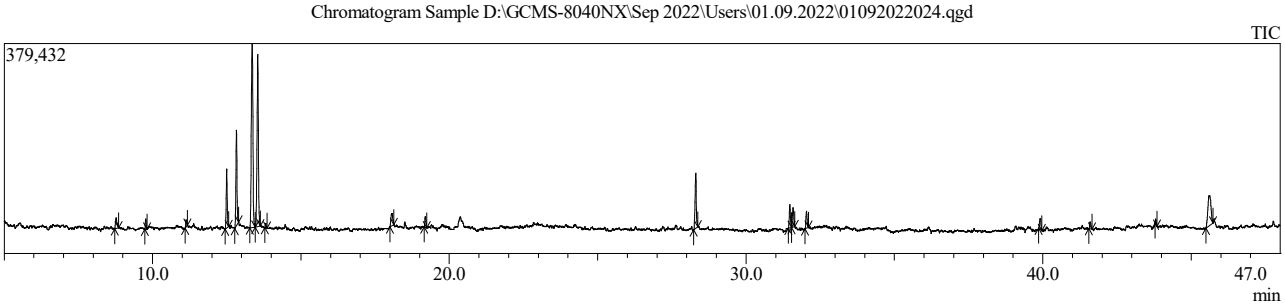
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 1:48:14 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 8-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 9
Injection Volume	: 5.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022024.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022024.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 11:06:55 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022024.qgd



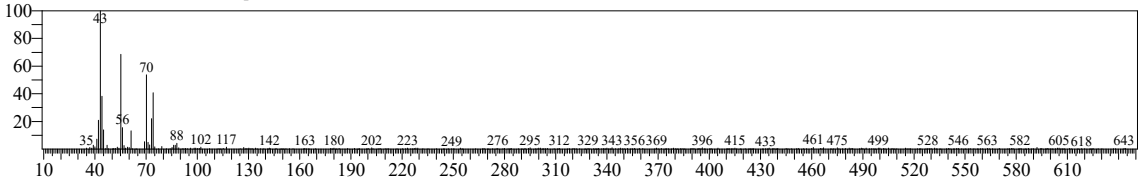
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.771	68410	1.59	18619	1.40	3.67	85	1-Butanol, 3-methyl-, acetate
2	9.772	37413	0.87	18664	1.41	2.00	94	Pentasiloxane, dodecamethyl-
3	11.133	31649	0.73	12487	0.94	2.53	38	Methyl arachidonate
4	12.498	255284	5.92	106376	8.02	2.40	74	2,5-Cyclohexadiene-1,4-dione, dioxime
5	12.826	429685	9.97	172959	13.04	2.48	74	1,3-Benzodioxol-5-ol
6	13.356	1226619	28.45	332274	25.06	3.69	53	Methyl cis-13,16-Docosadienate
7	13.546	988015	22.92	311525	23.50	3.17	53	Methyl cis-13,16-Docosadienate
8	13.818	19797	0.46	8125	0.61	2.44	77	Trisiloxane, octamethyl-
9	18.074	95002	2.20	21745	1.64	4.37	89	.beta.-D-Glucopyranose, 1,6-anhydro-
10	19.190	46547	1.08	19578	1.48	2.38	88	2,4-Di-tert-butylphenoxytrimethylsilane
11	28.305	289939	6.73	99588	7.51	2.91	95	n-Hexadecanoic acid
12	31.477	114688	2.66	42426	3.20	2.70	94	9,12-Octadecadienoic acid (Z,Z)-
13	31.584	105201	2.44	35020	2.64	3.00	87	7-Tetradecenal, (Z)-
14	32.037	87912	2.04	30621	2.31	2.87	93	Octadecanoic acid
15	39.914	61336	1.42	19695	1.49	3.11	94	Bis(2-ethylhexyl) phthalate
16	41.591	37459	0.87	12464	0.94	3.01	83	Tetracosamethyl-cyclododecasiloxane
17	43.808	17006	0.39	9636	0.73	1.76	81	Tetracosamethyl-cyclododecasiloxane
18	45.626	398820	9.25	54074	4.08	7.38	90	Diosgenin
		4310782	100.00	1325876	100.00			

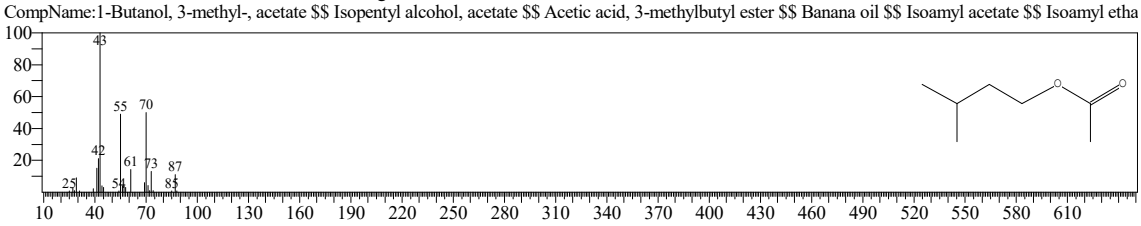
Library

TNAU

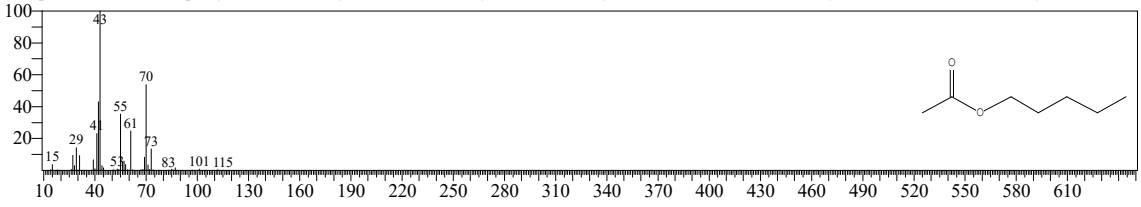
<< Target >>
Line#:1 R.Time:8.770(Scan#:755) MassPeaks:332
RawMode:Averaged 8.765-8.775(754-756) BasePeak:43.05(4144)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



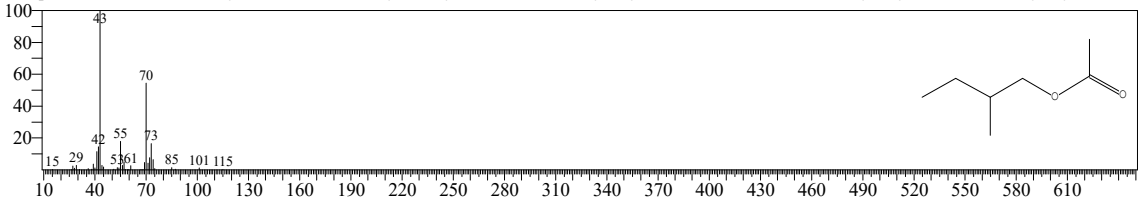
Hit#:1 Entry:6783 Library:NIST20R.lib
SI:85 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



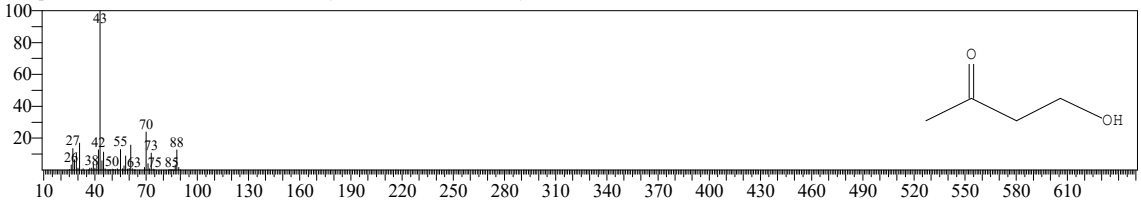
Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:83 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ An



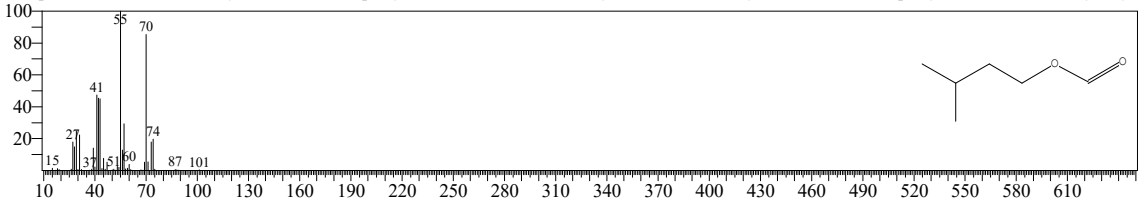
Hit#:3 Entry:6819 Library:NIST20R.lib
SI:82 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:1220 Library:NIST20R.lib
SI:80 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-

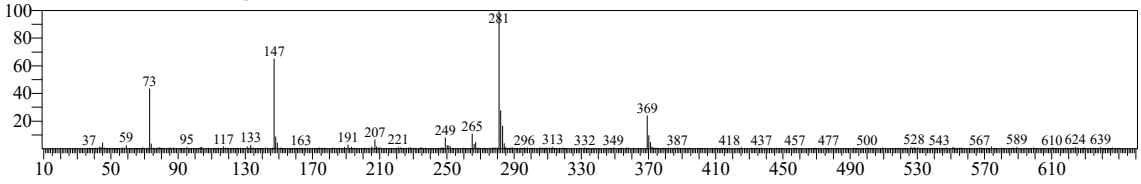


Hit#:5 Entry:4411 Library:NIST20R.lib
SI:79 Formula:C6H12O2 CAS:110-45-2 MolWeight:116 RetIndex:818
CompName:1-Butanol, 3-methyl-, formate $$ Isopentyl alcohol, formate $$ Isoamyl formate $$ Isoamyl methanoate $$ Isopentyl formate $$ 3-Methylbutyl

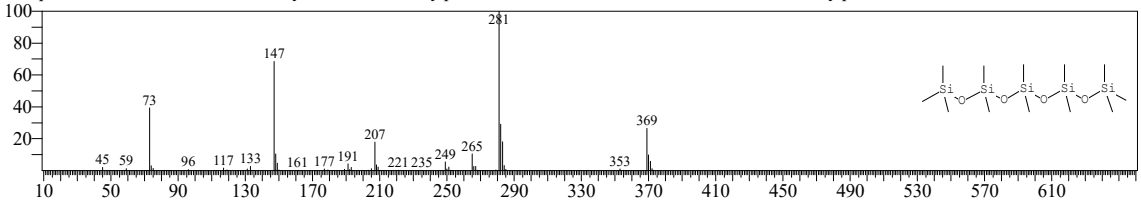


TNAU

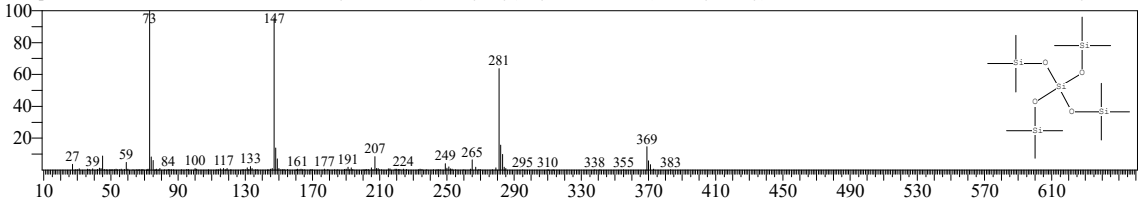
<< Target >>
Line#:2 R.Time:9.770(Scan#:955) MassPeaks:364
RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.00(4202)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



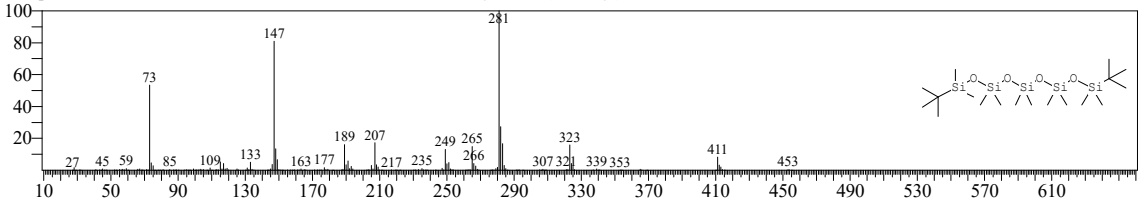
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:94 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



