TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022013.qgd

Peak Report TIC

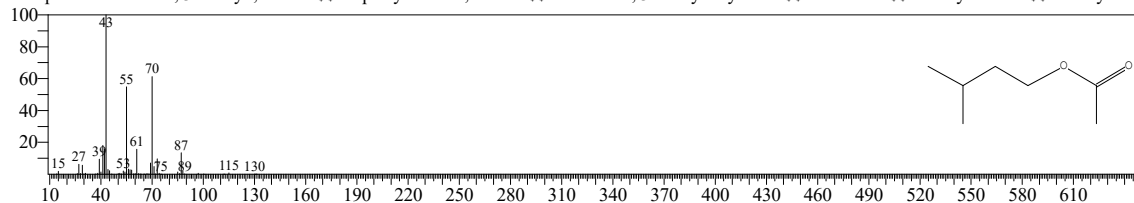| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.320	81312	3.41	18629	2.35	4.36	84	1-Butanol, 3-methyl-, acetate
2	9.765	50709	2.13	21901	2.77	2.32	95	Pentasiloxane, dodecamethyl-
3	12.498	20044	0.84	8358	1.06	2.40	34	Caffeine
4	12.825	59063	2.48	25223	3.19	2.34	74	1,3-Benzodioxol-5-ol
5	13.235	603496	25.31	223200	28.20	2.70	54	Methyl cis-13,16-Docosadienate
6	13.430	519887	21.81	195589	24.71	2.66	54	Methyl cis-13,16-Docosadienate
7	13.813	21923	0.92	9988	1.26	2.19	82	Trisiloxane, octamethyl-
8	19.194	97970	4.11	45484	5.75	2.15	94	2,4-Di-tert-butylphenoxytrimethylsilane
9	28.302	217805	9.14	81641	10.32	2.67	96	n-Hexadecanoic acid
10	31.483	198792	8.34	68146	8.61	2.92	95	9,12-Octadecadienoic acid (Z,Z)-
11	31.584	146122	6.13	43769	5.53	3.34	89	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
12	45.617	367089	15.40	49501	6.25	7.42	88	Diosgenin
		2384212	100.00	791429	100.00			

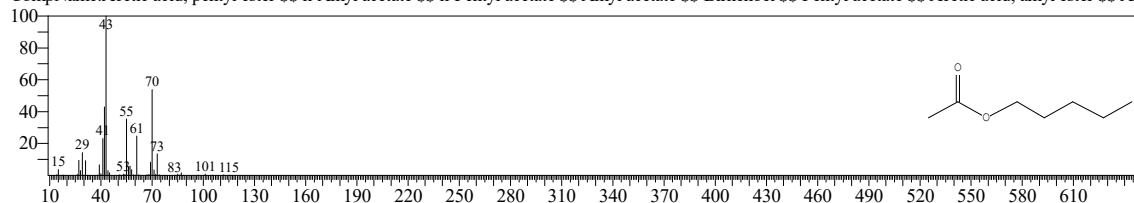Library

TNAU

<< Target >>
Line#:1 R.Time:8.320(Scan#:665) MassPeaks:394
RawMode:Averaged 8.315-8.325(664-666) BasePeak:43.00(3077)
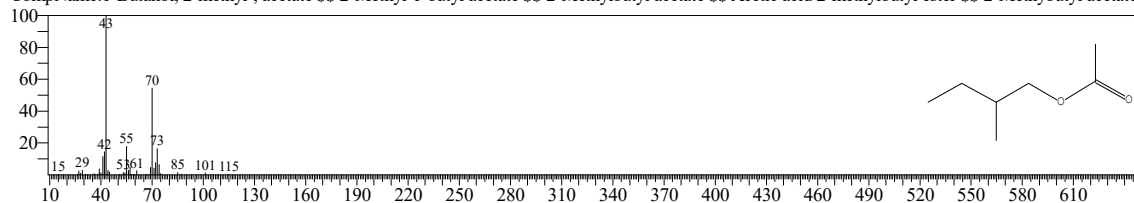BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:6784 Library:NIST20R.lib
SI:84 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha
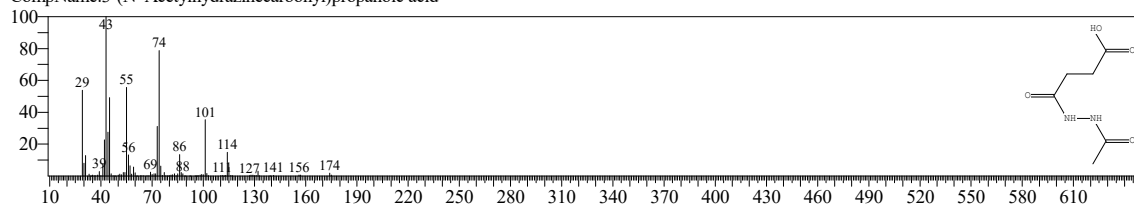

Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:82 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ Am
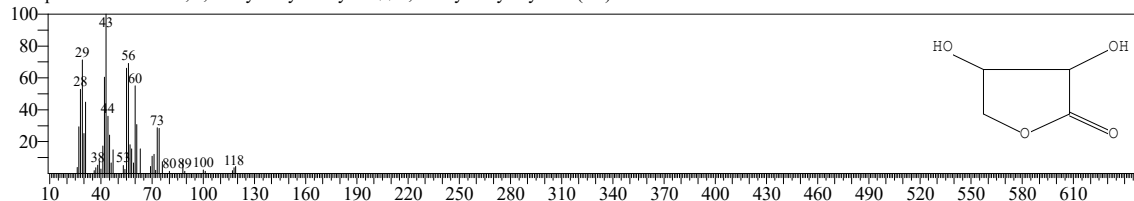

Hit#:3 Entry:6819 Library:NIST20R.lib
SI:80 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate

Hit#:4 Entry:32045 Library:NIST20M1.lib
SI:79 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid

Hit#:5 Entry:5225 Library:NIST20M1.lib
SI:79 Formula:C4H6O4 CAS:17675-99-9 MolWeight:118 RetIndex:1201
CompName:2-Furanone, 3,4-dihydroxytetrahydro $$ 3,4-Dihydroxydihydro-2(3H)-furanone #
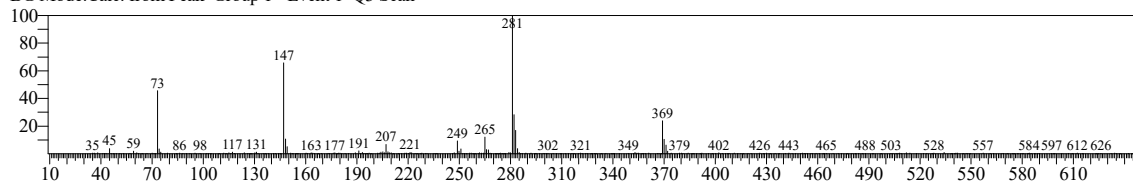
TNAU

