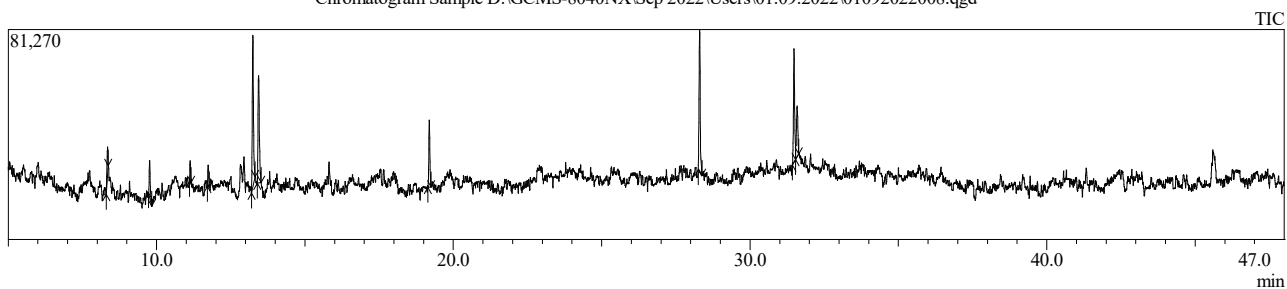


TNAU

Sample Information

Analyzed by : Admin
 Analyzed : 01-Sep-22 11:43:48 PM
 Sample Type : Unknown
 Level # : 1
 Sample Name : Sample
 Sample ID : 3-1
 IS Amount : [1]=1
 Sample Amount : 1
 Dilution Factor : 1
 Vial # : 4
 Injection Volume : 2.00
 Data File : D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022008.qgd
 Org Data File : D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022008.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 10:58:14 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022008.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.349	25263	3.20	10697	3.74	2.36	82	1-Butanol, 3-methyl-, acetate
2	9.768	34470	4.37	14210	4.96	2.43	93	Pentasiloxane, dodecamethyl-
3	11.133	13686	1.73	8297	2.90	1.65	52	Mevalonic lactone-TMS
4	11.738	18847	2.39	8376	2.93	2.25	59	Hypotaaurine-3TMS
5	13.244	165896	21.03	58618	20.47	2.83	54	Methyl cis-13,16-Docosadienate
6	13.438	128952	16.34	41525	14.50	3.11	54	Methyl cis-13,16-Docosadienate
7	19.192	64402	8.16	25958	9.07	2.48	92	2,4-Di-tert-butylphenoxytrimethylsilane
8	28.301	150353	19.06	55073	19.23	2.73	95	n-Hexadecanoic acid
9	31.483	122372	15.51	43871	15.32	2.79	95	10E,12Z-Octadecadienoic acid
10	31.585	64794	8.21	19729	6.89	3.28	86	7-Tetradecenal, (Z)-
		789035	100.00	286354	100.00			

Library

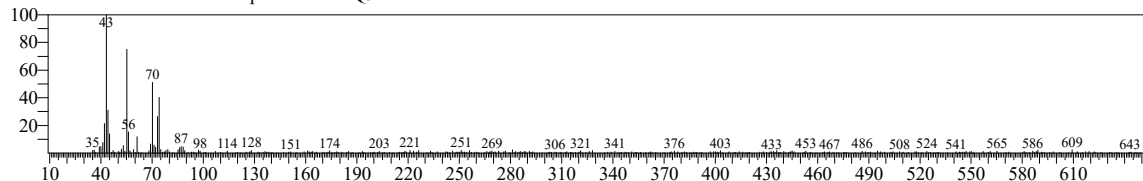
TNAU

<< Target >>

Line#:1 R.Time:8.350(Scan#:671) MassPeaks:330

RawMode:Averaged 8.345-8.355(670-672) BasePeak:43.05(1938)

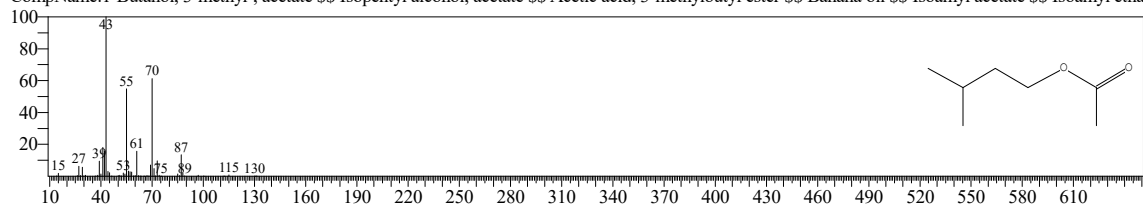
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:6784 Library:NIST20R.lib

SI:82 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820

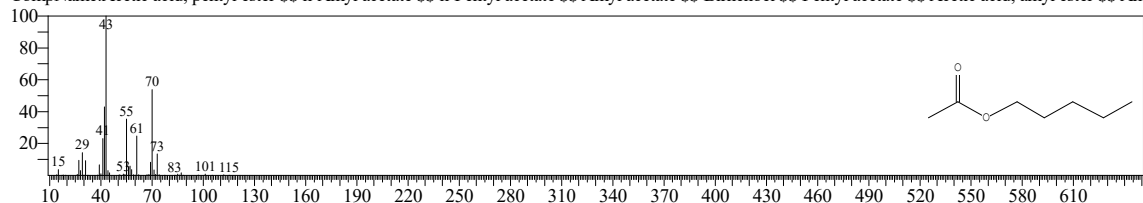
CompName:1-Butanol, 3-methyl-, acetate \$\$ Isopentyl alcohol, acetate \$\$ Acetic acid, 3-methylbutyl ester \$\$ Banana oil \$\$ Isoamyl acetate \$\$ Isoamyl etha



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

SI:79 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884

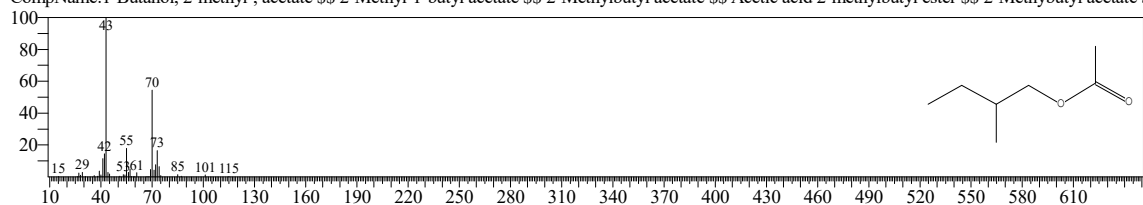
CompName:Acetic acid, pentyl ester \$\$ n-Amyl acetate \$\$ n-Pentyl acetate \$\$ Amyl acetate \$\$ Birnenöl \$\$ Pentyl acetate \$\$ Acetic acid, amyl ester \$\$ An



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

SI:79 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820

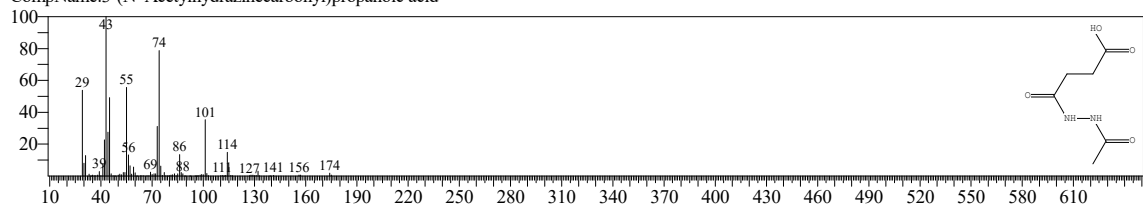
CompName:1-Butanol, 2-methyl-, acetate \$\$ 2-Methyl-1-butyl acetate \$\$ 2-Methylbutyl acetate \$\$ Acetic acid 2-methylbutyl ester \$\$ 2-Methylbutyl acetate :



