TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022002.qgd

Peak Report TIC

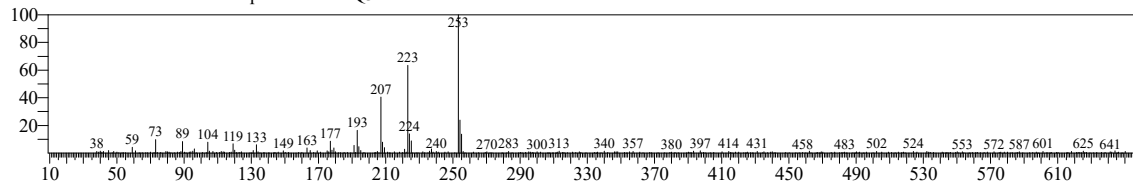| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	6.561	28470	3.95	12636	4.86	2.25	71	Methyl 6,6,8,8,10,10-hexamethyl-3-oxo-2,5,7,
2	9.772	40140	5.57	19645	7.56	2.04	93	Pentasiloxane, dodecamethyl-
3	11.140	20202	2.80	10619	4.09	1.90	62	Caproic acid-TMS
4	12.827	26541	3.68	13001	5.00	2.04	40	Caffeine
5	13.256	306538	42.55	104779	40.31	2.93	54	Methyl cis-13,16-Docosadienate
6	13.448	247192	34.31	76445	29.41	3.23	54	Methyl cis-13,16-Docosadienate
7	15.819	51388	7.13	22781	8.77	2.26	78	Malic acid 1-ethyl ester, 2TMS
		720471	100.00	259906	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:6.560(Scan#:313) MassPeaks:325
RawMode:Averaged 6.555-6.565(312-314) BasePeak:253.10(2935)
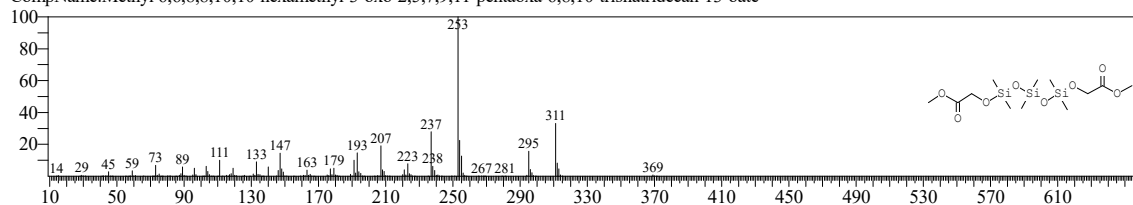BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:249268 Library:NIST20M1.lib
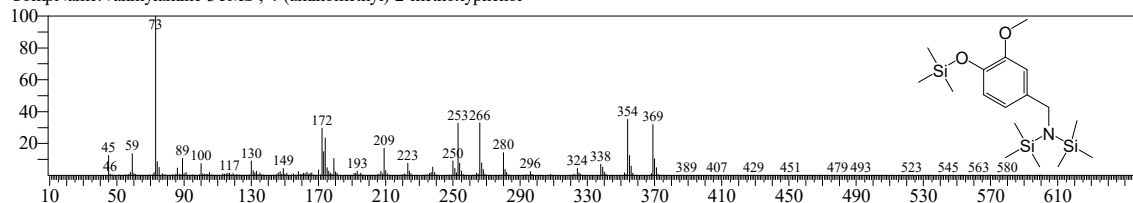SI:71 Formula:C12H28O8Si3 CAS:0-00-0 MolWeight:384 RetIndex:1582
CompName:Methyl 6,6,8,8,10,10-hexamethyl-3-oxo-2,5,7,9,11-pentaoxa-6,8,10-trisilatridecan-13-oate

Hit#:2 Entry:368 Library:OA_TMS_DB5_67min_V3.lib
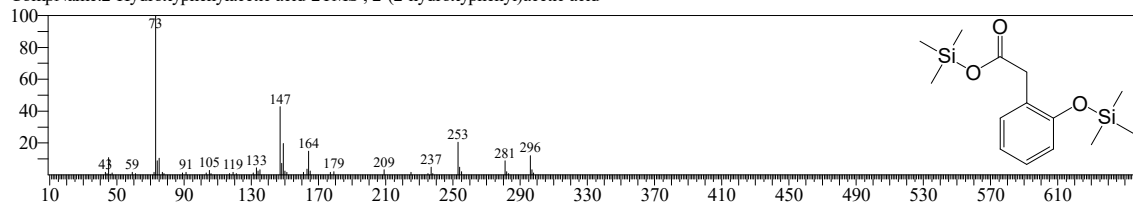SI:39 Formula:C17H35NO2Si3 CAS:1196-92-5 MolWeight:369 RetIndex:1899
CompName:Vanillylamine-3TMS ; 4-(aminomethyl)-2-methoxyphenol

