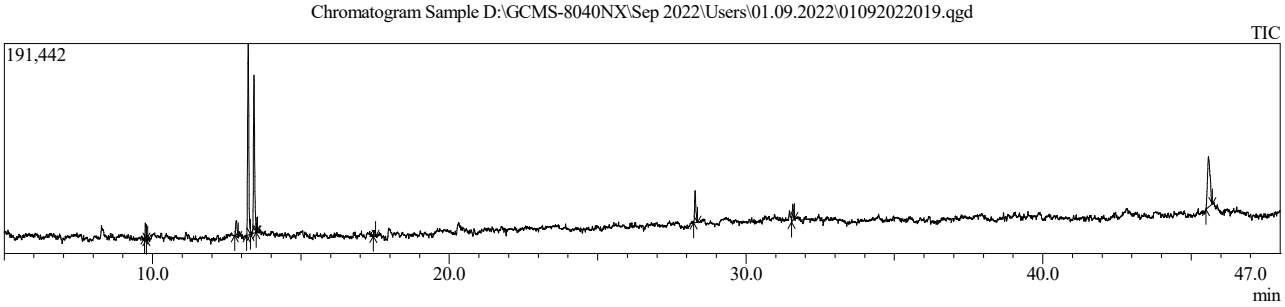
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 9:24:00 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 6-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 7
Injection Volume	: 2.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022019.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022019.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 11:04:00 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022019.qgd



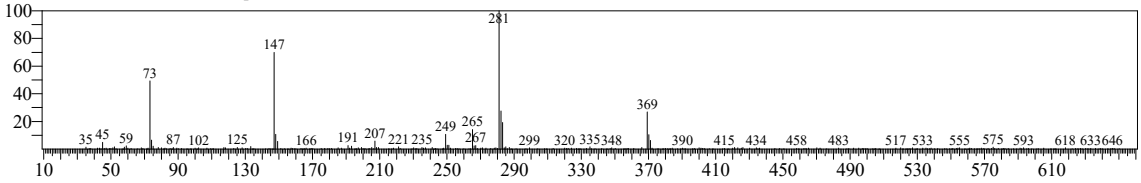
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.759	30002	2.15	14314	3.15	2.10	92	Pentasiloxane, dodecamethyl-
2	9.820	7544	0.54	4078	0.90	1.85	12	Phenol-TMS
3	12.825	50510	3.62	14465	3.18	3.49	70	2,5-Cyclohexadiene-1,4-dione, dioxime
4	13.223	471934	33.80	174460	38.40	2.71	54	Methyl cis-13,16-Docosadienate
5	13.419	401519	28.76	143996	31.70	2.79	54	Methyl cis-13,16-Docosadienate
6	13.510	13166	0.94	7378	1.62	1.78	20	2-Octenoic acid-TMS
7	17.459	15832	1.13	5389	1.19	2.94	17	Methyl cis-11,14,17-Icosatrienoate
8	28.284	82722	5.93	29197	6.43	2.83	93	n-Hexadecanoic acid
9	31.578	39807	2.85	15032	3.31	2.65	89	9-Octadecenoic acid, (E)-
10	45.582	283089	20.28	45975	10.12	6.16	91	Diosgenin
		1396125	100.00	454284	100.00			

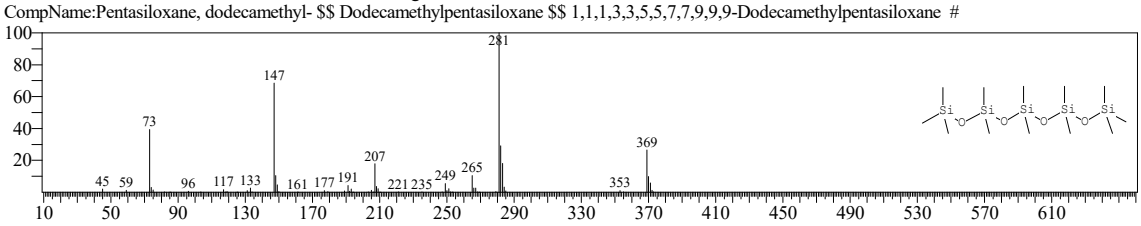
Library

TNAU

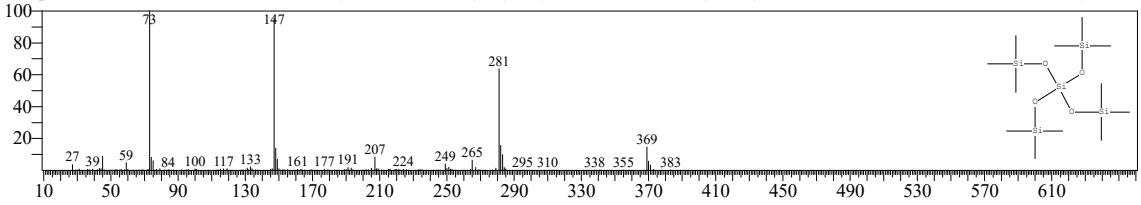
<< Target >>
Line#:1 R.Time:9.760(Scan#:953) MassPeaks:319
RawMode:Averaged 9.755-9.765(952-954) BasePeak:281.05(2843)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



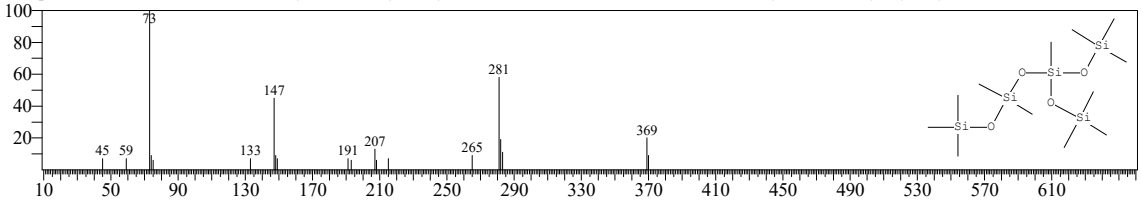
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:92 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



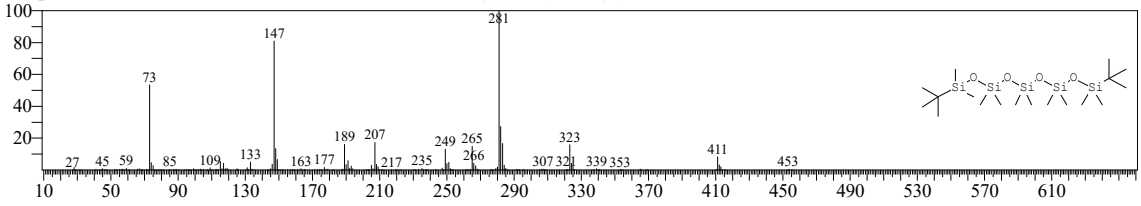
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



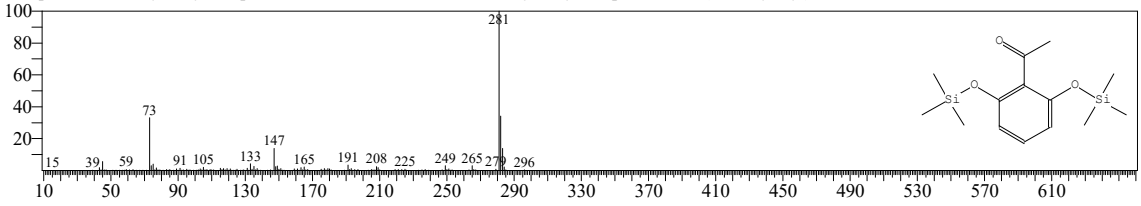
Hit#:3 Entry:249271 Library:NIST20M1.lib
SI:80 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



