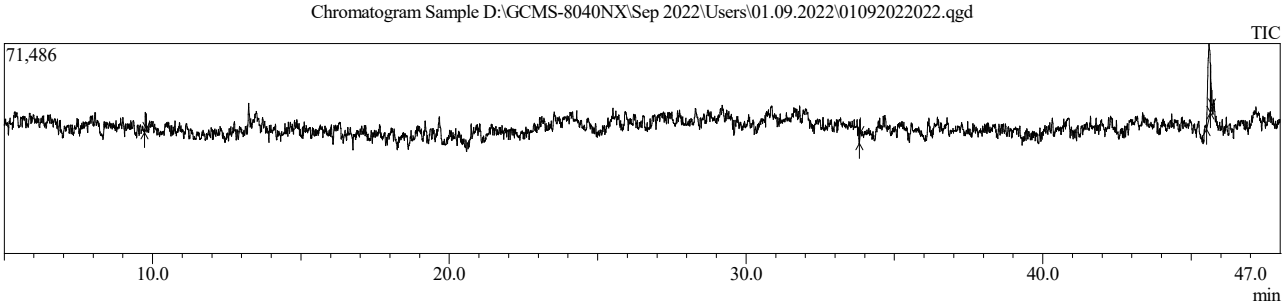
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 12:02:44 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 7-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 8
Injection Volume	: 2.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022022.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022022.qgd
Method File	: D:\GCMS-8040NX\Sep 2022\Method\Scan_methodfile.qgm
Org Method File	: D:\GCMS-8040NX\Sep 2022\Method\Scan_methodfile.qgm
Report File	:
Tuning File	: D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 25082022.qgt
Modified by	: Admin
Modified	: 05-Sep-22 11:05:04 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022022.qgd



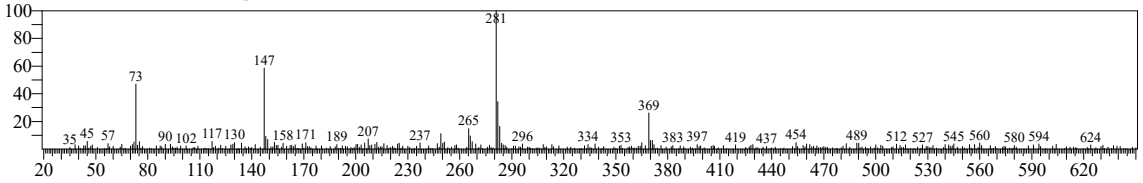
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.758	9953	5.66	6259	11.78	1.59	80	Pentasiloxane, dodecamethyl-
2	33.835	5995	3.41	5973	11.25	1.00	9	Cystathionine-4TMS
3	45.604	133648	76.06	25239	47.52	5.30	81	Diosgenin
4	45.655	26120	14.86	15643	29.45	1.67	15	Propionylglycine-2TMS
		175716	100.00	53114	100.00			

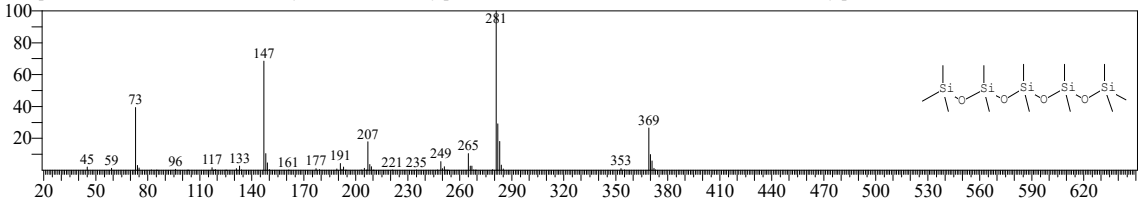
Library

TNAU

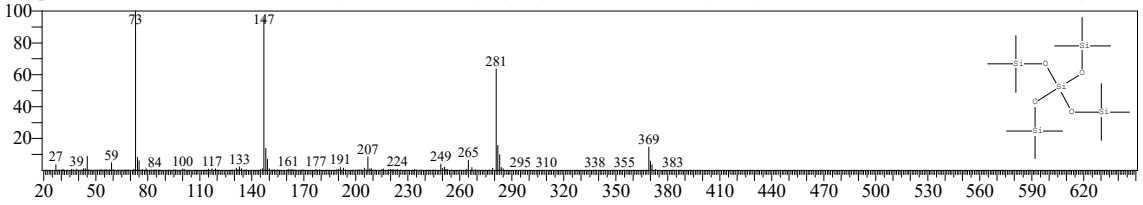
<< Target >>
Line#:1 R.Time:9.760(Scan#:953) MassPeaks:376
RawMode:Averaged 9.755-9.765(952-954) BasePeak:281.05(852)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