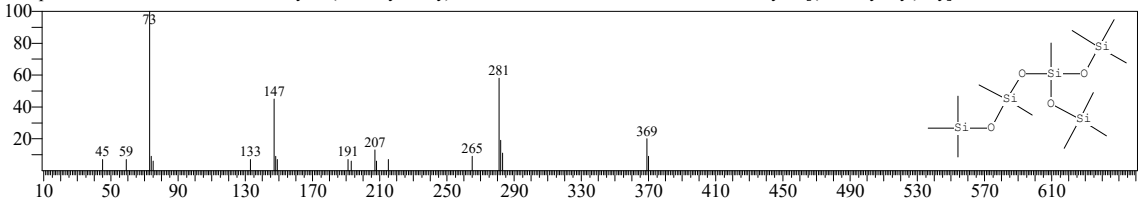
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



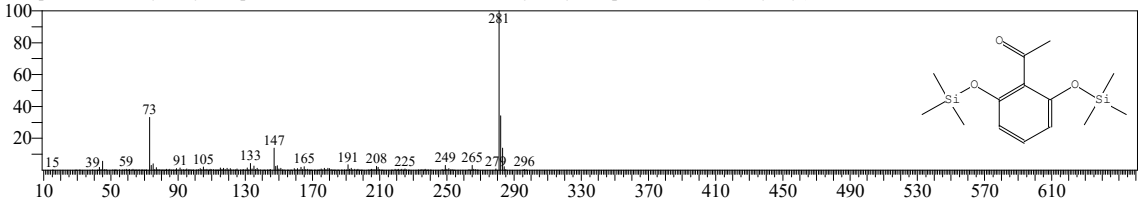
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:80 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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

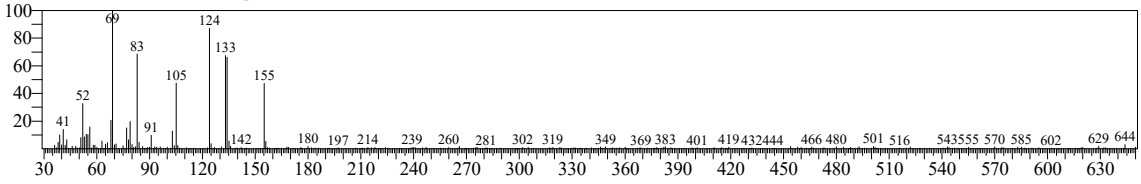


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

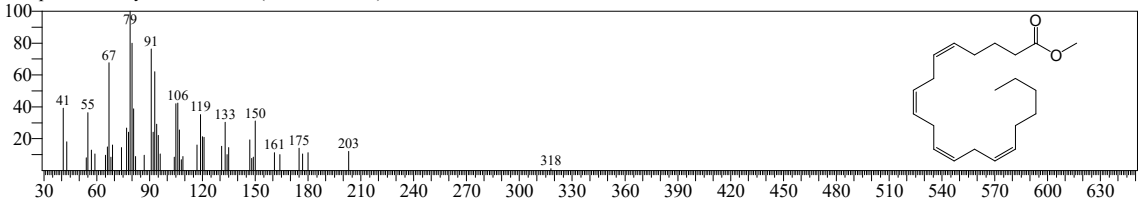


TNAU

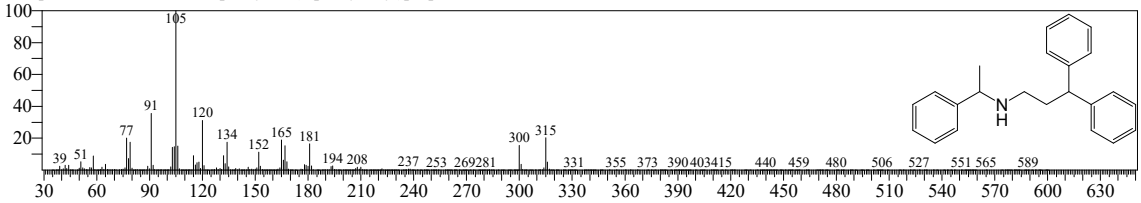
<< Target >>
Line#:3 R.Time:11.135(Scan#:1228) MassPeaks:266
RawMode:Averaged 11.130-11.140(1227-1229) BasePeak:69.00(1912)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



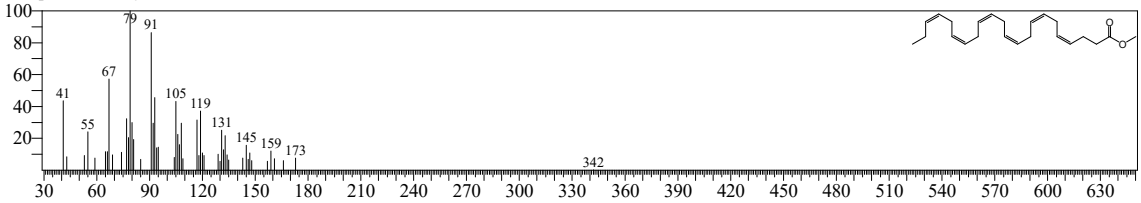
Hit#:1 Entry:33 Library:FA_ME_SP2560_EI_V3.lib
SI:38 Formula:C21H34O2 CAS:506-32-1 MolWeight:318 RetIndex:3109
CompName:Methyl arachidonate ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid



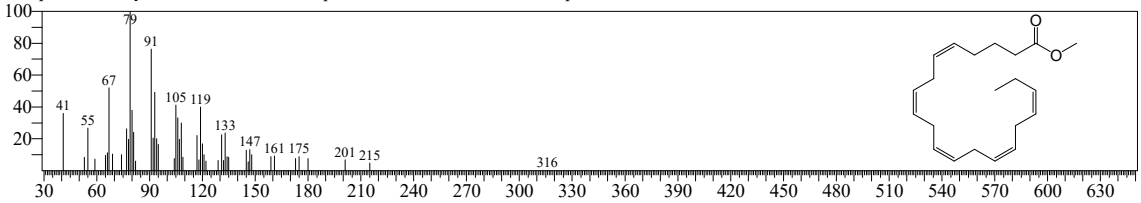
Hit#:2 Entry:530 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C23H25N CAS:13042-18-7 MolWeight:315 RetIndex:2545
CompName:Fendiline ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine



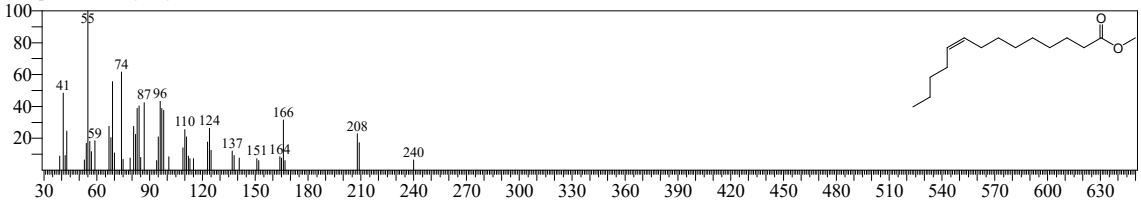
Hit#:3 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:37 Formula:C23H34O2 CAS:6217-54-5 MolWeight:342 RetIndex:3514
CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid



Hit#:4 Entry:36 Library:FA_ME_SP2560_EI_V3.lib
SI:37 Formula:C21H32O2 CAS:10417-94-4 MolWeight:316 RetIndex:3232
CompName:Methyl cis-5,8,11,14,17-Eicosapentaenoate ; Icosa-5,8,11,14,17-pentaenoic acid

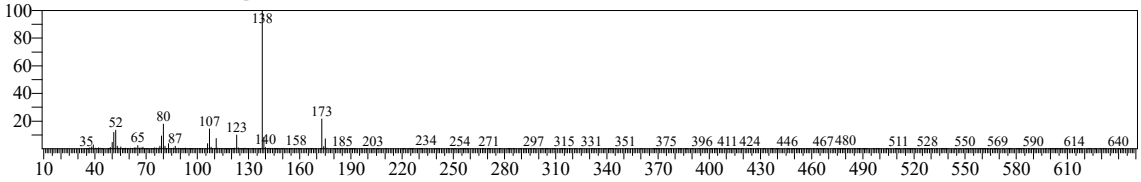


Hit#:5 Entry:9 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C15H28O2 CAS:544-64-9 MolWeight:240 RetIndex:2283
CompName:Methyl myristoleate ; ; (Z)-tetradec-9-enoic acid

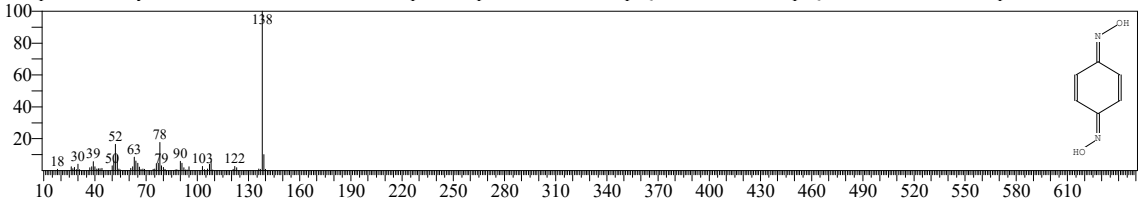


TNAU

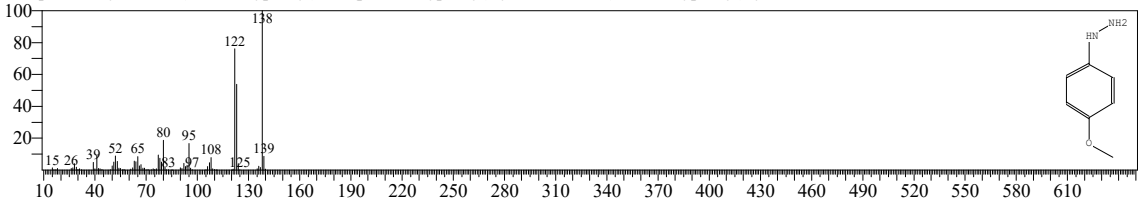
<< Target >>
Line#:4 R.Time:12.500(Scan#:1501) MassPeaks:329
RawMode:Averaged 12.495-12.505(1500-1502) BasePeak:138.05(37219)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



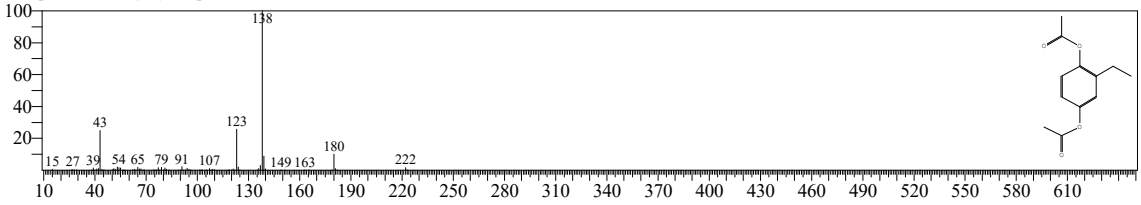
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:74 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



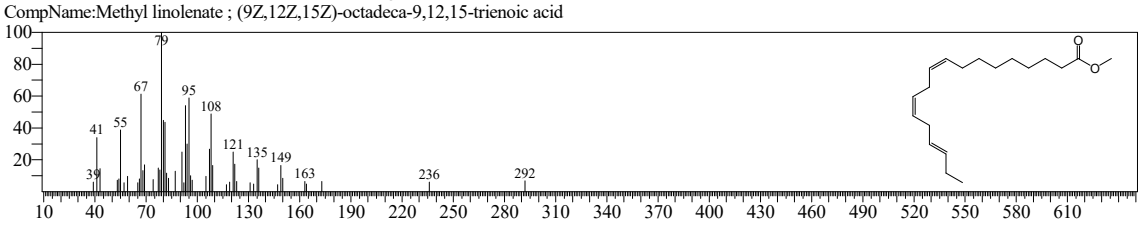
Hit#:2 Entry:11222 Library:NIST20M1.lib
SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #



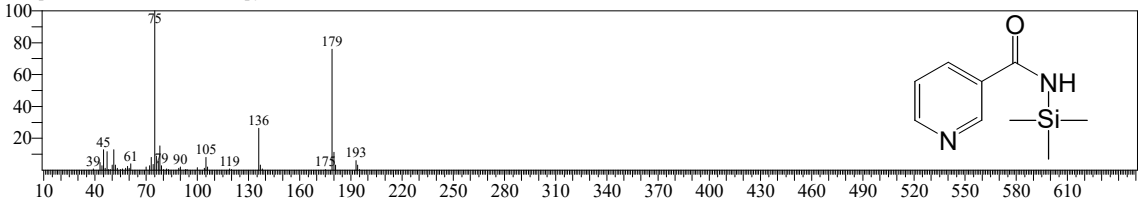
Hit#:3 Entry:74622 Library:NIST20M1.lib
SI:70 Formula:C12H14O4 CAS:57982-10-2 MolWeight:222 RetIndex:1653
CompName:2-Ethylhydroquinone, diacetate



