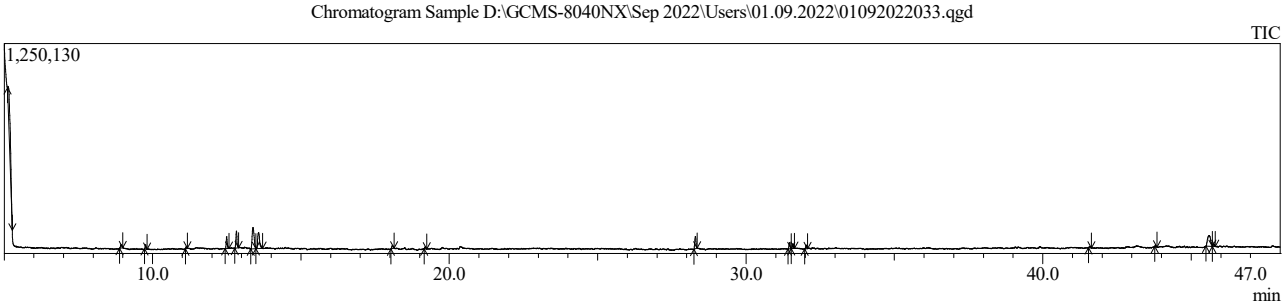
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 9:43:16 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 11-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 12
Injection Volume	: 5.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022033.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022033.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 11:11:35 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022033.qgd



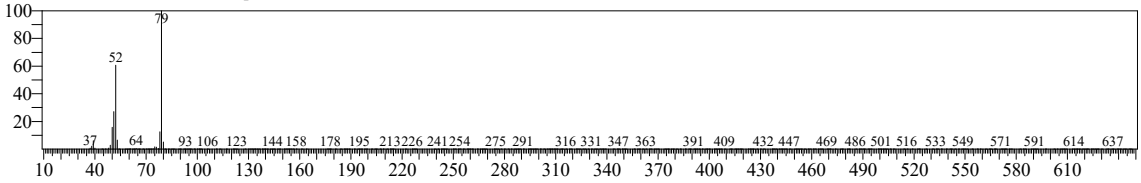
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	5.128	1347972	33.41	100619	12.17	13.40	98	Pyridine
2	8.942	67964	1.68	19921	2.41	3.41	81	1-Butanol, 3-methyl-, acetate
3	9.767	52986	1.31	24695	2.99	2.15	95	Pentasiloxane, dodecamethyl-
4	11.139	27297	0.68	11106	1.34	2.46	42	Fendiline
5	12.497	185299	4.59	71932	8.70	2.58	73	2,5-Cyclohexadiene-1,4-dione, dioxime
6	12.825	258389	6.40	100609	12.17	2.57	74	1,3-Benzodioxol-5-ol
7	13.381	585597	14.51	126682	15.32	4.62	51	Methyl cis-13,16-Docosadienate
8	13.573	433706	10.75	94192	11.39	4.60	53	Methyl cis-13,16-Docosadienate
9	18.090	56872	1.41	15935	1.93	3.57	90	.beta.-D-Glucopyranose, 1,6-anhydro-
10	19.193	30208	0.75	11242	1.36	2.69	84	2,4-Di-tert-butylphenoxytrimethylsilane
11	28.294	200364	4.97	73546	8.89	2.72	95	n-Hexadecanoic acid
12	31.467	102688	2.55	36308	4.39	2.83	95	9,12-Octadecadienoic acid (Z,Z)-
13	31.574	77332	1.92	26877	3.25	2.88	87	E,E,Z-1,3,12-Nonadecatriene-5,14-diol
14	32.025	52805	1.31	22083	2.67	2.39	91	Octadecanoic acid
15	41.593	28393	0.70	8406	1.02	3.38	83	Tetracosamethyl-cyclododecasiloxane
16	43.795	19638	0.49	10672	1.29	1.84	77	Tetracosamethyl-cyclododecasiloxane
17	45.613	464890	11.52	63642	7.70	7.30	90	Diosgenin
18	45.790	42177	1.05	8499	1.03	4.96	44	3,4-Dihydroxymandelic acid-4TMS
		4034577	100.00	826966	100.00			

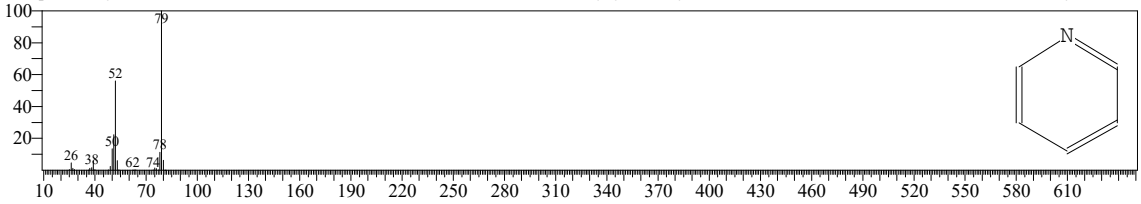
Library

TNAU

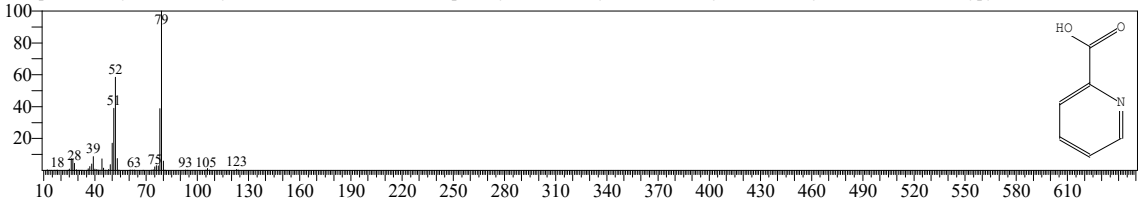
<< Target >>
Line#:1 R.Time:5.130(Scan#:27) MassPeaks:348
RawMode:Averaged 5.125-5.135(26-28) BasePeak:79.05(44966)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



