TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022034.qgd

Peak Report TIC

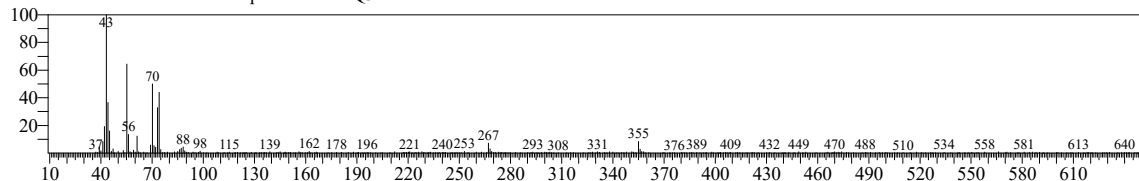| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.935	72276	2.80	21125	2.86	3.42	82	1-Butanol, 3-methyl-, acetate
2	9.767	49632	1.92	23423	3.17	2.12	95	Pentasiloxane, dodecamethyl-
3	12.498	173273	6.71	66730	9.04	2.60	73	2,5-Cyclohexadiene-1,4-dione, dioxime
4	12.825	231780	8.97	93497	12.66	2.48	73	2,5-Cyclohexadiene-1,4-dione, dioxime
5	13.387	531508	20.58	126006	17.06	4.22	51	Methyl cis-13,16-Docosadienate
6	13.570	374409	14.50	90064	12.20	4.16	53	Methyl cis-13,16-Docosadienate
7	18.089	40136	1.55	13759	1.86	2.92	88	.beta.-D-Glucopyranose, 1,6-anhydro-
8	19.193	25847	1.00	11138	1.51	2.32	84	2,4-Di-tert-butylphenoxytrimethylsilane
9	28.297	211864	8.20	78292	10.60	2.71	95	n-Hexadecanoic acid
10	31.468	106963	4.14	37556	5.09	2.85	95	9,12-Octadecadienoic acid (Z,Z)-
11	31.583	73036	2.83	25149	3.41	2.90	86	cis-9-Hexadecenal
12	32.030	75955	2.94	29258	3.96	2.60	92	Octadecanoic acid
13	39.072	24412	0.95	11214	1.52	2.18	81	Tetracosamethyl-cyclododecasiloxane
14	41.600	35354	1.37	13445	1.82	2.63	83	Tetracosamethyl-cyclododecasiloxane
15	43.798	46335	1.79	16665	2.26	2.78	84	Tetracosamethyl-cyclododecasiloxane
16	45.595	452739	17.53	66381	8.99	6.82	91	Diosgenin
17	45.774	57444	2.22	14734	2.00	3.90	82	Tetracosamethyl-cyclododecasiloxane
		2582963	100.00	738436	100.00			

Library

TNAU

<< Target >>
Line#:1 R.Time:8.935(Scan#:788) MassPeaks:330
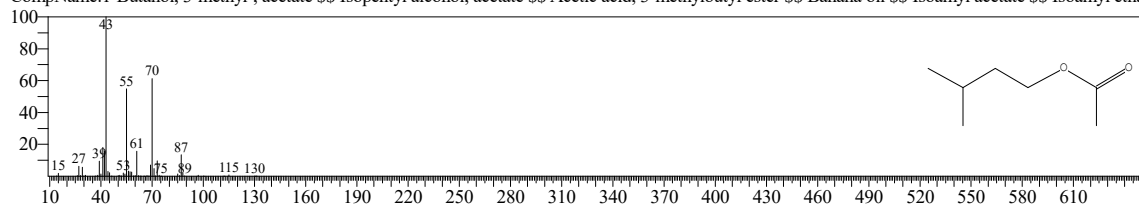RawMode:Averaged 8.930-8.940(787-789) BasePeak:43.05(4206)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:6784 Library:NIST20R.lib
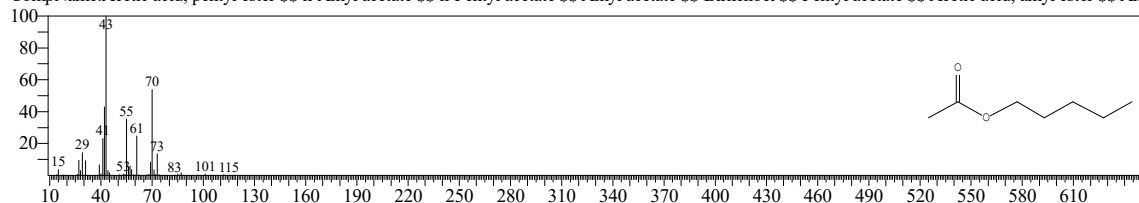SI:82 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha

Hit#:2 Entry:8685 Library:NIST20M1.lib
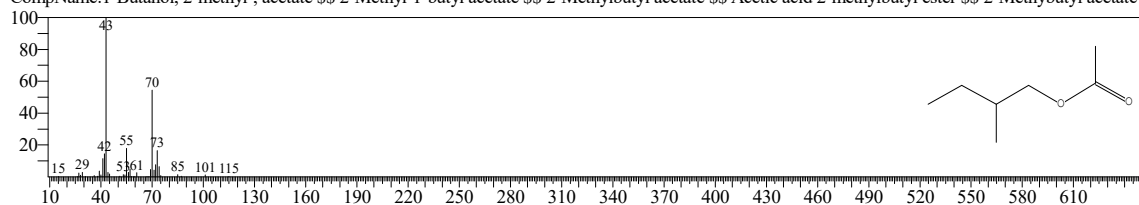SI:80 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ Am

Hit#:3 Entry:6819 Library:NIST20R.lib
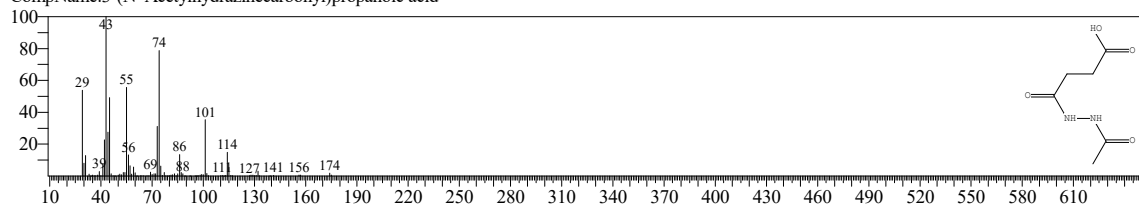SI:79 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate $

Hit#:4 Entry:32045 Library:NIST20M1.lib
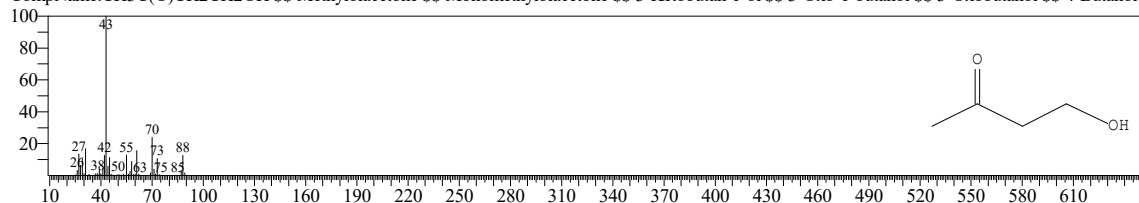SI:78 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid

Hit#:5 Entry:1220 Library:NIST20R.lib
SI:77 Formula:C4H8O2 CAS:590-90-9 MolWeight:88 RetIndex:798
CompName:CH3C(O)CH2CH2OH $$ Methylolacetone $$ Monomethylolacetone $$ 3-Ketobutan-1-ol $$ 3-Oxo-1-butanol $$ 3-Oxobutanol $$ 4-Butanol-
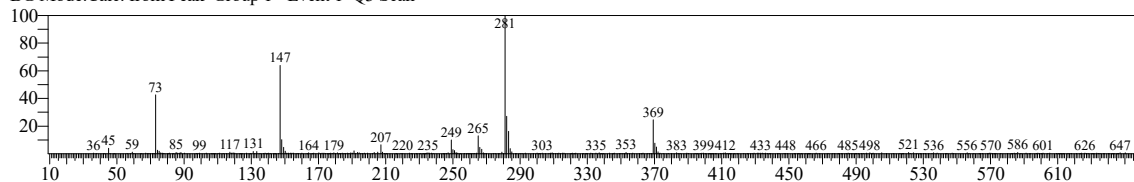
TNAU

<< Target >>
Line#:2   R.Time:9.765(Scan#:954) MassPeaks:370
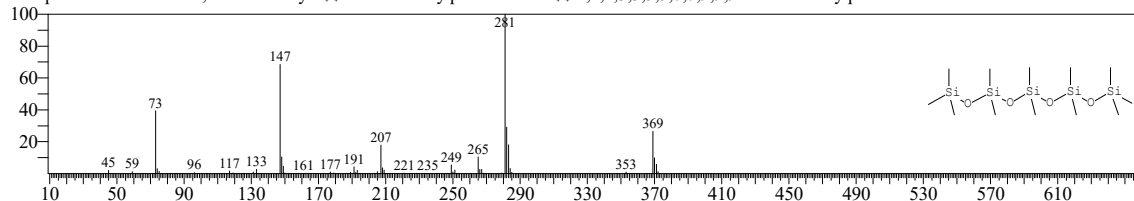RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.00(5434)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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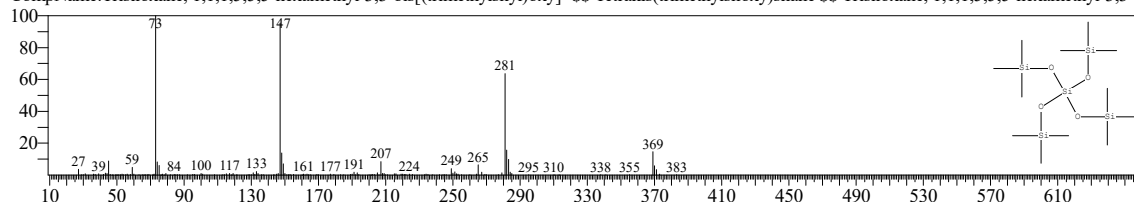SI:95 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

Hit#:2 Entry:249272 Library:NIST20M1.lib
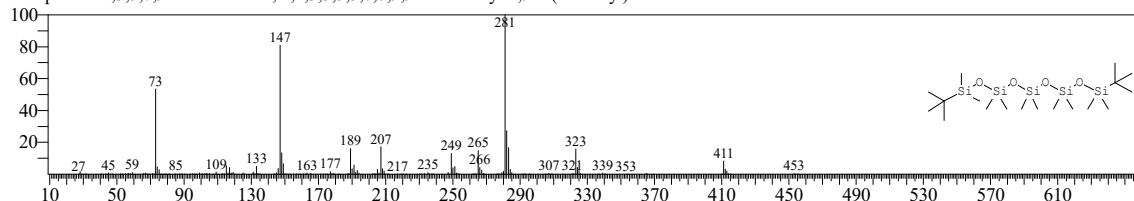SI:84 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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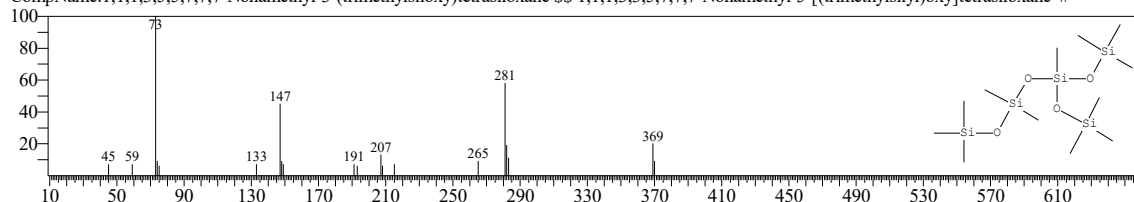SI:82 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

