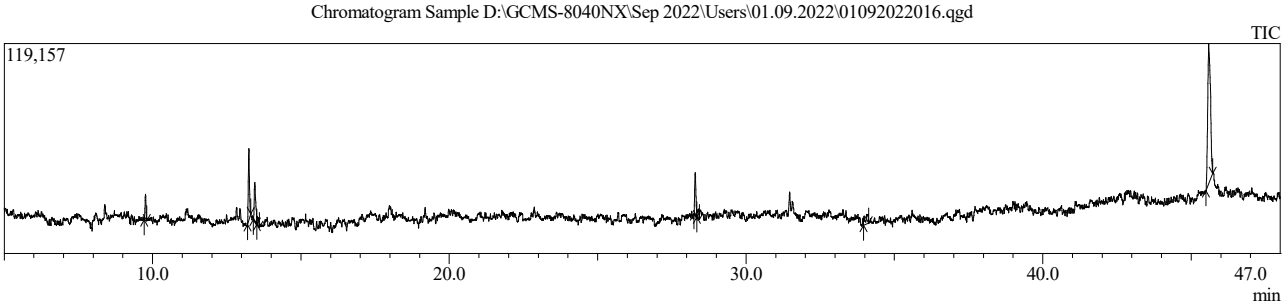
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 6:45:45 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 5-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 6
Injection Volume	: 2.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022016.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022016.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 11:02:55 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022016.qgd



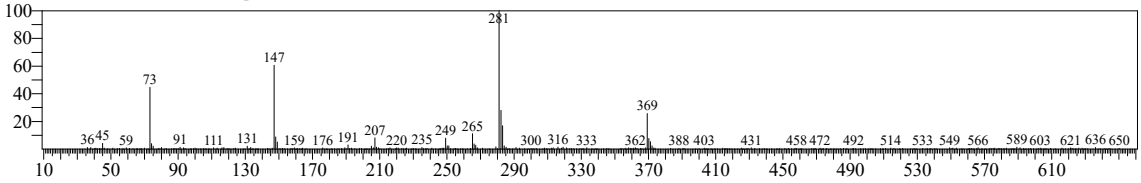
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.764	34611	3.96	14771	7.55	2.34	93	Pentasiloxane, dodecamethyl-
2	13.245	112155	12.83	40637	20.78	2.76	54	Methyl cis-13,16-Docosadienate
3	13.444	79623	9.11	22131	11.32	3.60	54	Methyl cis-13,16-Docosadienate
4	13.575	16229	1.86	4894	2.50	3.32	21	2-Octenoic acid-TMS
5	28.287	68015	7.78	24220	12.38	2.81	94	n-Hexadecanoic acid
6	28.410	17980	2.06	4132	2.11	4.35	21	S-Benzyl-Cysteine-4TMS
7	34.063	36023	4.12	5418	2.77	6.65	13	4-Cresol-TMS
8	45.592	509471	58.28	79360	40.58	6.42	90	Diosgenin
		874107	100.00	195563	100.00			

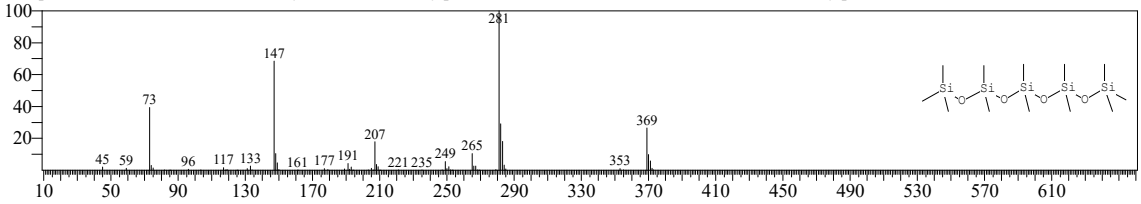
Library

TNAU

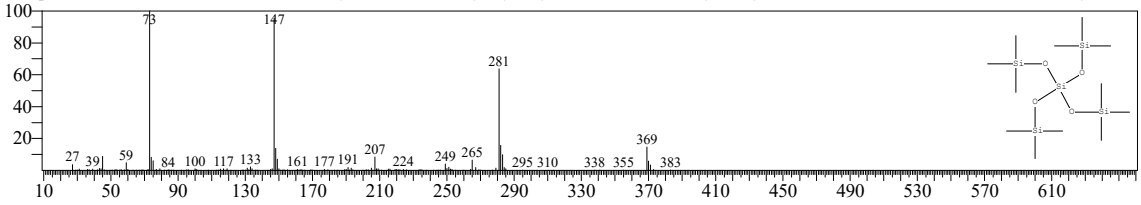
<< Target >>
Line#:1 R.Time:9.765(Scan#:954) MassPeaks:349
RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(3501)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



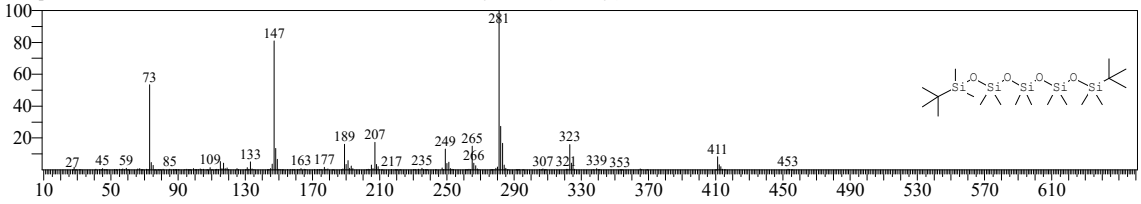
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



