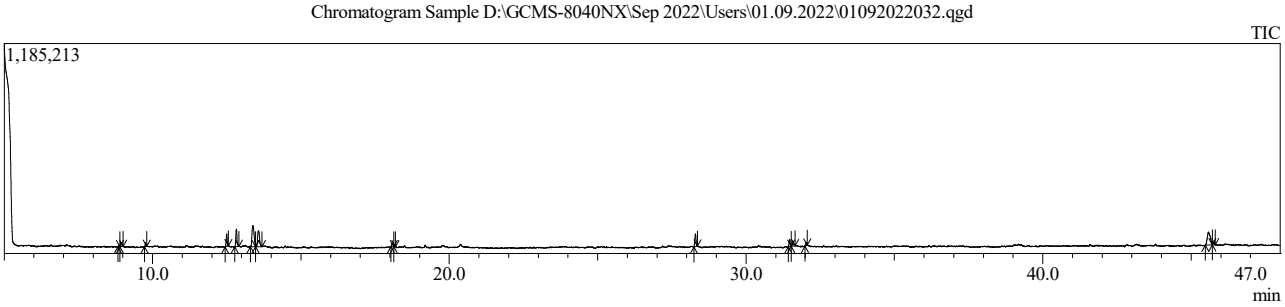
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 8:50:35 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 11-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 12
Injection Volume	: 5.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022032.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022032.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 11:11:08 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022032.qgd



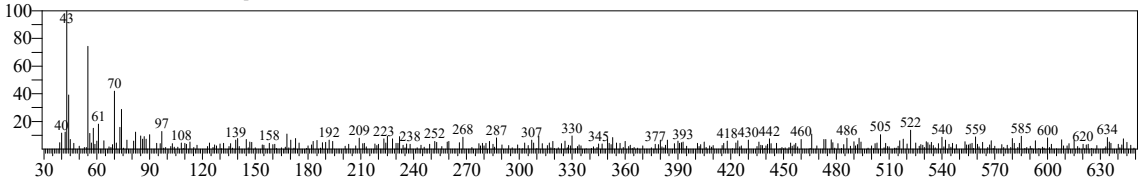
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.860	18697	0.71	6915	0.99	2.70	46	Methyl butanoate
2	8.938	77945	2.95	22599	3.25	3.45	82	1-Butanol, 3-methyl-, acetate
3	9.770	44187	1.67	20828	2.99	2.12	94	Pentasiloxane, dodecamethyl-
4	12.498	168908	6.39	69606	10.01	2.43	73	2,5-Cyclohexadiene-1,4-dione, dioxime
5	12.823	267649	10.13	99414	14.29	2.69	73	2,5-Cyclohexadiene-1,4-dione, dioxime
6	13.380	572820	21.68	118713	17.07	4.83	53	Methyl cis-13,16-Docosadienate
7	13.568	412452	15.61	88974	12.79	4.64	53	Methyl cis-13,16-Docosadienate
8	18.075	68498	2.59	20629	2.97	3.32	90	.beta.-D-Glucopyranose, 1,6-anhydro-
9	18.145	10347	0.39	6341	0.91	1.63	18	Methyl laurate
10	28.294	192212	7.27	72981	10.49	2.63	94	n-Hexadecanoic acid
11	31.469	117442	4.44	39482	5.68	2.97	95	(9E,11E)-Octadecadienoic acid
12	31.575	90920	3.44	29053	4.18	3.13	87	cis-9-Hexadecenal
13	32.030	42745	1.62	18671	2.68	2.29	91	Octadecanoic acid
14	45.582	515778	19.52	72975	10.49	7.07	89	Diosgenin
15	45.785	41707	1.58	8398	1.21	4.97	70	Tetracosamethyl-cyclododecasiloxane
		2642307	100.00	695579	100.00			

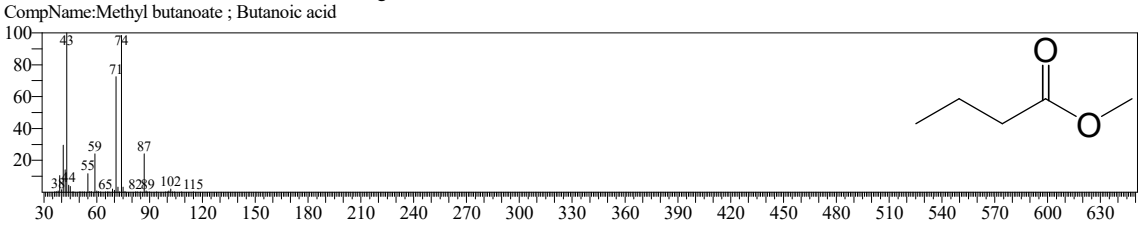
Library

TNAU

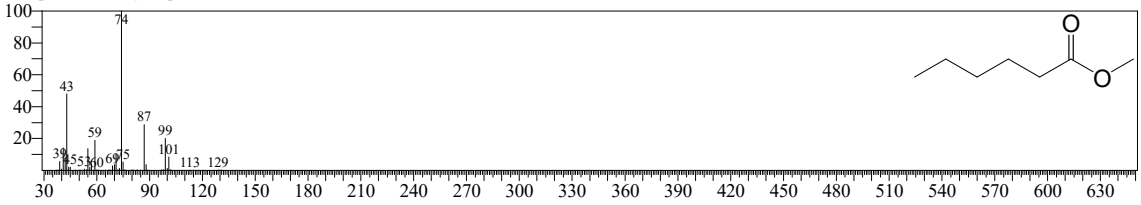
<< Target >>
Line#:1 R.Time:8.860(Scan#:773) MassPeaks:351
RawMode:Averaged 8.855-8.865(772-774) BasePeak:43.05(444)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



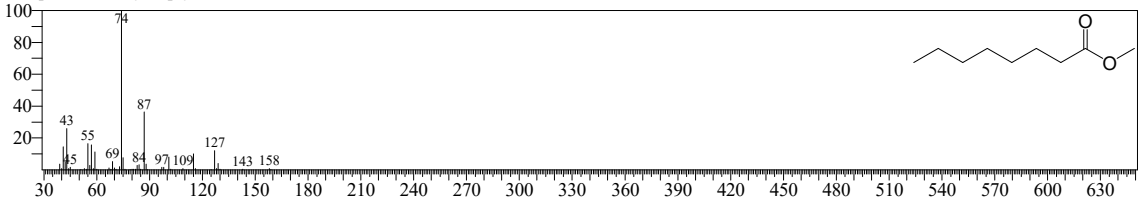
Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:46 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



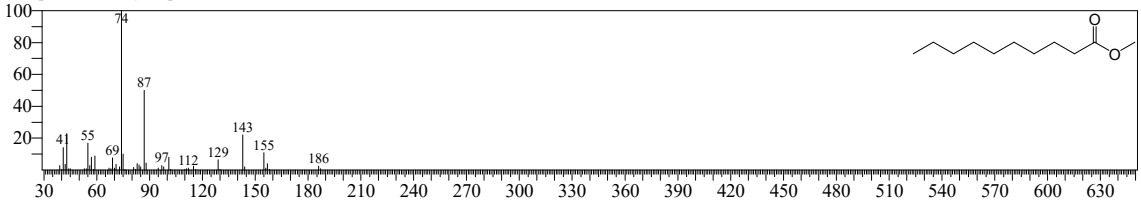
Hit#:2 Entry:2 Library:FA_ME_SP2560_EI_V3.lib
SI:43 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332
CompName:Methyl caproate ; Hexanoic acid



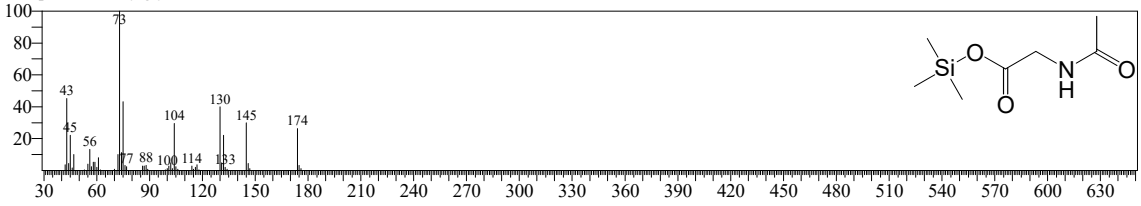
Hit#:3 Entry:3 Library:FA_ME_SP2560_EI_V3.lib
SI:40 Formula:C9H18O2 CAS:124-07-2 MolWeight:158 RetIndex:1550
CompName:Methyl caprylate ; Octanoic acid



Hit#:4 Entry:4 Library:FA_ME_SP2560_EI_V3.lib
SI:39 Formula:C11H22O2 CAS:334-48-5 MolWeight:186 RetIndex:1767
CompName:Methyl caprate ; Decanoic acid

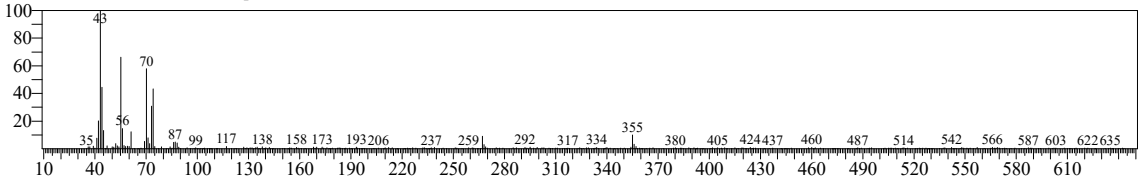


Hit#:5 Entry:78 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C7H15NO3Si CAS:543-24-8 MolWeight:189 RetIndex:1280
CompName:Acetylglycine-TMS ; 2-acetamidoacetic acid

