TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022011.qgd

Peak Report TIC

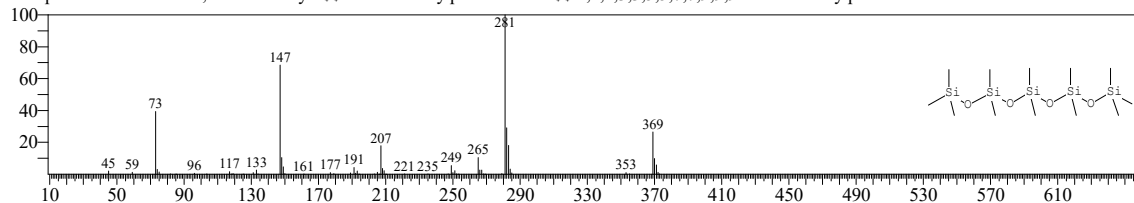| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.766	42174	1.94	21045	2.92	2.00	93	Pentasiloxane, dodecamethyl-
2	12.825	59131	2.71	24275	3.36	2.44	73	1,3-Benzodioxol-5-ol
3	13.240	597113	27.41	216535	29.99	2.76	54	Methyl cis-13,16-Docosadienate
4	13.436	517737	23.77	187885	26.02	2.76	54	Methyl cis-13,16-Docosadienate
5	13.812	25855	1.19	11918	1.65	2.17	80	Trisiloxane, octamethyl-
6	19.198	108392	4.98	42729	5.92	2.54	95	2,4-Di-tert-butylphenoxytrimethylsilane
7	28.305	195924	9.00	72365	10.02	2.71	96	n-Hexadecanoic acid
8	31.487	177996	8.17	61428	8.51	2.90	95	10E,12Z-Octadecadienoic acid
9	31.587	135735	6.23	36436	5.05	3.73	91	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
10	45.634	318061	14.60	47326	6.56	6.72	90	Diosgenin
		2178118	100.00	721942	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:9.765(Scan#:954) MassPeaks:325
RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(5031)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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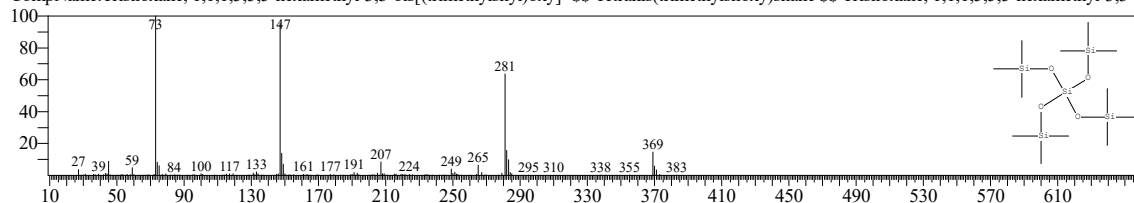SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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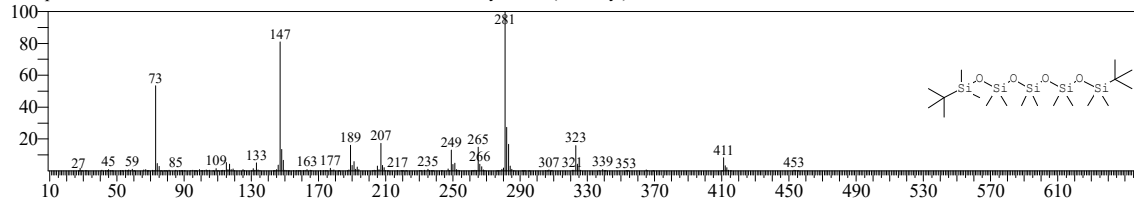SI:82 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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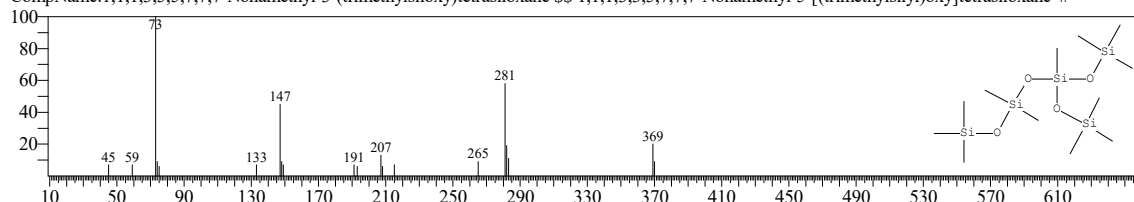CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

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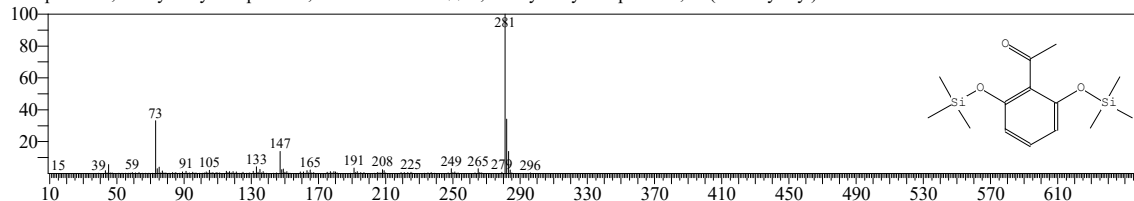SI:78 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

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
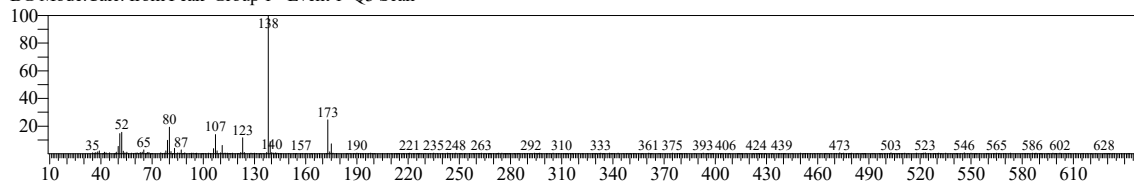
TNAU