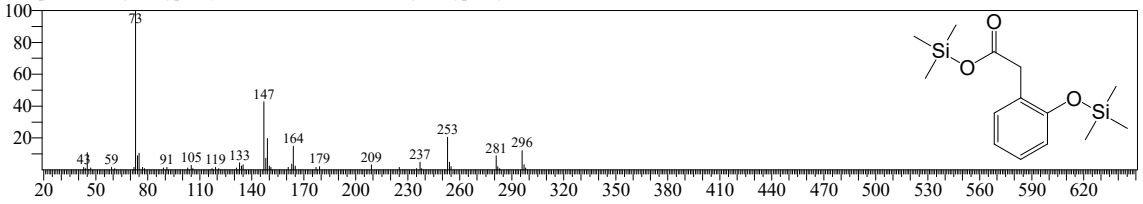
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:80 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



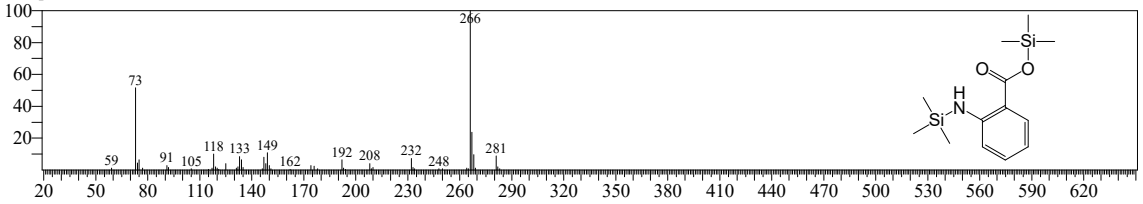
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:72 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



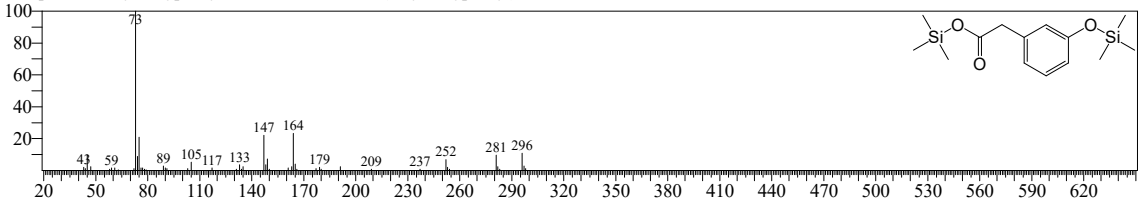
Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



Hit#:4 Entry:203 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C13H23NO2Si2 CAS:118-92-3 MolWeight:281 RetIndex:1623
CompName:Anthranilic acid-2TMS ; 2-aminobenzoic acid

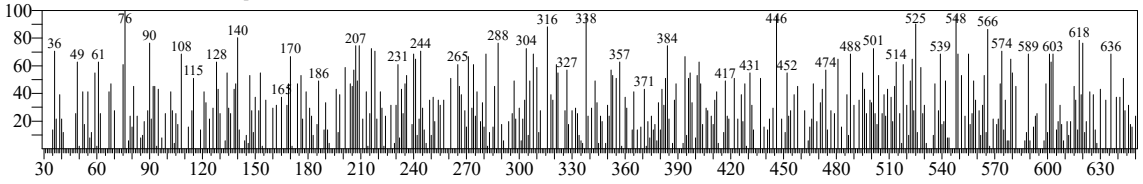


Hit#:5 Entry:200 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C14H24O3Si2 CAS:621-37-4 MolWeight:296 RetIndex:1617
CompName:3-Hydroxyphenylacetic acid-2TMS ; 2-(3-hydroxyphenyl)acetic acid