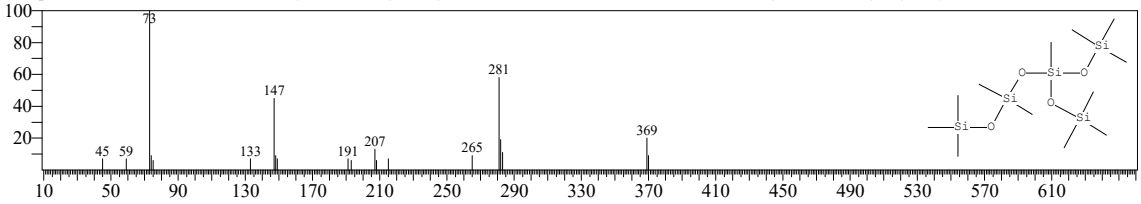
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:82 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



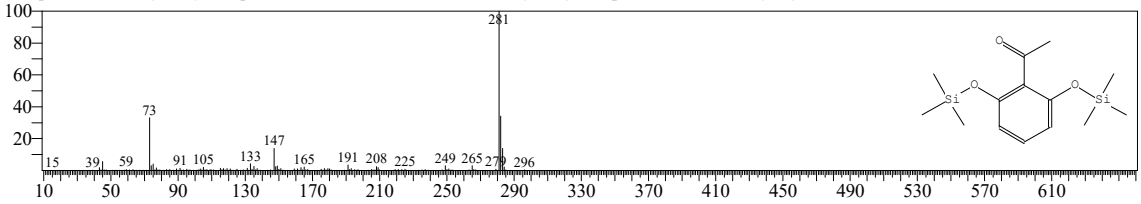
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:79 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



Hit#:4 Entry:249271 Library:NIST20M1.lib
SI:78 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

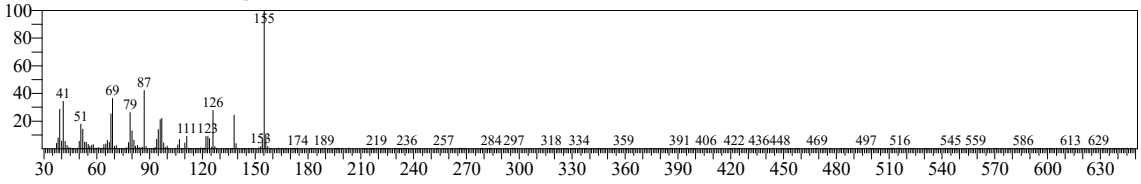


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

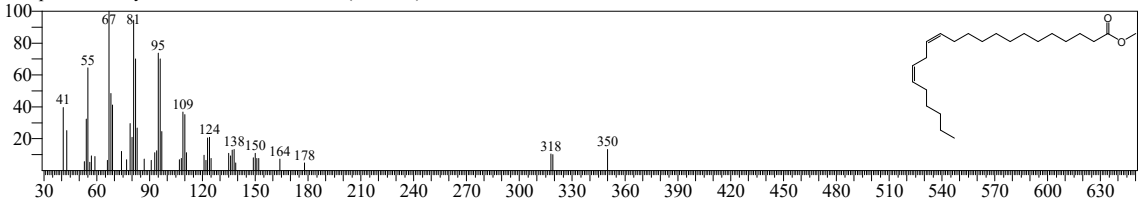


TNAU

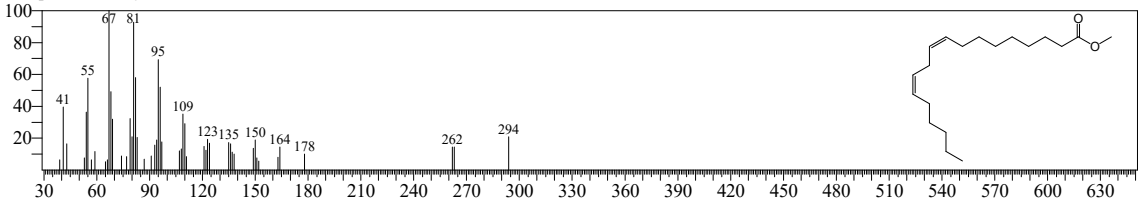
<< Target >>
Line#:2 R.Time:13.245(Scan#:1650) MassPeaks:340
RawMode:Averaged 13.240-13.250(1649-1651) BasePeak:155.10(6267)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



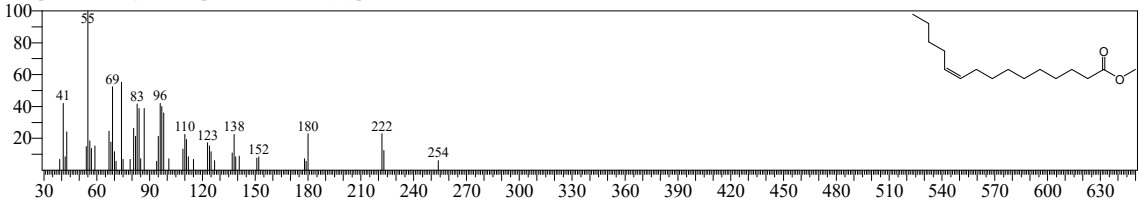
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



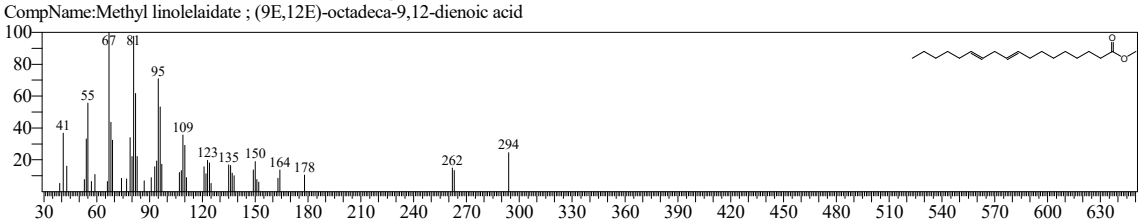
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