Hit#:3 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
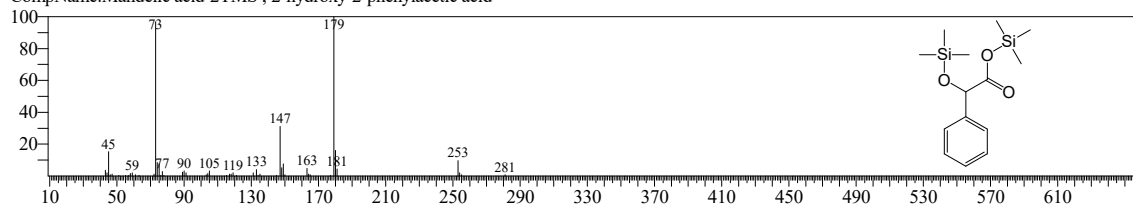CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid

Hit#:4 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
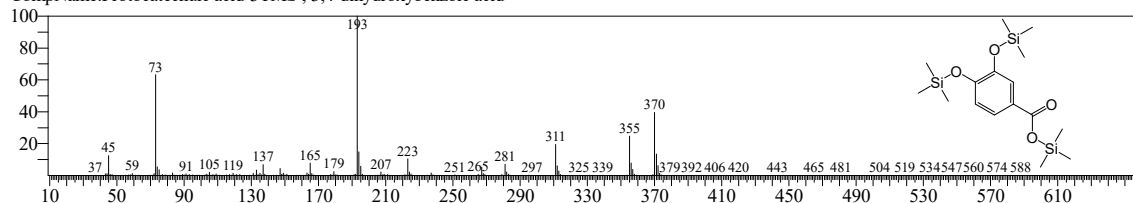SI:37 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid

Hit#:5 Entry:315 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C16H30O4Si3 CAS:99-50-3 MolWeight:370 RetIndex:1833
CompName:Protocatechuic acid-3TMS ; 3,4-dihydroxybenzoic acid
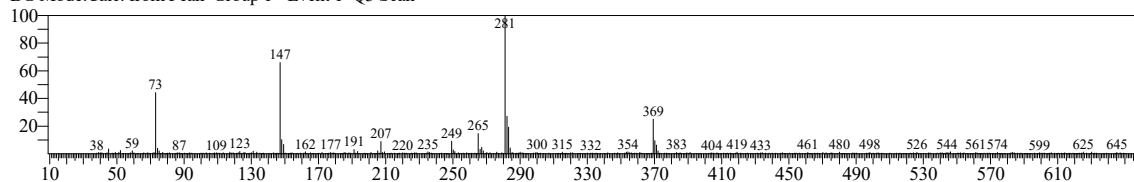
TNAU

<< Target >>
Line#:2   R.Time:9.770(Scan#:955) MassPeaks:421
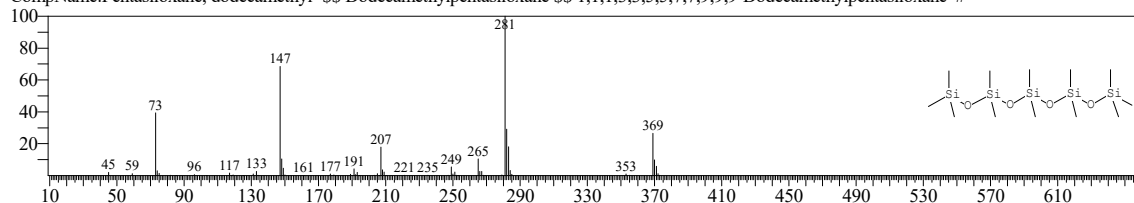RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.05(3705)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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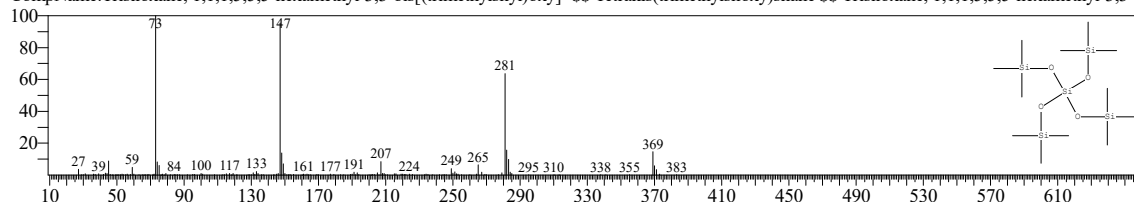CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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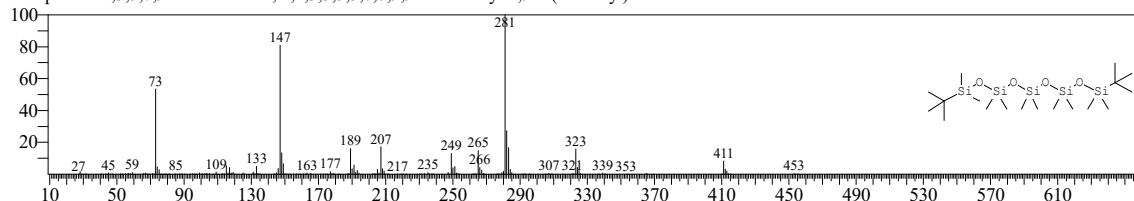SI:82 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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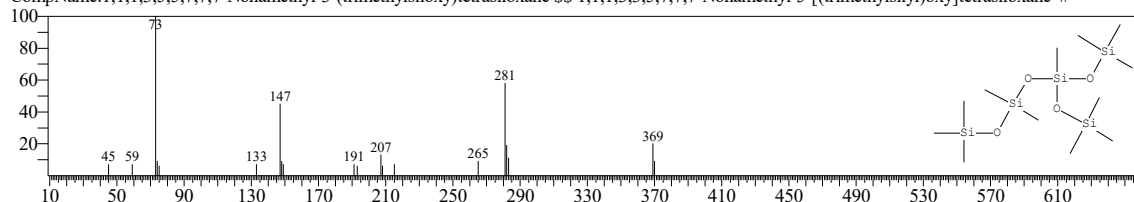CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