<< Target >>
Line#:2   R.Time:12.825(Scan#:1566) MassPeaks:352
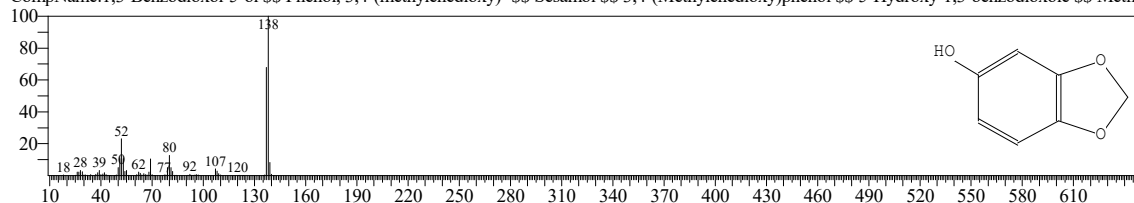RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(7780)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:11187 Library:NIST20M1.lib
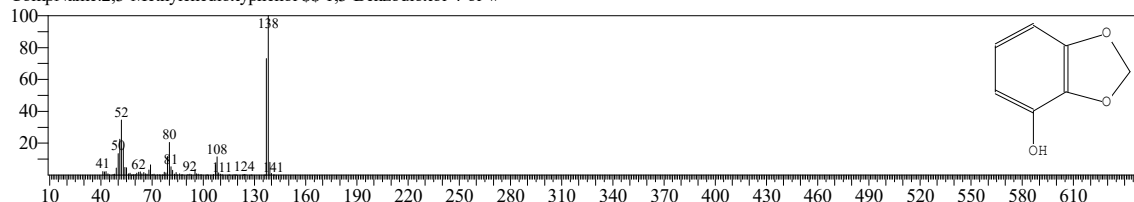SI:73 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy

Hit#:2 Entry:11188 Library:NIST20M1.lib
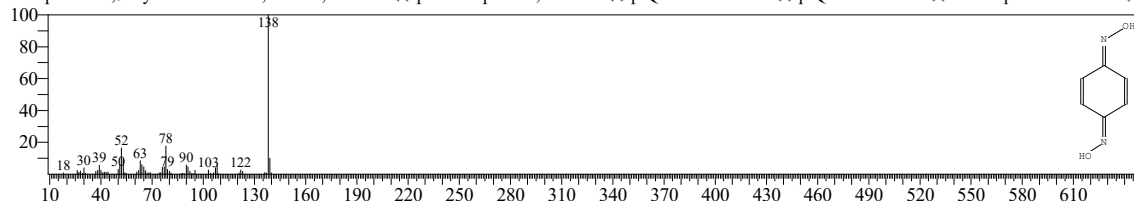SI:73 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #

Hit#:3 Entry:8360 Library:NIST20R.lib
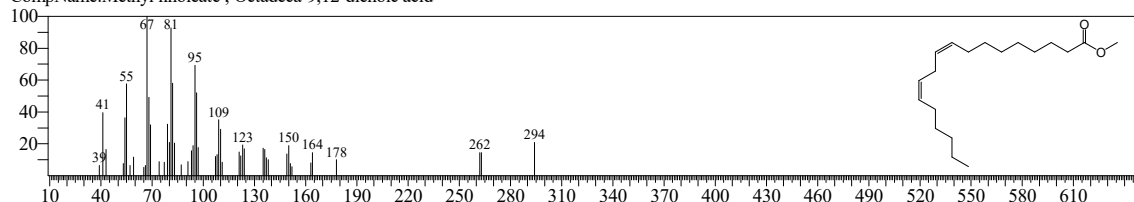SI:72 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

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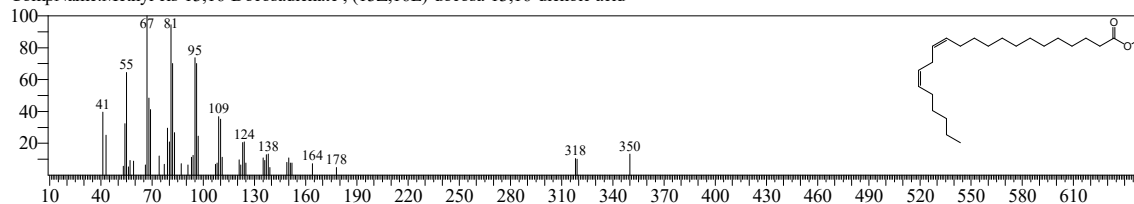CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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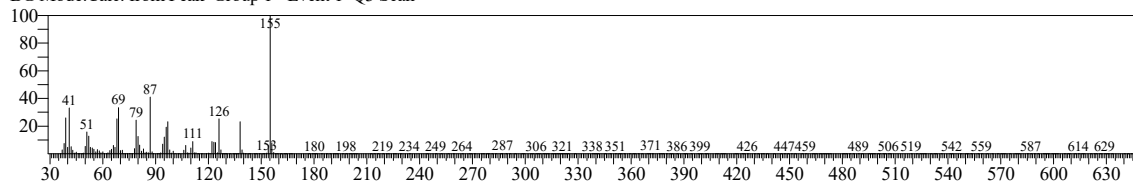CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