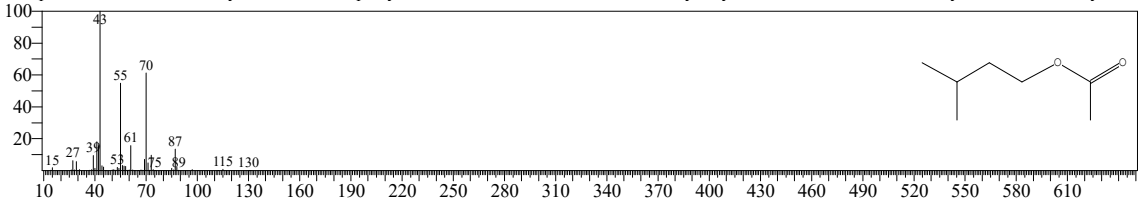


TNAU

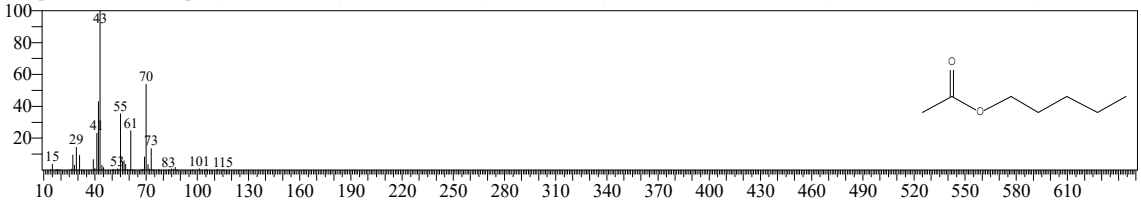
<< Target >>
Line#:2 R.Time:8.940(Scan#:789) MassPeaks:331
RawMode:Averaged 8.935-8.945(788-790) BasePeak:43.05(3527)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



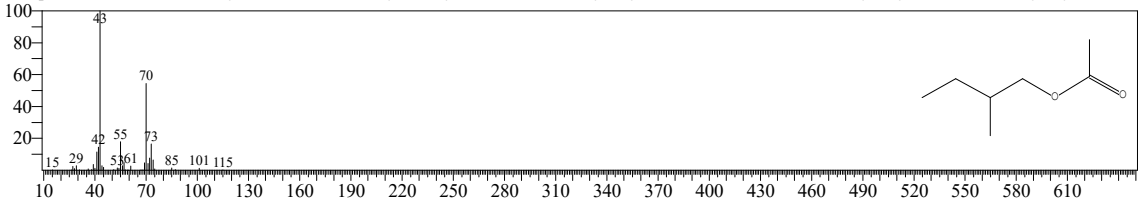
Hit#:1 Entry:6784 Library:NIST20R.lib
SI:82 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



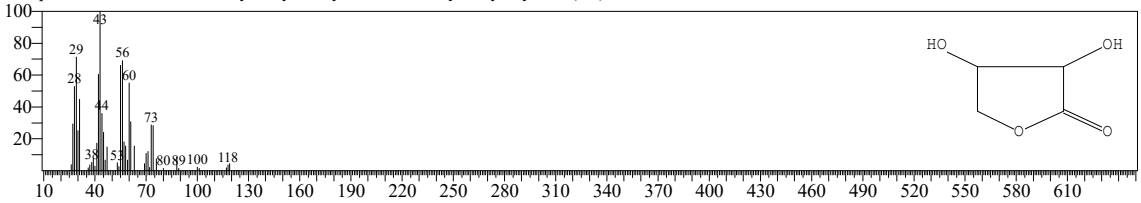
Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:79 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ Am



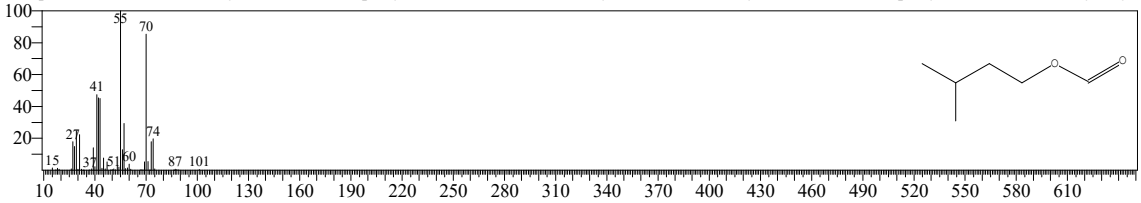
Hit#:3 Entry:6819 Library:NIST20R.lib
SI:78 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:5225 Library:NIST20M1.lib
SI:77 Formula:C4H6O4 CAS:17675-99-9 MolWeight:118 RetIndex:1201
CompName:2-Furanone, 3,4-dihydroxytetrahydro $$ 3,4-Dihydroxydihydro-2(3H)-furanone #

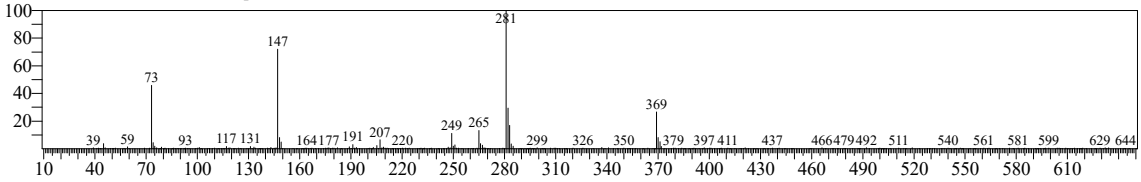


Hit#:5 Entry:4411 Library:NIST20R.lib
SI:77 Formula:C6H12O2 CAS:110-45-2 MolWeight:116 RetIndex:818
CompName:1-Butanol, 3-methyl-, formate $$ Isopentyl alcohol, formate $$ Isoamyl formate $$ Isoamyl methanoate $$ Isopentyl formate $$ 3-Methylbutyl

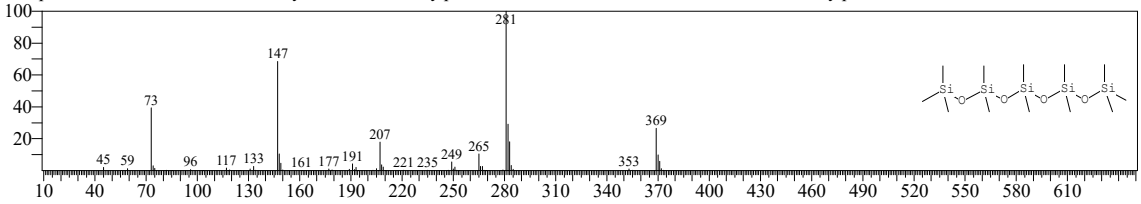


TNAU

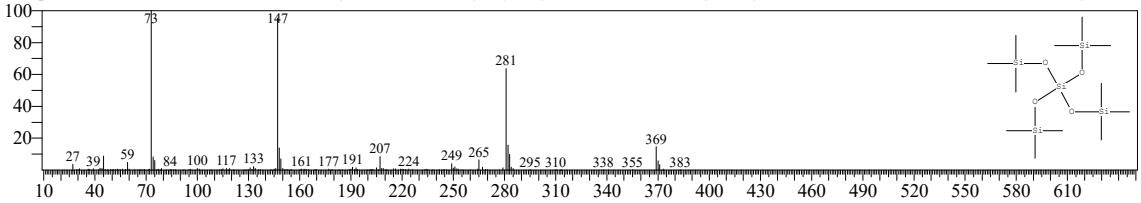
<< Target >>
Line#:3 R.Time:9.770(Scan#:955) MassPeaks:327
RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.00(5021)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



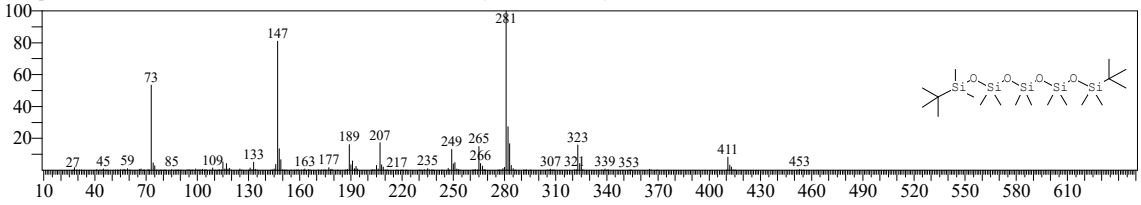
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:94 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



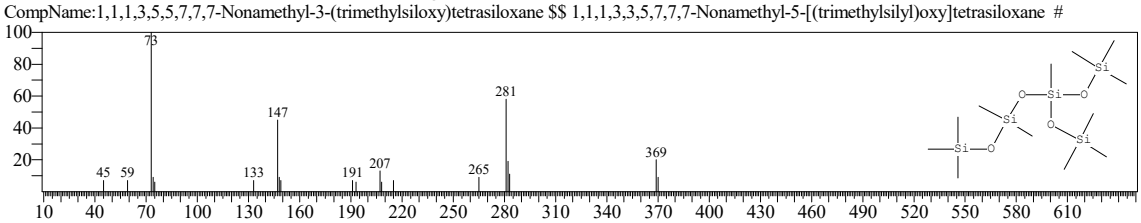
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:84 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



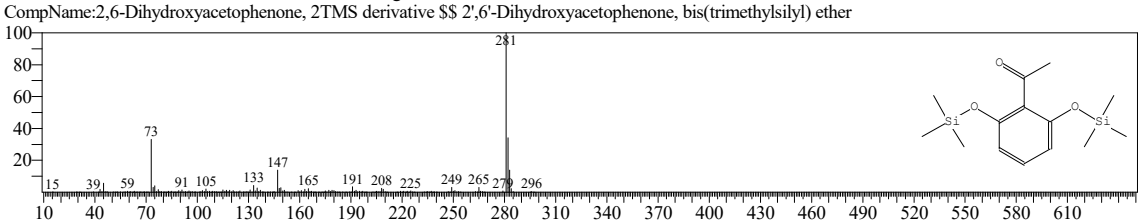
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:82 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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 #

