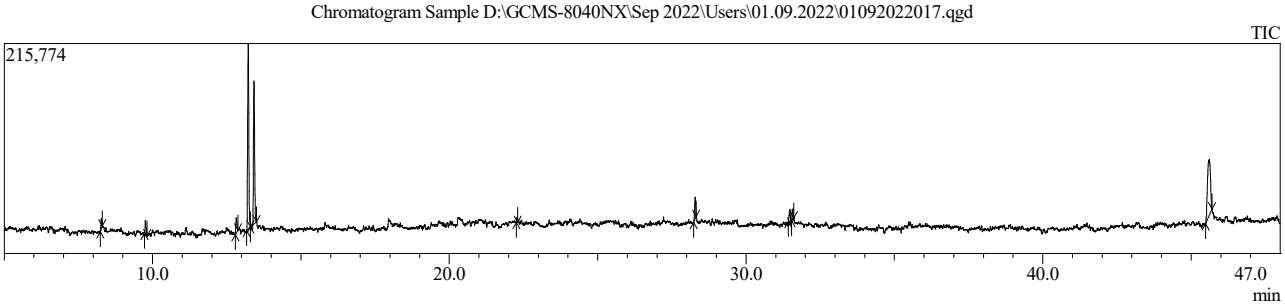
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 7:38:29 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 6-1
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\01092022017.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022017.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 11:03:17 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022017.qgd



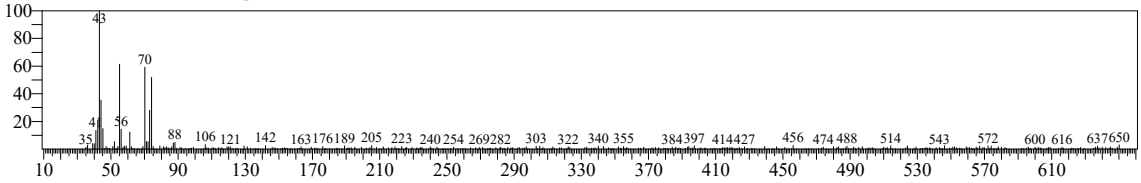
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.273	20350	1.36	10918	2.25	1.86	81	1-Butanol, 3-methyl-, acetate
2	9.760	31767	2.13	14502	2.98	2.19	93	Pentasiloxane, dodecamethyl-
3	12.820	38071	2.55	15386	3.17	2.47	71	2,5-Cyclohexadiene-1,4-dione, dioxime
4	13.224	500642	33.54	190458	39.18	2.63	54	Methyl cis-13,16-Docosadienate
5	13.419	379398	25.42	146987	30.24	2.58	54	Methyl cis-13,16-Docosadienate
6	22.284	7545	0.51	4863	1.00	1.55	17	Norvaline-TMS
7	28.287	53726	3.60	21928	4.51	2.45	92	n-Hexadecanoic acid
8	31.465	34866	2.34	13421	2.76	2.60	93	(9E,11E)-Octadecadienoic acid
9	31.580	21596	1.45	10283	2.12	2.10	87	9-Octadecenoic acid
10	45.613	404650	27.11	57349	11.80	7.06	89	Diosgenin
		1492611	100.00	486095	100.00			

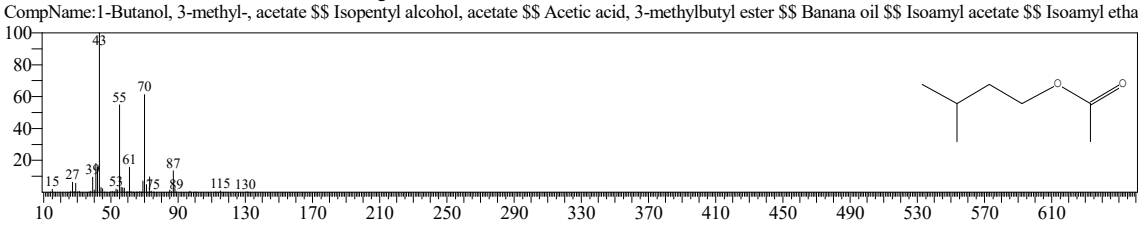
Library

TNAU

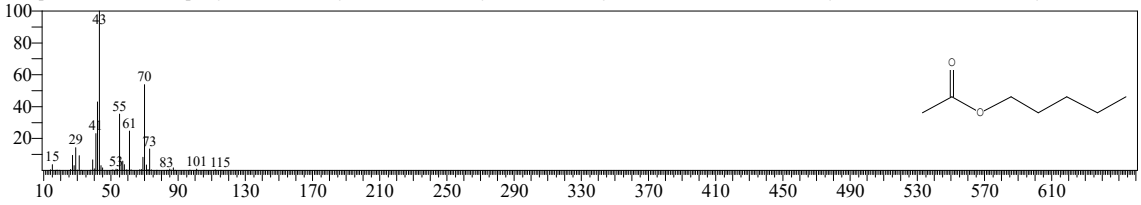
<< Target >>
Line#:1 R.Time:8.275(Scan#:656) MassPeaks:373
RawMode:Averaged 8.270-8.280(655-657) BasePeak:43.00(1631)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



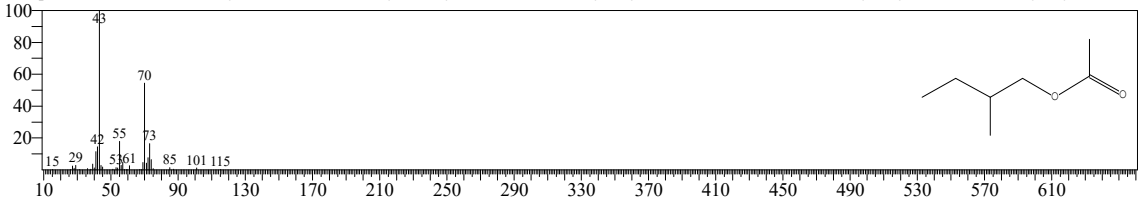
Hit#:1 Entry:6784 Library:NIST20R.lib
SI:81 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



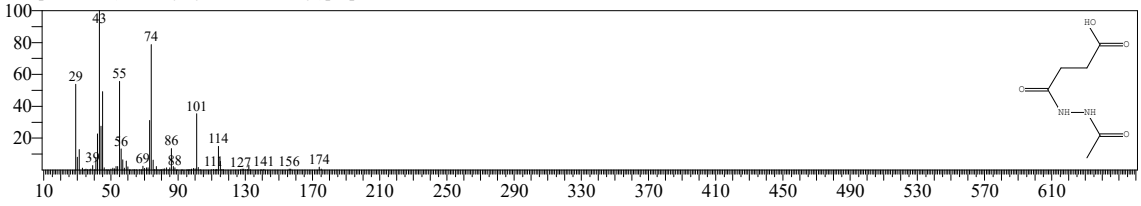
Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:78 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ An



