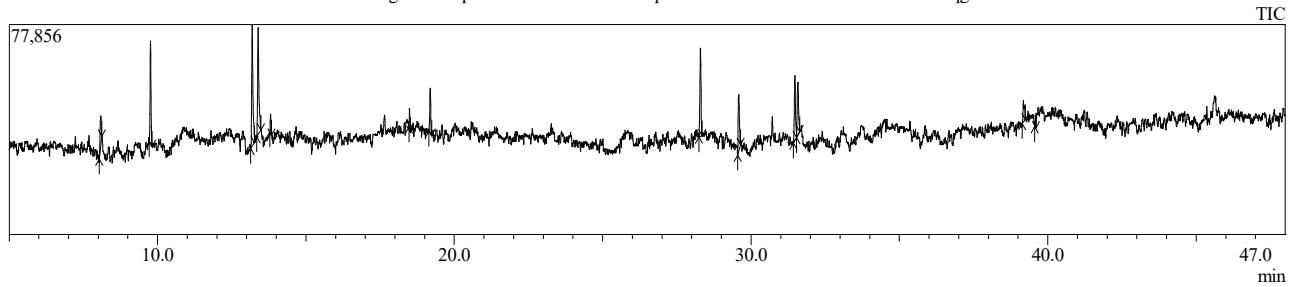


## Sample Information

Analyzed by : Admin  
 Analyzed : 01-Sep-22 10:51:00 PM  
 Sample Type : Unknown  
 Level # : 1  
 Sample Name : Sample  
 Sample ID : 2-3  
 IS Amount : [1]=1  
 Sample Amount : 1  
 Dilution Factor : 1  
 Vial # : 3  
 Injection Volume : 2.00  
 Data File : D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022007.qgd  
 Org Data File : D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022007.qgd  
 Method File : D:\GCMS-8040NX\Sep 2022\Method\Scan\_methodfile.qgm  
 Org Method File : D:\GCMS-8040NX\Sep 2022\Method\Scan\_methodfile.qgm  
 Report File :  
 Tuning File : D:\GCMS-8040NX\Aug 2022\Tuning Data\TUNING 25082022.qgt  
 Modified by : Admin  
 Modified : 05-Sep-22 10:57:45 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022007.qgd



Peak Report TIC

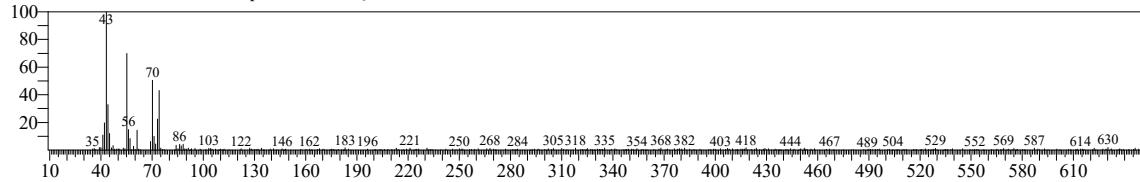
Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.087	32572	4.47	11001	4.01	2.96	83	1-Butanol, 3-methyl-, acetate
2	9.763	81477	11.18	38195	13.91	2.13	96	Pentasiloxane, dodecamethyl-
3	13.189	132850	18.23	45064	16.41	2.95	54	Methyl cis-13,16-Docosadienate
4	13.389	119788	16.44	39725	14.46	3.02	53	Methyl cis-13,16-Docosadienate
5	13.808	13239	1.82	7128	2.60	1.86	81	Trisiloxane, octamethyl-
6	18.491	11890	1.63	7682	2.80	1.55	77	2,4-Di-tert-butylphenol
7	19.189	38304	5.26	16718	6.09	2.29	92	2,4-Di-tert-butylphenoxytrimethylsilane
8	28.293	81099	11.13	32760	11.93	2.48	95	n-Hexadecanoic acid
9	29.587	59874	8.21	20644	7.52	2.90	87	Scyllo-Inositol, 6TMS
10	31.480	66824	9.17	23897	8.70	2.80	94	10E,12Z-Octadecadienoic acid
11	31.582	62701	8.60	19465	7.09	3.22	87	cis,cis,cis-7,10,13-Hexadecatrienal
12	39.177	23922	3.28	8006	2.91	2.99	59	Palmitic acid-TMS
13	39.579	4314	0.59	4394	1.60	0.98	14	Octadecanol-TMS
		728854	100.00	274679	100.00			

Library

# TNAU

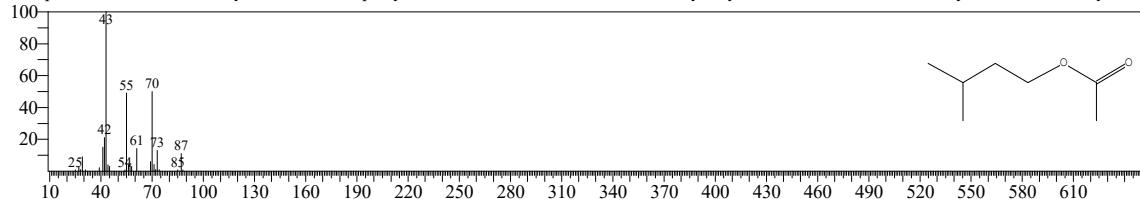
<<Target>>

Line#:1 R.Time:8.085(Scan#:618) MassPeaks:314  
 RawMode:Averaged 8.080-8.090(617-619) BasePeak:43.05(2407)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:6783 Library:NIST20R.lib

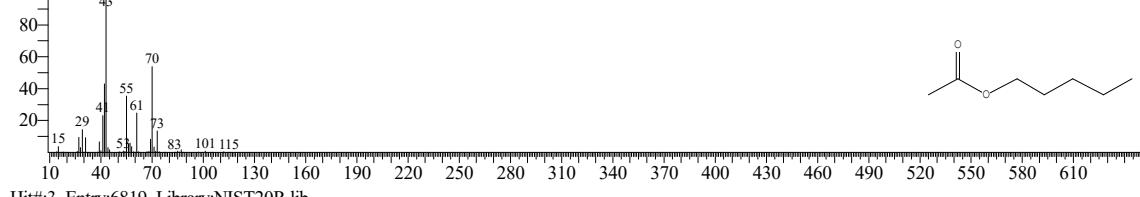
SI:83 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820  
 CompName:1-Butanol, 3-methyl-, acetate \$\$ Isopentyl alcohol, acetate \$\$ Acetic acid, 3-methylbutyl ester \$\$ Banana oil \$\$ Isoamyl acetate \$\$ Isoamyl etha



Hit#:2 Entry:8685 Library:NIST20M1.lib

SI:81 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884

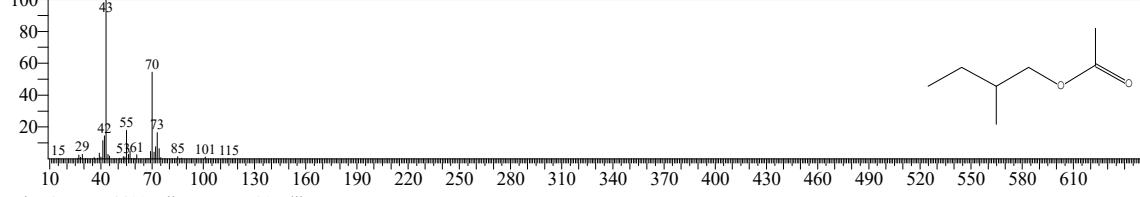
CompName:Acetic acid, pentyl ester \$\$ n-Amyl acetate \$\$ n-Pentyl acetate \$\$ Amyl acetate \$\$ Birnenoel \$\$ Pentyl acetate \$\$ Acetic acid, amyl ester \$\$ Ar



Hit#:3 Entry:6819 Library:NIST20R.lib

SI:80 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820

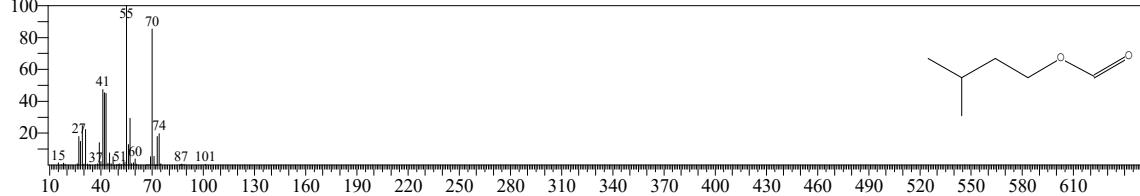
CompName:1-Butanol, 2-methyl-, acetate \$\$ 2-Methyl-1-butyl acetate \$\$ 2-Methylbutyl acetate \$\$ Acetic acid 2-methylbutyl ester \$\$ 2-Methybutyl acetate !