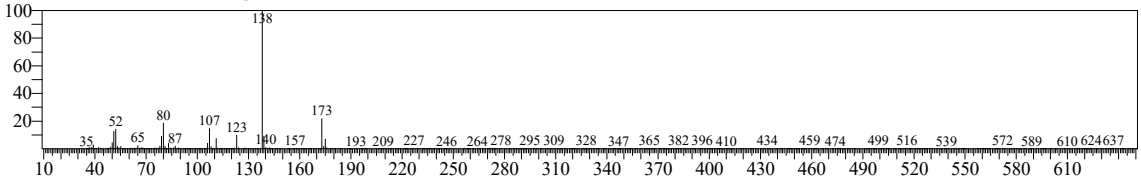


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

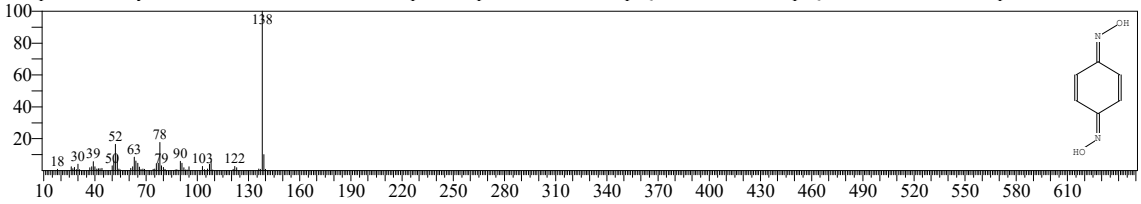


TNAU

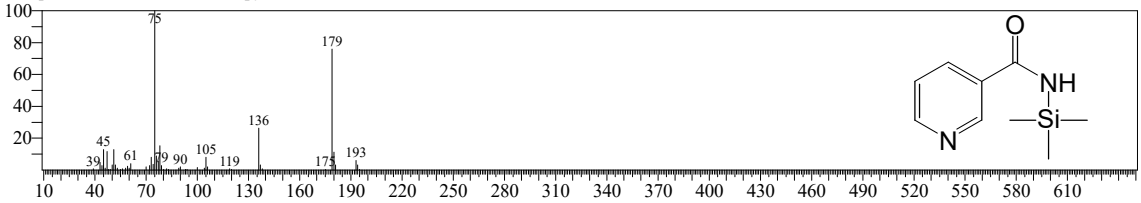
<< Target >>
Line#:4 R.Time:12.495(Scan#:1500) MassPeaks:373
RawMode:Averaged 12.490-12.500(1499-1501) BasePeak:138.05(24111)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



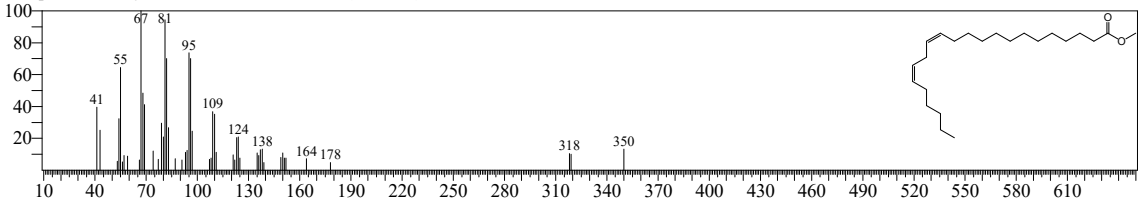
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



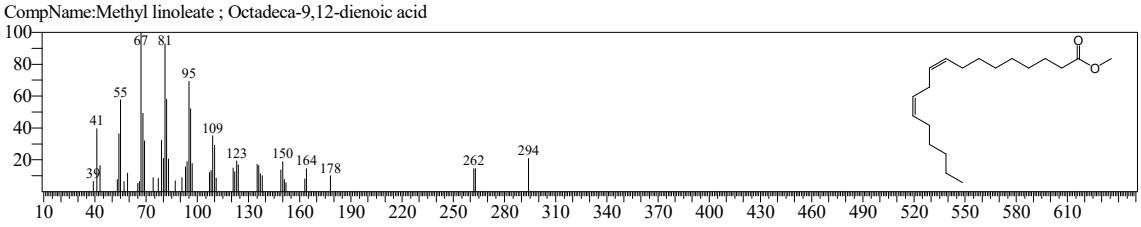
Hit#:2 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide



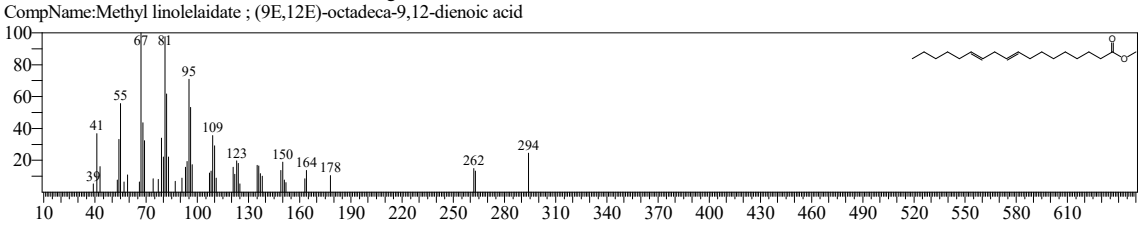
Hit#:3 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



Hit#:4 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

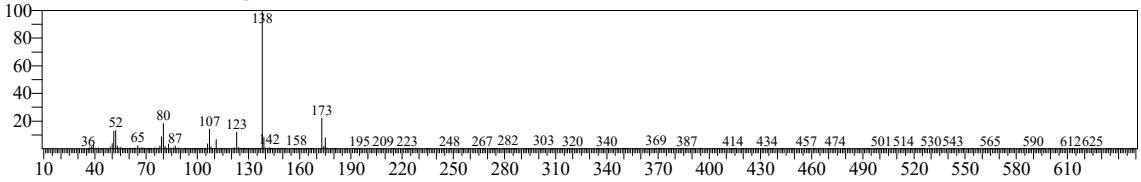


Hit#:5 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

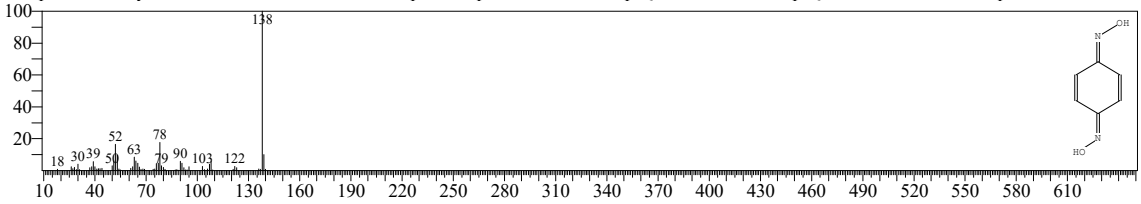


TNAU

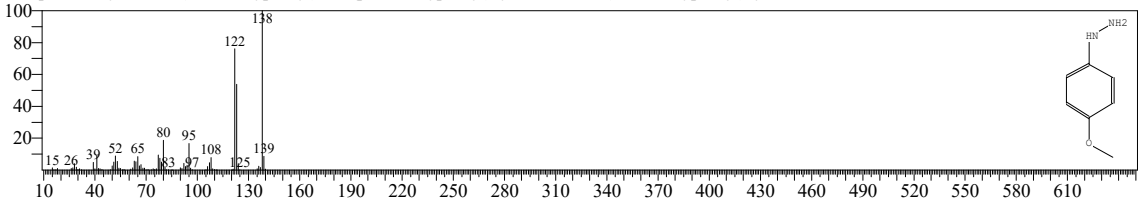
<< Target >>
Line#:5 R.Time:12.825(Scan#:1566) MassPeaks:323
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(35098)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



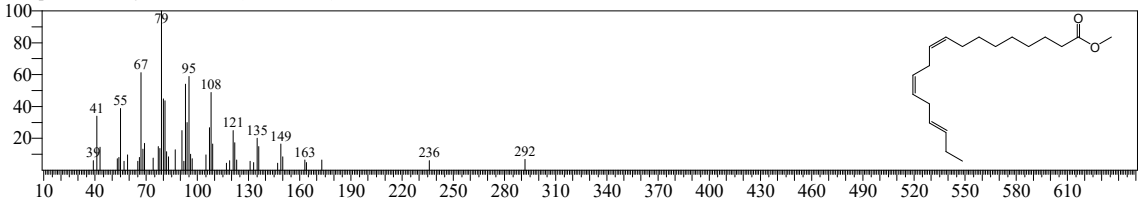
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



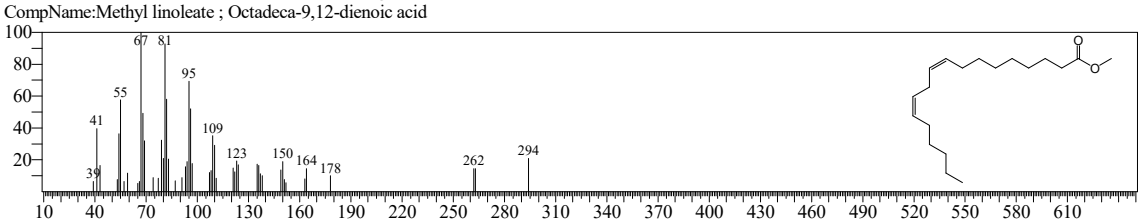
Hit#:2 Entry:11222 Library:NIST20M1.lib
SI:71 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #



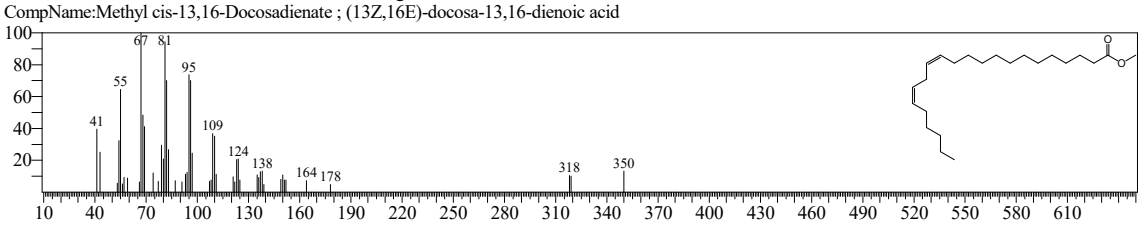
Hit#:3 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:34 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid



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

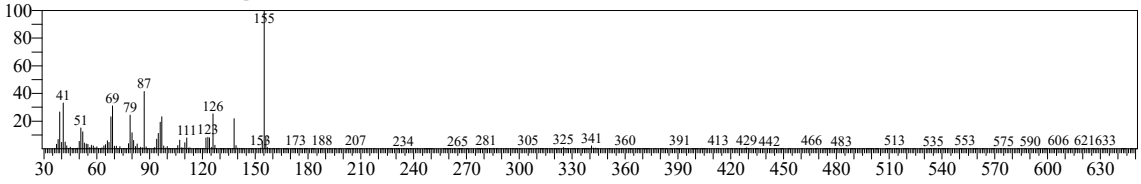


Hit#:5 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

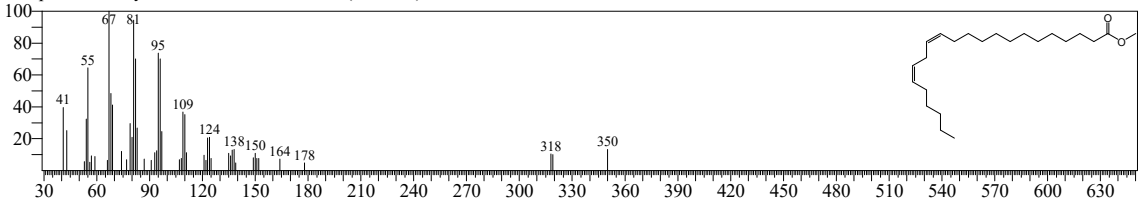


TNAU

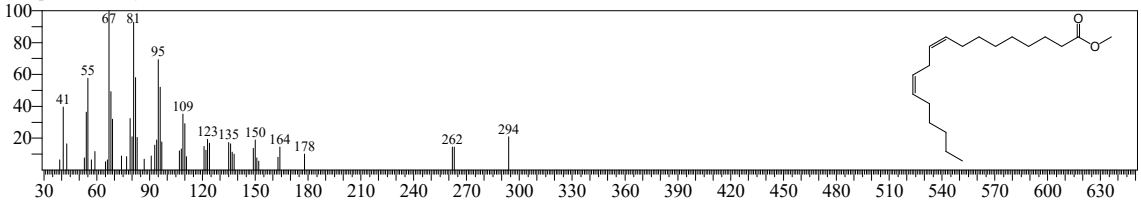
<< Target >>
Line#:6 R.Time:13.380(Scan#:1677) MassPeaks:341
RawMode:Averaged 13.375-13.385(1676-1678) BasePeak:155.05(19371)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