Hit#:4 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)-

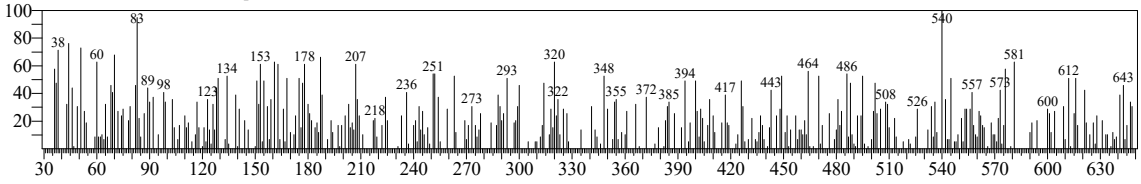


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:73 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

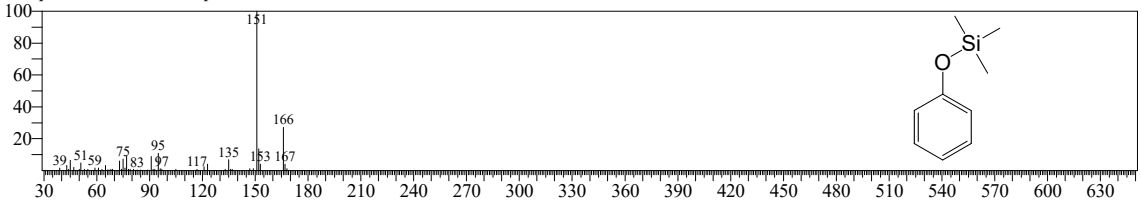


TNAU

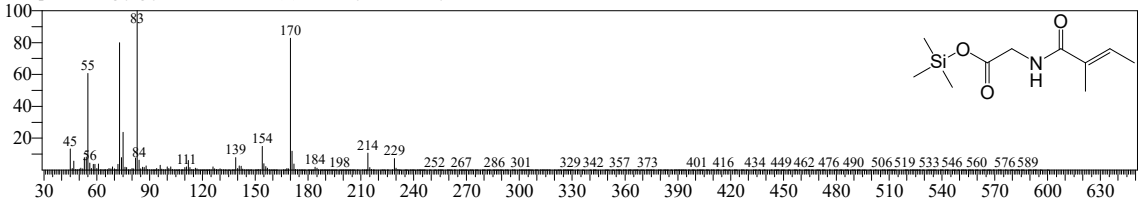
<< Target >>
Line#:2 R.Time:9.820(Scan#:965) MassPeaks:354
RawMode:Averaged 9.815-9.825(964-966) BasePeak:540.00(59)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



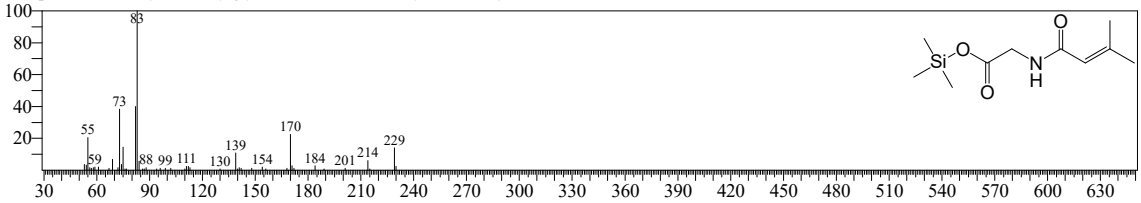
Hit#:1 Entry:7 Library:OA_TMS_DB5_67min_V3.lib
SI:12 Formula:C9H14OSi CAS:108-95-2 MolWeight:166 RetIndex:1060
CompName:Phenol-TMS ; phenol



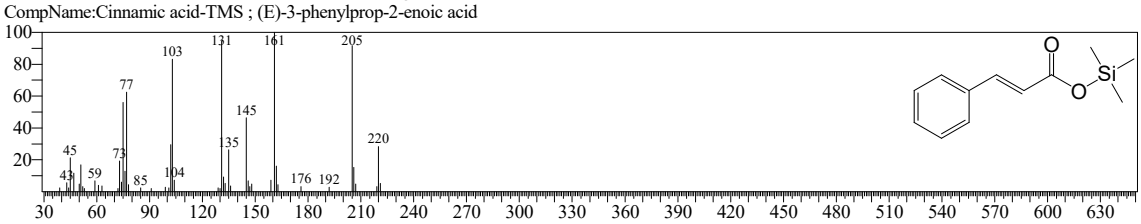
Hit#:2 Entry:178 Library:OA_TMS_DB5_67min_V3.lib
SI:10 Formula:C10H19NO3Si CAS:35842-45-6 MolWeight:229 RetIndex:1571
CompName:Tiglylglycine-TMS ; 2-[[(E)-2-methylbut-2-enoyl]amino]acetic acid



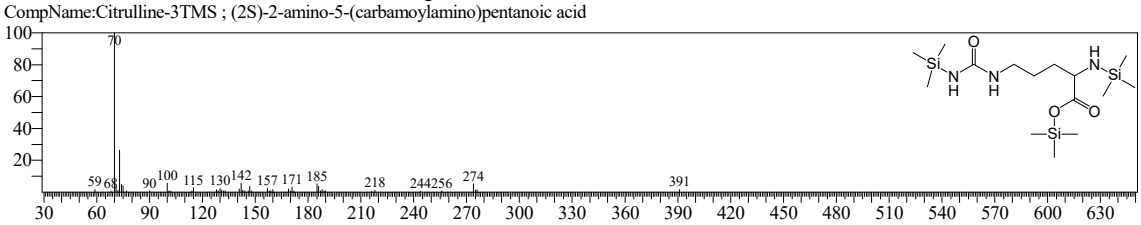
Hit#:3 Entry:175 Library:OA_TMS_DB5_67min_V3.lib
SI:10 Formula:C10H19NO3Si CAS:33008-07-0 MolWeight:229 RetIndex:1564
CompName:3-Methylcrotonoylglycine-TMS ; 2-(3-methylbut-2-enoylamino)acetic acid



Hit#:4 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
SI:10 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid

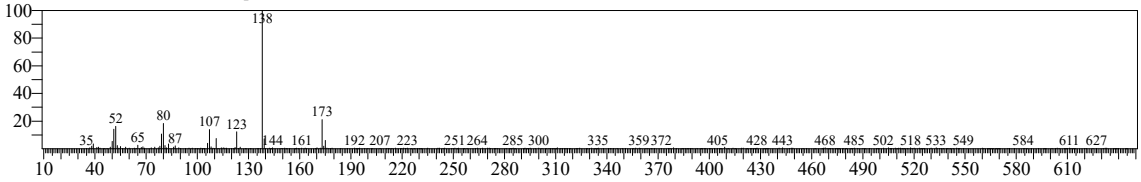


Hit#:5 Entry:459 Library:OA_TMS_DB5_67min_V3.lib
SI:8 Formula:C15H37N3O3Si3 CAS:372-75-8 MolWeight:391 RetIndex:2112
CompName:Citrulline-3TMS ; (2S)-2-amino-5-(carbamoylamino)pentanoic acid

