TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022012.qgd

Peak Report TIC

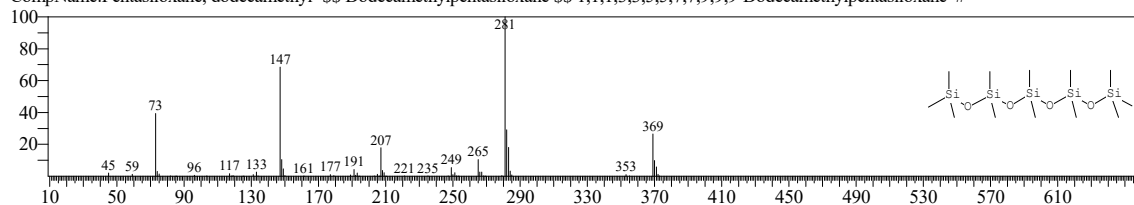| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.767	50092	2.18	21699	2.82	2.31	94	Pentasiloxane, dodecamethyl-
2	11.124	15209	0.66	8085	1.05	1.88	46	Pimelic acid-2TMS
3	12.487	19727	0.86	10350	1.35	1.91	31	Succinylacetone-ox-origin fragment
4	12.824	89804	3.91	28515	3.71	3.15	72	2,5-Cyclohexadiene-1,4-dione, dioxime
5	12.932	38595	1.68	15181	1.97	2.54	71	Morpholine, 4-methyl-, 4-oxide
6	13.239	633633	27.58	221892	28.86	2.86	54	Methyl cis-13,16-Docosadienate
7	13.434	523332	22.78	185556	24.13	2.82	54	Methyl cis-13,16-Docosadienate
8	13.816	20756	0.90	11085	1.44	1.87	84	Trisiloxane, octamethyl-
9	19.195	102182	4.45	43378	5.64	2.36	96	2,4-Di-tert-butylphenoxytrimethylsilane
10	28.305	224308	9.76	80135	10.42	2.80	95	n-Hexadecanoic acid
11	31.484	180444	7.85	62071	8.07	2.91	95	9,12-Octadecadienoic acid (Z,Z)-
12	31.586	138558	6.03	39159	5.09	3.54	90	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
13	45.626	231597	10.08	34968	4.55	6.62	88	Diosgenin
14	46.622	29364	1.28	6896	0.90	4.26	23	Linoleic acid-TMS
		2297601	100.00	768970	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:9.765(Scan#:954) MassPeaks:310
RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(5859)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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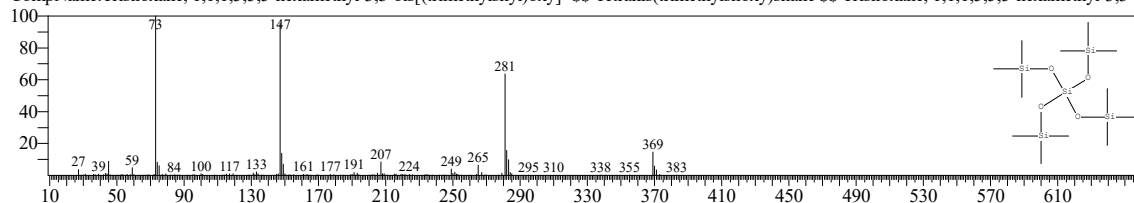SI:94 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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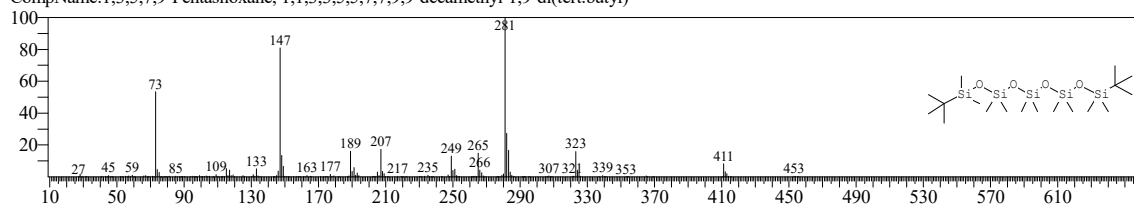SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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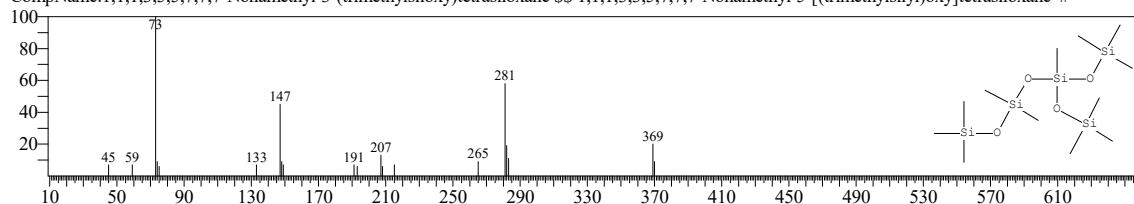SI:82 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

Hit#:4 Entry:249271 Library:NIST20M1.lib
SI:80 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
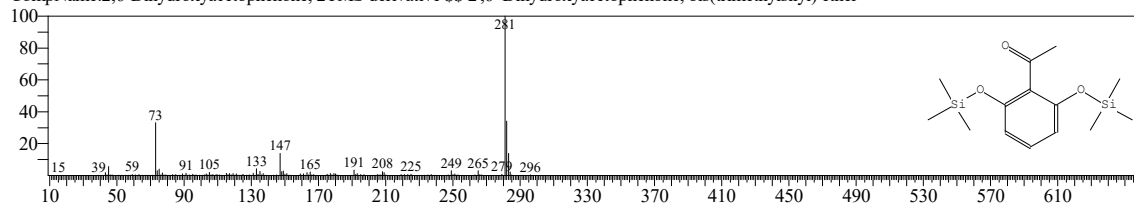CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:78 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether
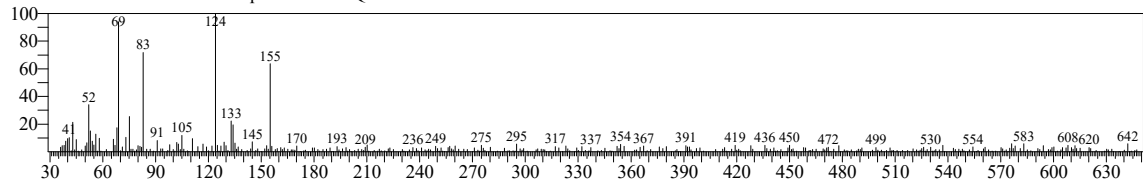
TNAU

<< Target >>
Line#:2   R.Time:11.125(Scan#:1226) MassPeaks:358
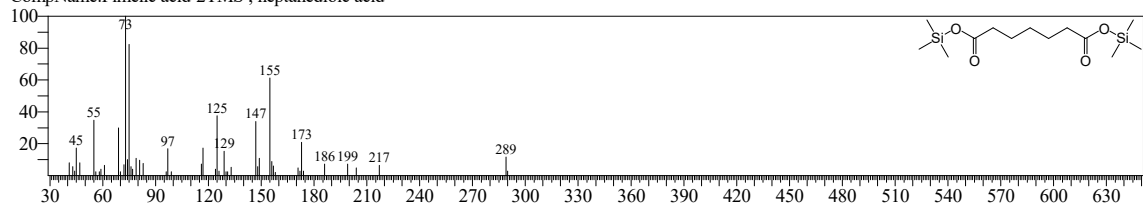RawMode:Averaged 11.120-11.130(1225-1227) BasePeak:124.05(782)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:196 Library:OA_TMS_DB5_67min_V3.lib
SI:46 Formula:C13H28O4Si2 CAS:111-16-0 MolWeight:304 RetIndex:1605
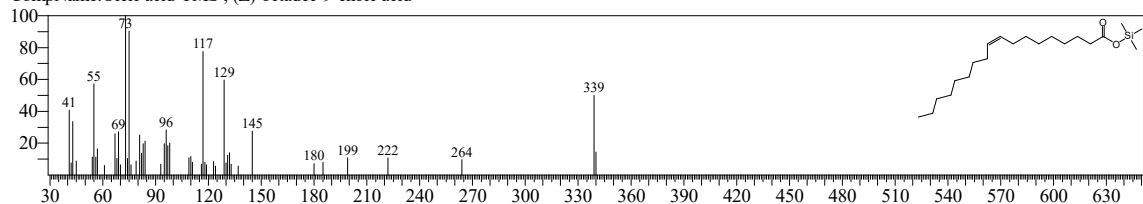CompName:Pimelic acid-2TMS ; heptanedioic acid

Hit#:2 Entry:485 Library:OA_TMS_DB5_67min_V3.lib
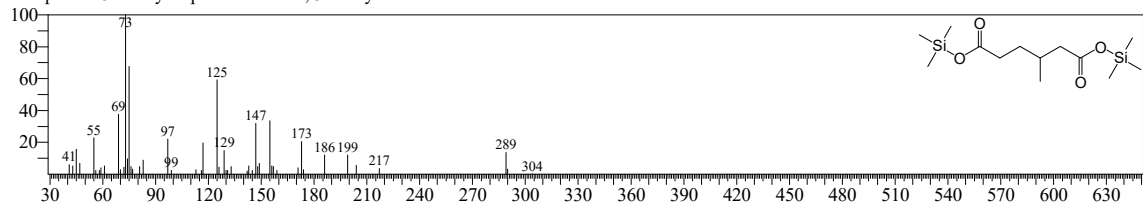SI:42 Formula:C21H42O2Si CAS:112-80-1 MolWeight:354 RetIndex:2222
CompName:Oleic acid-TMS ; (Z)-octadec-9-enoic acid