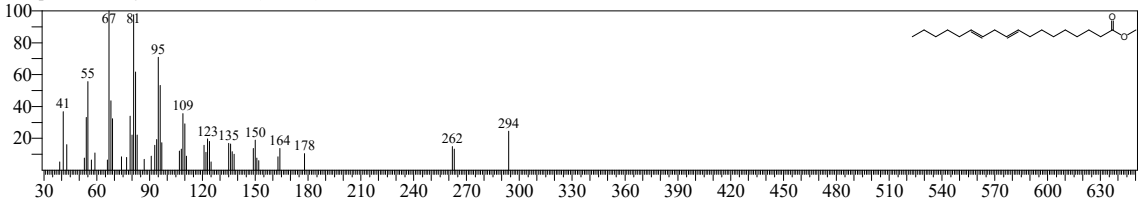
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



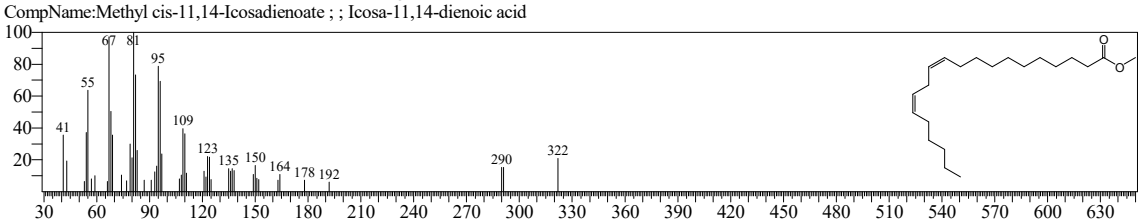
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



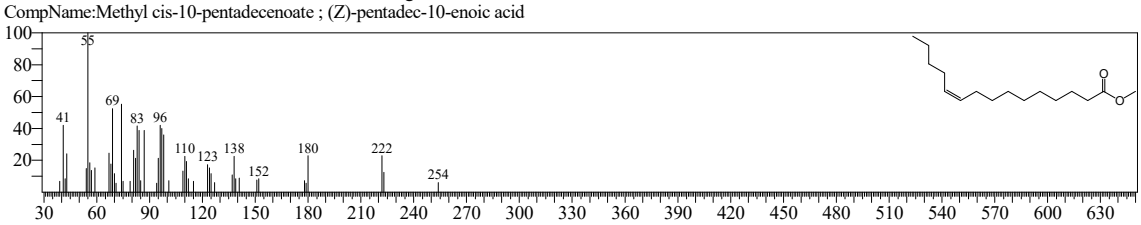
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

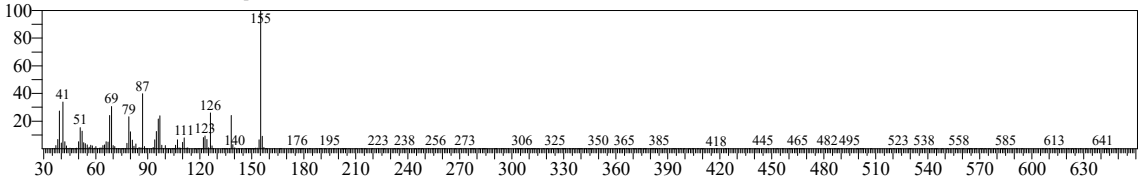


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

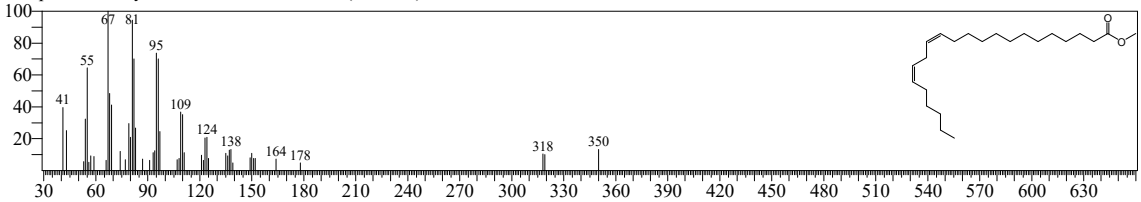


TNAU

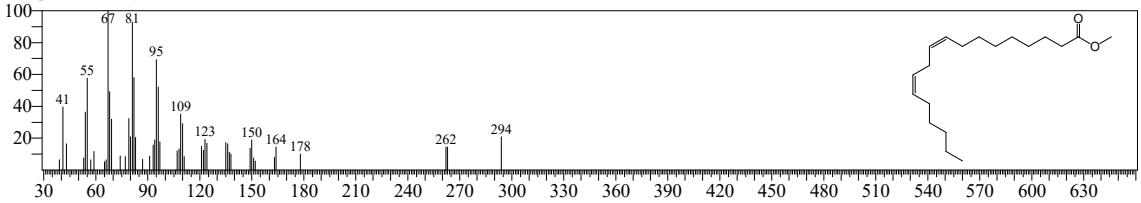
<< Target >>
Line#:7 R.Time:13.570(Scan#:1715) MassPeaks:327
RawMode:Averaged 13.565-13.575(1714-1716) BasePeak:155.05(14473)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



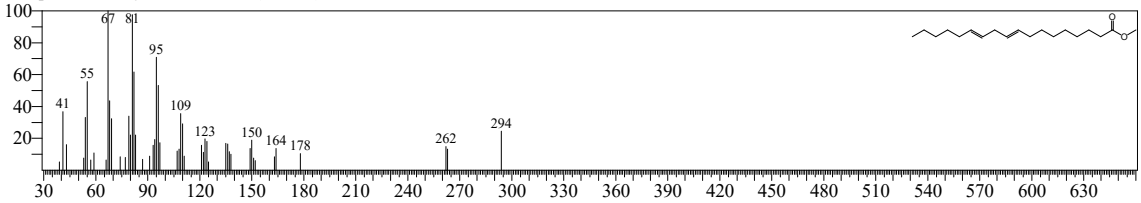
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



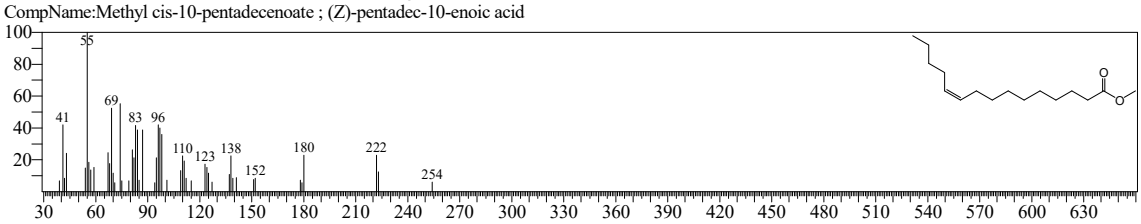
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



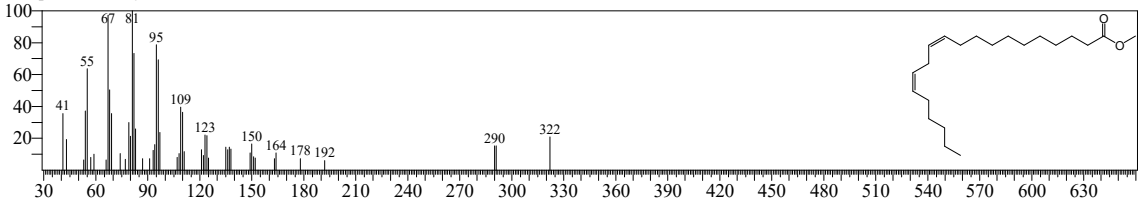
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

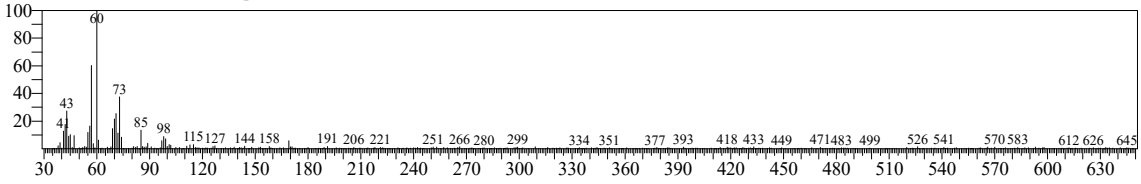


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

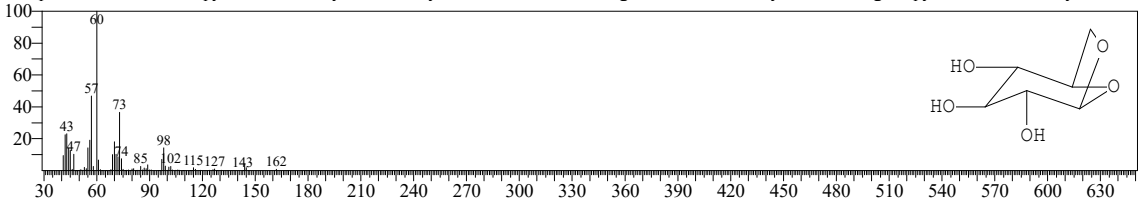


TNAU

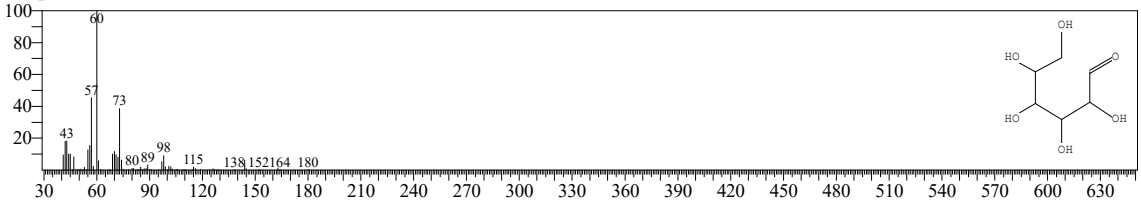
<< Target >>
Line#:8 R.Time:18.075(Scan#:2616) MassPeaks:362
RawMode:Averaged 18.070-18.080(2615-2617) BasePeak:60.00(3241)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



