TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022003.qgd

TIC

152,925

Peak Report TIC

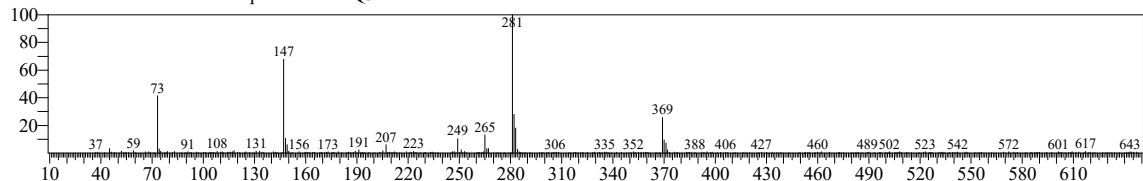| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	9.768	33941	4.52	15671	5.76	2.17	93	Pentasiloxane, dodecamethyl-
2	11.139	23882	3.18	9697	3.57	2.46	59	Decanoic acid-TMS
3	12.828	44478	5.92	18393	6.77	2.42	34	Methyl linoleate
4	13.253	345575	46.01	122546	45.08	2.82	54	Methyl cis-13,16-Docosadienate
5	13.448	256188	34.11	84440	31.06	3.03	54	Methyl cis-13,16-Docosadienate
6	14.845	9634	1.28	5207	1.92	1.85	19	Docosapentaenoic acid-TMS
7	15.815	37318	4.97	15877	5.84	2.35	78	Malic acid 1-ethyl ester, 2TMS
		751016	100.00	271831	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:9.770(Scan#:955) MassPeaks:322
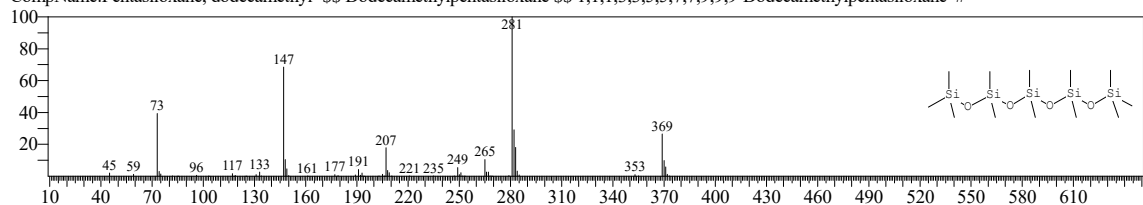RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.05(3679)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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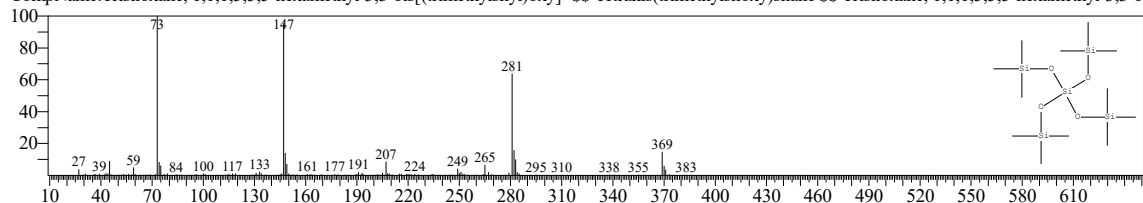SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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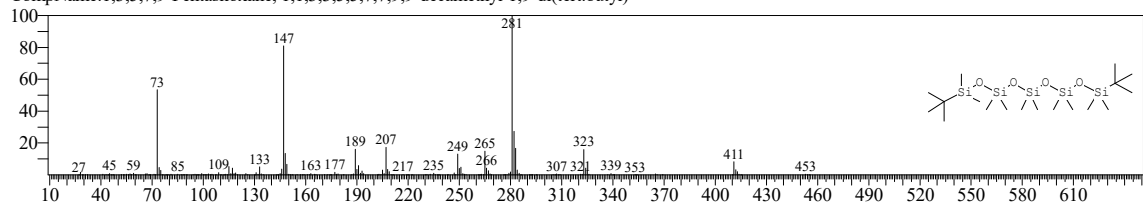SI:82 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

Hit#:3 Entry:27848 Library:NIST20M2.lib
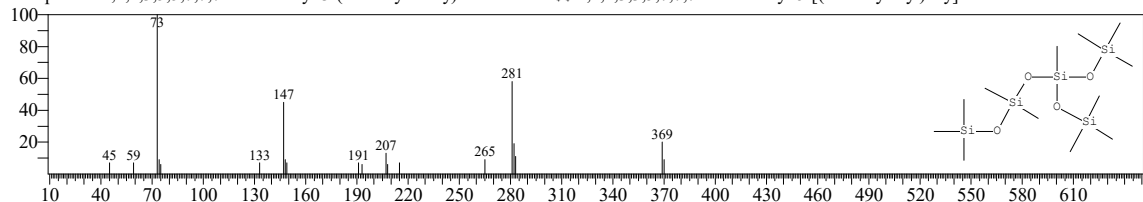SI:79 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