TNAU

<< Target >>
Line#:3 R.Time:13.240(Scan#:1649) MassPeaks:330
RawMode:Averaged 13.235-13.245(1648-1650) BasePeak:155.10(34645)
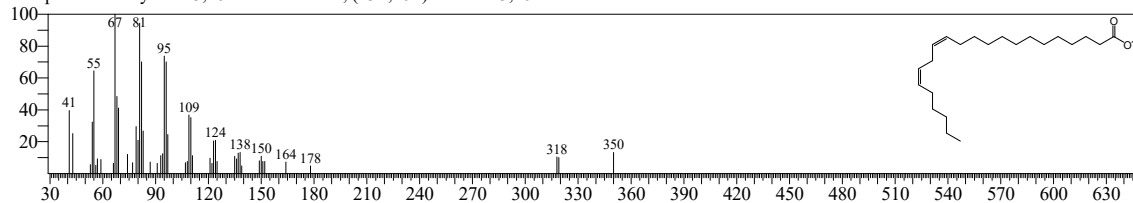BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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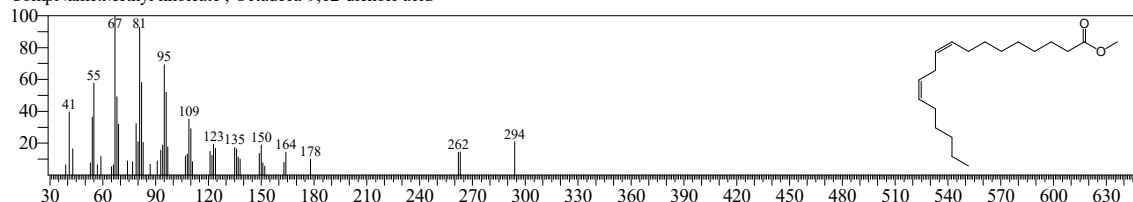SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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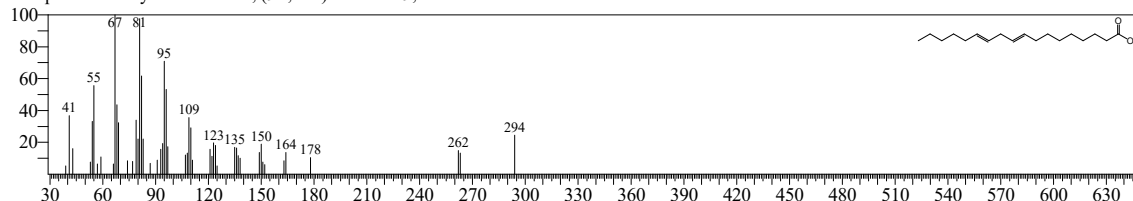SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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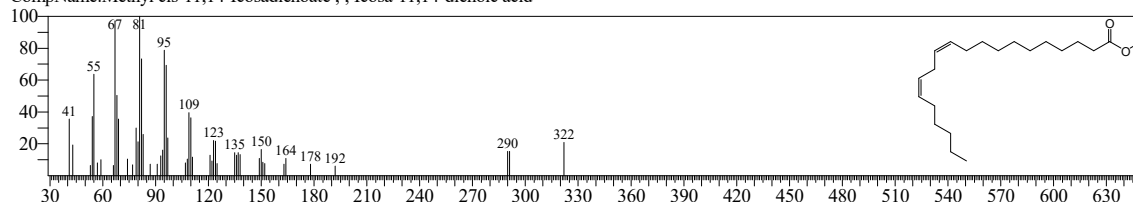CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
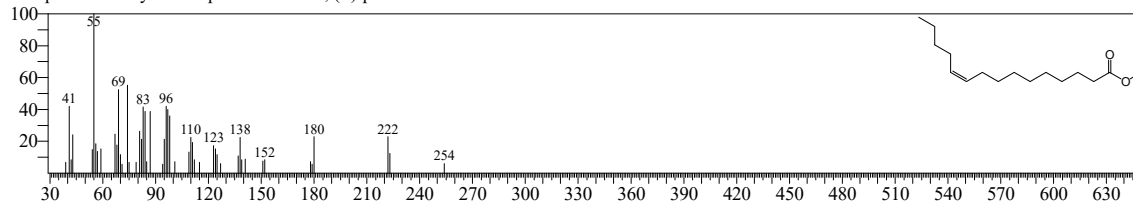SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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
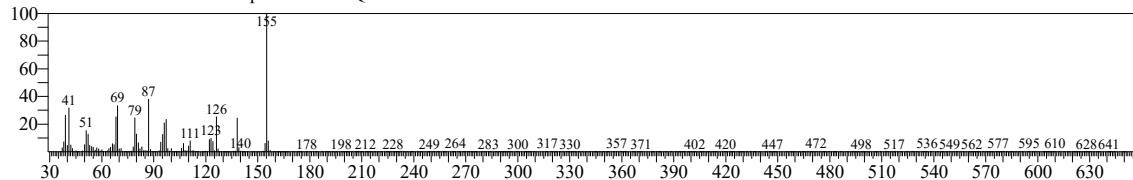
TNAU

<< Target >>
Line#:4 R.Time:13.435(Scan#:1688) MassPeaks:402
RawMode:Averaged 13.430-13.440(1687-1689) BasePeak:155.05(29699)
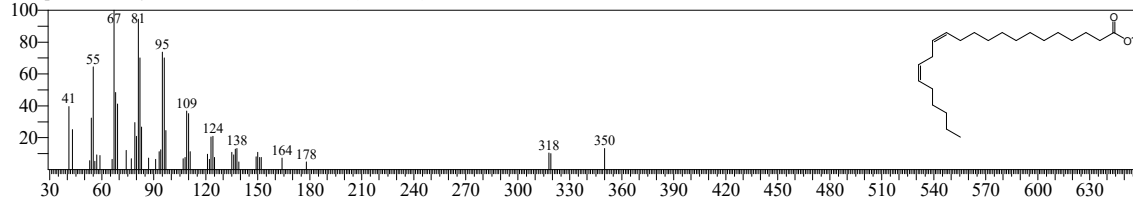BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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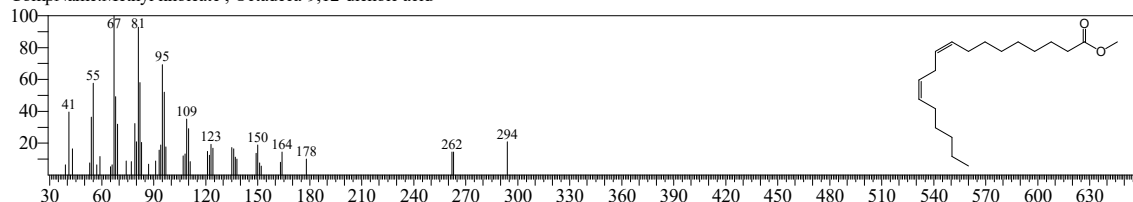SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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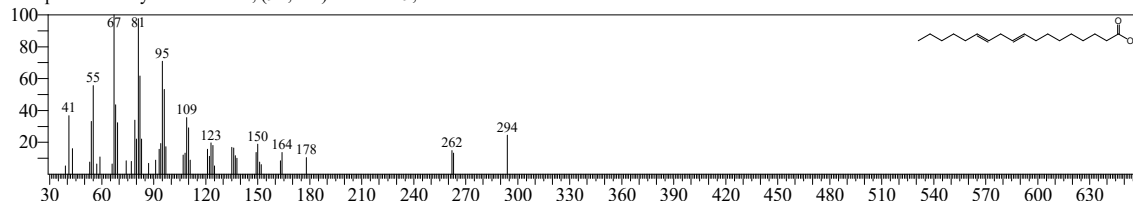SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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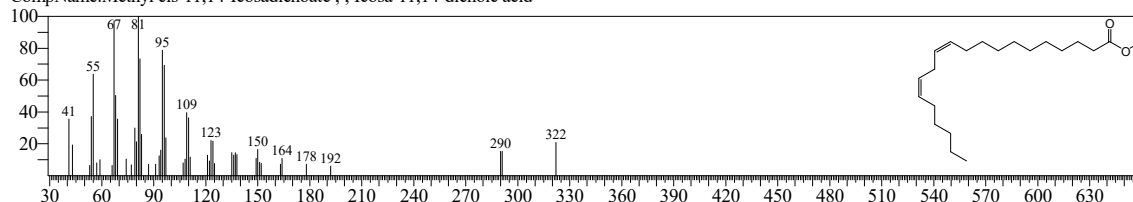CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
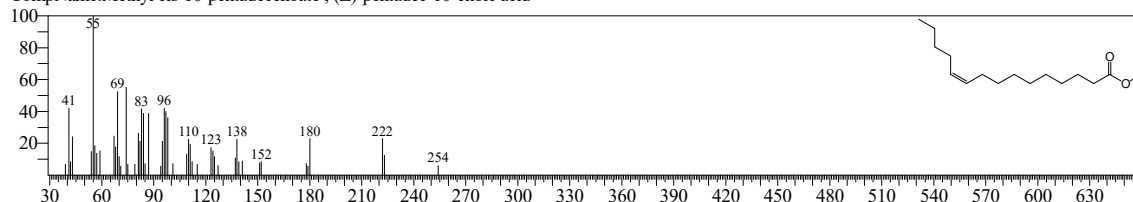SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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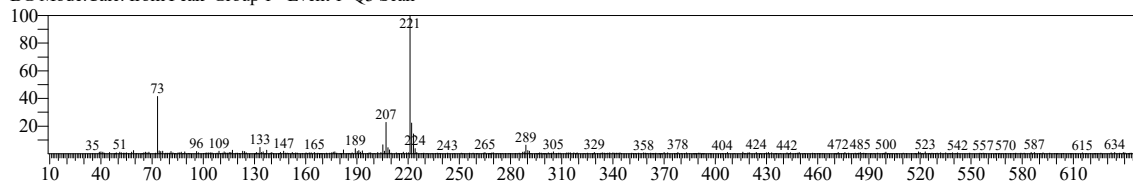CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:5   R.Time:13.810(Scan#:1763) MassPeaks:357
RawMode:Averaged 13.805-13.815(1762-1764) BasePeak:221.05(3464)
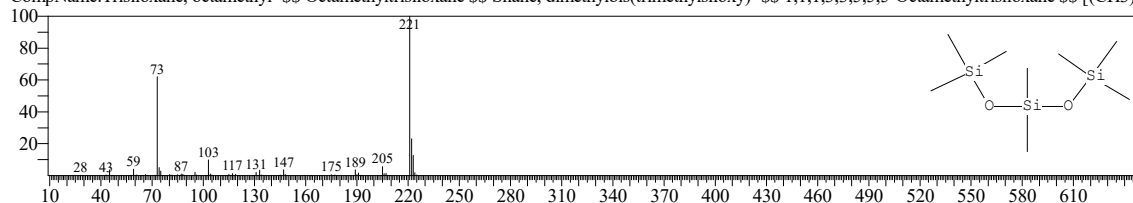BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:28950 Library:NIST20R.lib
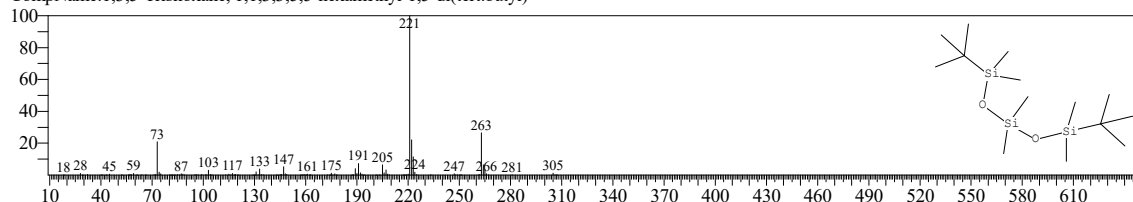SI:80 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3