<< Target >>
Line#:2 R.Time:9.765(Scan#:954) MassPeaks:317
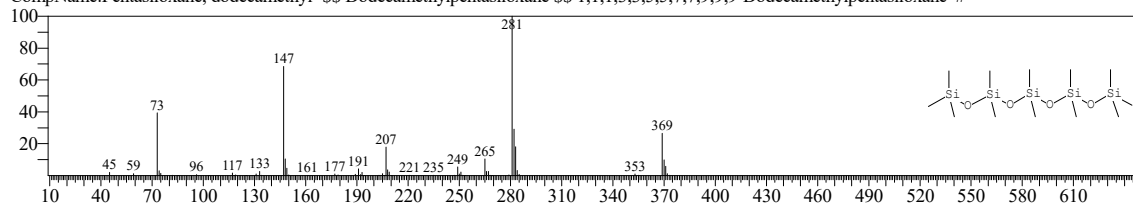RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(5747)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:40975 Library:NIST20R.lib
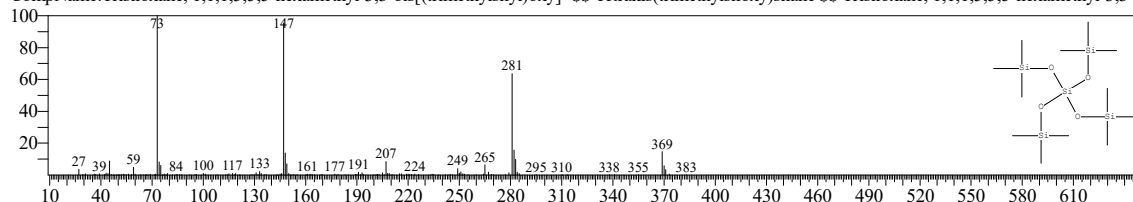SI:95 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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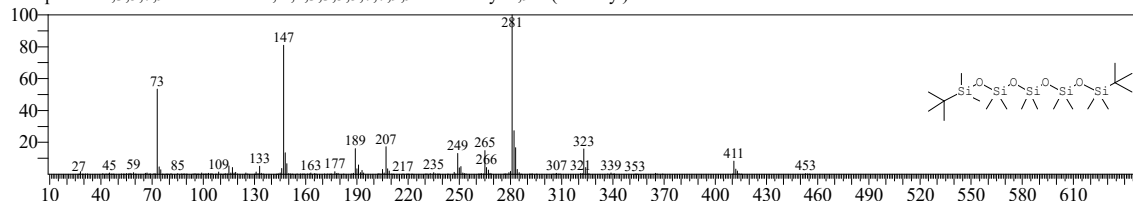SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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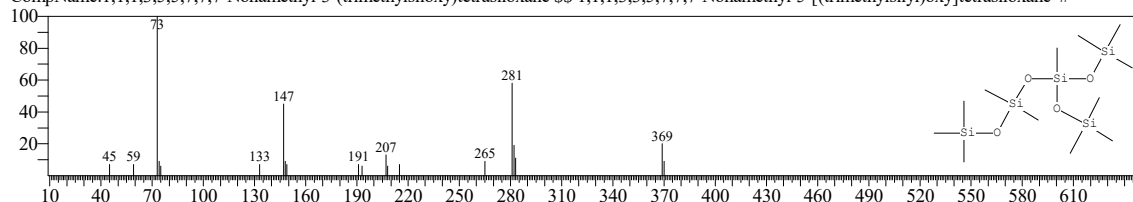CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

Hit#:4 Entry:249271 Library:NIST20M1.lib
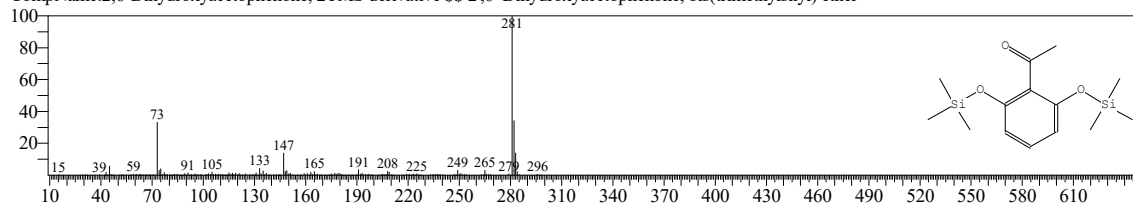SI:79 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

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
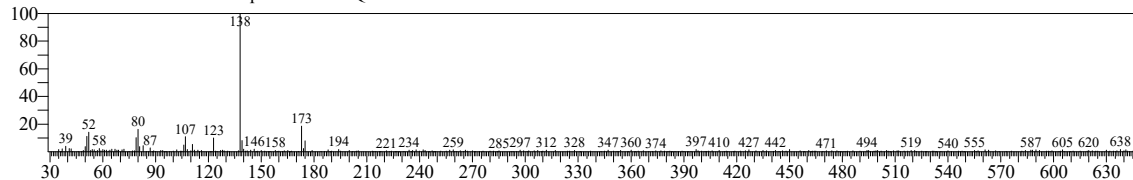
TNAU

<< Target >>
Line#:3 R.Time:12.500(Scan#:1501) MassPeaks:314
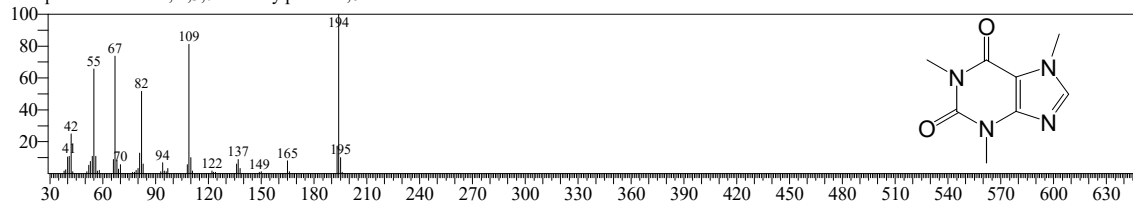RawMode:Averaged 12.495-12.505(1500-1502) BasePeak:138.05(2855)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:342 Library:OA_TMS_DB5_67min_V3.lib
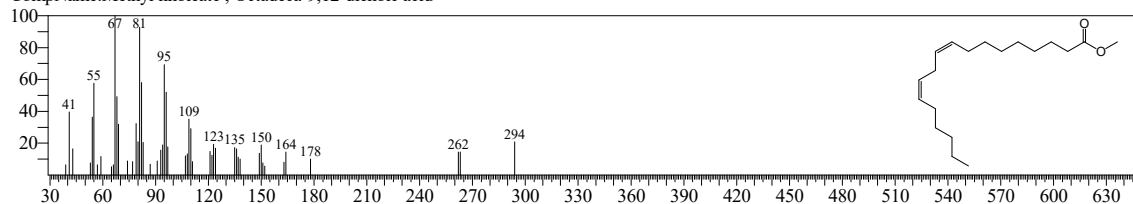SI:34 Formula:C8H10N4O2 CAS:58-08-2 MolWeight:194 RetIndex:1867
CompName:Caffeine ; 1,3,7-trimethylpurine-2,6-dione

Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
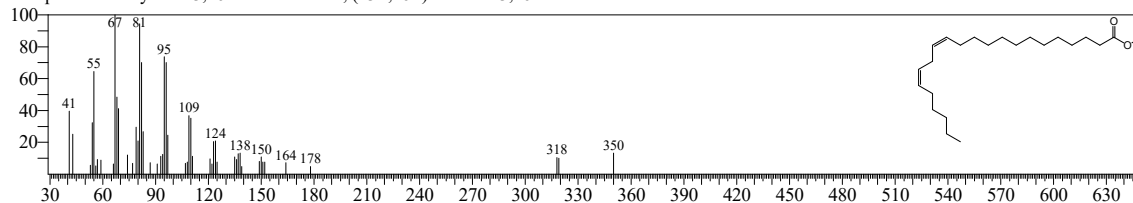SI:29 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:3 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:29 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
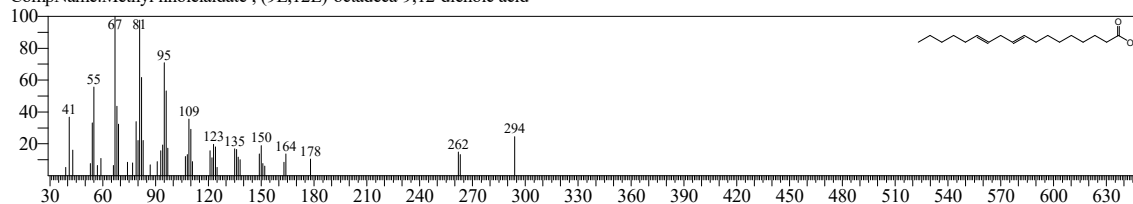CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:4 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
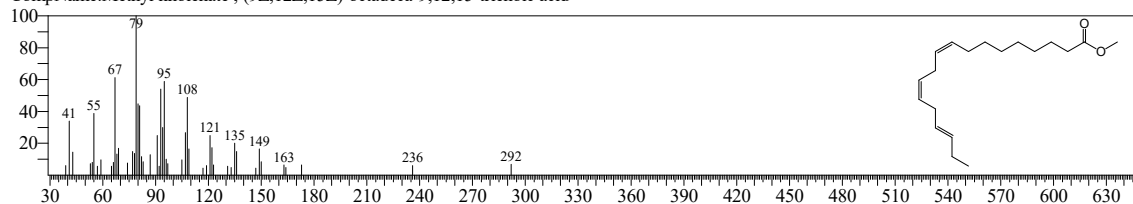SI:29 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:5 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:28 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid
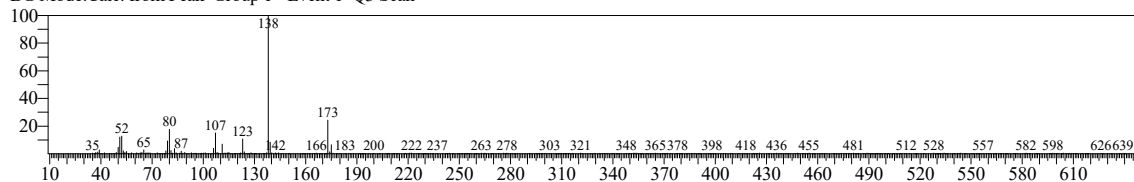
TNAU