Hit#:4 Entry:32045 Library:NIST20M1.lib

SI:78 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774

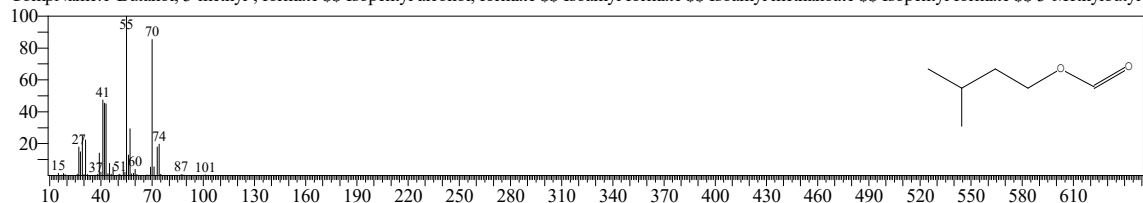
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid



Hit#:5 Entry:4411 Library:NIST20R.lib

SI:77 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



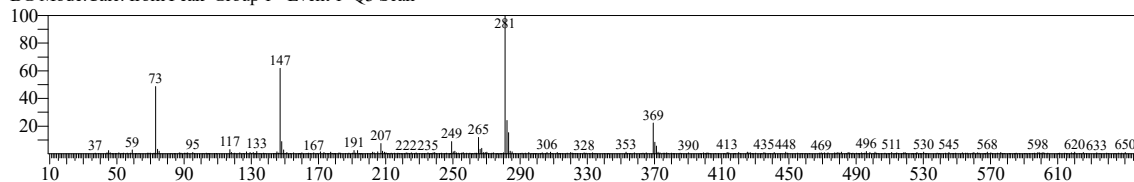
TNAU

<< Target >>

Line#2 R.Time:9.770(Scan#:955) MassPeaks:345

RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.05(3266)

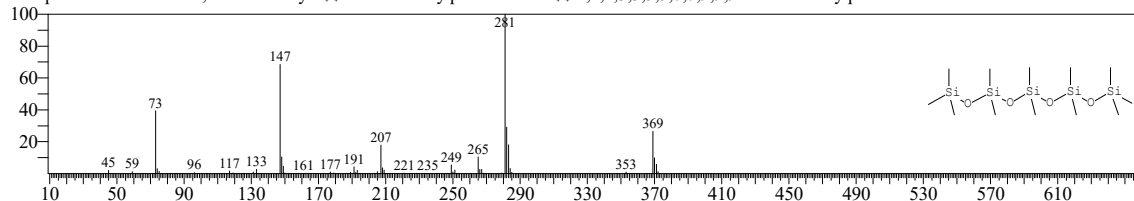
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#1 Entry:40975 Library:NIST20R.lib

SI:93 Formula:C₁₂H₃₆O₄Si₅ CAS:141-63-9 MolWeight:384 RetIndex:1068

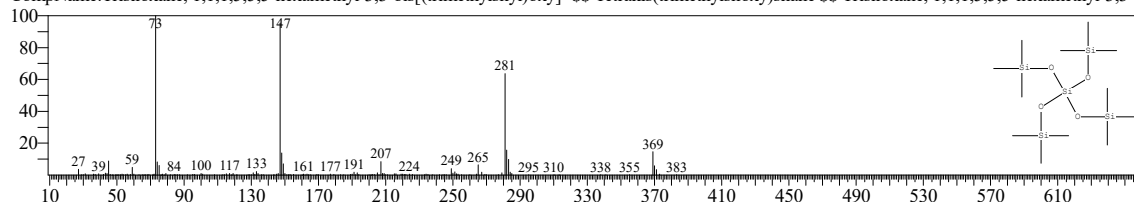
CompName:Pentasiloxane, dodecamethyl- \$S\$ Dodecamethylpentasiloxane \$S\$ 1,1,1,3,3,5,5,7,7,9,9-Dodecamethylpentasiloxane #



Hit#2 Entry:249272 Library:NIST20M1.lib

SI:83 Formula:C₁₂H₃₆O₄Si₅ CAS:3555-47-3 MolWeight:384 RetIndex:1068

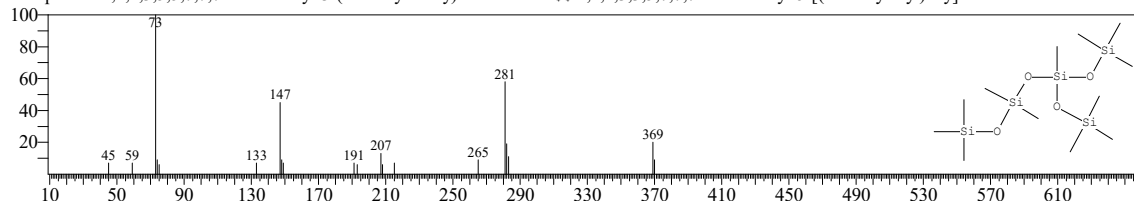
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- \$S\$ Tetrakis(trimethylsiloxy)silane \$S\$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



Hit#3 Entry:249271 Library:NIST20M1.lib

SI:80 Formula:C₁₂H₃₆O₄Si₅ CAS:38146-99-5 MolWeight:384 RetIndex:1068

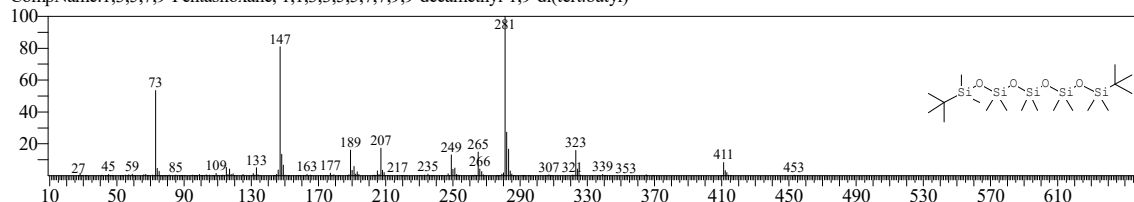
CompName:1,1,1,3,3,5,5,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane \$S\$ 1,1,1,3,3,5,5,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



Hit#4 Entry:27848 Library:NIST20M2.lib

SI:80 Formula:C₁₈H₄₈O₄Si₅ CAS:0-00-0 MolWeight:468 RetIndex:1495

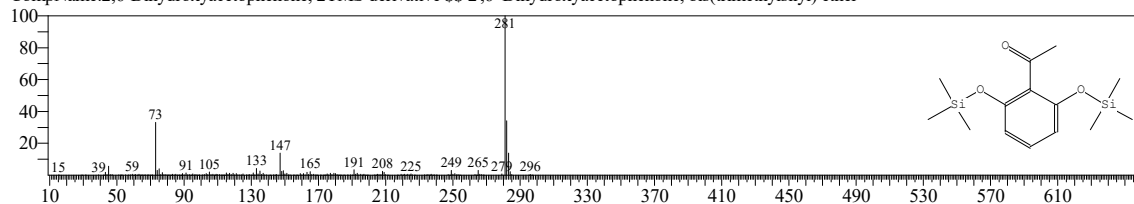
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9-decamethyl-1,9-di(tert-butyl)-



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 \$S\$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