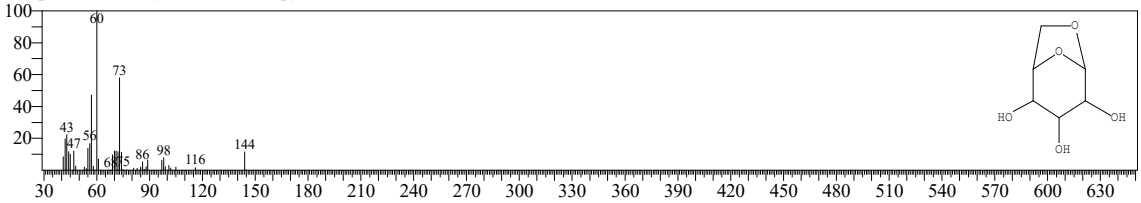
Hit#:1 Entry:13905 Library:NIST20R.lib
SI:90 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-



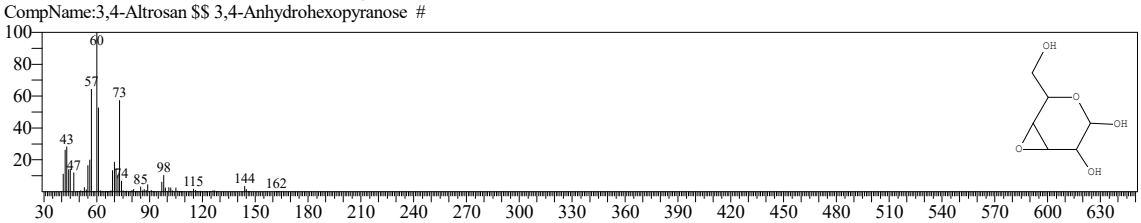
Hit#:2 Entry:36240 Library:NIST20M1.lib
SI:90 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #



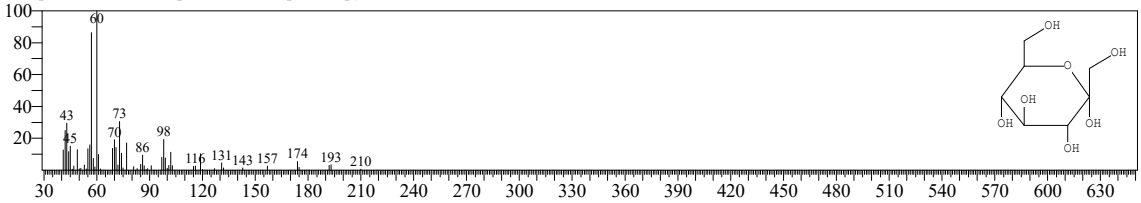
Hit#:3 Entry:23812 Library:NIST20M1.lib
SI:89 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose



Hit#:4 Entry:23808 Library:NIST20M1.lib
SI:88 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1400
CompName:3,4-Altrosan $$ 3,4-Anhydrohexopyranose #

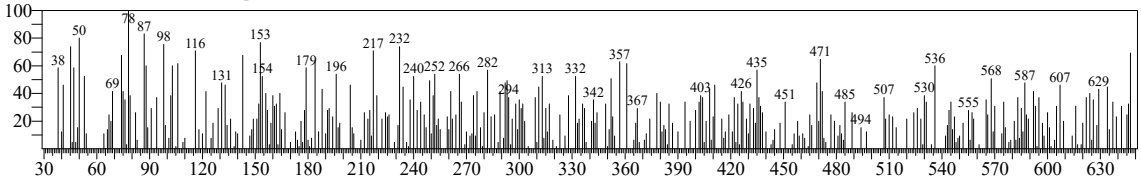


Hit#:5 Entry:62131 Library:NIST20M1.lib
SI:83 Formula:C7H14O7 CAS:0-00-0 MolWeight:210 RetIndex:2031
CompName:d-Gluco-heptulosan $$ Hept-2-ulopyranose #

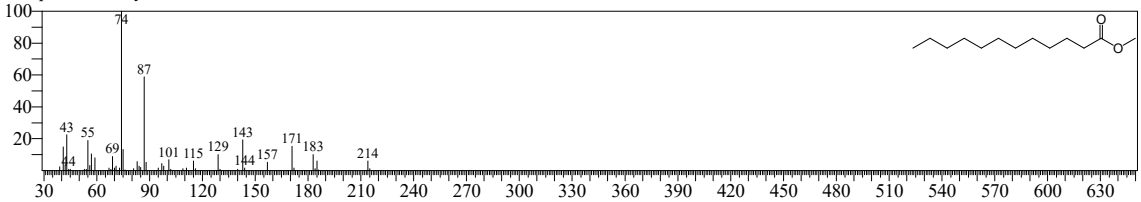


TNAU

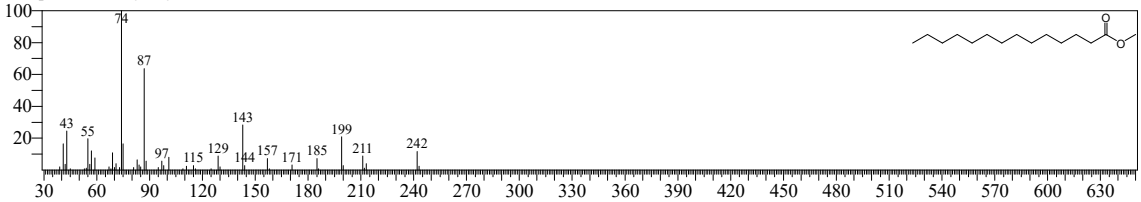
<< Target >>
Line#:9 R.Time:18.145(Scan#:2630) MassPeaks:350
RawMode:Averaged 18.140-18.150(2629-2631) BasePeak:78.00(65)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



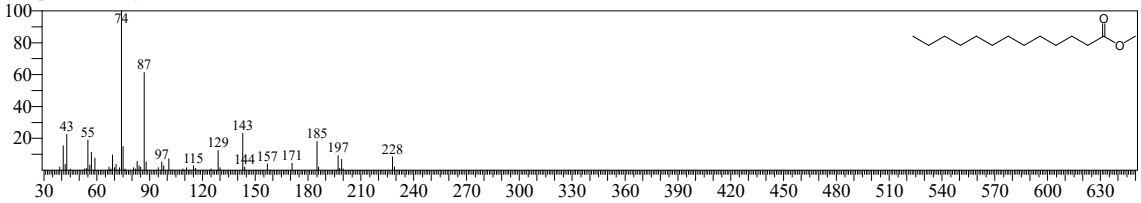
Hit#:1 Entry:6 Library:FA_ME_SP2560_EI_V3.lib
SI:18 Formula:C13H26O2 CAS:143-07-7 MolWeight:214 RetIndex:1983
CompName:Methyl laurate ; Dodecanoic acid



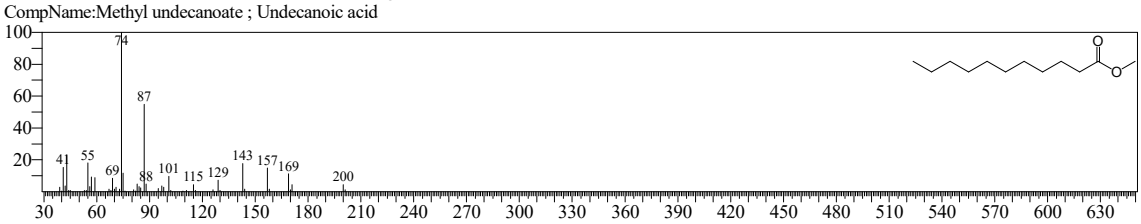
Hit#:2 Entry:8 Library:FA_ME_SP2560_EI_V3.lib
SI:18 Formula:C15H30O2 CAS:544-63-8 MolWeight:242 RetIndex:2194
CompName:Methyl myristate ; Tetradecanoic acid



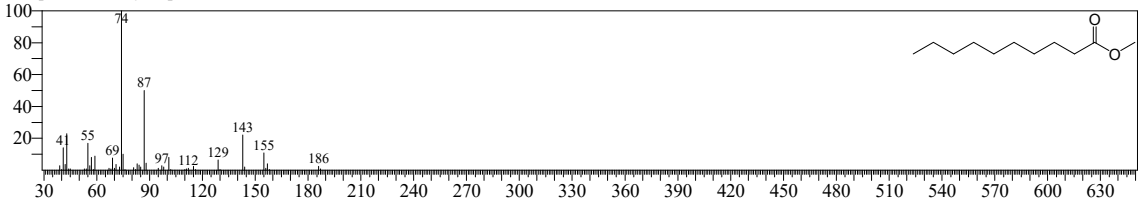
Hit#:3 Entry:7 Library:FA_ME_SP2560_EI_V3.lib
SI:18 Formula:C14H28O2 CAS:638-53-9 MolWeight:228 RetIndex:2089
CompName:Methyl tridecanoate ; Tridecanoic acid



Hit#:4 Entry:5 Library:FA_ME_SP2560_EI_V3.lib
SI:17 Formula:C12H24O2 CAS:112-37-8 MolWeight:200 RetIndex:1875
CompName:Methyl undecanoate ; Undecanoic acid

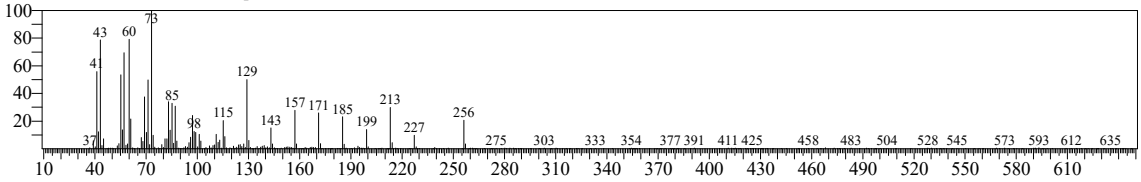


Hit#:5 Entry:4 Library:FA_ME_SP2560_EI_V3.lib
SI:17 Formula:C11H22O2 CAS:334-48-5 MolWeight:186 RetIndex:1767
CompName:Methyl caprate ; Decanoic acid