Hit#:4 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:34 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

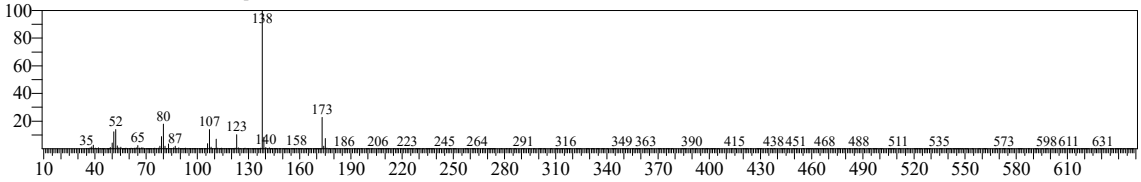


Hit#:5 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide

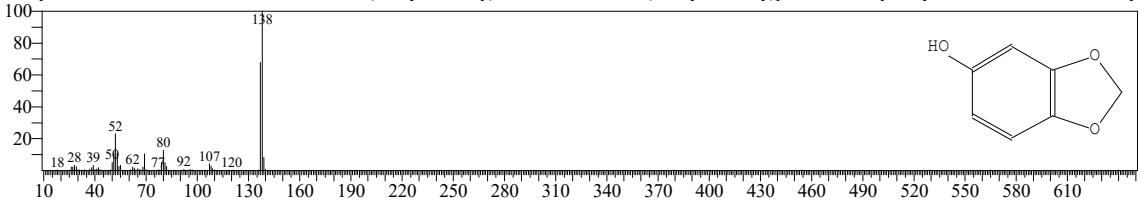


TNAU

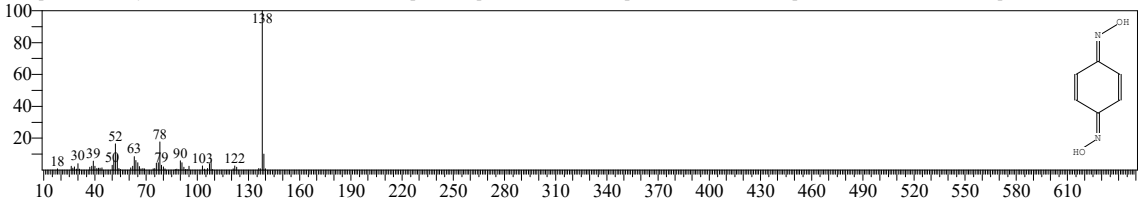
<< Target >>
Line#:5 R.Time:12.825(Scan#:1566) MassPeaks:378
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(60351)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



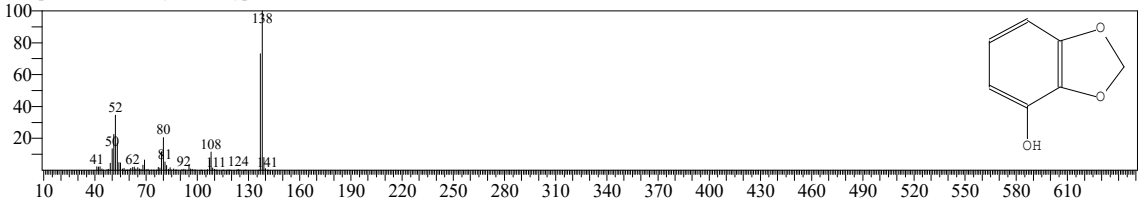
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



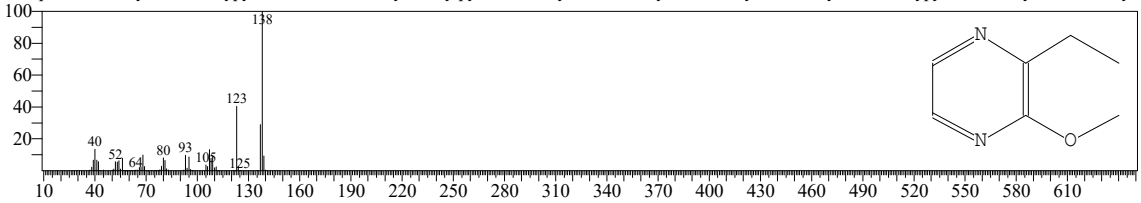
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



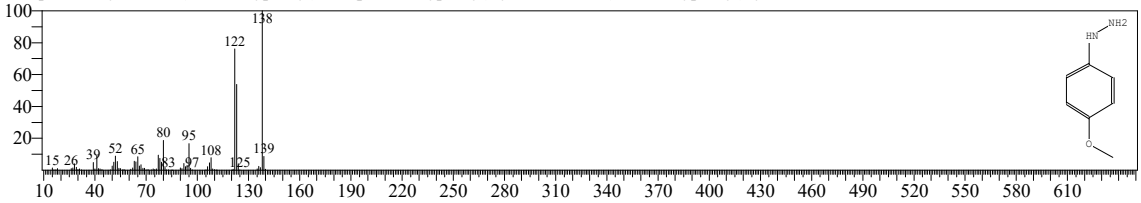
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:72 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



Hit#:4 Entry:8422 Library:NIST20R.lib
SI:71 Formula:C7H10N2O CAS:25680-58-4 MolWeight:138 RetIndex:1070
CompName:2-Ethyl-3-methoxypyrazine $$ 2-Methoxy-3-ethylpyrazine $$ Pyrazine, 2-ethyl-3-methoxy- $$ 3-Ethyl-2-methoxypyrazine $$ Pyrazine, 3-ethyl·

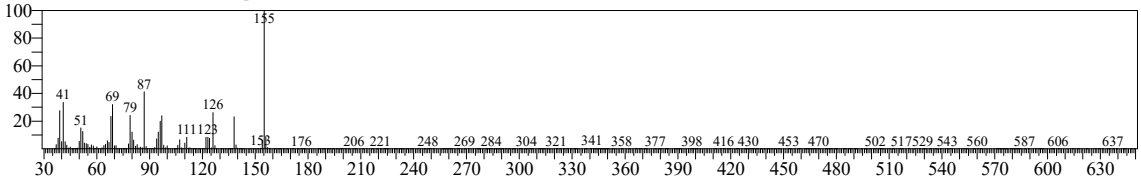


Hit#:5 Entry:11222 Library:NIST20M1.lib
SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

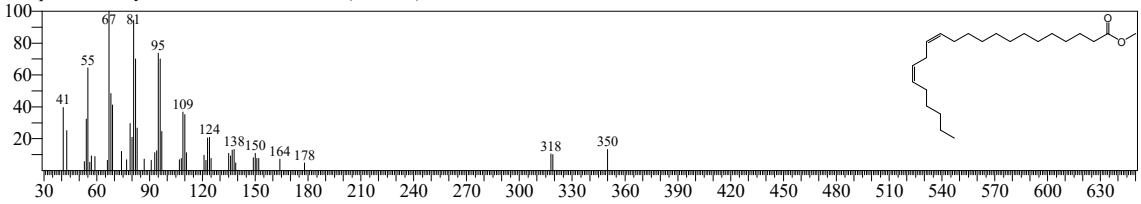


TNAU

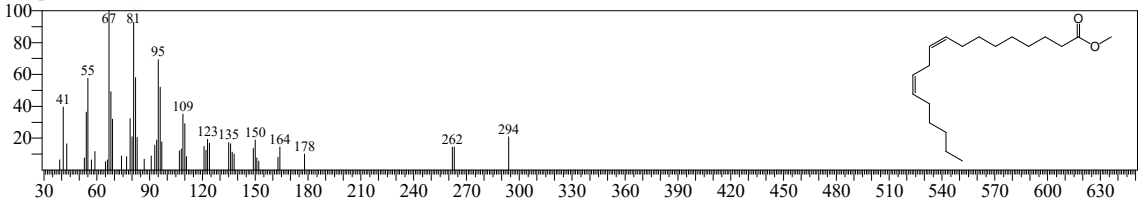
<< Target >>
Line#:6 R.Time:13.355(Scan#:1672) MassPeaks:340
RawMode:Averaged 13.350-13.360(1671-1673) BasePeak:155.05(54323)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



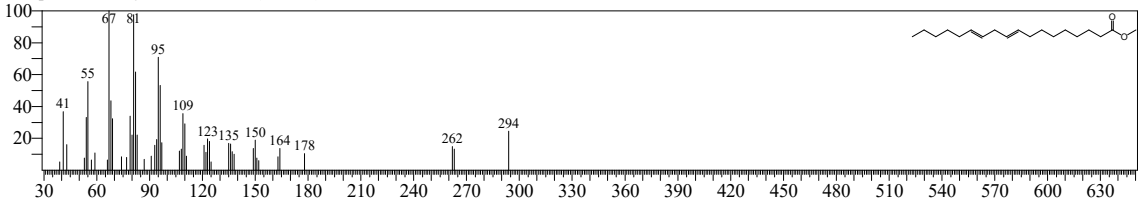
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



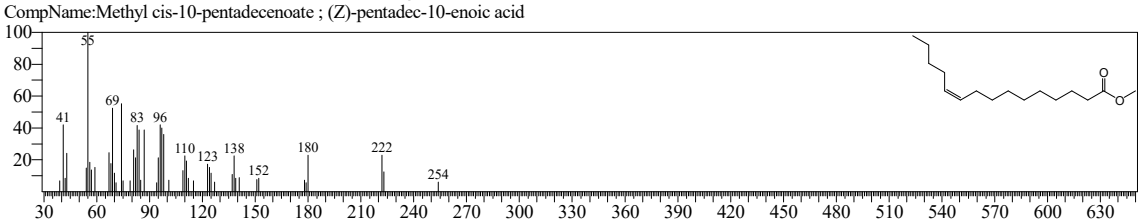
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



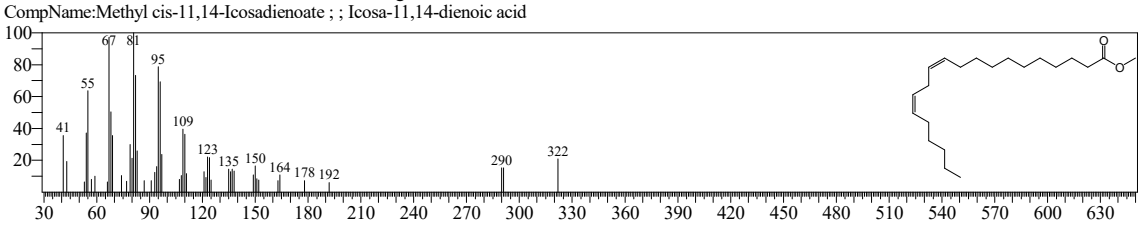
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

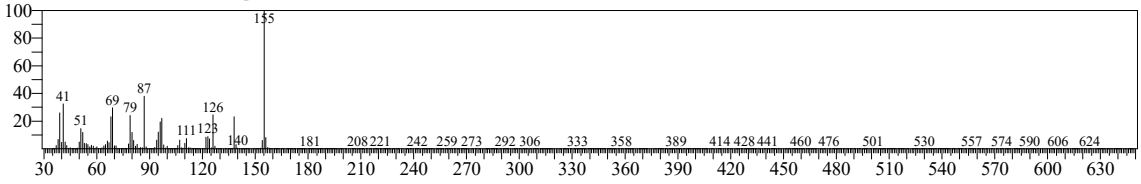


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

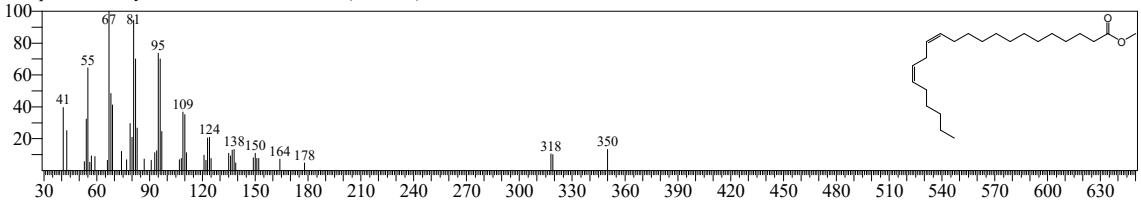


TNAU

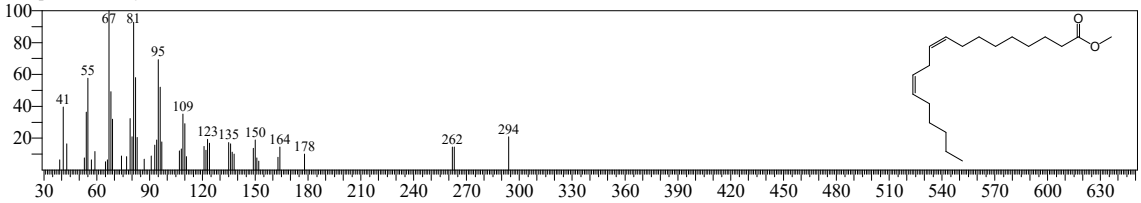
<< Target >>
Line#:7 R.Time:13.545(Scan#:1710) MassPeaks:433
RawMode:Averaged 13.540-13.550(1709-1711) BasePeak:155.05(51962)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