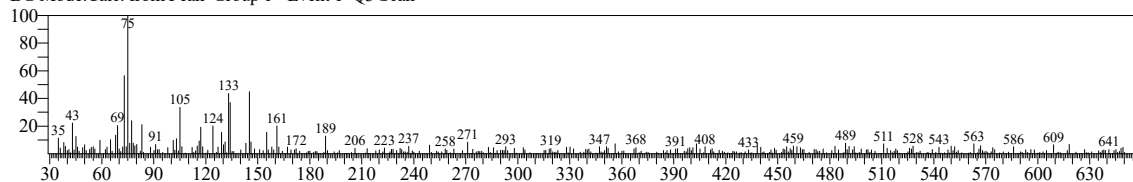
TNAU

<< Target >>

Line#:3 R.Time:11.135(Scan#:1228) MassPeaks:379

RawMode:Averaged 11.130-11.140(1227-1229) BasePeak:75.05(674)

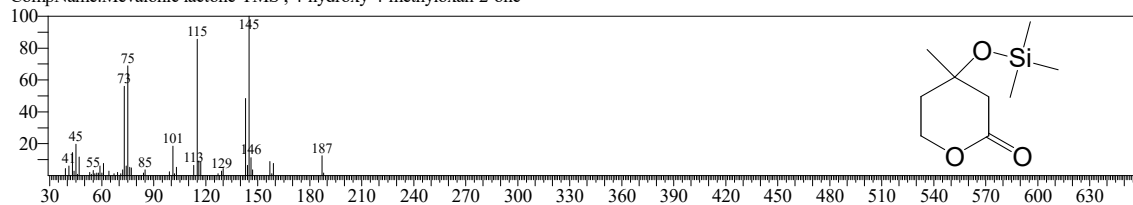
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:106 Library:OA_TMS_DB5_67min_V3.lib

SI:52 Formula:C₉H₁₈O₃Si CAS:503-48-0 MolWeight:202 RetIndex:1378

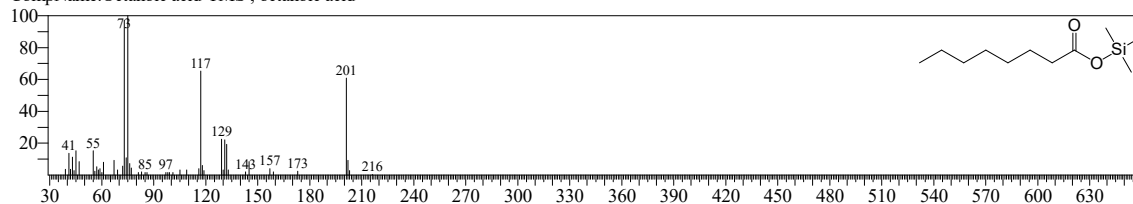
CompName:Mevalonic lactone-TMS ; 4-hydroxy-4-methyloxan-2-one



Hit#:2 Entry:70 Library:OA_TMS_DB5_67min_V3.lib

SI:51 Formula:C₁₁H₂₄O₂Si CAS:124-07-2 MolWeight:216 RetIndex:1263

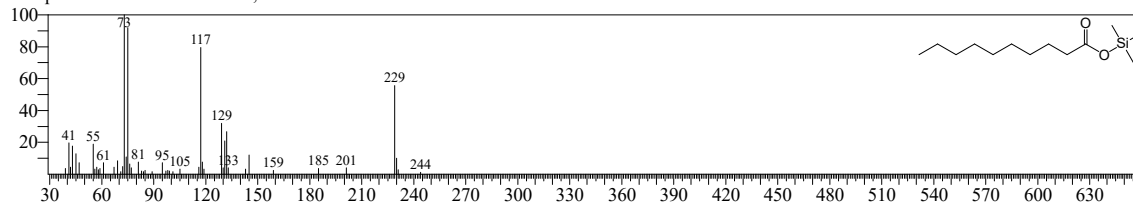
CompName:Octanoic acid-TMS ; octanoic acid



Hit#:3 Entry:129 Library:OA_TMS_DB5_67min_V3.lib

SI:51 Formula:C₁₃H₂₈O₂Si CAS:334-48-5 MolWeight:244 RetIndex:1457

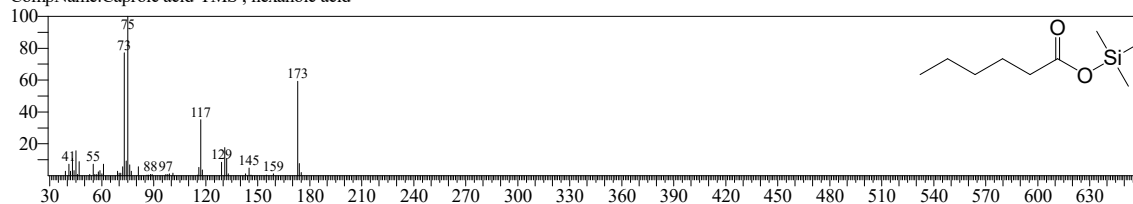
CompName:Decanoic acid-TMS ; decanoic acid



Hit#:4 Entry:11 Library:OA_TMS_DB5_67min_V3.lib

SI:50 Formula:C₉H₂₀O₂Si CAS:142-62-1 MolWeight:188 RetIndex:1071

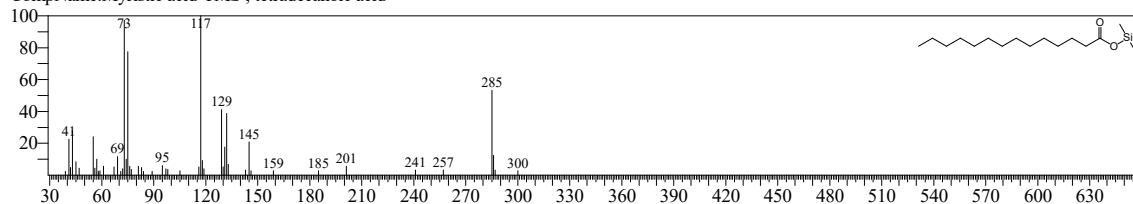
CompName:Caproic acid-TMS ; hexanoic acid



Hit#:5 Entry:331 Library:OA_TMS_DB5_67min_V3.lib

SI:50 Formula:C₁₇H₃₆O₂Si CAS:544-63-8 MolWeight:300 RetIndex:1850

CompName:Myristic acid-TMS ; tetradecanoic acid



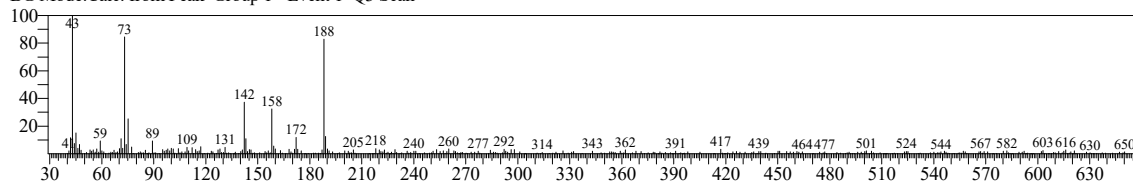
TNAU

<< Target >>

Line#:4 R.Time:11.740(Scan#:1349) MassPeaks:356

RawMode:Averaged 11.735-11.745(1348-1350) BasePeak:43.05(1236)

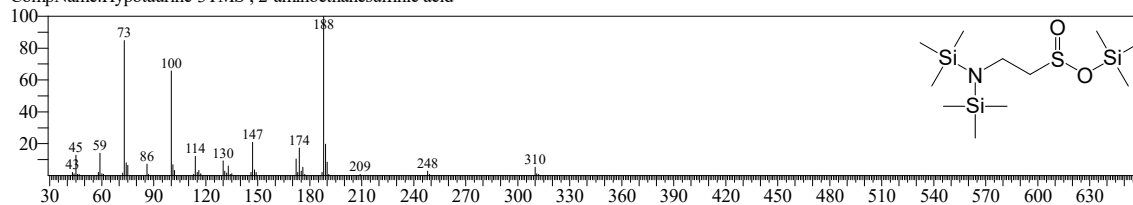
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:201 Library:OA_TMS_DB5_67min_V3.lib