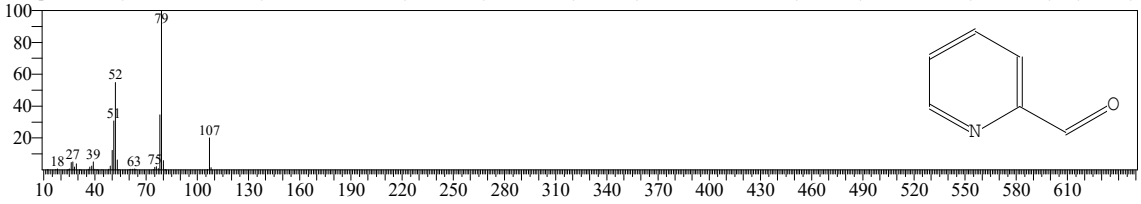
Hit#:1 Entry:498 Library:NIST20M1.lib
SI:98 Formula:C5H5N CAS:110-86-1 MolWeight:79 RetIndex:674
CompName:Pyridine $$ Azabenzene $$ Azine $$ NCI-C55301 $$ Piridina $$ Pirydyna $$ Pyridin $$ Rcra waste number U196 $$ UN 1282 $$ Pyr $$ CP



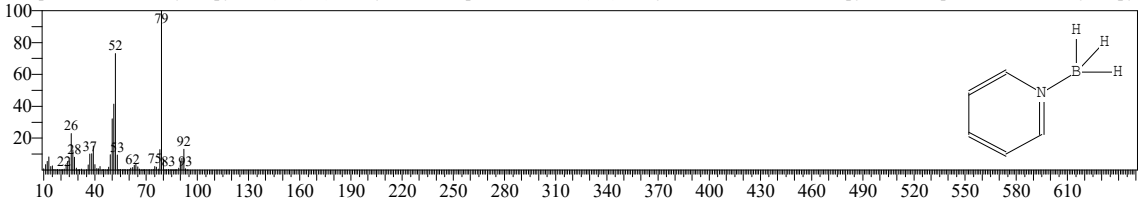
Hit#:2 Entry:6149 Library:NIST20M1.lib
SI:92 Formula:C6H5NO2 CAS:98-98-6 MolWeight:123 RetIndex:1144
CompName:2-Pyridinecarboxylic acid $$ Picolinic acid $$ .alpha.-Pyridinecarboxylic acid $$ o-Pyridinecarboxylic acid $$ 2-Carboxypyridine $$ 2-Picolini



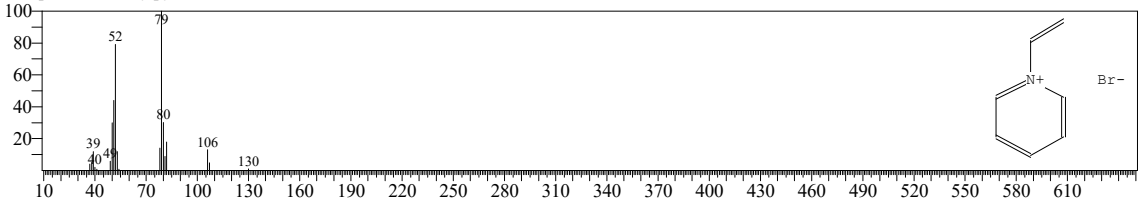
Hit#:3 Entry:2869 Library:NIST20M1.lib
SI:91 Formula:C6H5NO CAS:1121-60-4 MolWeight:107 RetIndex:976
CompName:2-Pyridinecarboxaldehyde $$ Picolinaldehyde $$ 2-Pyridinealdehyde $$ Pyridine-2-carboxaldehyde $$ Pyridine-2-aldehyde $$ 2-Pyridylaldehy



Hit#:4 Entry:1275 Library:NIST20M1.lib
SI:86 Formula:C5H8BN CAS:110-51-0 MolWeight:93 RetIndex:0
CompName:Boron, trihydro(pyridine)-, (T-4)- $$ Pyridine, compd. with borane (1:1) $$ Pyridine borane $$ Borane-pyridine complex $$ Boron, trihydro(py

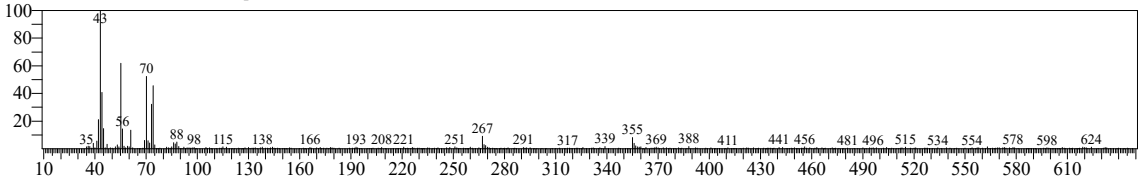


Hit#:5 Entry:40406 Library:NIST20M1.lib
SI:85 Formula:C7H8BrN CAS:0-00-0 MolWeight:185 RetIndex:0
CompName:N-Vinylpyridinium bromide