Hit#:3 Entry:165 Library:OA_TMS_DB5_67min_V3.lib
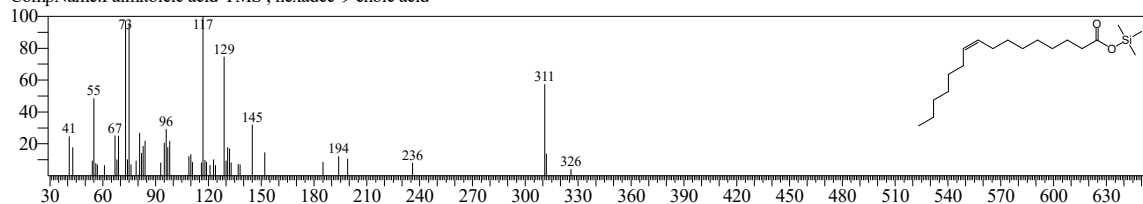SI:41 Formula:C13H28O4Si2 CAS:3058-01-3 MolWeight:304 RetIndex:1539
CompName:3-Methyladipic acid-2TMS ; 3-methylhexanedioic acid

Hit#:4 Entry:442 Library:OA_TMS_DB5_67min_V3.lib
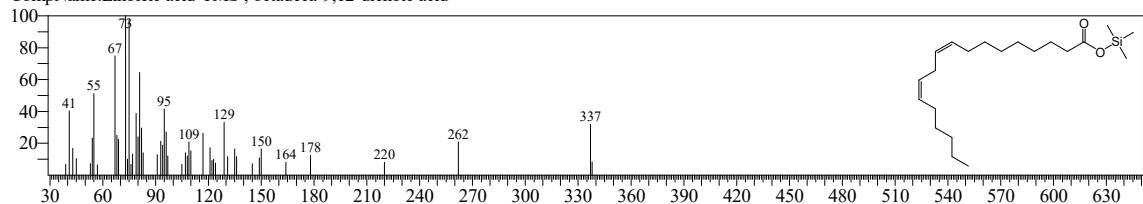SI:40 Formula:C19H38O2Si CAS:373-49-9 MolWeight:326 RetIndex:2028
CompName:Palmitoleic acid-TMS ; hexadec-9-enoic acid

Hit#:5 Entry:484 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C21H40O2Si CAS:60-33-3 MolWeight:352 RetIndex:2218
CompName:Linoleic acid-TMS ; octadeca-9,12-dienoic acid
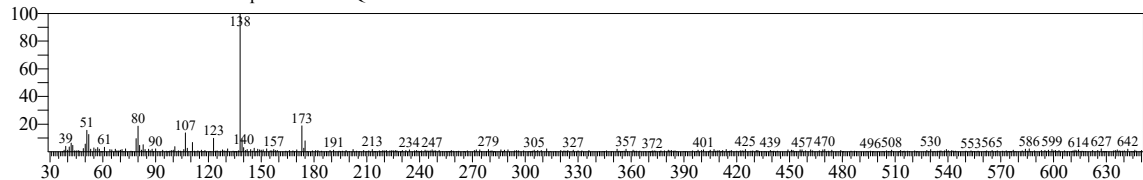
TNAU

<< Target >>
Line#:3 R.Time:12.485(Scan#:1498) MassPeaks:379
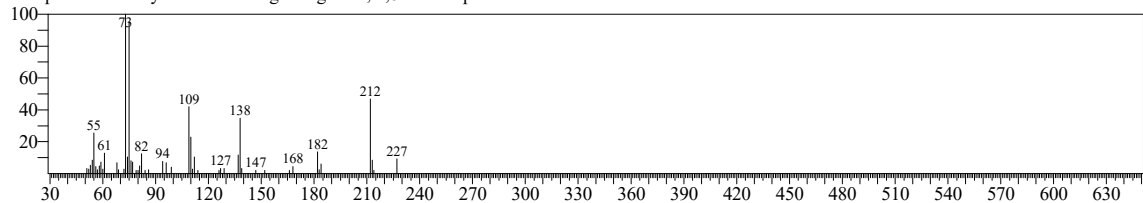RawMode:Averaged 12.480-12.490(1497-1499) BasePeak:138.05(2027)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:127 Library:OA_TMS_DB5_67min_V3.lib
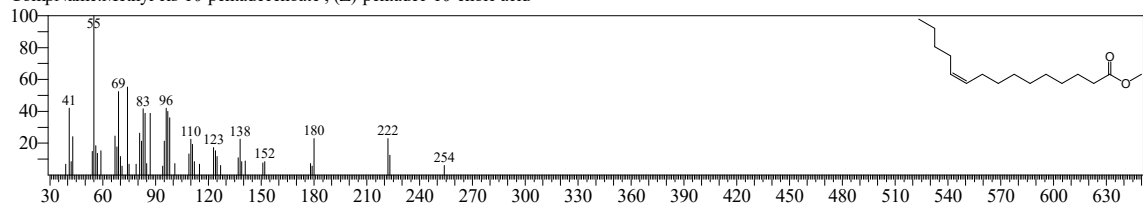SI:31 Formula: CAS:51568-18-4 MolWeight:0 RetIndex:1453
CompName:Succinylacetone-ox-origin fragment ; 4,6-dioxoheptanoic acid

Hit#:2 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
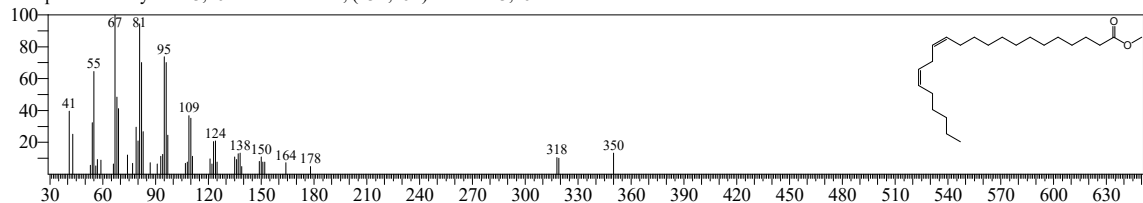SI:30 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

Hit#:3 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
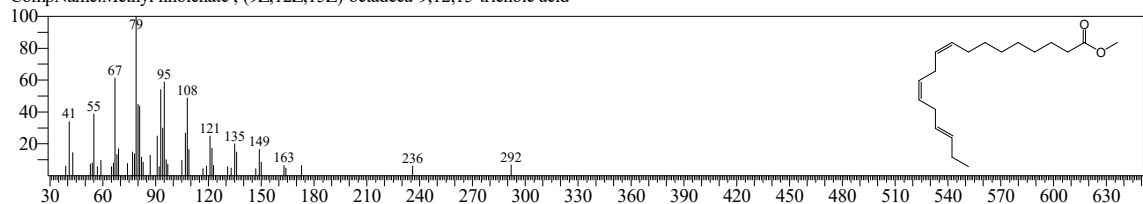SI:30 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:4 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
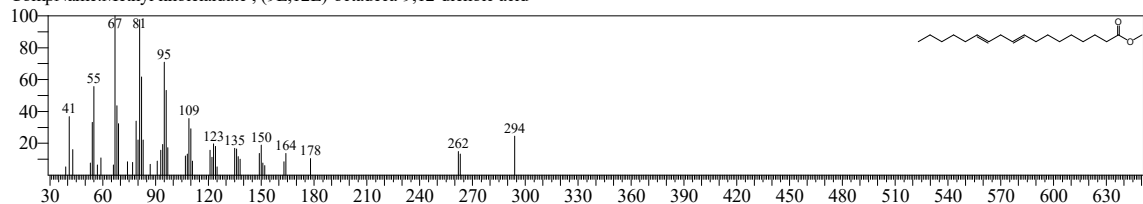SI:29 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

Hit#:5 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:29 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
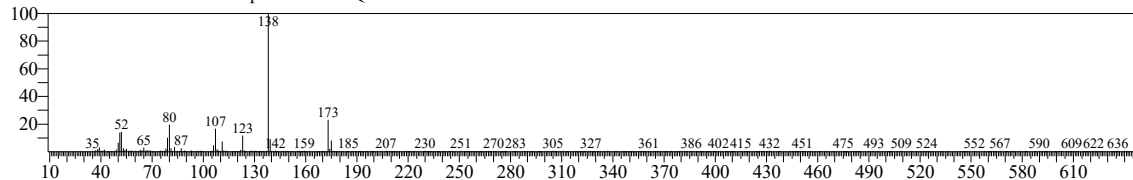CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

TNAU

<< Target >>
Line#:4 R.Time:12.825(Scan#:1566) MassPeaks:374
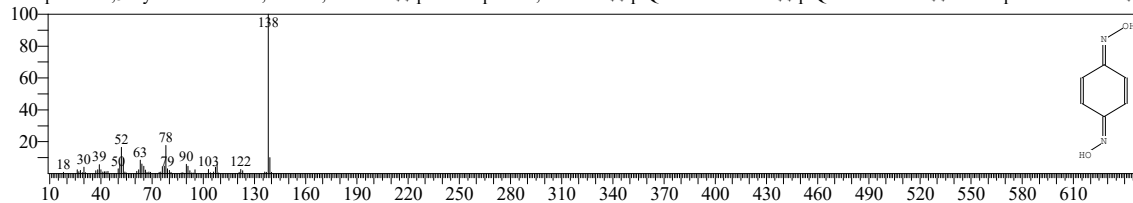RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.10(8471)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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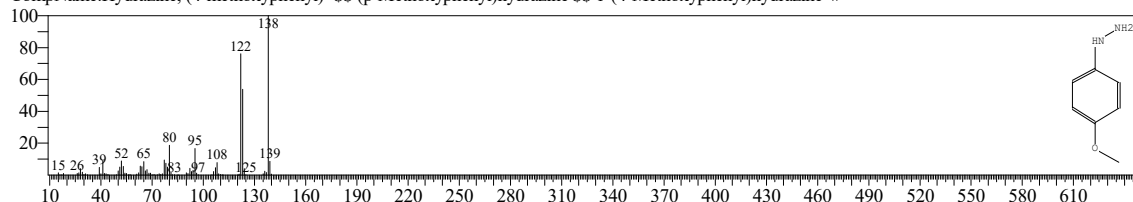CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