SI:59 Formula:C11H31NO2SSi3 CAS:300-84-5 MolWeight:325 RetIndex:1617

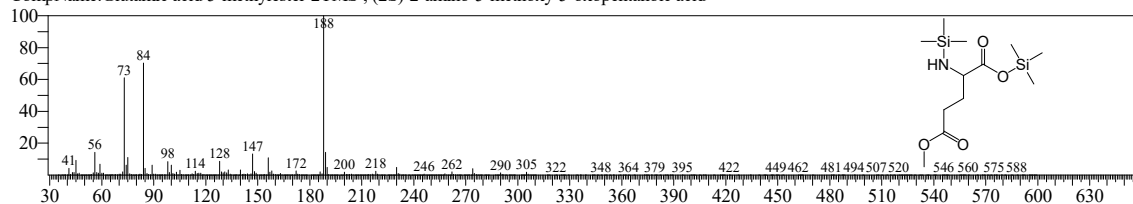
CompName:Hypotaaurine-3TMS ; 2-aminoethanesulfonic acid



Hit#:2 Entry:153 Library:OA_TMS_DB5_67min_V3.lib

SI:58 Formula:C12H27NO4Si2 CAS:1499-55-4 MolWeight:305 RetIndex:1519

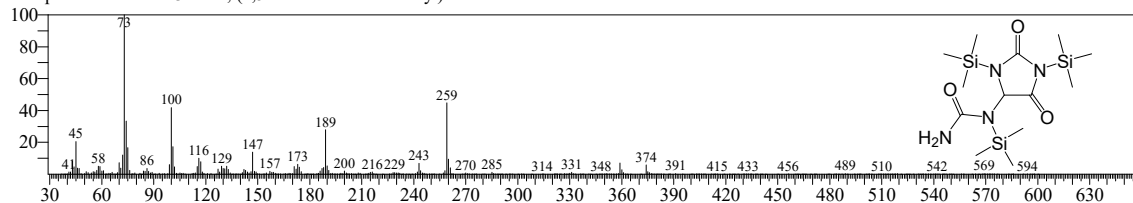
CompName:Glutamic acid 5-methylester-2TMS ; (2S)-2-amino-5-methoxy-5-oxopentanoic acid



Hit#:3 Entry:453 Library:OA_TMS_DB5_67min_V3.lib

SI:57 Formula:C13H30N4O3Si3 CAS:97-59-6 MolWeight:374 RetIndex:2087

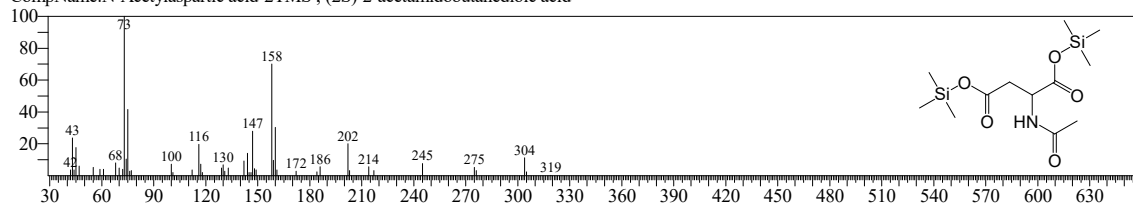
CompName:Allantoin-3TMS ; (2,5-dioxoimidazolidin-4-yl)urea



Hit#:4 Entry:229 Library:OA_TMS_DB5_67min_V3.lib

SI:56 Formula:C12H25NO5Si2 CAS:997-55-7 MolWeight:319 RetIndex:1665

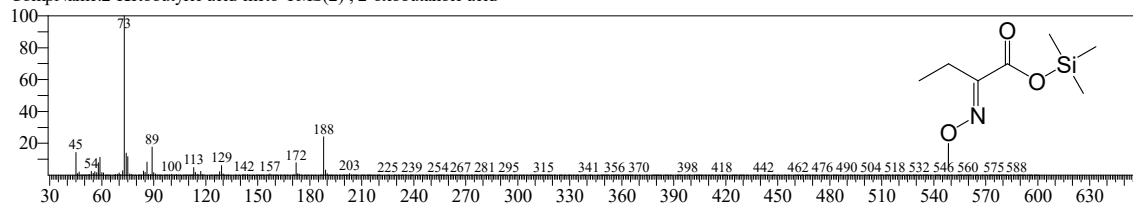
CompName:N-Acetylaspartic acid-2TMS ; (2S)-2-acetamidobutanedioic acid



Hit#:5 Entry:15 Library:OA_TMS_DB5_67min_V3.lib

SI:56 Formula:C8H17NO3Si CAS:600-18-0 MolWeight:203 RetIndex:1103

CompName:2-Ketobutyric acid-meto-TMS(2) ; 2-oxobutanoic acid



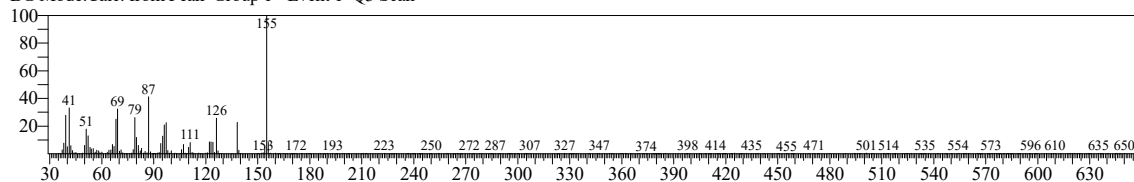
TNAU

<< Target >>

Line#:5 R.Time:13.245(Scan#:1650) MassPeaks:280

RawMode:Averaged 13.240-13.250(1649-1651) BasePeak:155.05(9706)

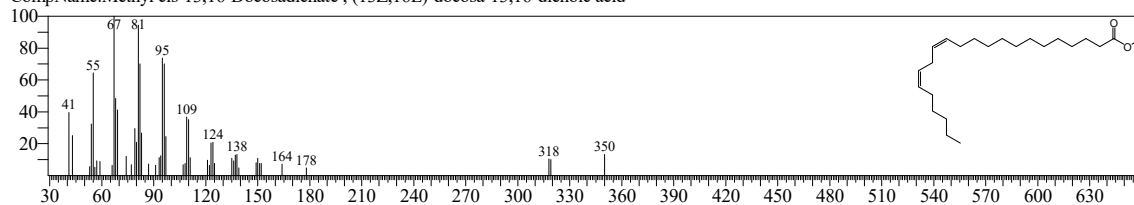
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib

SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169

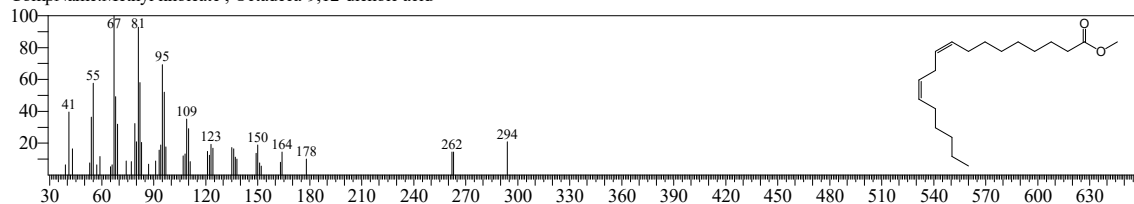
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib

SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775

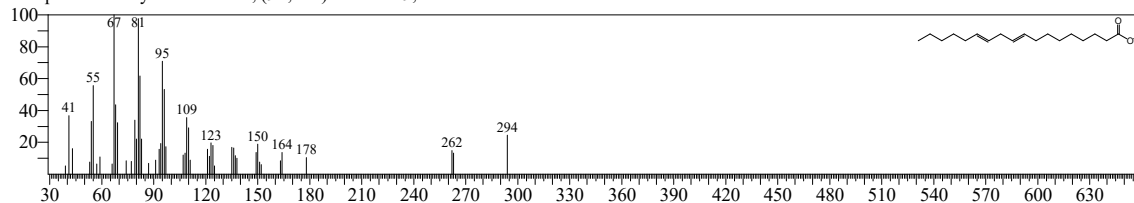
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib

SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727

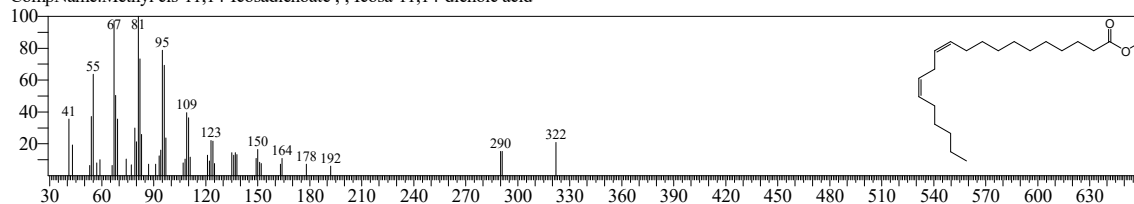
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib

SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973

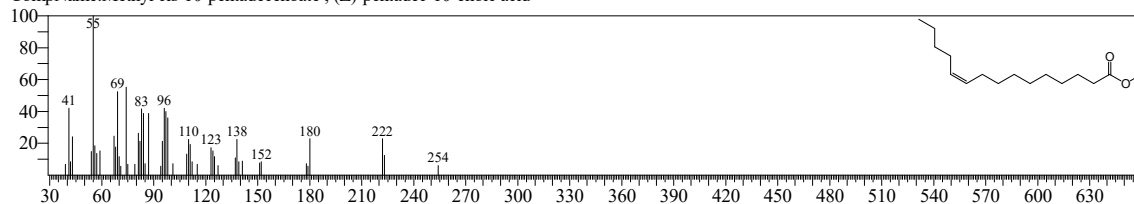
CompName:Methyl cis-11,14-Icosadienoate ; Icosa-11,14-dienoic acid



Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib

SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388

CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid



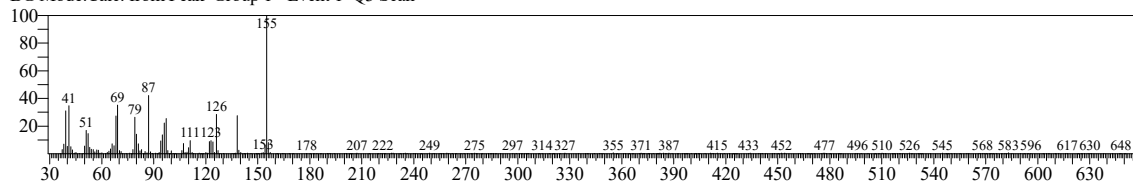
TNAU

<< Target >>

Line#:6 R.Time:13.440(Scan#:1689) MassPeaks:306

RawMode:Averaged 13.435-13.445(1688-1690) BasePeak:155.10(6530)

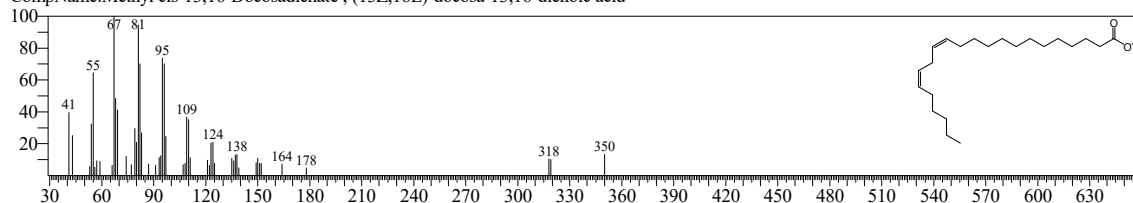
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib

SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169

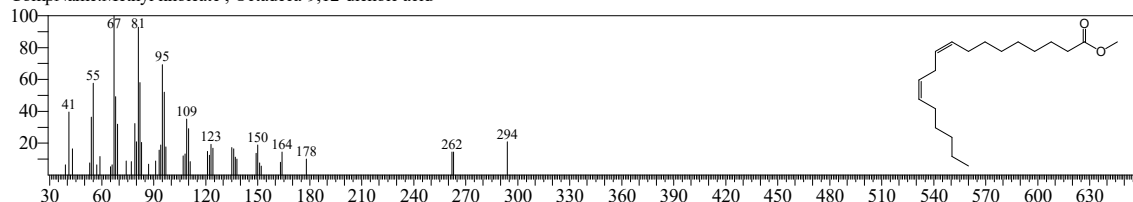
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib

SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775

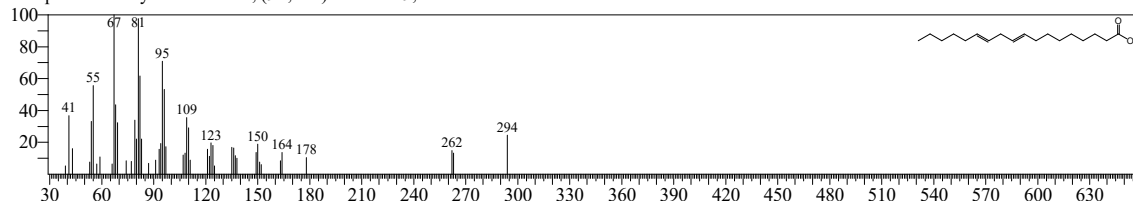
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib

SI:53 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727

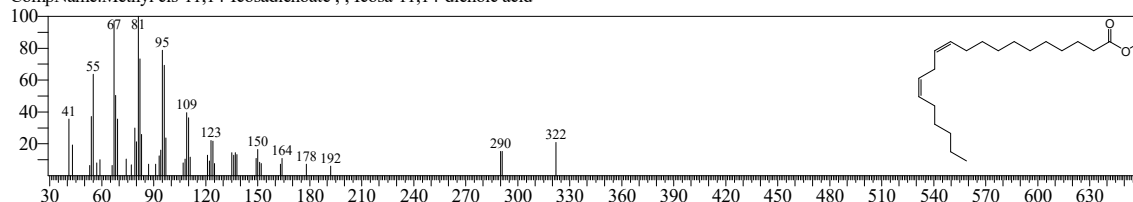
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib

SI:53 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973

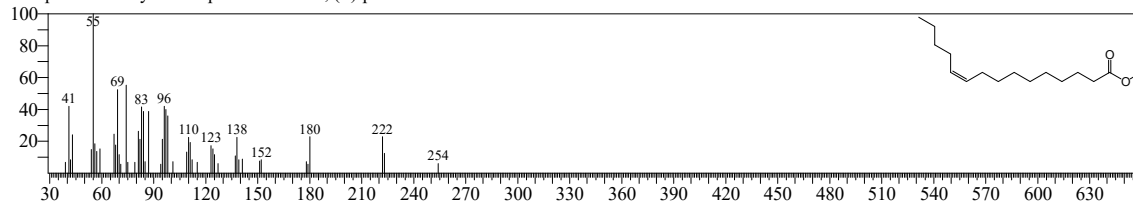
CompName:Methyl cis-11,14-Icosadienoate ; Icosa-11,14-dienoic acid