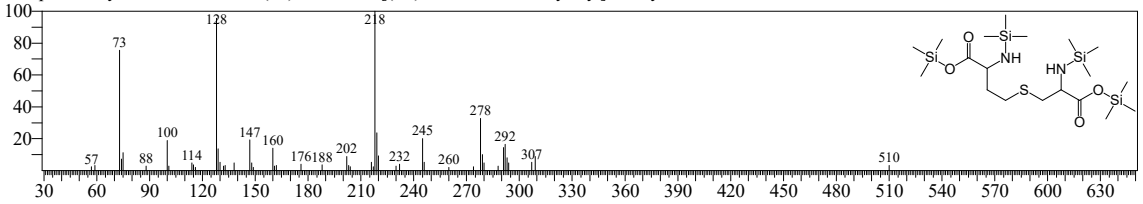


TNAU

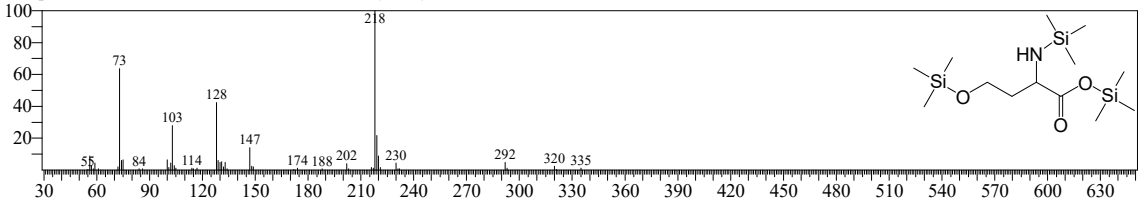
<< Target >>
Line#:2 R.Time:33.835(Scan#:5768) MassPeaks:408
RawMode:Averaged 33.830-33.840(5767-5769) BasePeak:76.00(51)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



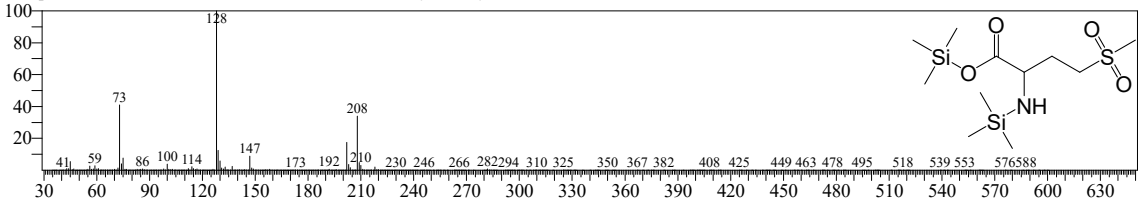
Hit#:1 Entry:489 Library:OA_TMS_DB5_67min_V3.lib
SI:9 Formula:C19H46N2O4SSi4 CAS:56-88-2 MolWeight:510 RetIndex:2233
CompName:Cystathionine-4TMS ; (2S)-2-amino-4-[(2R)-2-amino-2-carboxyethyl]sulfanylbutanoic acid



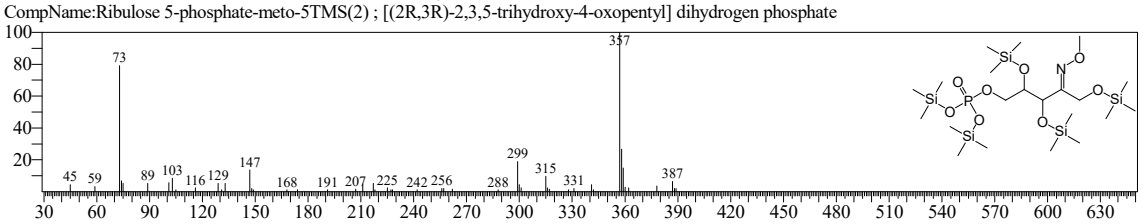
Hit#:2 Entry:130 Library:OA_TMS_DB5_67min_V3.lib
SI:9 Formula:C13H33NO3Si3 CAS:672-15-1 MolWeight:335 RetIndex:1458
CompName:Homoserine-3TMS ; (2S)-2-amino-4-hydroxybutanoic acid