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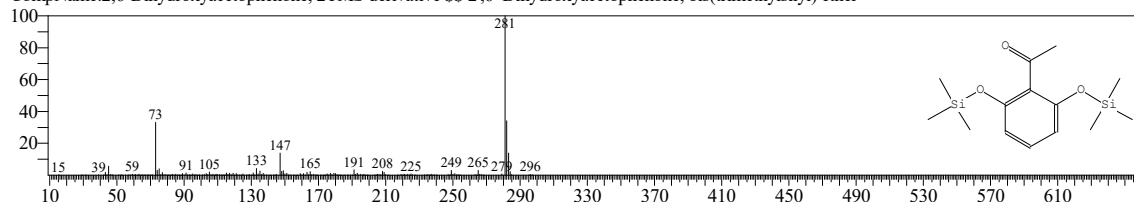SI:79 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:77 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether
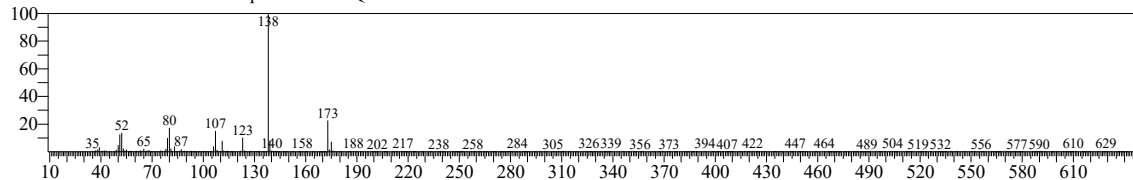
TNAU

<< Target >>
Line#:3 R.Time:12.495(Scan#:1500) MassPeaks:331
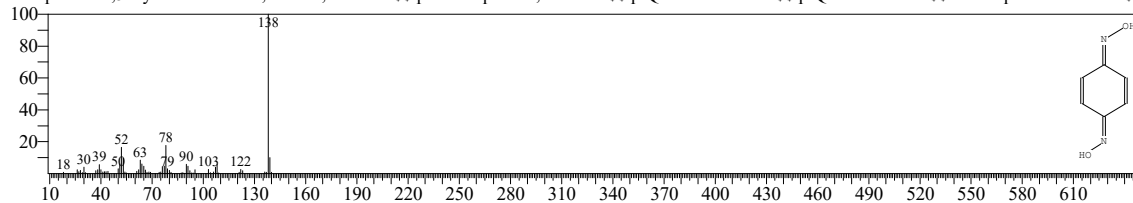RawMode:Averaged 12.490-12.500(1499-1501) BasePeak:138.05(24056)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:8360 Library:NIST20R.lib
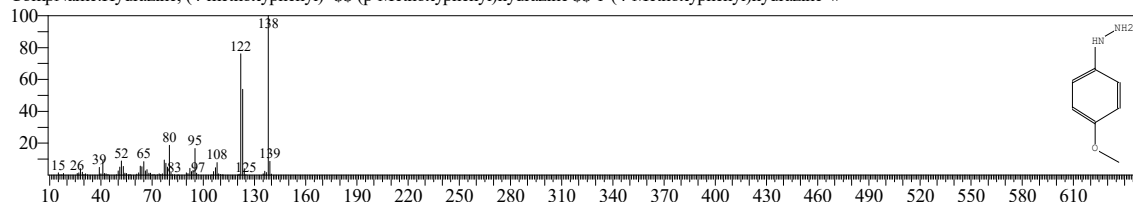SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

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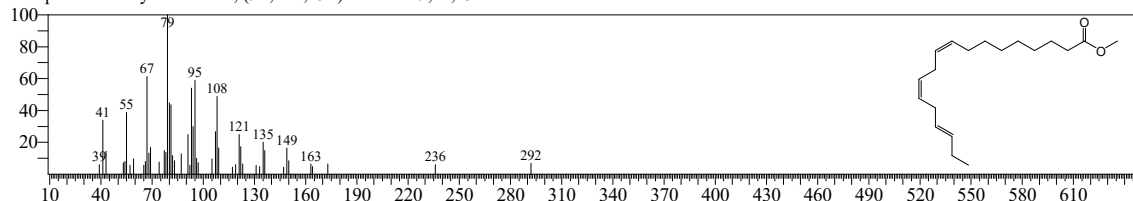SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

Hit#:3 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
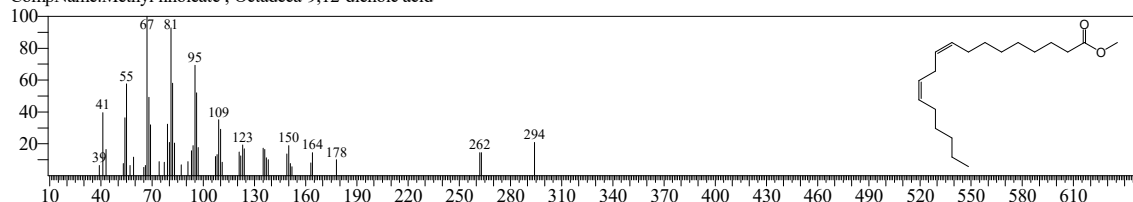SI:35 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

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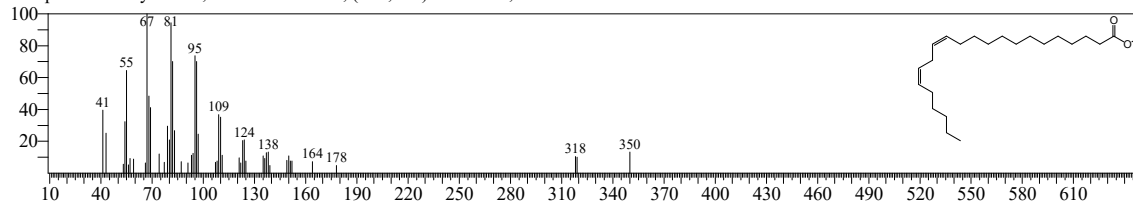SI:34 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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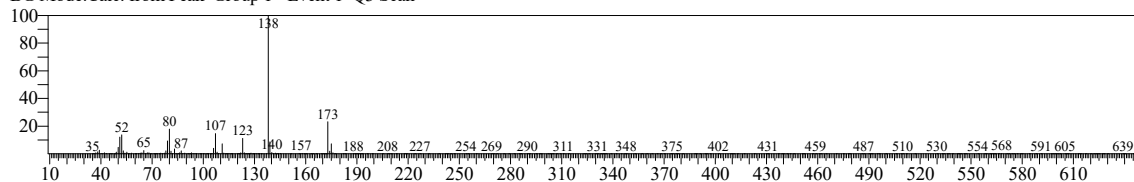
TNAU

<< Target >>
Line#:4 R.Time:12.825(Scan#:1566) MassPeaks:290
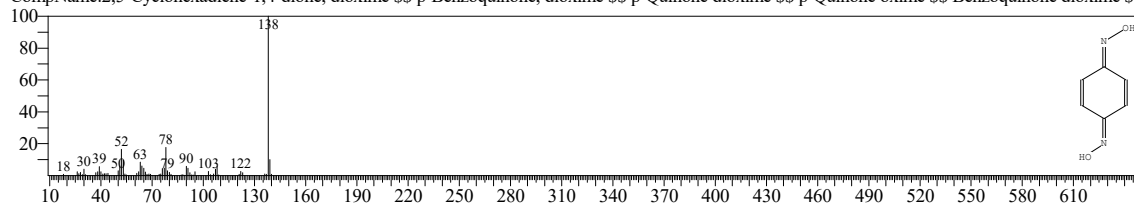RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(33639)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
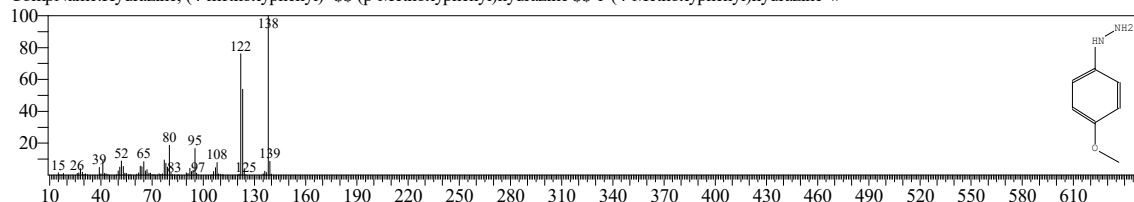CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

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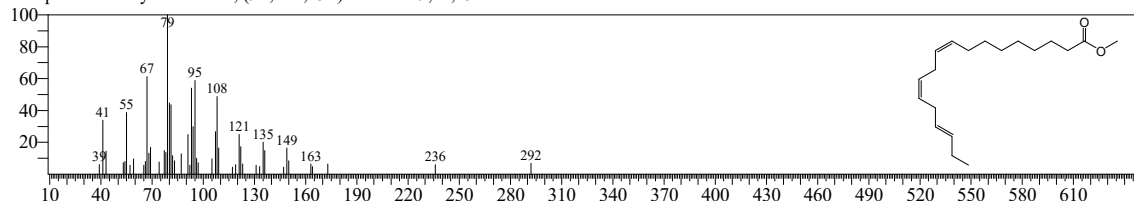CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

Hit#:3 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
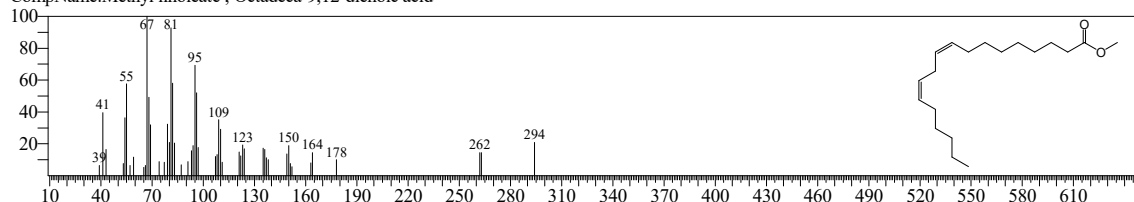SI:33 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