Hit#:2 Entry:11222 Library:NIST20M1.lib
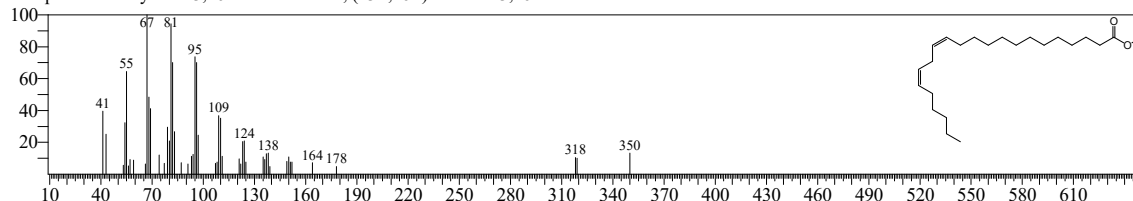SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

Hit#:3 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
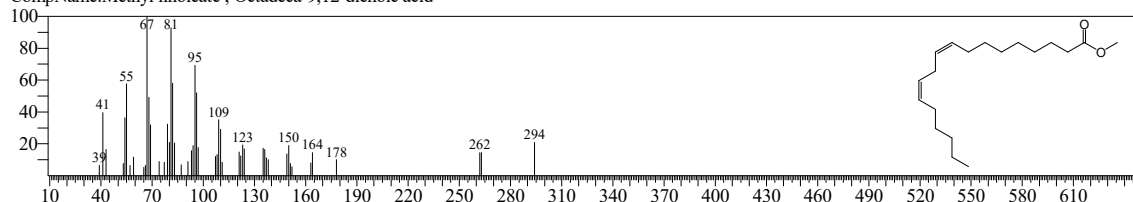SI:36 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:4 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
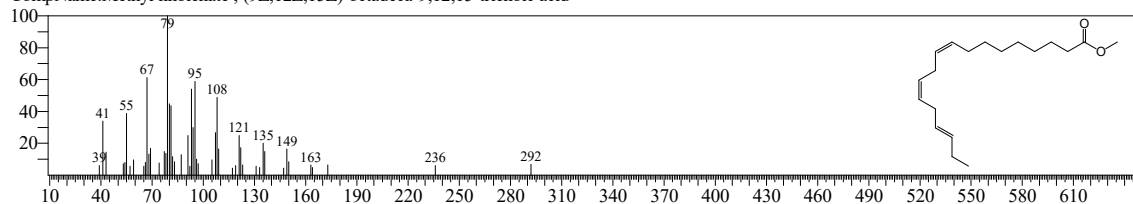CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:5 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
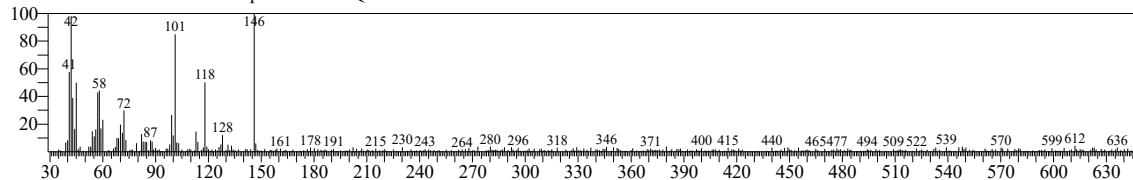CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

TNAU

<< Target >>
Line#:5 R.Time:12.930(Scan#:1587) MassPeaks:400
RawMode:Averaged 12.925-12.935(1586-1588) BasePeak:146.10(1066)
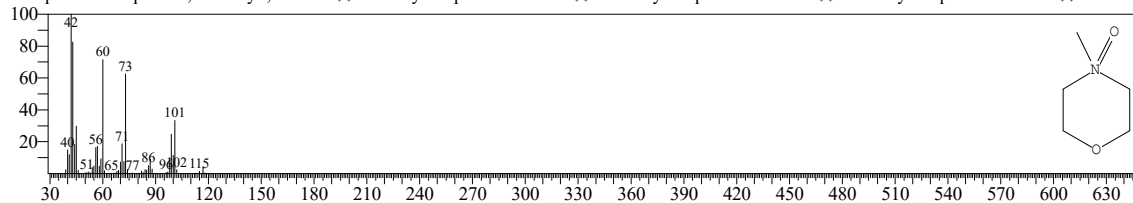BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:5109 Library:NIST20M1.lib
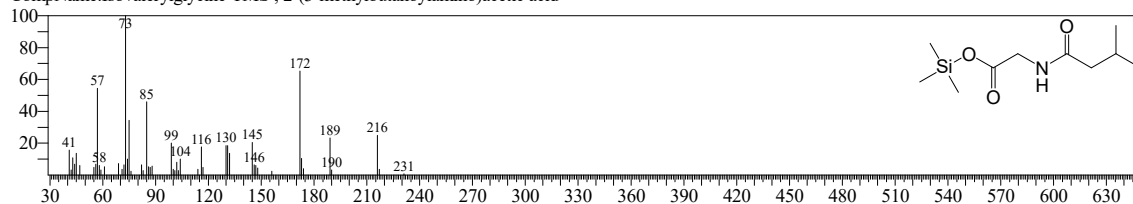SI:71 Formula:C5H11NO2 CAS:7529-22-8 MolWeight:117 RetIndex:0
CompName:Morpholine, 4-methyl-, 4-oxide $$ 4-Methylmorpholine 4-oxide $$ N-Methylmorpholine N-oxide $$ N-Methylmorpholine 4-oxide $$ N-Methy

Hit#:2 Entry:139 Library:OA_TMS_DB5_67min_V3.lib
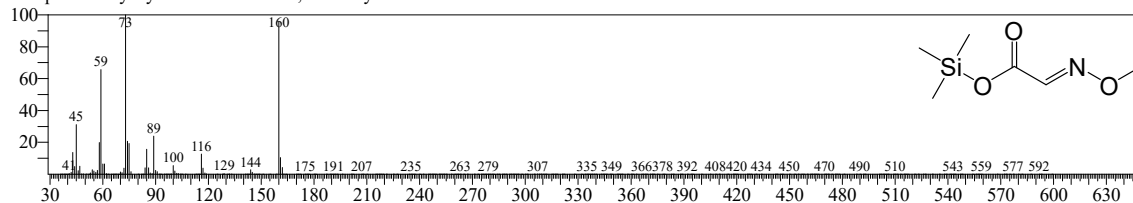SI:48 Formula:C10H21NO3Si CAS:16284-60-9 MolWeight:231 RetIndex:1487
CompName:Isovalerylglycine-TMS ; 2-(3-methylbutanoylamino)acetic acid

Hit#:3 Entry:2 Library:OA_TMS_DB5_67min_V3.lib
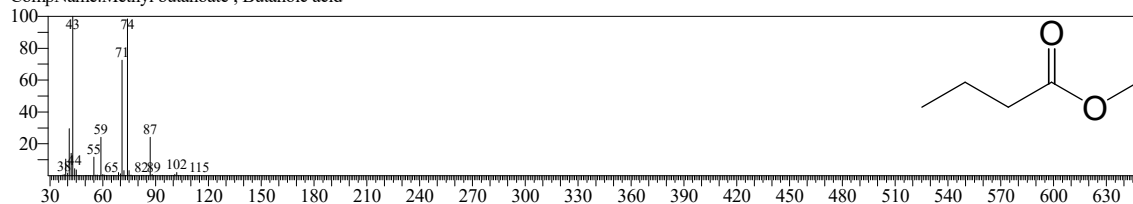SI:47 Formula:C6H13NO3Si CAS:298-12-4 MolWeight:175 RetIndex:990
CompName:Glyoxylic acid-meto-TMS ; oxaldehydic acid

Hit#:4 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
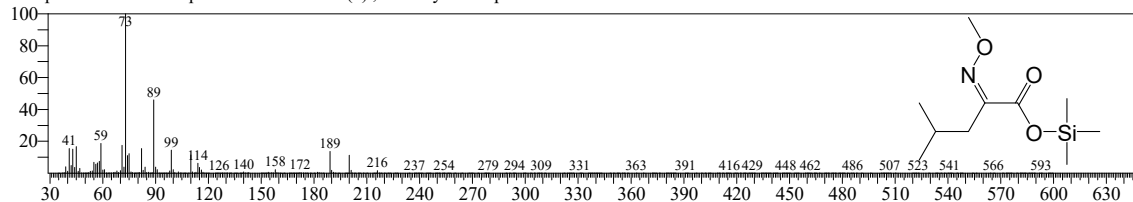SI:47 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid

Hit#:5 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:45 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
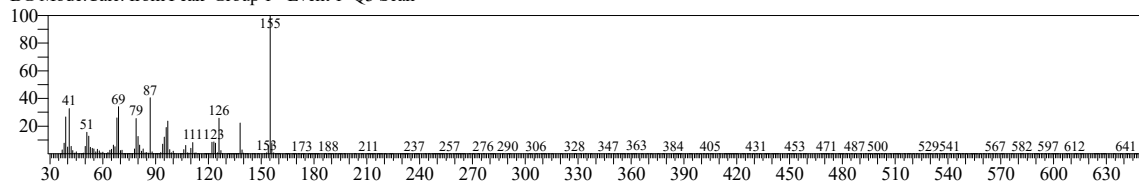CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid