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



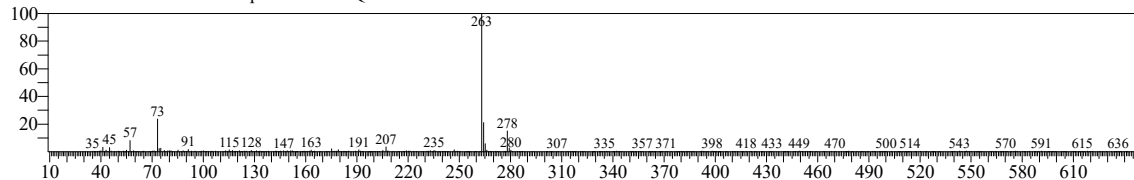
TNAU

<< Target >>

Line#:7 R.Time:19.190(Scan#:2839) MassPeaks:383

RawMode:Averaged 19.185-19.195(2838-2840) BasePeak:263.20(9444)

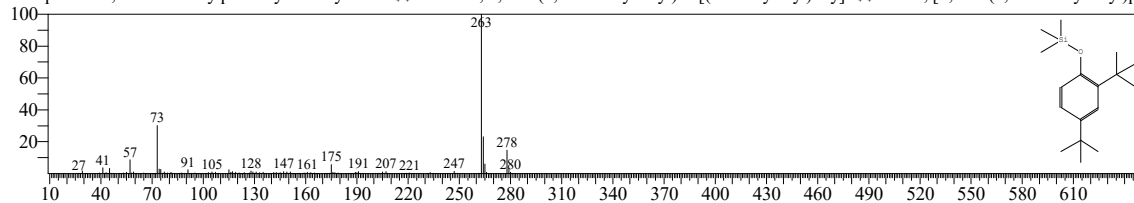
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:137399 Library:NIST20M1.lib

SI:92 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632

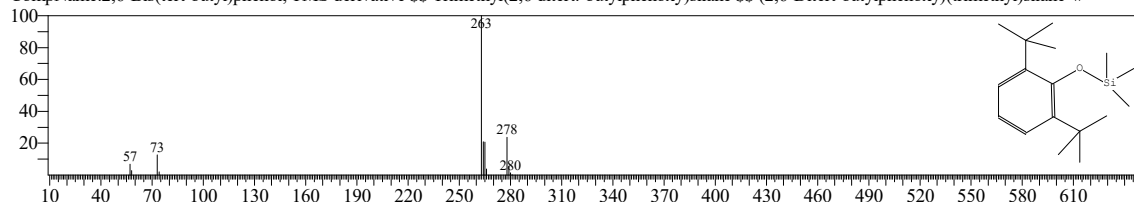
CompName:2,4-Di-tert-butylphenoxytrimethylsilane \$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- \$ Silane, [2,4-bis(1,1-dimethylethyl)ph



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

SI:84 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632

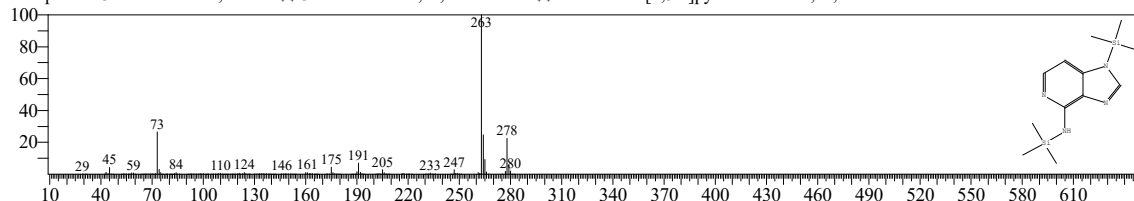
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative \$ Trimethyl(2,6 ditert-butylphenoxy)silane \$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #



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

SI:84 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703

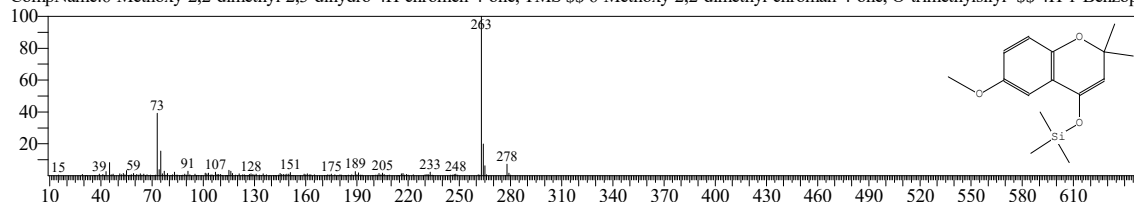
CompName:3-Deazaadenine, 2TMS \$ 3-Deazaadenine, N,N'-bis-TMS \$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



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

SI:80 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736

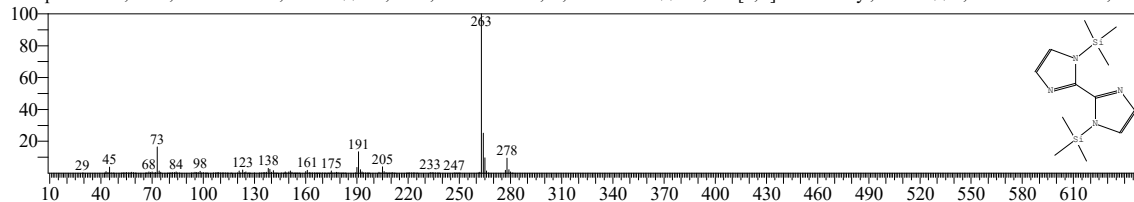
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS \$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- \$ 4H-1-Benzopy



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, 2TMS



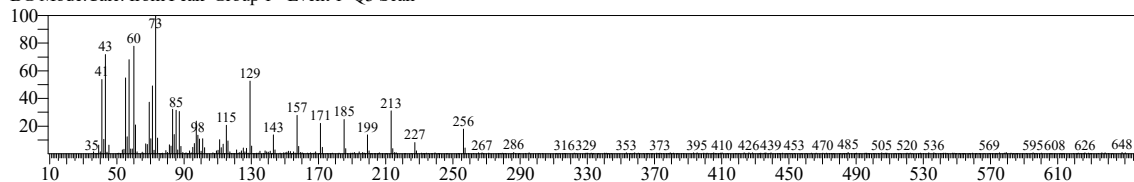
TNAU

<< Target >>

Line#:8 R.Time:28.300(Scan#:4661) MassPeaks:349

RawMode:Averaged 28.295-28.305(4660-4662) BasePeak:73.05(4532)

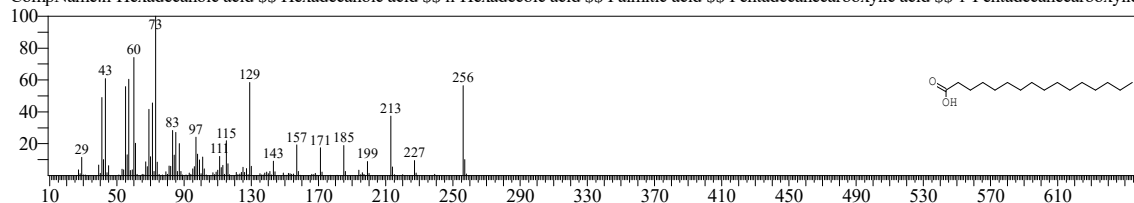
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:31600 Library:NIST20R.lib

SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968

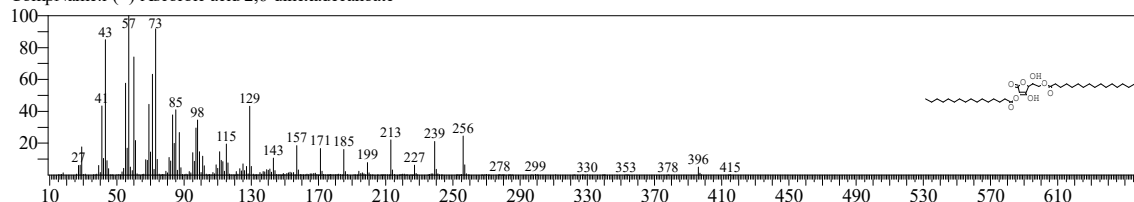
CompName:n-Hexadecanoic acid \$ Hexadecanoic acid \$ n-Hexadecoic acid \$ Palmitic acid \$ Pentadecanecarboxylic acid \$ 1-Pentadecanecarboxylic