Hit#:4 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
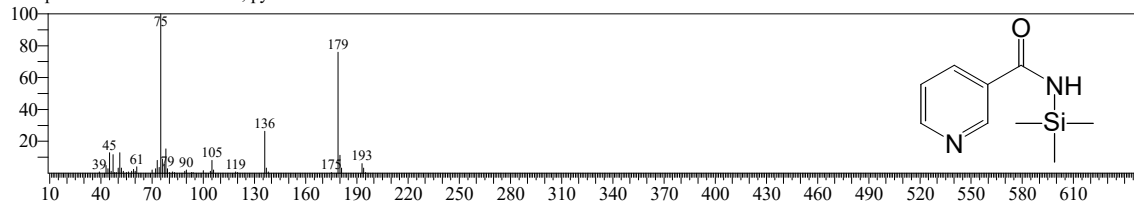SI:32 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:5 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
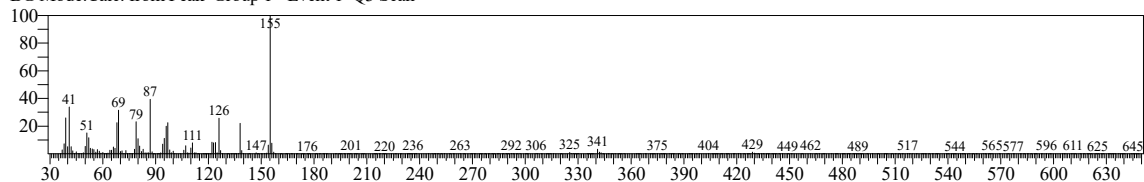CompName:Niacinamide-TMS ; pyridine-3-carboxamide

TNAU

<< Target >>
Line#:5 R.Time:13.385(Scan#:1678) MassPeaks:352
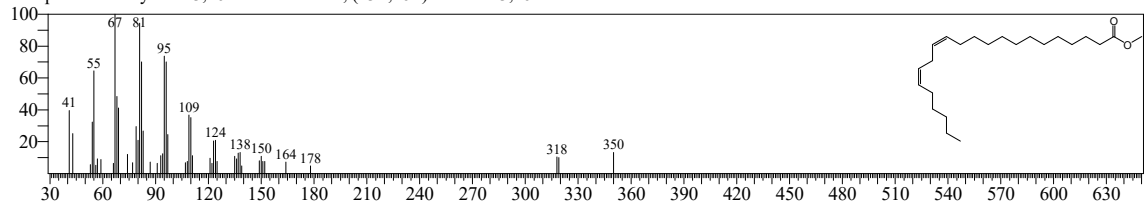RawMode:Averaged 13.380-13.390(1677-1679) BasePeak:155.05(20855)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
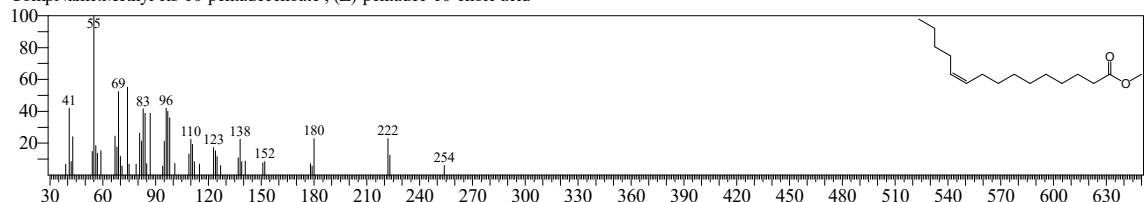SI:51 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:2 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
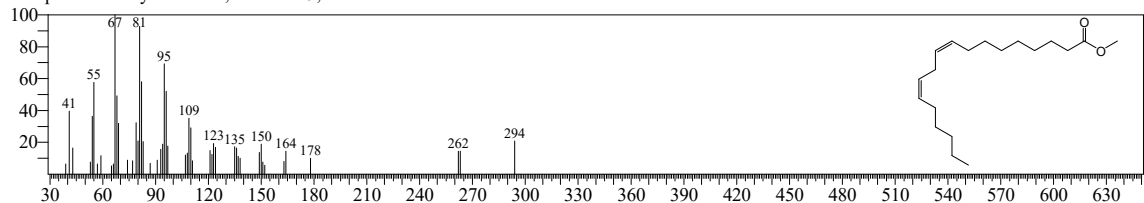SI:50 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

Hit#:3 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
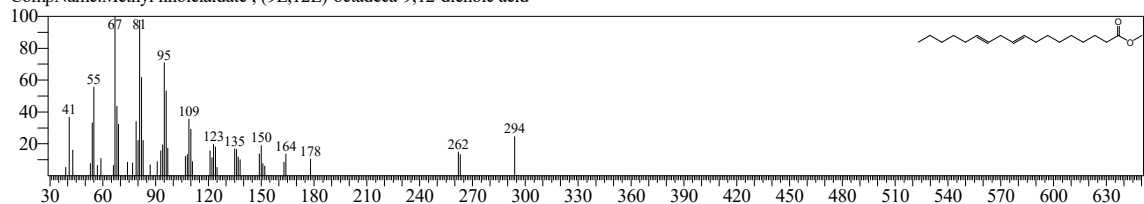SI:50 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:4 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:49 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
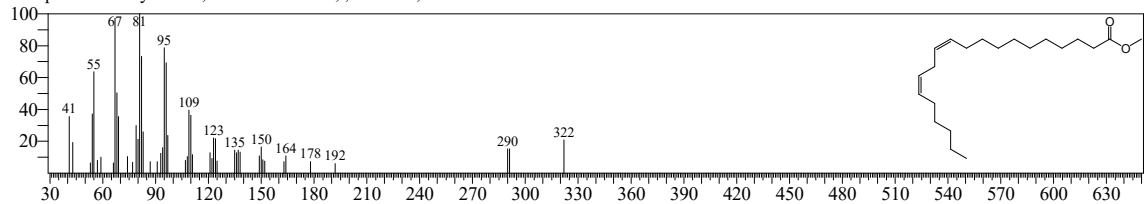CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:49 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid
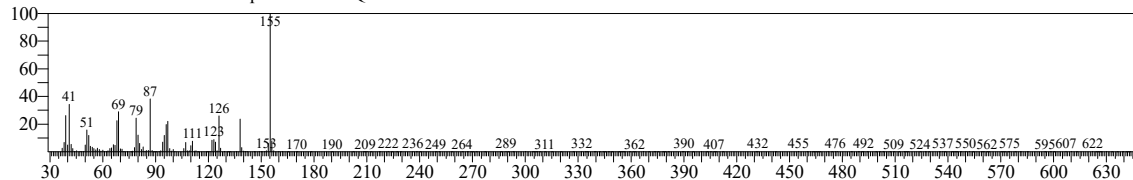
TNAU

<< Target >>
Line#:6   R.Time:13.570(Scan#:1715) MassPeaks:248
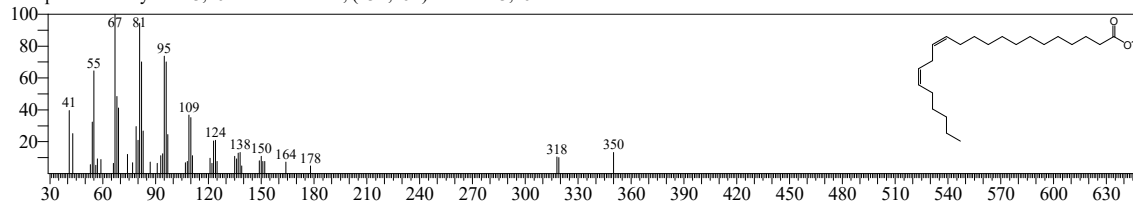RawMode:Averaged 13.565-13.575(1714-1716) BasePeak:155.05(15923)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
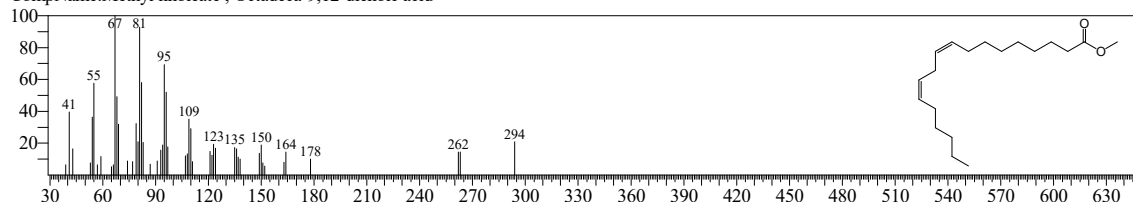SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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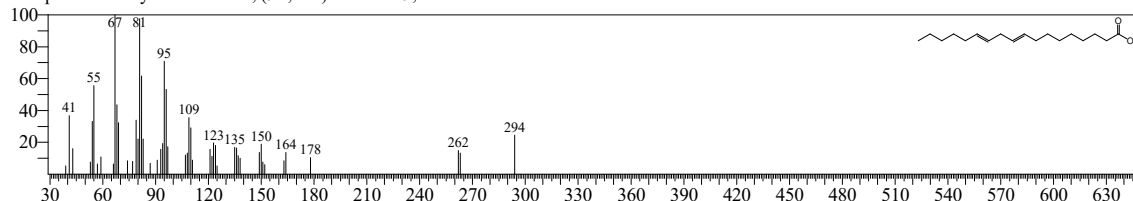SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
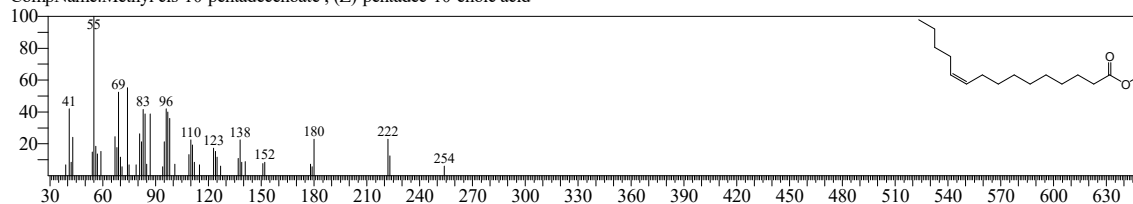CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
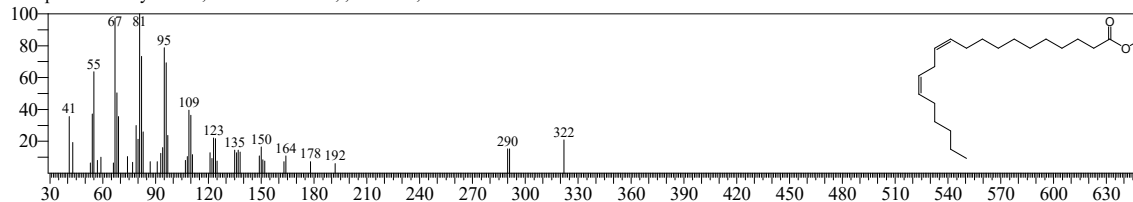SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid
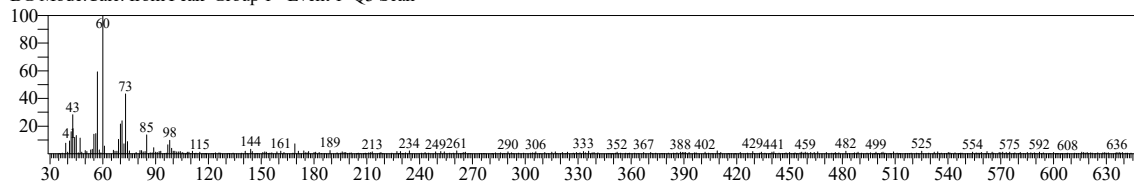
TNAU