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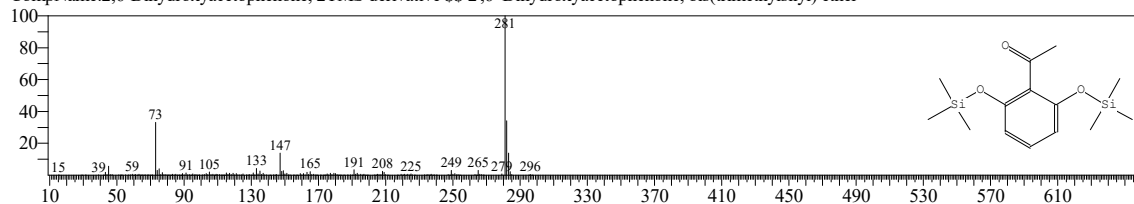SI:78 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

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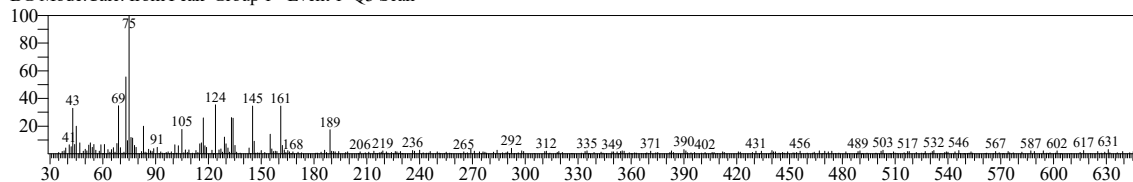
TNAU

<< Target >>
Line#:3   R.Time:11.140(Scan#:1229) MassPeaks:328
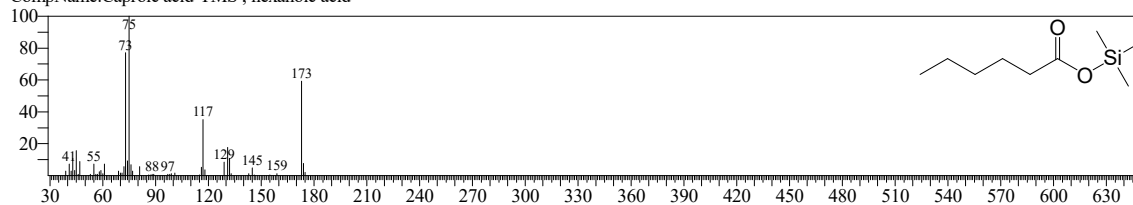RawMode:Averaged 11.135-11.145(1228-1230) BasePeak:75.05(1329)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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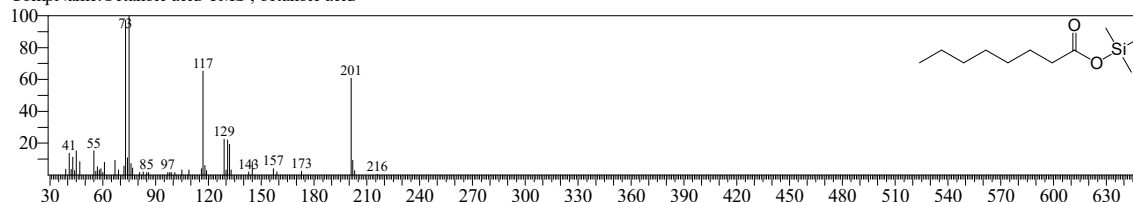SI:62 Formula:C9H20O2Si CAS:142-62-1 MolWeight:188 RetIndex:1071
CompName:Caproic acid-TMS ; hexanoic acid