Hit#:4 Entry:4411 Library:NIST20R.lib

SI:78 Formula:C6H12O2 CAS:110-45-2 MolWeight:116 RetIndex:818

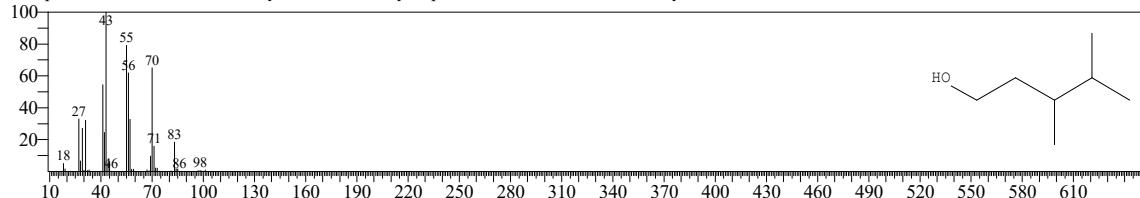
CompName:1-Butanol, 3-methyl-, formate \$\$ Isopentyl alcohol, formate \$\$ Isoamyl formate \$\$ Isoamyl methanoate \$\$ Isopentyl formate \$\$ 3-Methylbutyl



Hit#:5 Entry:5029 Library:NIST20M1.lib

SI:78 Formula:C7H16O CAS:6570-87-2 MolWeight:116 RetIndex:832

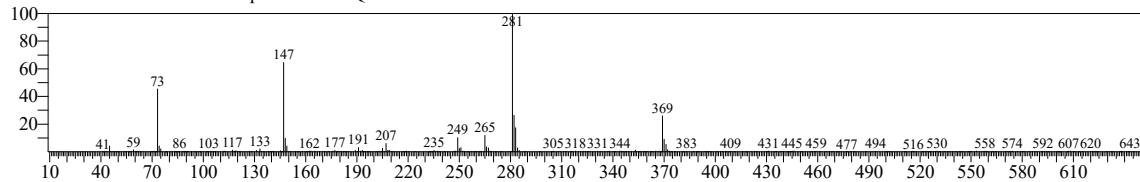
CompName:1-Pentanol, 3,4-dimethyl- \$\$ 3,4-Dimethyl-1-pentanol \$\$ Pentanol, 3,4-dimethyl



# TNAU

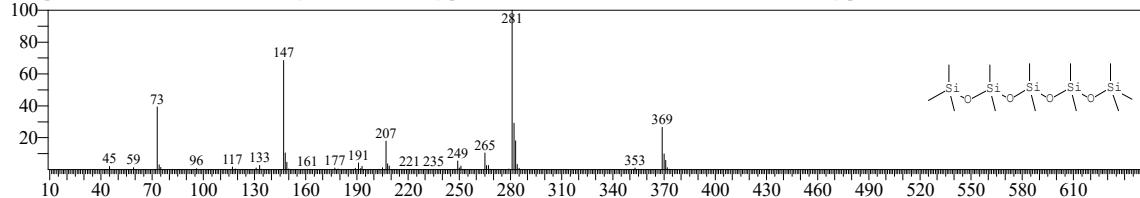
<<Target >>

Line#2 R.Time:9.765(Scan#:954) MassPeaks:326  
 RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(9358)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



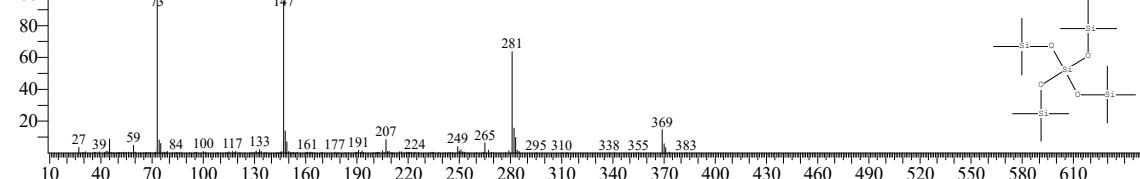
Hit#1 Entry:40975 Library:NIST20R.lib

SI:96 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068  
 CompName:Pentasiloxane, dodecamethyl- \$\$ Dodecamethylpentasiloxane #



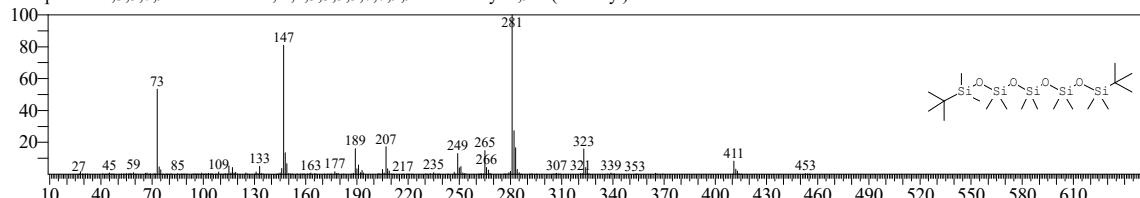
Hit#2 Entry:249272 Library:NIST20M1.lib

SI:84 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068  
 CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsiloxy)oxy] \$\$ Tetrakis(trimethylsiloxy)silane \$\$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



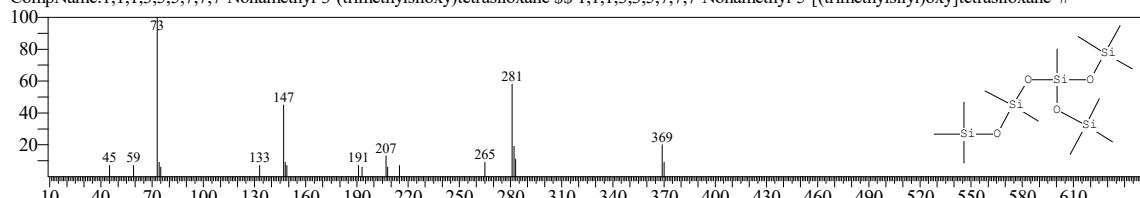
Hit#3 Entry:27848 Library:NIST20M2.lib

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



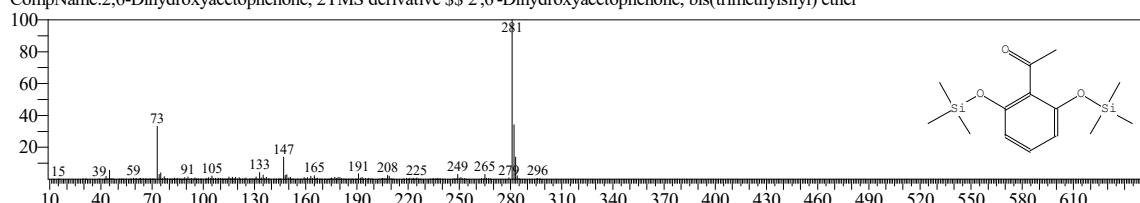
Hit#4 Entry:249271 Library:NIST20M1.lib

SI:80 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068  
 CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane \$\$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



Hit#5 Entry:158097 Library:NIST20M1.lib

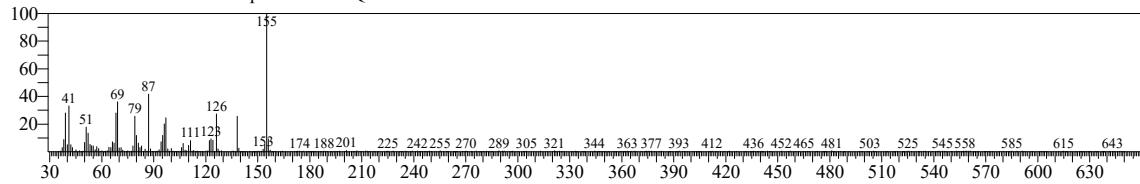
SI:77 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625  
 CompName:2,6-Dihydroxyacetophenone, 2TMS derivative \$\$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



# TNAU

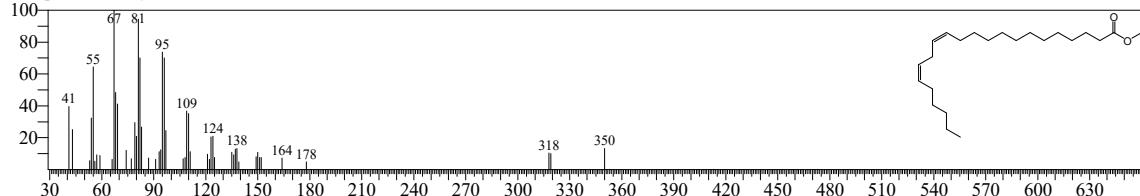
<<Target >>

Line#3 R.Time:13.190(Scan#:1639) MassPeaks:385  
 RawMode:Averaged 13.185-13.195(1638-1640) BasePeak:155.05(6596)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



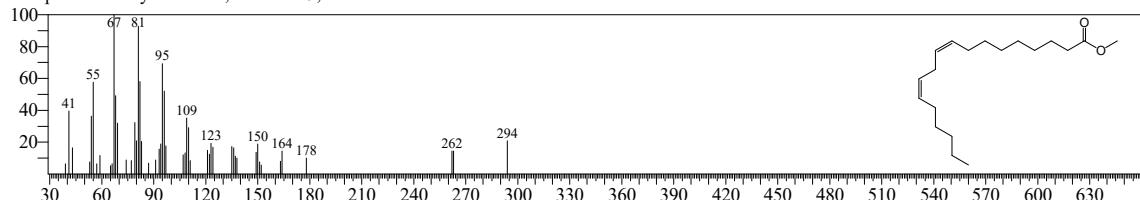
Hit#1 Entry:34 Library:FA\_ME\_SP2560 EI\_V3.lib

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



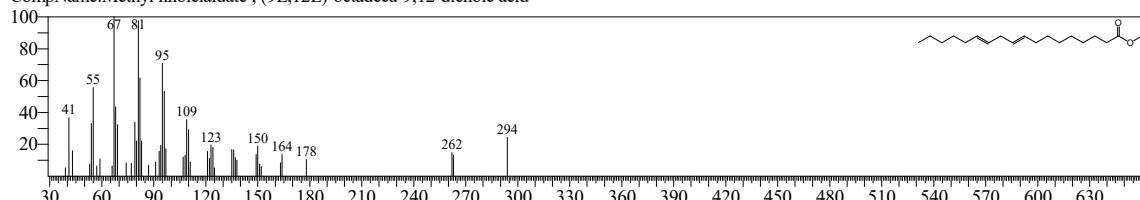
Hit#2 Entry:21 Library:FA\_ME\_SP2560 EI\_V3.lib

SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775  
 CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



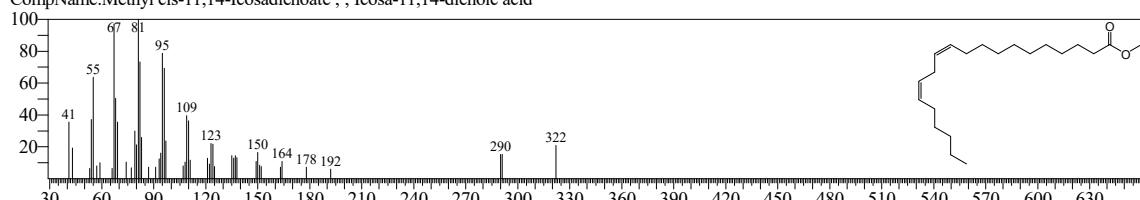
Hit#3 Entry:20 Library:FA\_ME\_SP2560 EI\_V3.lib

SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727  
 CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