Hit#:2 Entry:44286 Library:NIST20M2.lib

SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765

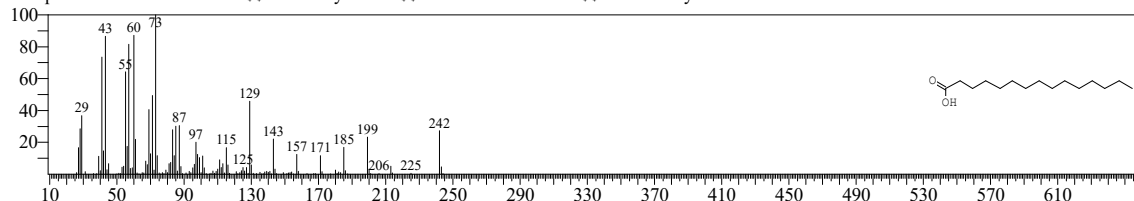
CompName:L-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:3 Entry:29890 Library:NIST20R.lib

SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869

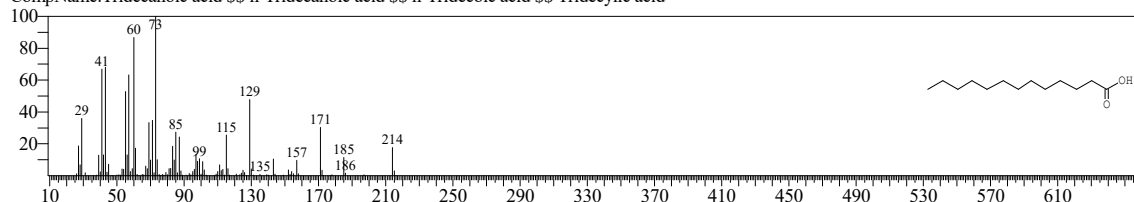
CompName:Pentadecanoic acid \$ Pentadecylic acid \$ n-Pentadecanoic acid \$ n-Pentadecylic acid



Hit#:4 Entry:25643 Library:NIST20R.lib

SI:89 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670

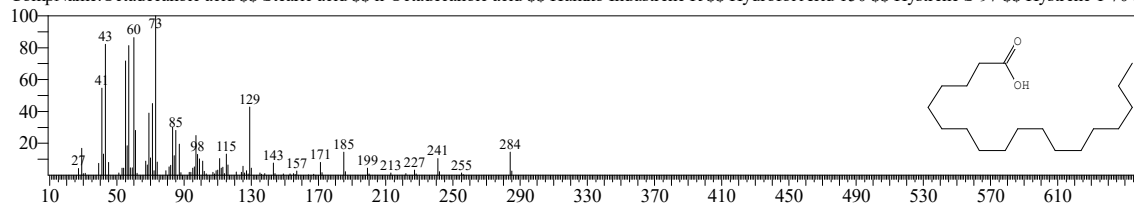
CompName:Tridecanoic acid \$ n-Tridecanoic acid \$ n-Tridecoic acid \$ Tridecyllic acid



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 Industriene R \$ Hydrofol Acid 150 \$ Hystrene S-97 \$ Hystrene T-70 \$



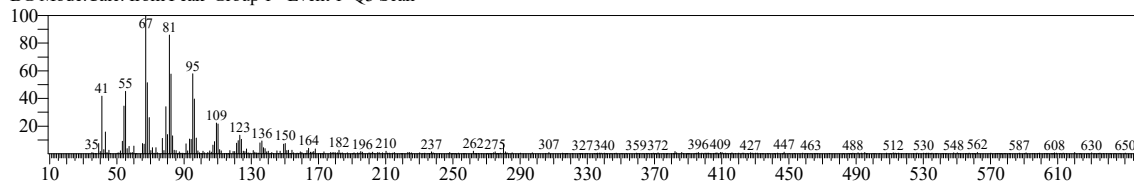
TNAU

<< Target >>

Line# 9 R.Time: 31.485 (Scan#: 5298) MassPeaks: 361

RawMode: Averaged 31.480-31.490 (5297-5299) BasePeak: 67.05 (3987)

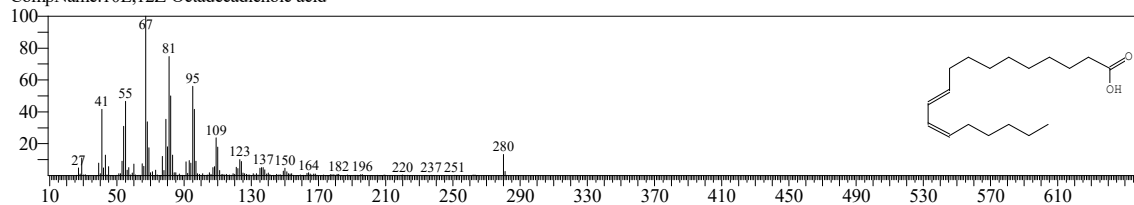
BG Mode: Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#: 1 Entry: 139646 Library: NIST20M1.lib

SI: 95 Formula: C₁₈H₃₂O₂ CAS: 2420-56-6 MolWeight: 280 RetIndex: 2183

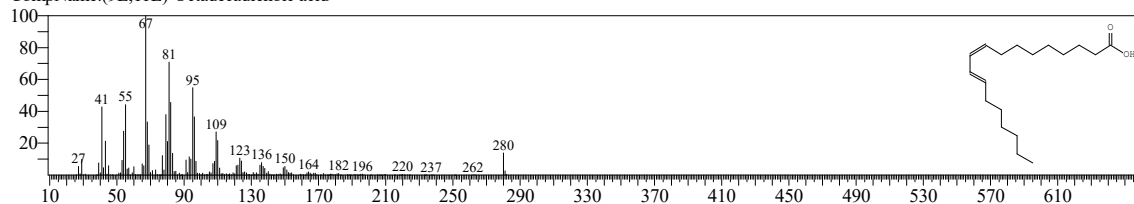
CompName: 10E, 12Z-Octadecadienoic acid



Hit#: 2 Entry: 139651 Library: NIST20M1.lib

SI: 95 Formula: C₁₈H₃₂O₂ CAS: 544-71-8 MolWeight: 280 RetIndex: 2183

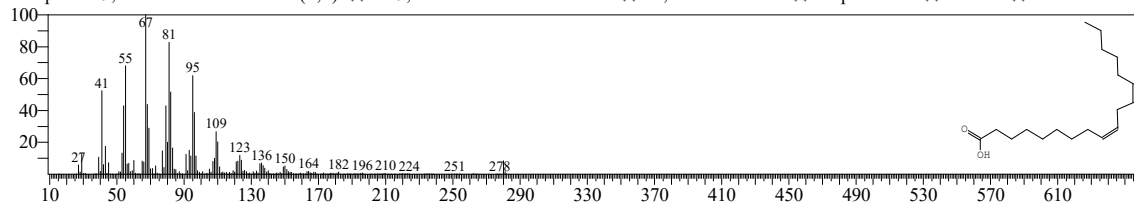
CompName: (9E, 11E)-Octadecadienoic acid