<< Target >>
Line#:7 R.Time:18.090(Scan#:2619) MassPeaks:365
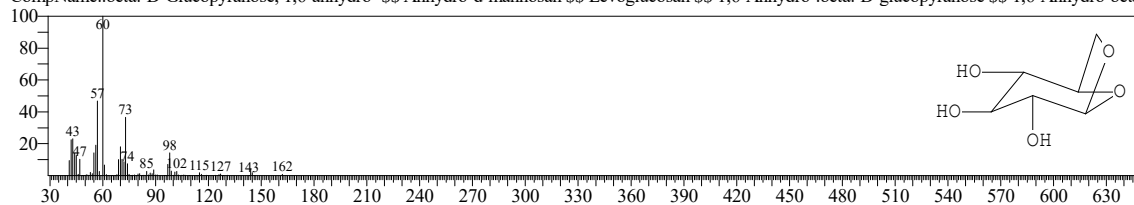RawMode:Averaged 18.085-18.095(2618-2620) BasePeak:60.05(2255)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:13905 Library:NIST20R.lib
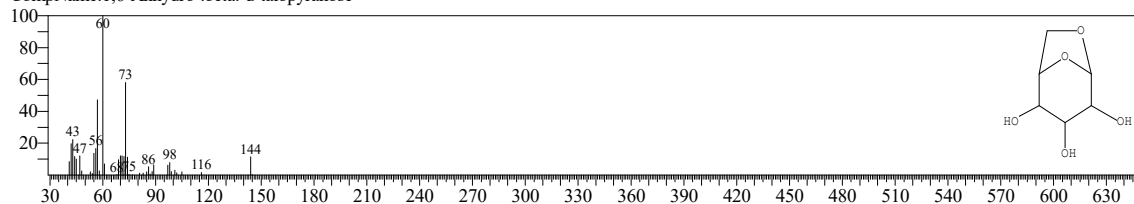SI:88 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-

Hit#:2 Entry:23812 Library:NIST20M1.lib
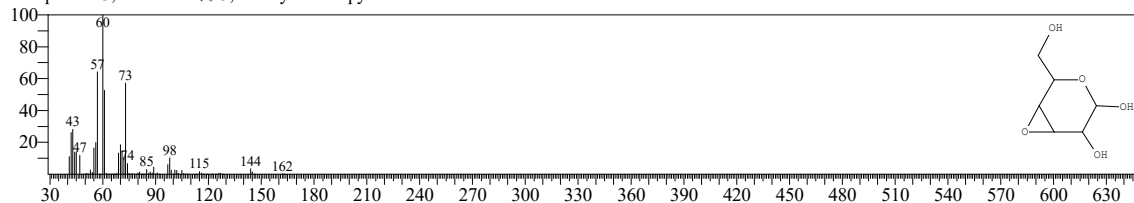SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose

Hit#:3 Entry:23808 Library:NIST20M1.lib
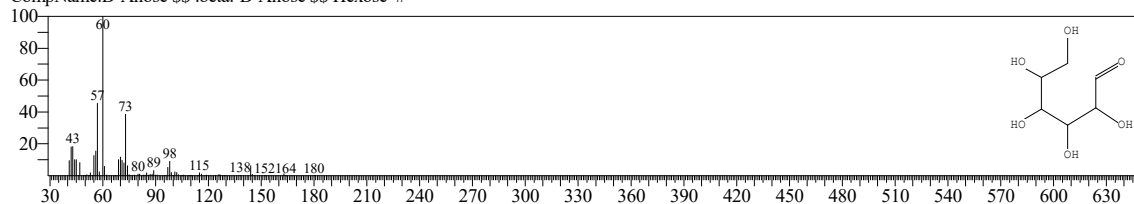SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1400
CompName:3,4-Altrosan $$ 3,4-Anhydrohexopyranose #

Hit#:4 Entry:36240 Library:NIST20M1.lib
SI:87 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
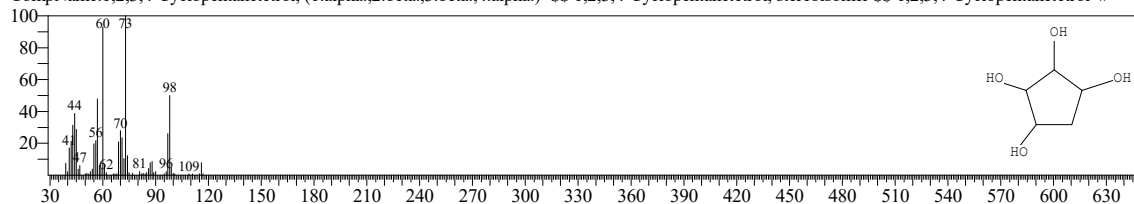CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #

Hit#:5 Entry:9697 Library:NIST20M1.lib
SI:82 Formula:C5H10O4 CAS:14003-71-5 MolWeight:134 RetIndex:1352
CompName:1,2,3,4-Cyclopentanetetrol, (1.alpha.,2.beta.,3.beta.,4.alpha.)- $$ 1,2,3,4-Cyclopentanetetrol, stereoisomer $$ 1,2,3,4-Cyclopentanetetrol #
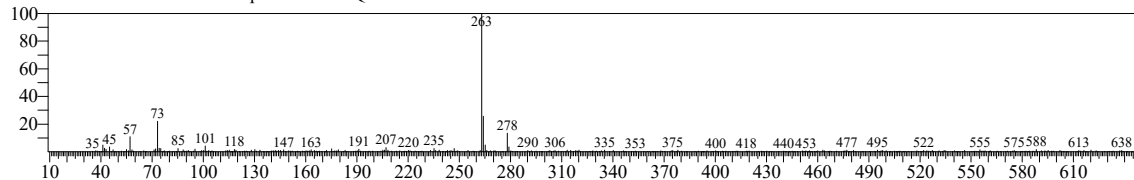
TNAU

<< Target >>
Line#:8 R.Time:19.195(Scan#:2840) MassPeaks:369
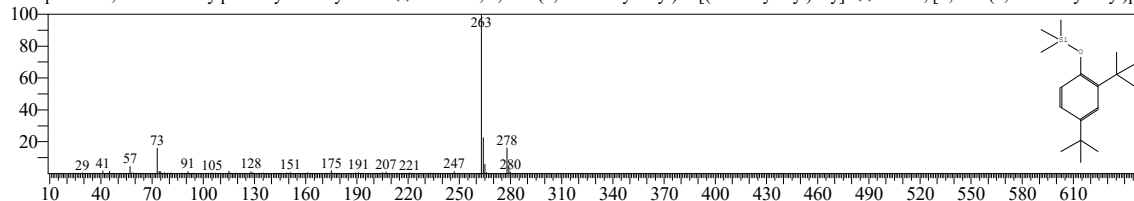RawMode:Averaged 19.190-19.200(2839-2841) BasePeak:263.15(3577)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:33874 Library:NIST20R.lib
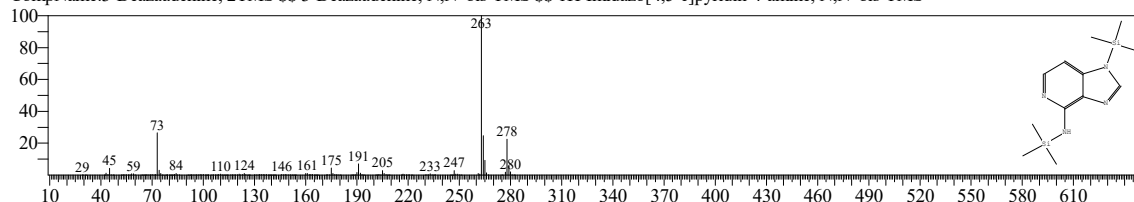SI:84 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph

Hit#:2 Entry:136557 Library:NIST20M1.lib
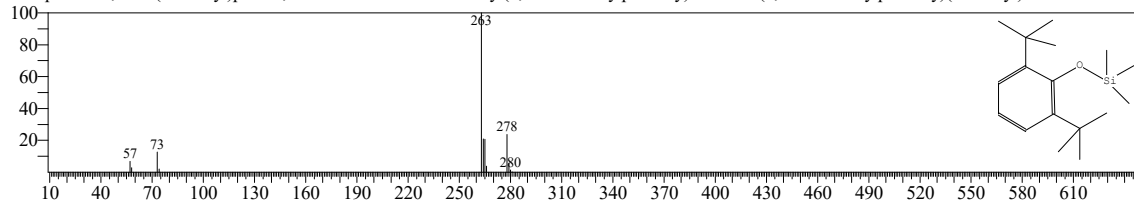SI:78 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS

Hit#:3 Entry:33871 Library:NIST20R.lib
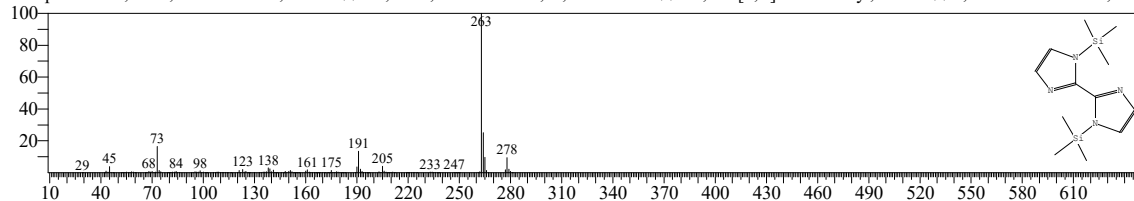SI:78 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #

Hit#:4 Entry:136556 Library:NIST20M1.lib
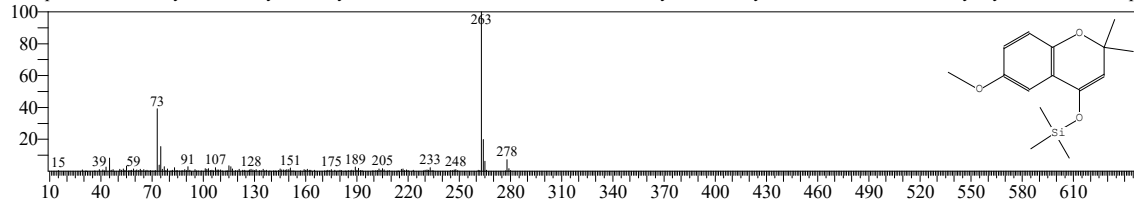SI:75 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM

Hit#:5 Entry:137020 Library:NIST20M1.lib
SI:73 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy
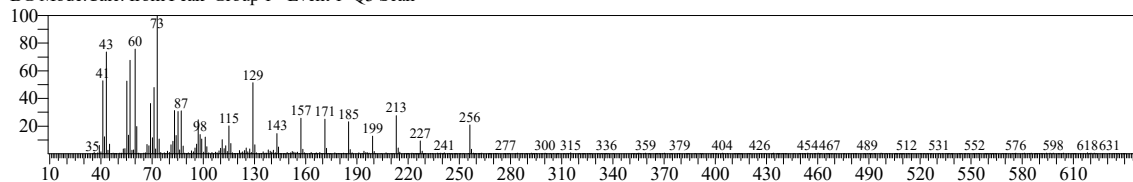
TNAU