Hit#:2 Entry:186590 Library:NIST20M1.lib
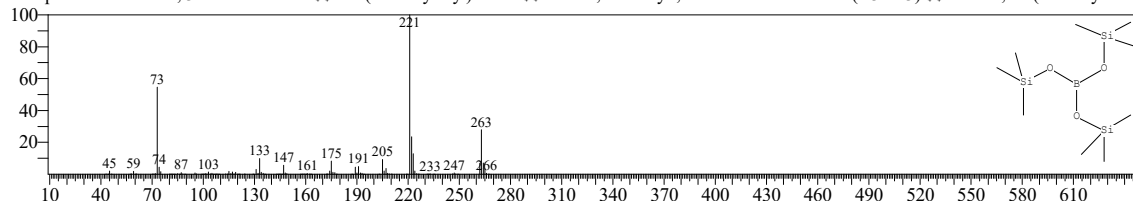SI:76 Formula:C14H36O2Si3 CAS:0-00-0 MolWeight:320 RetIndex:1126
CompName:1,3,5-Trisiloxane, 1,1,3,3,5,5-hexamethyl-1,5-di(tert.butyl)-

Hit#:3 Entry:33791 Library:NIST20R.lib
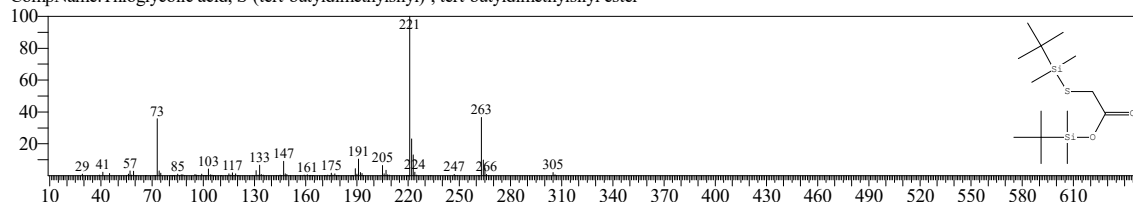SI:75 Formula:C9H27BO3Si3 CAS:4325-85-3 MolWeight:278 RetIndex:0
CompName:Boric acid, 3TMS derivative $$ Tris(trimethylsilyl)borate $$ Silanol, trimethyl-, triester with boric acid (H3BO3) $$ Borane, tris(trimethylsiloxy

Hit#:4 Entry:186586 Library:NIST20M1.lib
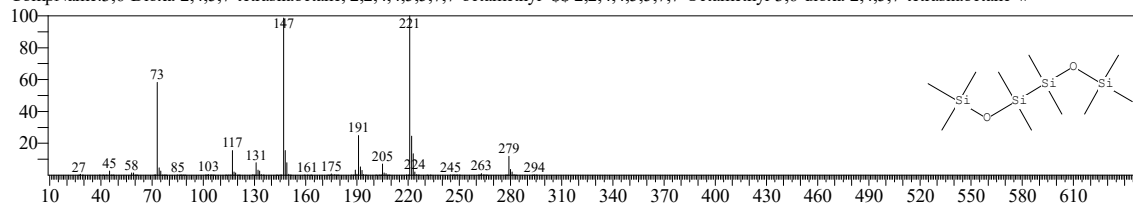SI:75 Formula:C14H32O2SSi2 CAS:82112-29-6 MolWeight:320 RetIndex:1482
CompName:Thioglycolic acid, S-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Hit#:5 Entry:155460 Library:NIST20M1.lib
SI:71 Formula:C10H30O2Si4 CAS:4342-25-0 MolWeight:294 RetIndex:807
CompName:3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl- $$ 2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane #
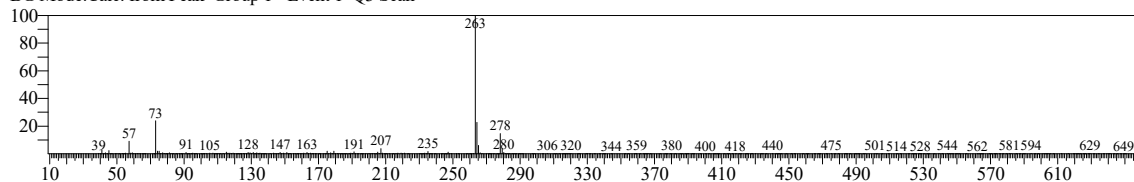
TNAU