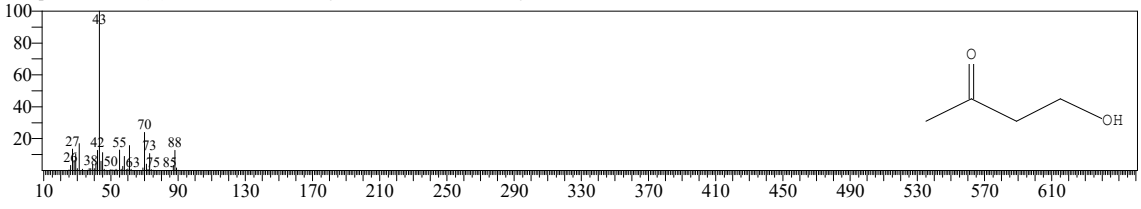
Hit#:3 Entry:6819 Library:NIST20R.lib
SI:77 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:32045 Library:NIST20M1.lib
SI:75 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid

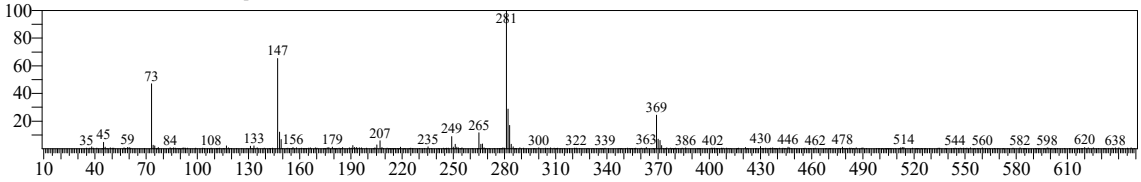


Hit#:5 Entry:1220 Library:NIST20R.lib
SI:75 Formula:C4H8O2 CAS:590-90-9 MolWeight:88 RetIndex:798
CompName:CH3C(O)CH2CH2OH $$ Methylolacetone $$ Monomethylolacetone $$ 3-Ketobutan-1-ol $$ 3-Oxo-1-butanol $$ 3-Oxobutanol $$ 4-Butanol-

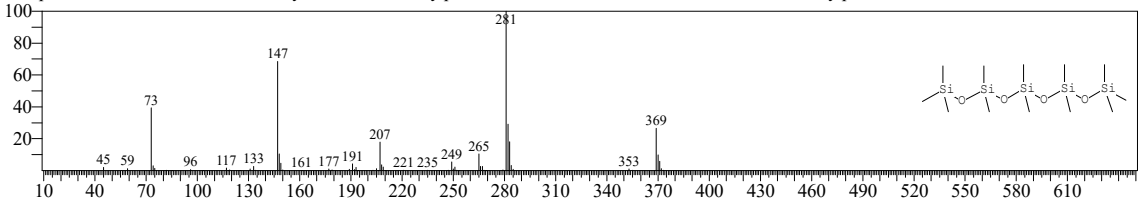


TNAU

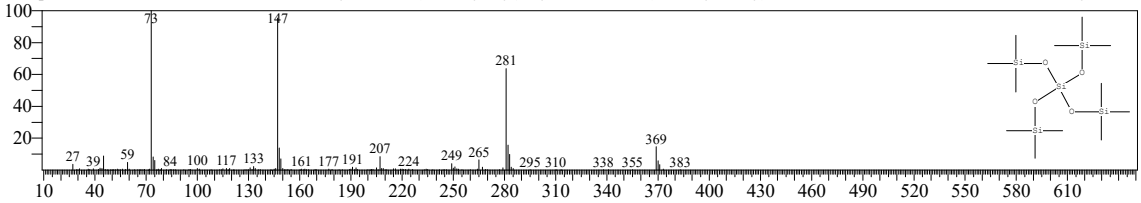
<< Target >>
Line#:2 R.Time:9.760(Scan#:953) MassPeaks:327
RawMode:Averaged 9.755-9.765(952-954) BasePeak:281.05(3499)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



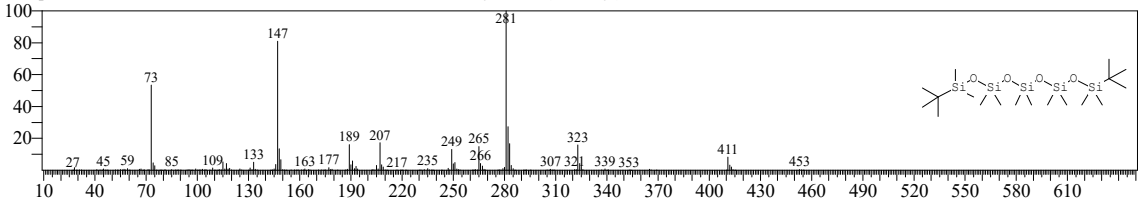
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



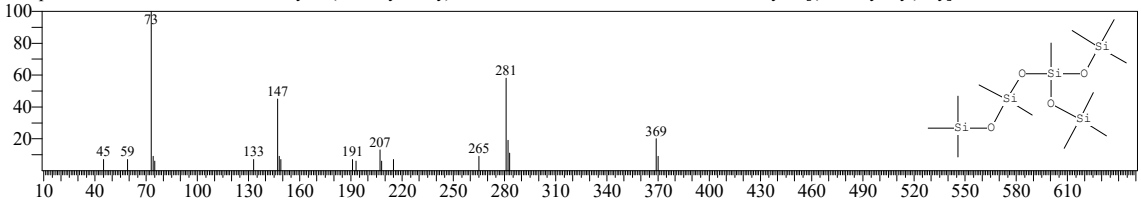
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



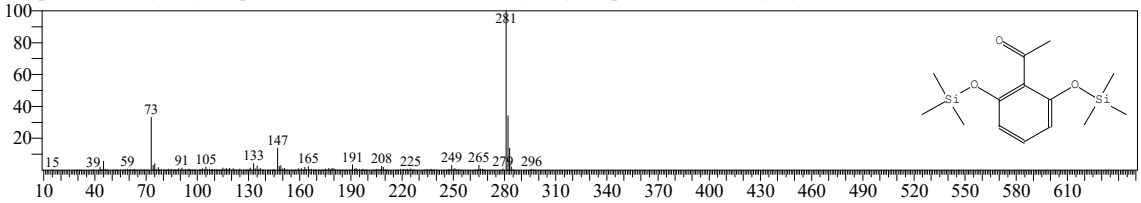
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:80 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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 #