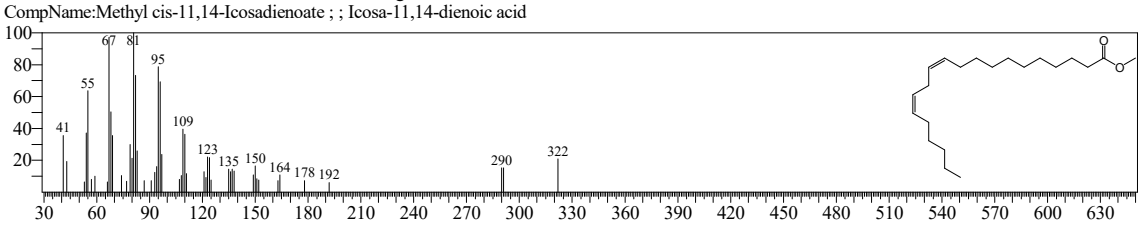
Hit#:3 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid



Hit#:4 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

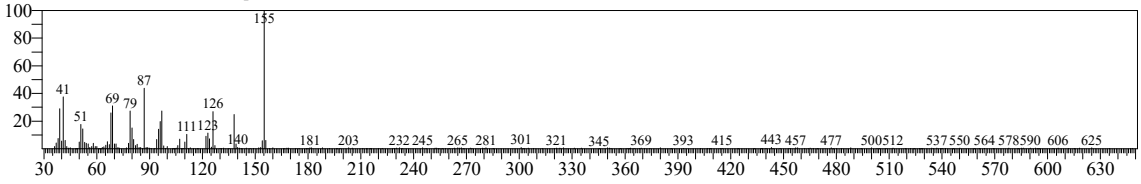


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

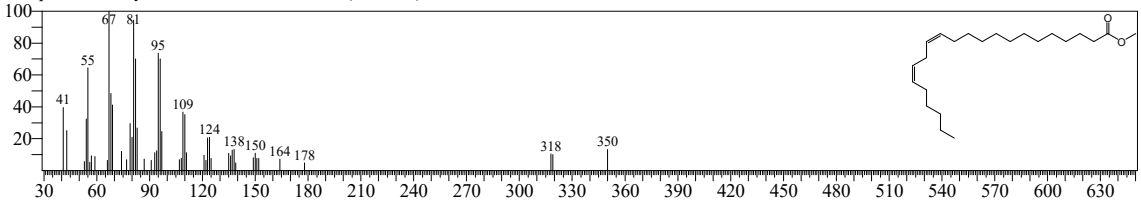


TNAU

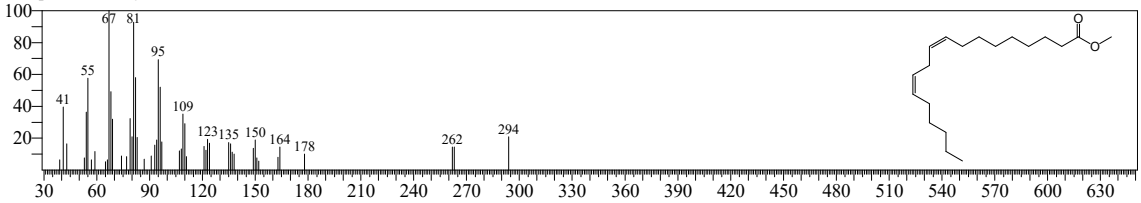
<< Target >>
Line#:3 R.Time:13.445(Scan#:1690) MassPeaks:239
RawMode:Averaged 13.440-13.450(1689-1691) BasePeak:155.05(3710)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



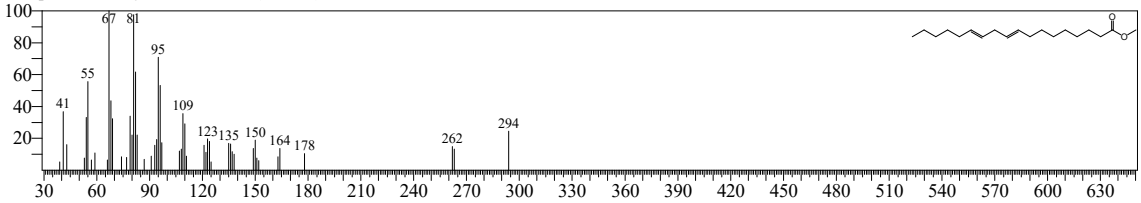
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



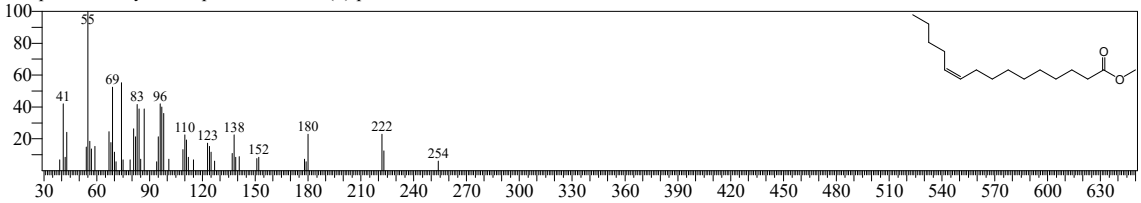
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



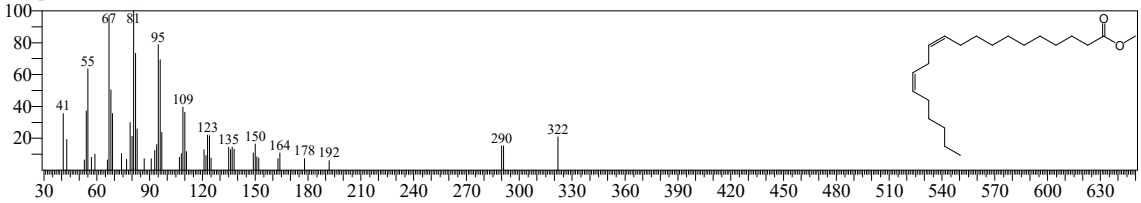
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