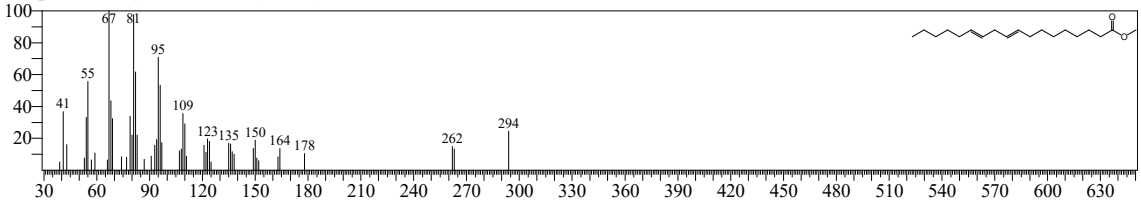
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



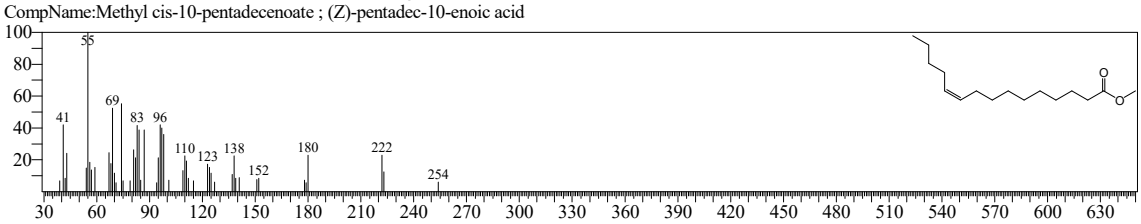
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



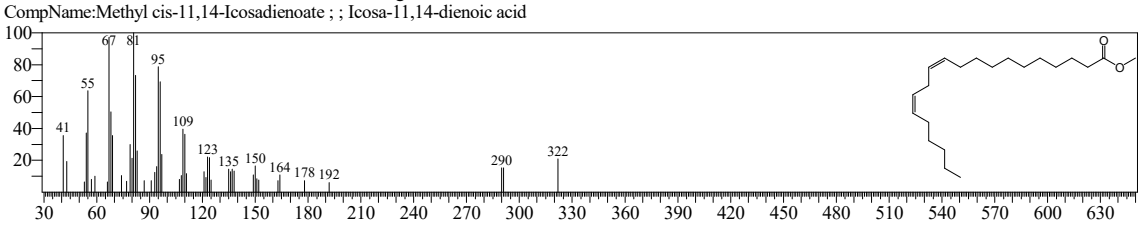
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

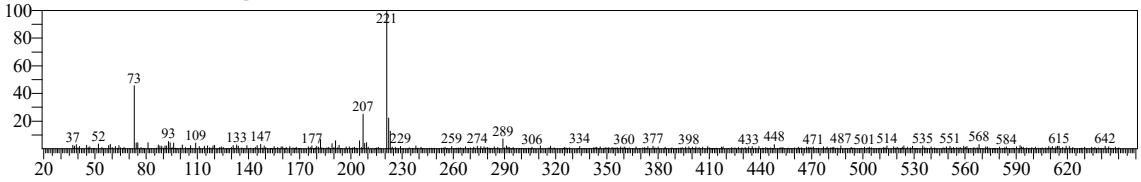


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

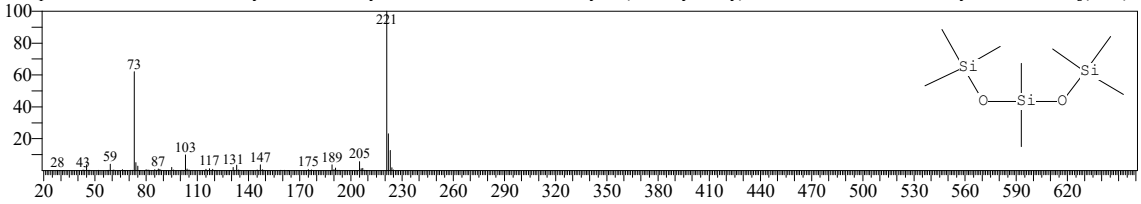


TNAU

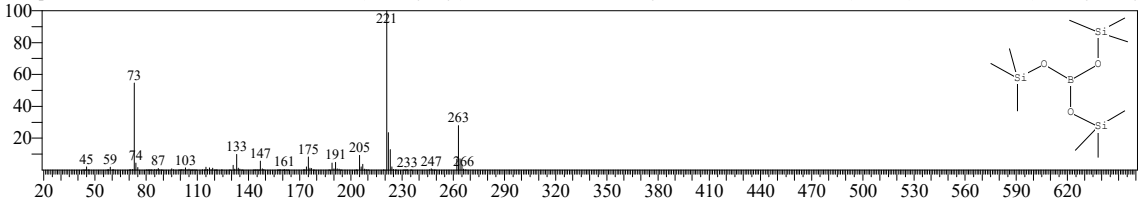
<< Target >>
Line#:8 R.Time:13.820(Scan#:1765) MassPeaks:390
RawMode:Averaged 13.815-13.825(1764-1766) BasePeak:221.05(1784)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



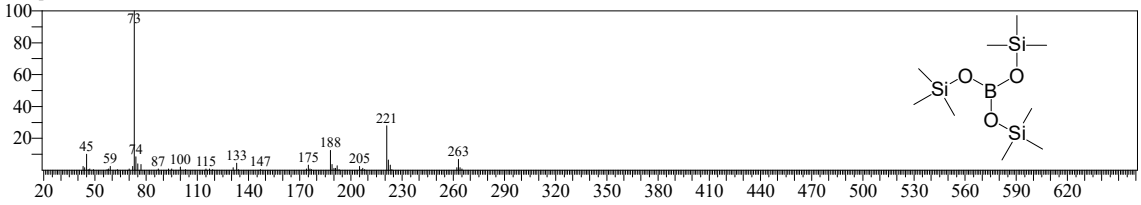
Hit#:1 Entry:28950 Library:NIST20R.lib
SI:77 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3



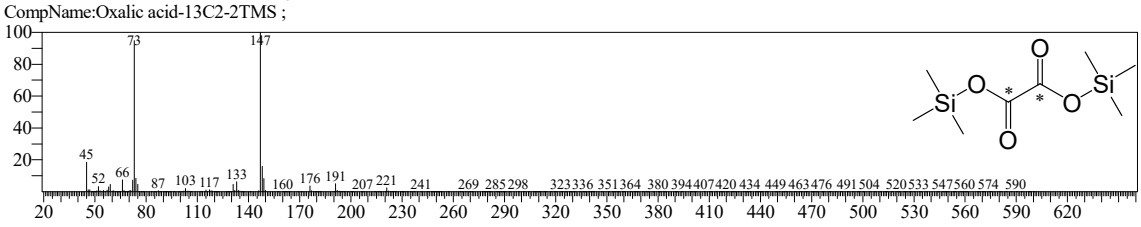
Hit#:2 Entry:33791 Library:NIST20R.lib
SI:71 Formula:C9H27BO3Si3 CAS:4325-85-3 MolWeight:278 RetIndex:0
CompName:Boric acid, 3TMS derivative $$ Tris(trimethylsilyl)borate $$ Silanol, trimethyl-, triester with boric acid (H3BO3) $$ Borane, tris(trimethylsiloxy



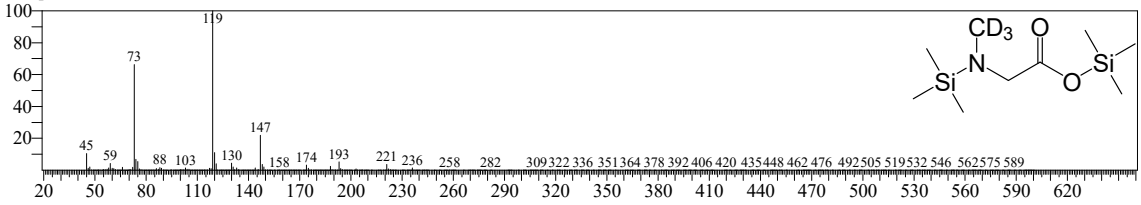
Hit#:3 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
SI:58 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid



Hit#:4 Entry:24 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula: CAS:0-00-0 MolWeight:236 RetIndex:1130
CompName:Oxalic acid-13C2-2TMS ;

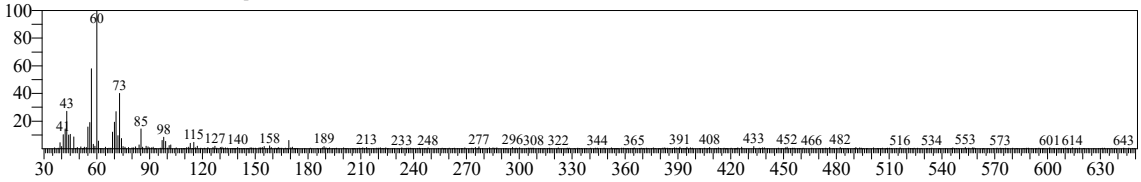


Hit#:5 Entry:28 Library:OA_TMS_DB5_67min_V3.lib
SI:49 Formula: CAS:347840-04-4 MolWeight:236 RetIndex:1140
CompName:Sarcosine-d3-2TMS ;

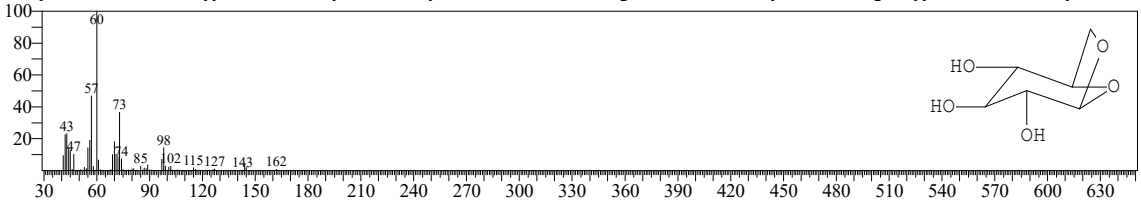


TNAU

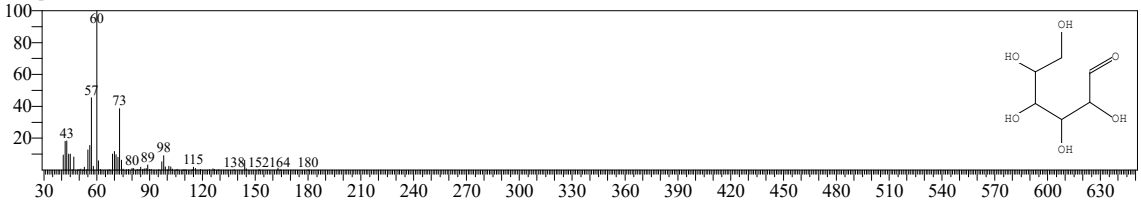
<< Target >>
Line#:9 R.Time:18.075(Scan#:2616) MassPeaks:373
RawMode:Averaged 18.070-18.080(2615-2617) BasePeak:60.00(3769)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



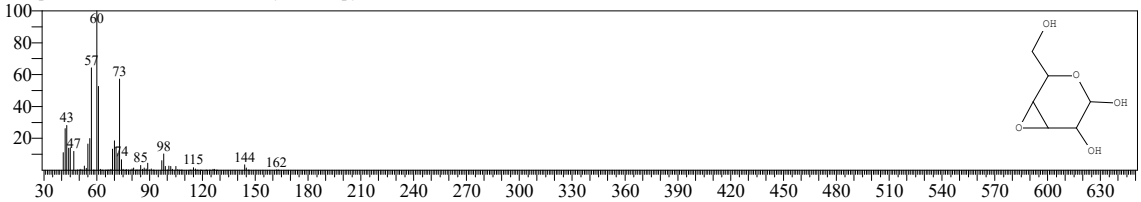
Hit#:1 Entry:13905 Library:NIST20R.lib
SI:89 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-