<< Target >>
Line#:6 R.Time:19.200(Scan#:2841) MassPeaks:367
RawMode:Averaged 19.195-19.205(2840-2842) BasePeak:263.20(17619)
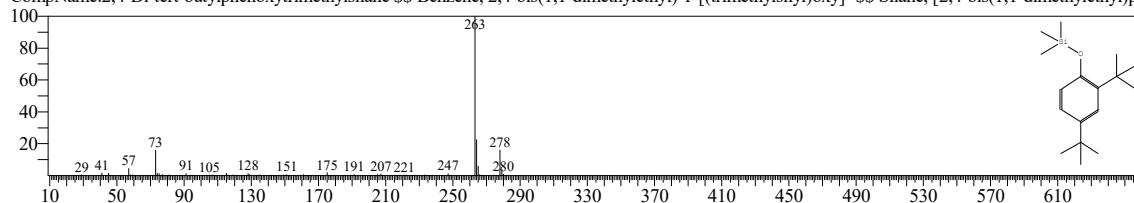BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:33874 Library:NIST20R.lib
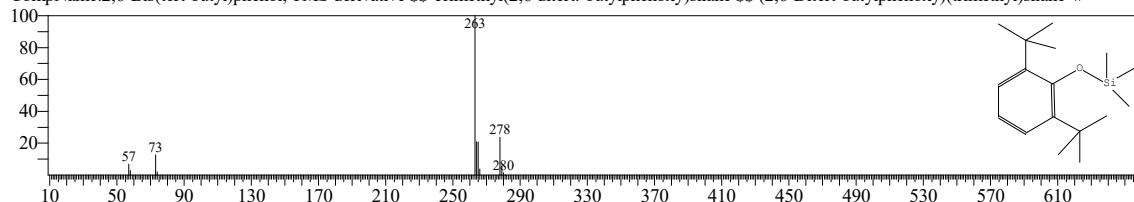SI:95 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph

Hit#:2 Entry:33871 Library:NIST20R.lib
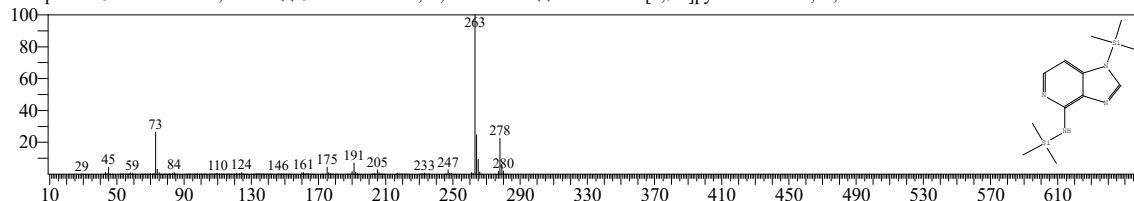SI:85 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #

Hit#:3 Entry:136557 Library:NIST20M1.lib
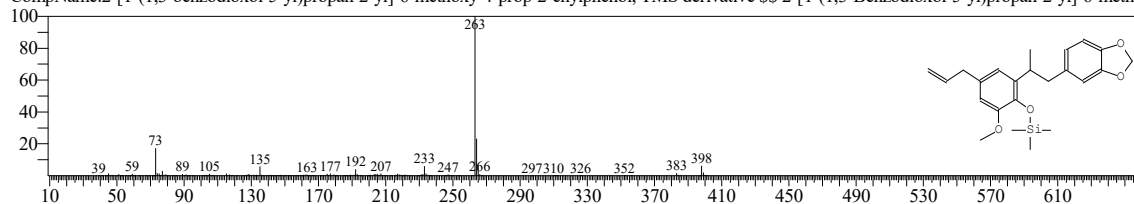SI:84 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS

Hit#:4 Entry:259338 Library:NIST20M1.lib
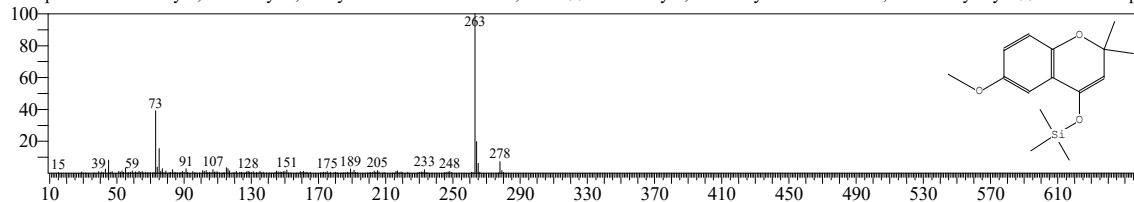SI:81 Formula:C23H30O4Si CAS:0-00-0 MolWeight:398 RetIndex:2735
CompName:2-[1-(1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-prop-2-enylphenol, TMS derivative $$ 2-[1-(1,3-Benzodioxol-5-yl)propan-2-yl]-6-metho

Hit#:5 Entry:137020 Library:NIST20M1.lib
SI:80 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy
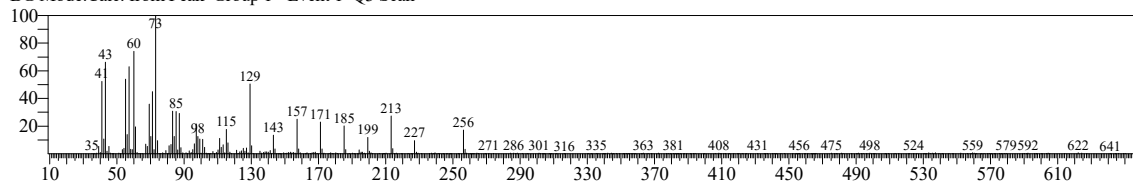
TNAU