Hit#:4 Entry:249271 Library:NIST20M1.lib
SI:77 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
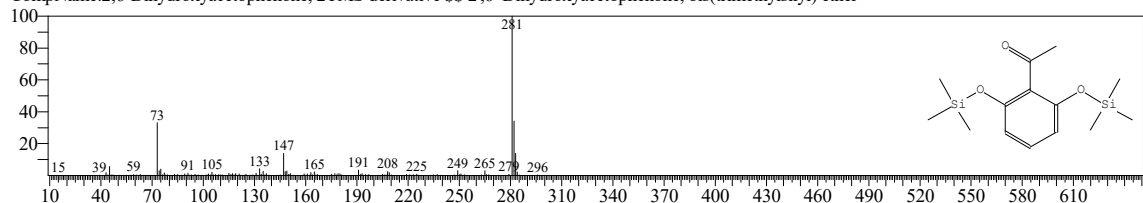CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:74 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether
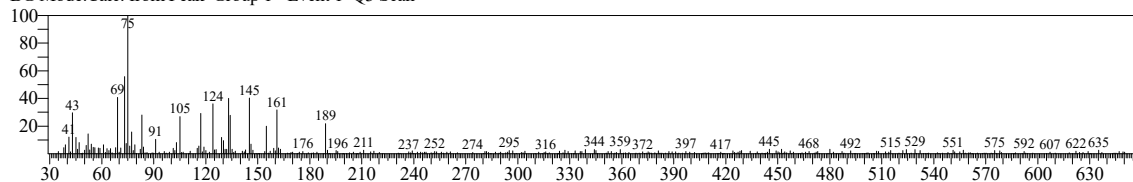
TNAU

<< Target >>
Line#:2 R.Time:11.140(Scan#:1229) MassPeaks:337
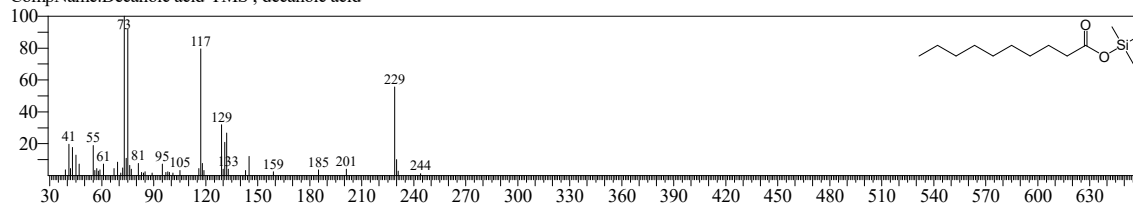RawMode:Averaged 11.135-11.145(1228-1230) BasePeak:75.05(1241)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:129 Library:OA_TMS_DB5_67min_V3.lib
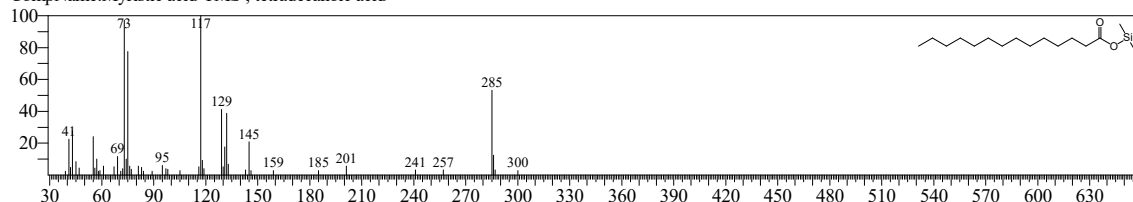SI:59 Formula:C13H28O2Si CAS:334-48-5 MolWeight:244 RetIndex:1457
CompName:Decanoic acid-TMS ; decanoic acid

Hit#:2 Entry:331 Library:OA_TMS_DB5_67min_V3.lib
SI:58 Formula:C17H36O2Si CAS:544-63-8 MolWeight:300 RetIndex:1850
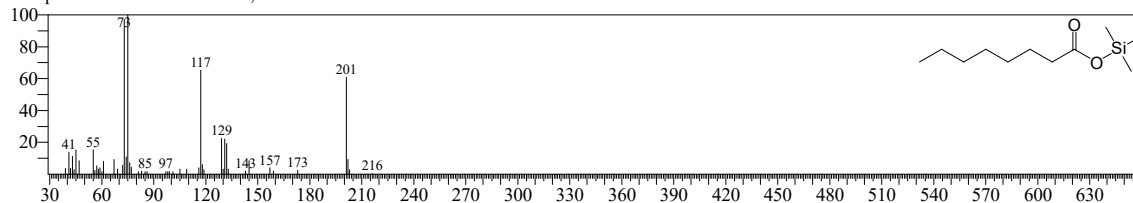CompName:Myristic acid-TMS ; tetradecanoic acid