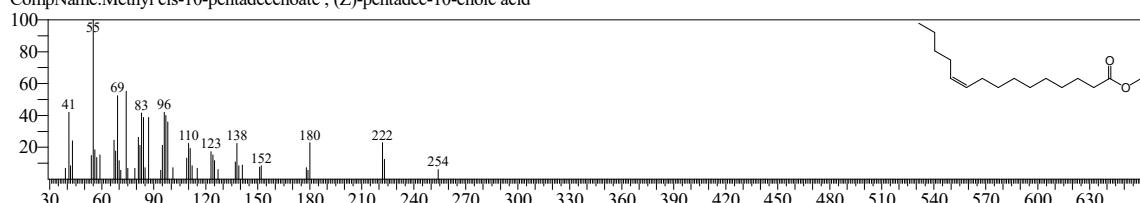
Hit#4 Entry:27 Library:FA\_ME\_SP2560 EI\_V3.lib

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

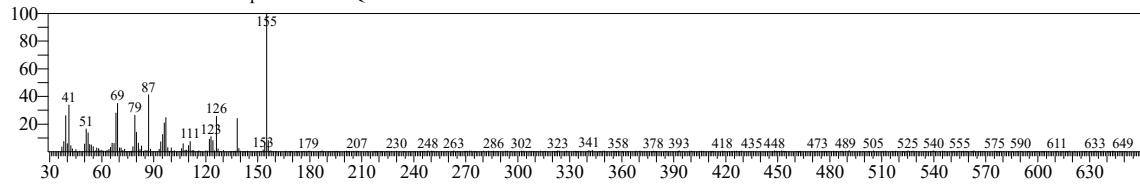
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388  
 CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid



# TNAU

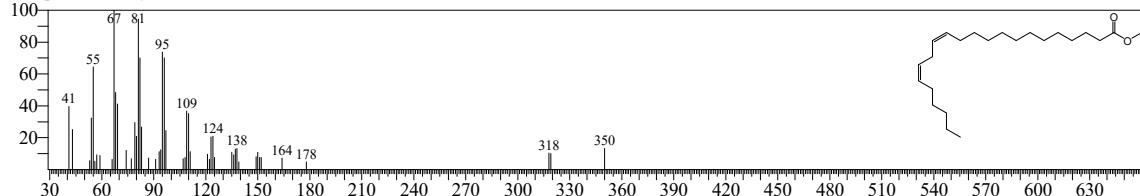
<<Target >>

Line#4 R.Time:13.390(Scan#:1679) MassPeaks:347  
 RawMode:Averaged 13.385-13.395(1678-1680) BasePeak:155.10(5941)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



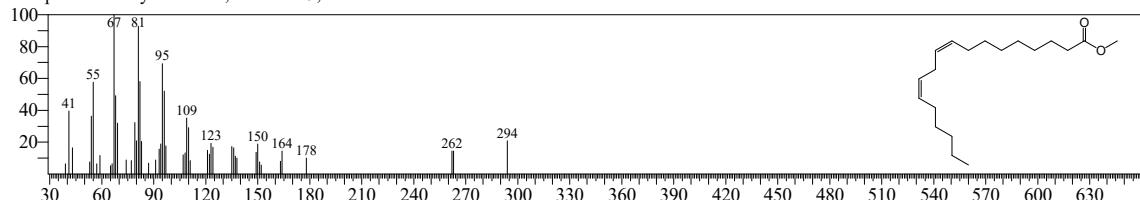
Hit#1 Entry:34 Library:FA\_ME\_SP2560 EI\_V3.lib

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



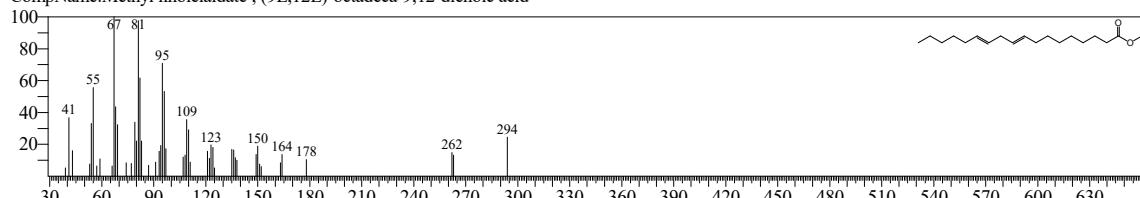
Hit#2 Entry:21 Library:FA\_ME\_SP2560 EI\_V3.lib

SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775  
 CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



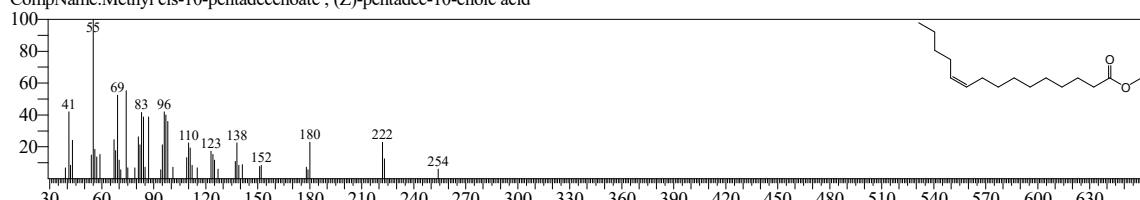
Hit#3 Entry:20 Library:FA\_ME\_SP2560 EI\_V3.lib

SI:51 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727  
 CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



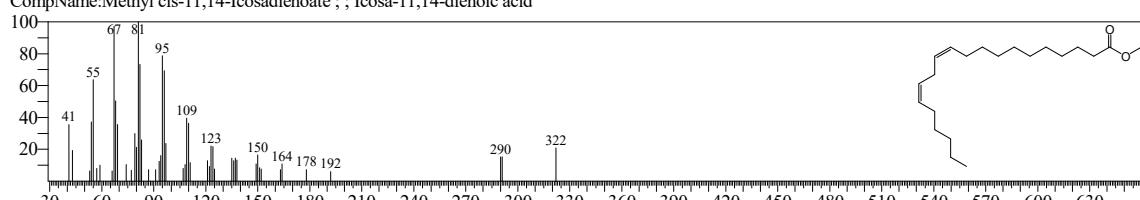
Hit#4 Entry:11 Library:FA\_ME\_SP2560 EI\_V3.lib

SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388  
 CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enonic 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



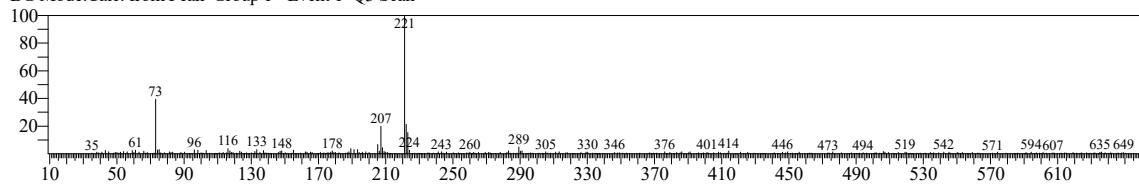
# TNAU

<<Target>>

Line#5 R.Time:13.810(Scan#:1763) MassPeaks:340

RawMode:Averaged 13.805-13.815(1762-1764) BasePeak:221.10(2228)

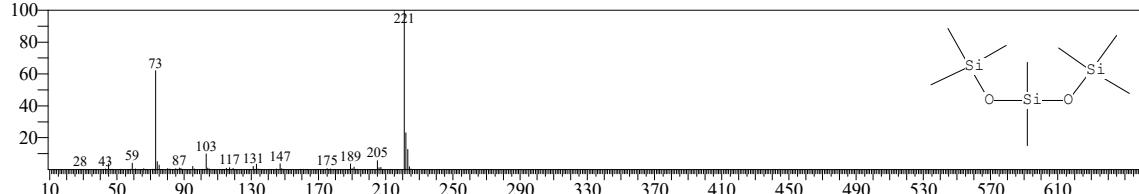
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:28950 Library:NIST20R.lib

SI:81 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698

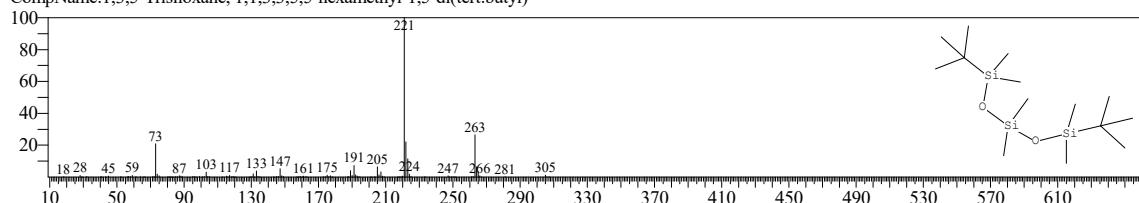
CompName:Trisiloxane, octamethyl- \$\$ Octamethyltrisiloxane \$\$ Silane, dimethylbis(trimethylsiloxy)- \$\$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane \$\$ [(CH<sub>3</sub>)<sub>3</sub>SiO)<sub>2</sub>Si(CH<sub>3</sub>)<sub>2</sub>]<sub>2</sub>



Hit#2 Entry:186590 Library:NIST20M1.lib

SI:75 Formula:C14H36O2Si3 CAS:0-0-0 MolWeight:320 RetIndex:1126

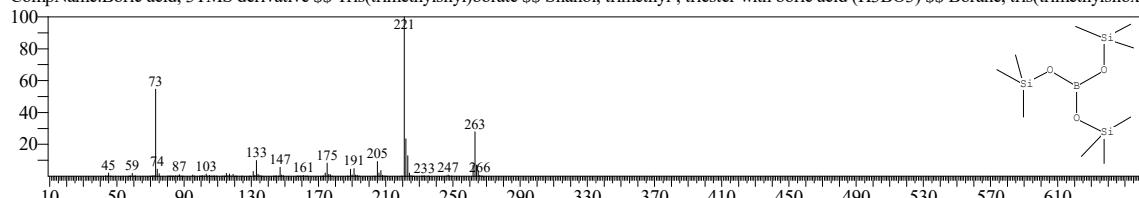
CompName:1,3,5-Trisiloxane, 1,1,3,3,5,5-hexamethyl-1,5-di(tert.butyl)-