<< Target >>
Line#:7 R.Time:28.305(Scan#:4662) MassPeaks:331
RawMode:Averaged 28.300-28.310(4661-4663) BasePeak:73.05(6341)
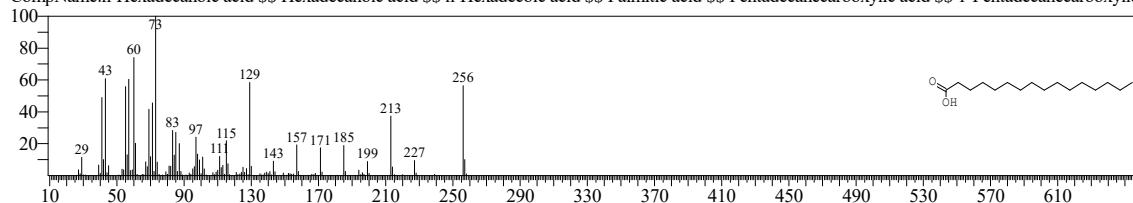BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:31600 Library:NIST20R.lib
SI:96 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
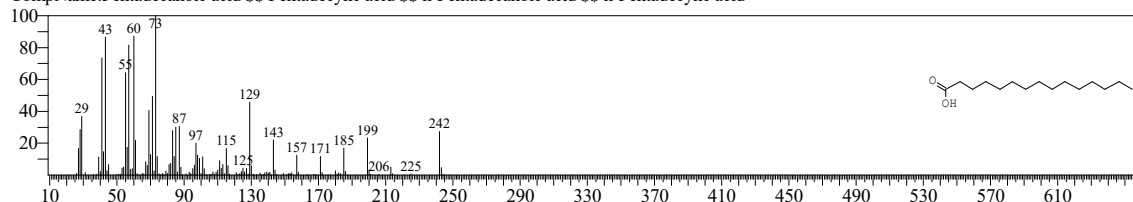CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic $$ 1-Pentadecanecarboxylic

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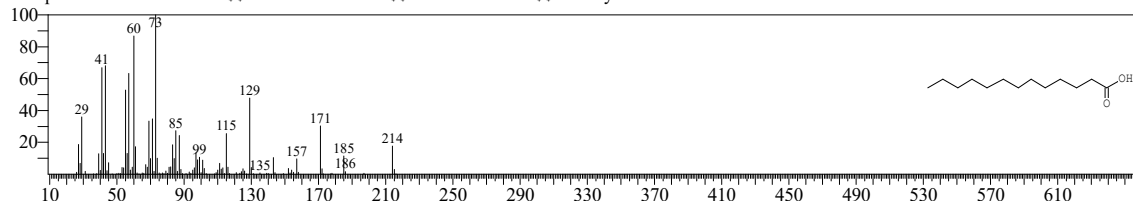SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

Hit#:3 Entry:25643 Library:NIST20R.lib
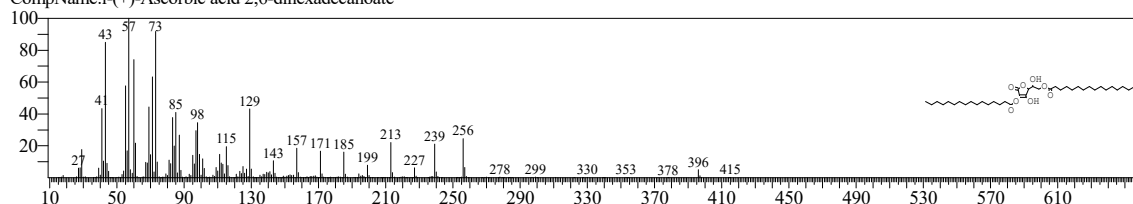SI:91 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

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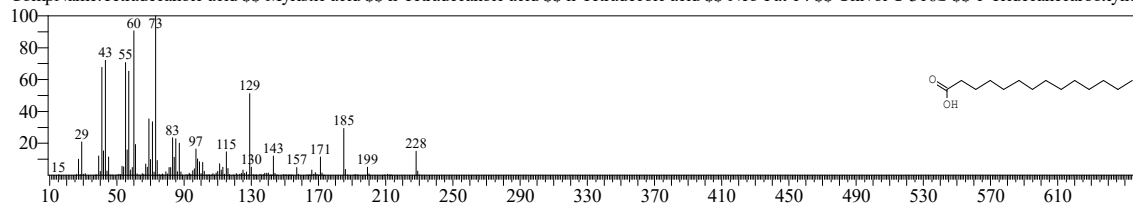CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:90 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
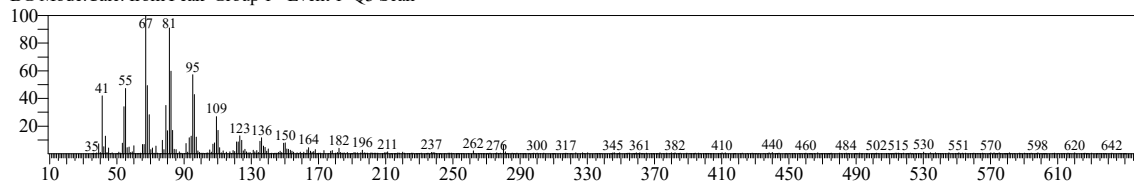
<< Target >>
Line#:8   R.Time:31.485(Scan#:5298) MassPeaks:427
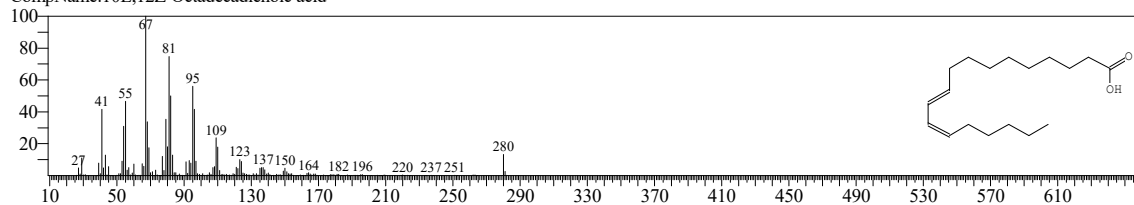RawMode:Averaged 31.480-31.490(5297-5299) BasePeak:67.05(5341)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:139646 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
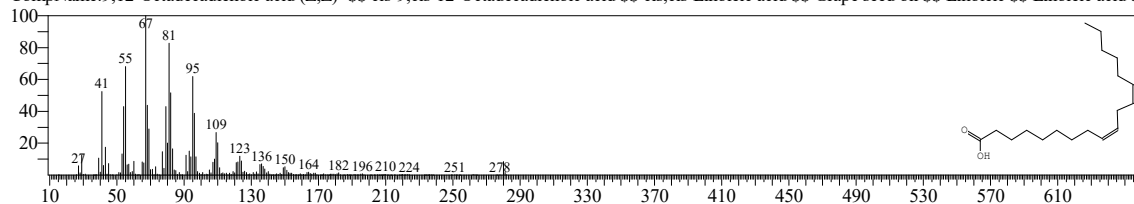CompName:10E,12Z-Octadecadienoic acid