Hit#:2 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
SI:61 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
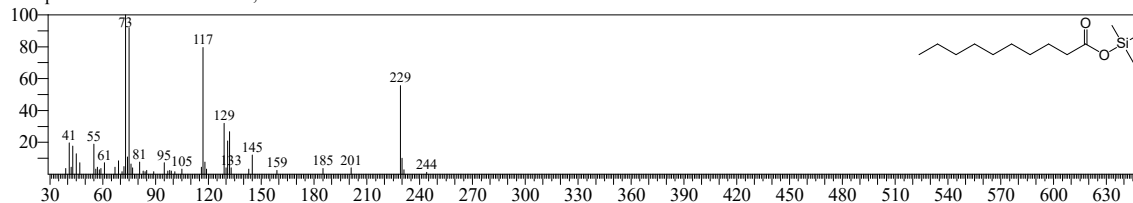CompName:Octanoic acid-TMS ; octanoic acid

Hit#:3 Entry:129 Library:OA_TMS_DB5_67min_V3.lib
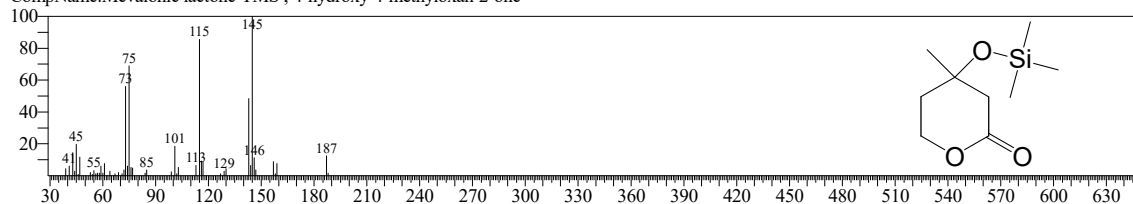SI:61 Formula:C13H28O2Si CAS:334-48-5 MolWeight:244 RetIndex:1457
CompName:Decanoic acid-TMS ; decanoic acid

Hit#:4 Entry:106 Library:OA_TMS_DB5_67min_V3.lib
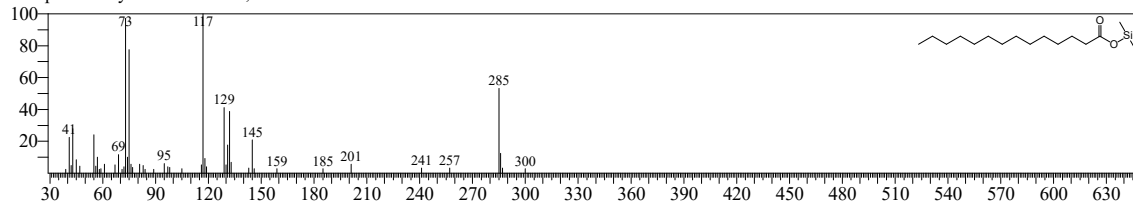SI:60 Formula:C9H18O3Si CAS:503-48-0 MolWeight:202 RetIndex:1378
CompName:Mevalonic lactone-TMS ; 4-hydroxy-4-methyloxan-2-one

Hit#:5 Entry:331 Library:OA_TMS_DB5_67min_V3.lib
SI:60 Formula:C17H36O2Si CAS:544-63-8 MolWeight:300 RetIndex:1850
CompName:Myristic acid-TMS ; tetradecanoic acid
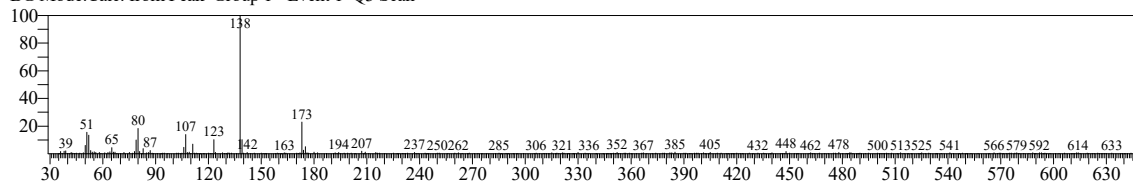
TNAU