<< Target >>
Line#:9 R.Time:28.295(Scan#:4660) MassPeaks:391
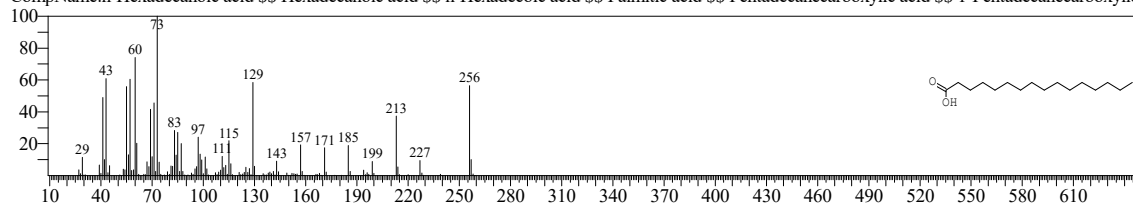RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.00(6374)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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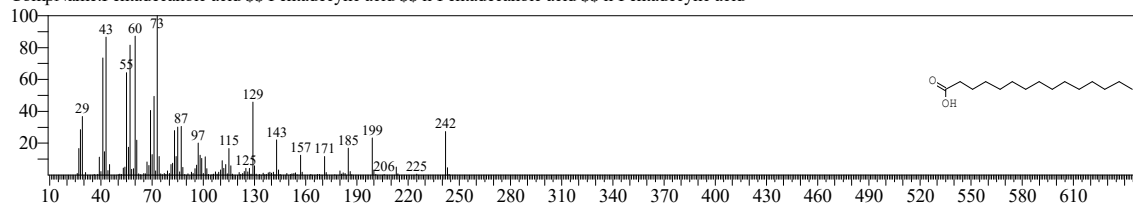SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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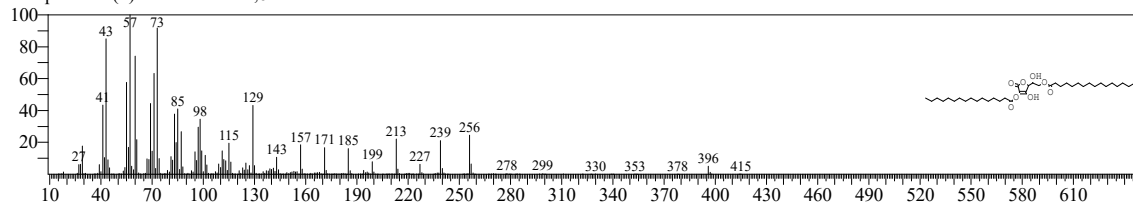SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

Hit#:3 Entry:44286 Library:NIST20M2.lib
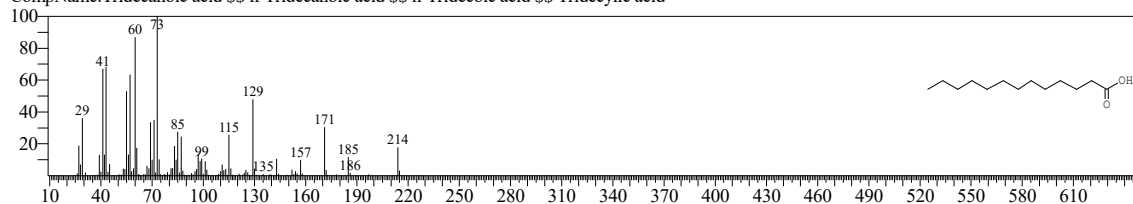SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

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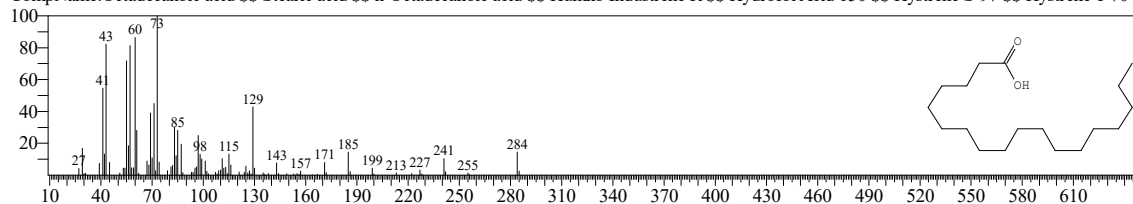SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

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 $
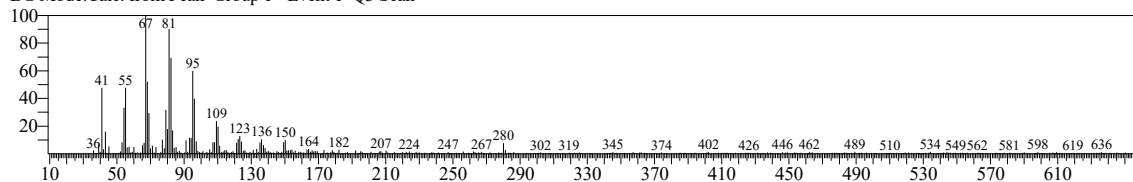
TNAU

<< Target >>
Line#:10   R.Time:31.470(Scan#:5295) MassPeaks:381
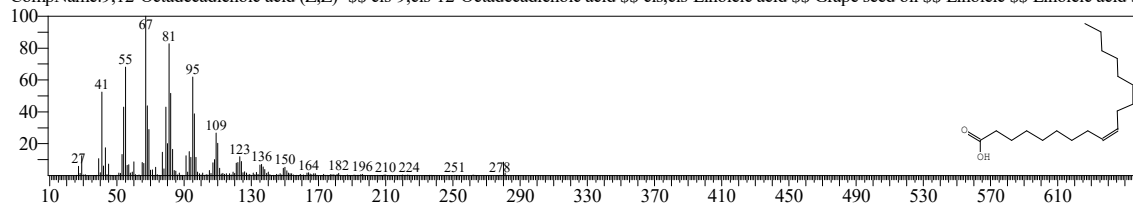RawMode:Averaged 31.465-31.475(5294-5296) BasePeak:67.05(3381)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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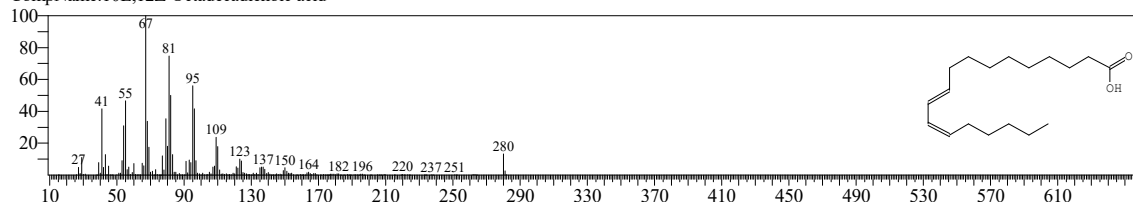SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$

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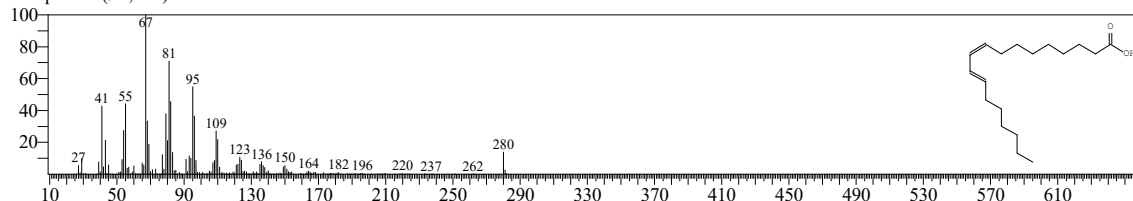SI:94 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid

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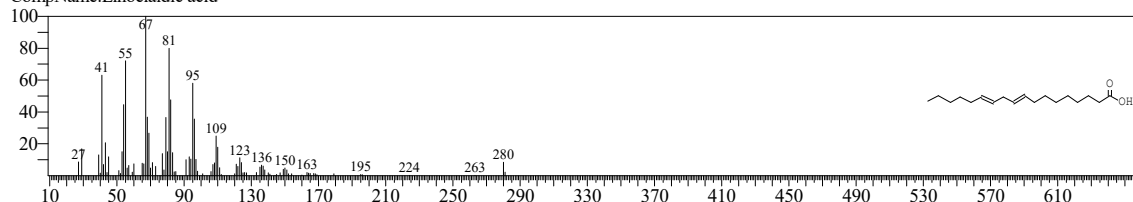SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid

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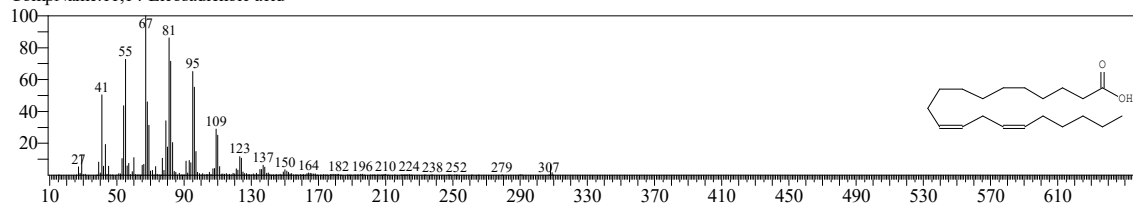SI:94 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

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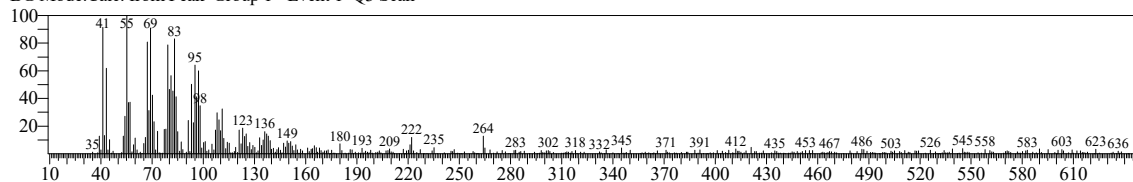CompName:11,14-Eicosadienoic acid