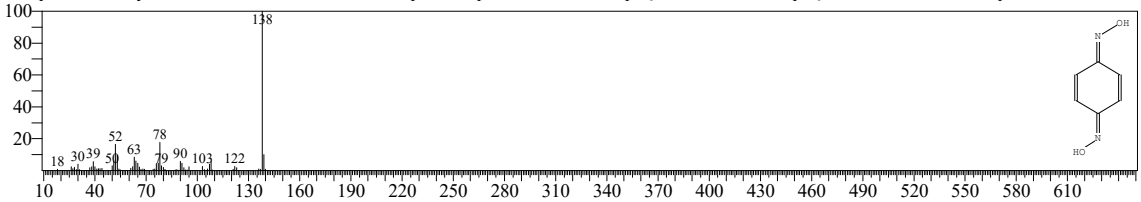


TNAU

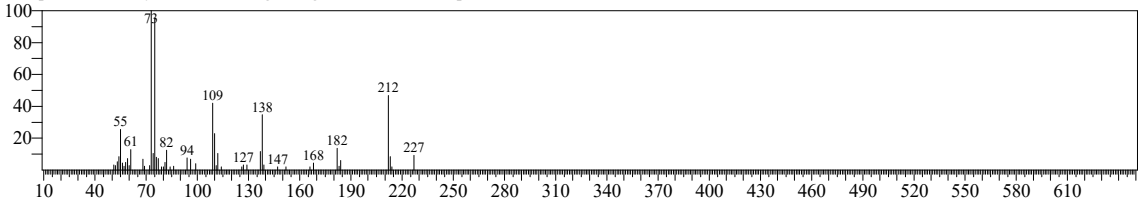
<< Target >>
Line#:3 R.Time:12.825(Scan#:1566) MassPeaks:332
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(5138)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



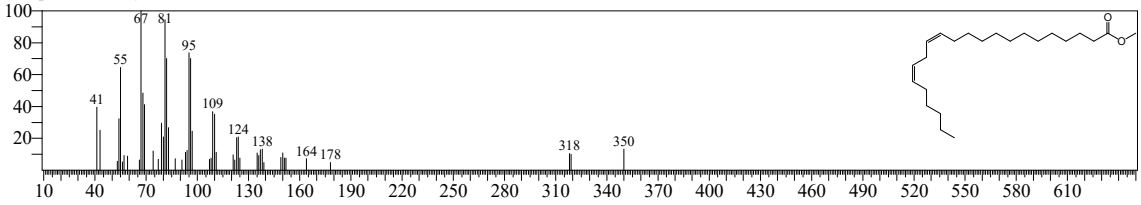
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:70 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



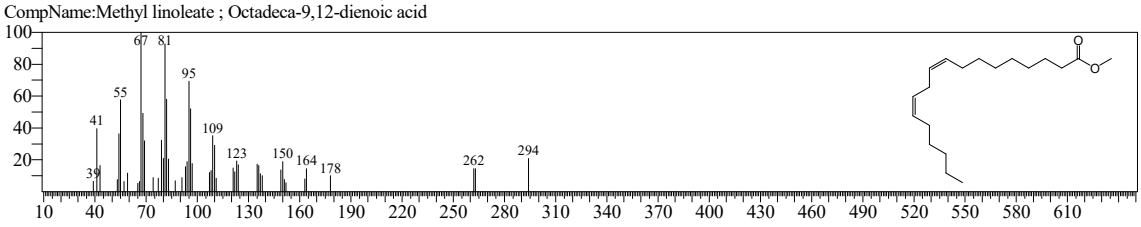
Hit#:2 Entry:127 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula: CAS:51568-18-4 MolWeight:0 RetIndex:1453
CompName:Succinylacetone-ox-origin fragment ; 4,6-dioxoheptanoic acid



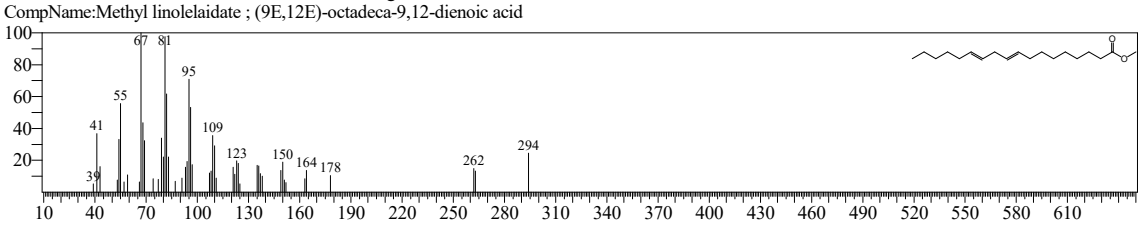
Hit#:3 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:34 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



Hit#:4 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:34 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

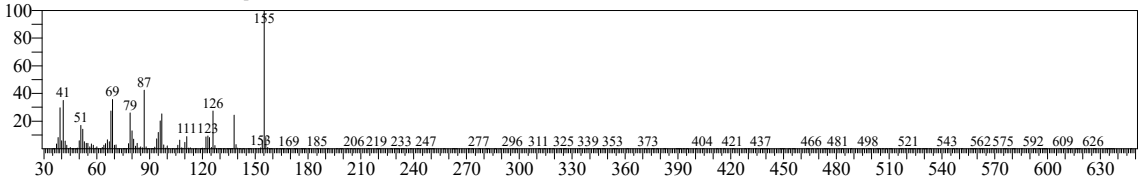


Hit#:5 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

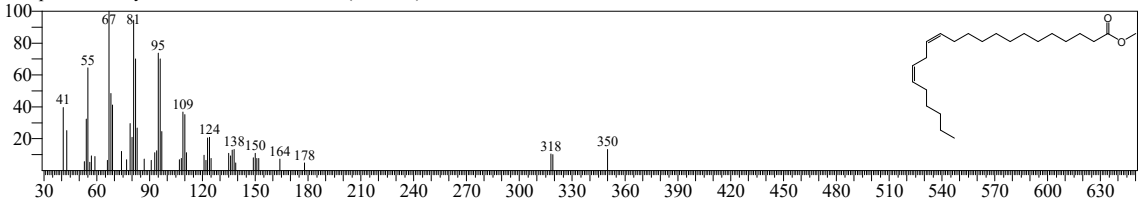


TNAU

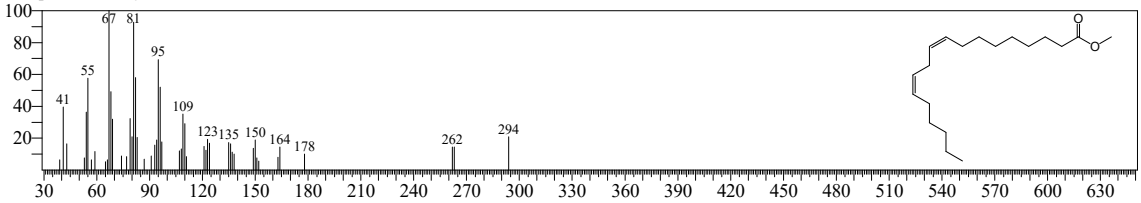
<< Target >>
Line#:4 R.Time:13.225(Scan#:1646) MassPeaks:283
RawMode:Averaged 13.220-13.230(1645-1647) BasePeak:155.05(26843)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