Hit#3 Entry:33791 Library:NIST20R.lib

SI:74 Formula:C9H27BO3Si3 CAS:4325-85-3 MolWeight:278 RetIndex:0

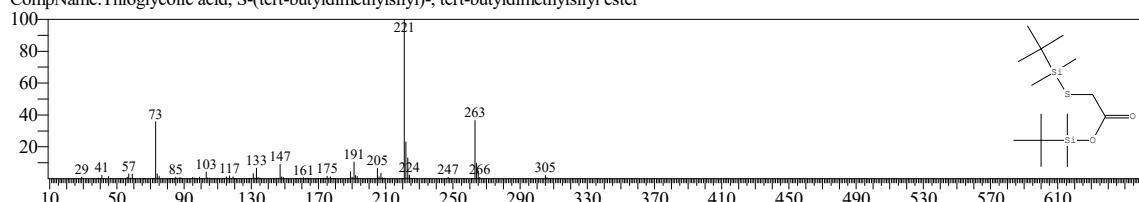
CompName:Boric acid, 3TMS derivative \$\$ Tris(trimethylsilyl)borate \$\$ Silanol, trimethyl-, triester with boric acid (H<sub>3</sub>BO<sub>3</sub>) \$\$ Borane, tris(trimethylsiloxy



Hit#4 Entry:186586 Library:NIST20M1.lib

SI:74 Formula:C14H32O2Si2 CAS:82112-29-6 MolWeight:320 RetIndex:1482

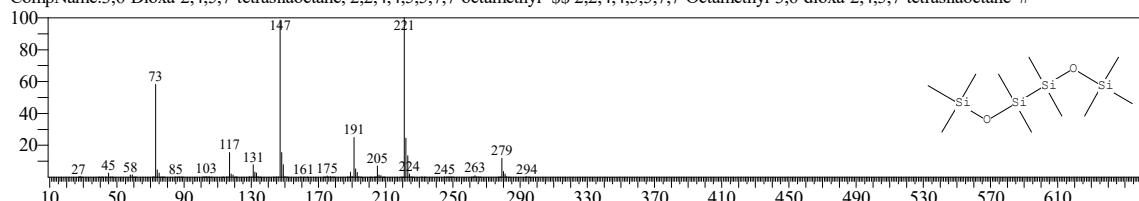
CompName:Thioglycolic acid, S-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester



Hit#5 Entry:155460 Library:NIST20M1.lib

SI:72 Formula:C10H30O2Si4 CAS:4342-25-0 MolWeight:294 RetIndex:807

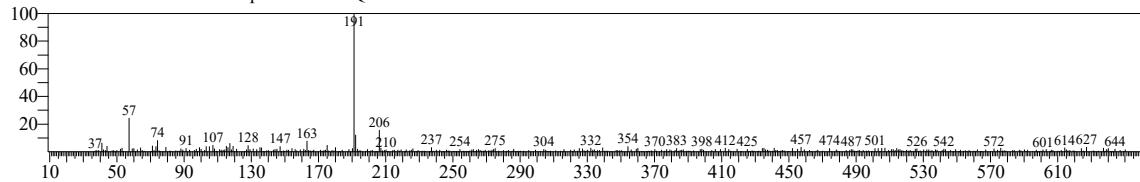
CompName:3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl- \$\$ 2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane #



# TNAU

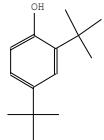
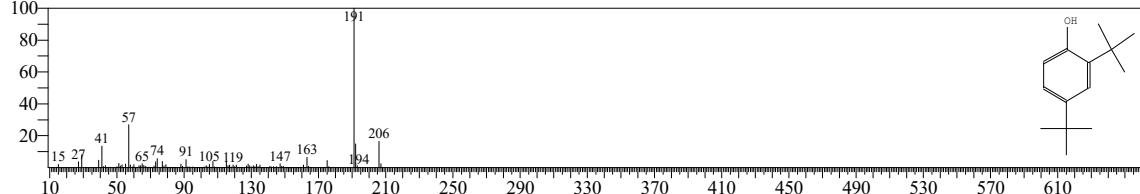
<<Target >>

Line#6 R.Time:18.490(Scan#:2699) MassPeaks:404  
 RawMode:Averaged 18.485-18.495(2698-2700) BasePeak:191.15(1585)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



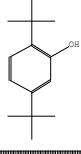
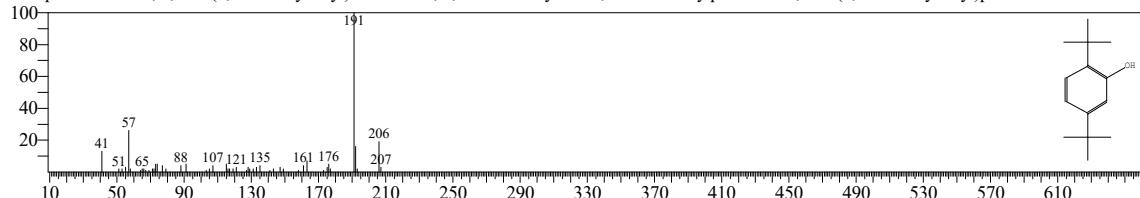
Hit#1 Entry:24086 Library:NIST20R.lib

SI:77 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555  
 CompName:2,4-Di-tert-butylphenol \$\$ Phenol, 2,4-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,4-di-tert-butyl- \$\$ 2,4-di-t-Butylphenol \$\$ 1-Hydroxy-2,4-di-tert-bu



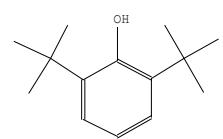
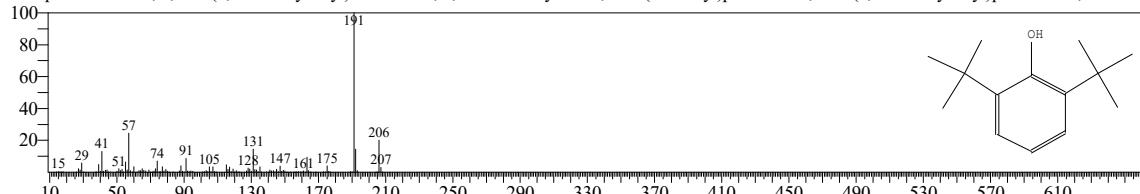
Hit#2 Entry:24098 Library:NIST20R.lib

SI:75 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555  
 CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,5-di-tert-butyl- \$\$ 2,5-Di-tert-butylphenol \$\$ 2,5-bis(1,1-Dimethylethyl)phenol



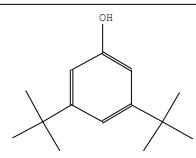
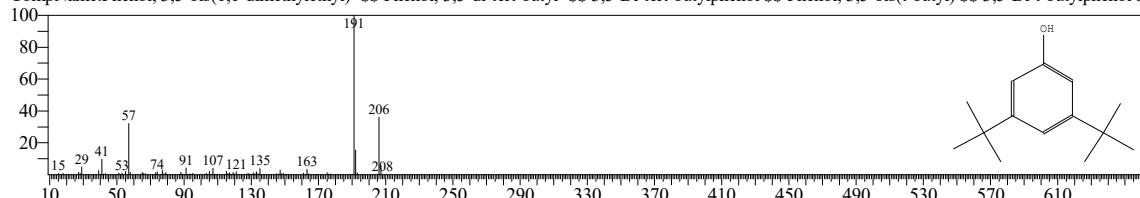
Hit#3 Entry:59031 Library:NIST20M1.lib

SI:74 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555  
 CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,6-di-tert-butyl- \$\$ 2,6-Bis(tert-butyl)phenol \$\$ 2,6-Bis(1,1-dimethylethyl)phenol \$\$ 2,6-Di-tert



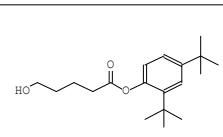
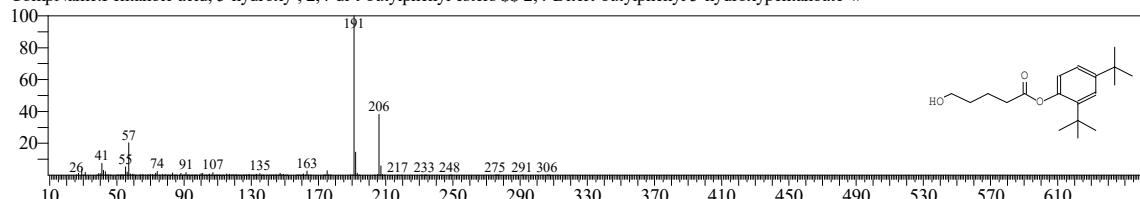
Hit#4 Entry:24110 Library:NIST20R.lib

SI:74 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555  
 CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- \$\$ Phenol, 3,5-di-tert-butyl- \$\$ 3,5-Di-tert-butylphenol \$\$ Phenol, 3,5-bis(t-butyl) \$\$ 3,5-Di-t-butylphenol \$



Hit#5 Entry:170993 Library:NIST20M1.lib

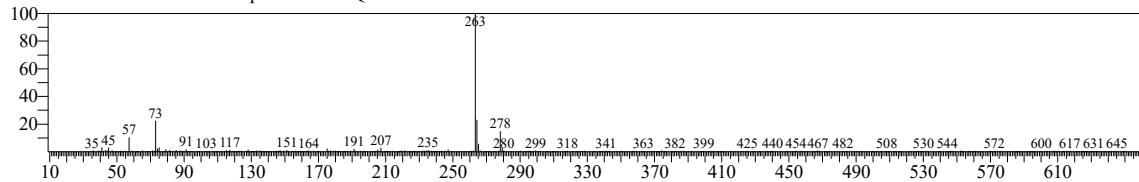
SI:73 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255  
 CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters \$\$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #



# TNAU

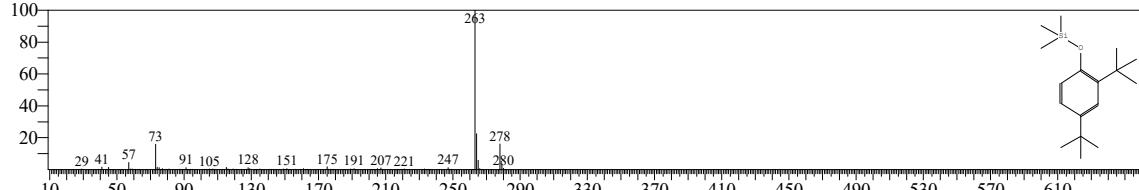
<<Target >>

Line#:7 R.Time:19.190(Scan#:2839) MassPeaks:341  
 RawMode:Averaged 19.185-19.195(2838-2840) BasePeak:263.20(7056)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



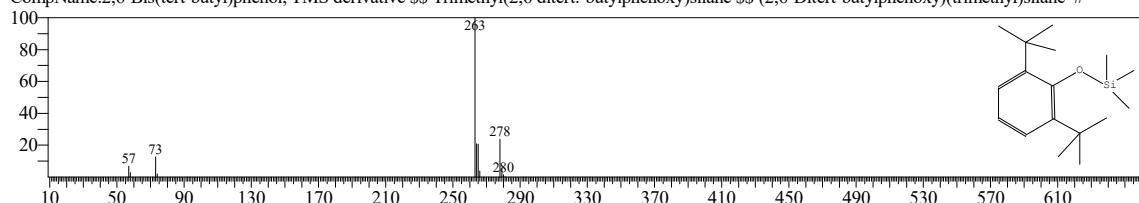
Hit#:1 Entry:33874 Library:NIST20R.lib

SI:92 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)phenoxy]trimethylsilane



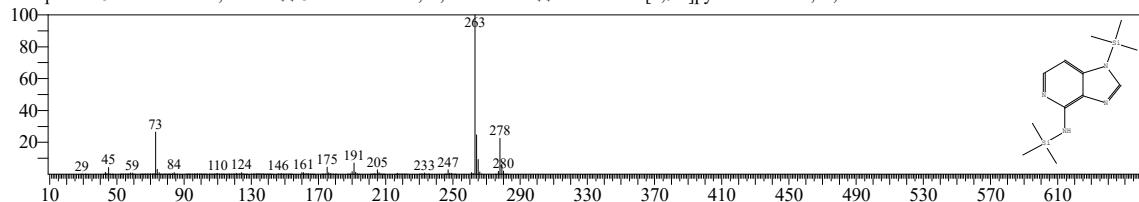
Hit#:2 Entry:33871 Library:NIST20R.lib

SI:84 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 #



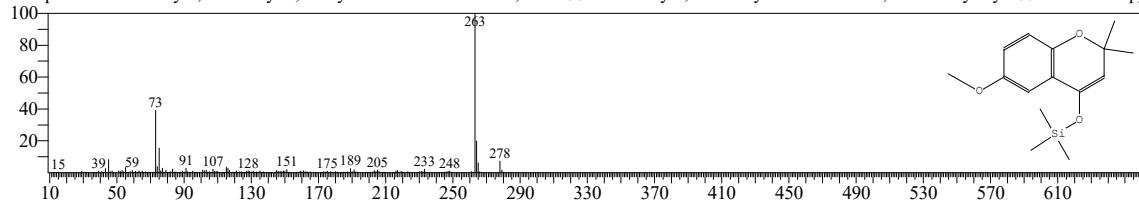
Hit#:3 Entry:136557 Library:NIST20M1.lib

SI:83 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703  
 CompName:3-Deazaadenine, 2TMS \$\$ 3-Deazaadenine, N,N'-bis-TMS \$\$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



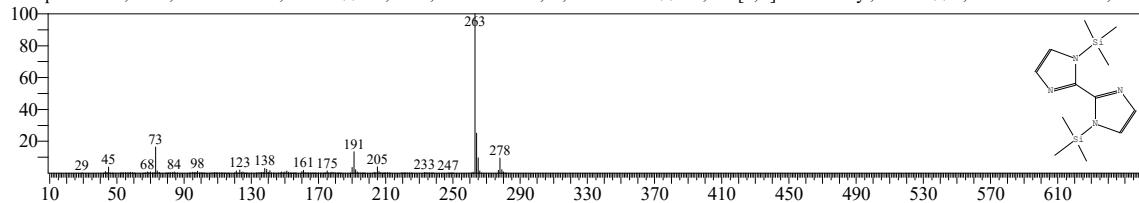
Hit#:4 Entry:137020 Library:NIST20M1.lib

SI:79 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736  
 CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS \$\$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- \$\$ 4H-1-Benzopy



Hit#:5 Entry:136556 Library:NIST20M1.lib

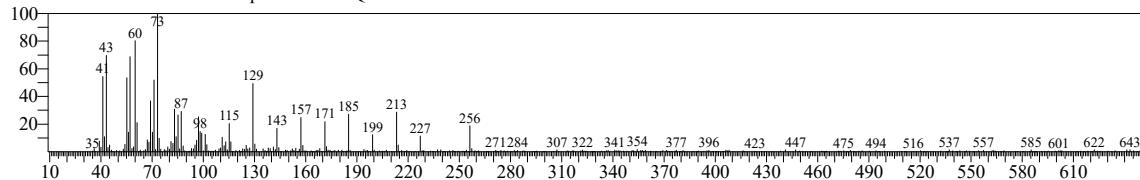
SI:79 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606  
 CompName:1H,1'H-2,2'-Biimidazole, 2TMS \$\$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS \$\$ 1H,1'H-[2,2']Biimidazolyl, 2TMS \$\$ 2,2'-Bi-1H-imidazole, 2T



# TNAU

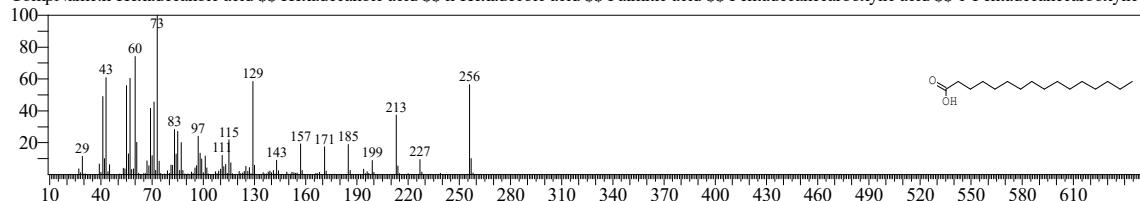
<<Target >>

Line#8 R.Time:28.295(Scan#:4660) MassPeaks:342  
 RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.05(2693)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



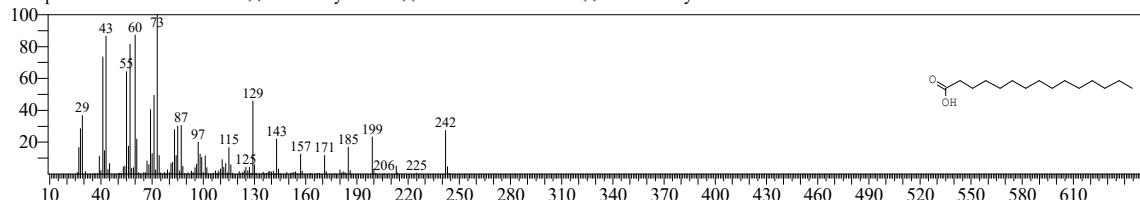
Hit#1 Entry:31600 Library:NIST20R.lib

SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968  
 CompName:n-Hexadecanoic acid \$\$ Hexadecanoic acid \$\$ n-Hexadecenoic acid \$\$ Palmitic acid \$\$ Pentadecanecarboxylic acid \$\$ 1-Pentadecanecarboxylic



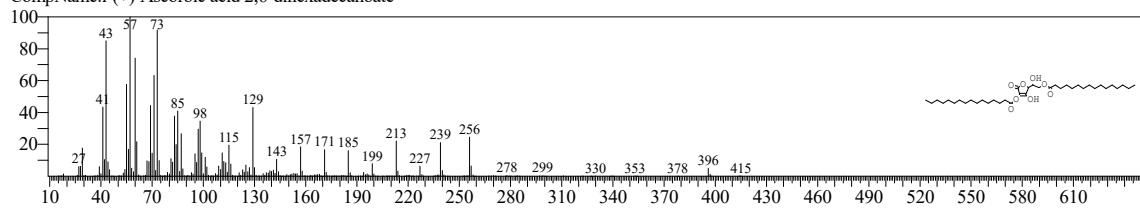
Hit#2 Entry:29890 Library:NIST20R.lib

SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869  
 CompName:Pentadecanoic acid \$\$ Pentadecyclic acid \$\$ n-Pentadecanoic acid \$\$ n-Pentadecylic acid



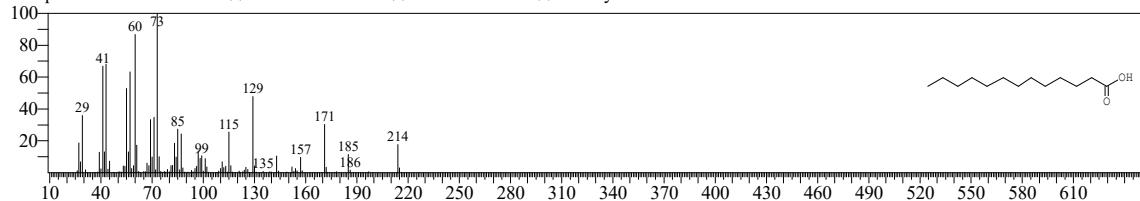
Hit#3 Entry:44286 Library:NIST20M2.lib

SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765  
 CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



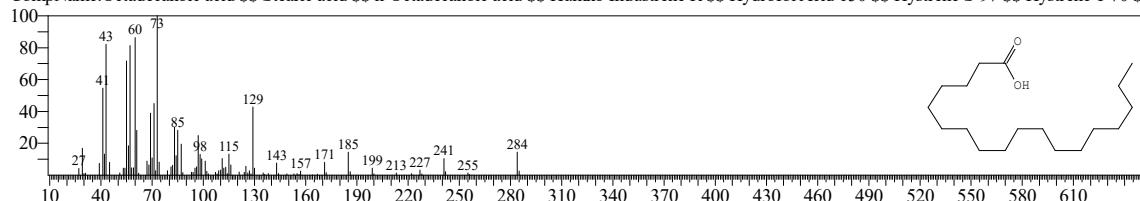
Hit#4 Entry:25643 Library:NIST20R.lib

SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670  
 CompName:Tridecanoic acid \$\$ n-Tridecanoic acid \$\$ n-Tridecoic acid \$\$ Tridecyclic acid