<< Target >>
Line#:4 R.Time:12.825(Scan#:1566) MassPeaks:379
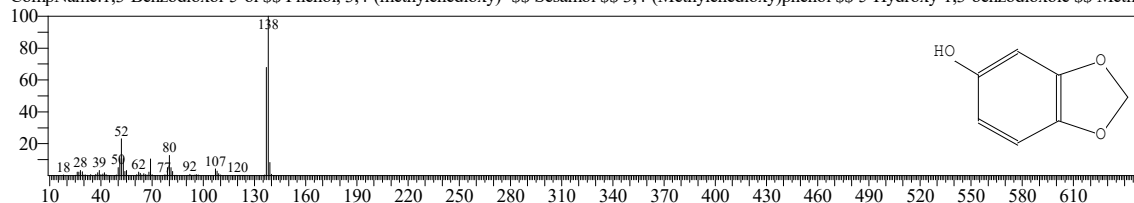RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(8023)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

138
173
52 80 107 123
35 65 87 142 166 183 200 222 237 263 278 303 321 348 365 378 398 418 436 455 481 512 528 557 582 598 626 639

Hit#:1 Entry:11187 Library:NIST20M1.lib
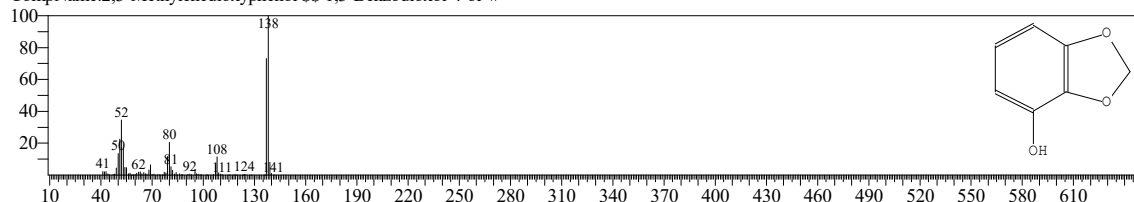SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy

138
52
80
18 28 39 50 62 71 92 107 120

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

138
52
50
80
108
41 62 81 92 111 124 141

Hit#:3 Entry:8360 Library:NIST20R.lib
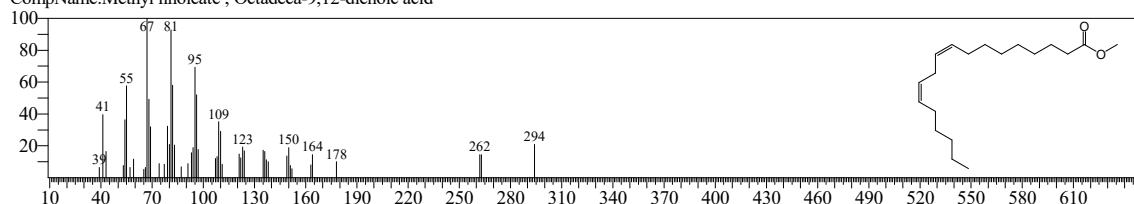SI:71 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

138
52 78
18 30 39 50 63 79 90 103 122

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

67 81
95
55
41 109
39 123 150 164 178 262 294

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

67 81
95
55
41 109
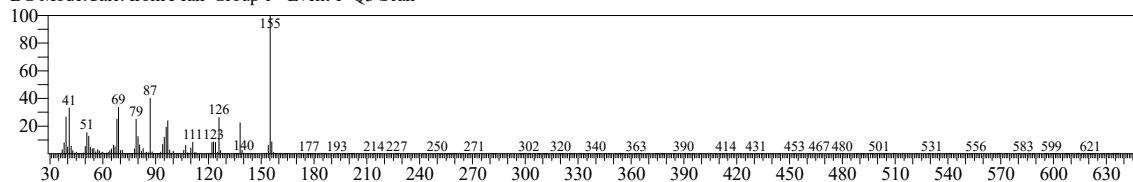124 138 164 178 318 350

TNAU

<< Target >>
Line#:5 R.Time:13.235(Scan#:1648) MassPeaks:259
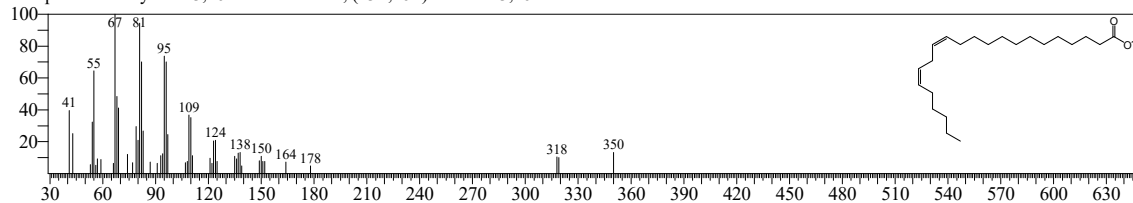RawMode:Averaged 13.230-13.240(1647-1649) BasePeak:155.05(36250)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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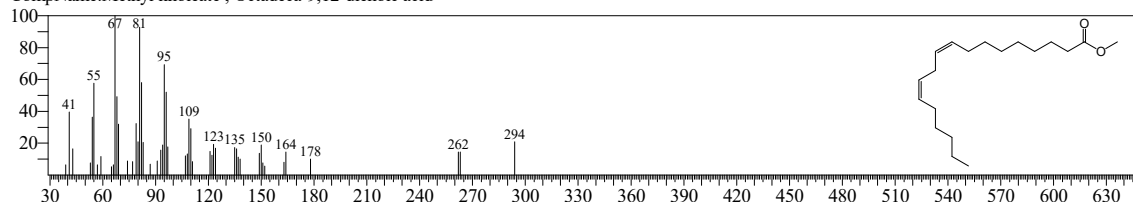SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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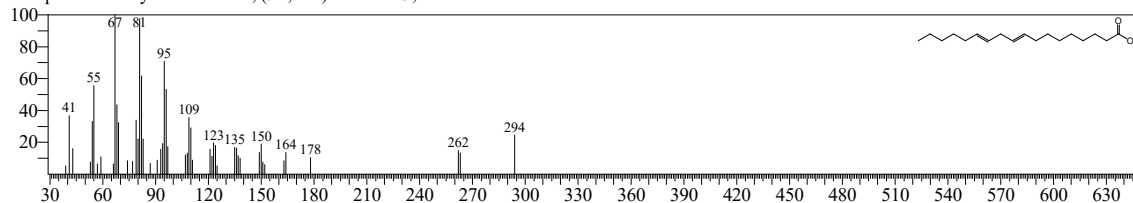CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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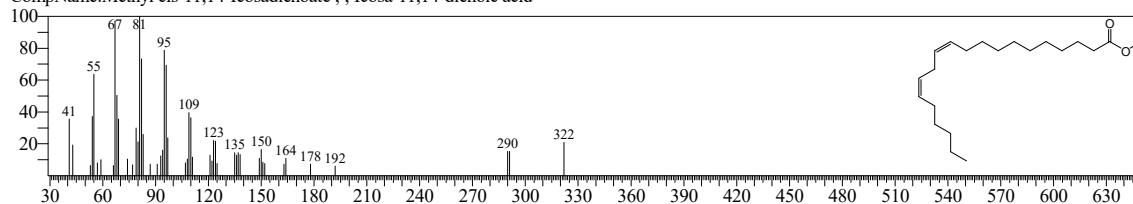CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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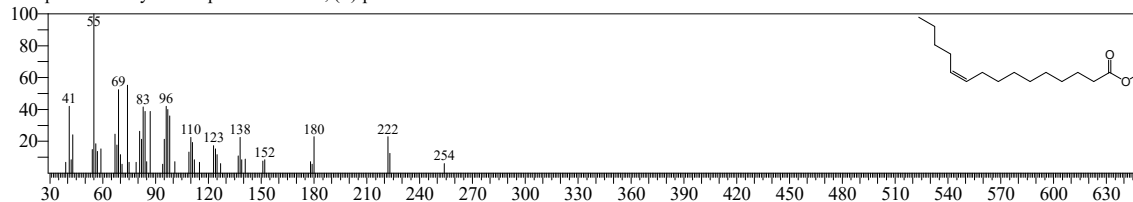SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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
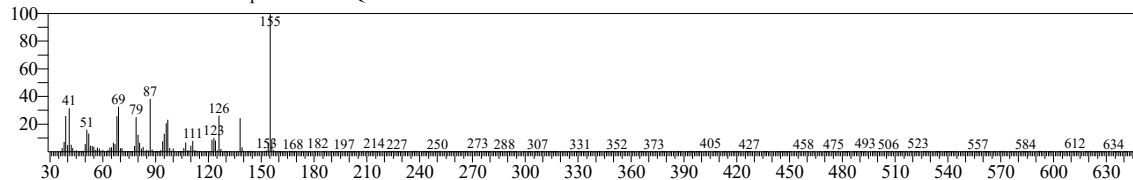
TNAU