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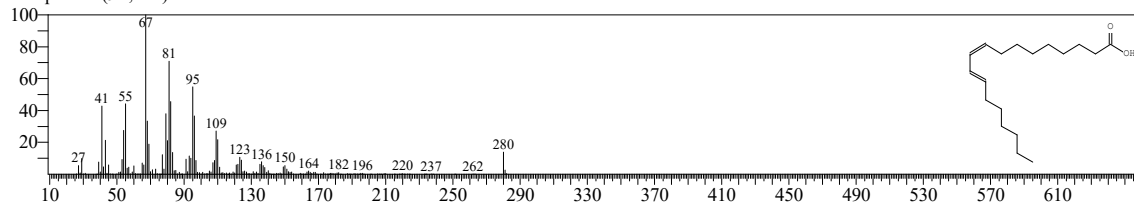CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$

Hit#:3 Entry:139651 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
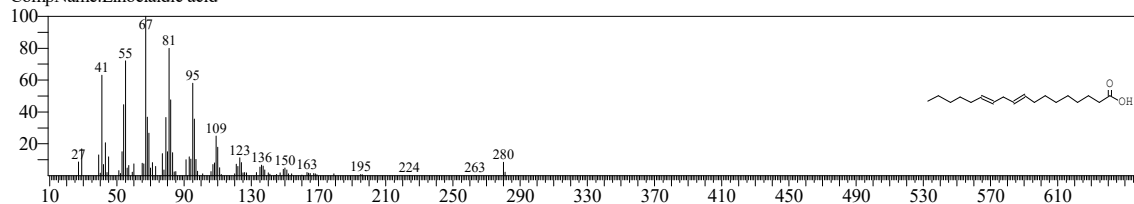CompName:(9E,11E)-Octadecadienoic acid

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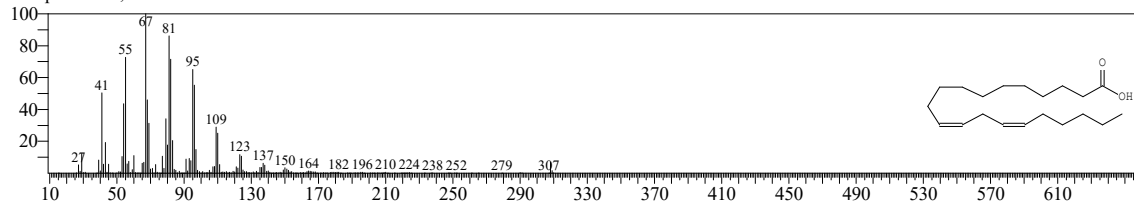CompName:Linoelaidic acid

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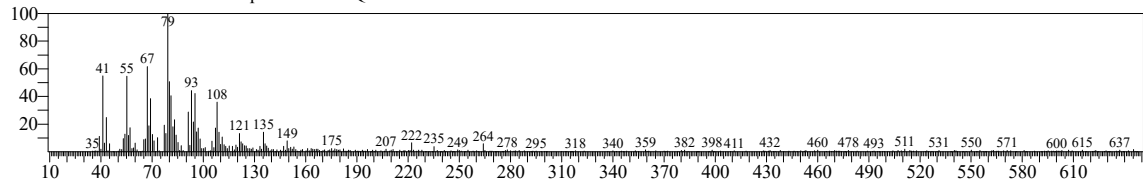CompName:11,14-Eicosadienoic acid

TNAU

<< Target >>
Line#:9   R.Time:31.585(Scan#:5318) MassPeaks:353
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:79.10(2799)
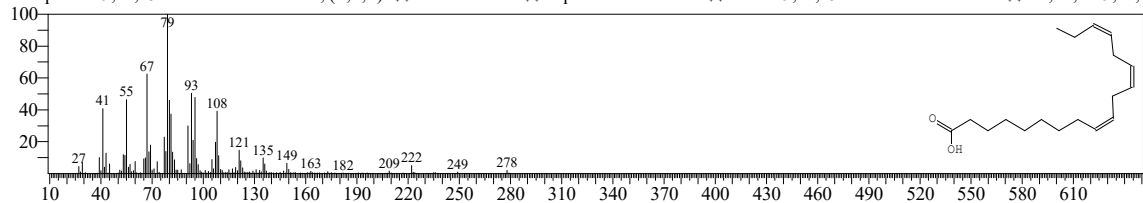BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:137464 Library:NIST20M1.lib
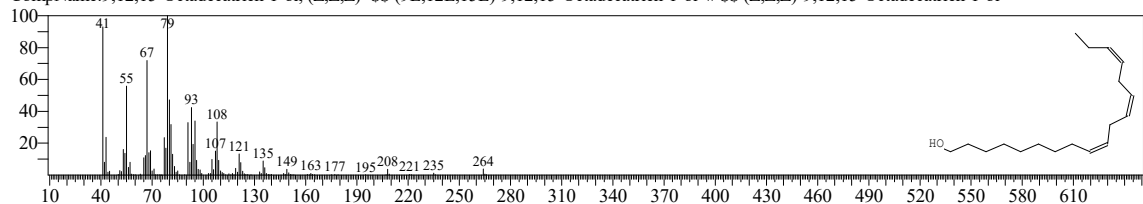SI:91 Formula:C18H30O2 CAS:463-40-1 MolWeight:278 RetIndex:2191
CompName:9,12,15-Octadecatrienoic acid, (Z,Z,Z)- $$ Linolenic acid $$ .alpha.-Linolenic acid $$ All-cis-9,12,15-Octadecatrienoic acid $$ cis,cis,cis-9,12,1

Hit#:2 Entry:32465 Library:NIST20R.lib
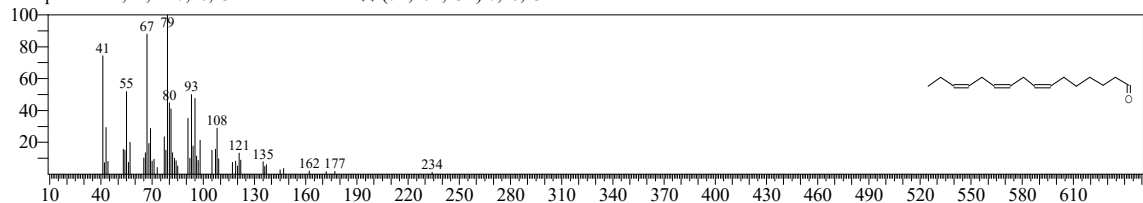SI:89 Formula:C18H32O CAS:506-44-5 MolWeight:264 RetIndex:2077
CompName:9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- $$ (9E,12E,15E)-9,12,15-Octadecatrien-1-ol # $$ (Z,Z,Z)-9,12,15-Octadecatrien-1-ol