<< Target >>
Line#:4 R.Time:12.825(Scan#:1566) MassPeaks:339
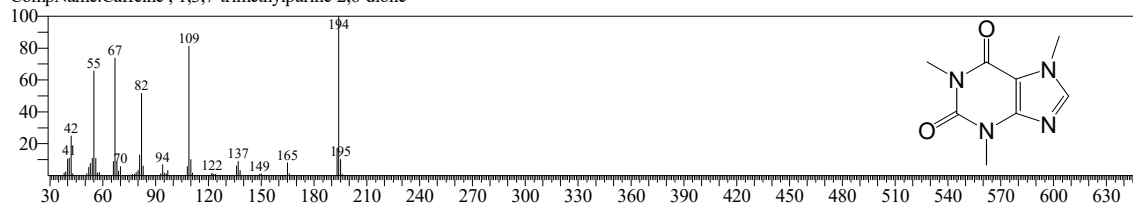RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(4188)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:342 Library:OA_TMS_DB5_67min_V3.lib
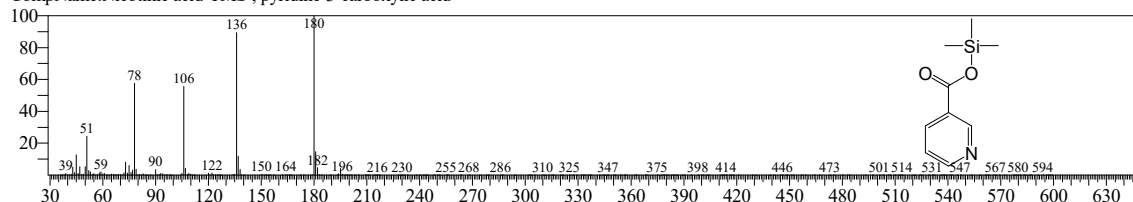SI:40 Formula:C8H10N4O2 CAS:58-08-2 MolWeight:194 RetIndex:1867
CompName:Caffeine ; 1,3,7-trimethylpurine-2,6-dione

Hit#:2 Entry:84 Library:OA_TMS_DB5_67min_V3.lib
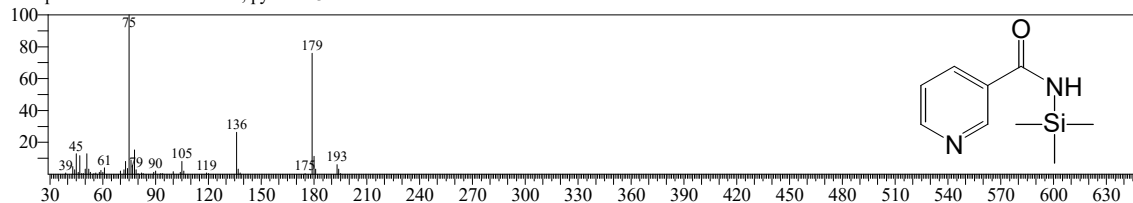SI:39 Formula:C9H13NO2Si CAS:59-67-6 MolWeight:195 RetIndex:1300
CompName:Nicotinic acid-TMS ; pyridine-3-carboxylic acid

Hit#:3 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
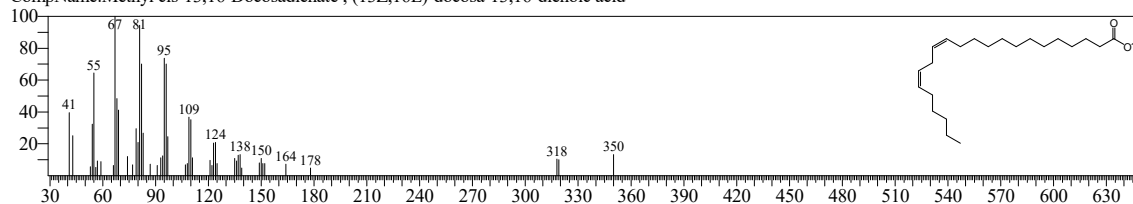SI:32 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide

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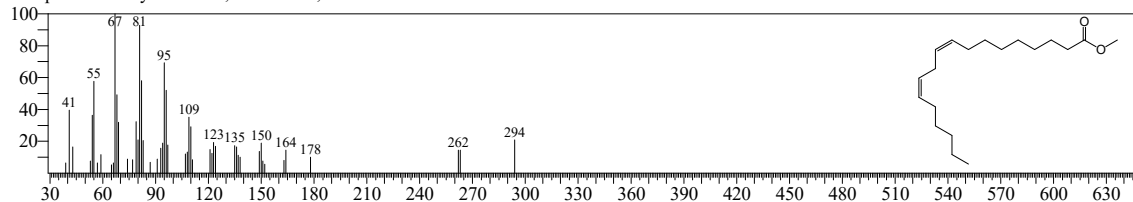CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:5 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:30 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
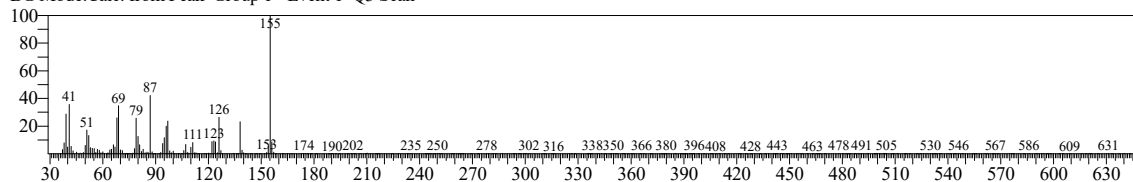CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