<< Target >>
Line#:6 R.Time:13.430(Scan#:1687) MassPeaks:408
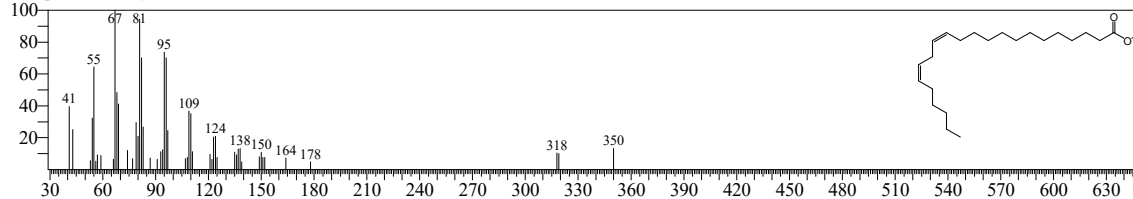RawMode:Averaged 13.425-13.435(1686-1688) BasePeak:155.05(31173)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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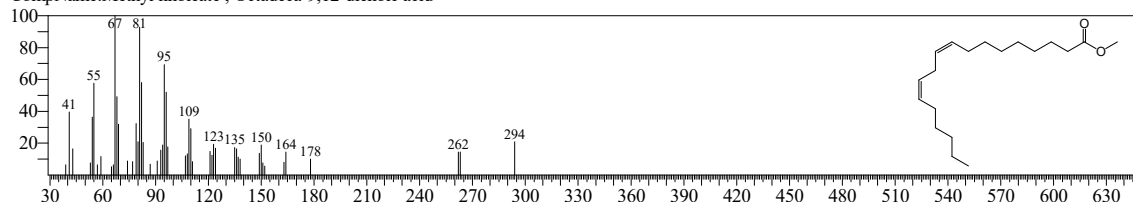SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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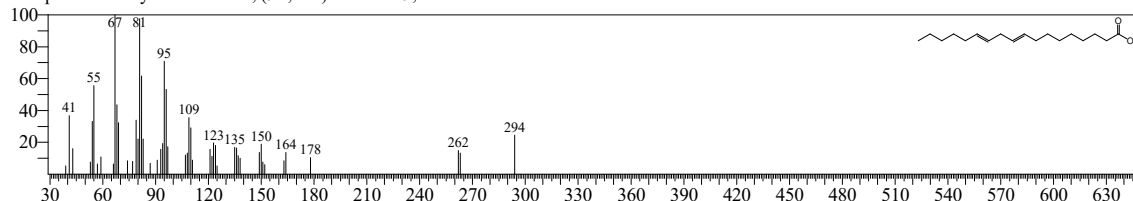SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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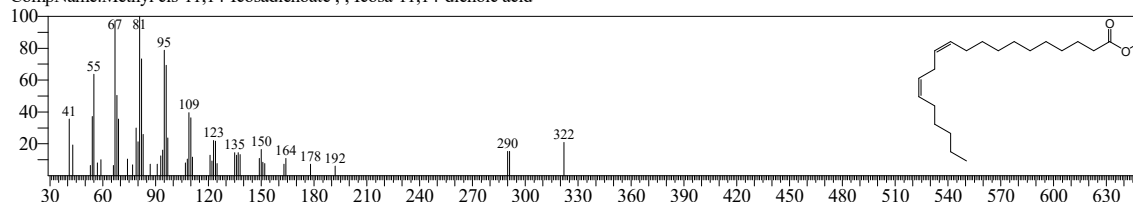CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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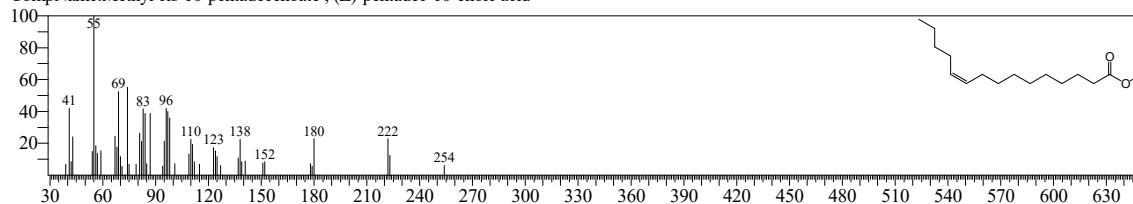SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

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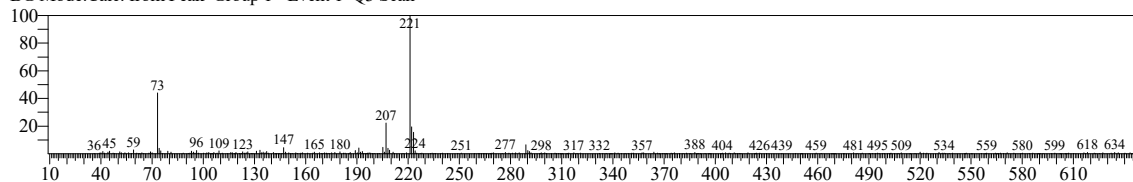CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