TNAU

<< Target >>
Line#:6 R.Time:13.240(Scan#:1649) MassPeaks:342
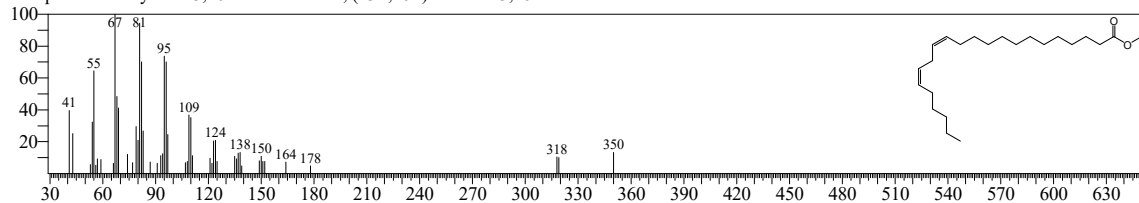RawMode:Averaged 13.235-13.245(1648-1650) BasePeak:155.05(35297)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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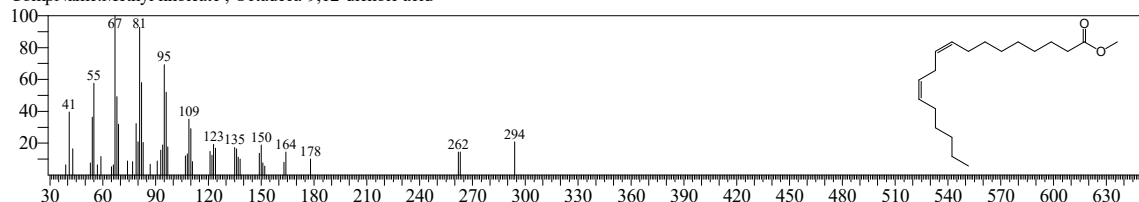SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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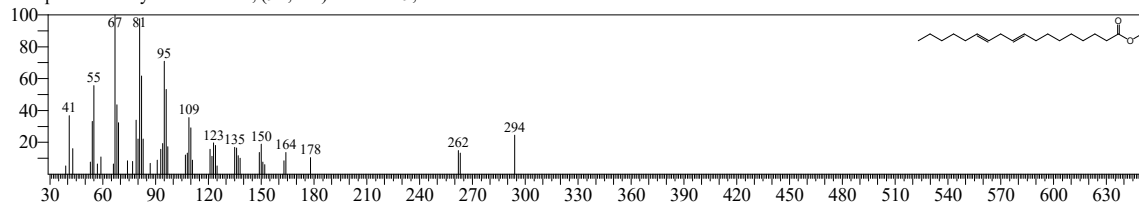SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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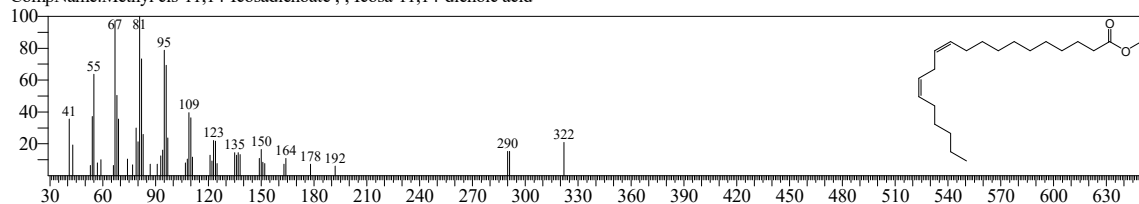CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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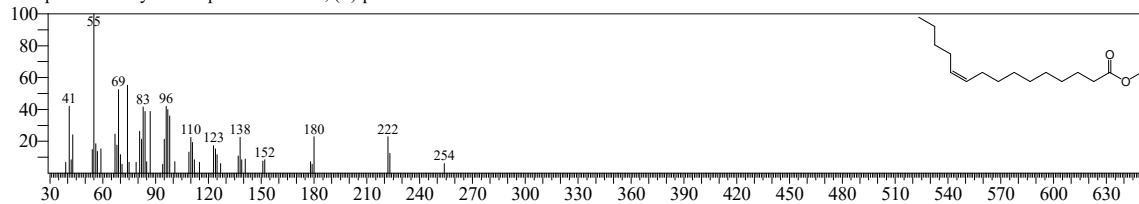CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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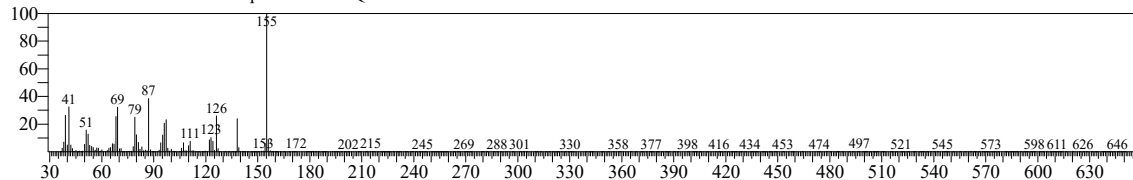CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:7   R.Time:13.435(Scan#:1688) MassPeaks:369
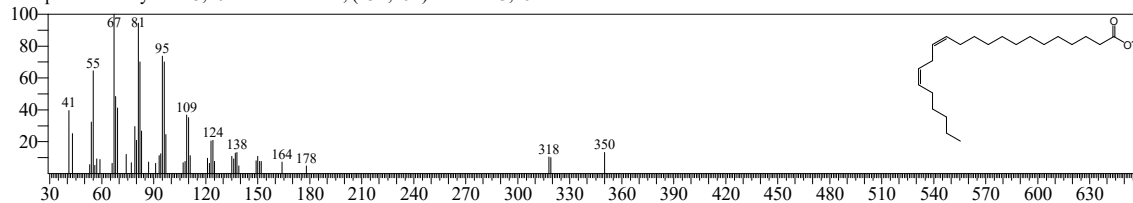RawMode:Averaged 13.430-13.440(1687-1689) BasePeak:155.05(29377)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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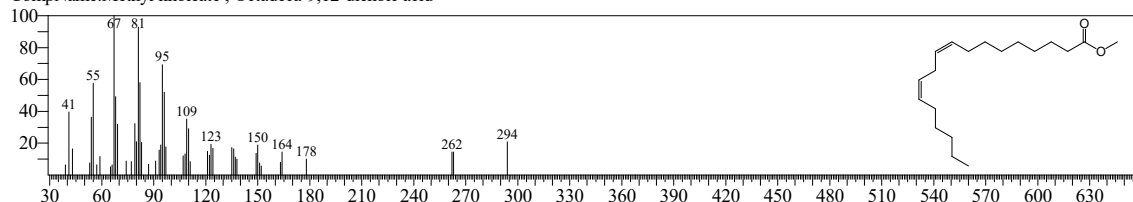SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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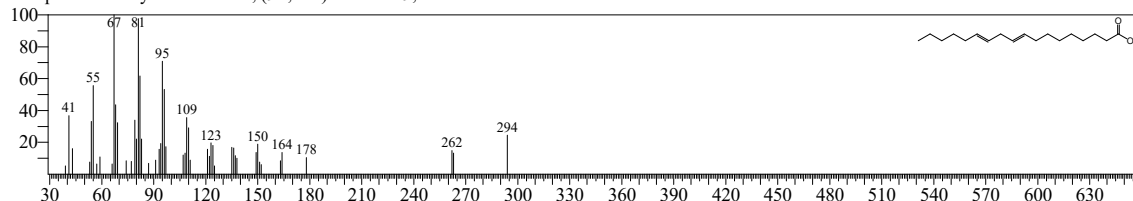SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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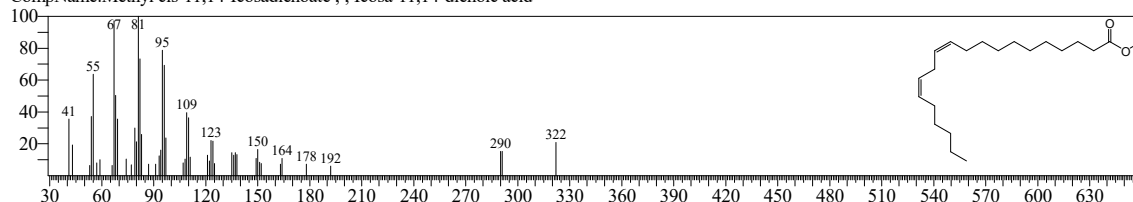CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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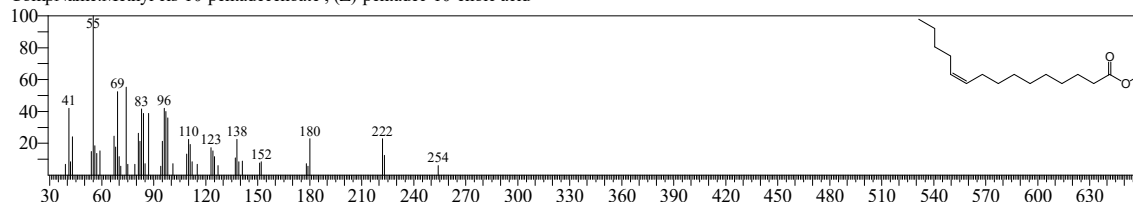SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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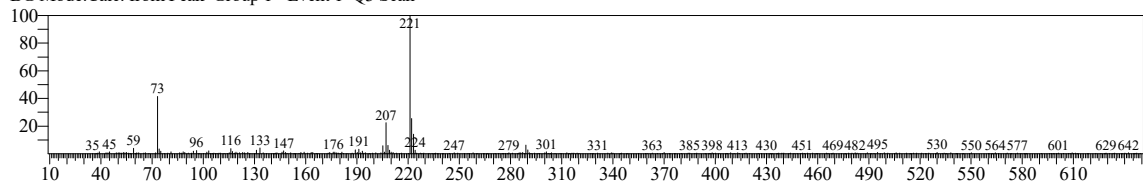CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:8 R.Time:13.815(Scan#:1764) MassPeaks:313
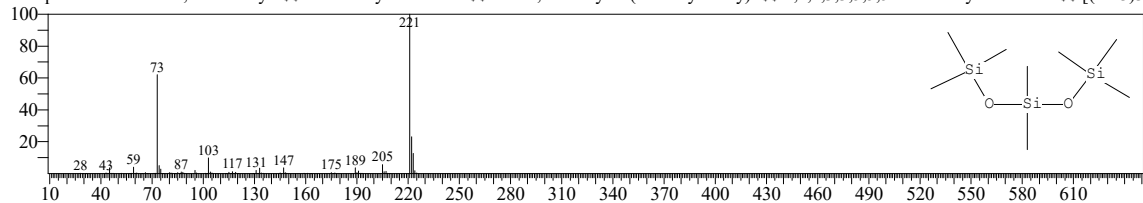RawMode:Averaged 13.810-13.820(1763-1765) BasePeak:221.10(3580)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:28950 Library:NIST20R.lib
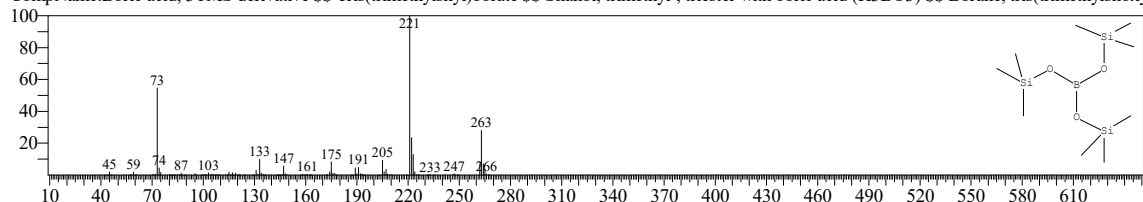SI:84 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3