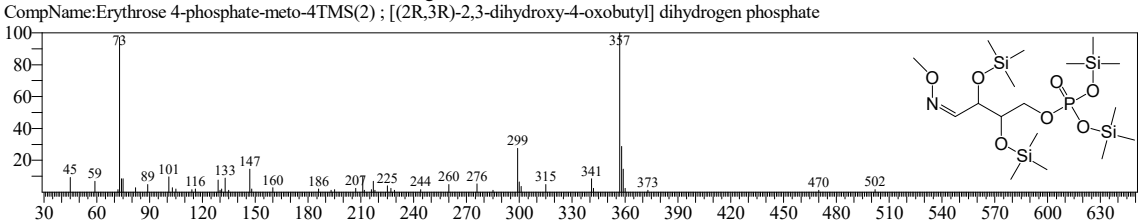
Hit#:3 Entry:329 Library:OA_TMS_DB5_67min_V3.lib
SI:8 Formula:C11H27NO4SSi2 CAS:820-10-0 MolWeight:325 RetIndex:1848
CompName:Methionine sulfone-2TMS ; 2-amino-4-methylsulfonylbutanoic acid



Hit#:4 Entry:476 Library:OA_TMS_DB5_67min_V3.lib
SI:8 Formula:C21H54NO8PSi5 CAS:4151-19-3 MolWeight:619 RetIndex:2152
CompName:Ribulose 5-phosphate-meto-5TMS(2) ; [(2R,3R)-2,3,5-trihydroxy-4-oxopentyl] dihydrogen phosphate

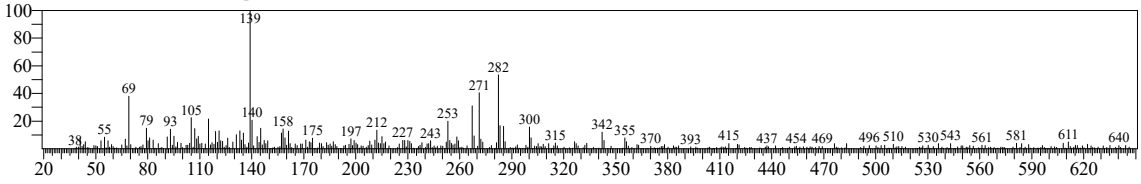


Hit#:5 Entry:394 Library:OA_TMS_DB5_67min_V3.lib
SI:7 Formula:C17H44NO7PSi4 CAS:585-18-2 MolWeight:517 RetIndex:1935
CompName:Erythrose 4-phosphate-meto-4TMS(2) ; [(2R,3R)-2,3-dihydroxy-4-oxobutyl] dihydrogen phosphate

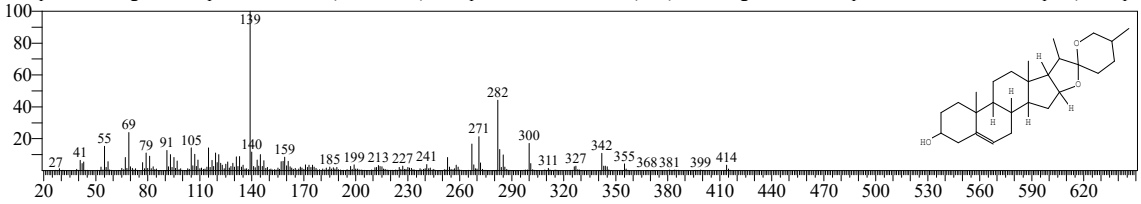


TNAU

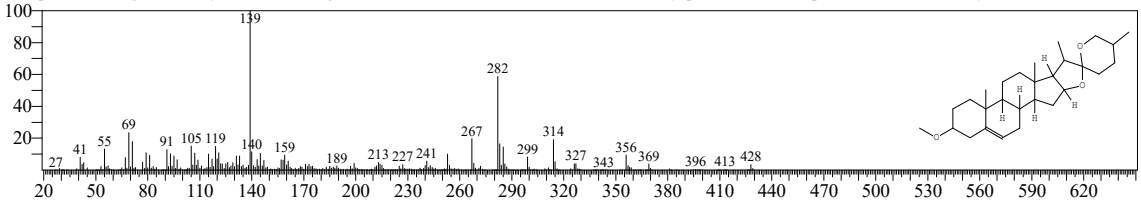
<< Target >>
Line#:3 R.Time:45.605(Scan#:8122) MassPeaks:403
RawMode:Averaged 45.600-45.610(8121-8123) BasePeak:139.10(1103)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