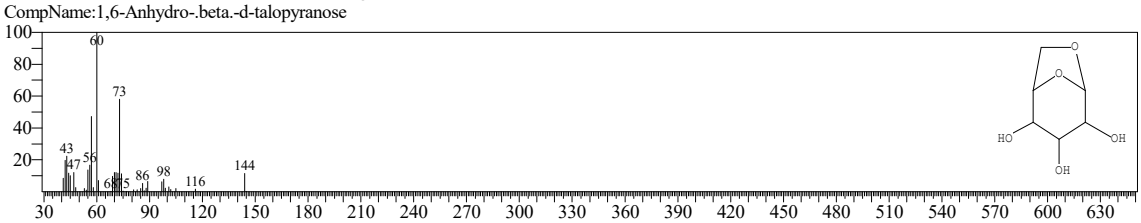
Hit#:2 Entry:36240 Library:NIST20M1.lib
SI:89 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #



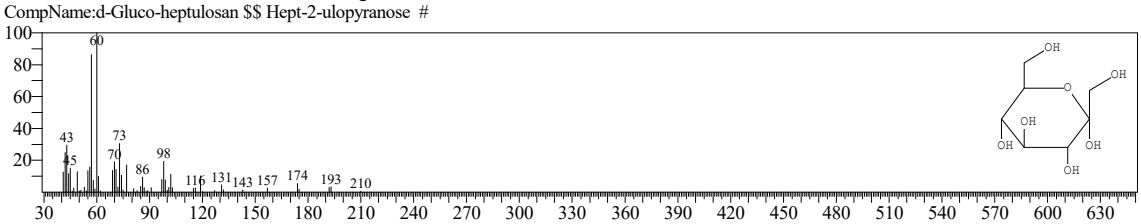
Hit#:3 Entry:23808 Library:NIST20M1.lib
SI:88 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1400
CompName:3,4-Altrosan $$ 3,4-Anhydrohexopyranose #



Hit#:4 Entry:23812 Library:NIST20M1.lib
SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose

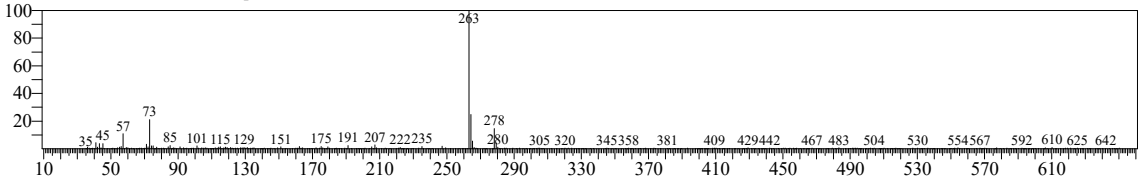


Hit#:5 Entry:62131 Library:NIST20M1.lib
SI:82 Formula:C7H14O7 CAS:0-00-0 MolWeight:210 RetIndex:2031
CompName:d-Gluco-heptulosan $$ Hept-2-ulopyranose #

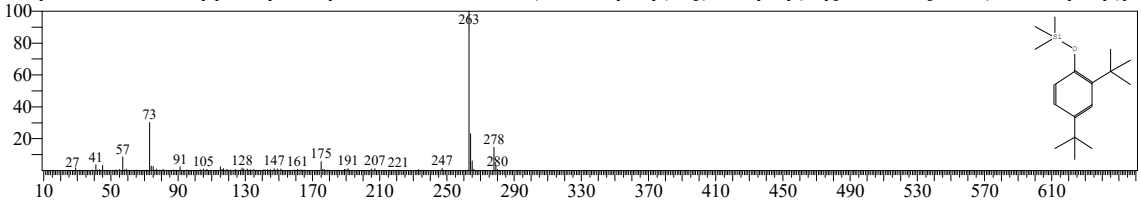


TNAU

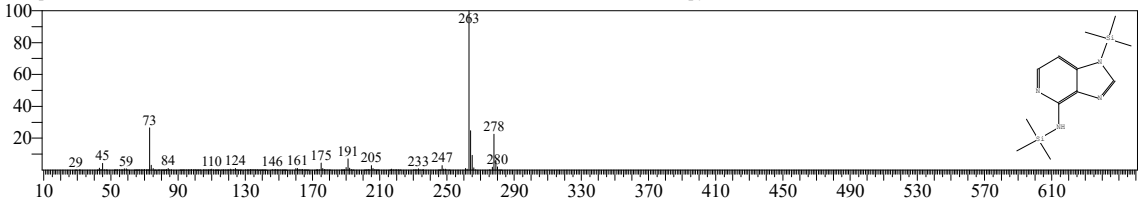
<< Target >>
Line#:10 R.Time:19.190(Scan#:2839) MassPeaks:386
RawMode:Averaged 19.185-19.195(2838-2840) BasePeak:263.15(6589)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



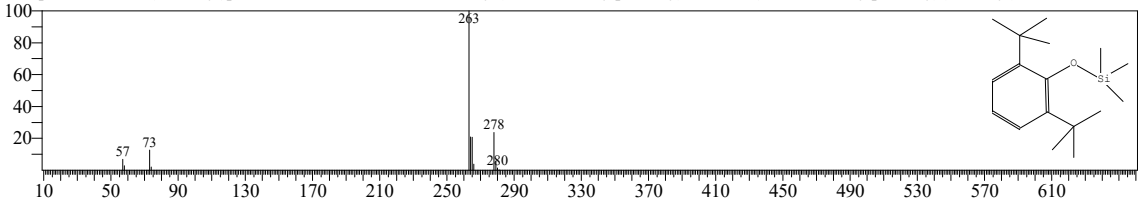
Hit#:1 Entry:137399 Library:NIST20M1.lib
SI:88 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph



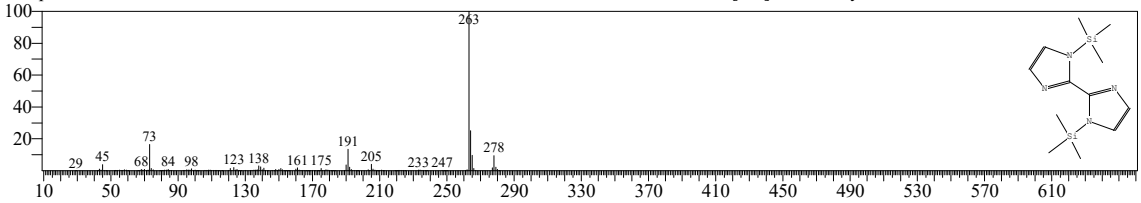
Hit#:2 Entry:136557 Library:NIST20M1.lib
SI:82 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



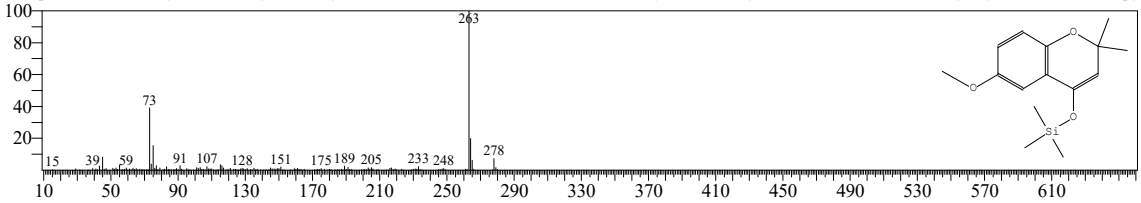
Hit#:3 Entry:33871 Library:NIST20R.lib
SI:80 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #



Hit#:4 Entry:136556 Library:NIST20M1.lib
SI:78 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

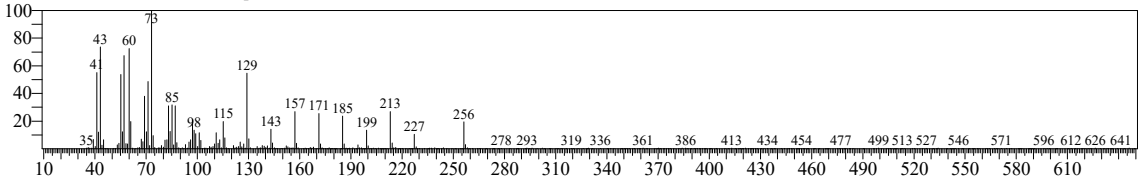


Hit#:5 Entry:137020 Library:NIST20M1.lib
SI:77 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy

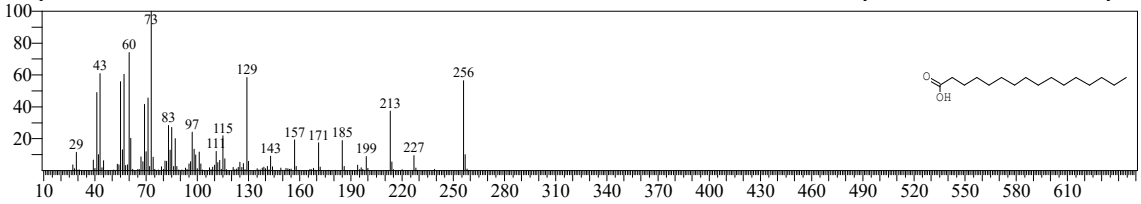


TNAU

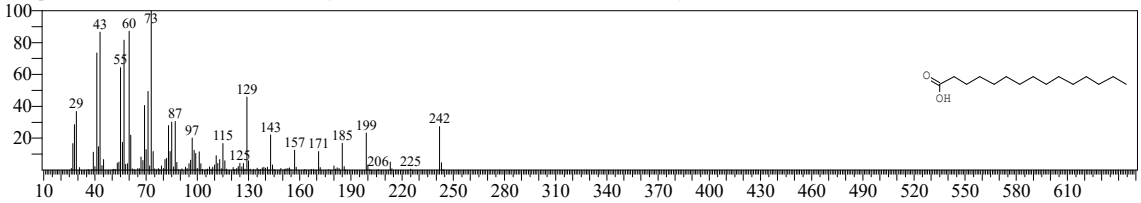
<< Target >>
Line#:11 R.Time:28.305(Scan#:4662) MassPeaks:391
RawMode:Averaged 28.300-28.310(4661-4663) BasePeak:73.05(8095)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



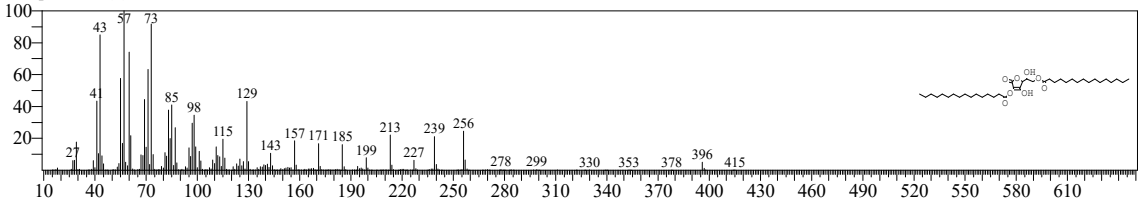
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



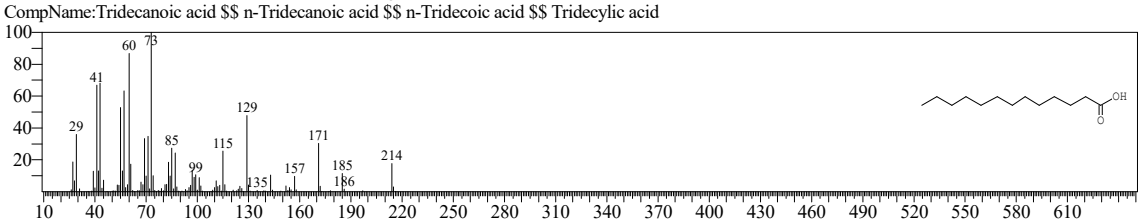
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:91 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



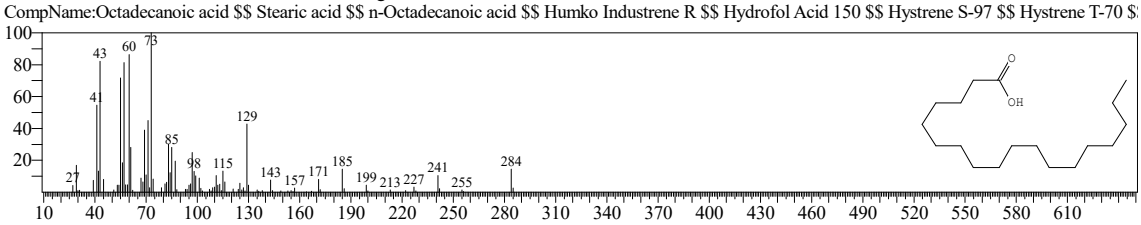
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:90 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