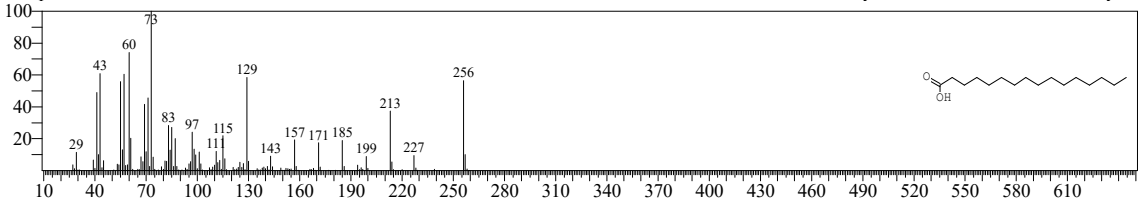


TNAU

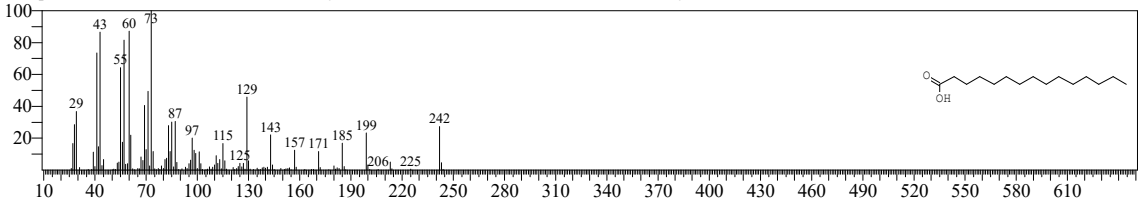
<< Target >>
Line#:10 R.Time:28.295(Scan#:4660) MassPeaks:312
RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.05(5970)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



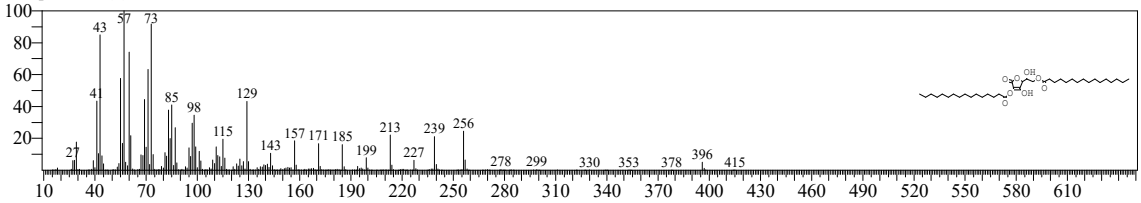
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:94 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



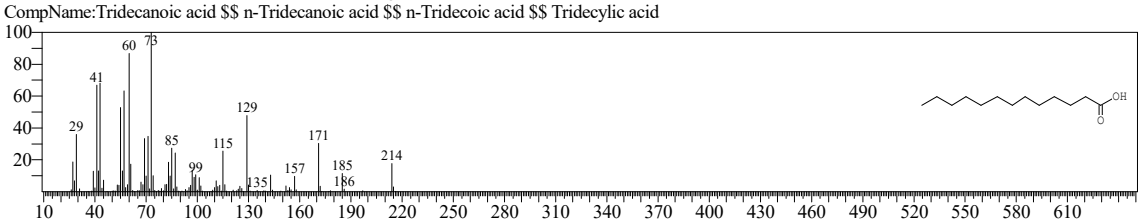
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



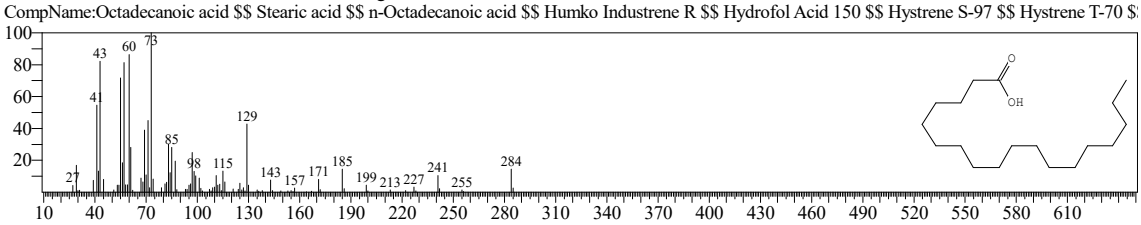
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:4 Entry:25643 Library:NIST20R.lib
SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

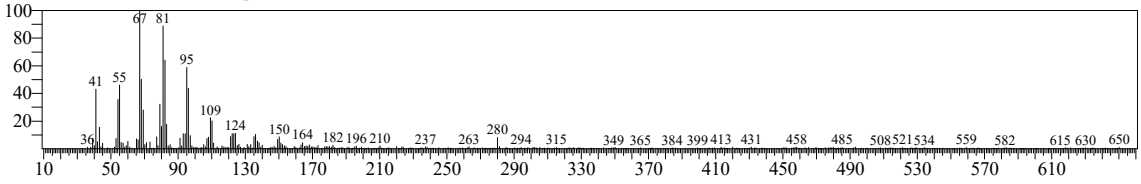


Hit#:5 Entry:144781 Library:NIST20M1.lib
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $

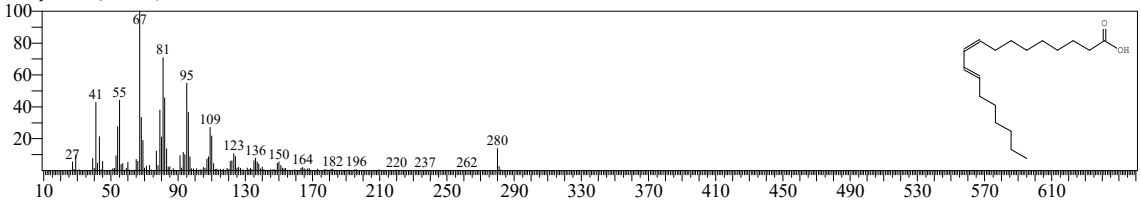


TNAU

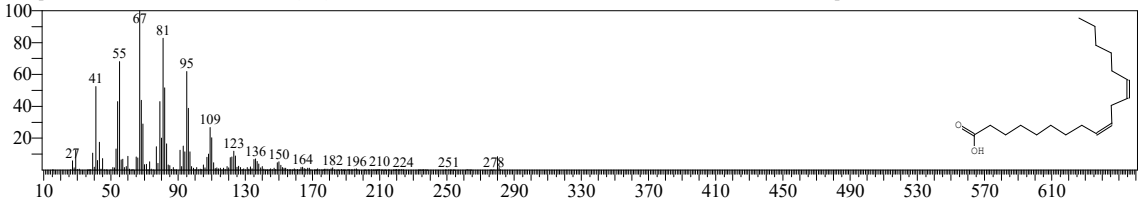
<< Target >>
Line#:11 R.Time:31.470(Scan#:5295) MassPeaks:386
RawMode:Averaged 31.465-31.475(5294-5296) BasePeak:67.05(3493)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



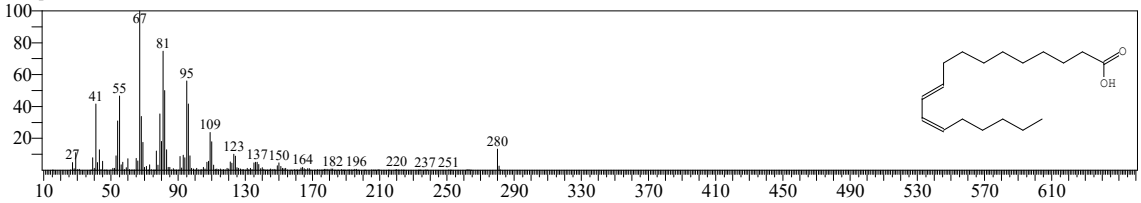
Hit#:1 Entry:139651 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



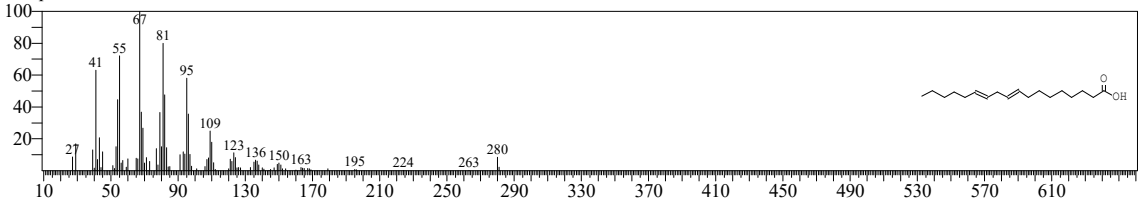
Hit#:2 Entry:34035 Library:NIST20R.lib
SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



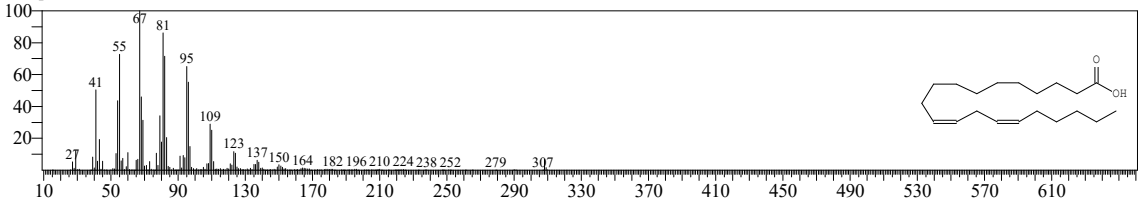
Hit#:3 Entry:139646 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid



Hit#:4 Entry:139661 Library:NIST20M1.lib
SI:94 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