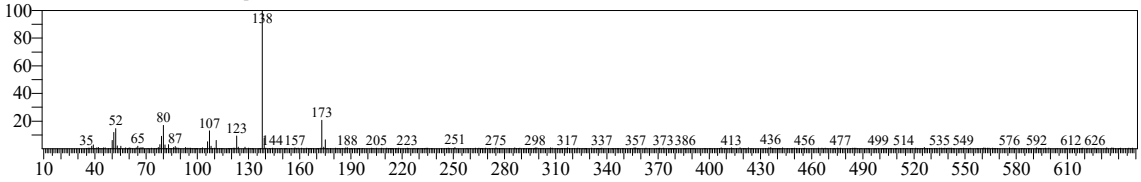


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

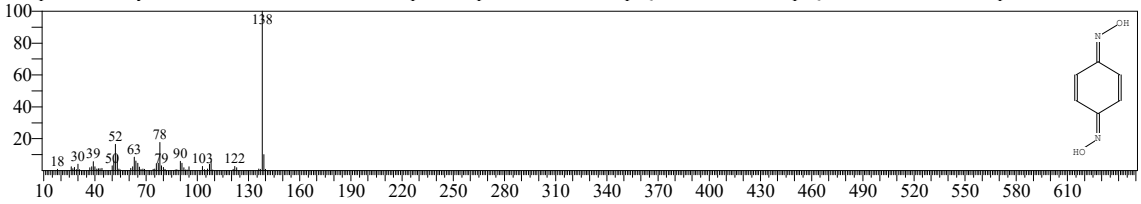


TNAU

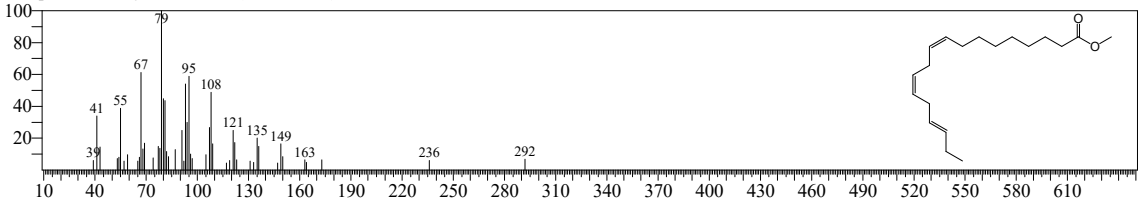
<< Target >>
Line#:3 R.Time:12.820(Scan#:1565) MassPeaks:369
RawMode:Averaged 12.815-12.825(1564-1566) BasePeak:138.05(4919)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



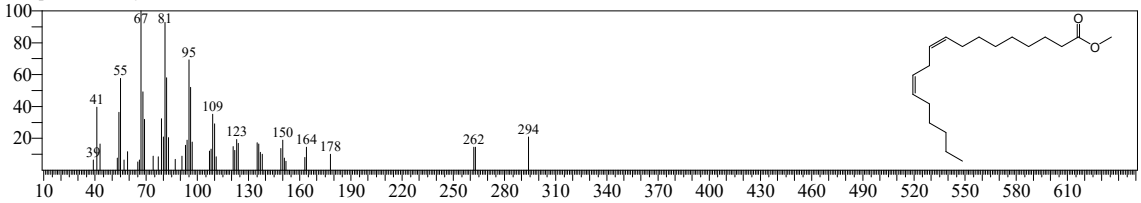
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:71 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



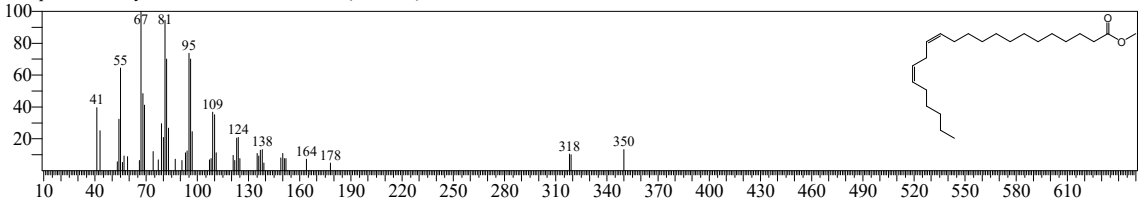
Hit#:2 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid



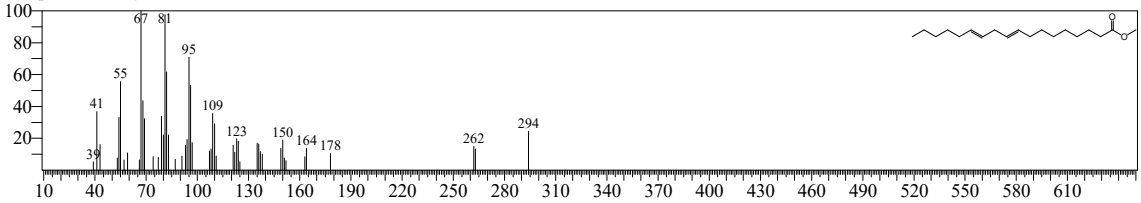
Hit#:3 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



Hit#:4 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:31 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

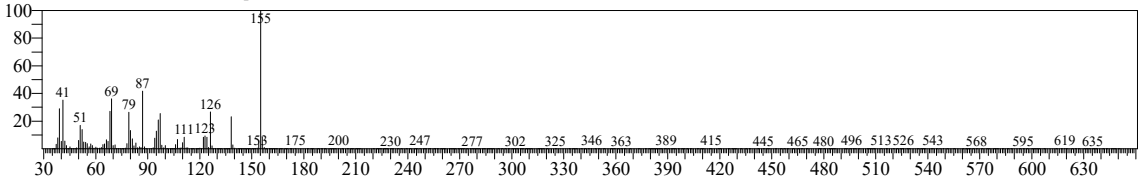


Hit#:5 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:31 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

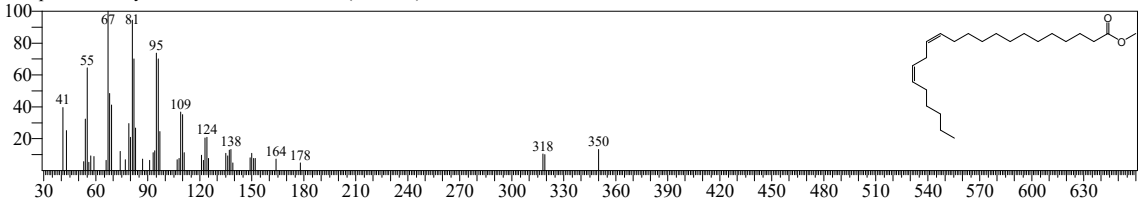


TNAU

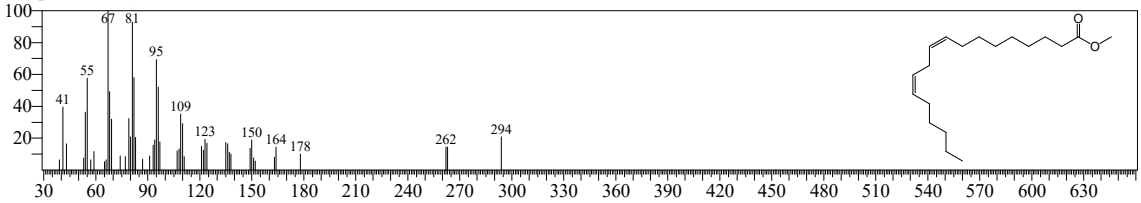
<< Target >>
Line#:4 R.Time:13.225(Scan#:1646) MassPeaks:362
RawMode:Averaged 13.220-13.230(1645-1647) BasePeak:155.05(28677)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