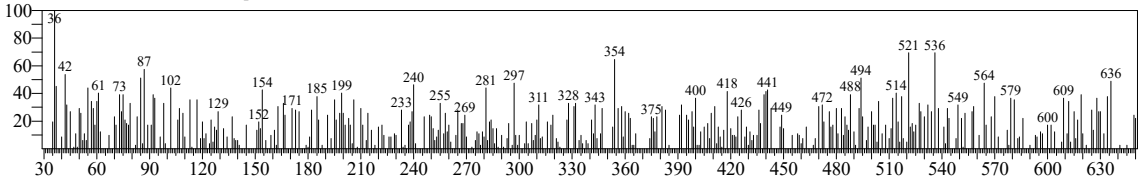


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

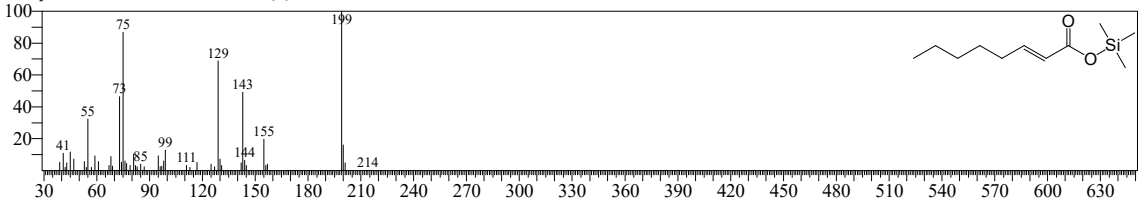


TNAU

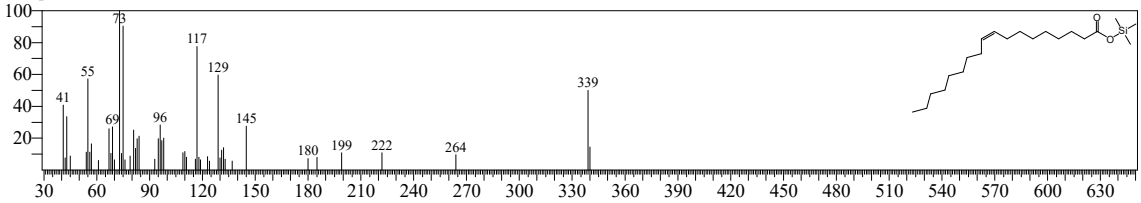
<< Target >>
Line#:4 R.Time:13.575(Scan#:1716) MassPeaks:373
RawMode:Averaged 13.570-13.580(1715-1717) BasePeak:36.00(82)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



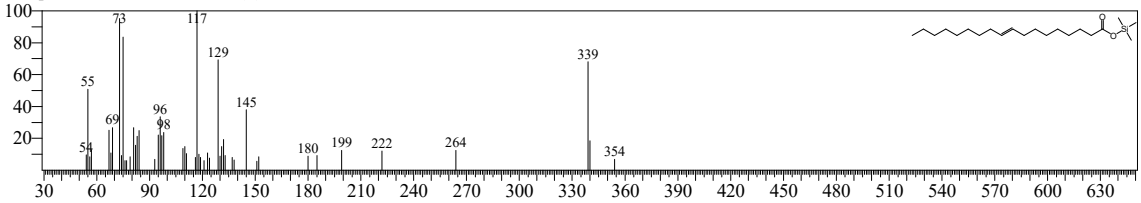
Hit#:1 Entry:91 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula:C11H22O2Si CAS:1871-67-6 MolWeight:214 RetIndex:1313
CompName:2-Octenoic acid-TMS ; (E)-oct-2-enoic acid



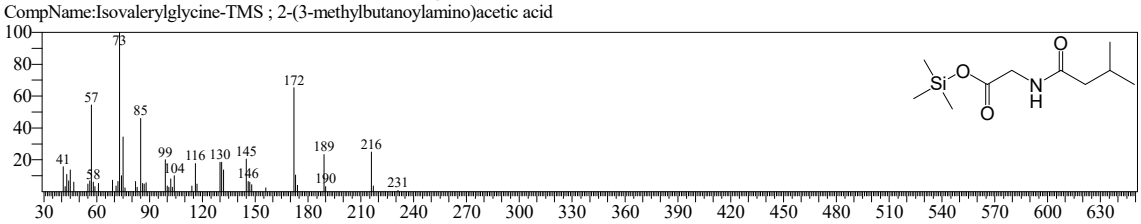
Hit#:2 Entry:485 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C21H42O2Si CAS:112-80-1 MolWeight:354 RetIndex:2222
CompName:Oleic acid-TMS ; (Z)-octadec-9-enoic acid



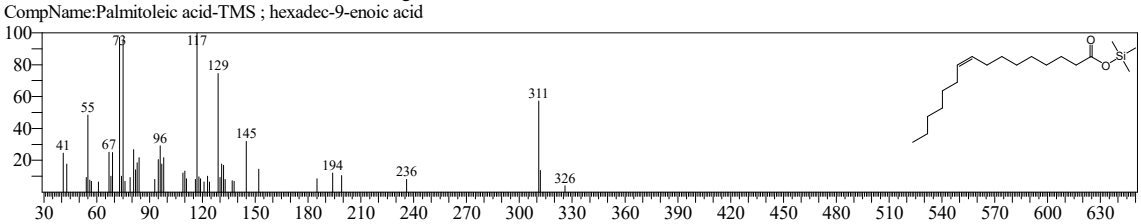
Hit#:3 Entry:487 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C21H42O2Si CAS:112-79-8 MolWeight:354 RetIndex:2227
CompName:Elaidic acid-TMS ; (E)-octadec-9-enoic acid