TNAU

<< Target >>
Line#:5 R.Time:13.255(Scan#:1652) MassPeaks:310
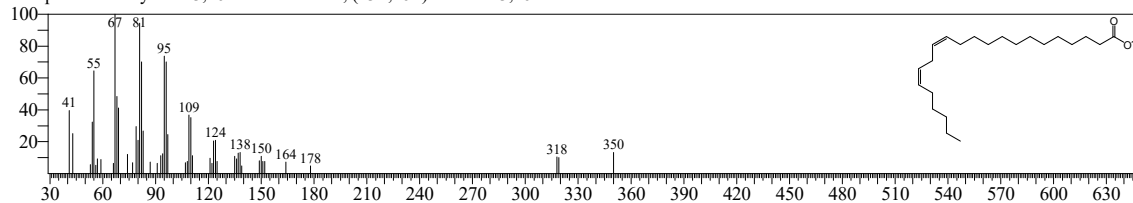RawMode:Averaged 13.250-13.260(1651-1653) BasePeak:155.10(16094)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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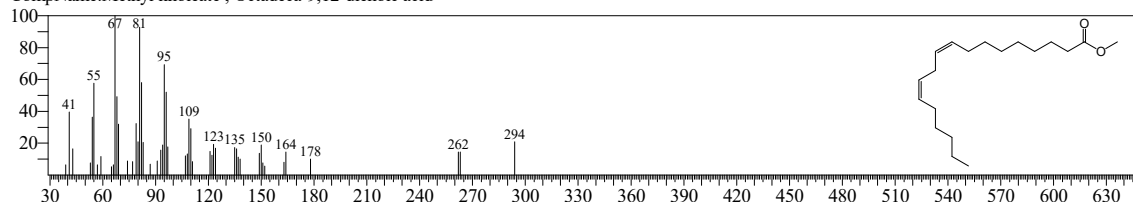SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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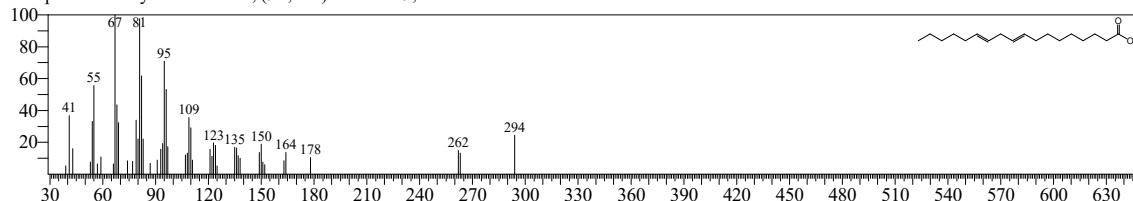SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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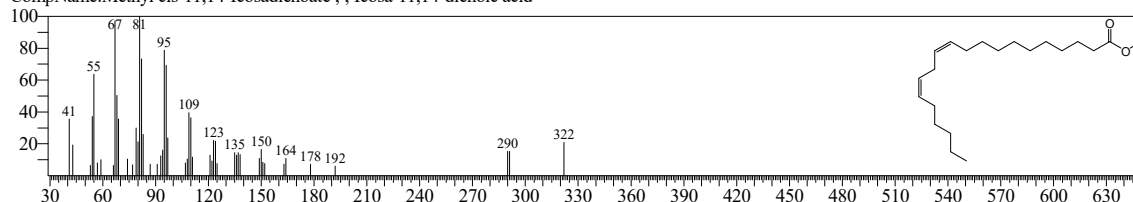SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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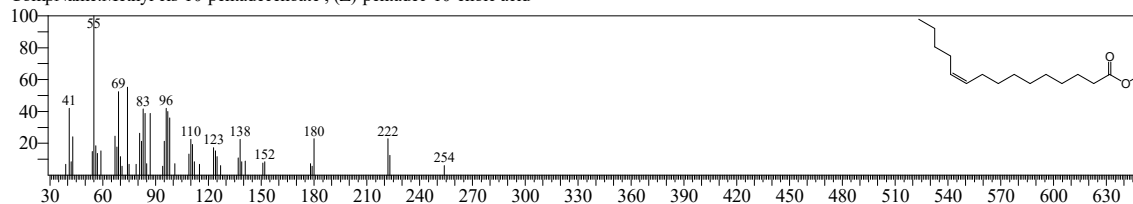SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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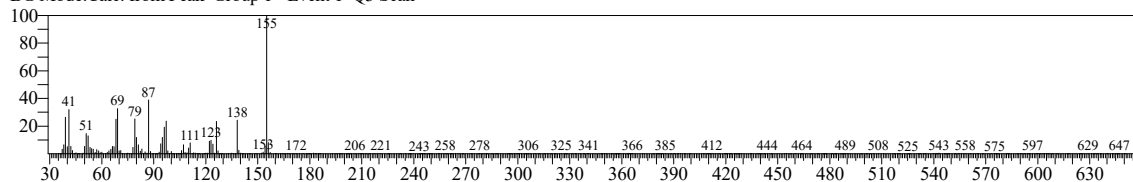CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:6   R.Time:13.450(Scan#:1691) MassPeaks:337