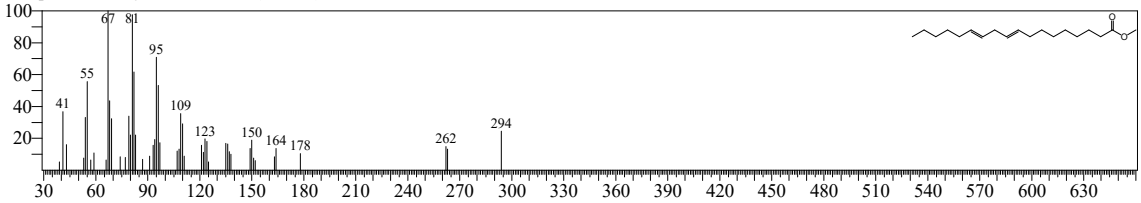
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



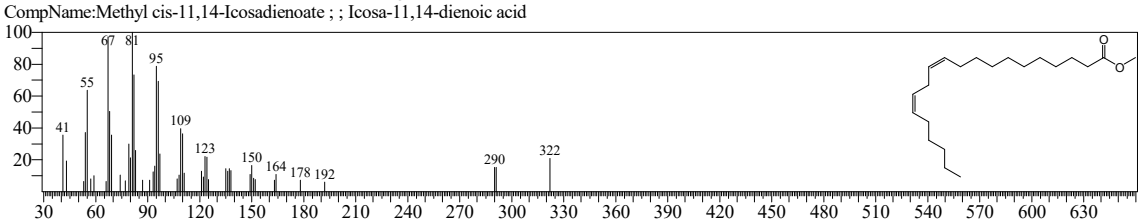
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



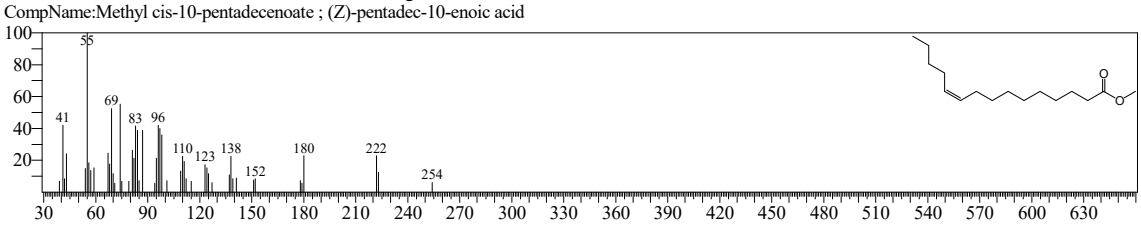
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

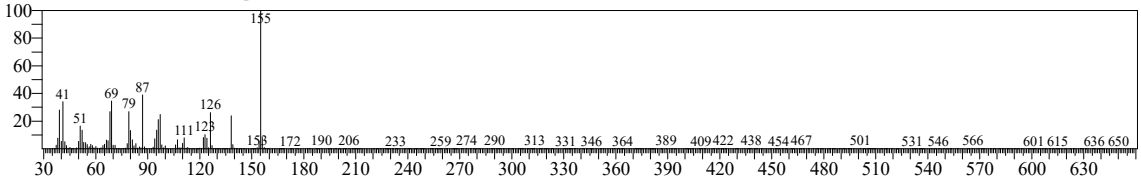


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

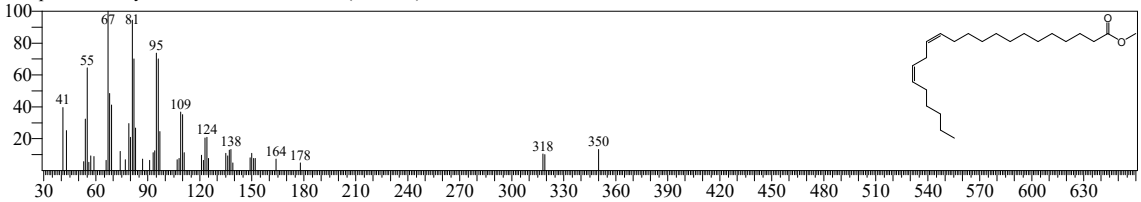


TNAU

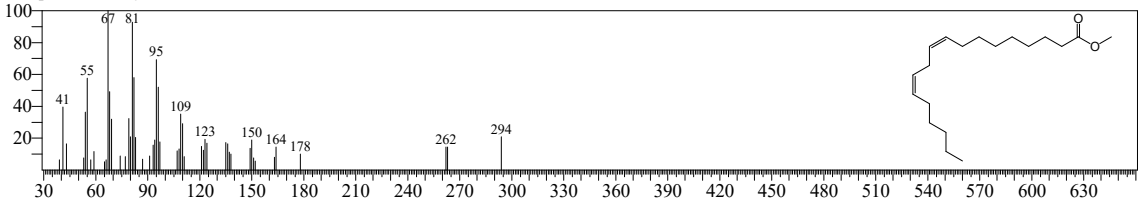
<< Target >>
Line#:5 R.Time:13.420(Scan#:1685) MassPeaks:327
RawMode:Averaged 13.415-13.425(1684-1686) BasePeak:155.05(22884)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



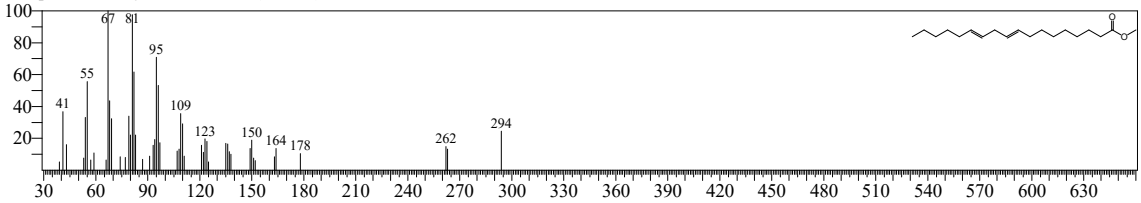
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



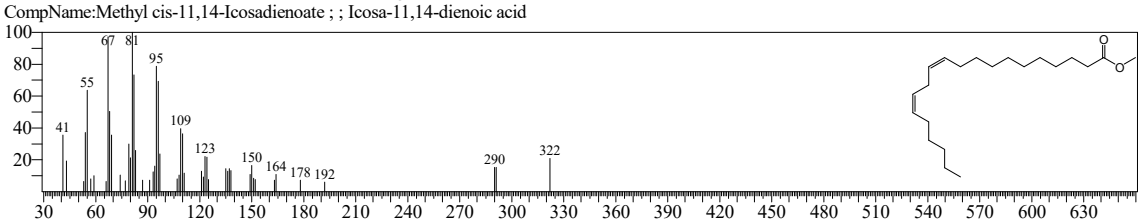
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