Hit#:4 Entry:139 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C10H21NO3Si CAS:16284-60-9 MolWeight:231 RetIndex:1487
CompName:Isovalerylglycine-TMS ; 2-(3-methylbutanoylamino)acetic acid

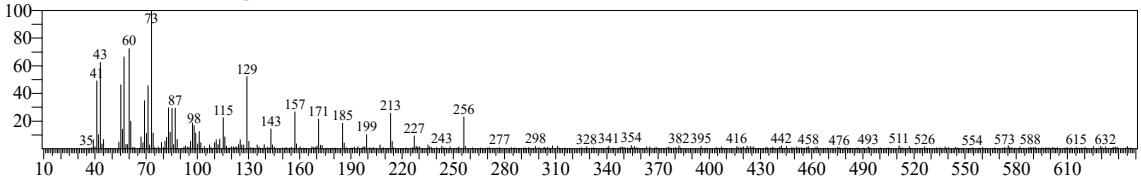


Hit#:5 Entry:442 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C19H38O2Si CAS:373-49-9 MolWeight:326 RetIndex:2028
CompName:Palmitoleic acid-TMS ; hexadec-9-enoic acid

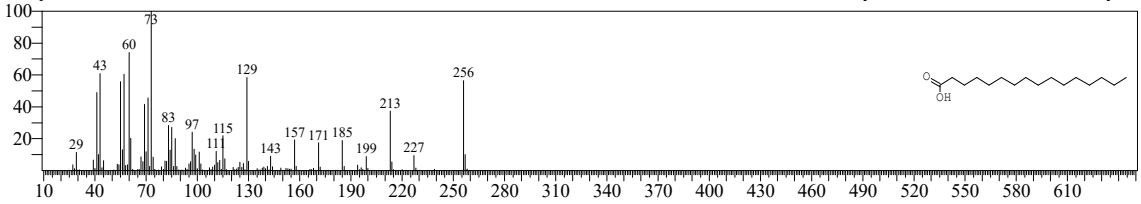


TNAU

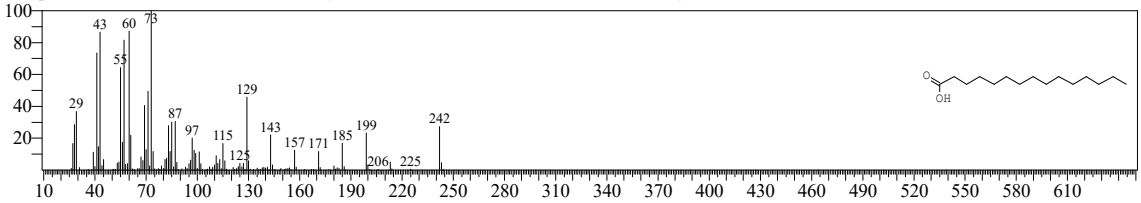
<< Target >>
Line#:5 R.Time:28.285(Scan#:4658) MassPeaks:359
RawMode:Averaged 28.280-28.290(4657-4659) BasePeak:73.05(1868)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



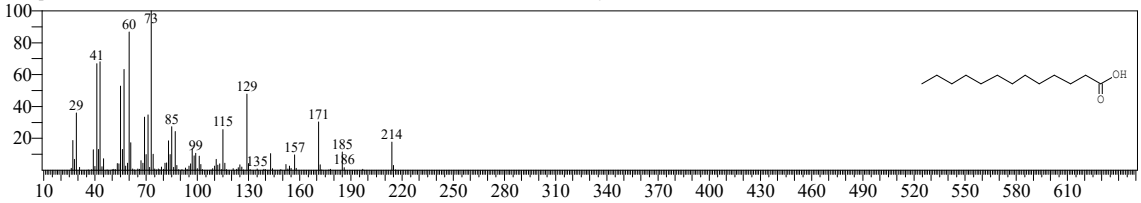
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:94 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



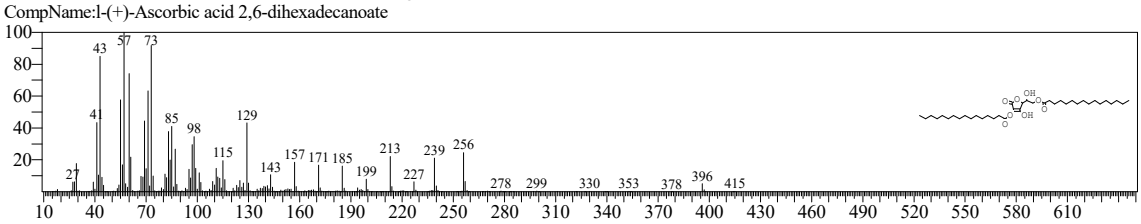
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:90 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



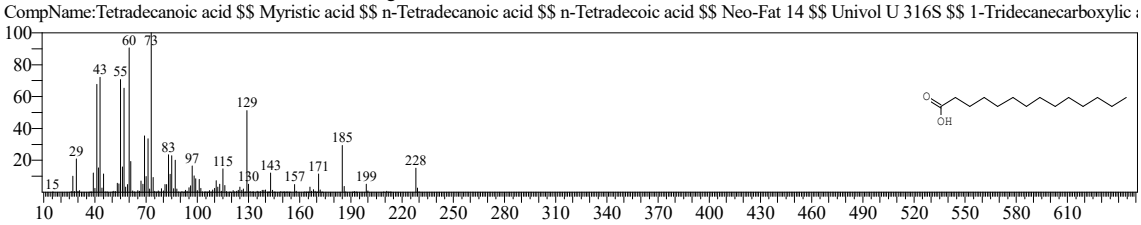
Hit#:3 Entry:25643 Library:NIST20R.lib
SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid



Hit#:4 Entry:44286 Library:NIST20M2.lib
SI:89 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