RawMode:Averaged 13.445-13.455(1690-1692) BasePeak:155.10(12162)
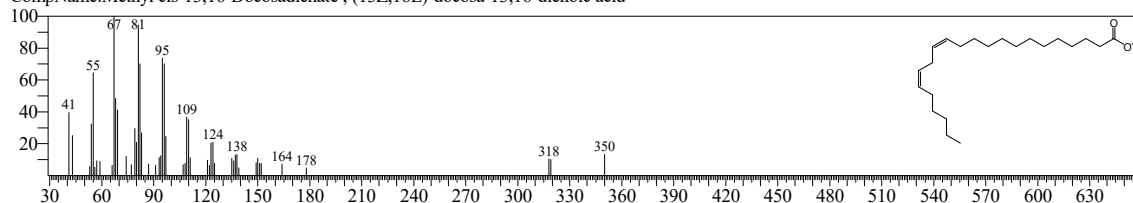BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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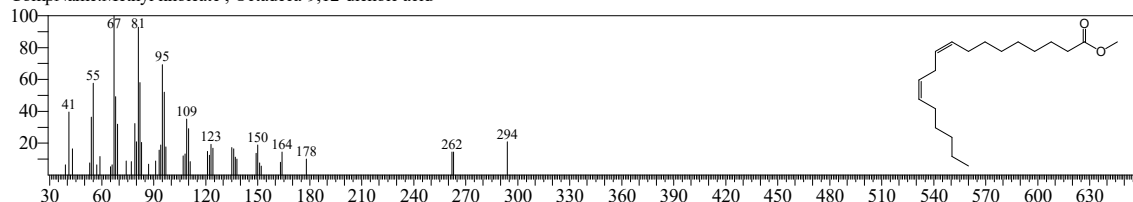SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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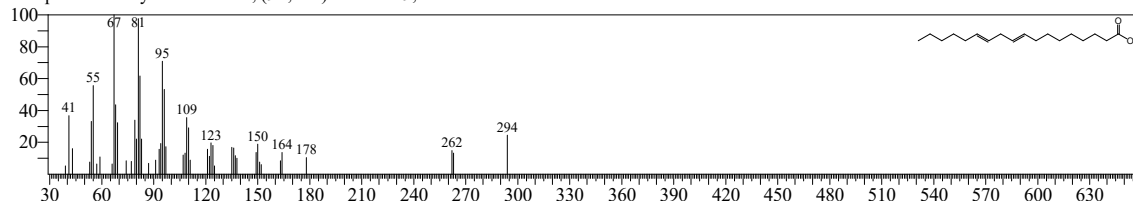SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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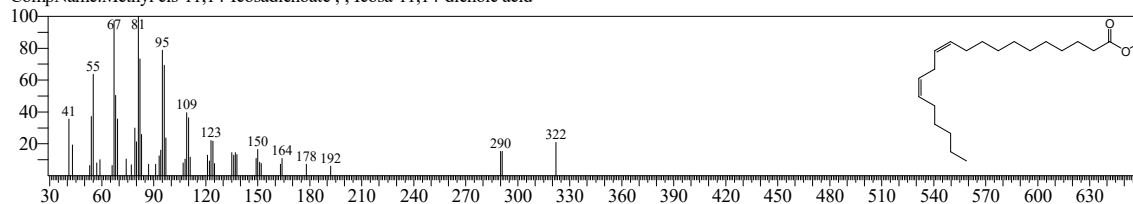CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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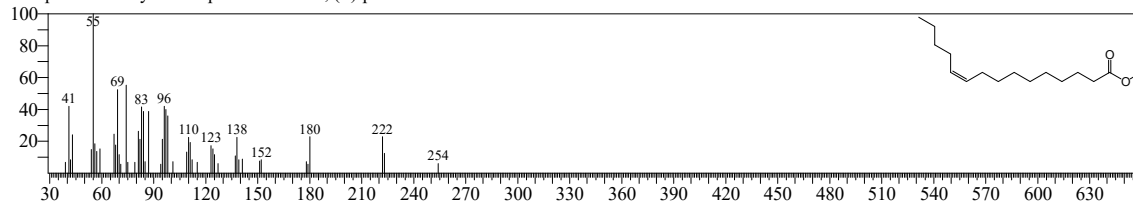SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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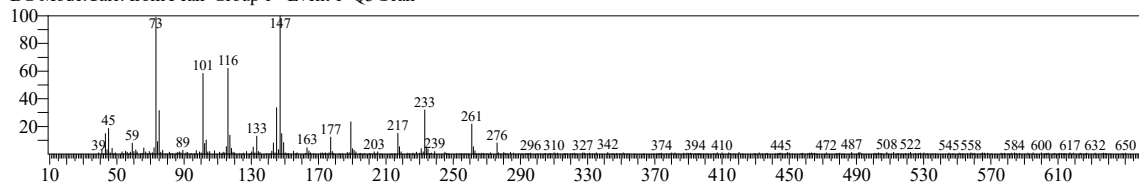CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