Hit#:3 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
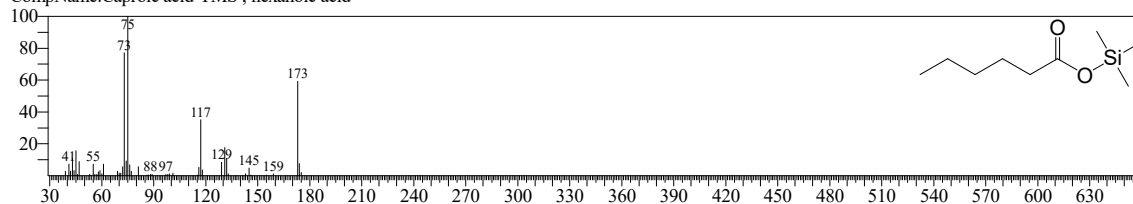SI:58 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
CompName:Octanoic acid-TMS ; octanoic acid

Hit#:4 Entry:11 Library:OA_TMS_DB5_67min_V3.lib
SI:57 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
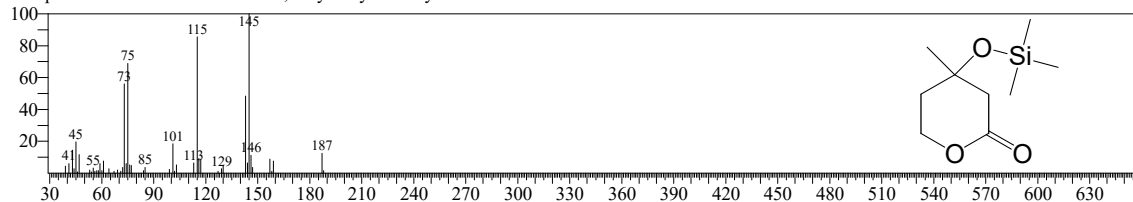CompName:Caproic acid-TMS ; hexanoic acid

Hit#:5 Entry:106 Library:OA_TMS_DB5_67min_V3.lib
SI:57 Formula:C9H18O3Si CAS:503-48-0 MolWeight:202 RetIndex:1378
CompName:Mevalonic lactone-TMS ; 4-hydroxy-4-methyloxan-2-one
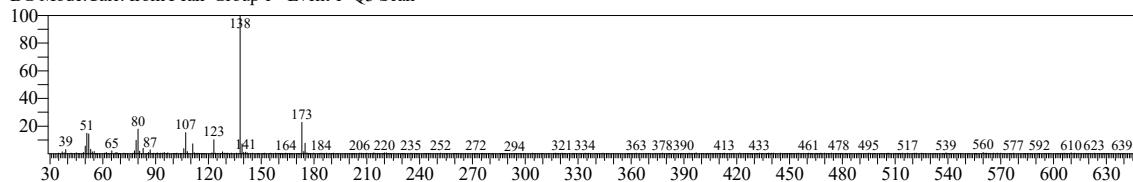
TNAU

<< Target >>
Line#:3   R.Time:12.830(Scan#:1567) MassPeaks:368
RawMode:Averaged 12.825-12.835(1566-1568) BasePeak:138.10(5717)
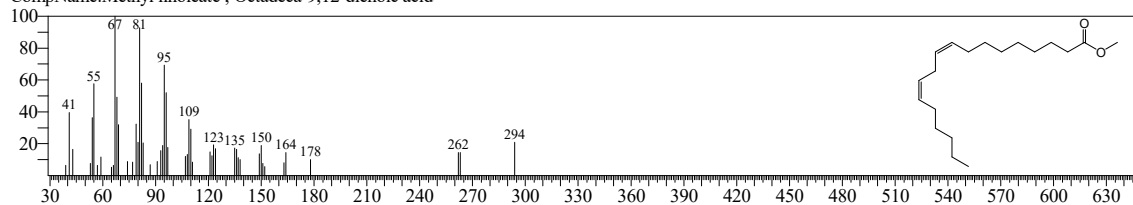BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
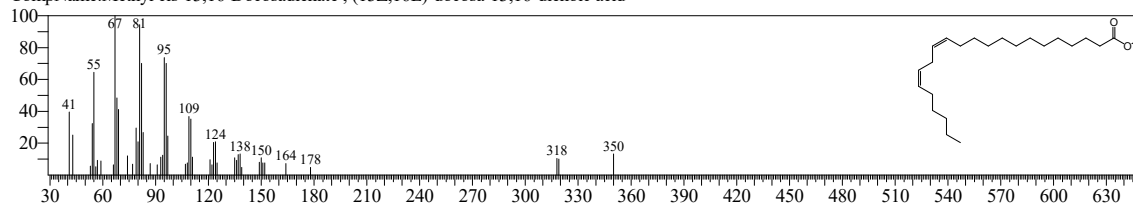SI:34 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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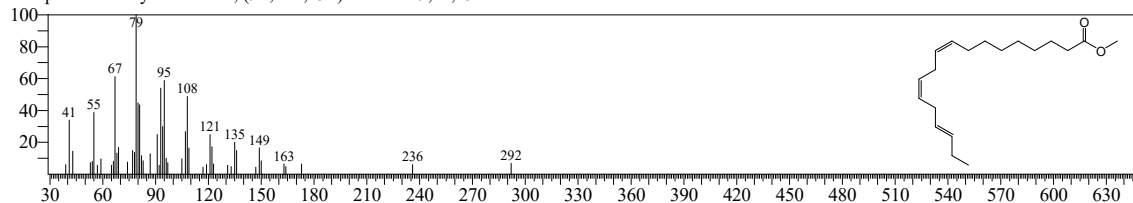SI:34 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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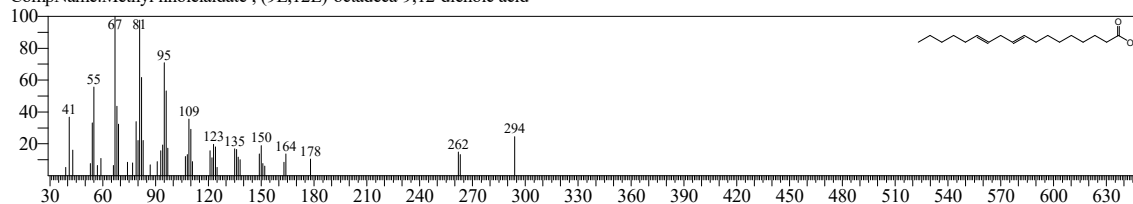CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