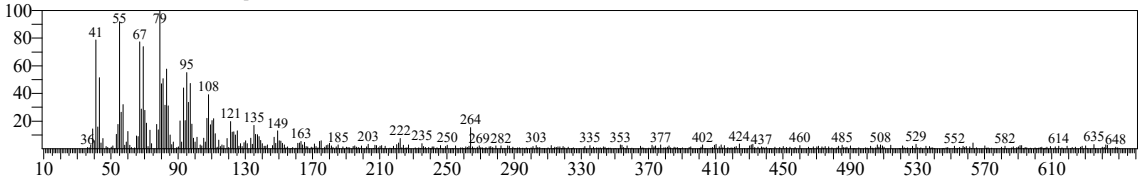


Hit#:5 Entry:173215 Library:NIST20M1.lib
SI:93 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382
CompName:11,14-Eicosadienoic acid

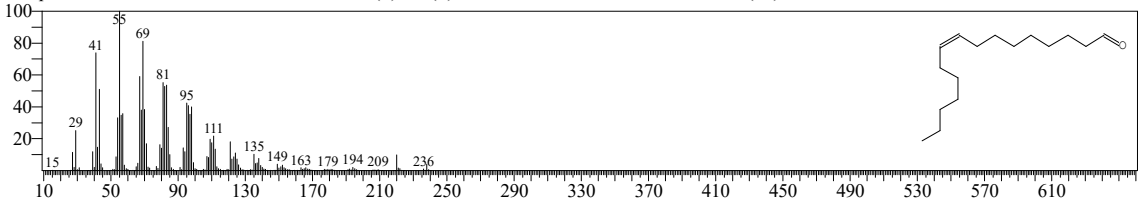


TNAU

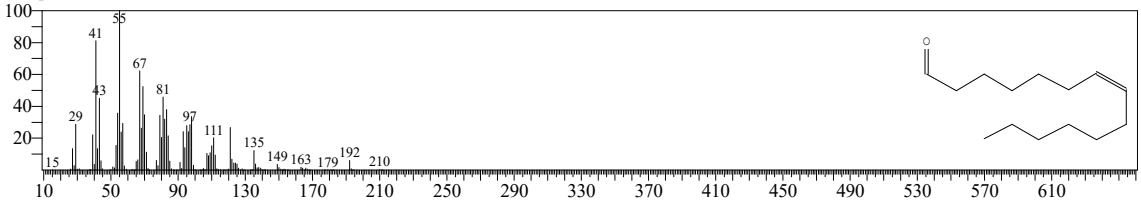
<< Target >>
Line#:12 R.Time:31.575(Scan#:5316) MassPeaks:423
RawMode:Averaged 31.570-31.580(5315-5317) BasePeak:79.05(1360)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



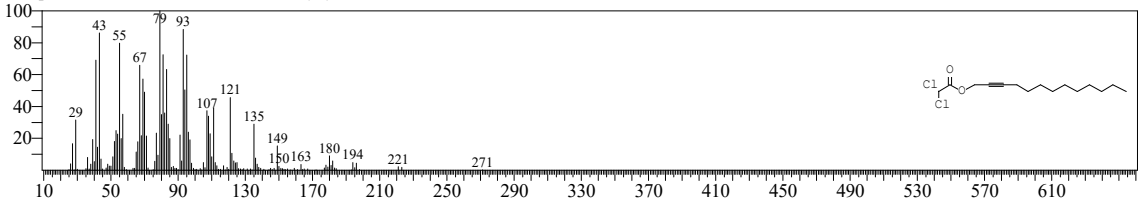
Hit#:1 Entry:92244 Library:NIST20M1.lib
SI:87 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #



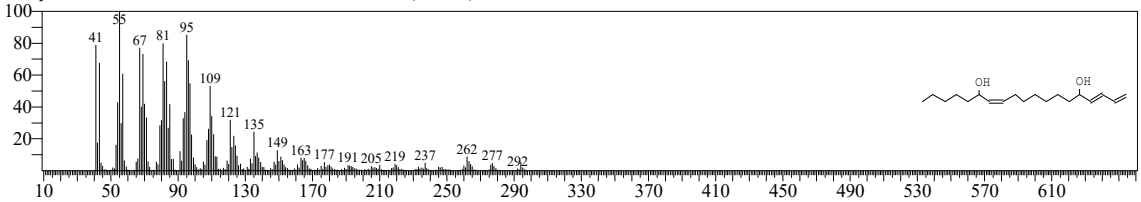
Hit#:2 Entry:63176 Library:NIST20M1.lib
SI:87 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #



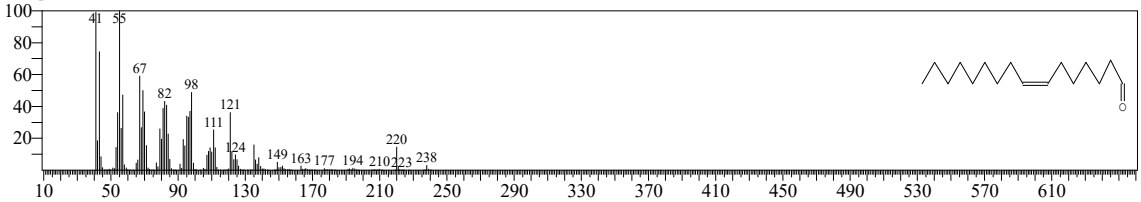
Hit#:3 Entry:170238 Library:NIST20M1.lib
SI:87 Formula:C15H24Cl2O2 CAS:0-00-0 MolWeight:306 RetIndex:2042
CompName:Dichloroacetic acid, tridec-2-ynyl ester



Hit#:4 Entry:156549 Library:NIST20M1.lib
SI:87 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #

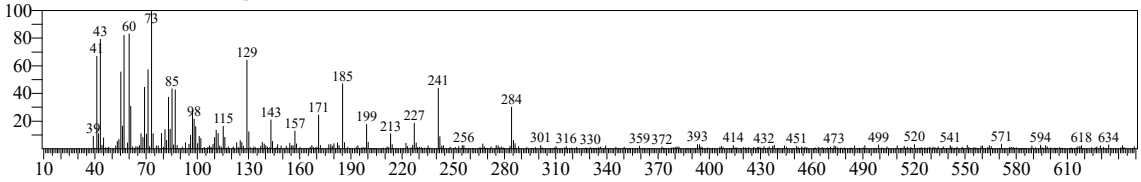


Hit#:5 Entry:92227 Library:NIST20M1.lib
SI:86 Formula:C16H30O CAS:56797-40-1 MolWeight:238 RetIndex:1808
CompName:7-Hexadecenal, (Z)- $$ (Z)-7-Hexadecenal $$ Z-7-Hexadecenal $$ (7Z)-7-Hexadecenal #

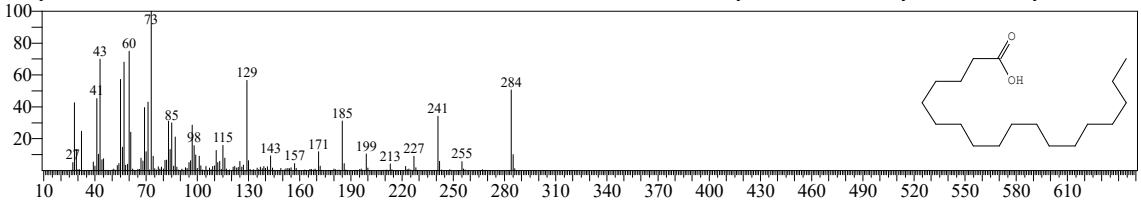


TNAU

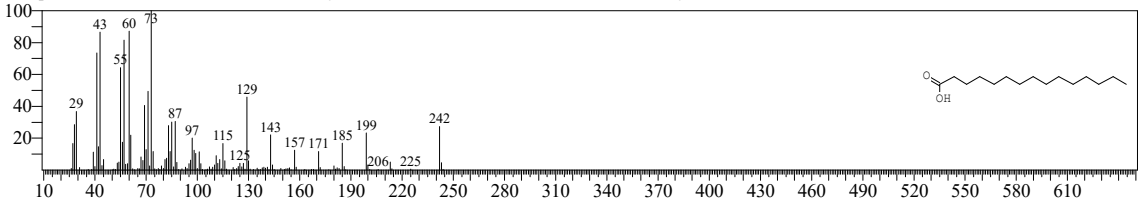
<< Target >>
Line#:13 R.Time:32.030(Scan#:5407) MassPeaks:346
RawMode:Averaged 32.025-32.035(5406-5408) BasePeak:73.05(1203)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



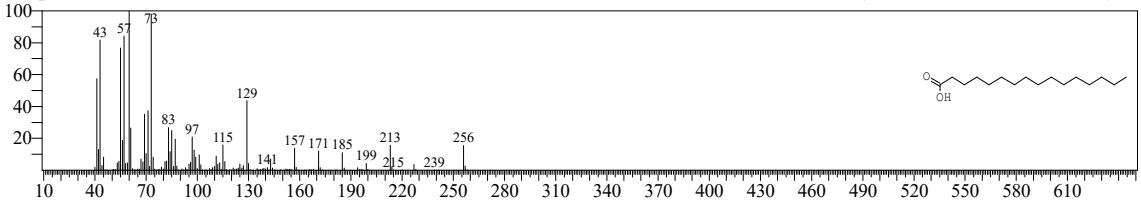
Hit#:1 Entry:34463 Library:NIST20R.lib
SI:91 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



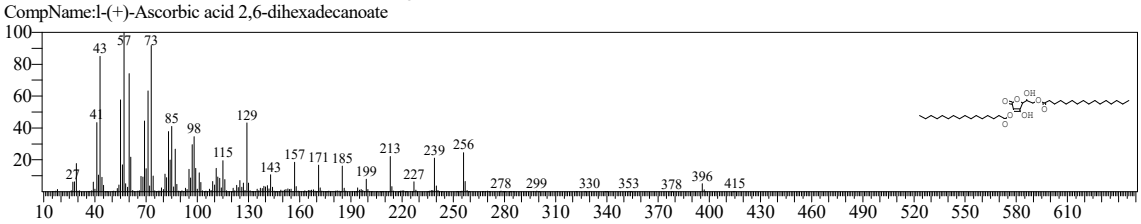
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:89 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



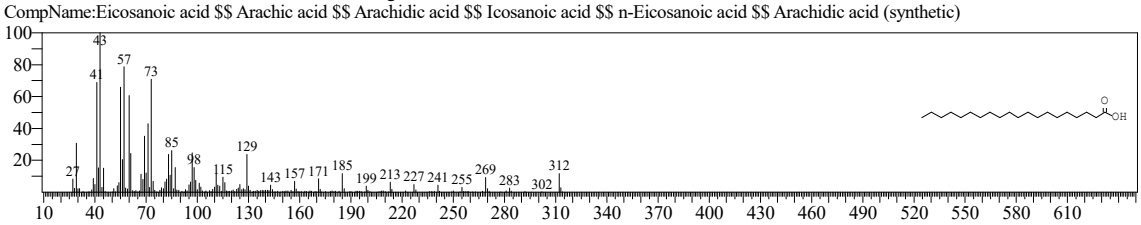
Hit#:3 Entry:31599 Library:NIST20R.lib
SI:86 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