Hit#5 Entry:144781 Library:NIST20M1.lib

SI:90 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 \$\$



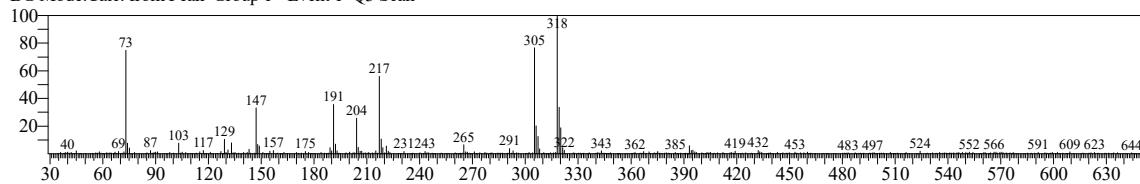
# TNAU

<<Target >>

Line#9 R.Time:29.585(Scan#:4918) MassPeaks:388

RawMode:Averaged 29.580-29.590(4917-4919) BasePeak:318.15(2809)

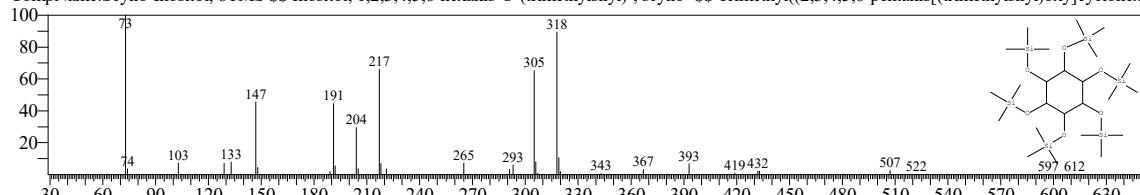
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:43144 Library:NIST20M2.lib

SI:87 Formula:C24H60O6Si6 CAS:14251-18-4 MolWeight:612 RetIndex:2194

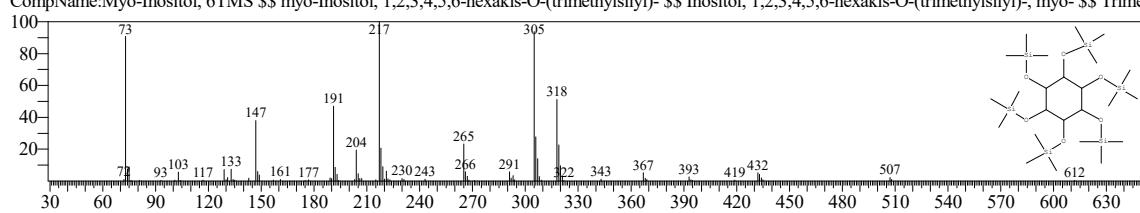
CompName:Scyllo-Inositol, 6TMS \$\$ Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, scyllo- \$\$ Trimethyl((2,3,4,5,6-pentakis[(trimethylsilyl)oxy]cyclohex-



Hit#2 Entry:43552 Library:NIST20R.lib

SI:87 Formula:C24H60O6Si6 CAS:2582-79-8 MolWeight:612 RetIndex:2194

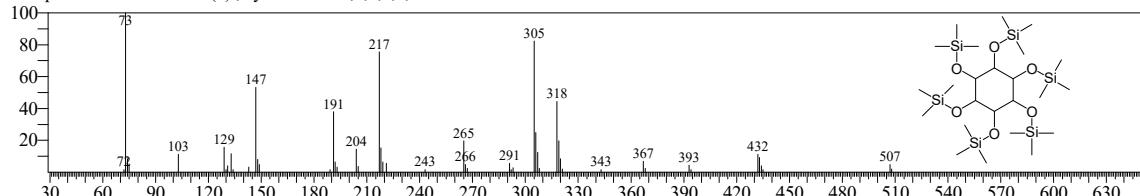
CompName:Myo-Inositol, 6TMS \$\$ myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)- \$\$ Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, myo- \$\$ Trime



Hit#3 Entry:465 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:86 Formula:C24H60O6Si6 CAS:87-89-8 MolWeight:612 RetIndex:2132

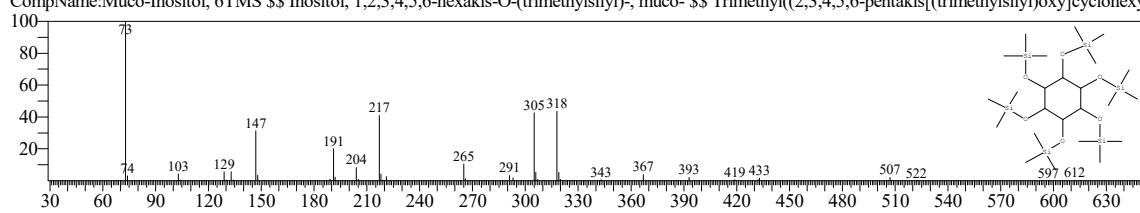
CompName:Inositol-6TMS(2) ; cyclohexane-1,2,3,4,5,6-hexol



Hit#4 Entry:43145 Library:NIST20M2.lib

SI:79 Formula:C24H60O6Si6 CAS:29412-26-8 MolWeight:612 RetIndex:2194

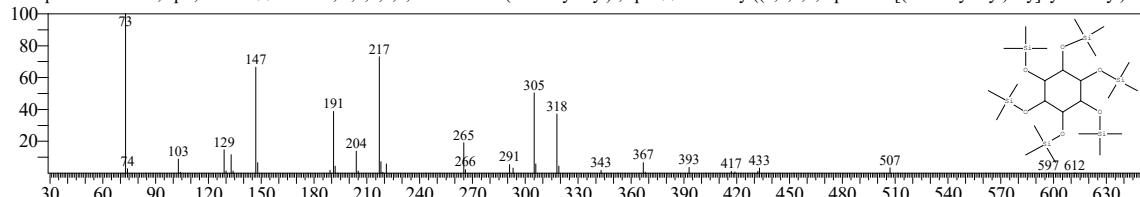
CompName:Muco-Inositol, 6TMS \$\$ Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, muco- \$\$ Trimethyl((2,3,4,5,6-pentakis[(trimethylsilyl)oxy]cyclohexy



Hit#5 Entry:43146 Library:NIST20M2.lib

SI:79 Formula:C24H60O6Si6 CAS:29267-01-4 MolWeight:612 RetIndex:2194

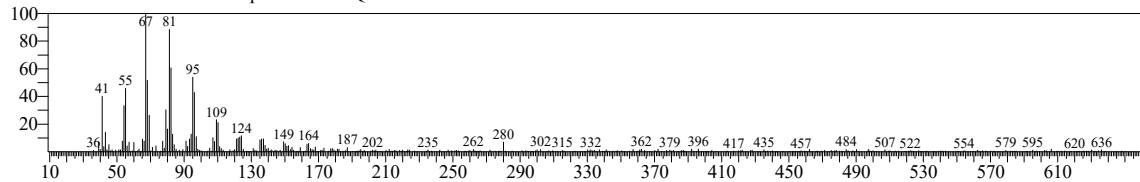
CompName:Inositol, epi-, 6TMS \$\$ Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-, epi- \$\$ Trimethyl((2,3,4,5,6-pentakis[(trimethylsilyl)oxy]cyclohexyl)ox



# TNAU

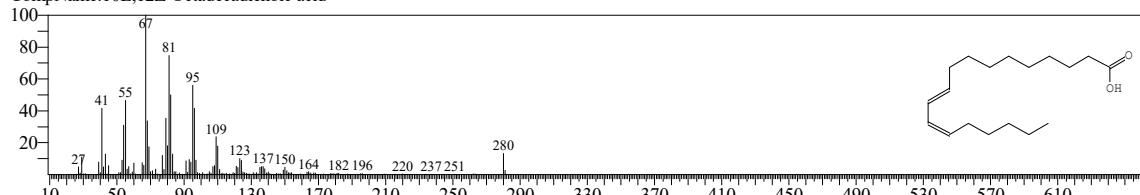
<<Target >>

Line#:10 R.Time:31.480(Scan#:5297) MassPeaks:359  
 RawMode:Averaged 31.475-31.485(5296-5298) BasePeak:67.10(2276)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



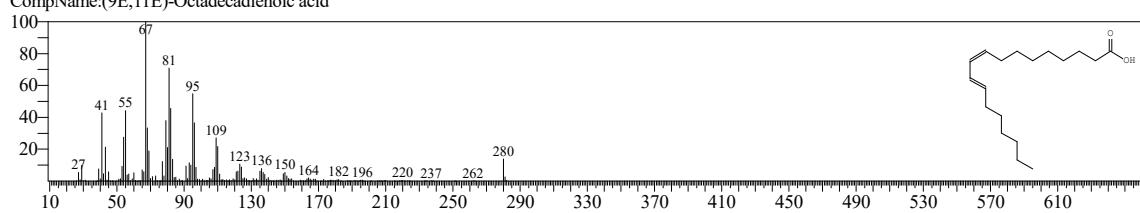
Hit#1 Entry:139646 Library:NIST20M1.lib

SI:94 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183  
 CompName:10E,12Z-Octadecadienoic acid



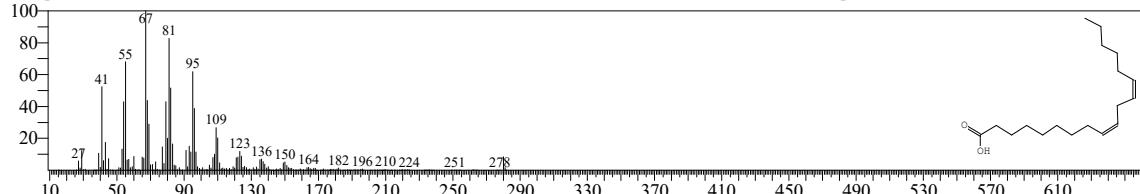
Hit#2 Entry:139651 Library:NIST20M1.lib

SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183  
 CompName:(9E,11E)-Octadecadienoic acid