Hit#:4 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
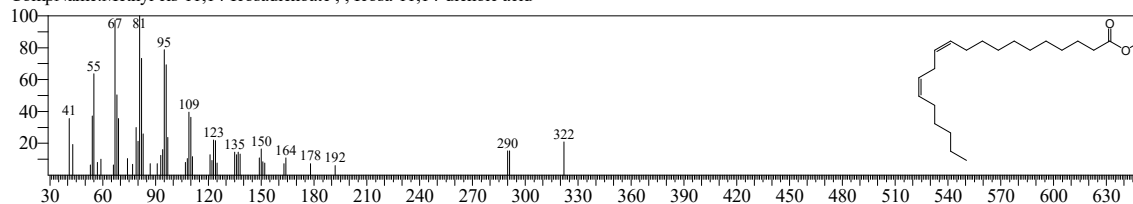SI:34 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
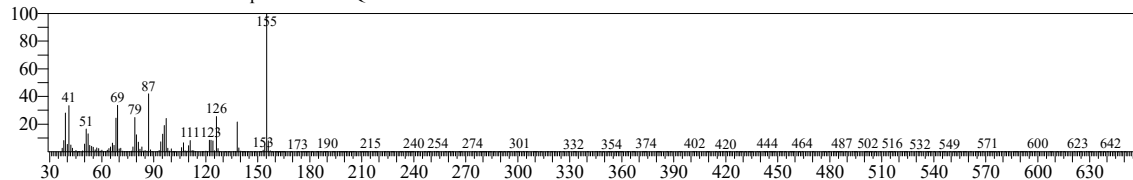CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