Hit#:2 Entry:33791 Library:NIST20R.lib
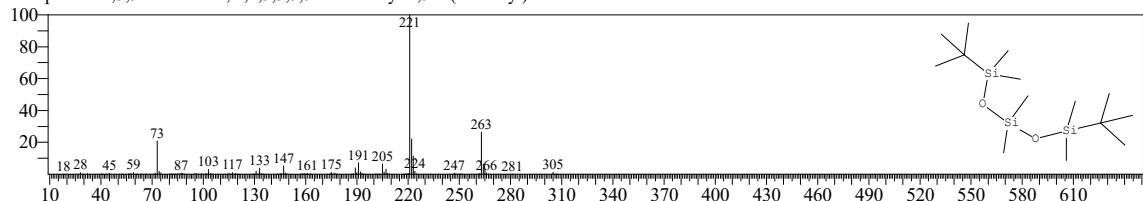SI:78 Formula:C9H27BO3Si3 CAS:4325-85-3 MolWeight:278 RetIndex:0
CompName:Boric acid, 3TMS derivative $$ Tris(trimethylsilyl)borate $$ Silanol, trimethyl-, triester with boric acid (H3BO3) $$ Borane, tris(trimethylsiloxy

Hit#:3 Entry:186590 Library:NIST20M1.lib
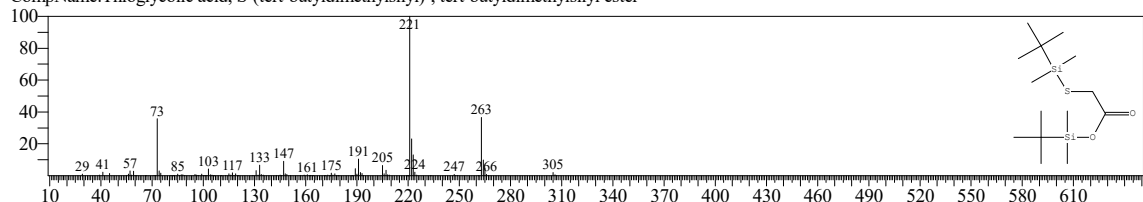SI:77 Formula:C14H36O2Si3 CAS:0-00-0 MolWeight:320 RetIndex:1126
CompName:1,3,5-Trisiloxane, 1,1,3,3,5,5-hexamethyl-1,5-di(tert.butyl)-

Hit#:4 Entry:186586 Library:NIST20M1.lib
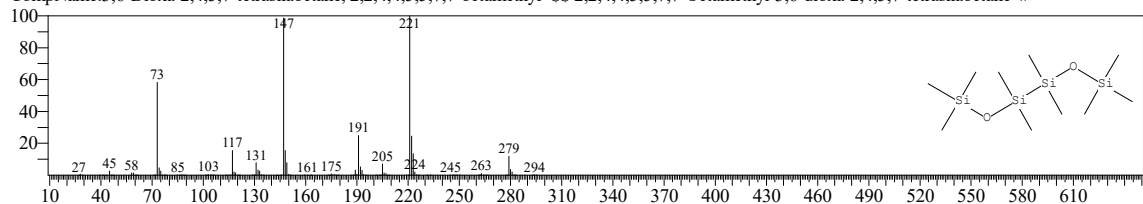SI:77 Formula:C14H32O2SSi2 CAS:82112-29-6 MolWeight:320 RetIndex:1482
CompName:Thioglycolic acid, S-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Hit#:5 Entry:155460 Library:NIST20M1.lib
SI:74 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 #
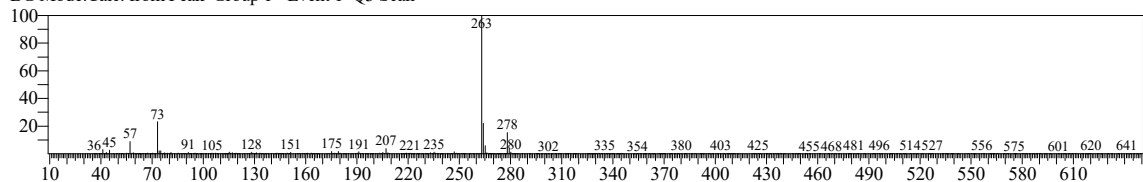
TNAU

<< Target >>
Line#:9 R.Time:19.195(Scan#:2840) MassPeaks:353
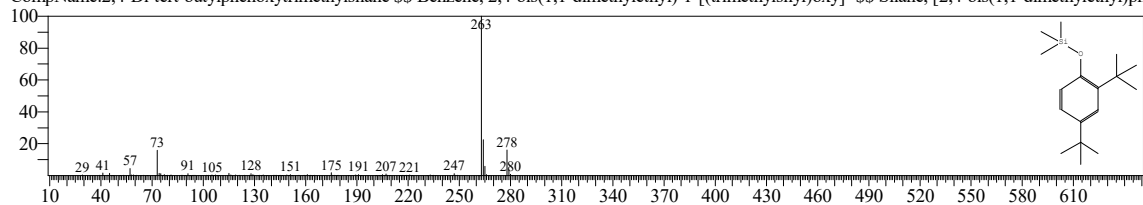RawMode:Averaged 19.190-19.200(2839-2841) BasePeak:263.20(17803)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:33874 Library:NIST20R.lib
SI:96 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
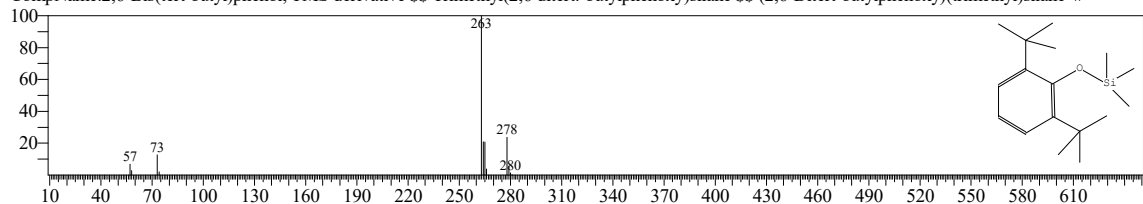CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph

Hit#:2 Entry:33871 Library:NIST20R.lib
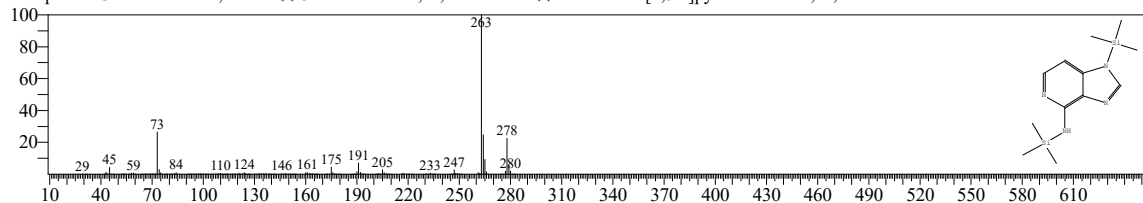SI:86 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #