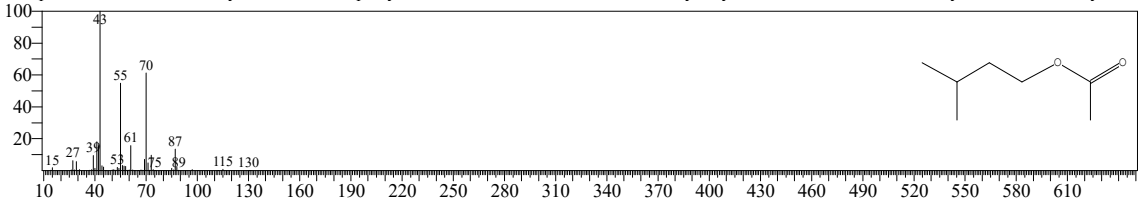


TNAU

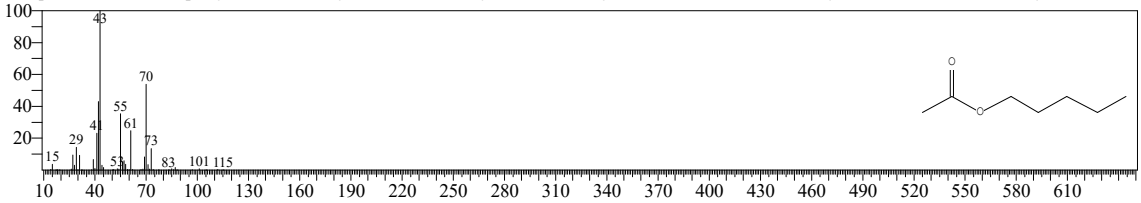
<< Target >>
Line#:2 R.Time:8.940(Scan#:789) MassPeaks:402
RawMode:Averaged 8.935-8.945(788-790) BasePeak:43.05(3373)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



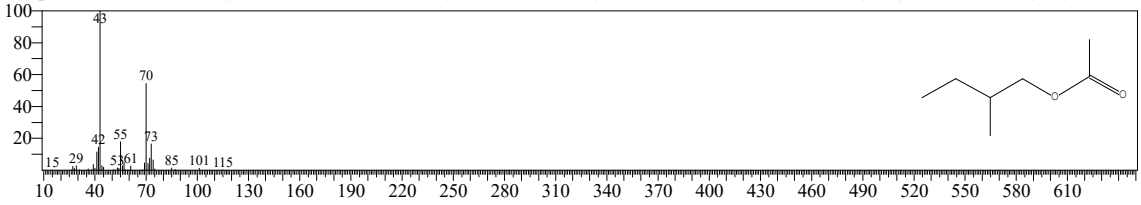
Hit#:1 Entry:6784 Library:NIST20R.lib
SI:81 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



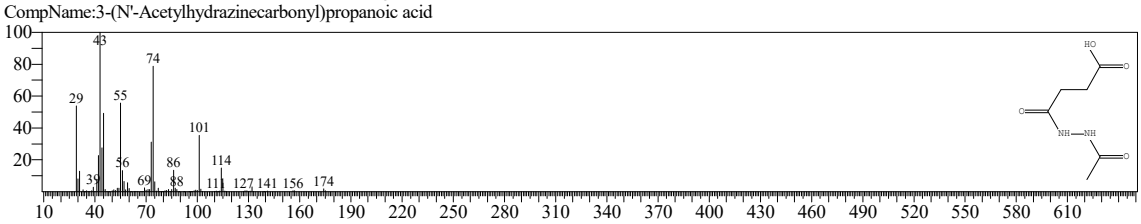
Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:78 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ An



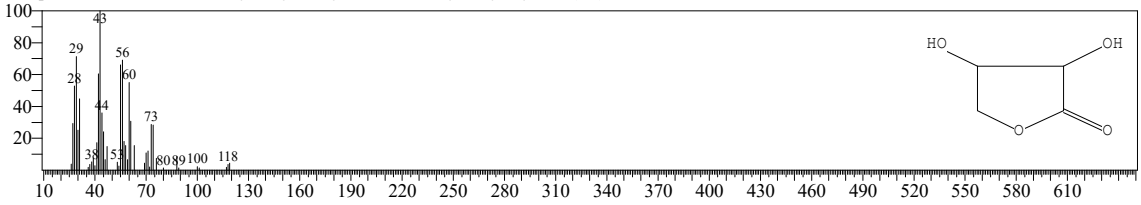
Hit#:3 Entry:6819 Library:NIST20R.lib
SI:78 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:32045 Library:NIST20M1.lib
SI:77 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid

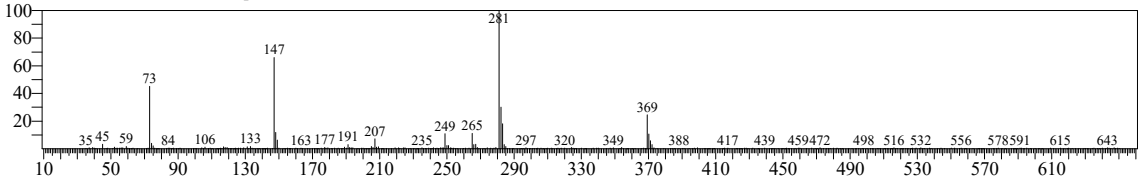


Hit#:5 Entry:5225 Library:NIST20M1.lib
SI:76 Formula:C4H6O4 CAS:17675-99-9 MolWeight:118 RetIndex:1201
CompName:2-Furanone, 3,4-dihydroxytetrahydro $$ 3,4-Dihydroxydihydro-2(3H)-furanone #

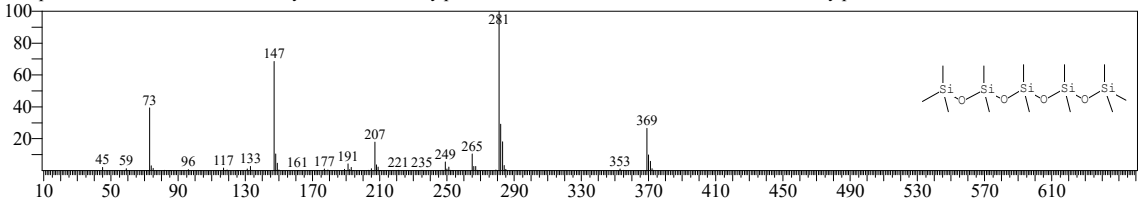


TNAU

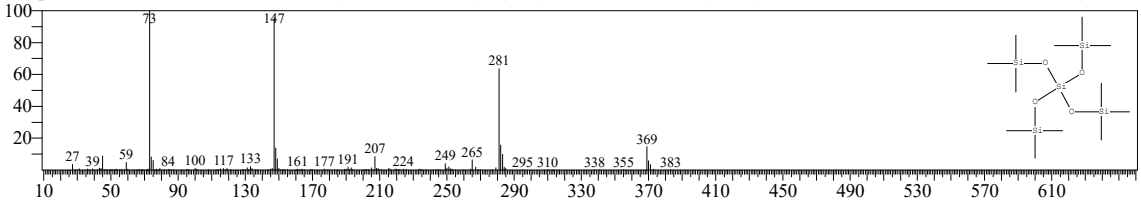
<< Target >>
Line#:3 R.Time:9.765(Scan#:954) MassPeaks:369
RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(5357)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