TNAU

<< Target >>
Line#:11 R.Time:31.585(Scan#:5318) MassPeaks:401
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:55.05(1114)
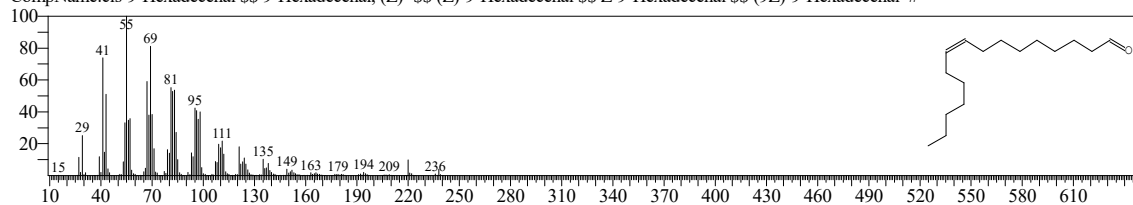BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:92244 Library:NIST20M1.lib
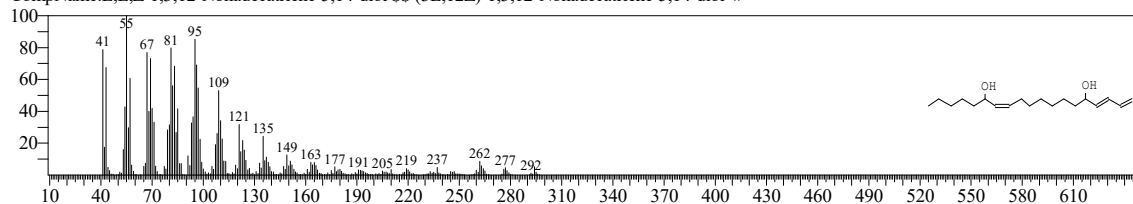SI:86 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #

Hit#:2 Entry:156549 Library:NIST20M1.lib
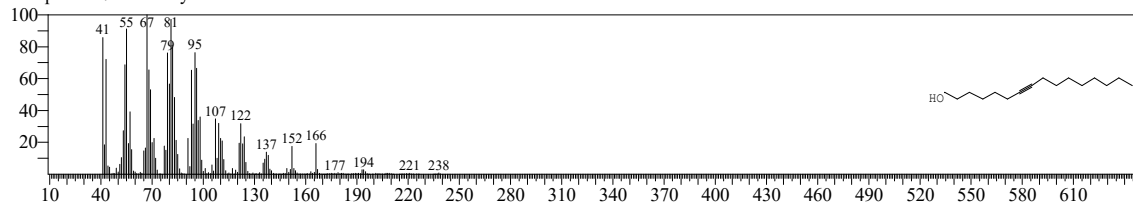SI:86 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #

Hit#:3 Entry:92246 Library:NIST20M1.lib
SI:86 Formula:C16H30O CAS:822-21-9 MolWeight:238 RetIndex:1872
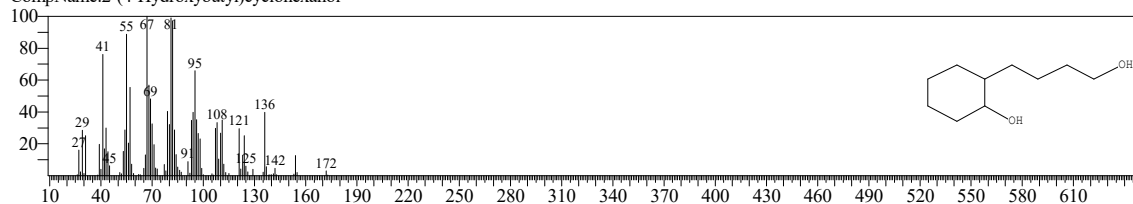CompName:7-Hexadecyn-1-ol

Hit#:4 Entry:31321 Library:NIST20M1.lib
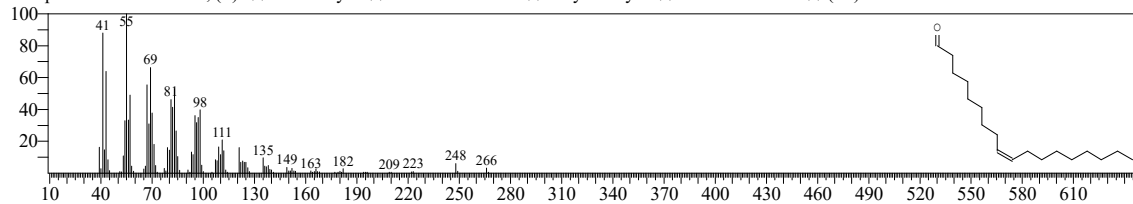SI:85 Formula:C10H20O2 CAS:0-00-0 MolWeight:172 RetIndex:1510
CompName:2-(4-Hydroxybutyl)cyclohexanol

Hit#:5 Entry:123421 Library:NIST20M1.lib
SI:85 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal #
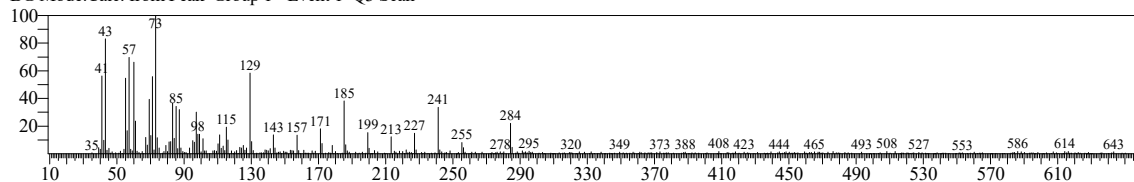
TNAU

<< Target >>
Line#:12 R.Time:32.030(Scan#:5407) MassPeaks:380
RawMode:Averaged 32.025-32.035(5406-5408) BasePeak:73.05(2009)
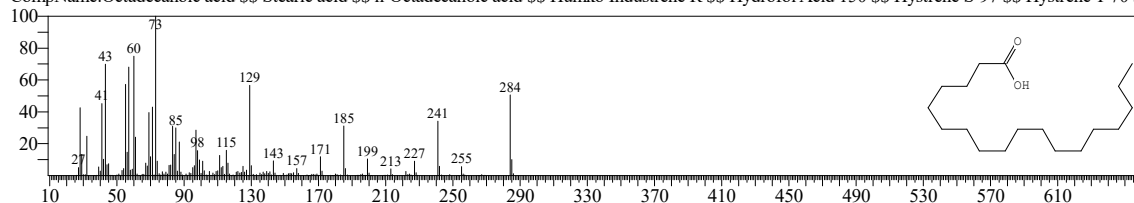BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34463 Library:NIST20R.lib
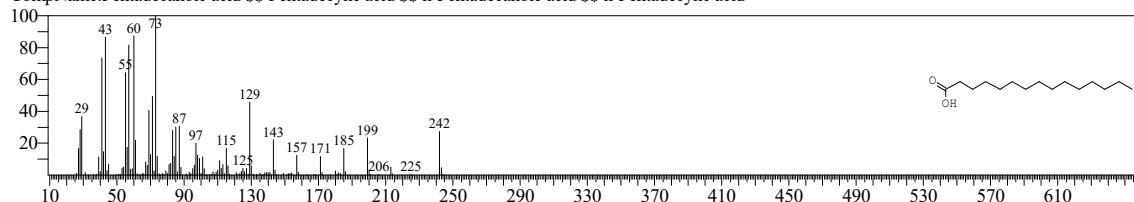SI:92 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $

Hit#:2 Entry:29890 Library:NIST20R.lib
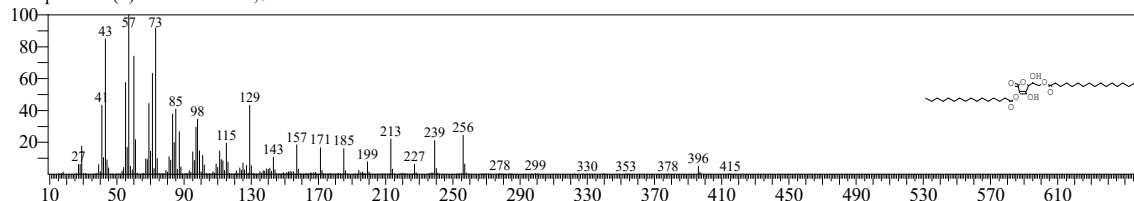SI:88 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:88 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
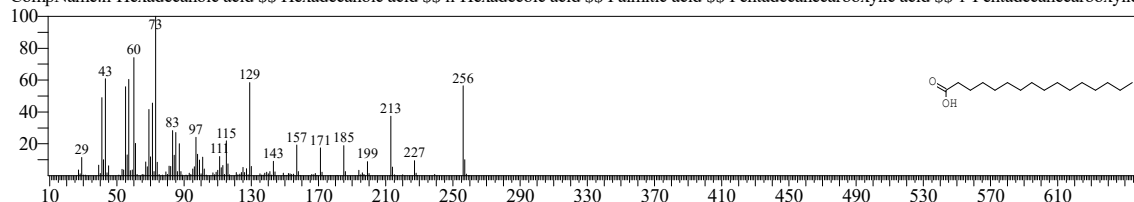CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

Hit#:4 Entry:31600 Library:NIST20R.lib
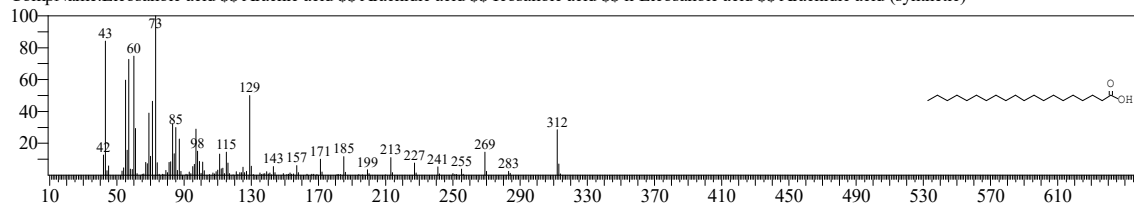SI:87 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

Hit#:5 Entry:178153 Library:NIST20M1.lib
SI:87 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)
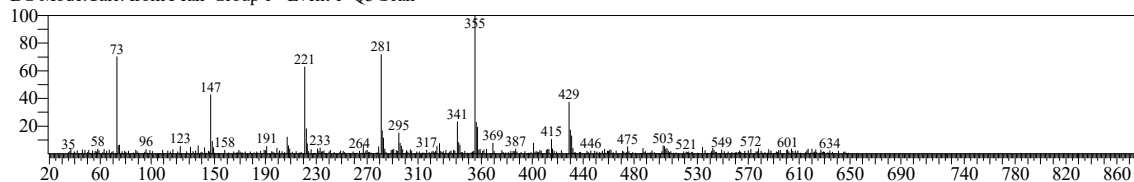
TNAU