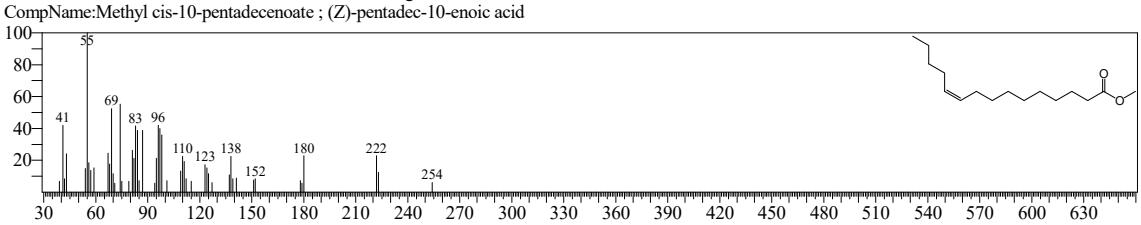
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

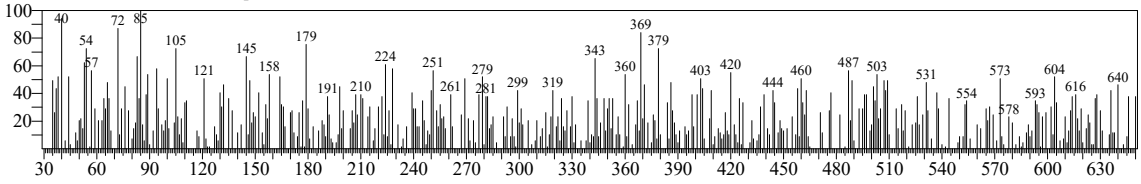


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

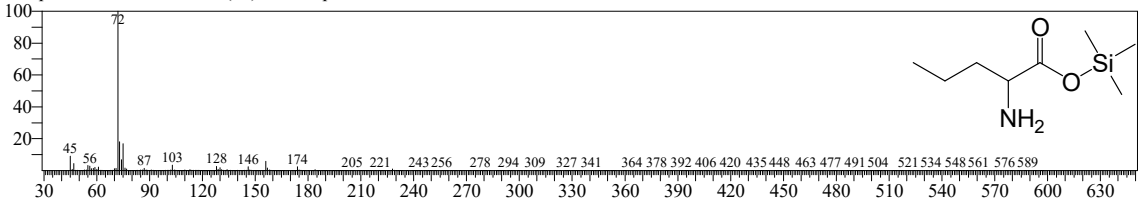


TNAU

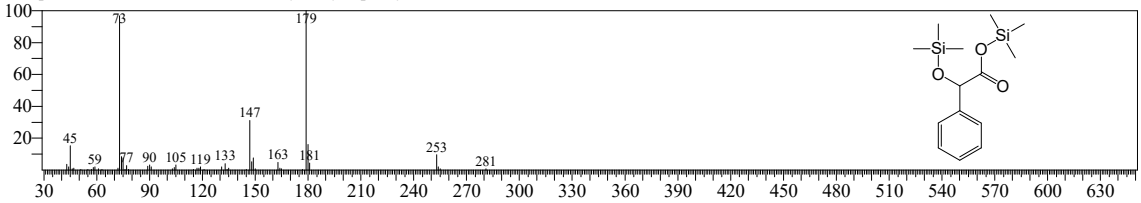
<< Target >>
Line#:6 R.Time:22.285(Scan#:3458) MassPeaks:413
RawMode:Averaged 22.280-22.290(3457-3459) BasePeak:85.00(69)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



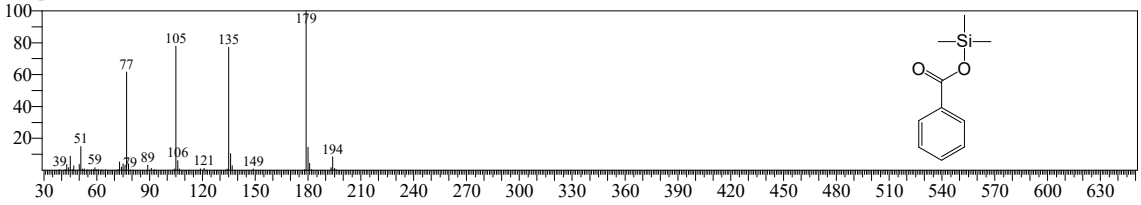
Hit#:1 Entry:18 Library:OA_TMS_DB5_67min_V3.lib
SI:17 Formula:C8H19NO2Si CAS:6600-40-4 MolWeight:189 RetIndex:1113
CompName:Norvaline-TMS ; (2S)-2-aminopentanoic acid



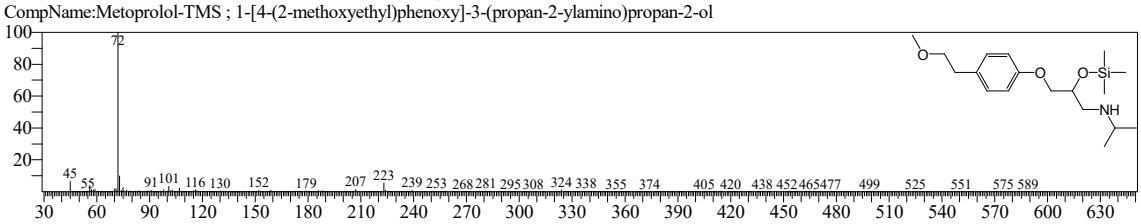
Hit#:2 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



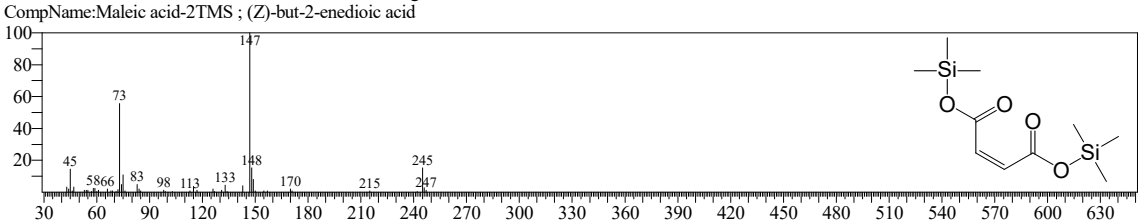
Hit#:3 Entry:66 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C10H14O2Si CAS:65-85-0 MolWeight:194 RetIndex:1252
CompName:Benzoic acid-TMS ; benzoic acid



Hit#:4 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:14 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

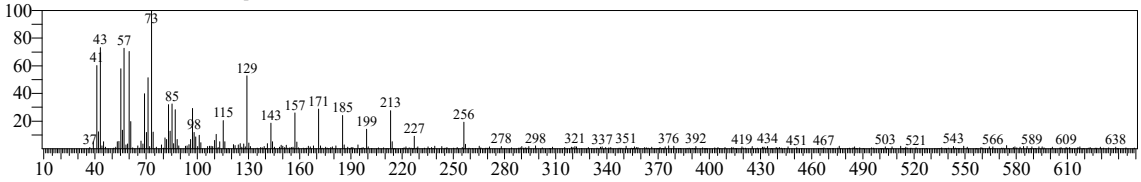


Hit#:5 Entry:90 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C10H20O4Si2 CAS:110-16-7 MolWeight:260 RetIndex:1306
CompName:Maleic acid-2TMS ; (Z)-but-2-enedioic acid