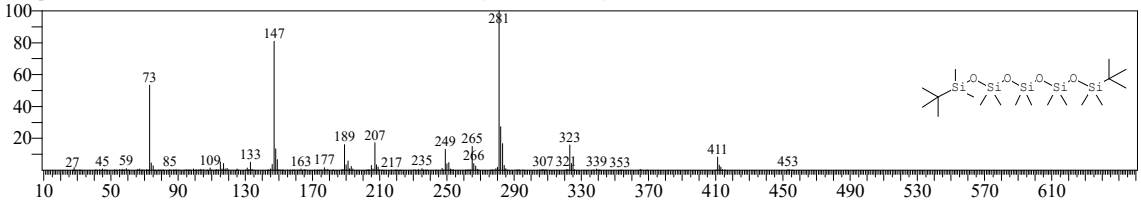
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:95 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



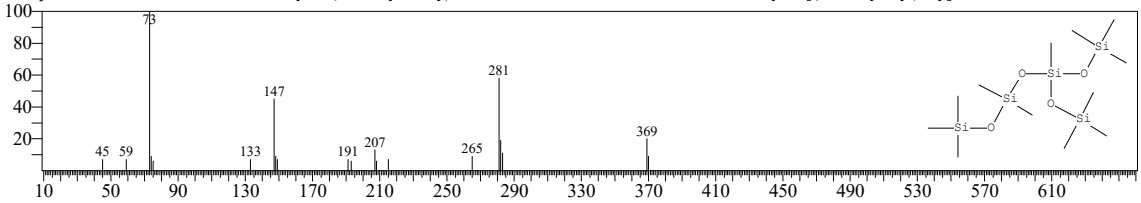
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:84 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



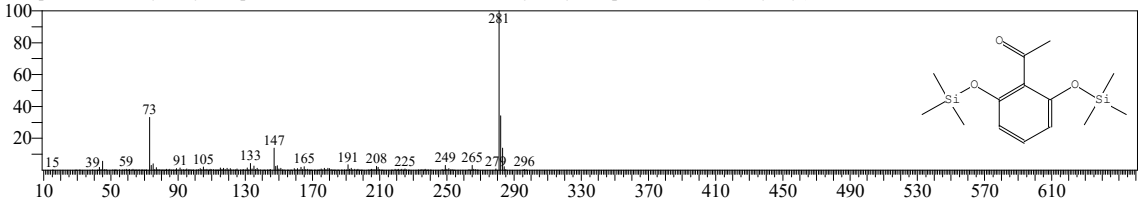
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:83 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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 #

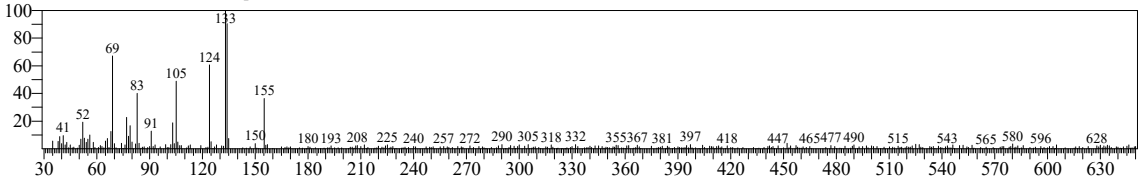


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

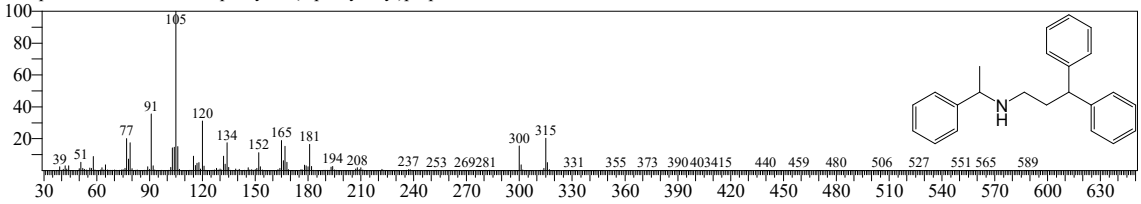


TNAU

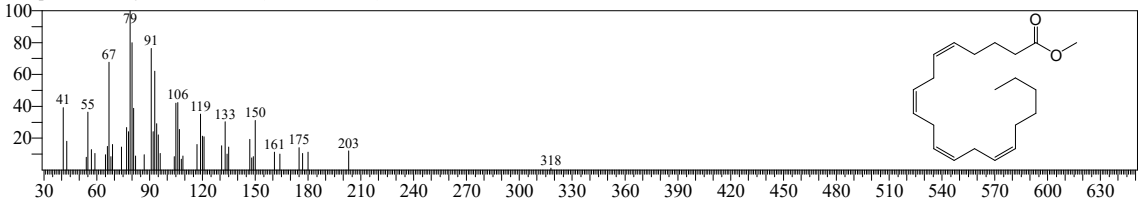
<< Target >>
Line#:4 R.Time:11.140(Scan#:1229) MassPeaks:379
RawMode:Averaged 11.135-11.145(1228-1230) BasePeak:133.05(1161)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