<< Target >>
Line#:13 R.Time:39.070(Scan#:6815) MassPeaks:380
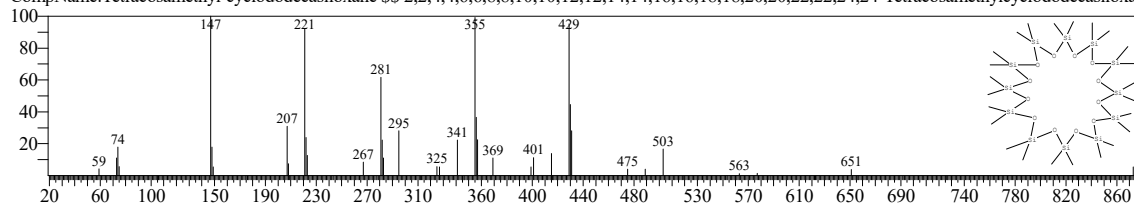RawMode:Averaged 39.065-39.075(6814-6816) BasePeak:355.00(1069)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
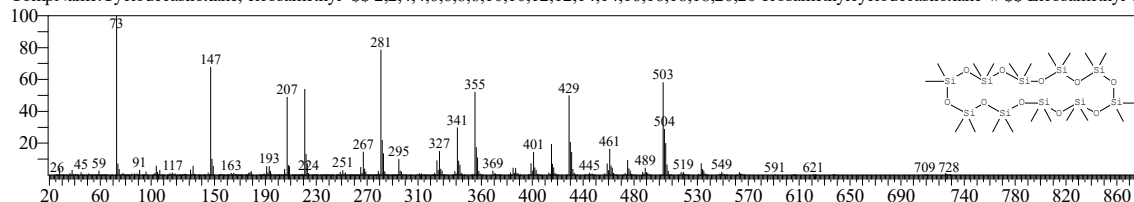SI:81 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
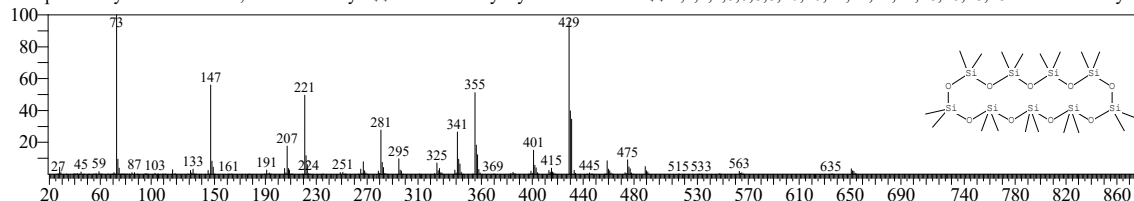SI:78 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
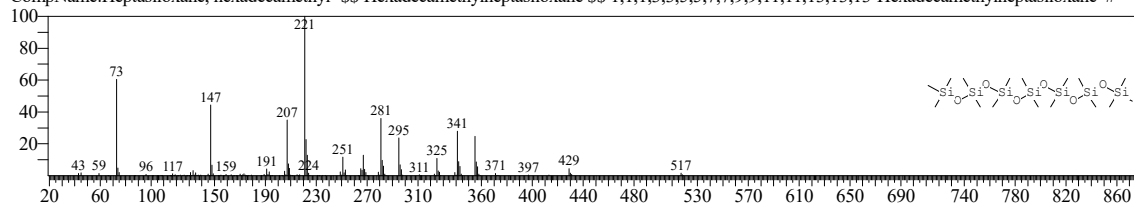SI:78 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:43312 Library:NIST20R.lib
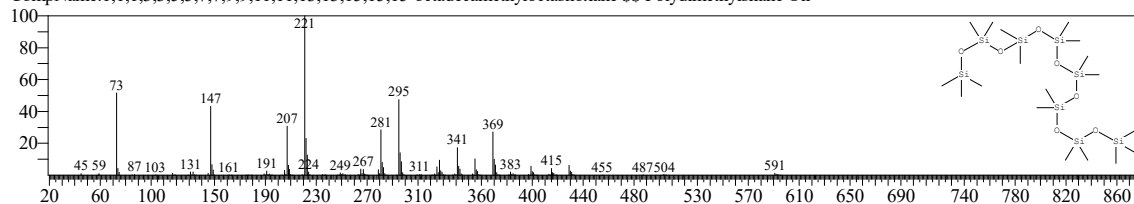SI:75 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

Hit#:5 Entry:42942 Library:NIST20M2.lib
SI:75 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil
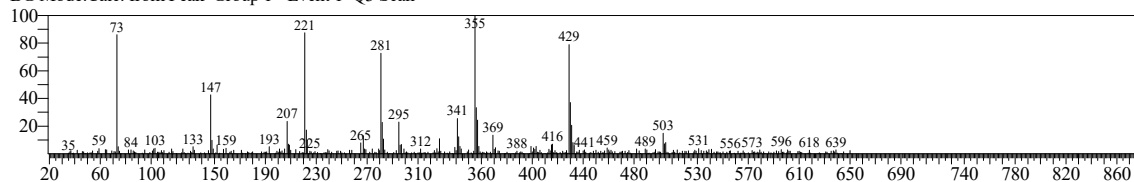
TNAU

<< Target >>
Line#:14 R.Time:41.600(Scan#:7321) MassPeaks:362
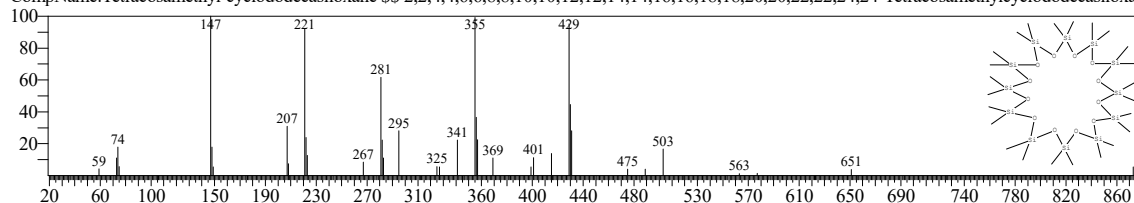RawMode:Averaged 41.595-41.605(7320-7322) BasePeak:355.05(1151)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
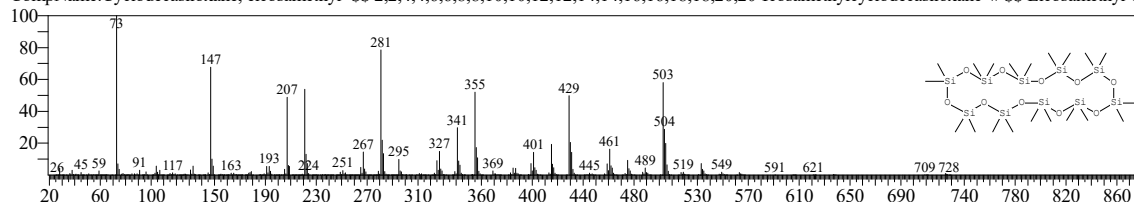SI:83 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
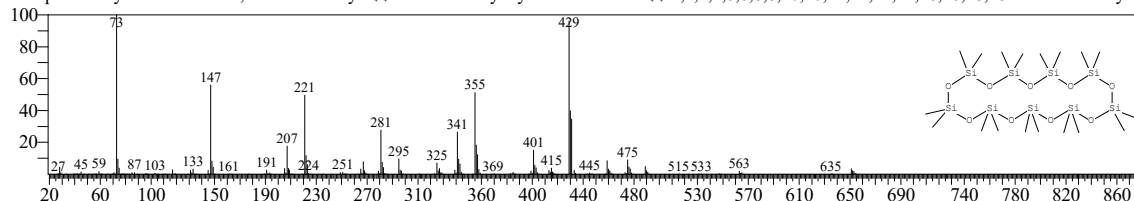SI:81 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
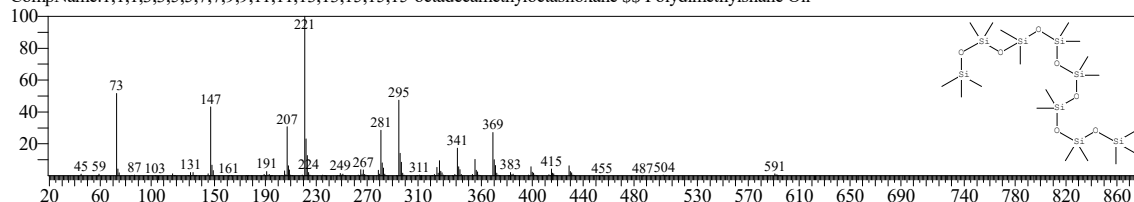SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:74 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
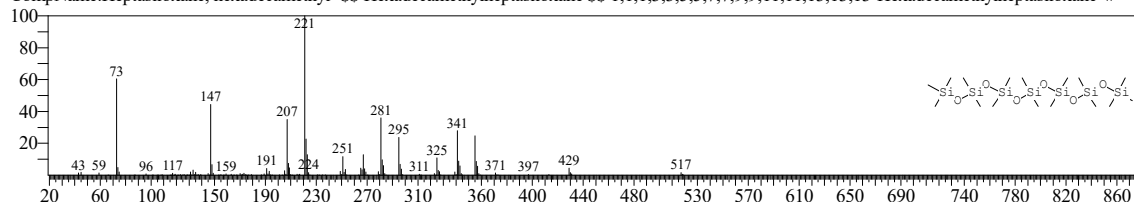CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:74 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
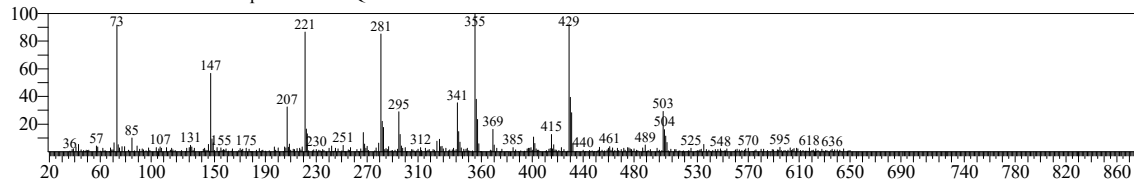
TNAU