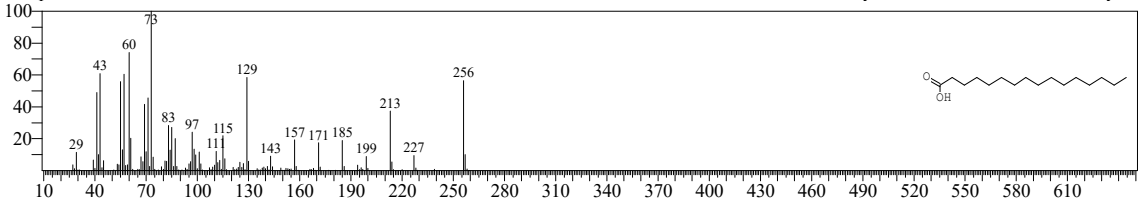


TNAU

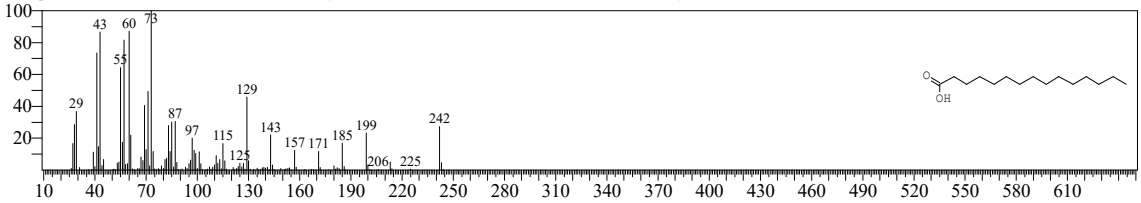
<< Target >>
Line#:7 R.Time:28.285(Scan#:4658) MassPeaks:333
RawMode:Averaged 28.280-28.290(4657-4659) BasePeak:73.05(1813)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



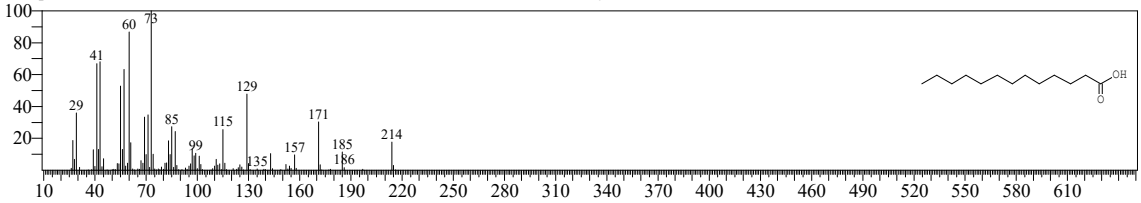
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:92 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



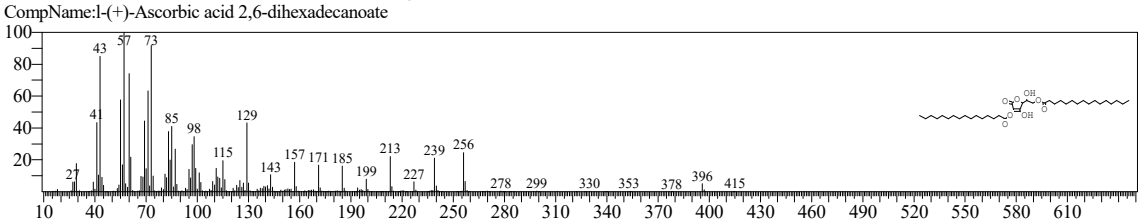
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



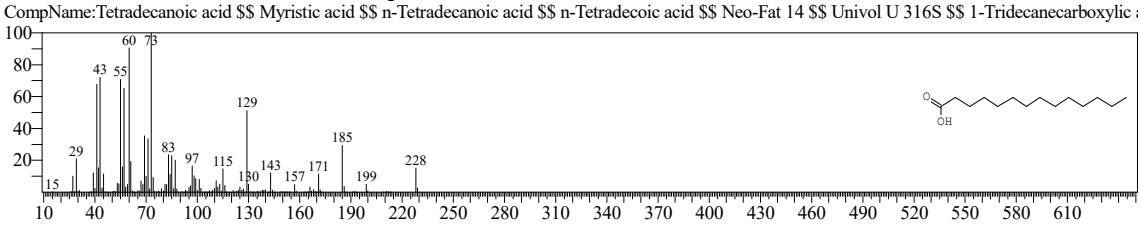
Hit#:3 Entry:25643 Library:NIST20R.lib
SI:89 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid



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

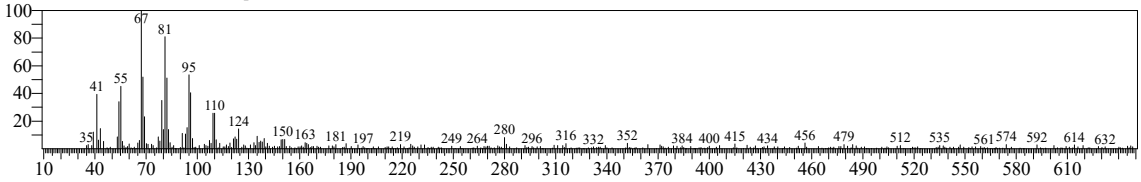


Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:88 Formula:C14H28O2 CAS:544-63-8 MolWeight:228 RetIndex:1769
CompName:Tetradecanoic acid $$ Myristic acid $$ n-Tetradecanoic acid $$ n-Tetradecoic acid $$ Neo-Fat 14 $$ Univol U 316S $$ 1-Tridecanecarboxylic

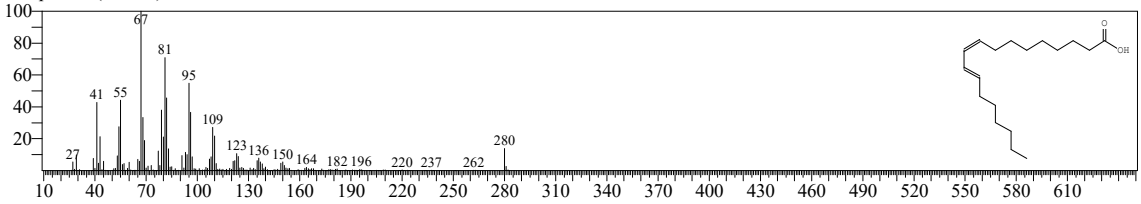


TNAU

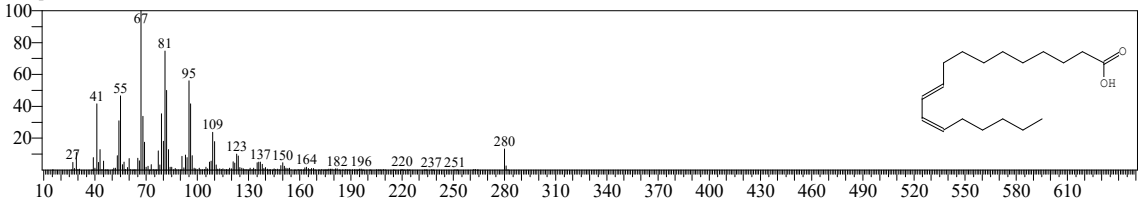
<< Target >>
Line#:8 R.Time:31.465(Scan#:5294) MassPeaks:357
RawMode:Averaged 31.460-31.470(5293-5295) BasePeak:67.05(1202)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