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

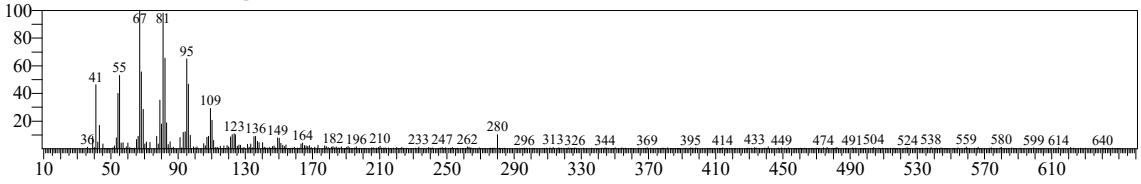


Hit#:5 Entry:144781 Library:NIST20M1.lib
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $

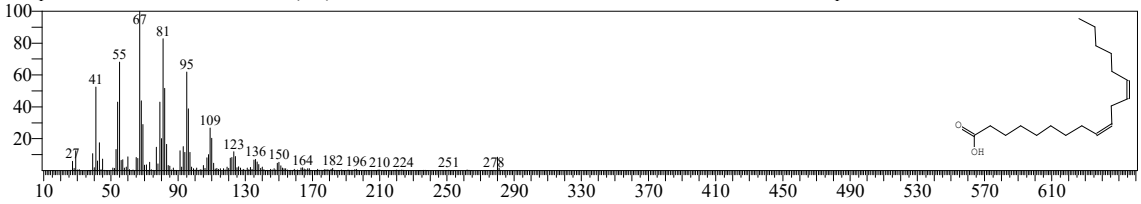


TNAU

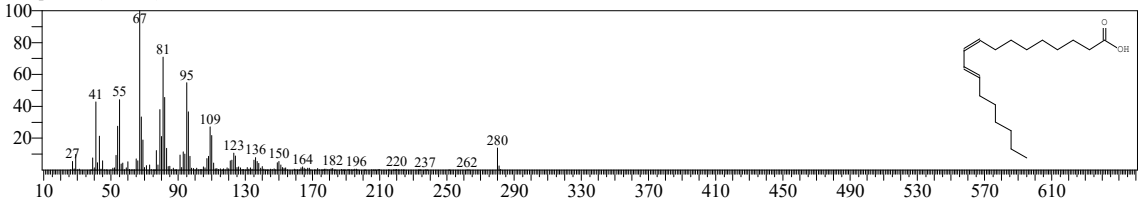
<< Target >>
Line#:12 R.Time:31.475(Scan#:5296) MassPeaks:383
RawMode:Averaged 31.470-31.480(5295-5297) BasePeak:67.05(3708)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



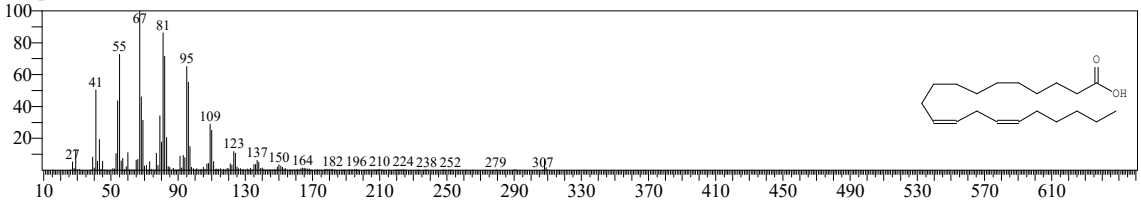
Hit#:1 Entry:34035 Library:NIST20R.lib
SI:94 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



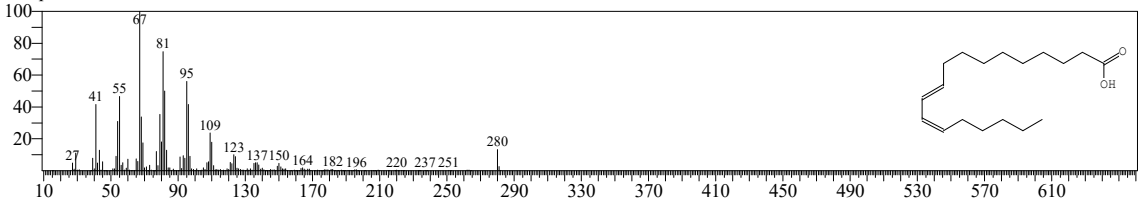
Hit#:2 Entry:139651 Library:NIST20M1.lib
SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



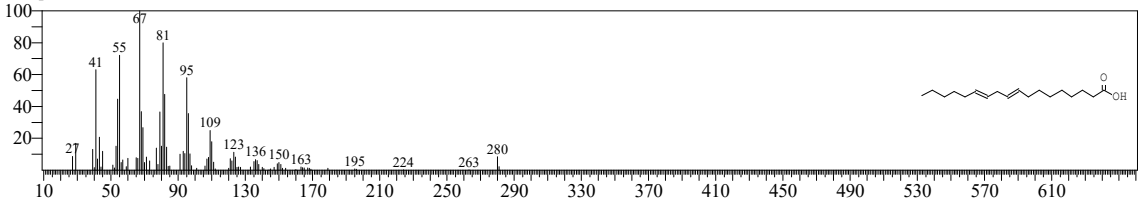
Hit#:3 Entry:173215 Library:NIST20M1.lib
SI:93 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382
CompName:11,14-Eicosadienoic acid



Hit#:4 Entry:139646 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid

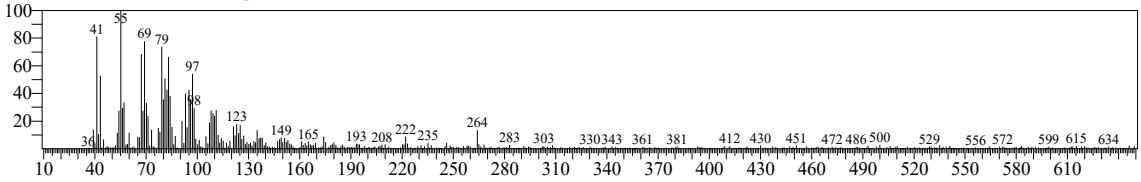


Hit#:5 Entry:139661 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

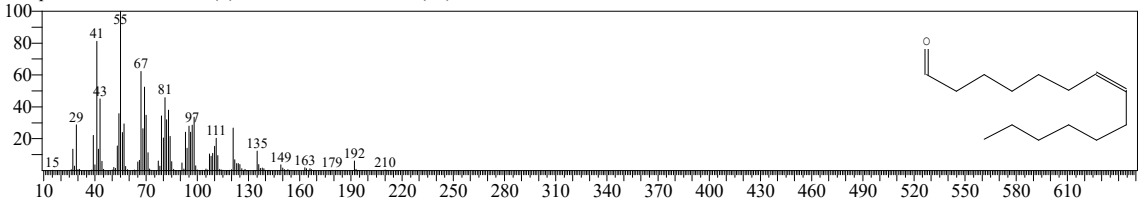


TNAU

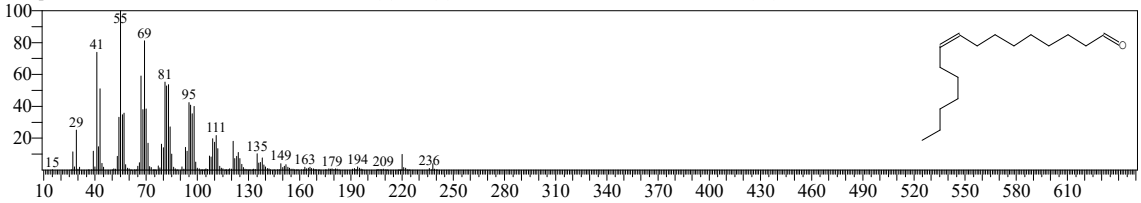
<< Target >>
Line#:13 R.Time:31.585(Scan#:5318) MassPeaks:405
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:55.10(1827)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



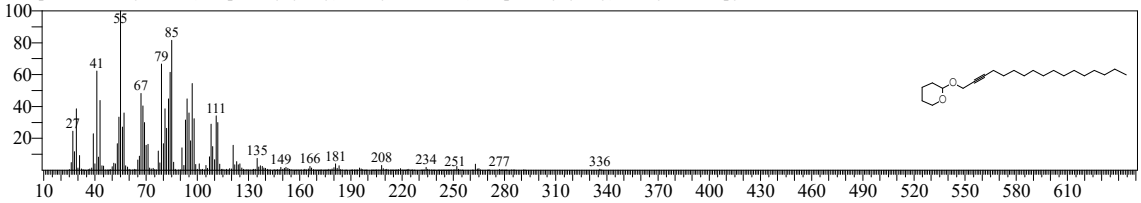
Hit#:1 Entry:63176 Library:NIST20M1.lib
SI:87 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #



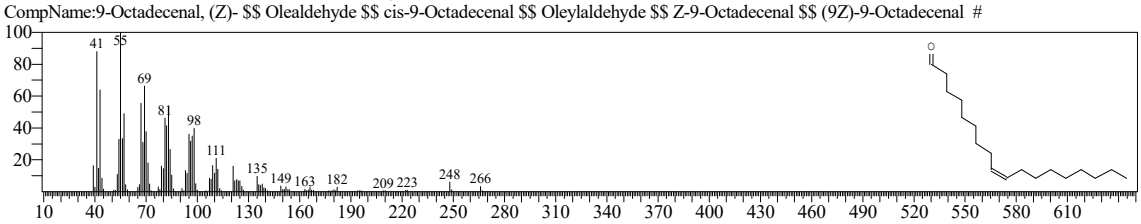
Hit#:2 Entry:92244 Library:NIST20M1.lib
SI:87 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #



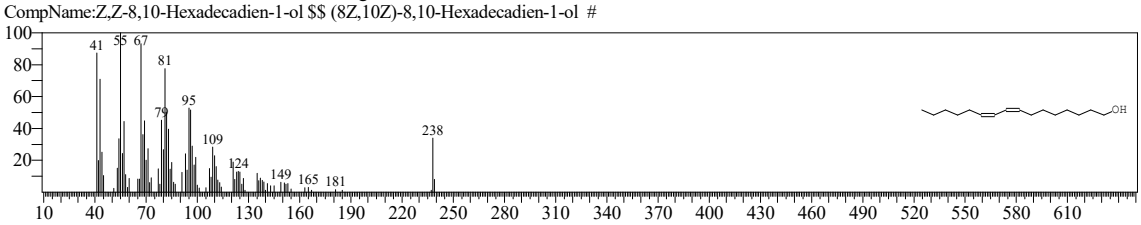
Hit#:3 Entry:205575 Library:NIST20M1.lib
SI:87 Formula:C22H40O2 CAS:69502-96-1 MolWeight:336 RetIndex:2453
CompName:2H-Pyran, 2-(2-heptadecynyloxy)tetrahydro- $$ 2-(2-Heptadecynyloxy)tetrahydro-2H-pyran #



Hit#:4 Entry:123421 Library:NIST20M1.lib
SI:86 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 #

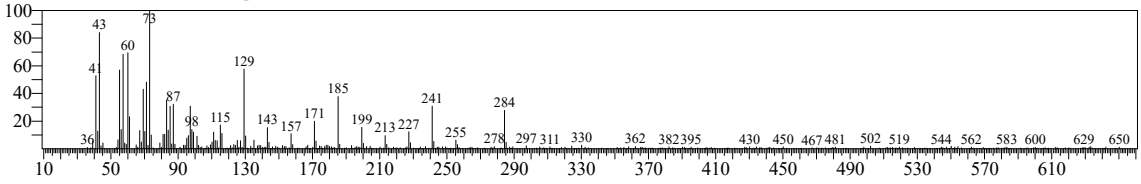


Hit#:5 Entry:92234 Library:NIST20M1.lib
SI:86 Formula:C16H30O CAS:0-00-0 MolWeight:238 RetIndex:1870
CompName:Z,Z-8,10-Hexadecadien-1-ol $$ (8Z,10Z)-8,10-Hexadecadien-1-ol #