Hit#:4 Entry:44286 Library:NIST20M2.lib
SI:86 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

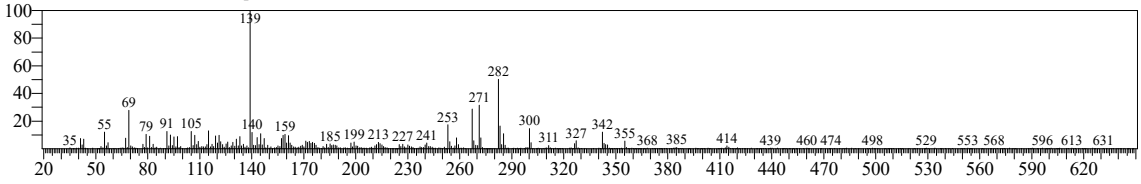


Hit#:5 Entry:36903 Library:NIST20R.lib
SI:85 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)

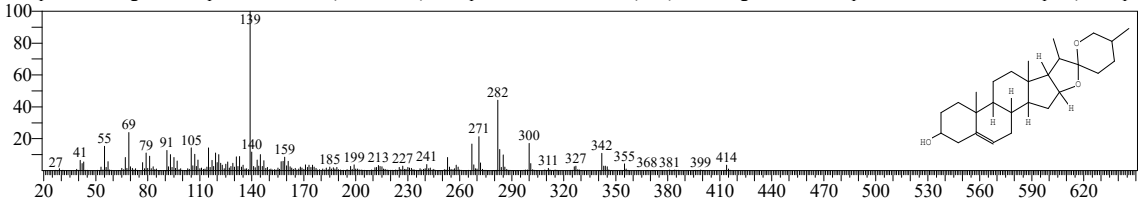


TNAU

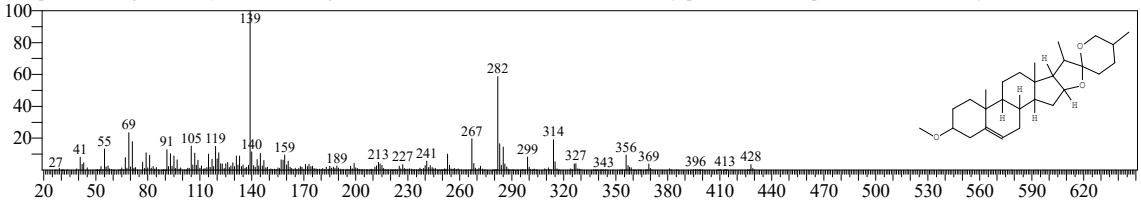
<< Target >>
Line#:14 R.Time:45.580(Scan#:8117) MassPeaks:447
RawMode:Averaged 45.575-45.585(8116-8118) BasePeak:139.10(7397)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



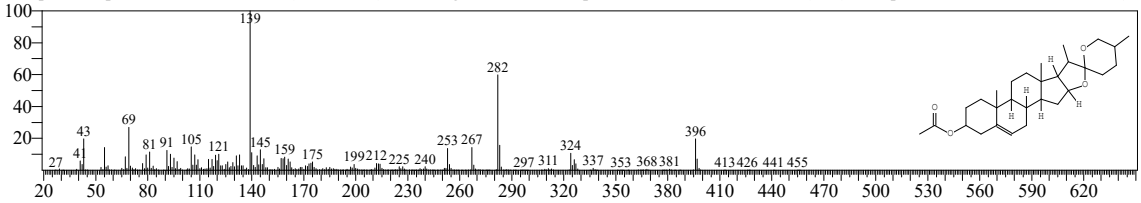
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:89 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



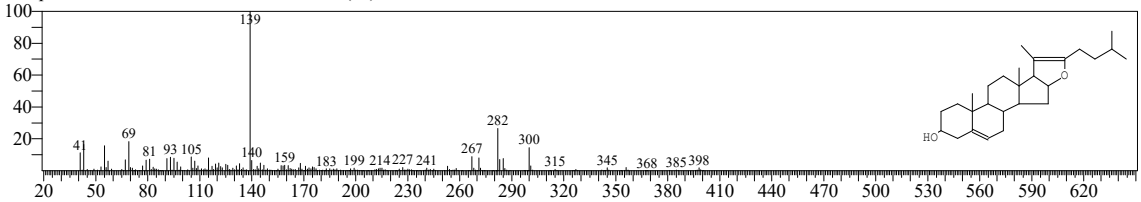
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:82 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



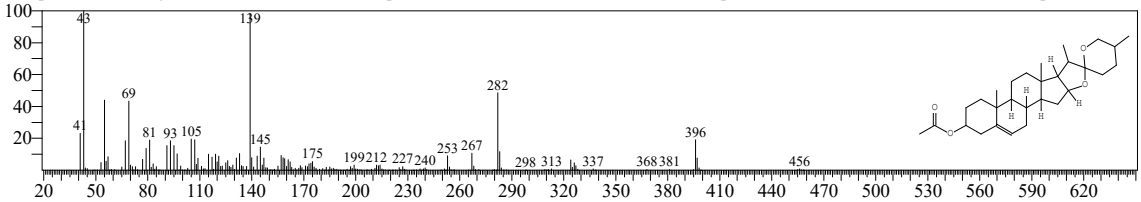
Hit#:3 Entry:24878 Library:NIST20M2.lib
SI:80 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (2



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 #

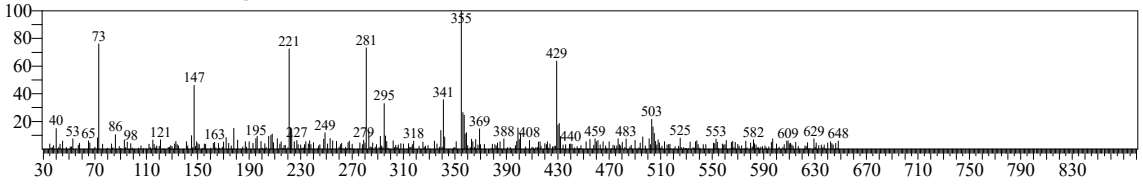


Hit#:5 Entry:42677 Library:NIST20R.lib
SI:73 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.

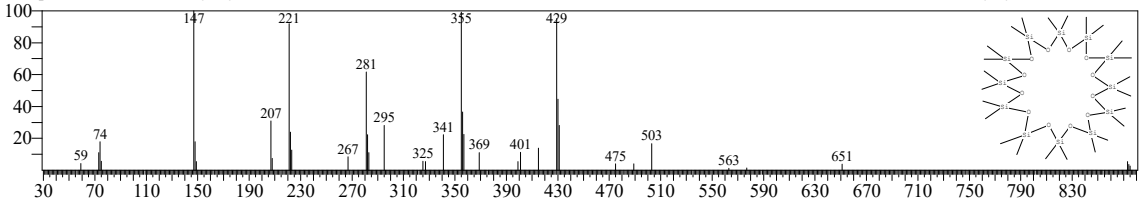


TNAU

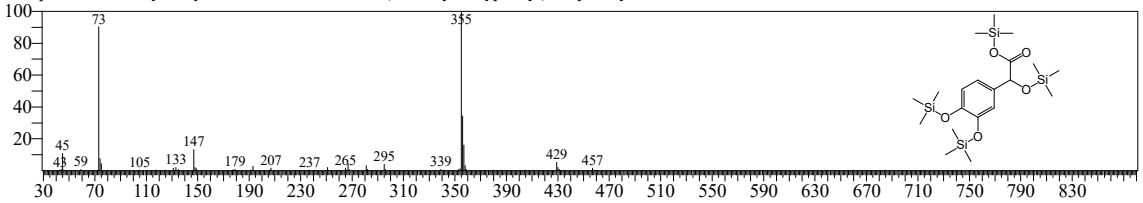
<< Target >>
Line#:15 R.Time:45.785(Scan#:8158) MassPeaks:367
RawMode:Averaged 45.780-45.790(8157-8159) BasePeak:355.05(479)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



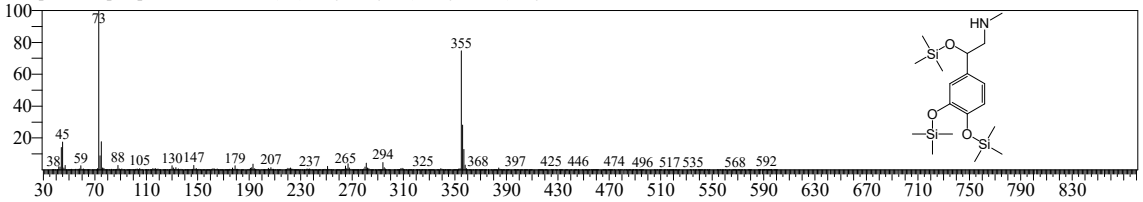
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:70 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



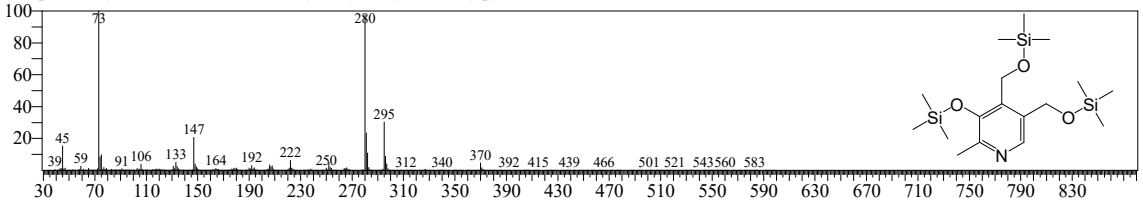
Hit#:2 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:52 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:384 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H35NO3Si3 CAS:65-23-6 MolWeight:385 RetIndex:1919
CompName:Pyridoxine-3TMS ; 4,5-bis(hydroxymethyl)-2-methylpyridin-3-ol



Hit#:5 Entry:443 Library:OA_TMS_DB5_67min_V3.lib
SI:31 Formula:C14H28N4O2Si3 CAS:69-89-6 MolWeight:368 RetIndex:2040
CompName:Xanthine-3TMS ; 3,7-dihydropurine-2,6-dione