Hit#:3 Entry:87848 Library:NIST20M1.lib
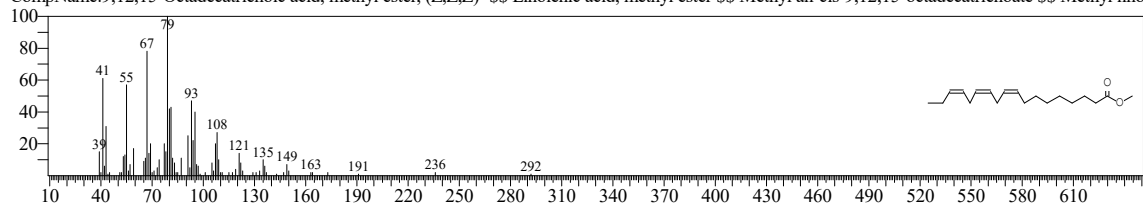SI:89 Formula:C16H26O CAS:56797-43-4 MolWeight:234 RetIndex:1824
CompName:cis,cis,cis-7,10,13-Hexadecatrienal $$ (7Z,10Z,13Z)-7,10,13-Hexadecatrienal #

Hit#:4 Entry:35226 Library:NIST20R.lib
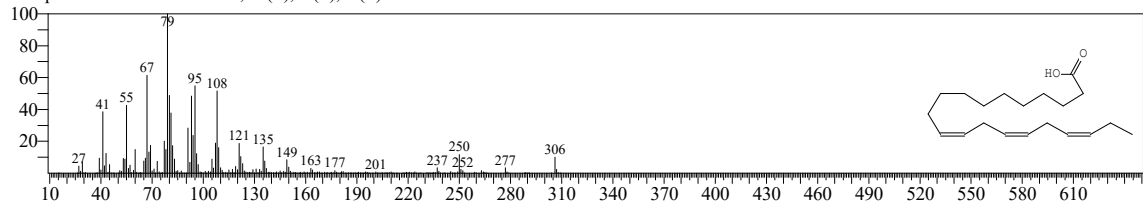SI:88 Formula:C19H32O2 CAS:301-00-8 MolWeight:292 RetIndex:2101
CompName:9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- $$ Linolenic acid, methyl ester $$ Methyl all-cis-9,12,15-octadecatrienoate $$ Methyl lino

Hit#:5 Entry:171056 Library:NIST20M1.lib
SI:88 Formula:C20H34O2 CAS:17046-59-2 MolWeight:306 RetIndex:2390
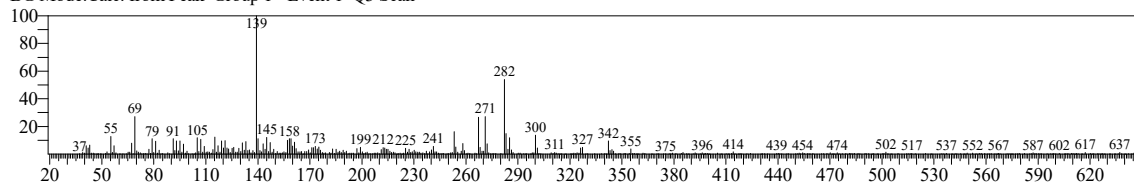CompName:Eicosatrienoic acid, 11(Z),14(Z),17(Z)

TNAU

<< Target >>
Line#:10 R.Time:45.635(Scan#:8128) MassPeaks:442
RawMode:Averaged 45.630-45.640(8127-8129) BasePeak:139.10(4926)
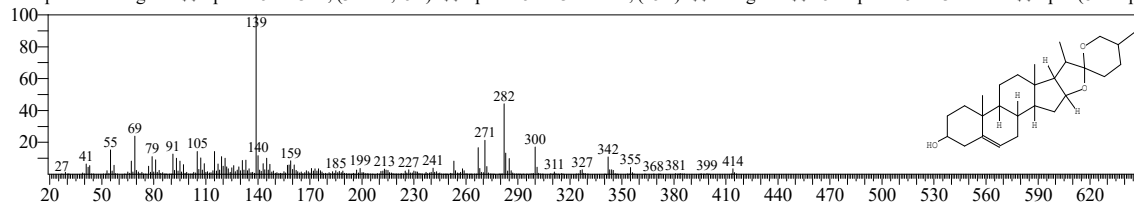BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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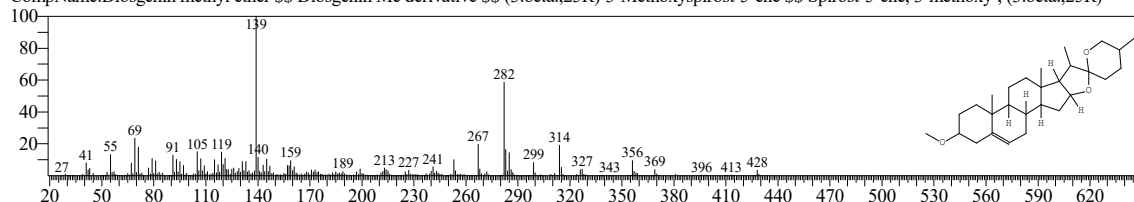SI:90 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

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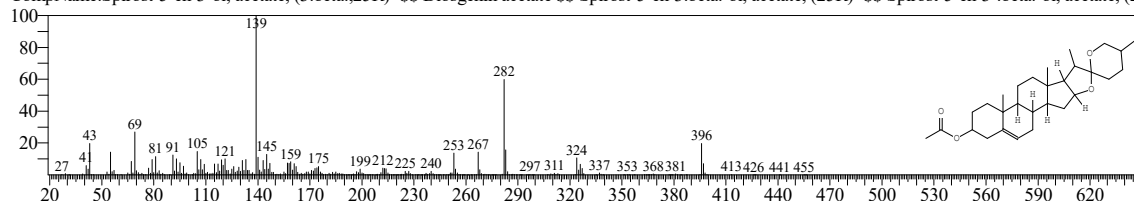SI:82 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:3 Entry:24878 Library:NIST20M2.lib
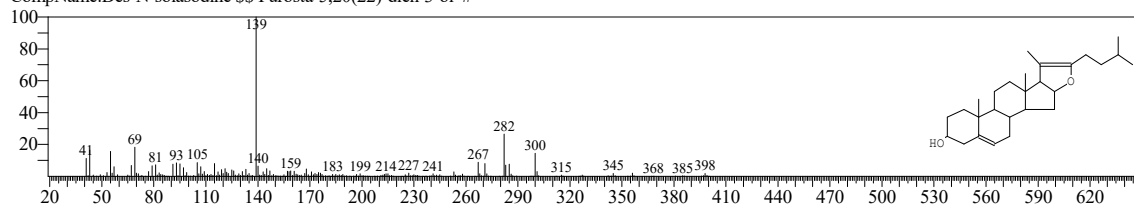SI:81 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (25

Hit#:4 Entry:41561 Library:NIST20R.lib
SI:80 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: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.