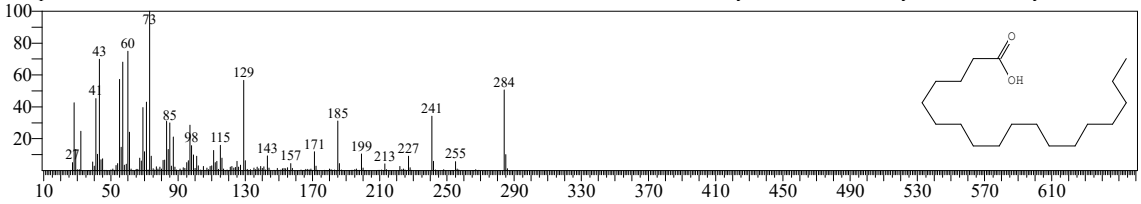


TNAU

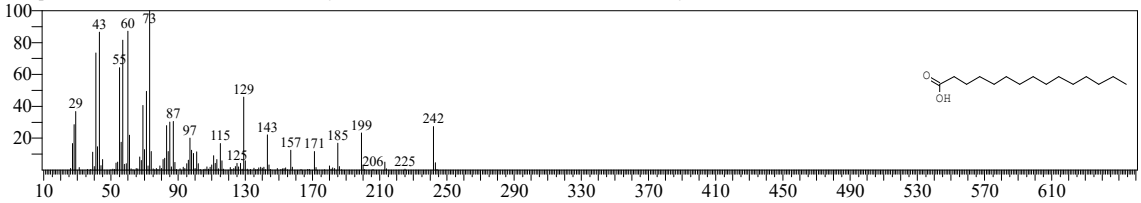
<< Target >>
Line#:14 R.Time:32.035(Scan#:5408) MassPeaks:370
RawMode:Averaged 32.030-32.040(5407-5409) BasePeak:73.05(2239)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



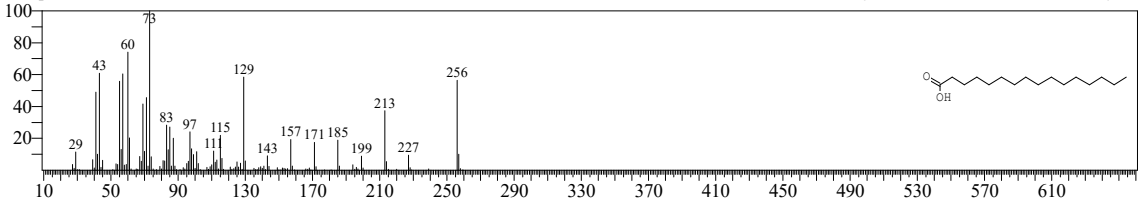
Hit#:1 Entry:34463 Library:NIST20R.lib
SI:93 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



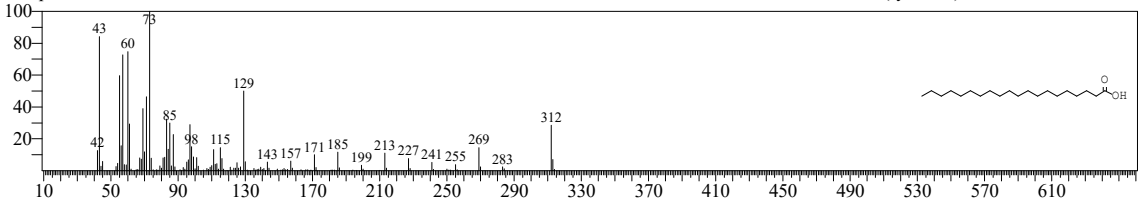
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:90 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



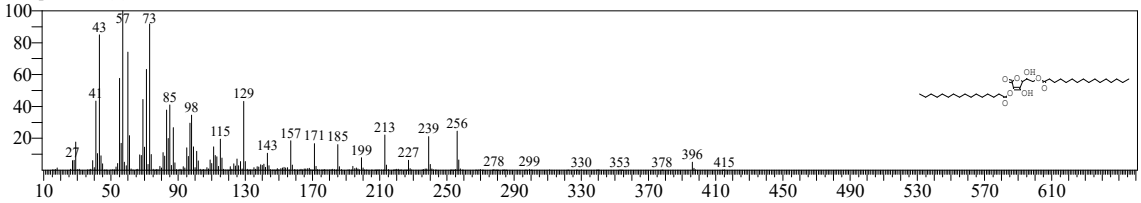
Hit#:3 Entry:31600 Library:NIST20R.lib
SI:88 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



Hit#:4 Entry:178153 Library:NIST20M1.lib
SI:88 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)

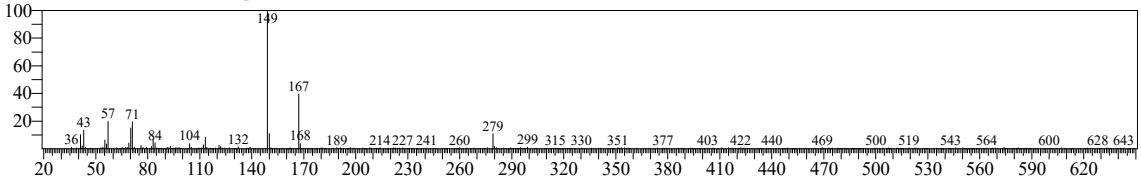


Hit#:5 Entry:44286 Library:NIST20M2.lib
SI:87 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

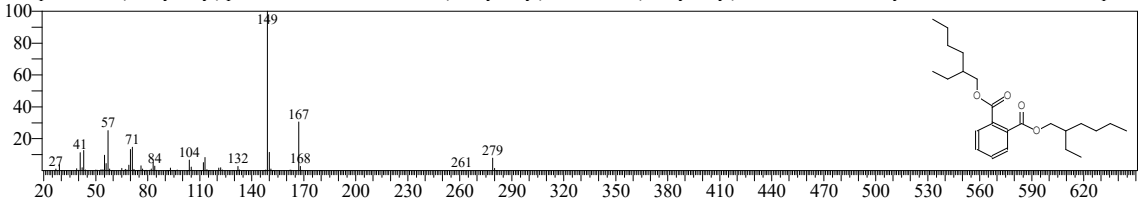


TNAU

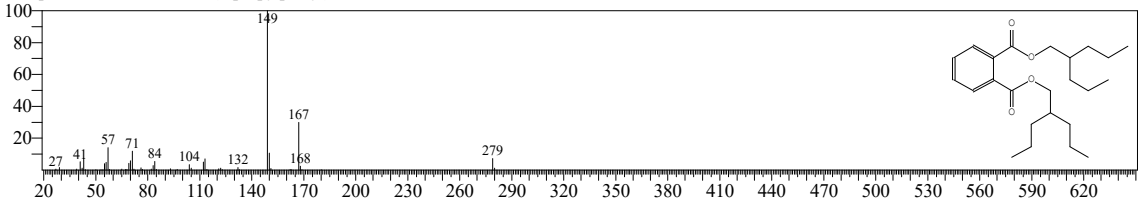
<< Target >>
Line#:15 R.Time:39.915(Scan#:6984) MassPeaks:369
RawMode:Averaged 39.910-39.920(6983-6985) BasePeak:149.00(5502)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



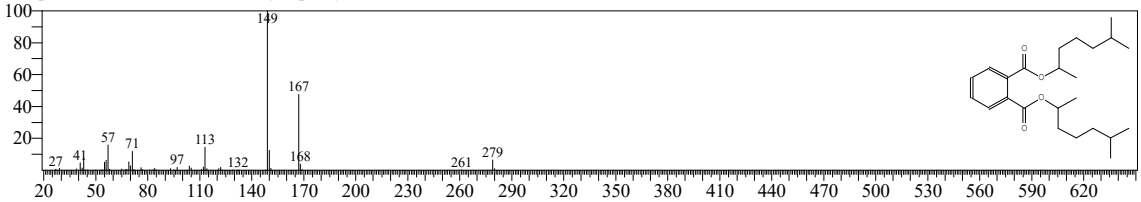
Hit#:1 Entry:41263 Library:NIST20R.lib
SI:94 Formula:C24H38O4 CAS:117-81-7 MolWeight:390 RetIndex:2704
CompName:Bis(2-ethylhexyl) phthalate $$ Phthalic acid, bis(2-ethylhexyl) ester $$ Bis(2-ethylhexyl) 1,2-benzenedicarboxylate $$ Bisoflex 81 $$ Compoun



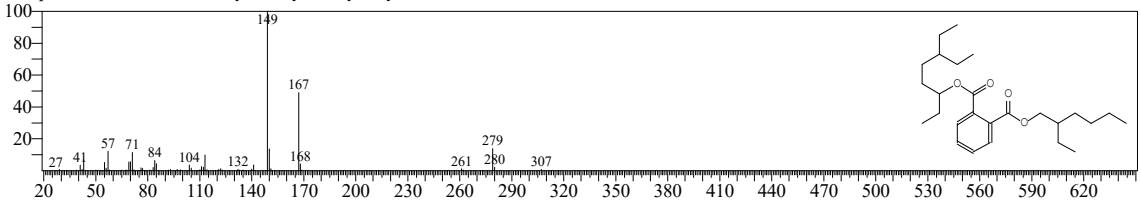
Hit#:2 Entry:254434 Library:NIST20M1.lib
SI:91 Formula:C24H38O4 CAS:0-00-0 MolWeight:390 RetIndex:2704
CompName:Phthalic acid, di(2-propylpentyl) ester



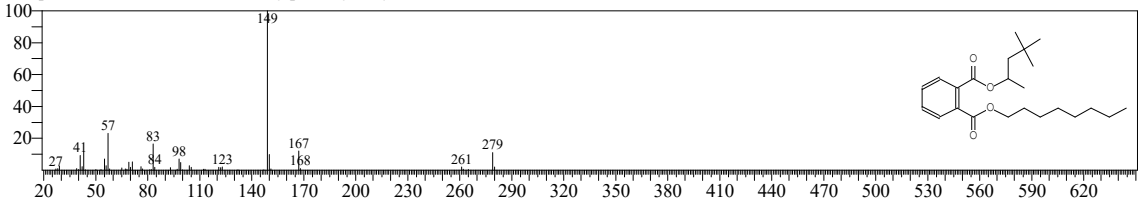
Hit#:3 Entry:254360 Library:NIST20M1.lib
SI:90 Formula:C24H38O4 CAS:0-00-0 MolWeight:390 RetIndex:2575
CompName:Phthalic acid, di(6-methylhept-2-yl) ester



Hit#:4 Entry:10247 Library:NIST20M2.lib
SI:88 Formula:C26H42O4 CAS:0-00-0 MolWeight:418 RetIndex:2838
CompName:Phthalic acid, 6-ethyloct-3-yl 2-ethylhexyl ester

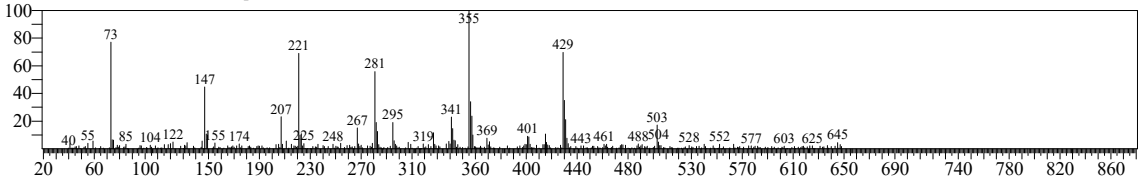


Hit#:5 Entry:244058 Library:NIST20M1.lib
SI:87 Formula:C23H36O4 CAS:0-00-0 MolWeight:376 RetIndex:2584
CompName:Phthalic acid, 4,4-dimethylpent-2-yl octyl ester

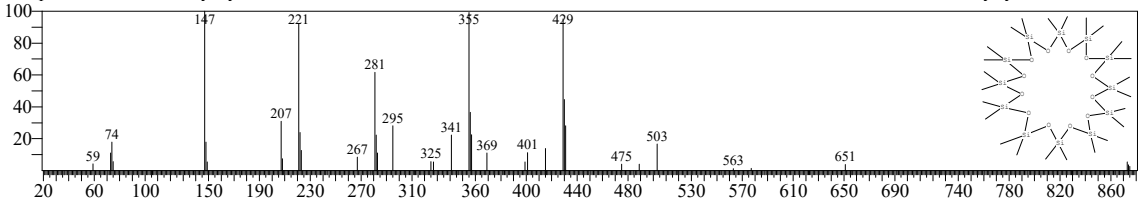


TNAU

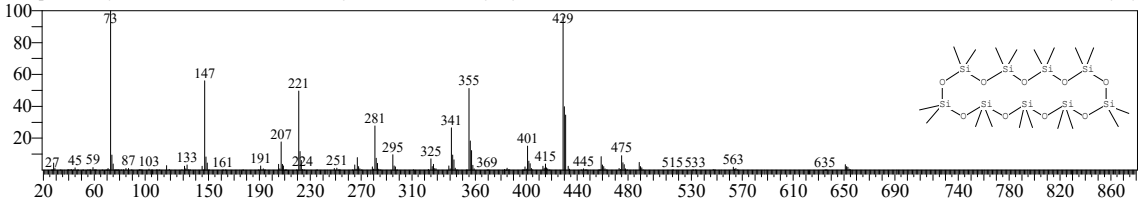
<< Target >>
Line#:16 R.Time:41.590(Scan#:7319) MassPeaks:363
RawMode:Averaged 41.585-41.595(7318-7320) BasePeak:355.05(1138)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