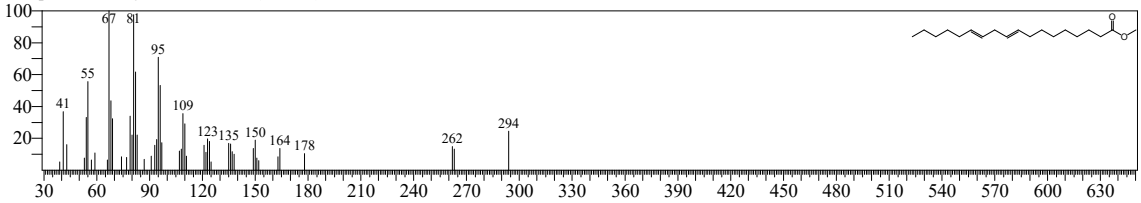
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



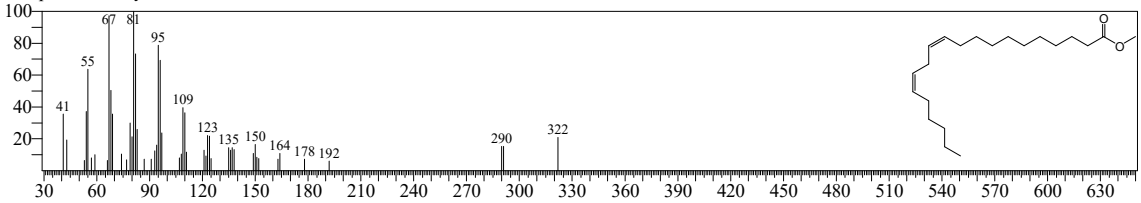
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



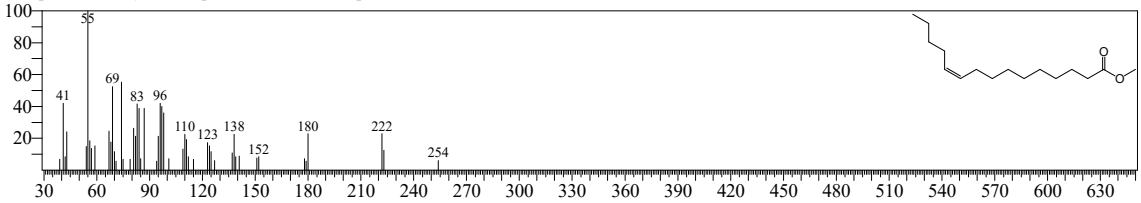
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry: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

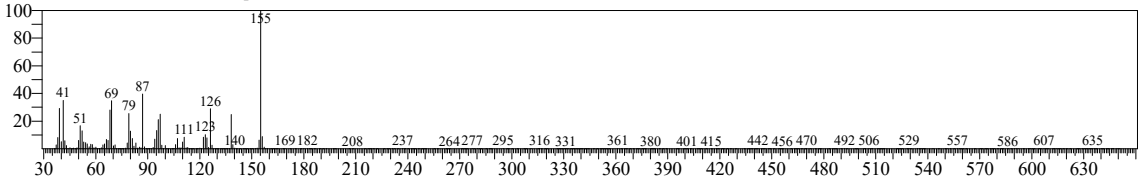


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

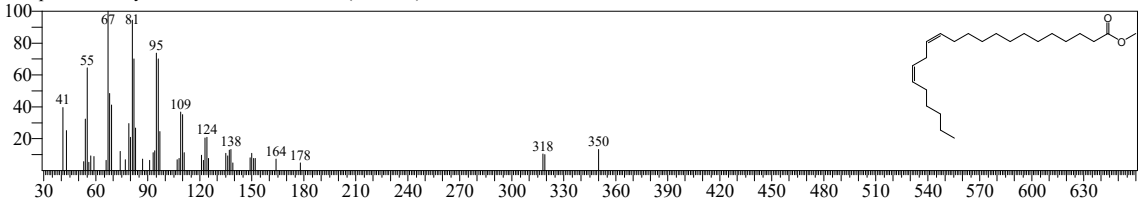


TNAU

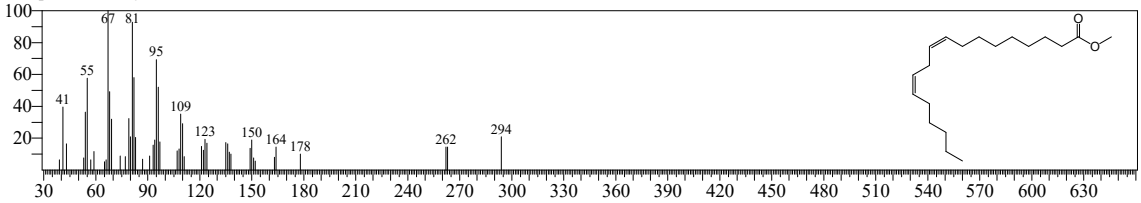
<< Target >>
Line#:5 R.Time:13.420(Scan#:1685) MassPeaks:375
RawMode:Averaged 13.415-13.425(1684-1686) BasePeak:155.10(20685)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



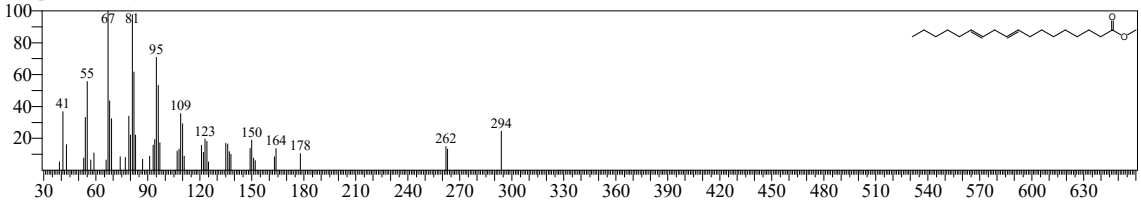
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



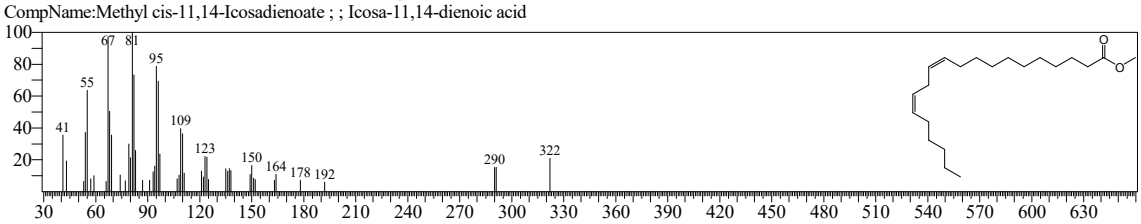
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