Hit#:3 Entry:136557 Library:NIST20M1.lib
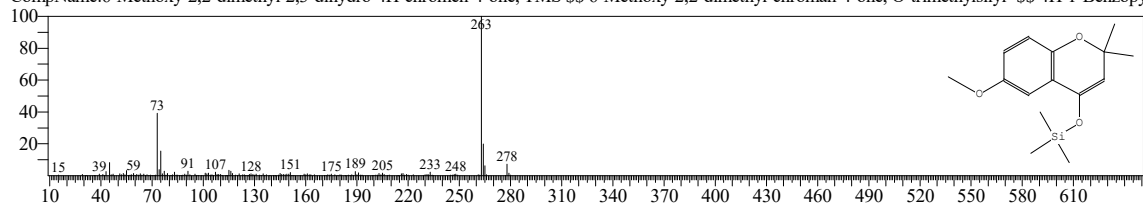SI:85 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS

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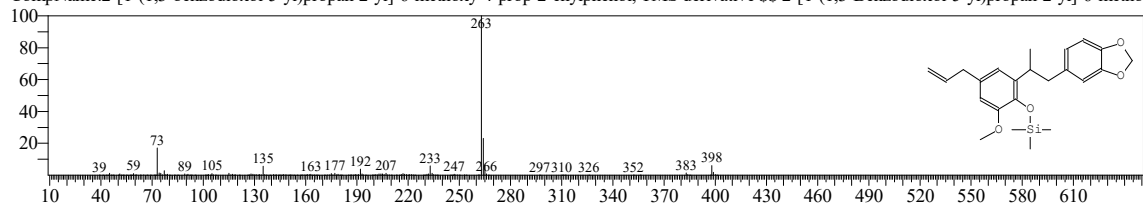SI:80 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy

Hit#:5 Entry:259338 Library:NIST20M1.lib
SI:80 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
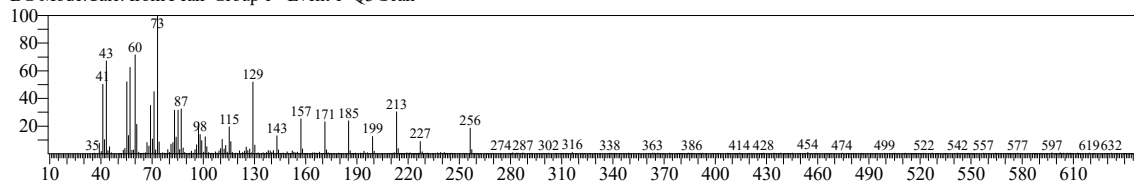
TNAU

<< Target >>
Line#:10 R.Time:28.305(Scan#:4662) MassPeaks:403
RawMode:Averaged 28.300-28.310(4661-4663) BasePeak:73.05(6615)
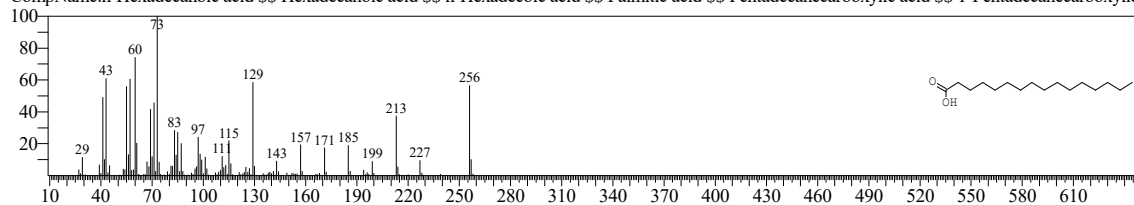BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:31600 Library:NIST20R.lib
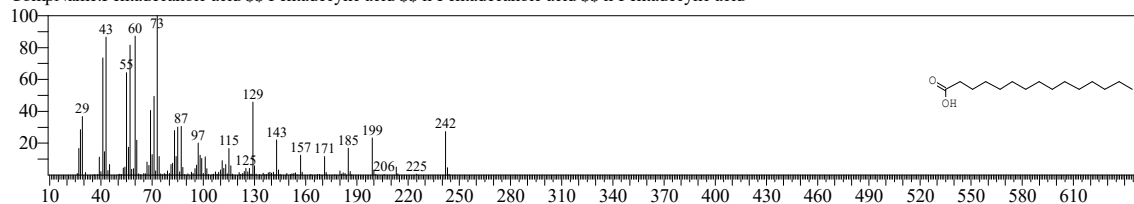SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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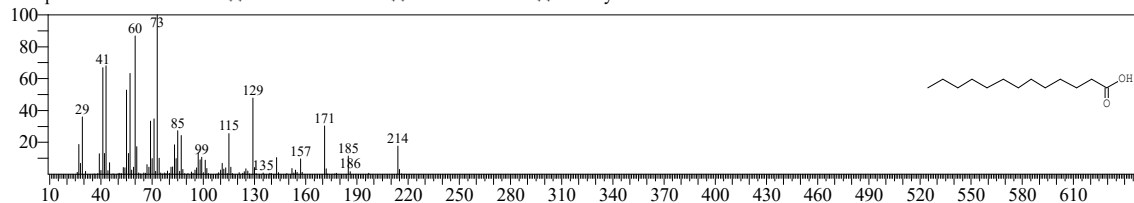SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

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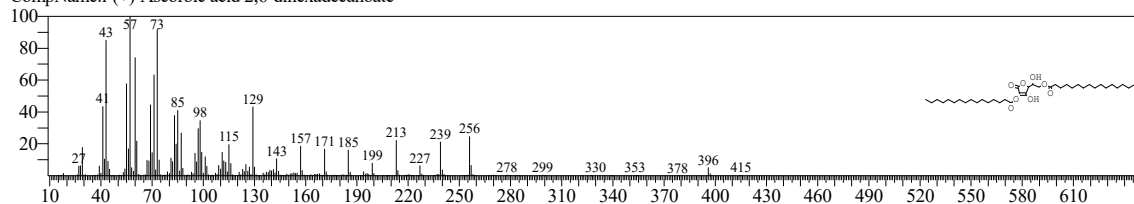SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

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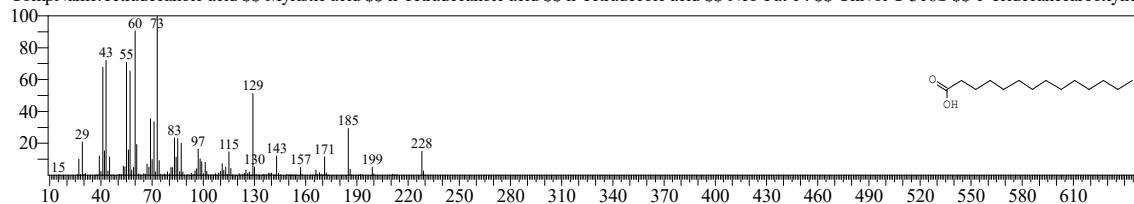SI:90 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

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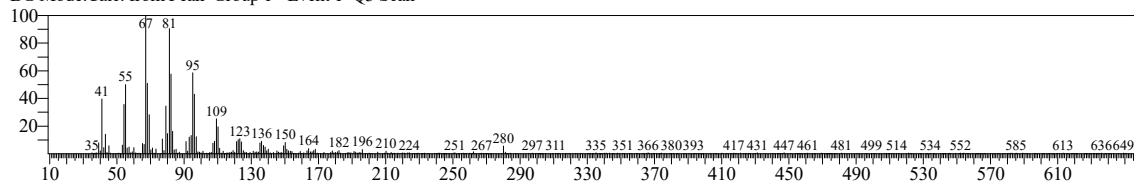
TNAU

<< Target >>
Line#:11 R.Time:31.485(Scan#:5298) MassPeaks:373
RawMode:Averaged 31.480-31.490(5297-5299) BasePeak:67.05(5326)
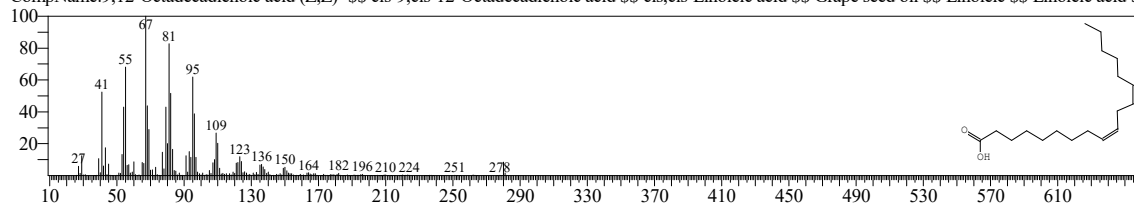BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34035 Library:NIST20R.lib
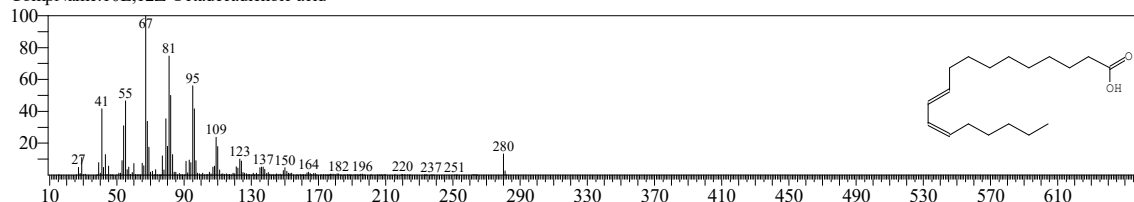SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$

Hit#:2 Entry:139646 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
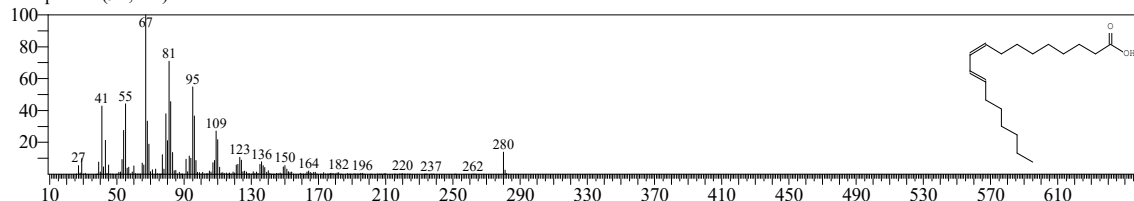CompName:10E,12Z-Octadecadienoic acid