TNAU

<< Target >>
Line#:4   R.Time:13.255(Scan#:1652) MassPeaks:361
RawMode:Averaged 13.250-13.260(1651-1653) BasePeak:155.05(19445)
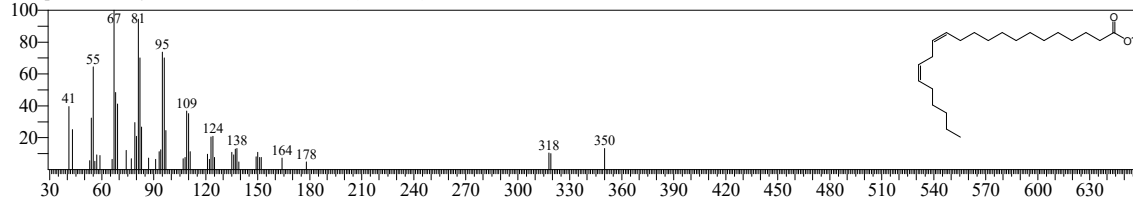BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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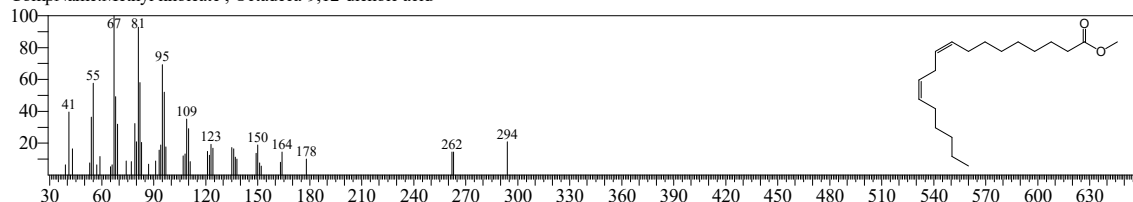SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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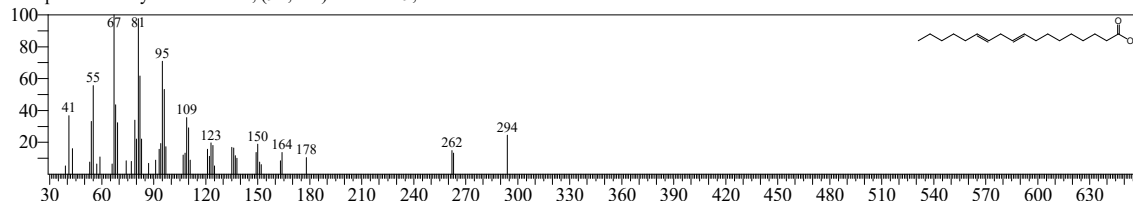SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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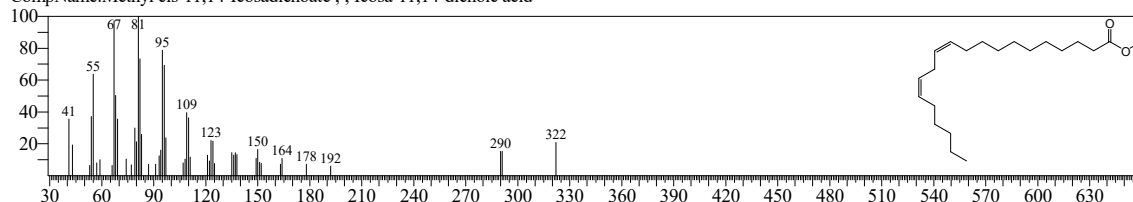CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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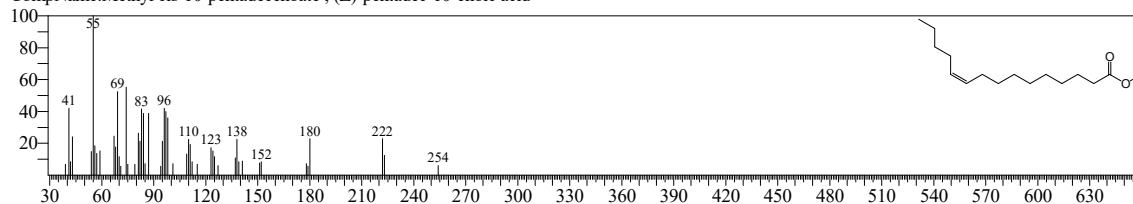SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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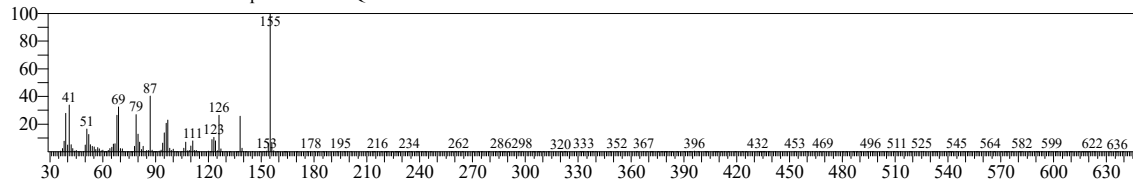CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:5 R.Time:13.450(Scan#:1691) MassPeaks:285
RawMode:Averaged 13.445-13.455(1690-1692) BasePeak:155.10(13749)