Hit#: 3 Entry: 34035 Library: NIST20R.lib

SI: 94 Formula: C₁₈H₃₂O₂ CAS: 60-33-3 MolWeight: 280 RetIndex: 2183

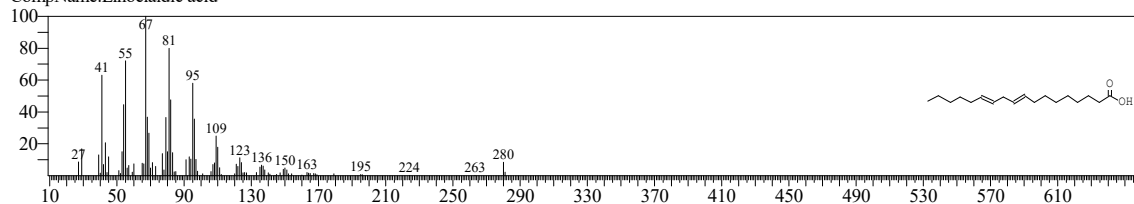
CompName: 9, 12-Octadecadienoic acid (Z, Z)- \$ cis-9, cis-12-Octadecadienoic acid \$ \$ cis-Linoleic acid \$ \$ Grape seed oil \$ \$ Linoleic \$ \$ Linoleic acid \$



Hit#: 4 Entry: 139661 Library: NIST20M1.lib

SI: 93 Formula: C₁₈H₃₂O₂ CAS: 506-21-8 MolWeight: 280 RetIndex: 2183

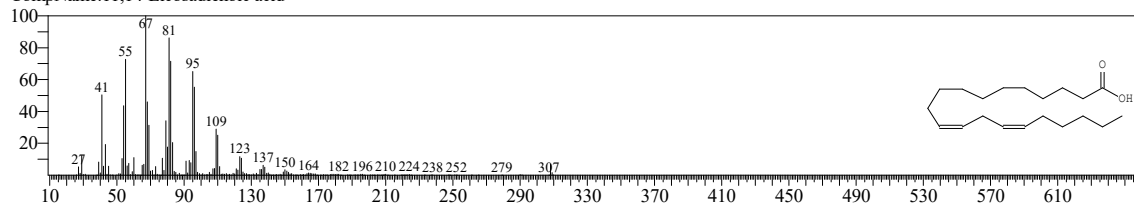
CompName: Linoelaidic acid



Hit#: 5 Entry: 173215 Library: NIST20M1.lib

SI: 92 Formula: C₂₀H₃₆O₂ CAS: 2091-39-6 MolWeight: 308 RetIndex: 2382

CompName: 11, 14-Eicosadienoic acid



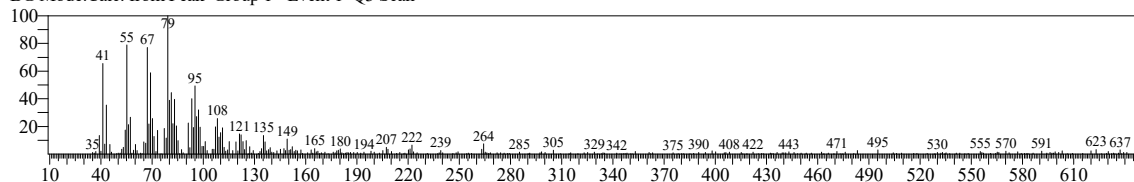
TNAU

<< Target >>

Line#:10 R.Time:31.585(Scan#:5318) MassPeaks:301

RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:79.05(1307)

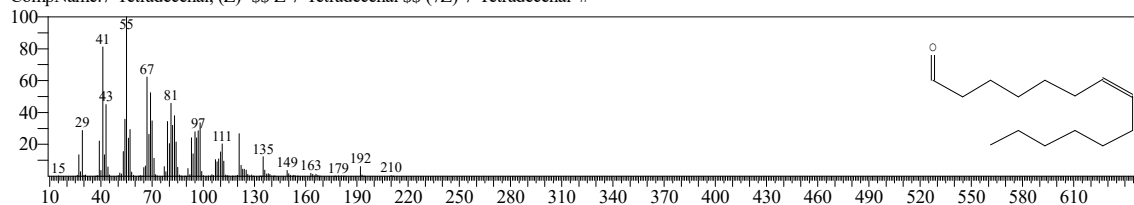
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Hit#:1 Entry:63176 Library:NIST20M1.lib

SI:86 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609

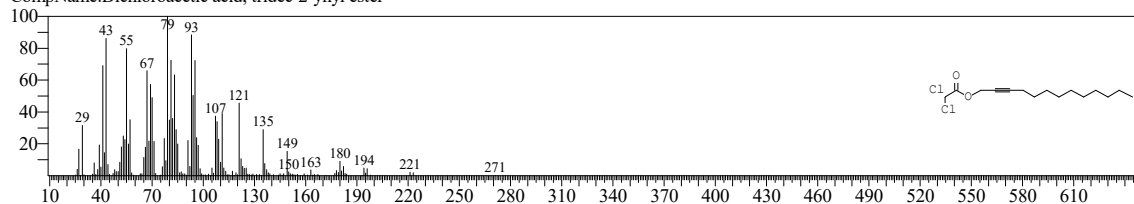
CompName:7-Tetradecenal, (Z)- \$\$ Z-7-Tetradecenal \$\$ (7Z)-7-Tetradecenal #



Hit#:2 Entry:170238 Library:NIST20M1.lib

SI:86 Formula:C15H24Cl2O2 CAS:0-00-0 MolWeight:306 RetIndex:2042

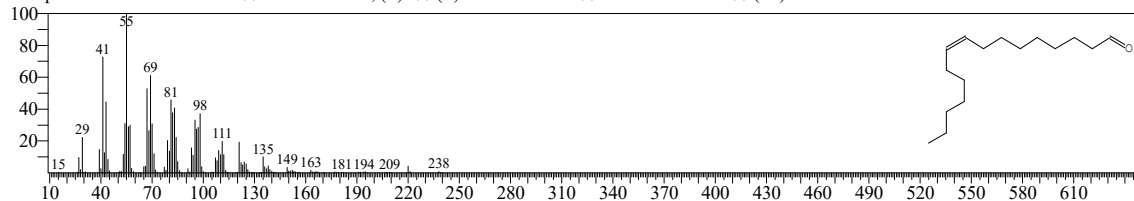
CompName:Dichloroacetic acid, tridec-2-ynyl ester



Hit#:3 Entry:29348 Library:NIST20R.lib

SI:85 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808

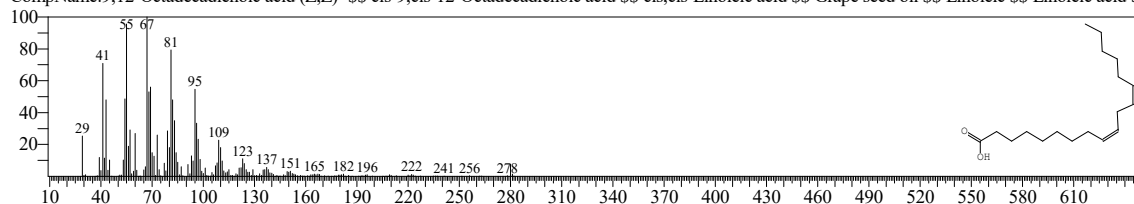
CompName:cis-9-Hexadecenal \$\$ 9-Hexadecenal, (Z)- \$\$ (Z)-9-Hexadecenal \$\$ Z-9-Hexadecenal \$\$ (9Z)-9-Hexadecenal #



Hit#:4 Entry:34034 Library:NIST20R.lib

SI:85 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#:5 Entry:39500 Library:NIST20R.lib

SI:85 Formula:C21H36O4 CAS:18465-99-1 MolWeight:352 RetIndex:2705

CompName:9,12,15-Octadecatrienoic acid, 2,3-dihydroxypropyl ester, (Z,Z,Z)- \$\$ Linolenin, 1-mono- \$\$.alpha.-Glyceryl linolenate \$\$ 2,3-Dihydroxypropyl