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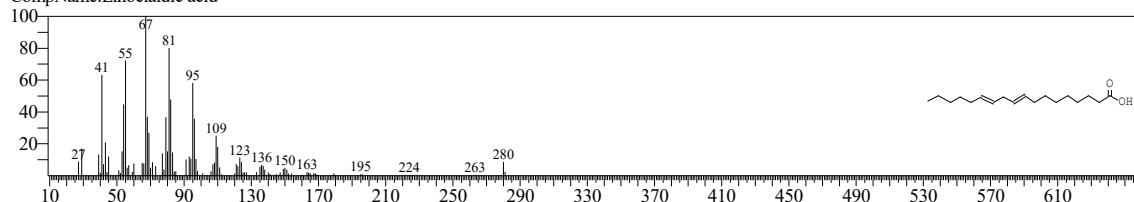CompName:(9E,11E)-Octadecadienoic acid

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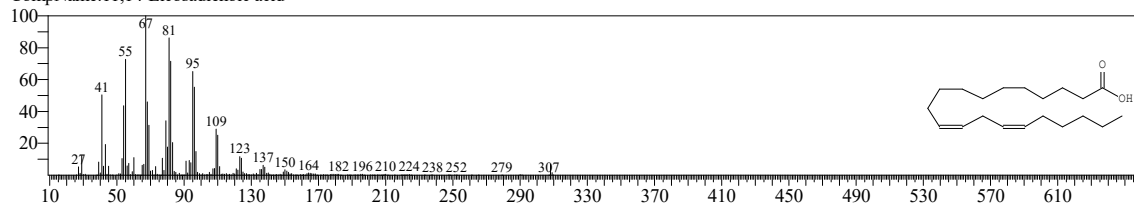CompName:Linoelaidic acid

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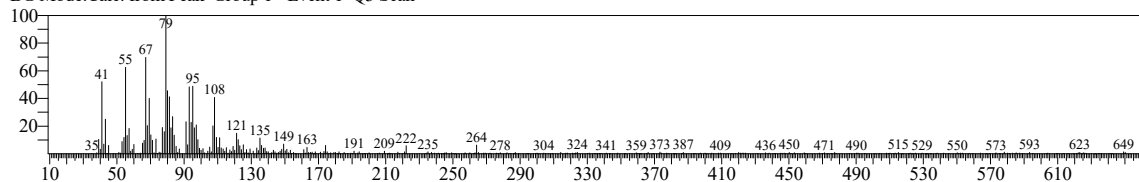CompName:11,14-Eicosadienoic acid

TNAU

<< Target >>
Line#:12   R.Time:31.585(Scan#:5318) MassPeaks:324
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:79.05(2799)
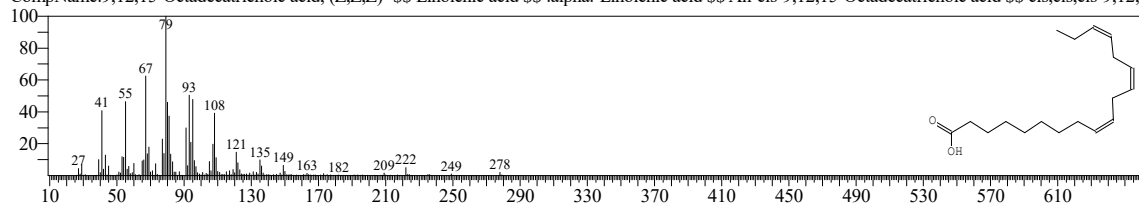BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:137464 Library:NIST20M1.lib
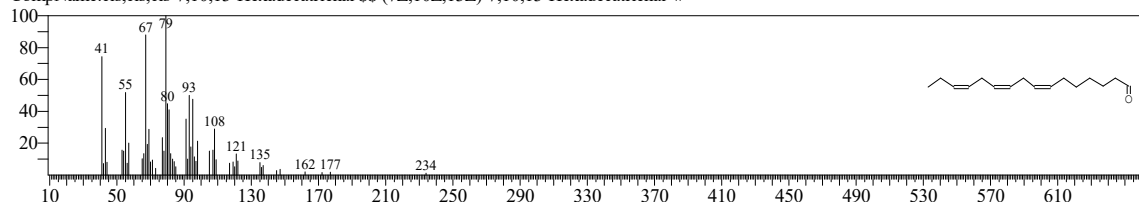SI:90 Formula:C18H30O2 CAS:463-40-1 MolWeight:278 RetIndex:2191
CompName:9,12,15-Octadecatrienoic acid, (Z,Z,Z)- $$ Linolenic acid $$ .alpha.-Linolenic acid $$ All-cis-9,12,15-Octadecatrienoic acid $$ cis,cis,cis-9,12,1

Hit#:2 Entry:87848 Library:NIST20M1.lib
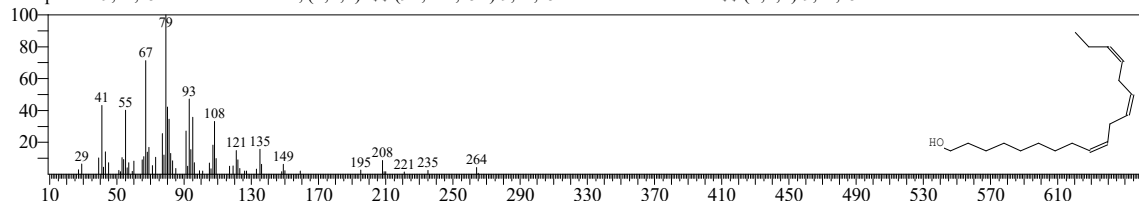SI:88 Formula:C16H26O CAS:56797-43-4 MolWeight:234 RetIndex:1824
CompName:cis,cis,cis-7,10,13-Hexadecatrienal $$ (7Z,10Z,13Z)-7,10,13-Hexadecatrienal #

Hit#:3 Entry:121160 Library:NIST20M1.lib
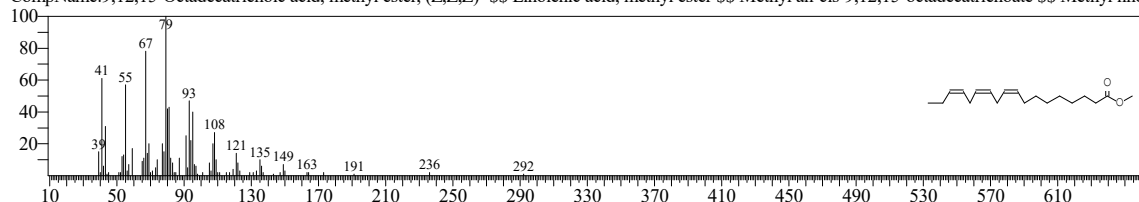SI:88 Formula:C18H32O CAS:506-44-5 MolWeight:264 RetIndex:2077
CompName:9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- $$ (9E,12E,15E)-9,12,15-Octadecatrien-1-ol # $$ (Z,Z,Z)-9,12,15-Octadecatrien-1-ol

Hit#:4 Entry:35226 Library:NIST20R.lib
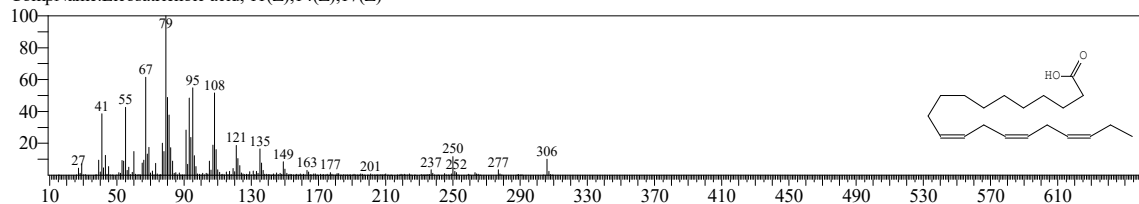SI:87 Formula:C19H32O2 CAS:301-00-8 MolWeight:292 RetIndex:2101
CompName:9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- $$ Linolenic acid, methyl ester $$ Methyl all-cis-9,12,15-octadecatrienoate $$ Methyl lino

Hit#:5 Entry:171056 Library:NIST20M1.lib
SI:87 Formula:C20H34O2 CAS:17046-59-2 MolWeight:306 RetIndex:2390
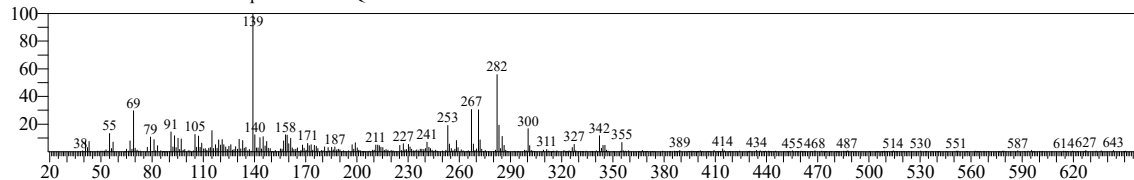CompName:Eicosatrienoic acid, 11(Z),14(Z),17(Z)