<< Target >>
Line#:7 R.Time:13.815(Scan#:1764) MassPeaks:301
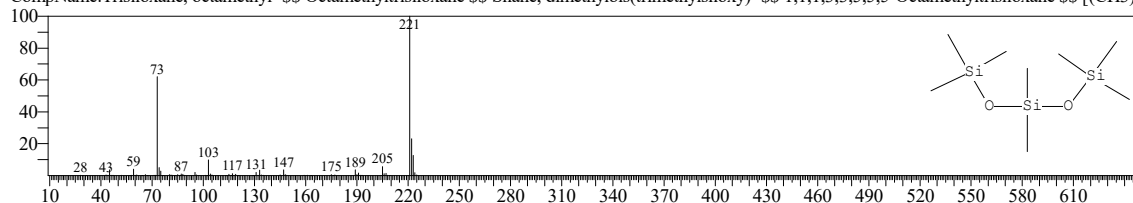RawMode:Averaged 13.810-13.820(1763-1765) BasePeak:221.10(3613)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:28950 Library:NIST20R.lib
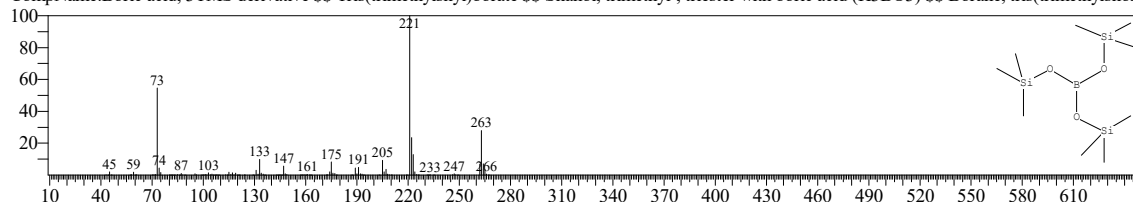SI:82 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3

Hit#:2 Entry:33791 Library:NIST20R.lib
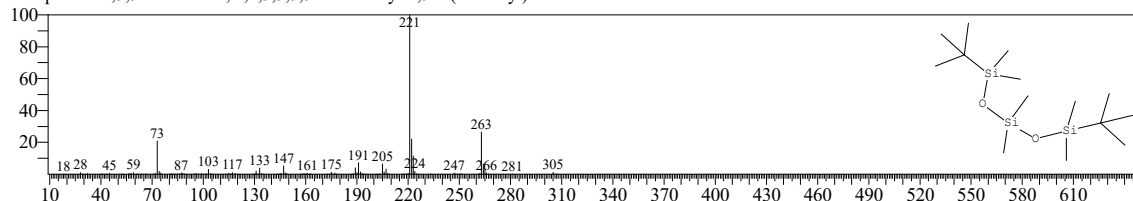SI:77 Formula:C9H27BO3Si3 CAS:4325-85-3 MolWeight:278 RetIndex:0
CompName:Boric acid, 3TMS derivative $$ Tris(trimethylsilyl)borate $$ Silanol, trimethyl-, triester with boric acid (H3BO3) $$ Borane, tris(trimethylsiloxy

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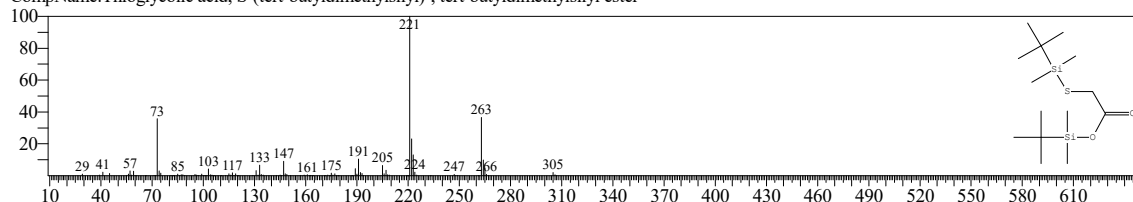CompName:1,3,5-Trisiloxane, 1,1,3,3,5,5-hexamethyl-1,5-di(tert.butyl)-

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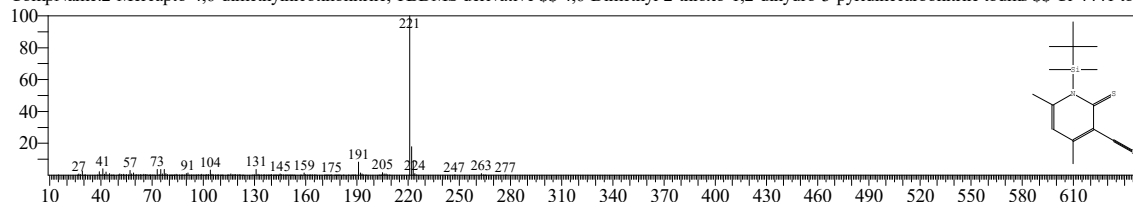CompName:Thioglycolic acid, S-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Hit#:5 Entry:136873 Library:NIST20M1.lib
SI:73 Formula:C14H22N2SSi CAS:0-00-0 MolWeight:278 RetIndex:1942
CompName:2-Mercapto-4,6-dimethylnicotinonitrile, TBDMS derivative $$ 4,6-Dimethyl-2-thioxo-1,2-dihydro-3-pyridinecarbonitrile tbdms $$ Cl-4441 tbd

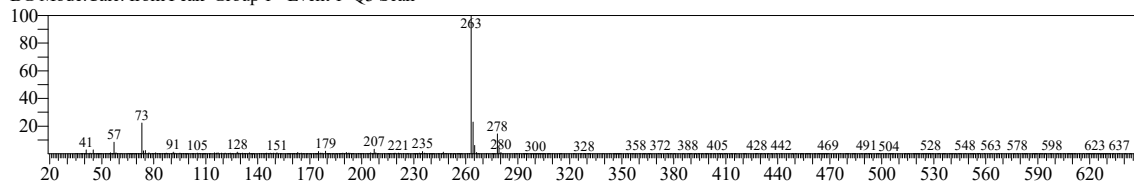# TNAU

<< Target >>
Line#:8   R.Time:19.195(Scan#:2840) MassPeaks:359
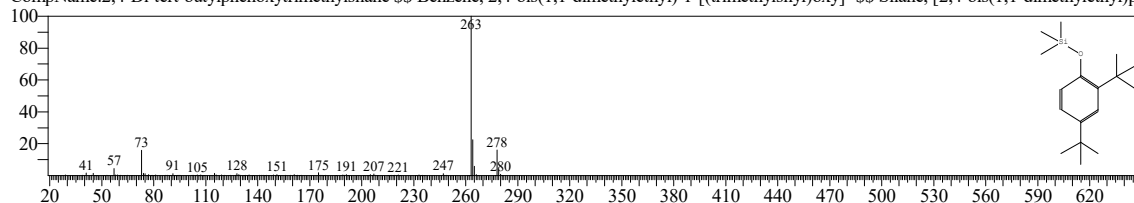RawMode:Averaged 19.190-19.200(2839-2841) BasePeak:263.15(18550)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:33874 Library:NIST20R.lib
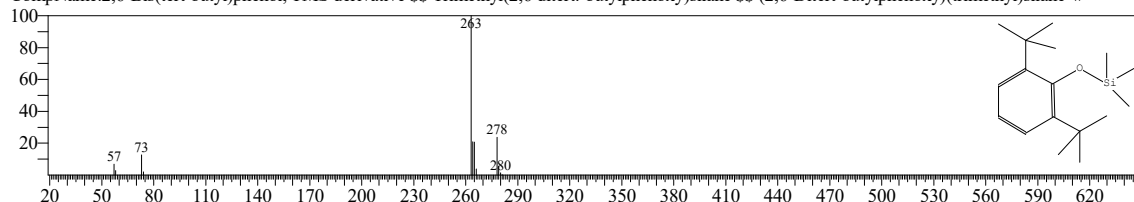SI:94 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph

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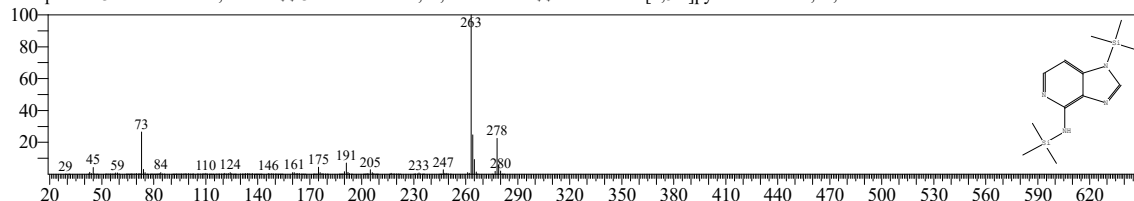SI:86 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #

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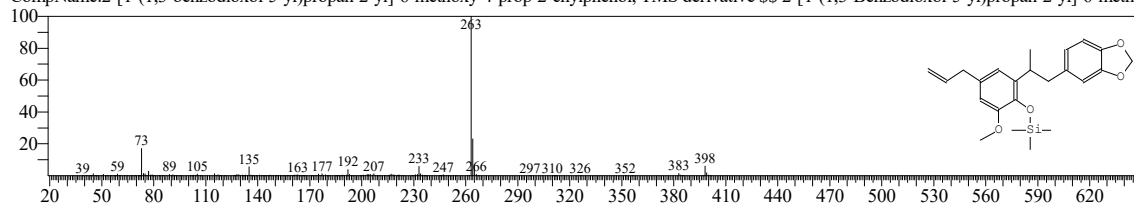CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS

Hit#:4 Entry:259338 Library:NIST20M1.lib
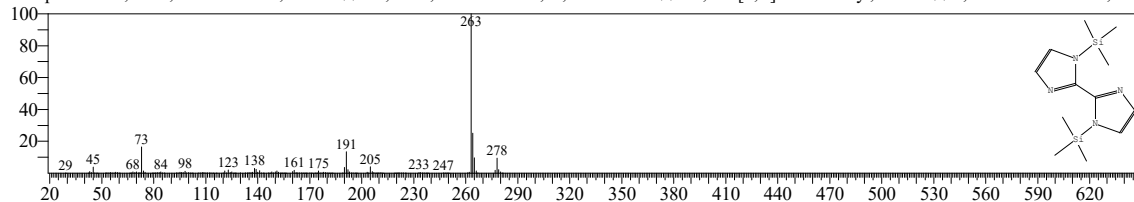SI:82 Formula:C23H30O4Si CAS:0-00-0 MolWeight:398 RetIndex:2735
CompName:2-[1-(1,3-benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-prop-2-enylphenol, TMS derivative $$ 2-[1-(1,3-Benzodioxol-5-yl)propan-2-yl]-6-metho

Hit#:5 Entry:136556 Library:NIST20M1.lib
SI:81 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM
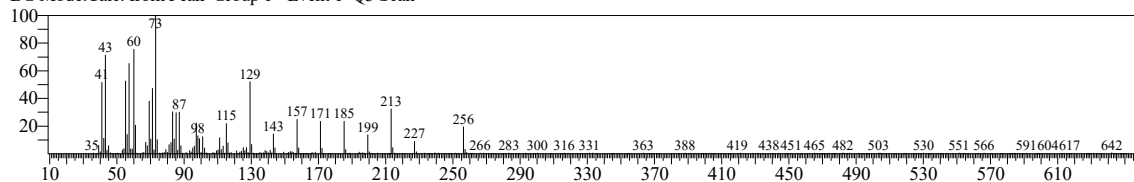
TNAU

<< Target >>
Line#:9   R.Time:28.300(Scan#:4661) MassPeaks:332
RawMode:Averaged 28.295-28.305(4660-4662) BasePeak:73.05(6914)
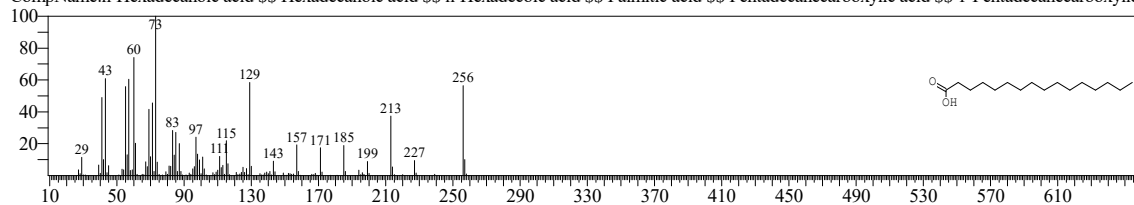BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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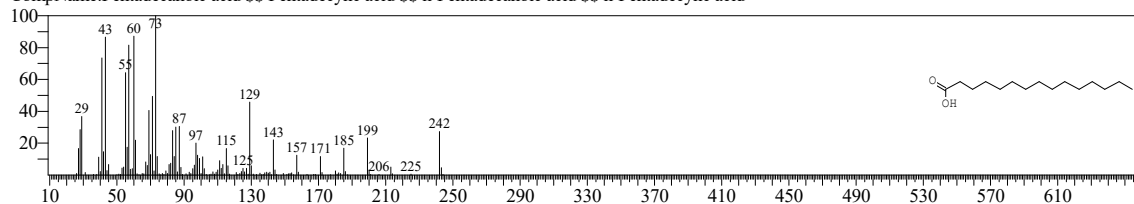SI:96 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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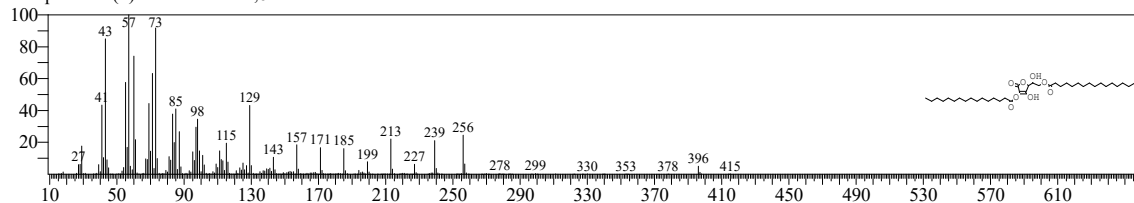SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

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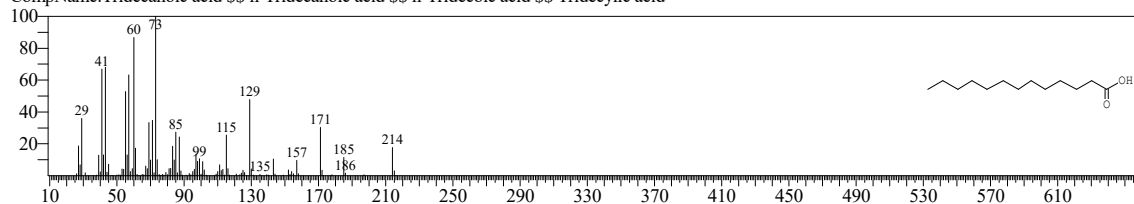CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

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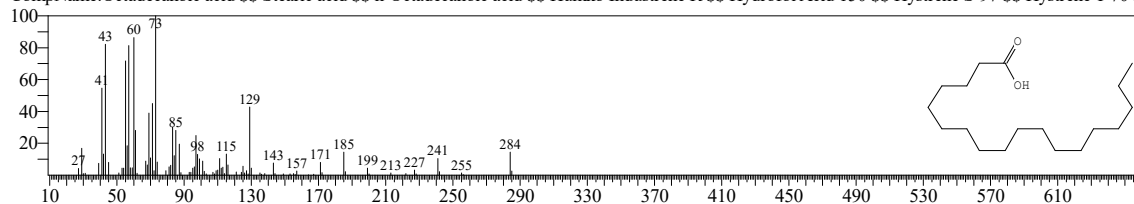SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

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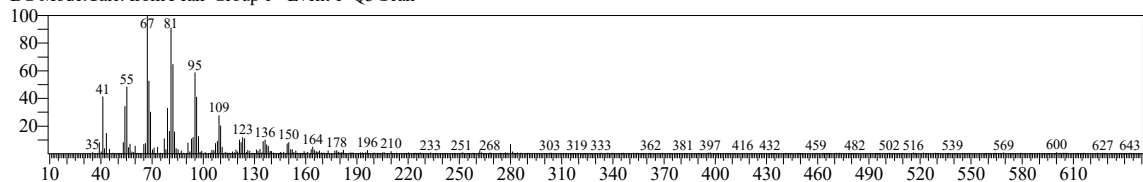
TNAU