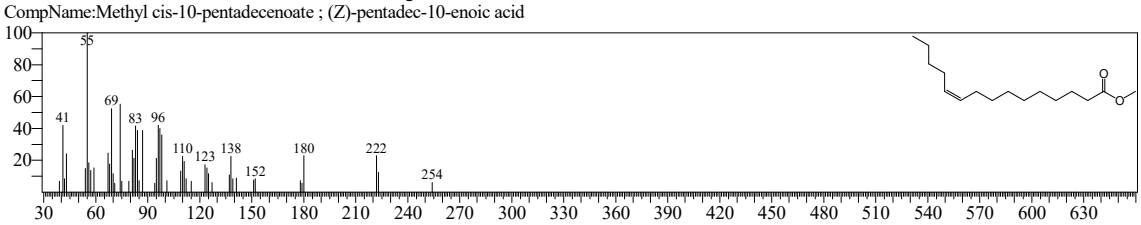
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry: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

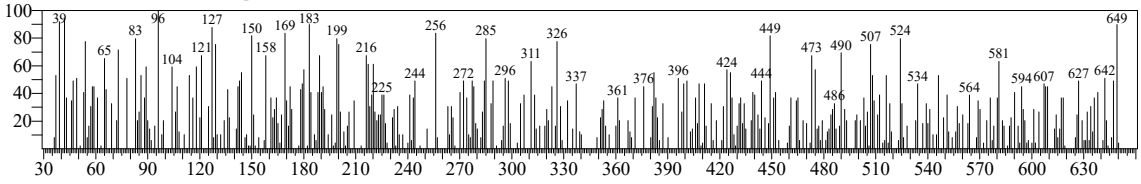


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

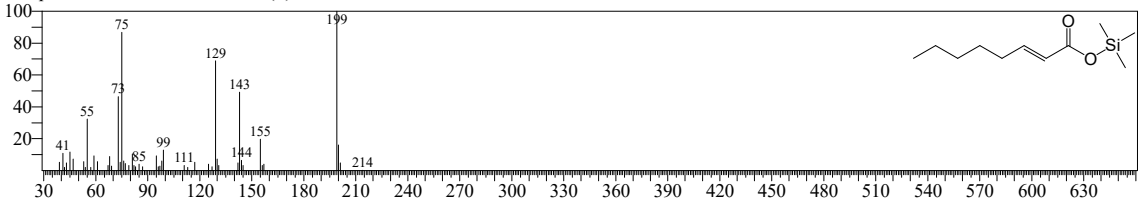


TNAU

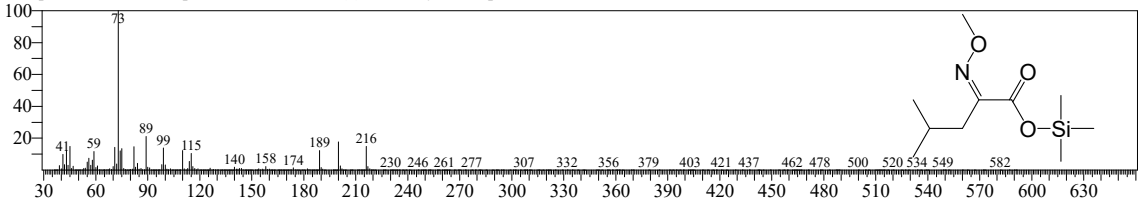
<< Target >>
Line#:6 R.Time:13.510(Scan#:1703) MassPeaks:371
RawMode:Averaged 13.505-13.515(1702-1704) BasePeak:96.00(49)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



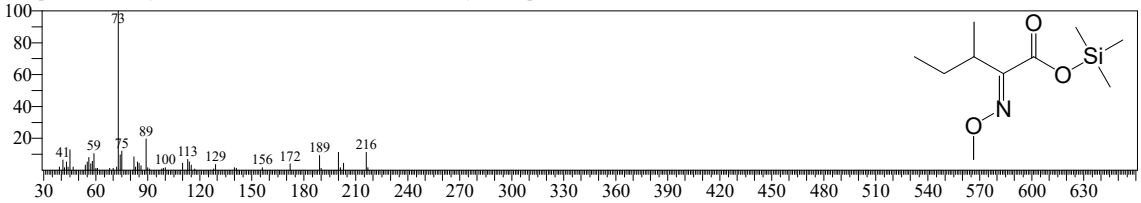
Hit#:1 Entry:91 Library:OA_TMS_DB5_67min_V3.lib
SI:20 Formula:C11H22O2Si CAS:1871-67-6 MolWeight:214 RetIndex:1313
CompName:2-Octenoic acid-TMS ; (E)-oct-2-enoic acid



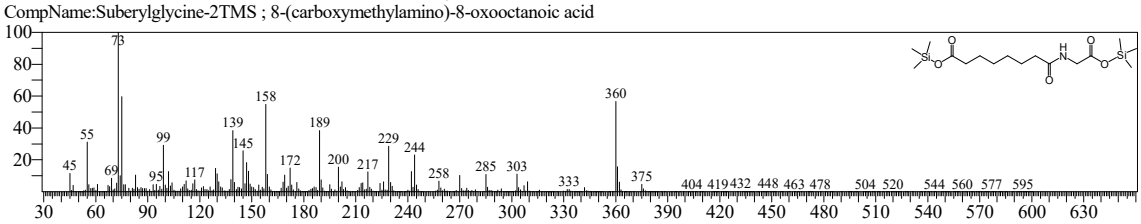
Hit#:2 Entry:51 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1217
CompName:2-Ketoisocaproic acid-meto-TMS(2) ; 4-methyl-2-oxopentanoic acid



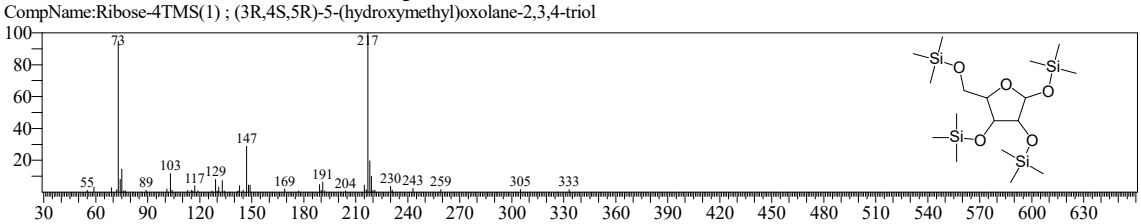
Hit#:3 Entry:42 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C10H21NO3Si CAS:1460-34-0 MolWeight:231 RetIndex:1204
CompName:3-Methyl-2-oxovaleric acid-meto-TMS(2) ; 3-methyl-2-oxopentanoic acid



Hit#:4 Entry:497 Library:OA_TMS_DB5_67min_V3.lib
SI:17 Formula:C16H33NO5Si2 CAS:60317-54-6 MolWeight:375 RetIndex:2271
CompName:Suberylglycine-2TMS ; 8-(carboxymethylamino)-8-oxooctanoic acid

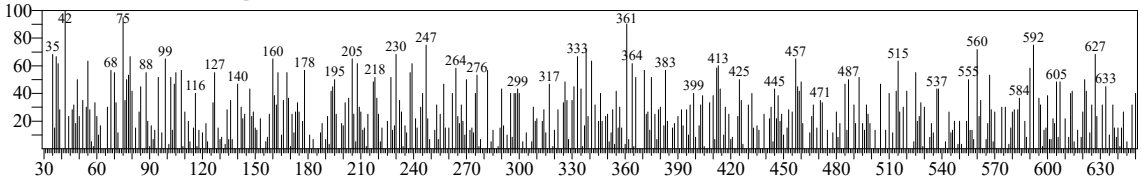


Hit#:5 Entry:227 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C17H42O5Si4 CAS:50-69-1 MolWeight:438 RetIndex:1657
CompName:Ribose-4TMS(1) ; (3R,4S,5R)-5-(hydroxymethyl)oxolane-2,3,4-triol