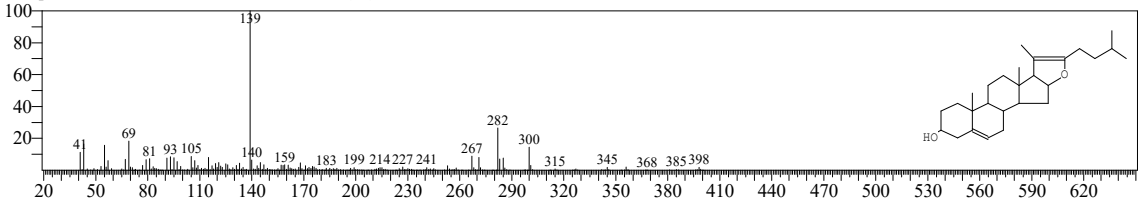
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:81 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



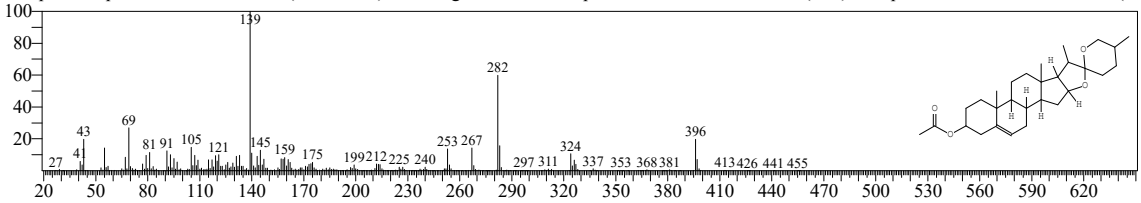
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:73 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



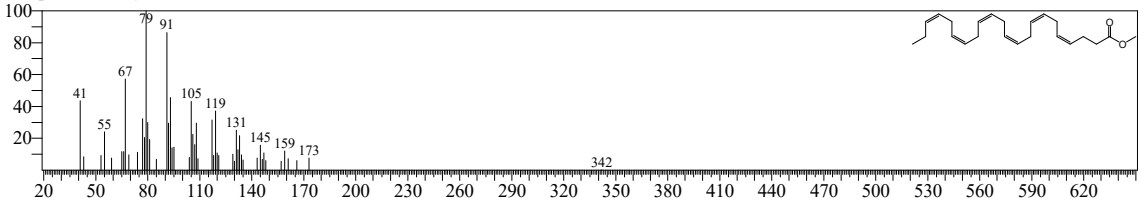
Hit#:3 Entry:41561 Library:NIST20R.lib
SI:72 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #



Hit#:4 Entry:24878 Library:NIST20M2.lib
SI:71 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (2

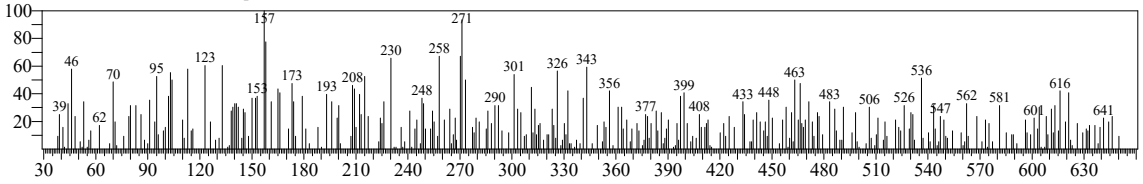


Hit#:5 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C23H34O2 CAS:6217-54-5 MolWeight:342 RetIndex:3514
CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid

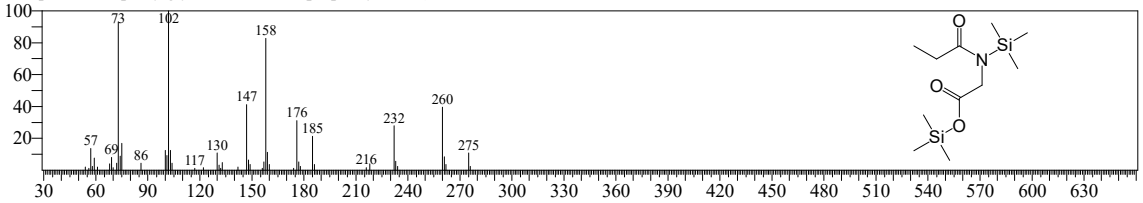


TNAU

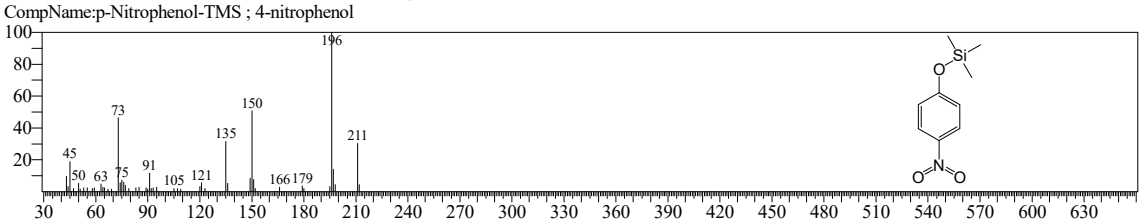
<< Target >>
Line#:4 R.Time:45.655(Scan#:8132) MassPeaks:326
RawMode:Averaged 45.650-45.660(8131-8133) BasePeak:157.10(76)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



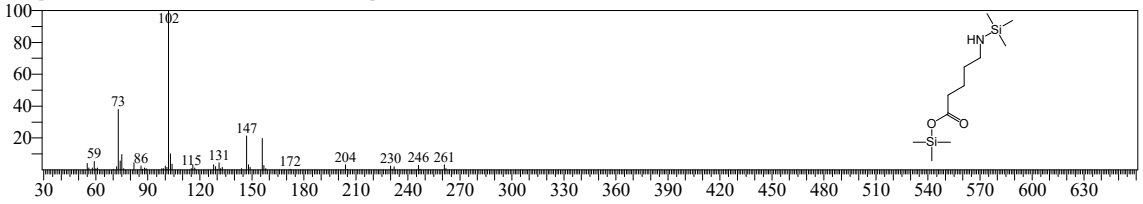
Hit#:1 Entry:120 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C11H25NO3Si2 CAS:21709-90-0 MolWeight:275 RetIndex:1428
CompName:Propionylglycine-2TMS ; 2-(propanoylamino)acetic acid



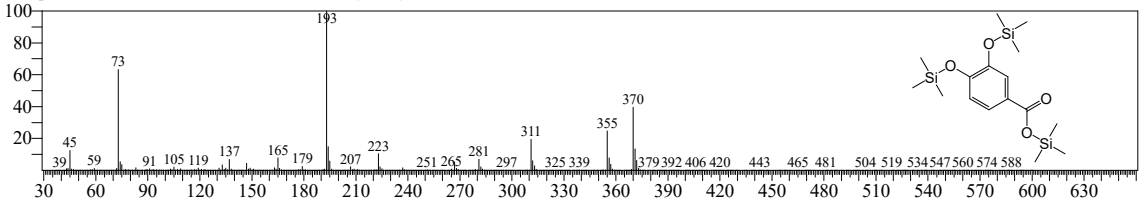
Hit#:2 Entry:151 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C9H13NO3Si CAS:100-02-7 MolWeight:211 RetIndex:1518
CompName:p-Nitrophenol-TMS ; 4-nitrophenol



Hit#:3 Entry:113 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C11H27NO2Si2 CAS:660-88-8 MolWeight:261 RetIndex:1400
CompName:5-Aminovaleric acid-2TMS ; 5-aminopentanoic acid



Hit#:4 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid



Hit#:5 Entry:76 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C12H29NO2Si2 CAS:61-90-5 MolWeight:275 RetIndex:1278
CompName:Leucine-2TMS ; (2S)-2-amino-4-methylpentanoic acid