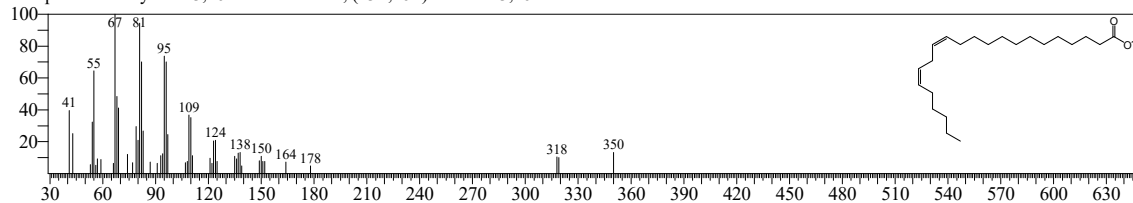BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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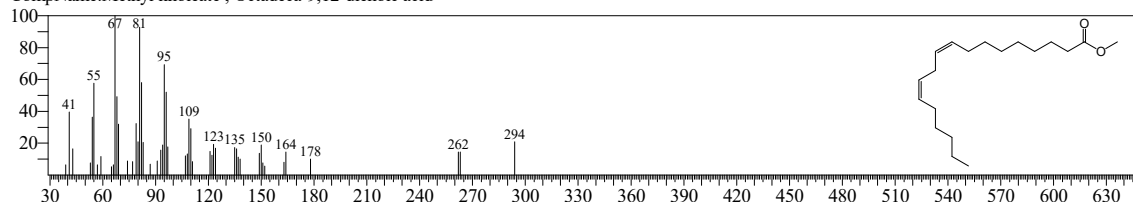SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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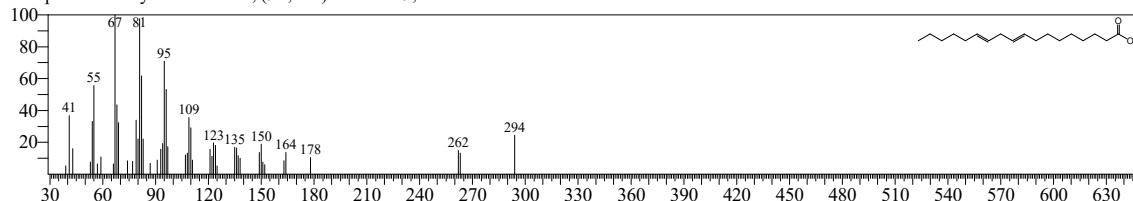CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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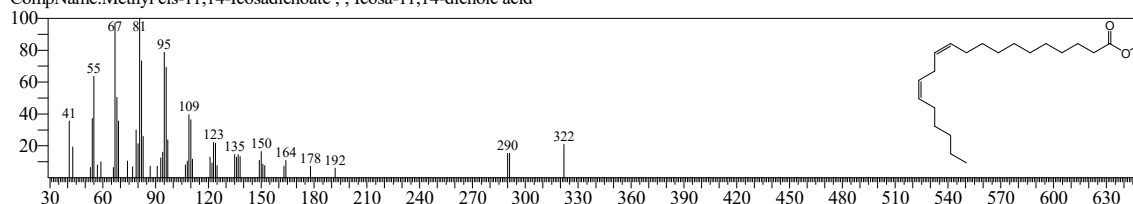CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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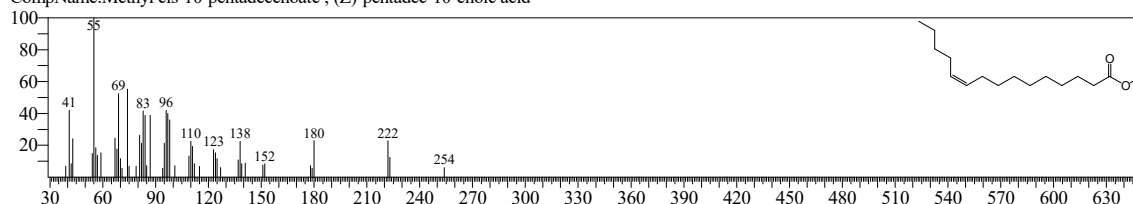SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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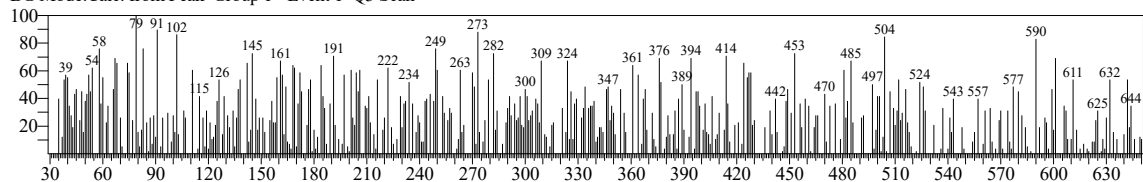CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:6 R.Time:14.845(Scan#:1970) MassPeaks:401
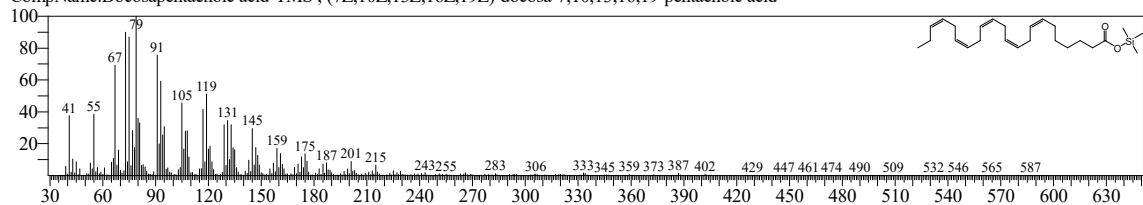RawMode:Averaged 14.840-14.850(1969-1971) BasePeak:79.00(58)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
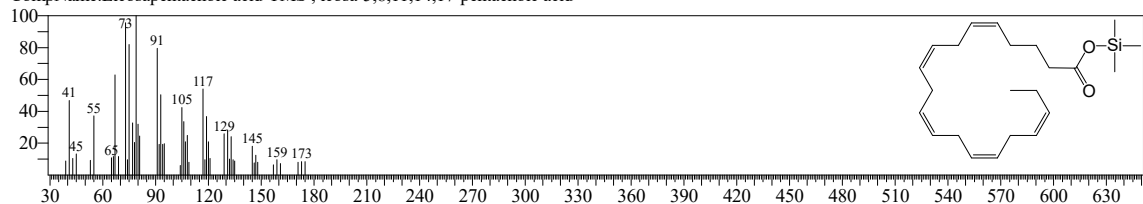SI:19 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid