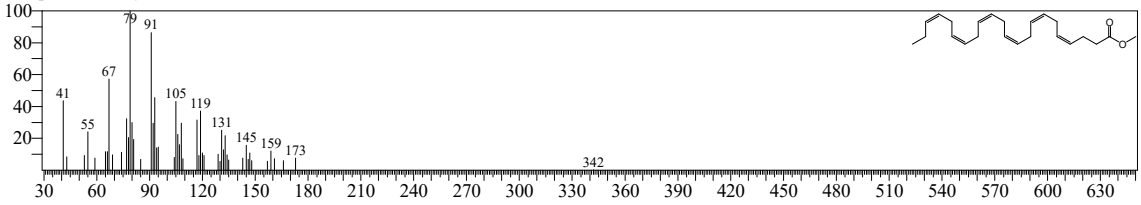
Hit#:1 Entry:530 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C23H25N CAS:13042-18-7 MolWeight:315 RetIndex:2545
CompName:Fendiline ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine



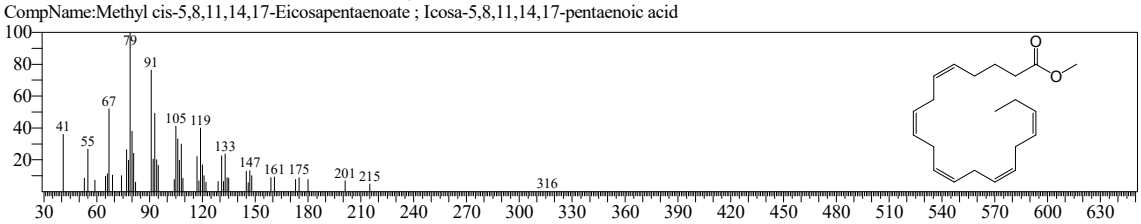
Hit#:2 Entry:33 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C21H34O2 CAS:506-32-1 MolWeight:318 RetIndex:3109
CompName:Methyl arachidonate ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid



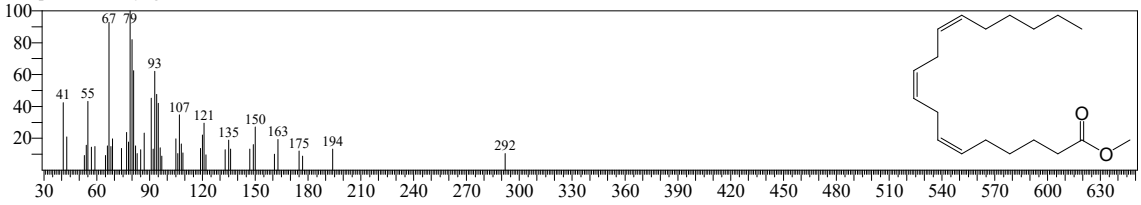
Hit#:3 Entry:38 Library:FA_ME_SP2560_EI_V3.lib
SI:40 Formula:C23H34O2 CAS:6217-54-5 MolWeight:342 RetIndex:3514
CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid



Hit#:4 Entry:36 Library:FA_ME_SP2560_EI_V3.lib
SI:40 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

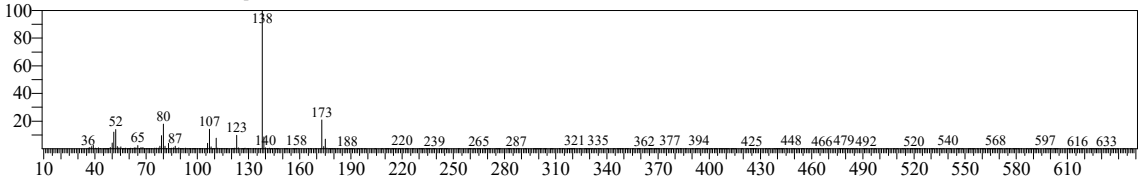


Hit#:5 Entry:23 Library:FA_ME_SP2560_EI_V3.lib
SI:36 Formula:C19H32O2 CAS:506-26-3 MolWeight:292 RetIndex:2852
CompName:Methyl ganma-linolenate ; ; Octadeca-6,9,12-trienoic acid

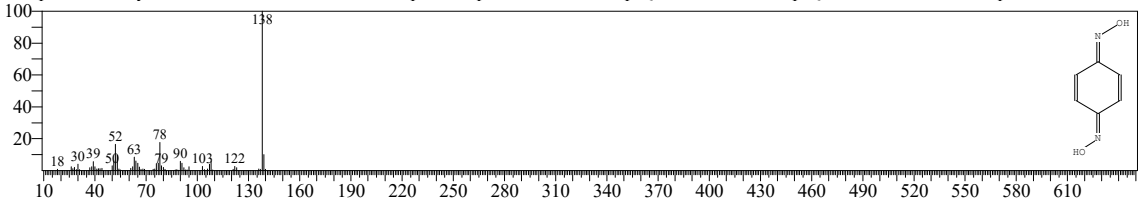


TNAU

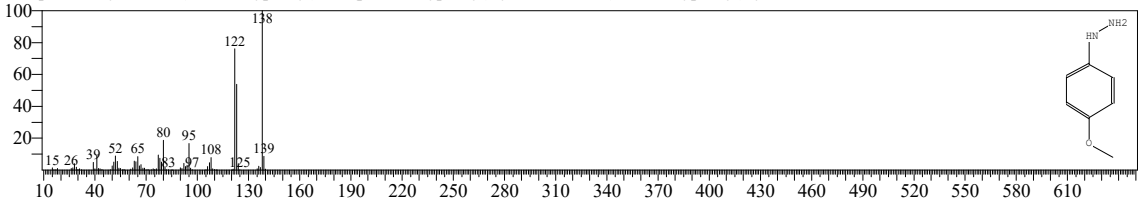
<< Target >>
Line#:5 R.Time:12.495(Scan#:1500) MassPeaks:378
RawMode:Averaged 12.490-12.500(1499-1501) BasePeak:138.05(25107)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