<< Target >>
Line#:13 R.Time:45.625(Scan#:8126) MassPeaks:386
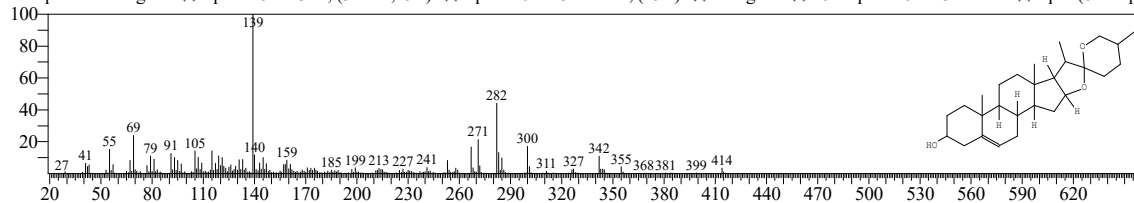RawMode:Averaged 45.620-45.630(8125-8127) BasePeak:139.10(3543)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:8297 Library:NIST20M2.lib
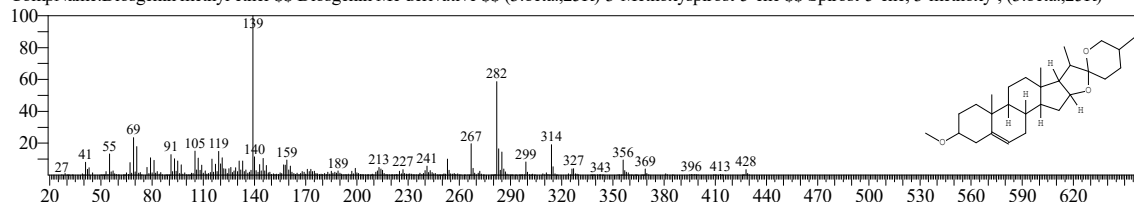SI:88 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

Hit#:2 Entry:14852 Library:NIST20M2.lib
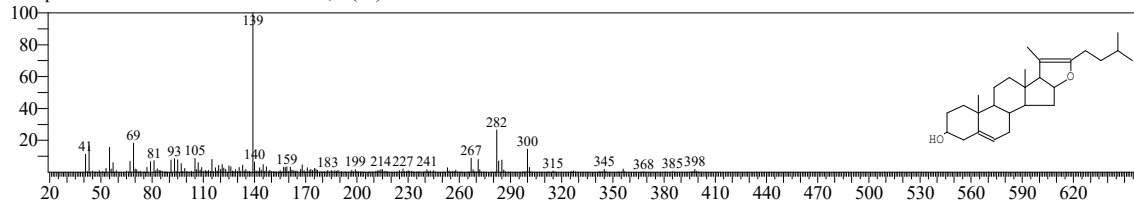SI:79 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:3 Entry:41561 Library:NIST20R.lib
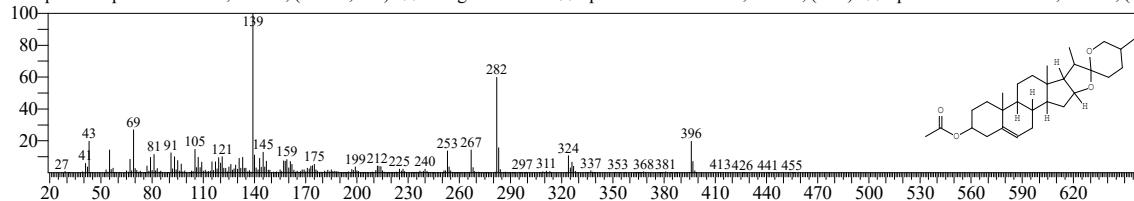SI:78 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #

Hit#:4 Entry:24878 Library:NIST20M2.lib
SI:76 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
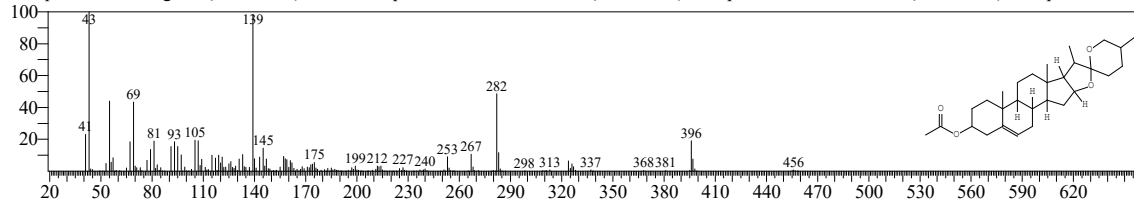CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (25

Hit#:5 Entry:42677 Library:NIST20R.lib
SI:72 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.
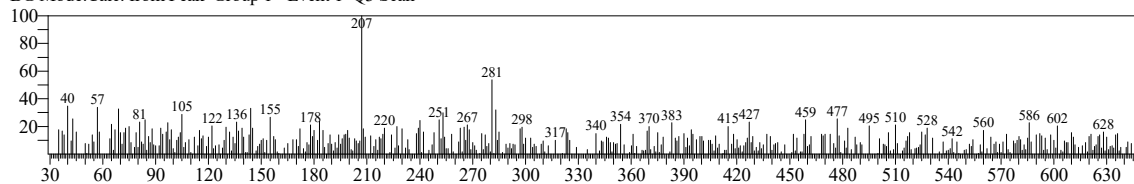
TNAU

<< Target >>
Line#:14 R.Time:46.620(Scan#:8325) MassPeaks:441
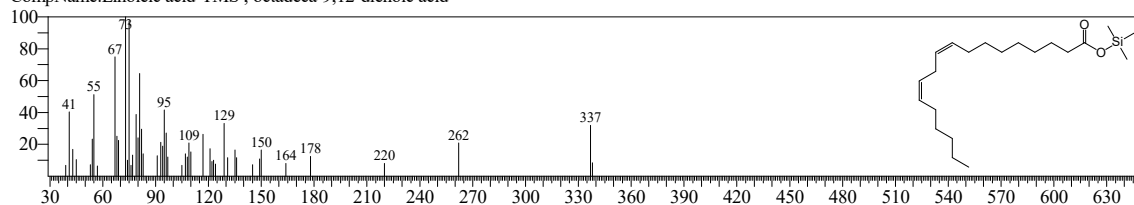RawMode:Averaged 46.615-46.625(8324-8326) BasePeak:207.05(181)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:484 Library:OA_TMS_DB5_67min_V3.lib
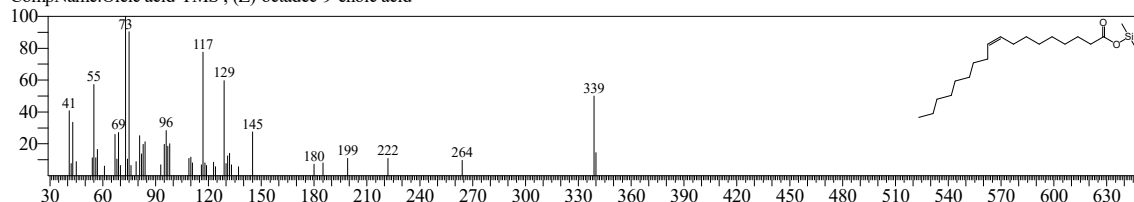SI:23 Formula:C21H40O2Si CAS:60-33-3 MolWeight:352 RetIndex:2218
CompName:Linoleic acid-TMS ; octadeca-9,12-dienoic acid

Hit#:2 Entry:485 Library:OA_TMS_DB5_67min_V3.lib
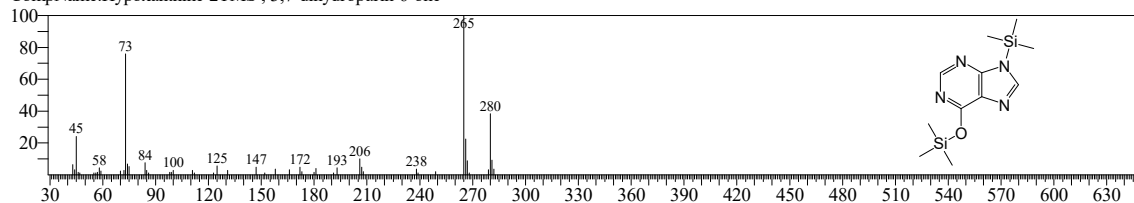SI:23 Formula:C21H42O2Si CAS:112-80-1 MolWeight:354 RetIndex:2222
CompName:Oleic acid-TMS ; (Z)-octadec-9-enoic acid

Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
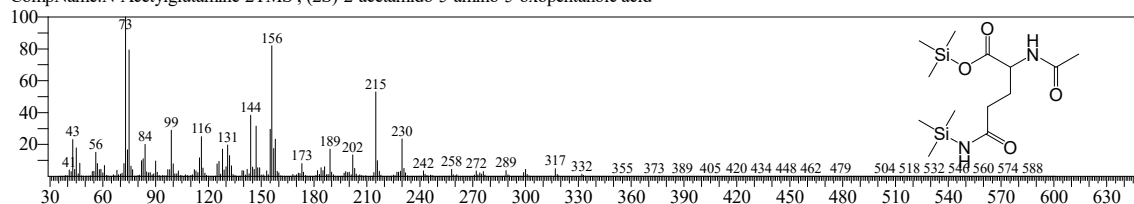SI:22 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one

Hit#:4 Entry:405 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C13H28N2O4Si2 CAS:2490-97-3 MolWeight:332 RetIndex:1948
CompName:N-Acetylglutamine-2TMS ; (2S)-2-acetamido-5-amino-5-oxopentanoic acid

Hit#:5 Entry:558 Library:OA_TMS_DB5_67min_V3.lib
SI:22 Formula:C19H39N2O8PSi3 CAS:365-07-1 MolWeight:538 RetIndex:2905
CompName:Thymidine monophosphate-3TMS ; [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxopyrimidin-1-yl)oxolan-2-yl]methyl dihydrogen phosph