Hit#:2 Entry:509 Library:OA_TMS_DB5_67min_V3.lib
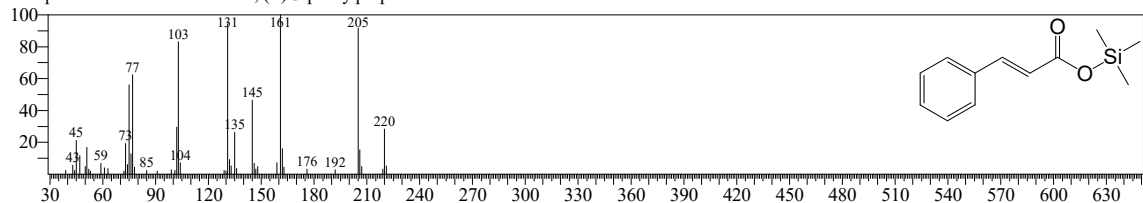SI:19 Formula:C23H38O2Si CAS:10417-94-4 MolWeight:374 RetIndex:2389
CompName:Eicosapentaenoic acid-TMS ; icosa-5,8,11,14,17-pentaenoic acid

Hit#:3 Entry:171 Library:OA_TMS_DB5_67min_V3.lib
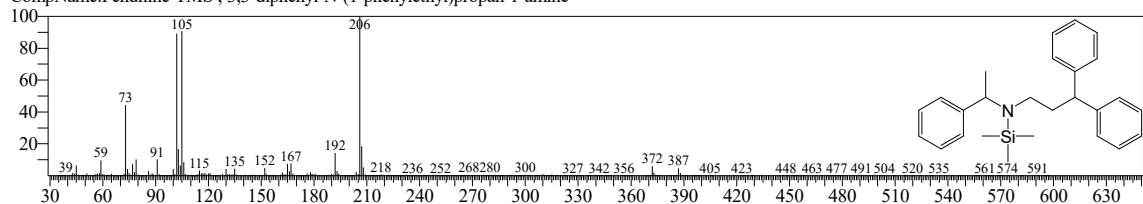SI:18 Formula:C12H16O2Si CAS:140-10-3 MolWeight:220 RetIndex:1552
CompName:Cinnamic acid-TMS ; (E)-3-phenylprop-2-enoic acid

Hit#:4 Entry:537 Library:OA_TMS_DB5_67min_V3.lib
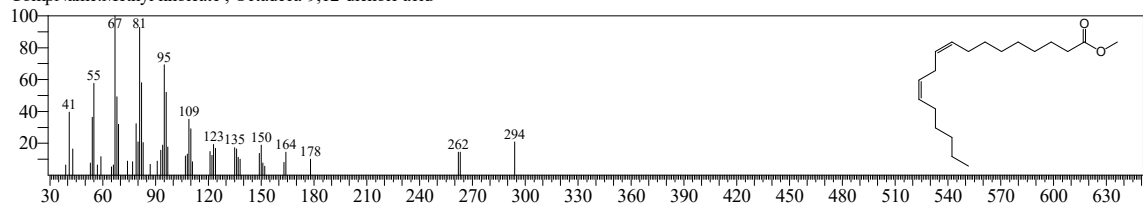SI:17 Formula:C26H33NSi CAS:13042-18-7 MolWeight:387 RetIndex:2646
CompName:Fendiline-TMS ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine

Hit#:5 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:17 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
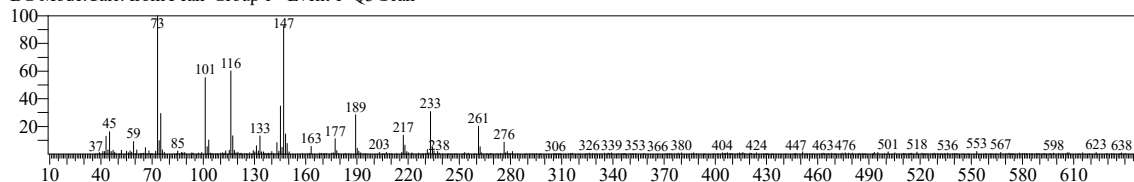CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