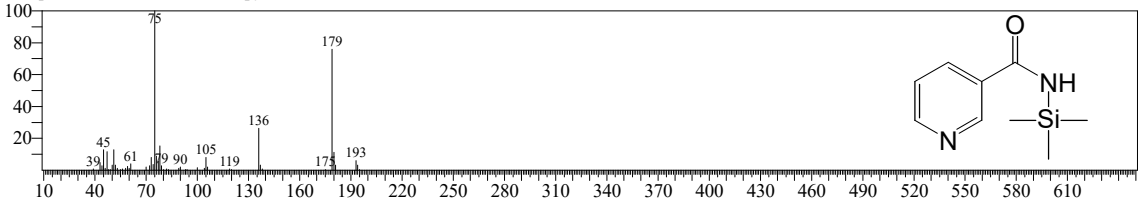
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



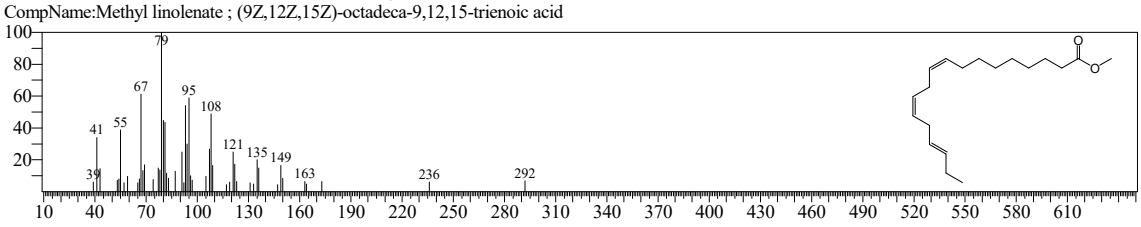
Hit#:2 Entry:11222 Library:NIST20M1.lib
SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #



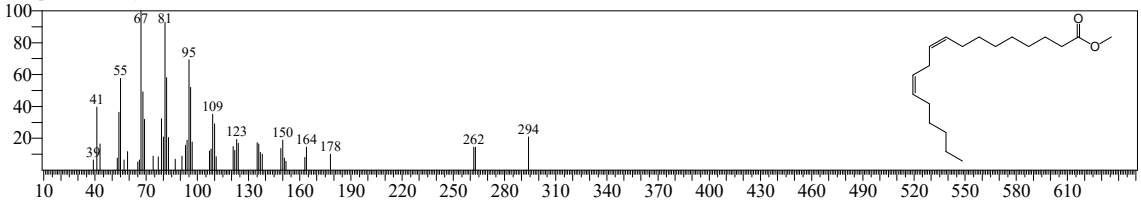
Hit#:3 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide



Hit#:4 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

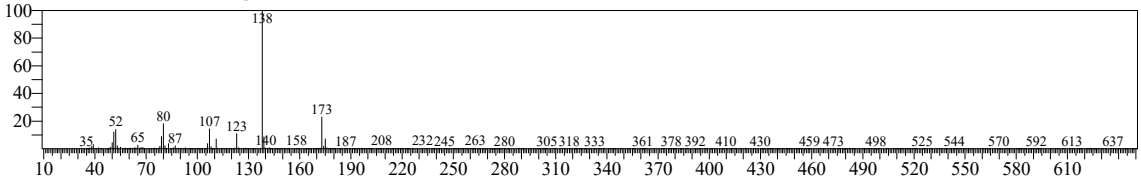


Hit#:5 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

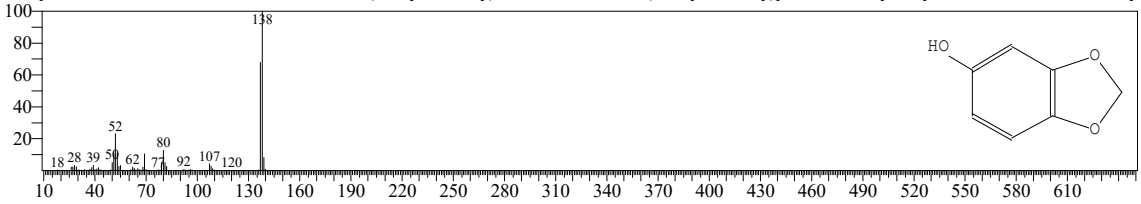


TNAU

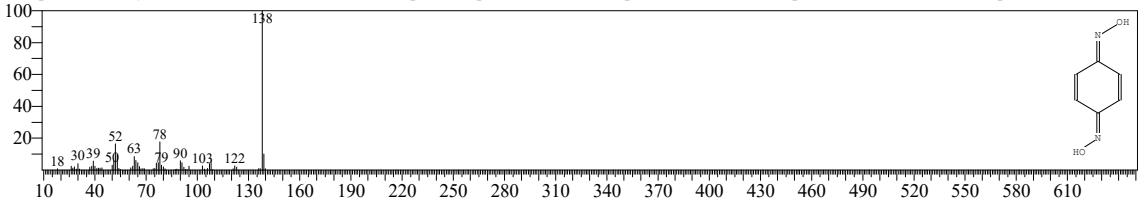
<< Target >>
Line#:6 R.Time:12.825(Scan#:1566) MassPeaks:353
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(34992)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