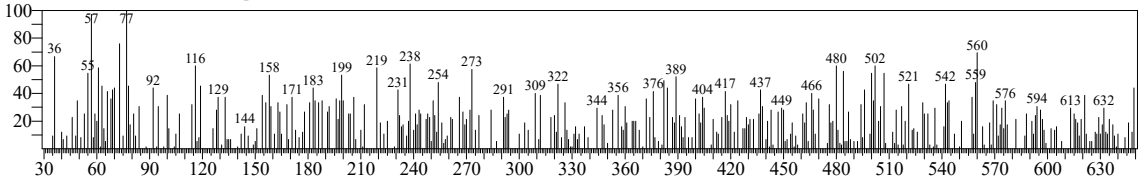


Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:89 Formula:C14H28O2 CAS:544-63-8 MolWeight:228 RetIndex:1769
CompName:Tetradecanoic acid $$ Myristic acid $$ n-Tetradecanoic acid $$ n-Tetradecoic acid $$ Neo-Fat 14 $$ Univol U 316S $$ 1-Tridecanecarboxylic

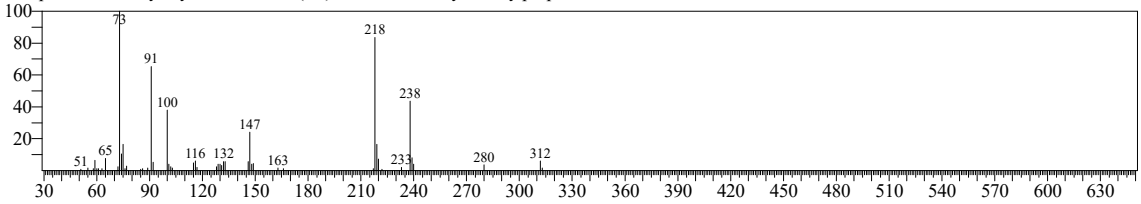


TNAU

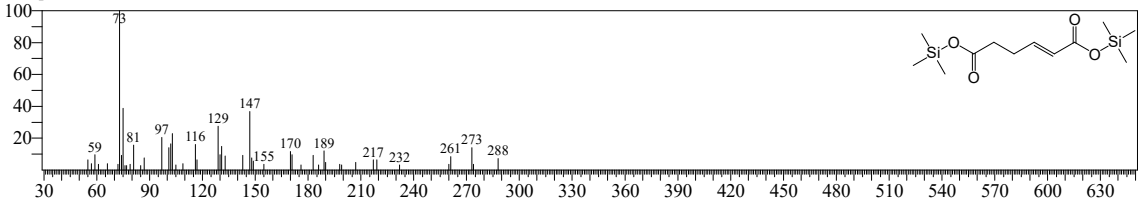
<< Target >>
Line#:6 R.Time:28.410(Scan#:4683) MassPeaks:352
RawMode:Averaged 28.405-28.415(4682-4684) BasePeak:77.00(75)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



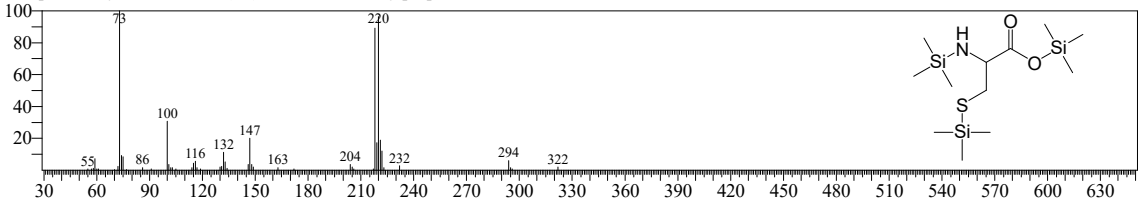
Hit#:1 Entry:440 Library:OA_TMS_DB5_67min_V3.lib
SI:21 Formula: CAS:3054-01-1 MolWeight:0 RetIndex:2015
CompName:S-Benzyl-Cysteine-4TMS ; (2R)-2-amino-3-benzylsulfanylpropanoic acid



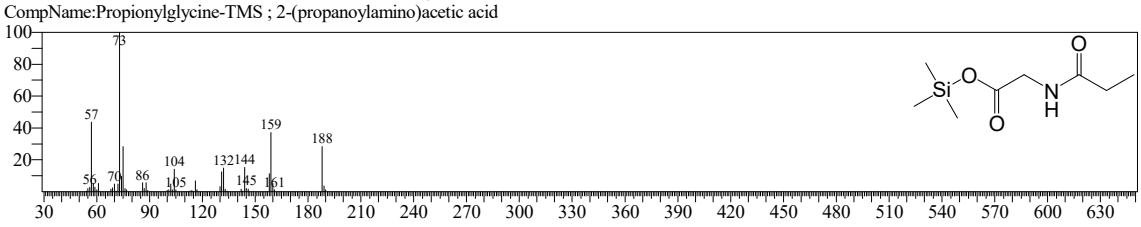
Hit#:2 Entry:156 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C12H24O4Si2 CAS:4440-68-0 MolWeight:288 RetIndex:1522
CompName:2-Hexenedioic acid-2TMS ; hex-2-enedioic acid



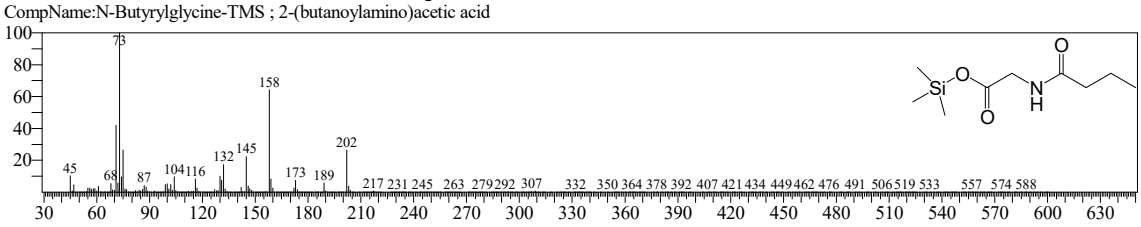
Hit#:3 Entry:177 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C12H31NO2SSi3 CAS:52-90-4 MolWeight:337 RetIndex:1568
CompName:Cysteine-3TMS ; (2R)-2-amino-3-sulfanylpropanoic acid