<< Target >>
Line#:10 R.Time:31.485(Scan#:5298) MassPeaks:345
RawMode:Averaged 31.480-31.490(5297-5299) BasePeak:67.10(5793)
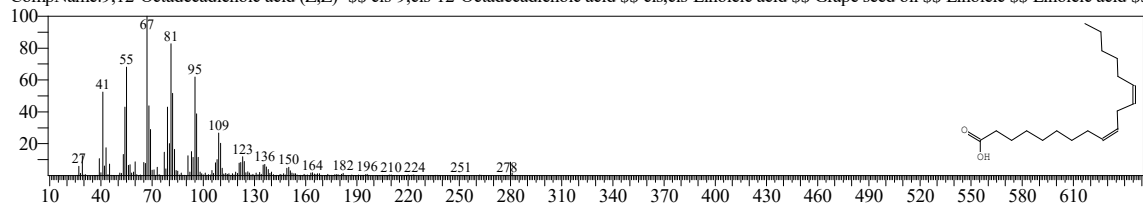BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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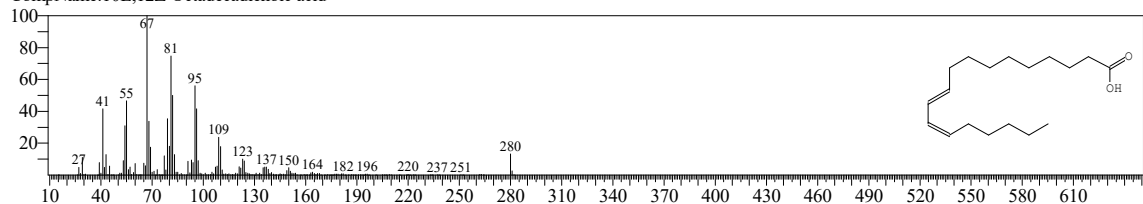SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$

Hit#:2 Entry:139646 Library:NIST20M1.lib
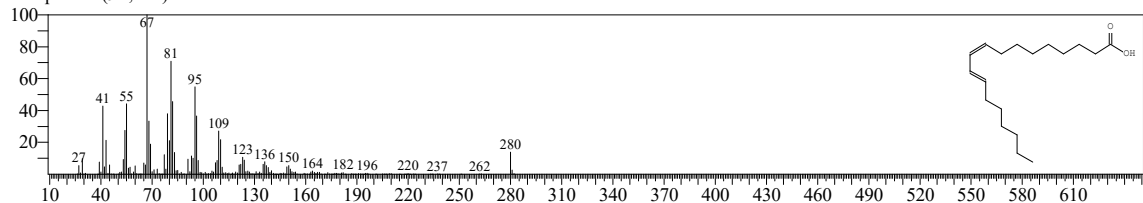SI:94 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid

Hit#:3 Entry:139651 Library:NIST20M1.lib
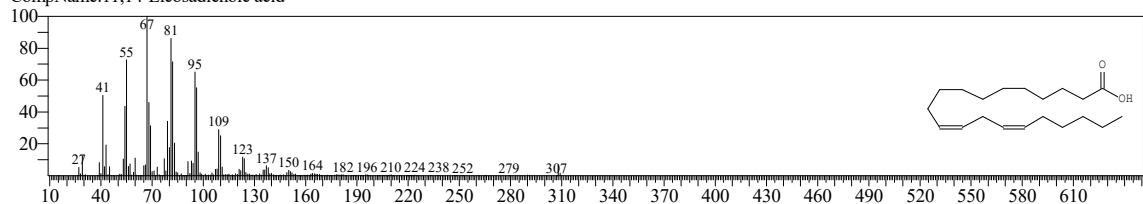SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid

Hit#:4 Entry:173215 Library:NIST20M1.lib
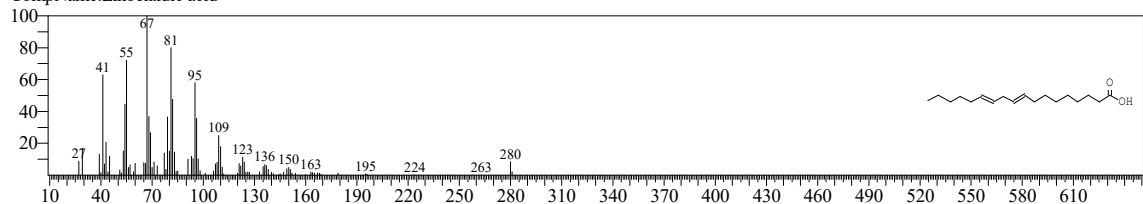SI:94 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382
CompName:11,14-Eicosadienoic acid

Hit#:5 Entry:139661 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
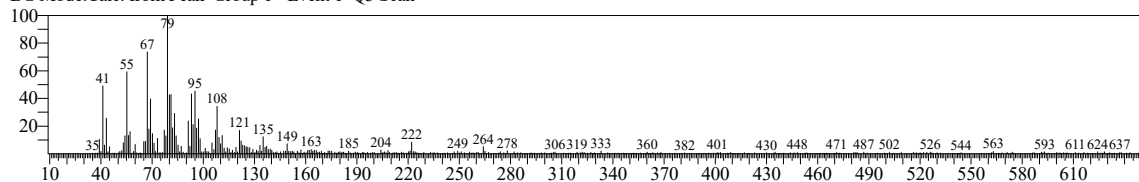CompName:Linoelaidic acid

TNAU

<< Target >>
Line#:11 R.Time:31.585(Scan#:5318) MassPeaks:393
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:79.05(2924)
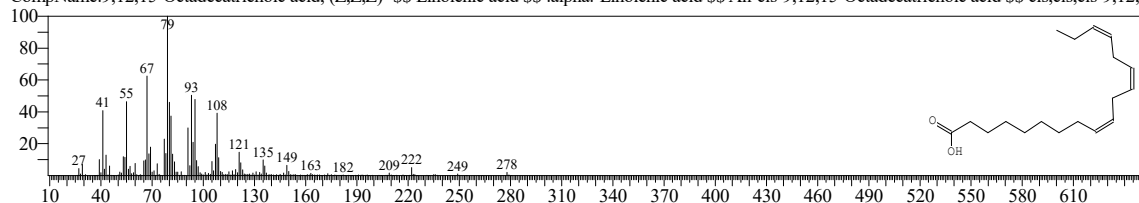BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:137464 Library:NIST20M1.lib
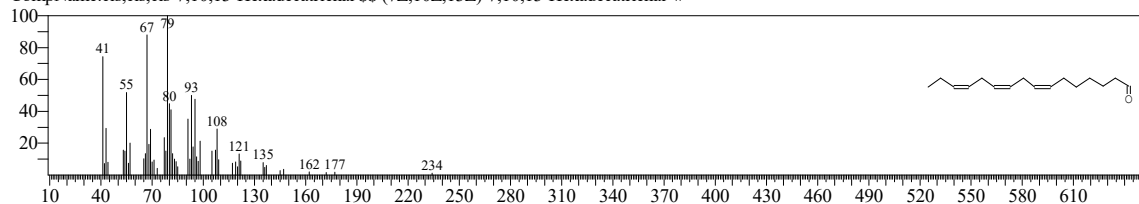SI:89 Formula:C18H30O2 CAS:463-40-1 MolWeight:278 RetIndex:2191
CompName:9,12,15-Octadecatrienoic acid, (Z,Z,Z)- $$ Linolenic acid $$ .alpha.-Linolenic acid $$ All-cis-9,12,15-Octadecatrienoic acid $$ cis,cis,cis-9,12,1