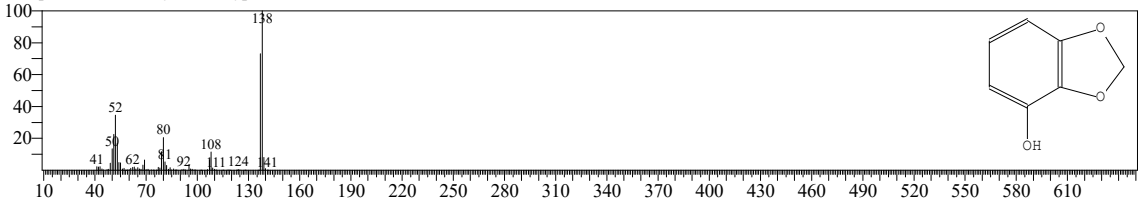
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



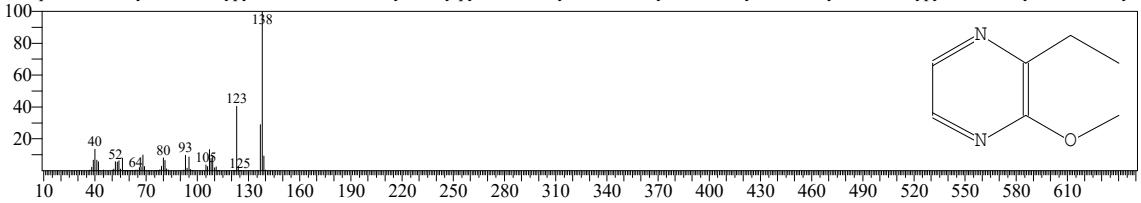
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



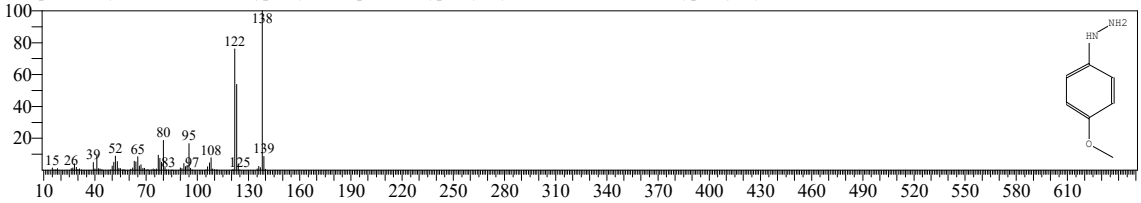
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:72 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



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·

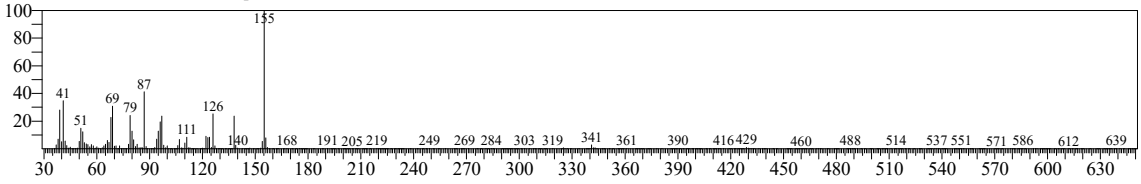


Hit#:5 Entry:11222 Library:NIST20M1.lib
SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

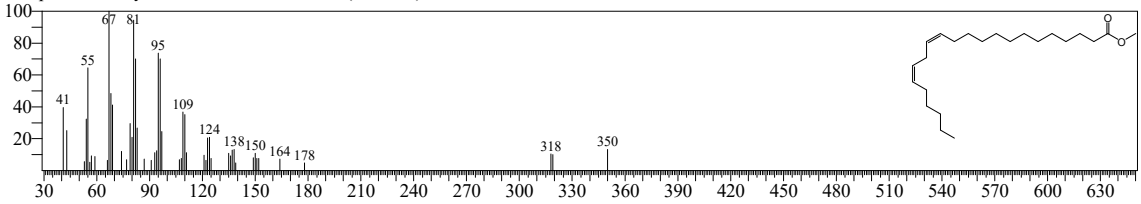


TNAU

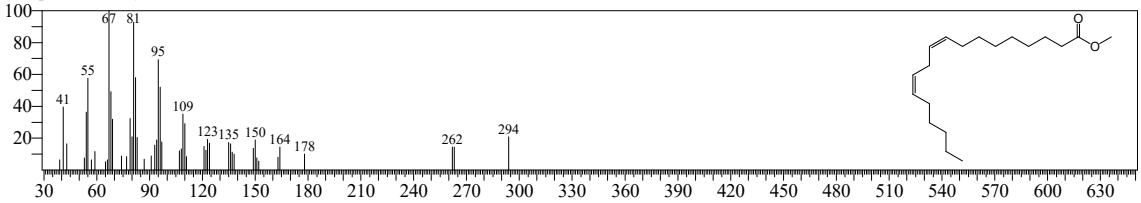
<< Target >>
Line#:7 R.Time:13.380(Scan#:1677) MassPeaks:385
RawMode:Averaged 13.375-13.385(1676-1678) BasePeak:155.05(19813)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



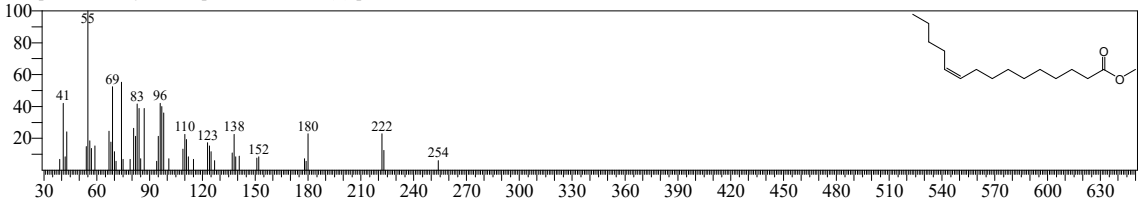
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