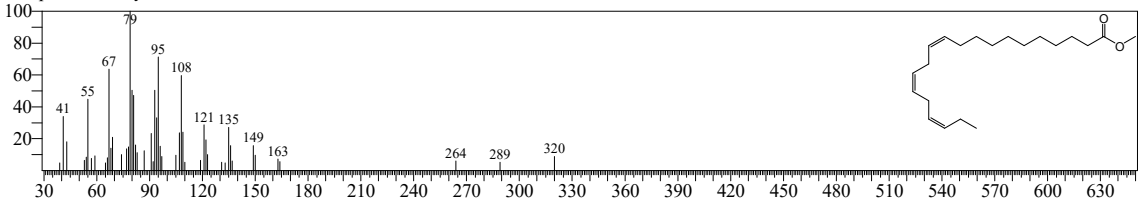


TNAU

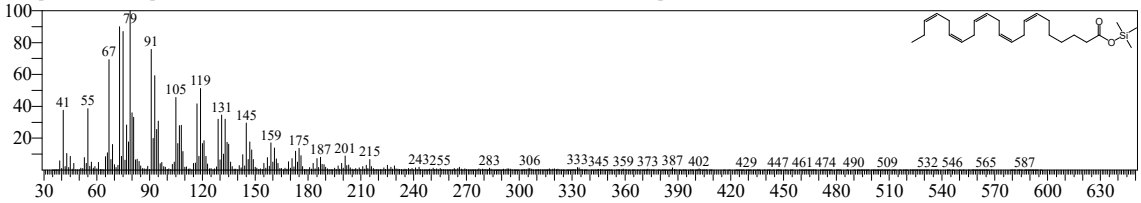
<< Target >>
Line#:7 R.Time:17.460(Scan#:2493) MassPeaks:415
RawMode:Averaged 17.455-17.465(2492-2494) BasePeak:42.00(60)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



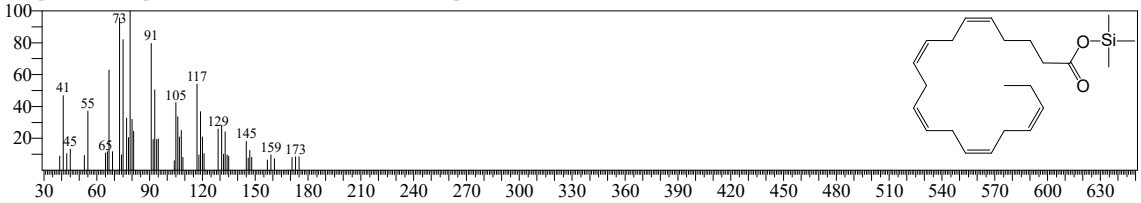
Hit#:1 Entry:31 Library:FA_ME_SP2560_EI_V3.lib
SI:17 Formula:C21H36O2 CAS:2091-27-2 MolWeight:320 RetIndex:3089
CompName:Methyl cis-11,14,17-Icosatrienoate ; Icosa-11,14,17-trienoic acid



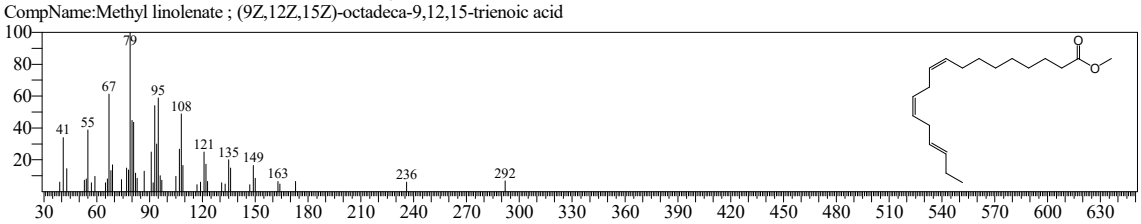
Hit#:2 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid



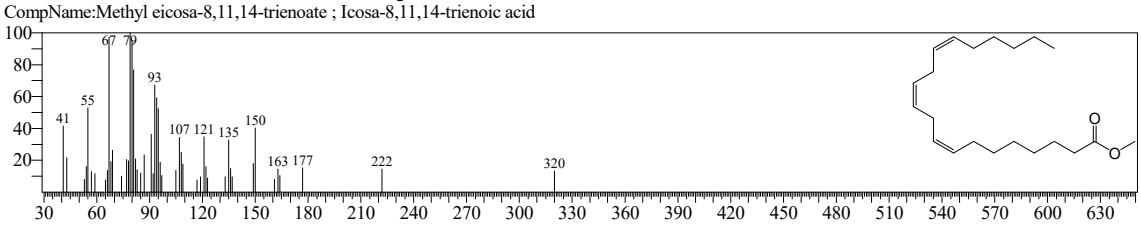
Hit#:3 Entry:509 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C23H38O2Si CAS:10417-94-4 MolWeight:374 RetIndex:2389
CompName:Eicosapentaenoic acid-TMS ; icosa-5,8,11,14,17-pentaenoic acid



Hit#:4 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:15 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

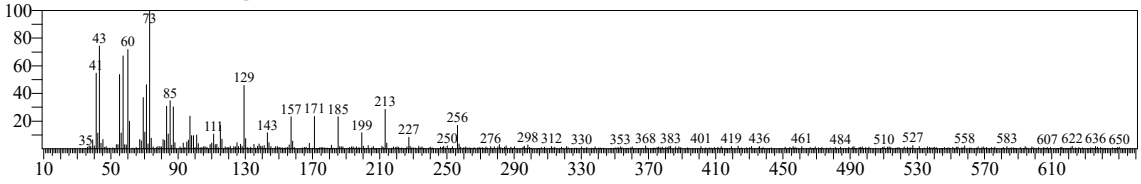


Hit#:5 Entry:29 Library:FA_ME_SP2560_EI_V3.lib
SI:14 Formula:C21H36O2 CAS:1783-84-2 MolWeight:320 RetIndex:3049
CompName:Methyl eicosa-8,11,14-trienoate ; Icosa-8,11,14-trienoic acid

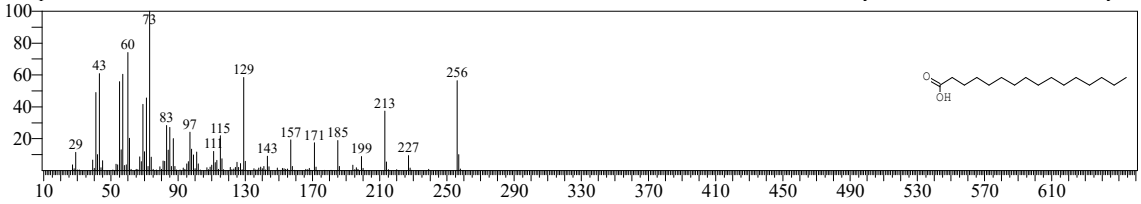


TNAU

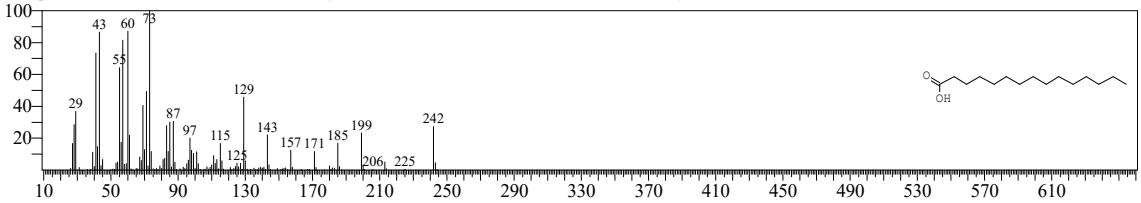
<< Target >>
Line#:8 R.Time:28.285(Scan#:4658) MassPeaks:439
RawMode:Averaged 28.280-28.290(4657-4659) BasePeak:73.05(2118)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