TNAU

<< Target >>
Line#:7 R.Time:15.815(Scan#:2164) MassPeaks:308
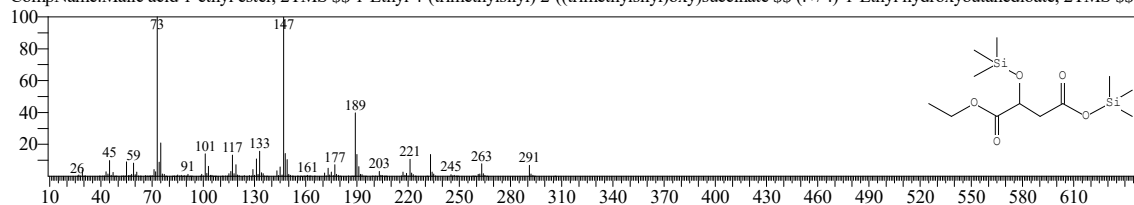RawMode:Averaged 15.810-15.820(2163-2165) BasePeak:73.05(2412)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:169946 Library:NIST20M1.lib
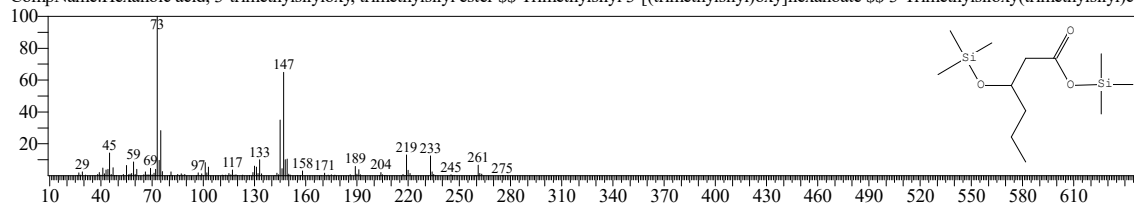SI:78 Formula:C12H26O5Si2 CAS:0-00-0 MolWeight:306 RetIndex:1380
CompName:Malic acid 1-ethyl ester, 2TMS $$ 1-Ethyl 4-(trimethylsilyl) 2-((trimethylsilyl)oxy)succinate $$ (.+/-.)-1-Ethyl hydroxybutanedioate, 2TMS $$ 1

Hit#:2 Entry:33630 Library:NIST20R.lib
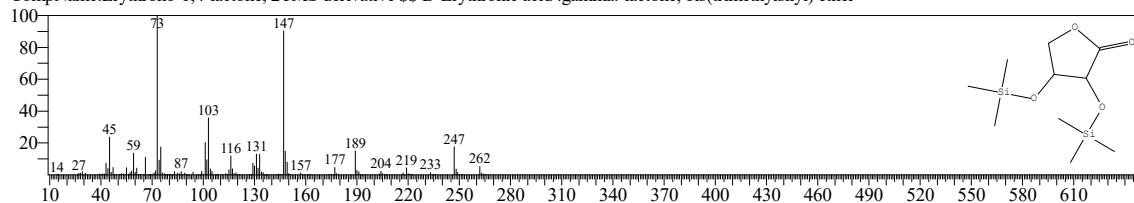SI:75 Formula:C12H28O3Si2 CAS:136788-82-4 MolWeight:276 RetIndex:1213
CompName:Hexanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester $$ Trimethylsilyl 3-[(trimethylsilyl)oxy]hexanoate $$ 3-Trimethylsiloxy(trimethylsilyl)ca

Hit#:3 Entry:117877 Library:NIST20M1.lib
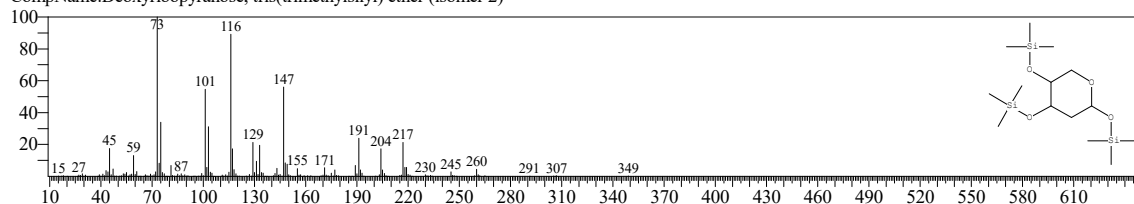SI:75 Formula:C10H22O4Si2 CAS:0-00-0 MolWeight:262 RetIndex:1317
CompName:Erythrono-1,4-lactone, 2TMS derivative $$ D-Erythronic acid .gamma.-lactone, bis(trimethylsilyl) ether

Hit#:4 Entry:219755 Library:NIST20M1.lib
SI:75 Formula:C14H34O4Si3 CAS:0-00-0 MolWeight:350 RetIndex:1446
CompName:Deoxyribopyranose, tris(trimethylsilyl) ether (isomer 2)

Hit#:5 Entry:219752 Library:NIST20M1.lib
SI:75 Formula:C14H34O4Si3 CAS:33648-76-9 MolWeight:350 RetIndex:1431
CompName:D-2-Deoxyribose, 3TMS derivative $$ 2-Deoxy ribose O,O',O''-tris(trimethylsilyl)- $$ 2-Deoxy-3,4,5-tris-O-(trimethylsilyl)pentose #