Hit#:4 Entry:103 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C8H17NO3Si CAS:21709-90-0 MolWeight:203 RetIndex:1359
CompName:Propionylglycine-TMS ; 2-(propanoylamino)acetic acid

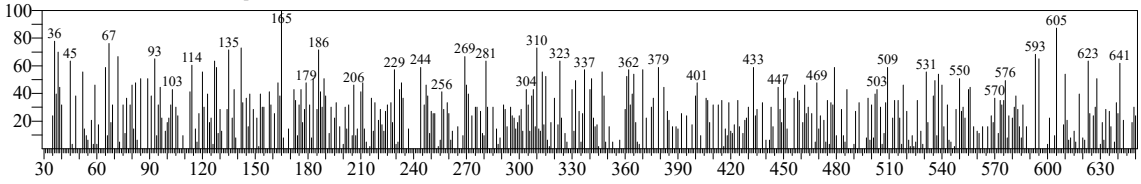


Hit#:5 Entry:125 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C9H19NO3Si CAS:20208-73-5 MolWeight:217 RetIndex:1446
CompName:N-Butyrylglycine-TMS ; 2-(butanoylamino)acetic acid

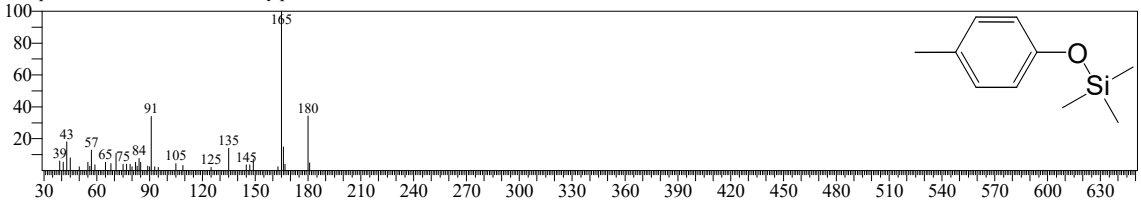


TNAU

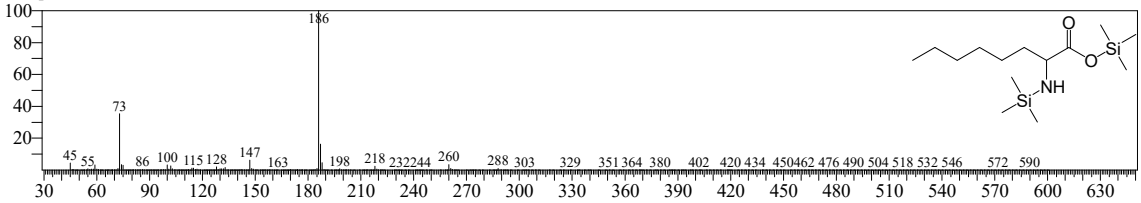
<< Target >>
Line#:7 R.Time:34.065(Scan#:5814) MassPeaks:416
RawMode:Averaged 34.060-34.070(5813-5815) BasePeak:165.00(63)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



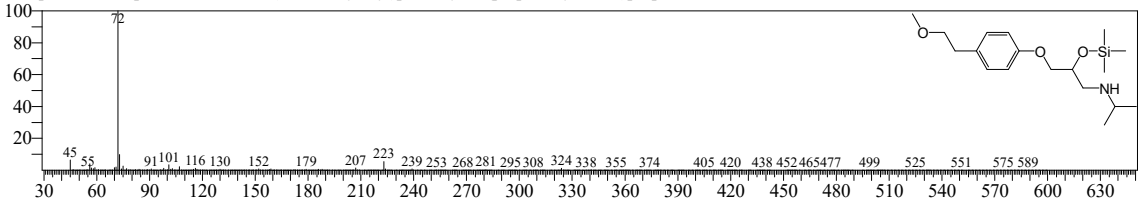
Hit#:1 Entry:34 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C10H16OSi CAS:106-44-5 MolWeight:180 RetIndex:1160
CompName:4-Cresol-TMS ; 4-methylphenol



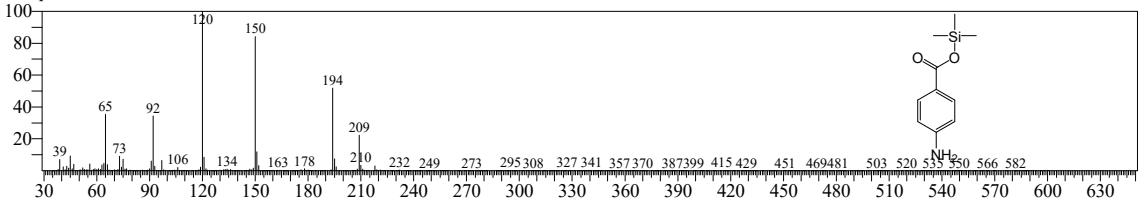
Hit#:2 Entry:145 Library:OA_TMS_DB5_67min_V3.lib
SI:11 Formula:C14H33NO2Si2 CAS:644-90-6 MolWeight:303 RetIndex:1500
CompName:2-Aminooctanoic acid-2TMS ; 2-aminooctanoic acid