Hit#:2 Entry:87848 Library:NIST20M1.lib
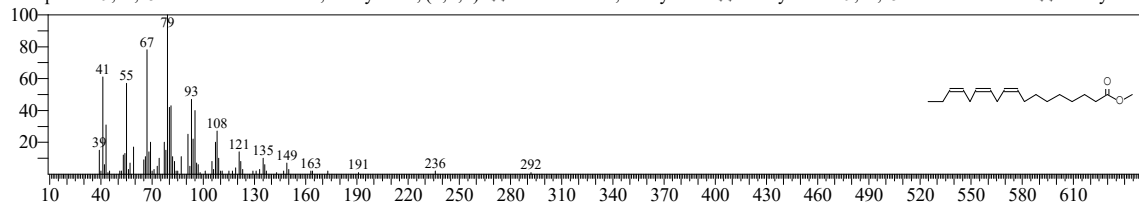SI:89 Formula:C16H26O CAS:56797-43-4 MolWeight:234 RetIndex:1824
CompName:cis,cis,cis-7,10,13-Hexadecatrienal $$ (7Z,10Z,13Z)-7,10,13-Hexadecatrienal #

Hit#:3 Entry:35226 Library:NIST20R.lib
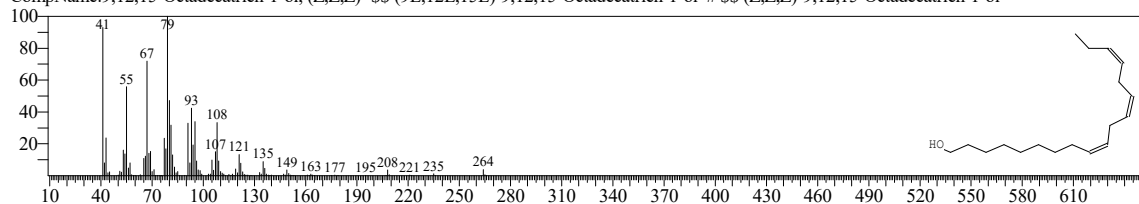SI:88 Formula:C19H32O2 CAS:301-00-8 MolWeight:292 RetIndex:2101
CompName:9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- $$ Linolenic acid, methyl ester $$ Methyl all-cis-9,12,15-octadecatrienoate $$ Methyl lino

Hit#:4 Entry:32465 Library:NIST20R.lib
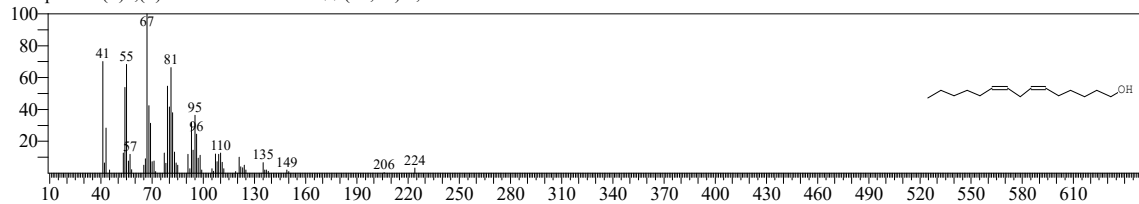SI:87 Formula:C18H32O CAS:506-44-5 MolWeight:264 RetIndex:2077
CompName:9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- $$ (9E,12E,15E)-9,12,15-Octadecatrien-1-ol # $$ (Z,Z,Z)-9,12,15-Octadecatrien-1-ol

Hit#:5 Entry:77474 Library:NIST20M1.lib
SI:86 Formula:C15H28O CAS:77899-11-7 MolWeight:224 RetIndex:1771
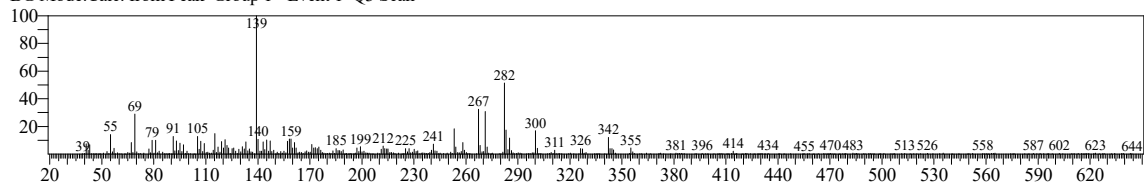CompName:(Z)6,(Z)9-Pentadecadien-1-ol $$ (6Z,9Z)-6,9-Pentadecadien-1-ol #

TNAU

<< Target >>
Line#:12 R.Time:45.615(Scan#:8124) MassPeaks:405
RawMode:Averaged 45.610-45.620(8123-8125) BasePeak:139.15(5285)
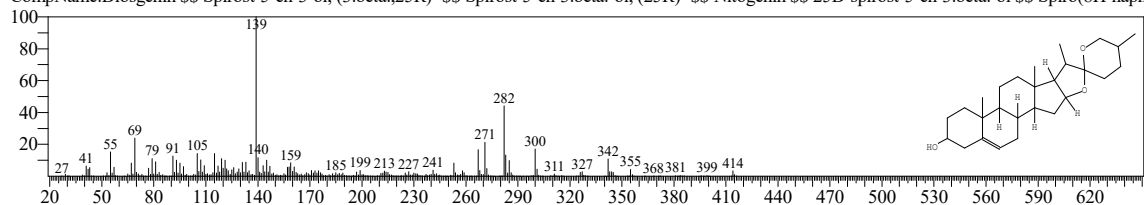BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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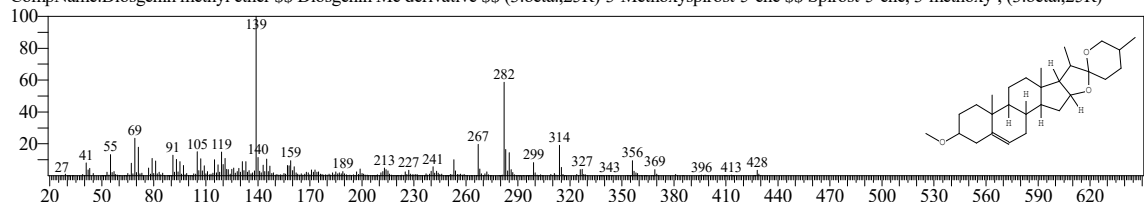SI:88 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:80 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
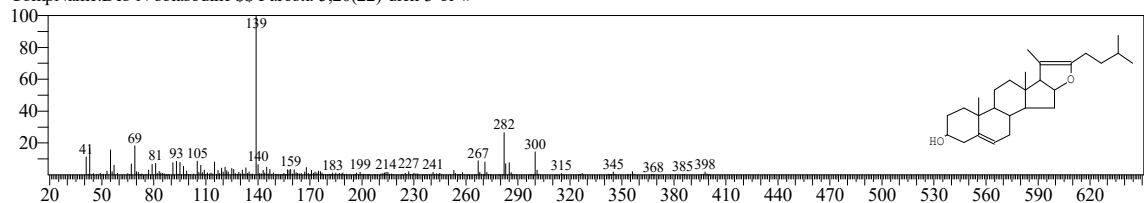CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:3 Entry:41561 Library:NIST20R.lib
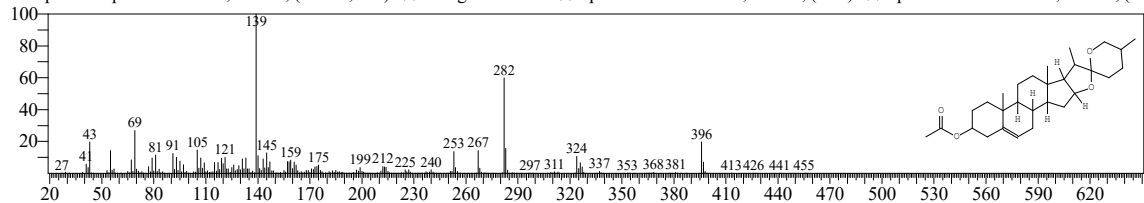SI:79 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #

Hit#:4 Entry:24878 Library:NIST20M2.lib
SI:79 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:74 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.