<< Target >>
Line#:15 R.Time:43.800(Scan#:7761) MassPeaks:382
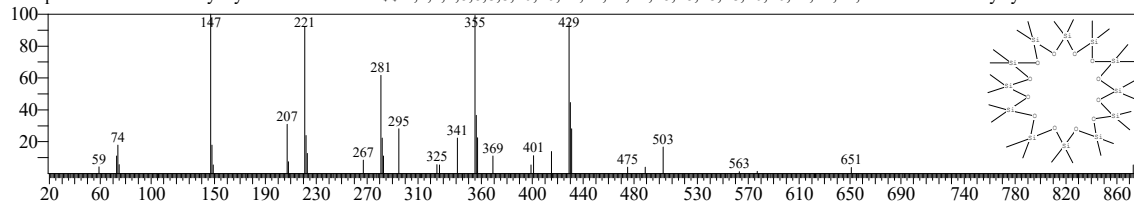RawMode:Averaged 43.795-43.805(7760-7762) BasePeak:355.00(1189)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
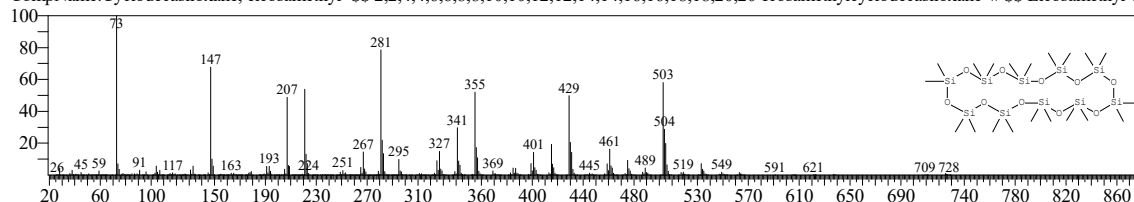SI:84 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
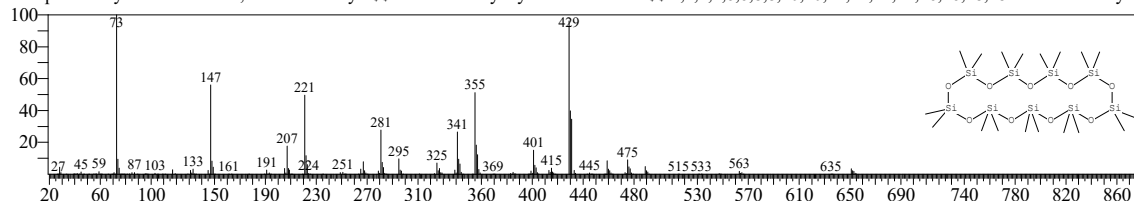SI:82 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
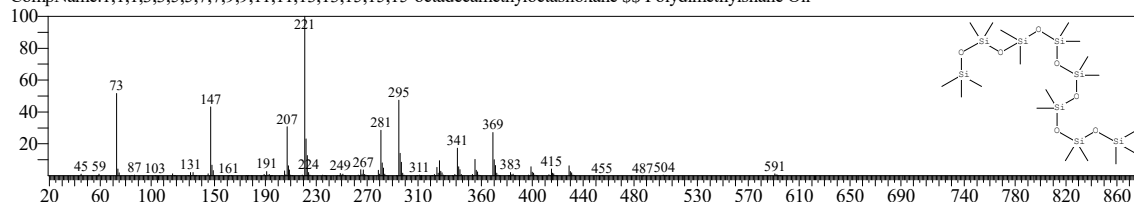SI:79 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:71 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
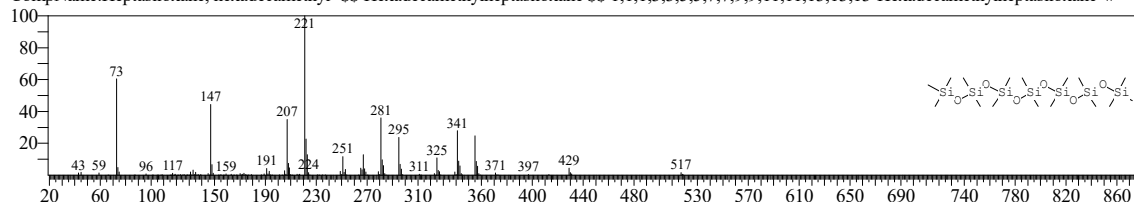CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:71 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
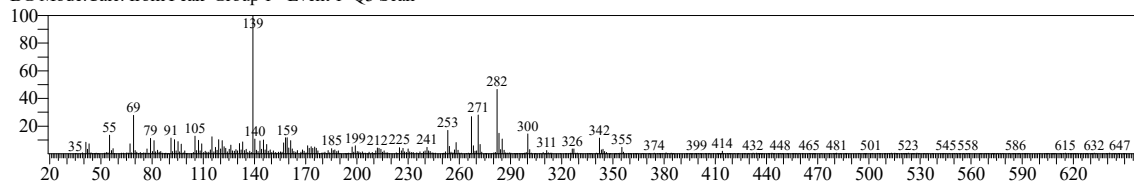
TNAU

Hit#:1 Entry:8297 Library:NIST20M2.lib
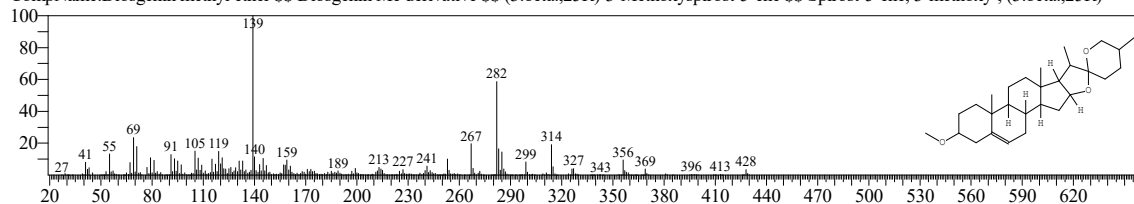SI:91 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

Hit#:2 Entry:14852 Library:NIST20M2.lib
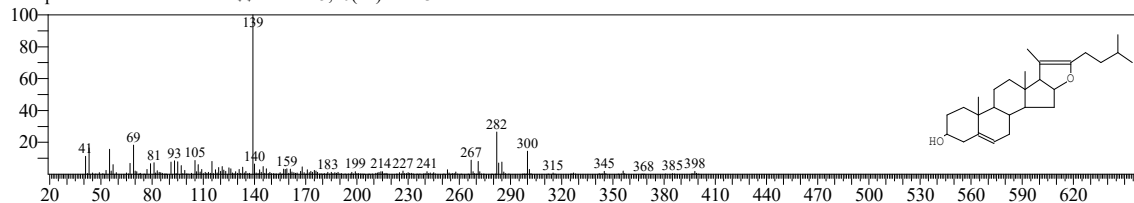SI:81 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:3 Entry:41561 Library:NIST20R.lib
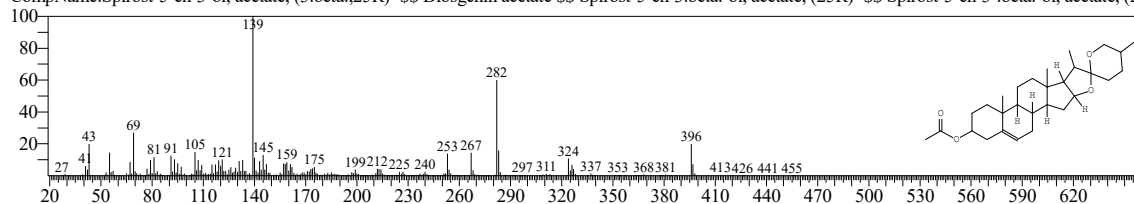SI:81 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #

Hit#:4 Entry:24878 Library:NIST20M2.lib
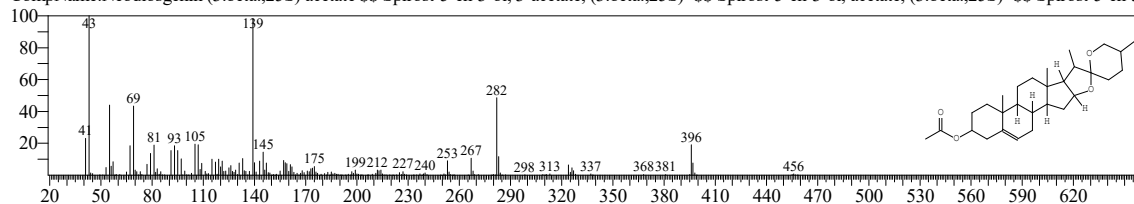SI:79 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (25

Hit#:5 Entry:42677 Library:NIST20R.lib
SI:75 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.
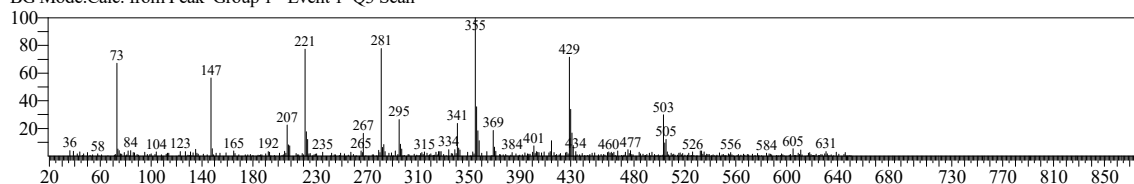
TNAU

<< Target >>
Line#:17 R.Time:45.775(Scan#:8156) MassPeaks:364
RawMode:Averaged 45.770-45.780(8155-8157) BasePeak:355.05(1107)
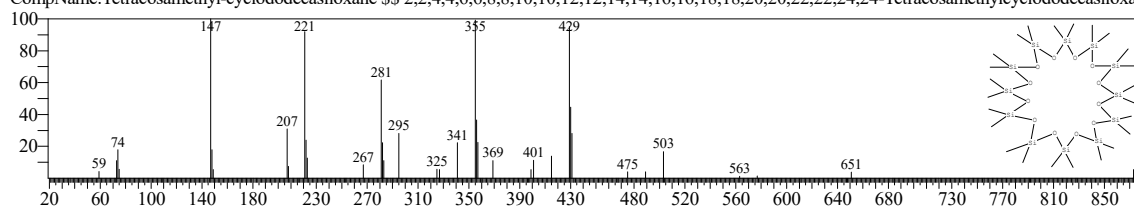BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
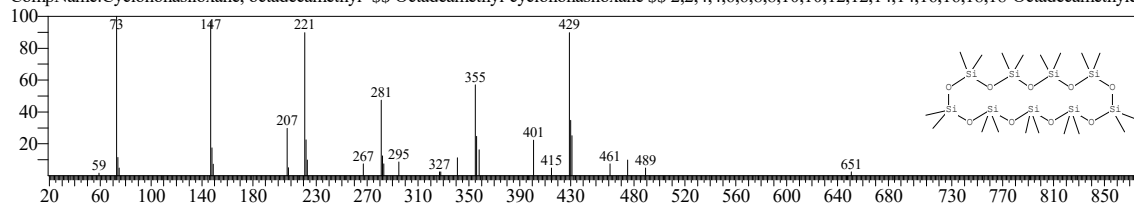SI:82 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:43658 Library:NIST20R.lib
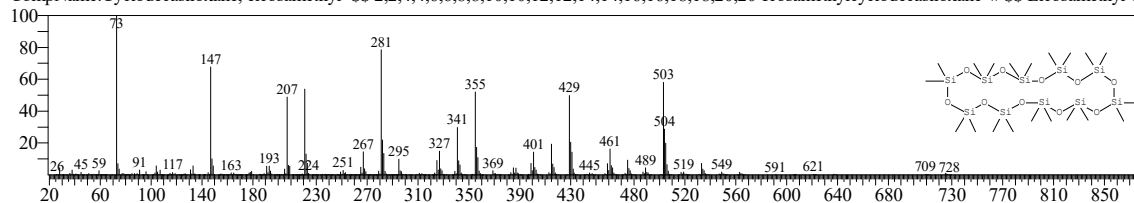SI:78 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:77 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
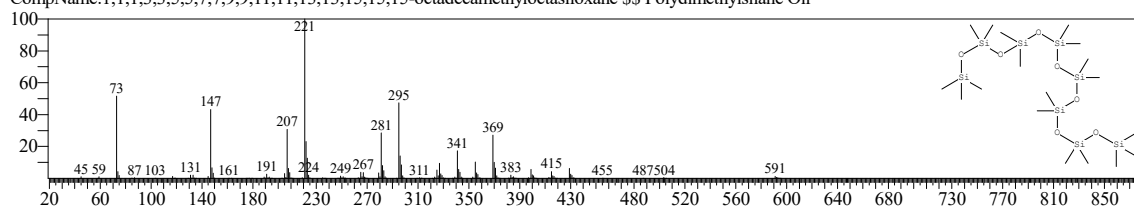CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:72 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:45794 Library:NIST20M2.lib
SI:72 Formula:C22H66O9Si10 CAS:556-70-7 MolWeight:754 RetIndex:1991
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,17,17,19,19,19-docosamethyldecasiloxane $$ Polydimethylsilane Oil