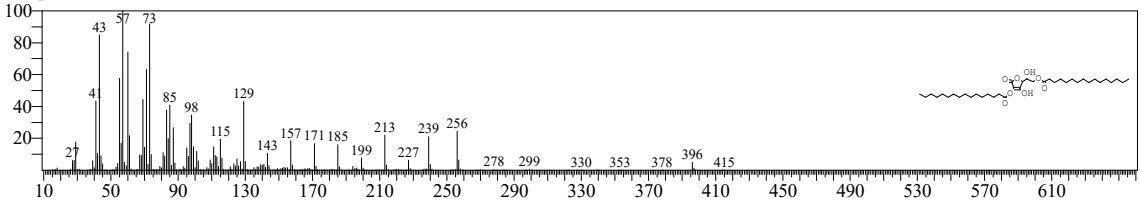
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:93 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



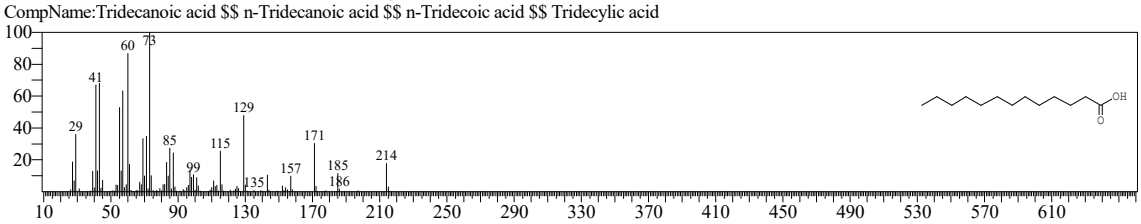
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:90 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



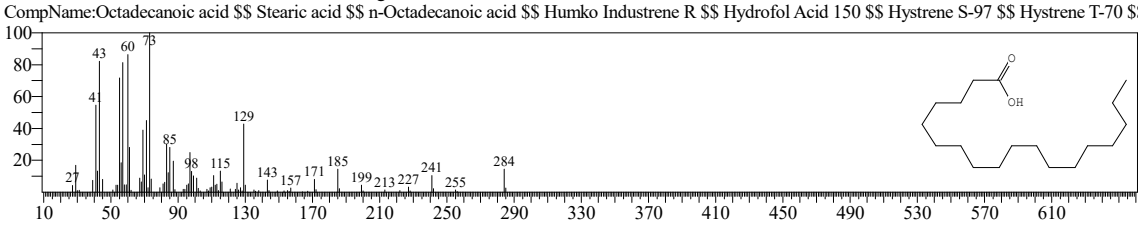
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:90 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:4 Entry:25643 Library:NIST20R.lib
SI:89 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

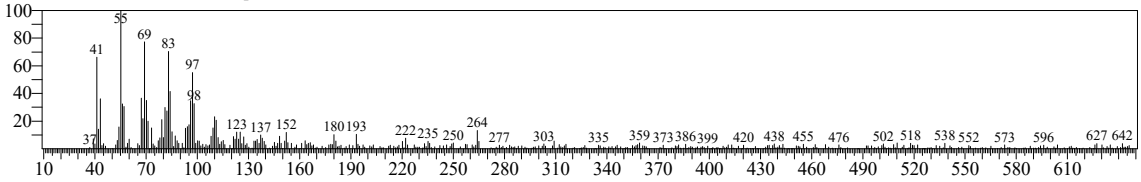


Hit#:5 Entry:144781 Library:NIST20M1.lib
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $

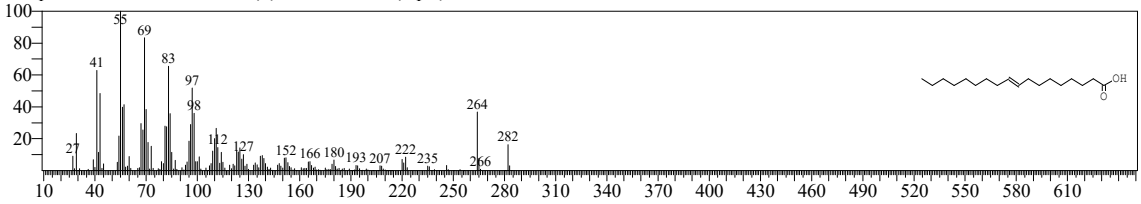


TNAU

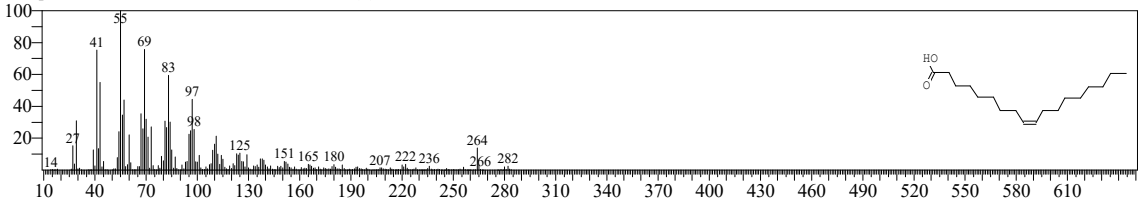
<< Target >>
Line#:9 R.Time:31.580(Scan#:5317) MassPeaks:404
RawMode:Averaged 31.575-31.585(5316-5318) BasePeak:55.05(936)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



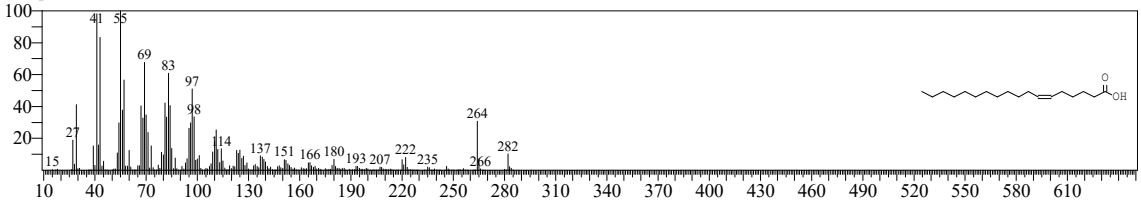
Hit#:1 Entry:34243 Library:NIST20R.lib
SI:89 Formula:C18H34O2 CAS:112-79-8 MolWeight:282 RetIndex:2175
CompName:9-Octadecenoic acid, (E)- $$ trans-.delta.(sup 9)-Octadecenoic acid $$ trans-.delta.9-Octadecenoic acid $$ trans-Octadec-9-enoic acid $$ trans-