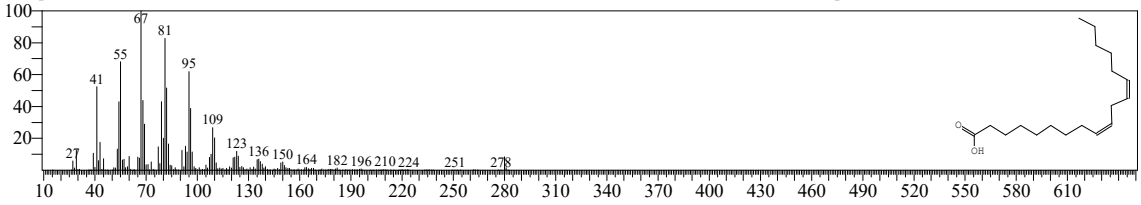
Hit#:1 Entry:139651 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



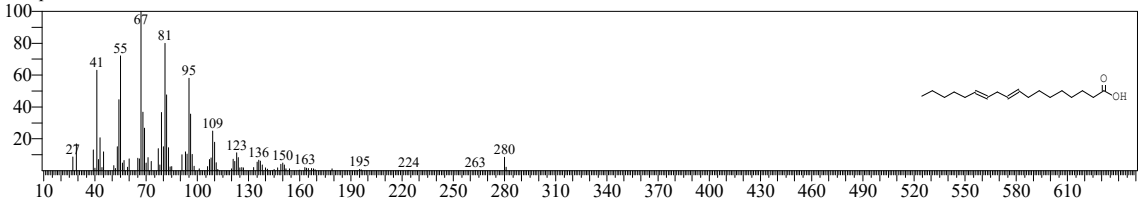
Hit#:2 Entry:139646 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid



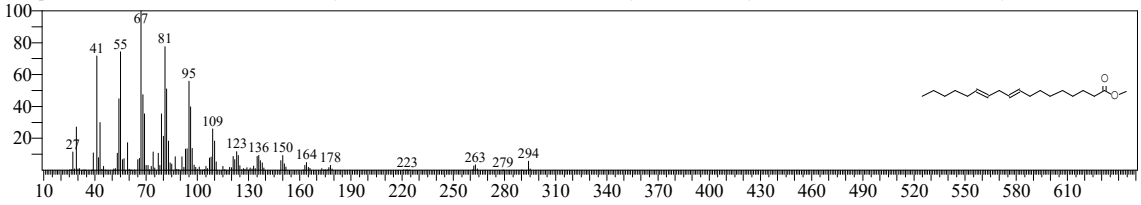
Hit#:3 Entry:34035 Library:NIST20R.lib
SI:92 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



Hit#:4 Entry:139661 Library:NIST20M1.lib
SI:91 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

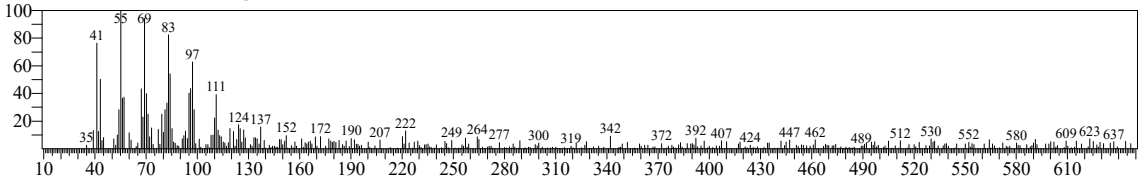


Hit#:5 Entry:156597 Library:NIST20M1.lib
SI:90 Formula:C19H34O2 CAS:2462-85-3 MolWeight:294 RetIndex:2093
CompName:9,12-Octadecadienoic acid, methyl ester $$ 9,12-Octadecenoic acid, methyl ester $$ Methyl octadeca-9,12-dienoate $$ Methyl 9,12-octadecadi

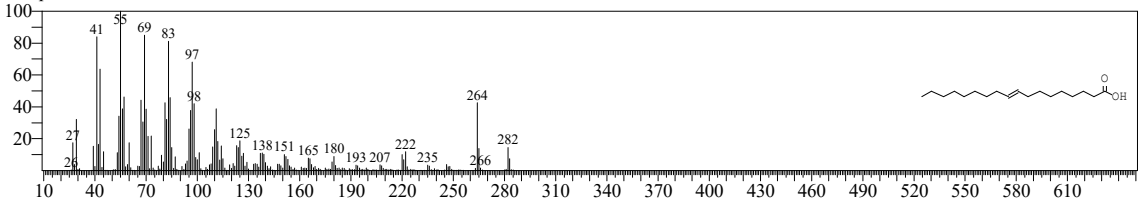


TNAU

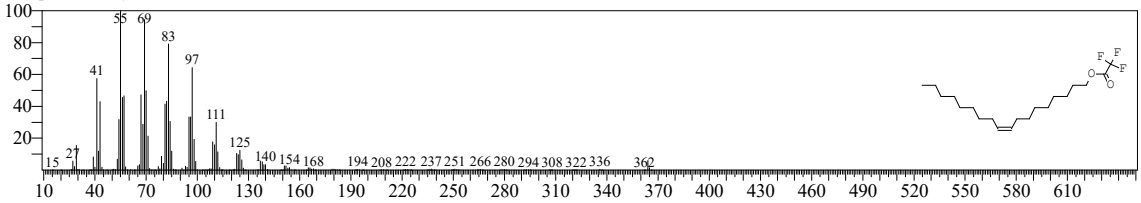
<< Target >>
Line#:9 R.Time:31.580(Scan#:5317) MassPeaks:367
RawMode:Averaged 31.575-31.585(5316-5318) BasePeak:55.10(565)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



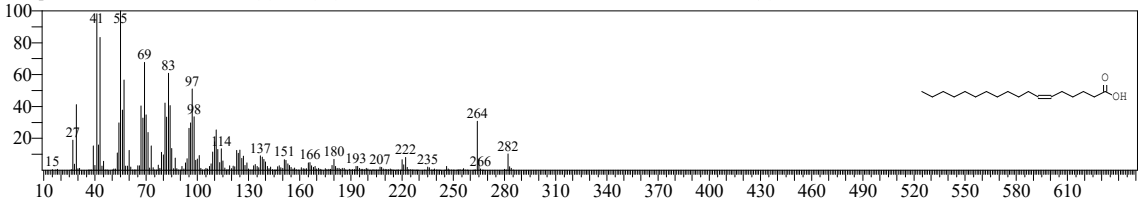
Hit#:1 Entry:142172 Library:NIST20M1.lib
SI:87 Formula:C18H34O2 CAS:2027-47-6 MolWeight:282 RetIndex:2175
CompName:9-Octadecenoic acid