TNAU

<< Target >>
Line#:7 R.Time:15.820(Scan#:2165) MassPeaks:333
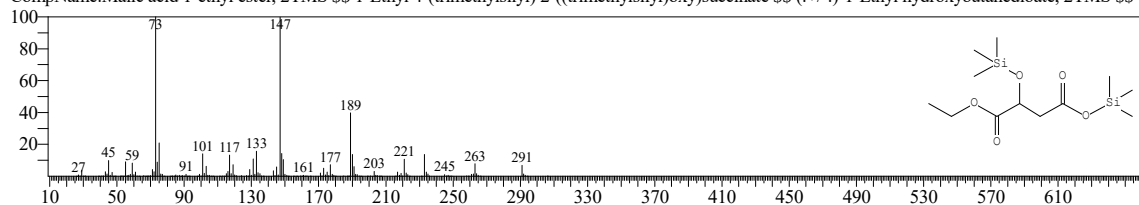RawMode:Averaged 15.815-15.825(2164-2166) BasePeak:147.05(2886)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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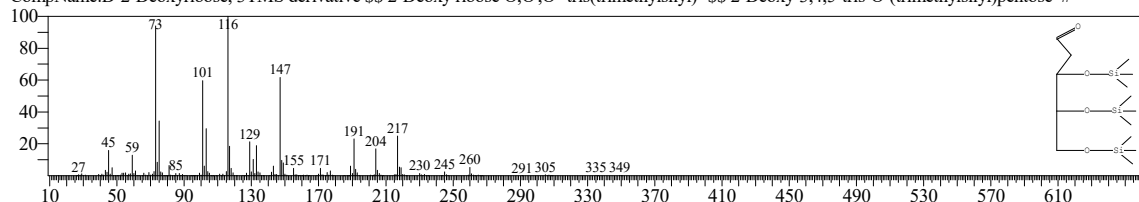SI:78 Formula:C12H26O5Si2 CAS:0-00-0 MolWeight:306 RetIndex:1380
CompName:Malic acid 1-ethyl ester, 2TMS $$ 1-Ethyl 4-(trimethylsilyl) 2-((trimethylsilyl)oxy)succinate $$ (.+/-.)-1-Ethyl hydroxybutanedioate, 2TMS $$ 1

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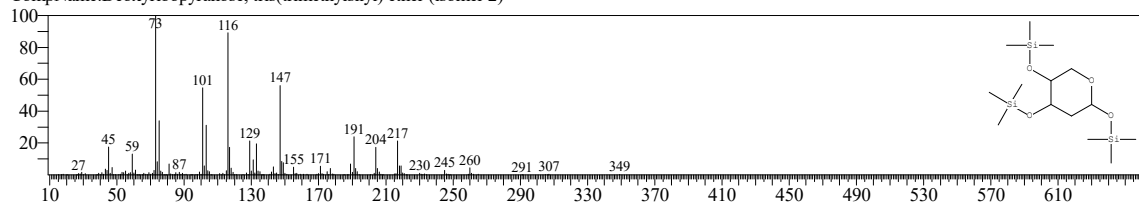SI:76 Formula:C14H34O4Si3 CAS:33648-76-9 MolWeight:350 RetIndex:1431
CompName:D-2-Deoxyribose, 3TMS derivative $$ 2-Deoxy ribose O,O',O''-tris(trimethylsilyl)- $$ 2-Deoxy-3,4,5-tris-O-(trimethylsilyl)pentose #

Hit#:3 Entry:219755 Library:NIST20M1.lib
SI:75 Formula:C14H34O4Si3 CAS:0-00-0 MolWeight:350 RetIndex:1446
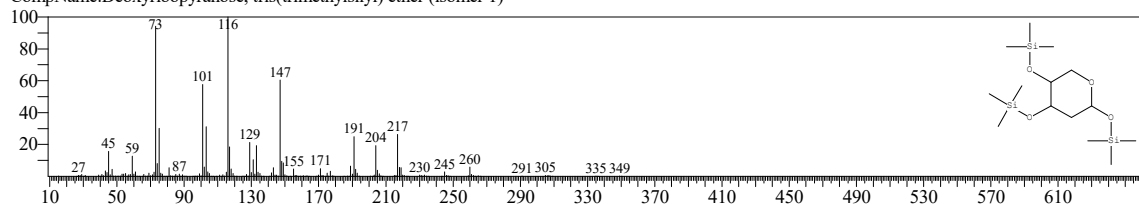CompName:Deoxyribopyranose, tris(trimethylsilyl) ether (isomer 2)

Hit#:4 Entry:219754 Library:NIST20M1.lib
SI:75 Formula:C14H34O4Si3 CAS:0-00-0 MolWeight:350 RetIndex:1446
CompName:Deoxyribopyranose, tris(trimethylsilyl) ether (isomer 1)

Hit#:5 Entry:33630 Library:NIST20R.lib
SI:74 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