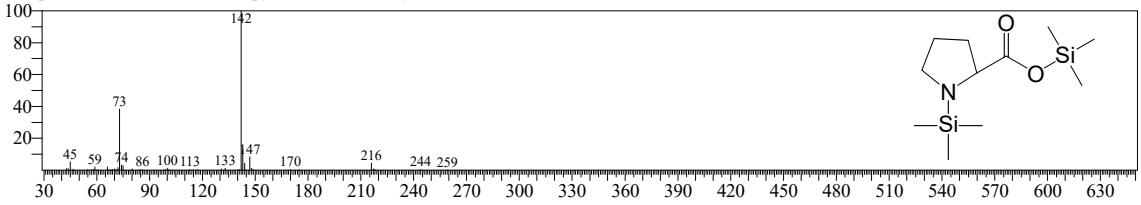
Hit#:3 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:11 Formula:C18H33NO3Si CAS:37350-58-6 MolWeight:339 RetIndex:2094
CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol



Hit#:4 Entry:228 Library:OA_TMS_DB5_67min_V3.lib
SI:10 Formula:C10H15NO2Si CAS:150-13-0 MolWeight:209 RetIndex:1661
CompName:4-Aminobenzoic acid-TMS ; 4-aminobenzoic acid

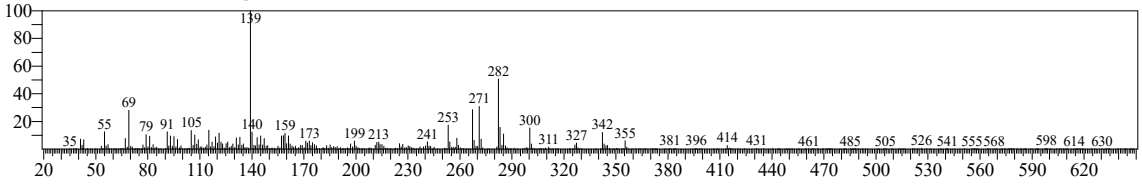


Hit#:5 Entry:89 Library:OA_TMS_DB5_67min_V3.lib
SI:10 Formula:C11H25NO2Si2 CAS:147-85-3 MolWeight:259 RetIndex:1306
CompName:Proline-2TMS ; (2S)-pyrrolidine-2-carboxylic acid

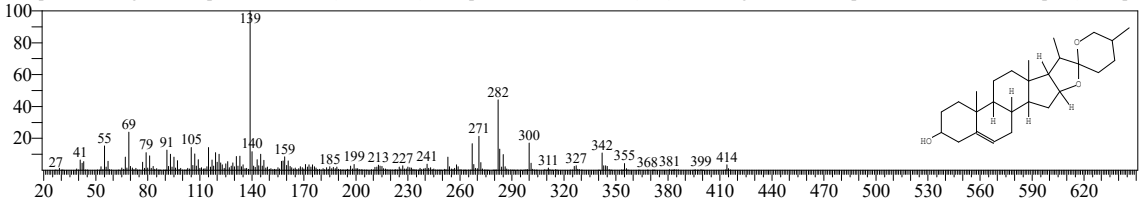


TNAU

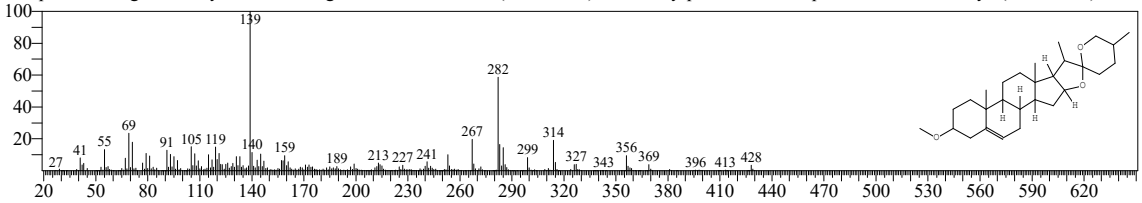
<< Target >>
Line#:8 R.Time:45.590(Scan#:8119) MassPeaks:395
RawMode:Averaged 45.585-45.595(8118-8120) BasePeak:139.15(8533)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



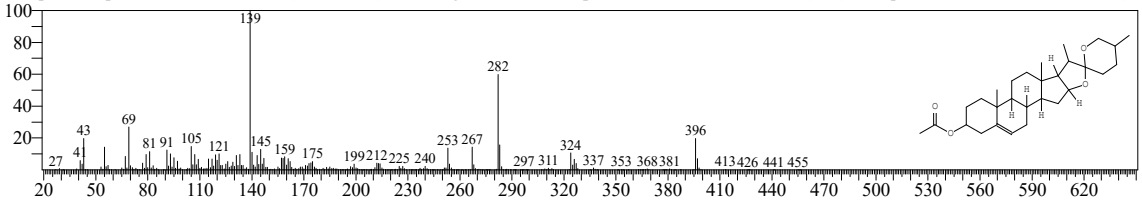
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:90 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



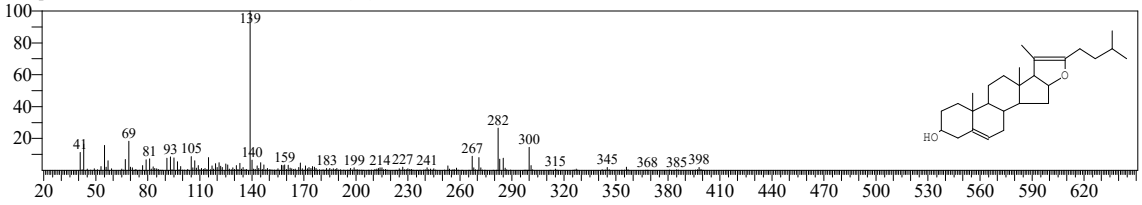
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:82 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#:3 Entry:24878 Library:NIST20M2.lib
SI:80 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#:4 Entry:41561 Library:NIST20R.lib
SI:79 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #



Hit#:5 Entry:42677 Library:NIST20R.lib
SI:74 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.