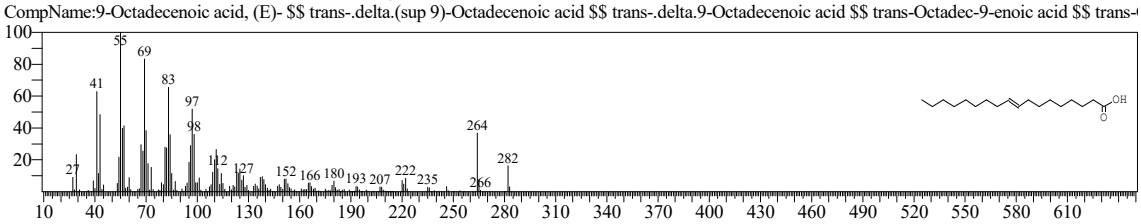
Hit#:2 Entry:233277 Library:NIST20M1.lib
SI:86 Formula:C20H35F3O2 CAS:0-00-0 MolWeight:364 RetIndex:2019
CompName:Oleyl alcohol, trifluoroacetate



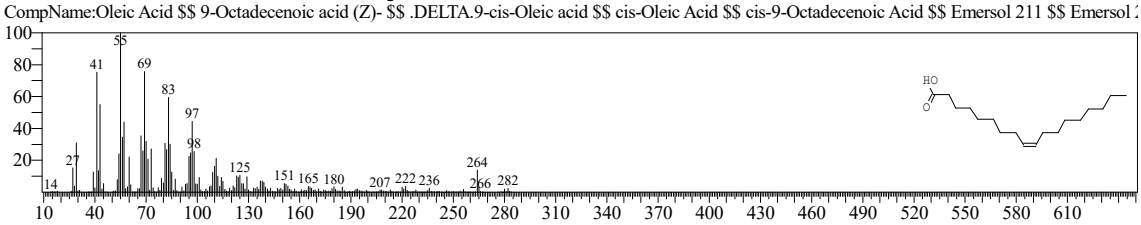
Hit#:3 Entry:142103 Library:NIST20M1.lib
SI:86 Formula:C18H34O2 CAS:593-39-5 MolWeight:282 RetIndex:2175
CompName:6-Octadecenoic acid, (Z)- $$ (6Z)-6-Octadecenoic acid # $$ cis- -6-Octadecenoic acid $$ (Z)-Octadec-6-enoic acid $$ Petroselinic acid



Hit#:4 Entry:34243 Library:NIST20R.lib
SI:86 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-

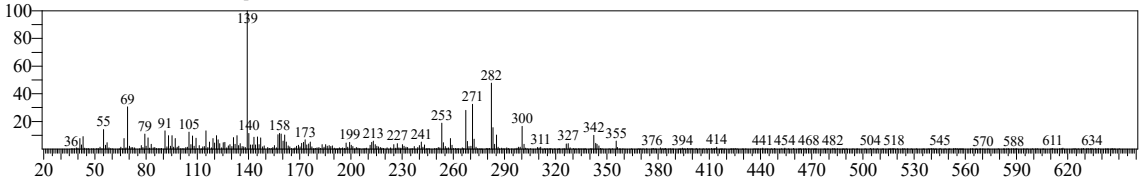


Hit#:5 Entry:34244 Library:NIST20R.lib
SI:85 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .DELTA.9-cis-Oleic acid $$ cis-Oleic Acid $$ cis-9-Octadecenoic Acid $$ Emersol 211 $$ Emersol

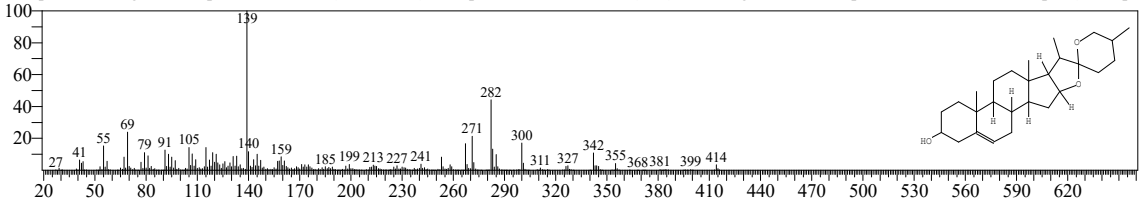


TNAU

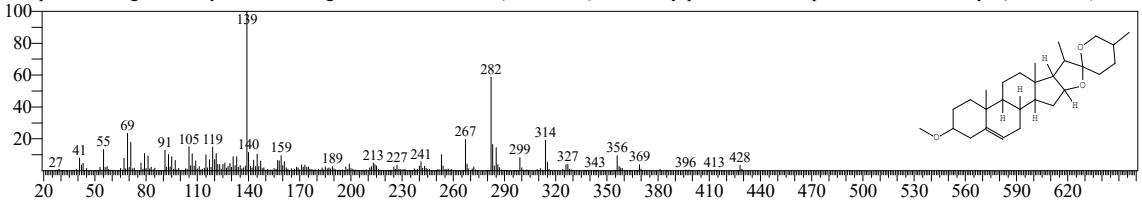
<< Target >>
Line#:10 R.Time:45.615(Scan#:8124) MassPeaks:427
RawMode:Averaged 45.610-45.620(8123-8125) BasePeak:139.10(5968)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



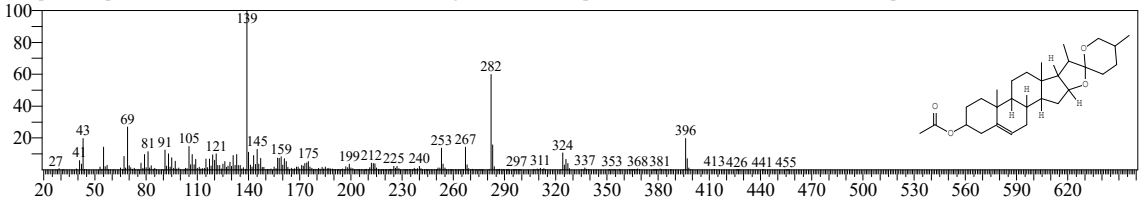
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:89 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



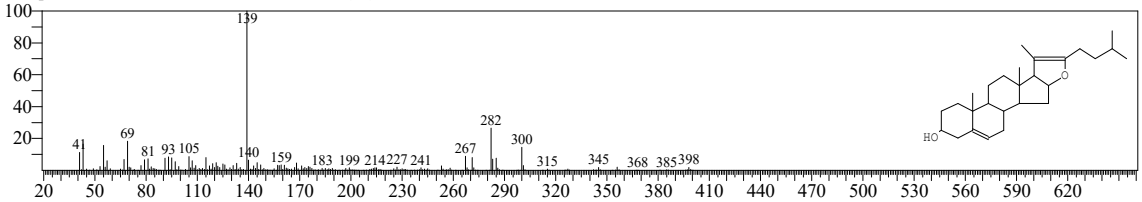
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:80 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#:3 Entry:24878 Library:NIST20M2.lib
SI: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#:4 Entry:41561 Library:NIST20R.lib
SI:78 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.