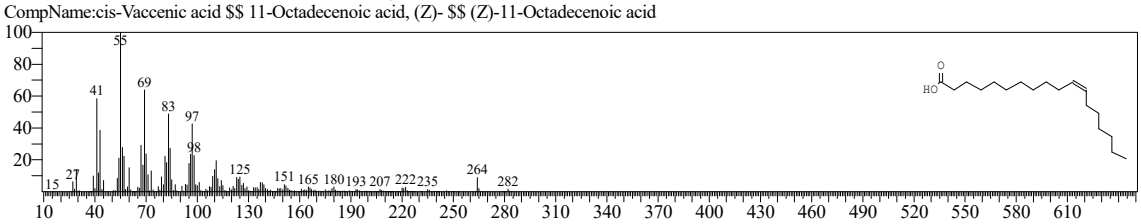
Hit#:2 Entry:34244 Library:NIST20R.lib
SI:88 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .DELTA.9-cis-Oleic acid $$ cis-Oleic Acid $$ cis-9-Octadecenoic Acid $$ Emersol 211 $$ Emersol



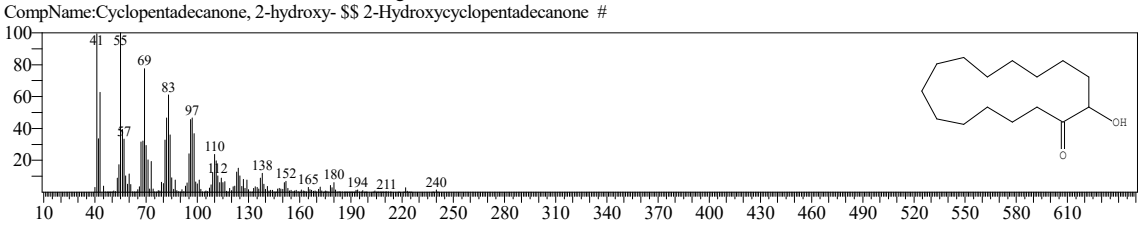
Hit#:3 Entry:142103 Library:NIST20M1.lib
SI:87 Formula:C18H34O2 CAS:593-39-5 MolWeight:282 RetIndex:2175
CompName:6-Octadecenoic acid, (Z)- $$ (6Z)-6-Octadecenoic acid # $$ cis- -6-Octadecenoic acid $$ (Z)-Octadec-6-enoic acid $$ Petroselinic acid



Hit#:4 Entry:142158 Library:NIST20M1.lib
SI:87 Formula:C18H34O2 CAS:506-17-2 MolWeight:282 RetIndex:2175
CompName:cis-Vaccenic acid $$ 11-Octadecenoic acid, (Z)- $$ (Z)-11-Octadecenoic acid

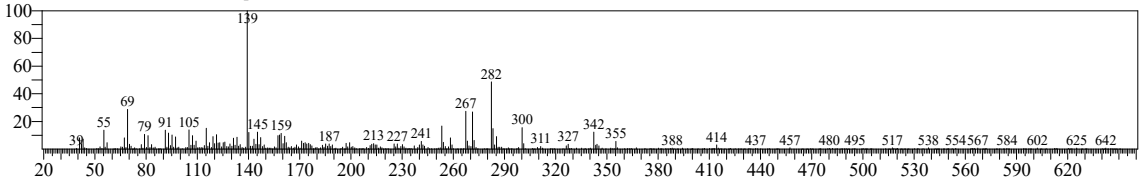


Hit#:5 Entry:94376 Library:NIST20M1.lib
SI:87 Formula:C15H28O2 CAS:4727-18-8 MolWeight:240 RetIndex:2158
CompName:Cyclopentadecanone, 2-hydroxy- $$ 2-Hydroxycyclopentadecanone #

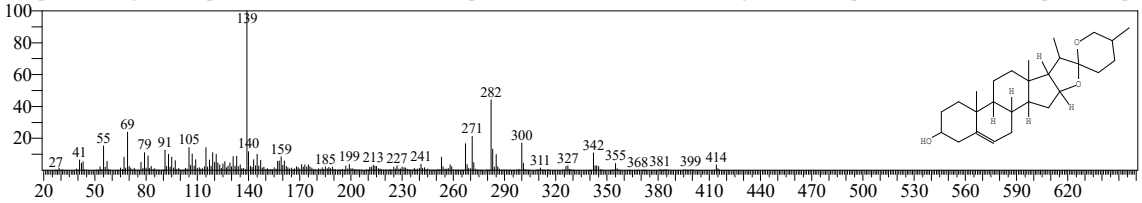


TNAU

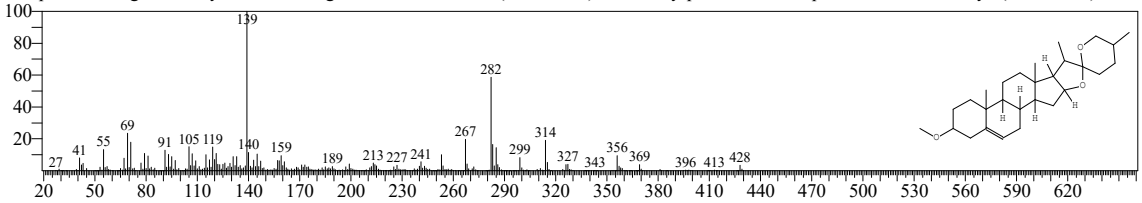
<< Target >>
Line#:10 R.Time:45.580(Scan#:8117) MassPeaks:392
RawMode:Averaged 45.575-45.585(8116-8118) BasePeak:139.15(4990)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



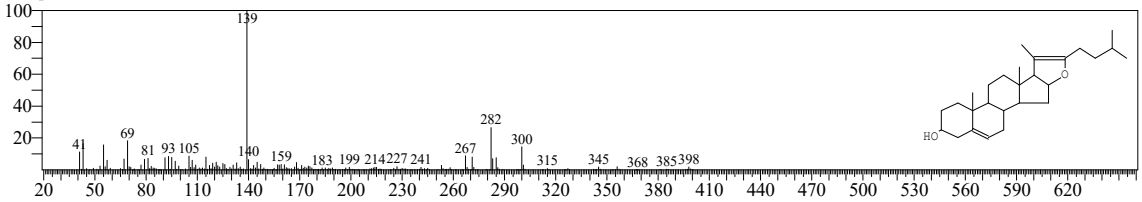
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:91 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



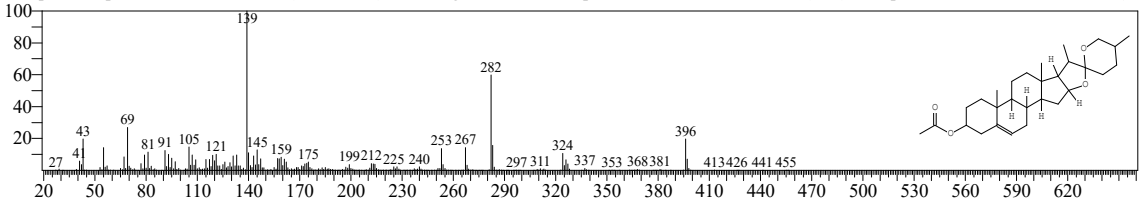
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:82 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#:3 Entry:41561 Library:NIST20R.lib
SI:81 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:79 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:42677 Library:NIST20R.lib
SI:76 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.