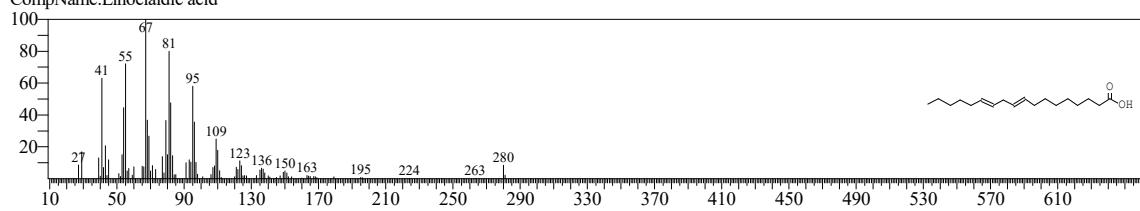
Hit#3 Entry:34035 Library:NIST20R.lib

SI:93 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 acid \$\$ Linoleic acid \$\$



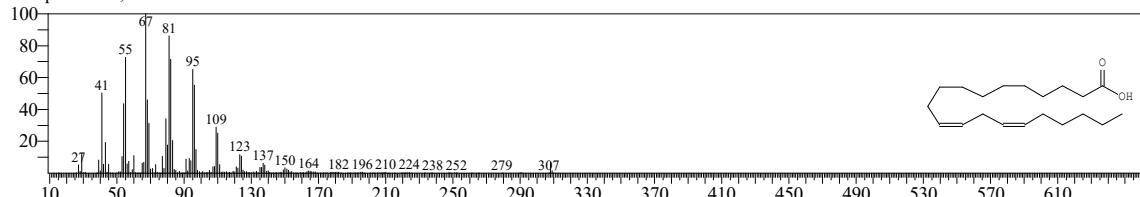
Hit#4 Entry:139661 Library:NIST20M1.lib

SI:92 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183  
 CompName:Linoelaidic acid



Hit#5 Entry:173215 Library:NIST20M1.lib

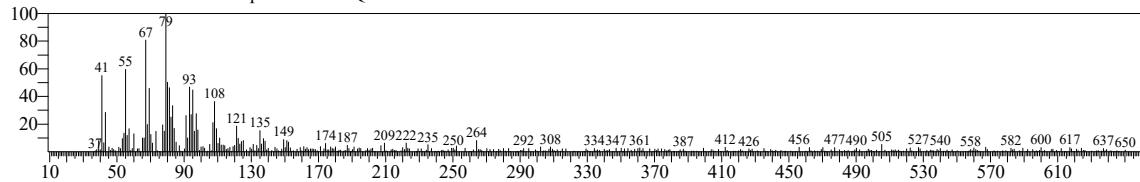
SI:92 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382  
 CompName:11,14-Eicosadienoic acid



# TNAU

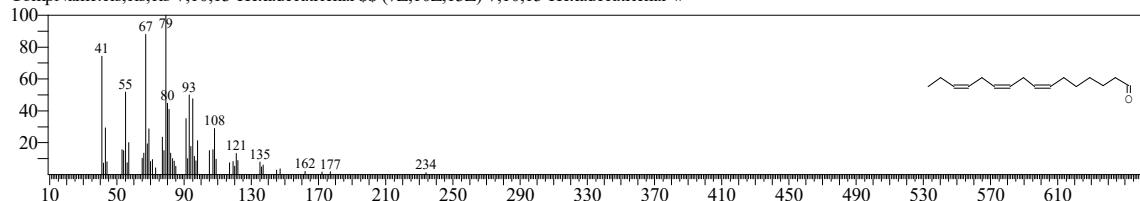
<<Target >>

Line#:11 R.Time:31.580(Scan#:5317) MassPeaks:406  
 RawMode:Averaged 31.575-31.585(5316-5318) BasePeak:79.10(1254)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:87848 Library:NIST20M1.lib

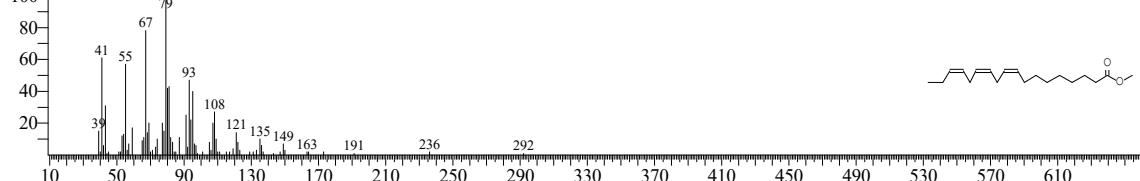
SI:87 Formula:C16H26O CAS:56797-43-4 MolWeight:234 RetIndex:1824  
 CompName:cis,cis,cis-7,10,13-Hexadecatrienal \$\$ (7Z,10Z,13Z)-7,10,13-Hexadecatrienal #



Hit#:2 Entry:35226 Library:NIST20R.lib

SI:85 Formula:C19H32O2 CAS:301-00-8 MolWeight:292 RetIndex:2101

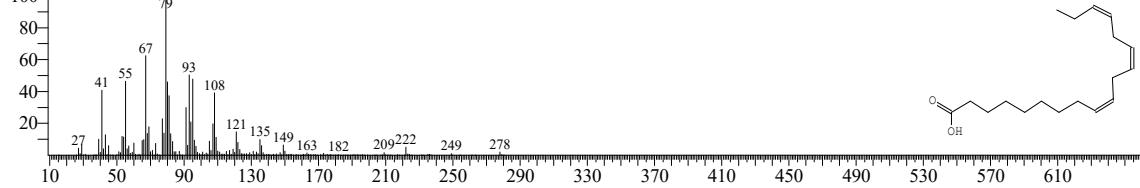
CompName:9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- \$\$ Linolenic acid, methyl ester \$\$ Methyl all-cis-9,12,15-octadecatrienoate \$\$ Methyl lino



Hit#:3 Entry:137464 Library:NIST20M1.lib

SI:85 Formula:C18H30O2 CAS:463-40-1 MolWeight:278 RetIndex:2191

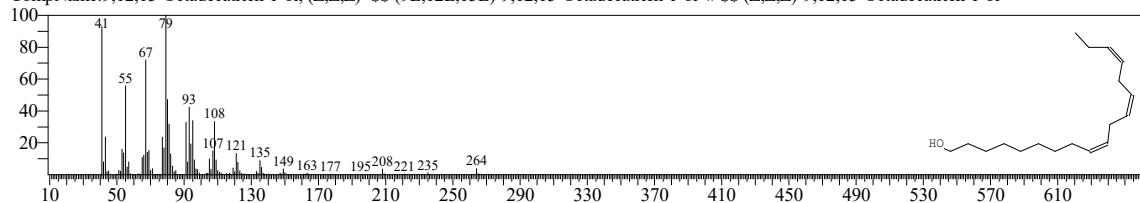
CompName:9,12,15-Octadecatrienoic acid, (Z,Z,Z)- \$\$ Linolenic acid \$\$ .alpha.-Linolenic acid \$\$ All-cis-9,12,15-Octadecatrienoic acid \$\$ cis,cis,cis-9,12,1



Hit#:4 Entry:32465 Library:NIST20R.lib

SI:84 Formula:C18H32O CAS:506-44-5 MolWeight:264 RetIndex:2077

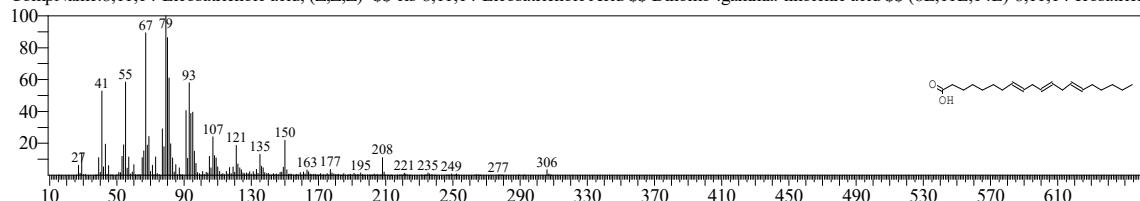
CompName:9,12,15-Octadecatrien-1-ol, (Z,Z,Z)- \$\$ (9E,12E,15E)-9,12,15-Octadecatrien-1-ol # \$\$ (Z,Z,Z)-9,12,15-Octadecatrien-1-ol



Hit#:5 Entry:171074 Library:NIST20M1.lib

SI:84 Formula:C20H34O2 CAS:1783-84-2 MolWeight:306 RetIndex:2390

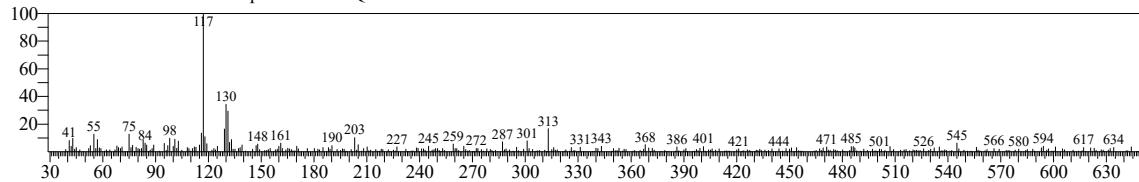
CompName:8,11,14-Eicosatrienoic acid, (Z,Z,Z)- \$\$ cis-8,11,14-Eicosatrienoic Acid \$\$ Dihomo-gamma.-linolenic acid \$\$ (8E,11E,14E)-8,11,14-Icosatrien



# TNAU

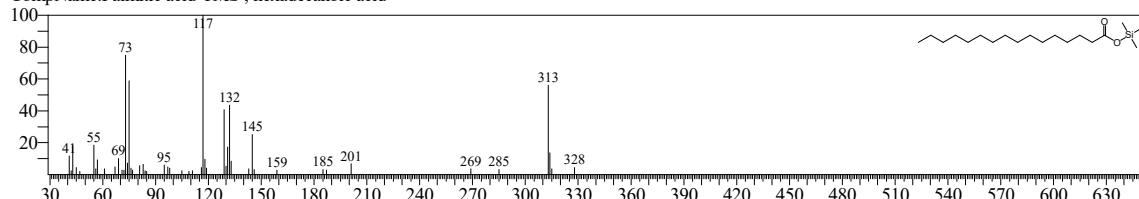
<<Target >>

Line#:12 R.Time:39.175(Scan#:6836) MassPeaks:376  
 RawMode:Averaged 39.170-39.180(6835-6837) BasePeak:117.05(1071)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