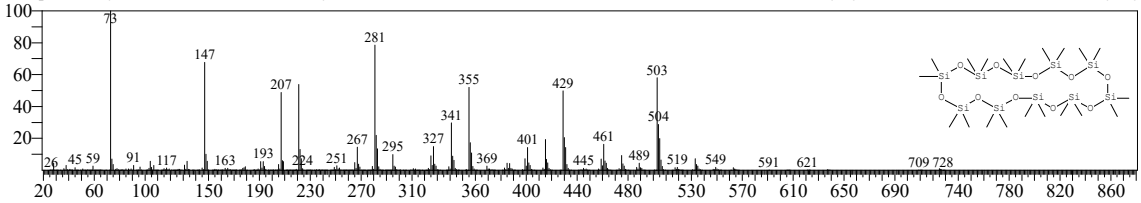
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:83 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



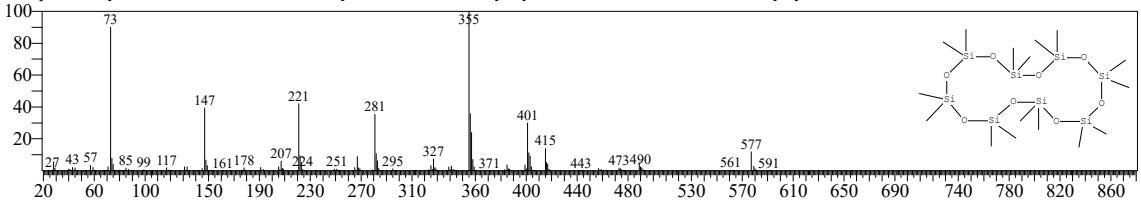
Hit#:2 Entry:44570 Library:NIST20M2.lib
SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



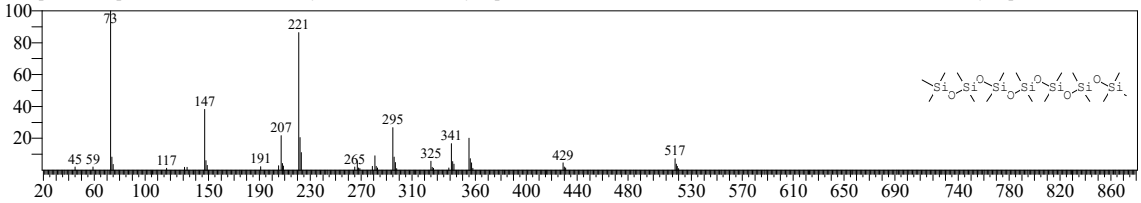
Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:77 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



Hit#:4 Entry:42384 Library:NIST20M2.lib
SI:71 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12

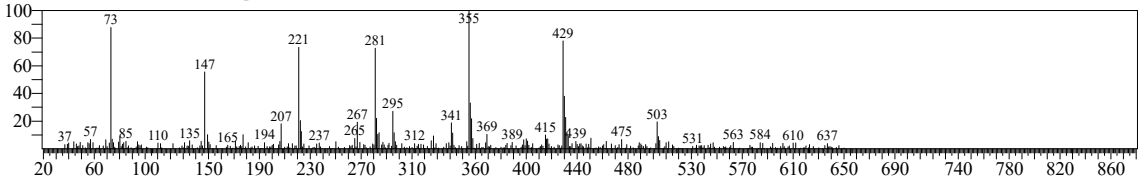


Hit#:5 Entry:38404 Library:NIST20M2.lib
SI:71 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #

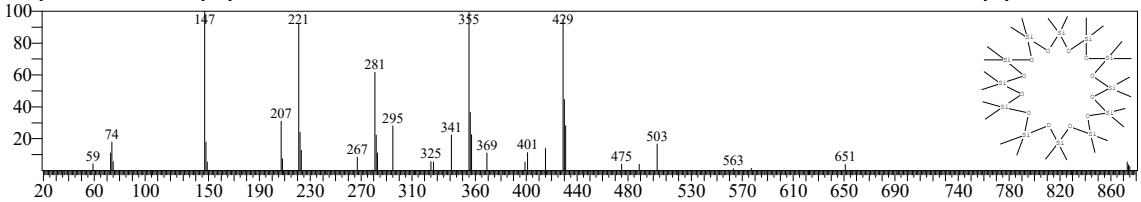


TNAU

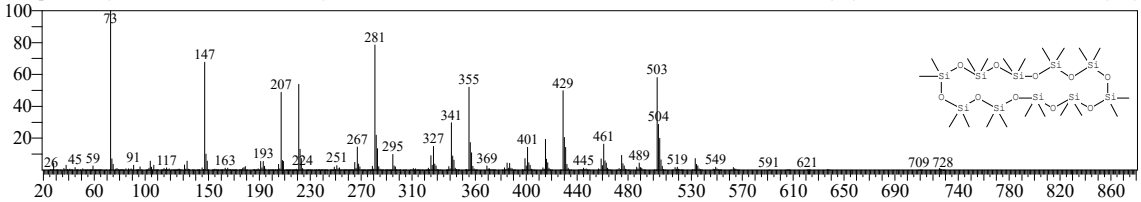
<< Target >>
Line#:17 R.Time:43.810(Scan#:7763) MassPeaks:350
RawMode:Averaged 43.805-43.815(7762-7764) BasePeak:355.00(762)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



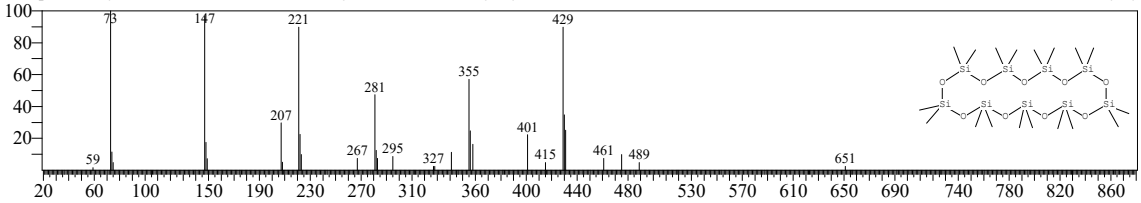
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:81 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



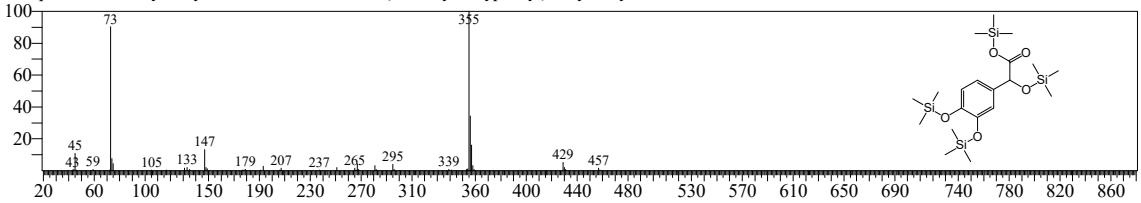
Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:78 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



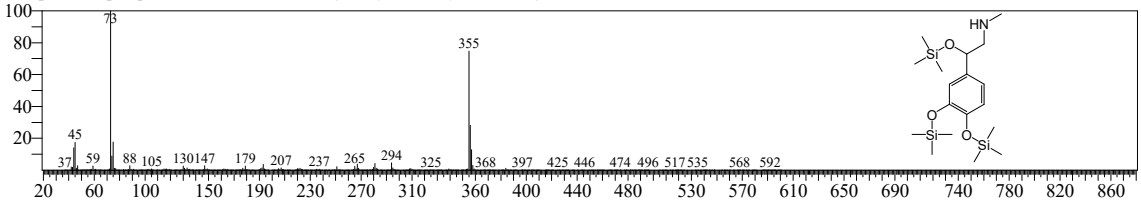
Hit#:3 Entry:43658 Library:NIST20R.lib
SI:77 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:59 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

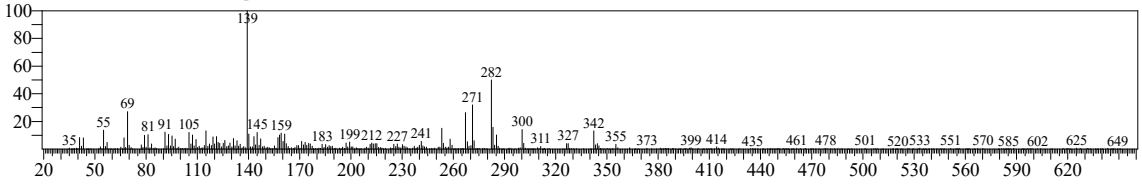


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:47 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

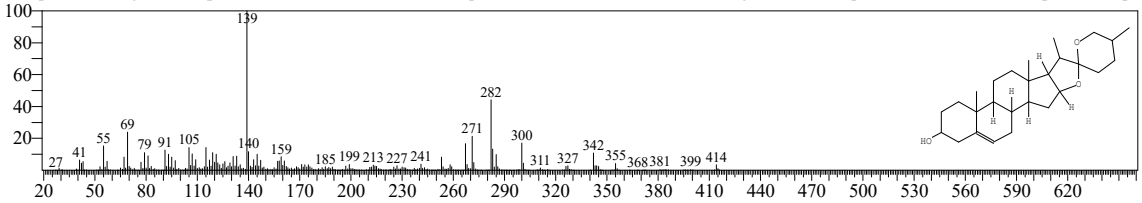


TNAU

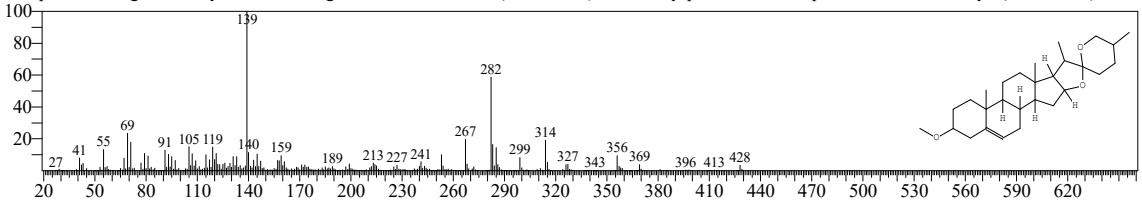
<< Target >>
Line#:18 R.Time:45.625(Scan#:8126) MassPeaks:412
RawMode:Averaged 45.620-45.630(8125-8127) BasePeak:139.10(5937)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



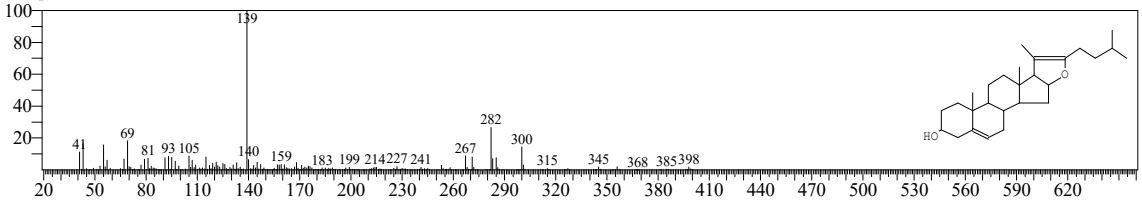
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:90 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



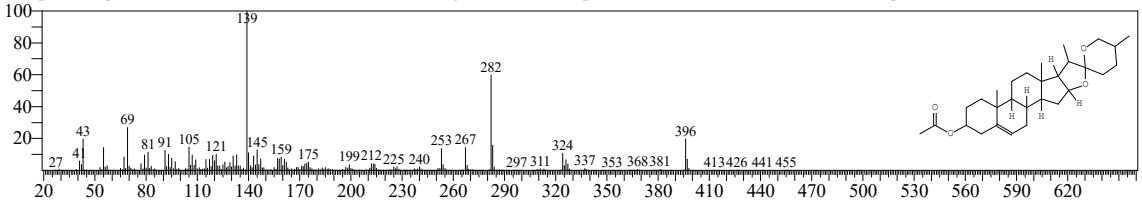
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:81 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#:3 Entry:41561 Library:NIST20R.lib
SI:80 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, (2



Hit#:5 Entry:42677 Library:NIST20R.lib
SI:74 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.