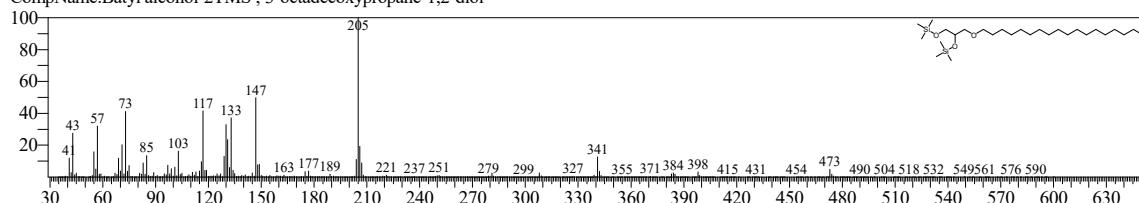
Hit#:1 Entry:446 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:59 Formula:C19H40O2Si CAS:57-10-3 MolWeight:328 RetIndex:2046  
 CompName:Palmitic acid-TMS ; hexadecanoic acid



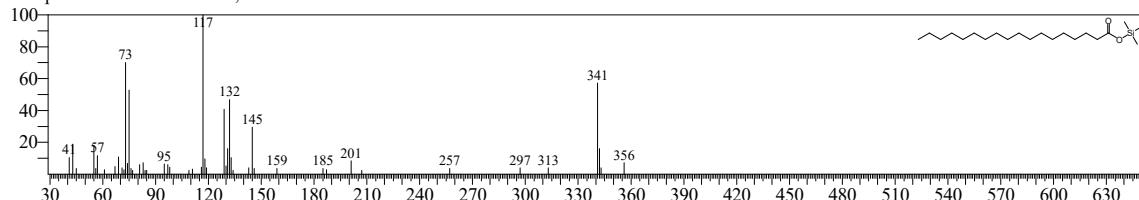
Hit#:2 Entry:539 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:57 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684  
 CompName:Butyl alcohol-2TMS ; 3-octadecoxyp propane-1,2-diol



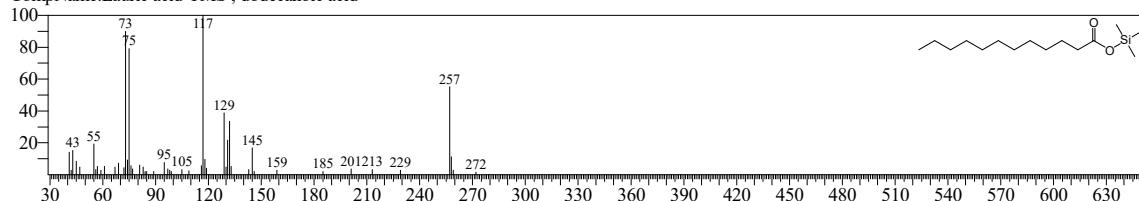
Hit#:3 Entry:491 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:55 Formula:C21H44O2Si CAS:57-11-4 MolWeight:356 RetIndex:2244  
 CompName:Stearic acid-TMS ; octadecanoic acid



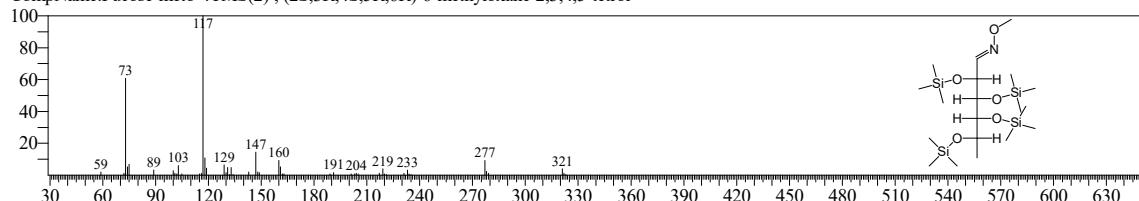
Hit#:4 Entry:223 Library:OA\_TMS\_DB5\_67min\_V3.lib

SI:54 Formula:C15H32O2Si CAS:143-07-7 MolWeight:272 RetIndex:1653  
 CompName:Lauric acid-TMS ; dodecanoic acid



Hit#:5 Entry:287 Library:OA\_TMS\_DB5\_67min\_V3.lib

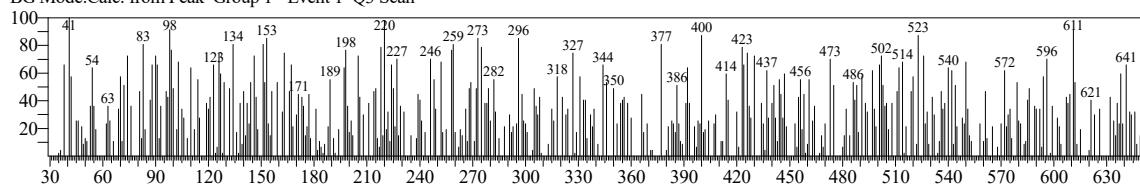
SI:54 Formula:C19H47NO5Si4 CAS:3615-37-0 MolWeight:481 RetIndex:1768  
 CompName:Fucose-meto-4TMS(2) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol



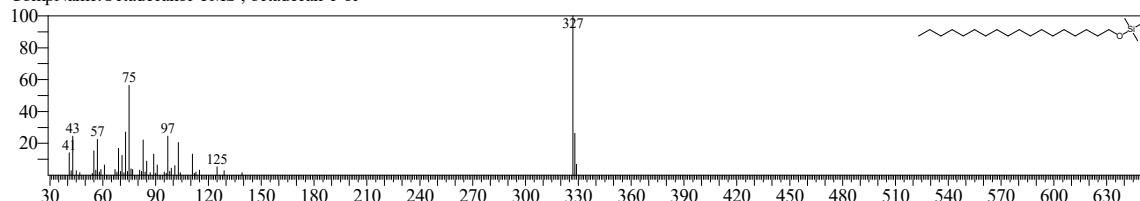
# TNAU

<<Target >>

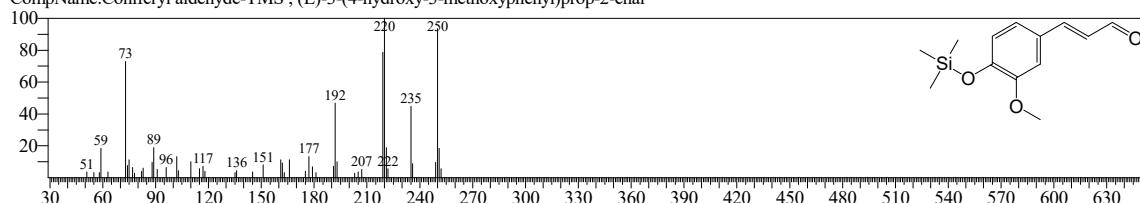
Line#:13 R.Time:39.580(Scan#:6917) MassPeaks:384  
 RawMode:Averaged 39.575-39.585(6916-6918) BasePeak:41.00(47)  
 BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



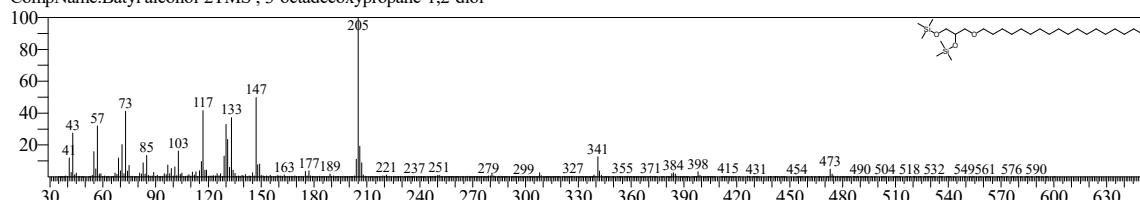
Hit#:1 Entry:477 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:14 Formula:C21H46Osi CAS:112-92-5 MolWeight:342 RetIndex:2156  
 CompName:Octadecanol-TMS ; octadecan-1-ol



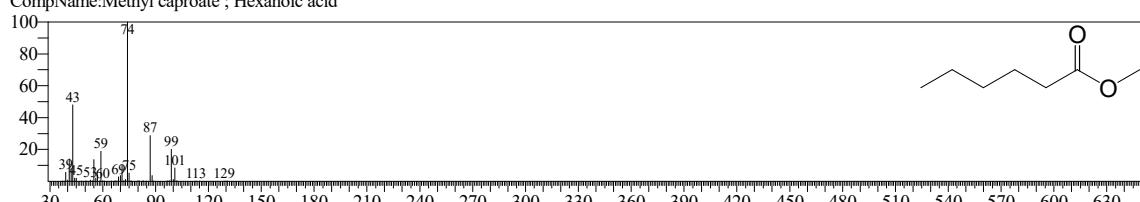
Hit#:2 Entry:339 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:13 Formula:C13H18O3Si CAS:458-36-6 MolWeight:250 RetIndex:1859  
 CompName:Coniferyl aldehyde-TMS ; (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal



Hit#:3 Entry:539 Library:OA\_TMS\_DB5\_67min\_V3.lib  
 SI:12 Formula:C27H60O3Si2 CAS:544-62-7 MolWeight:488 RetIndex:2684  
 CompName:Batyl alcohol-2TMS ; 3-octadecyloxypropane-1,2-diol



Hit#:4 Entry:2 Library:FA\_ME\_SP2560\_EI\_V3.lib  
 SI:11 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332  
 CompName:Methyl caproate ; Hexanoic acid



Hit#:5 Entry:22 Library:FA\_ME\_SP2560\_EI\_V3.lib  
 SI:11 Formula:C21H42O2 CAS:506-30-9 MolWeight:326 RetIndex:2809  
 CompName:Methyl arachisate ; Icosanoic acid