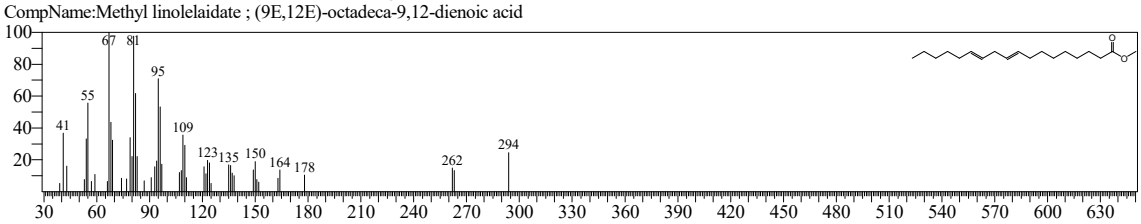
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



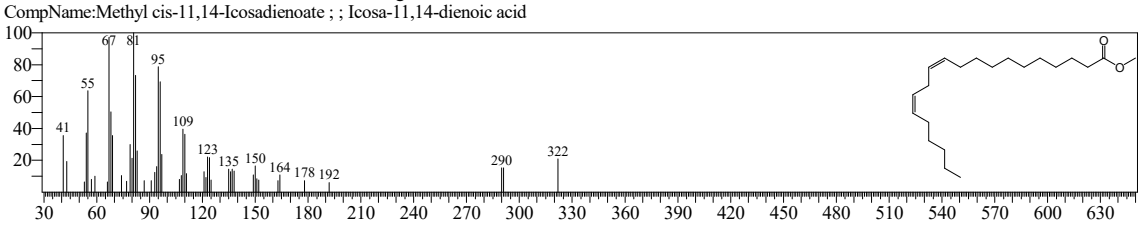
Hit#:3 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:50 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid



Hit#:4 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:50 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

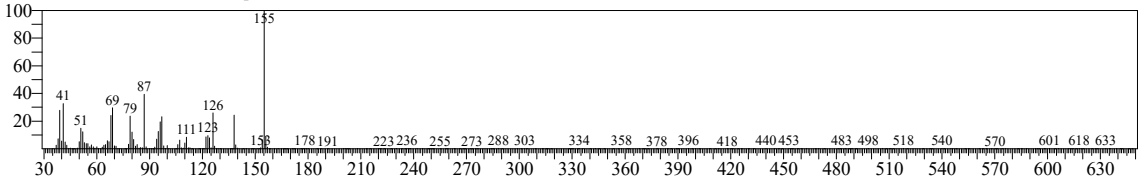


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:49 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

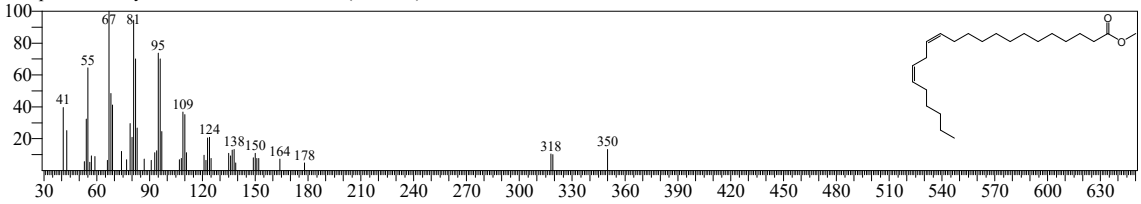


TNAU

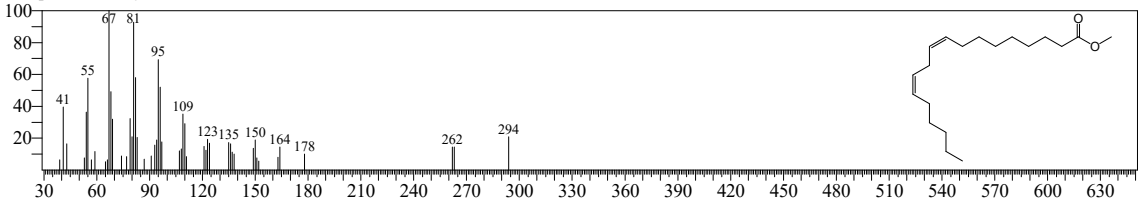
<< Target >>
Line#:8 R.Time:13.575(Scan#:1716) MassPeaks:277
RawMode:Averaged 13.570-13.580(1715-1717) BasePeak:155.05(15220)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



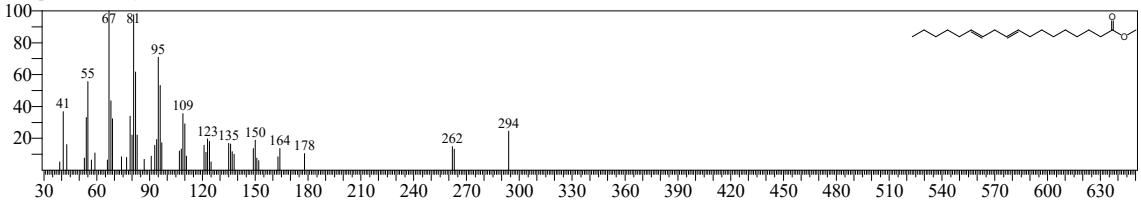
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



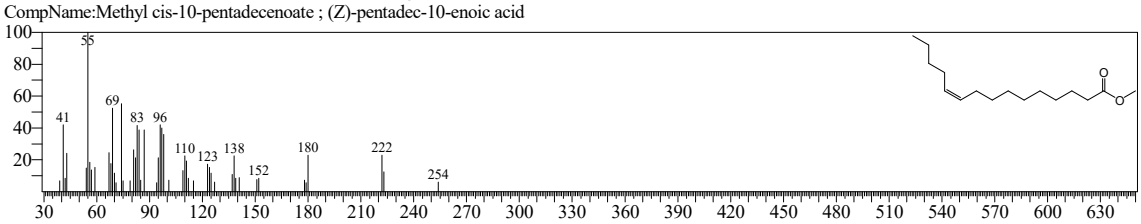
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



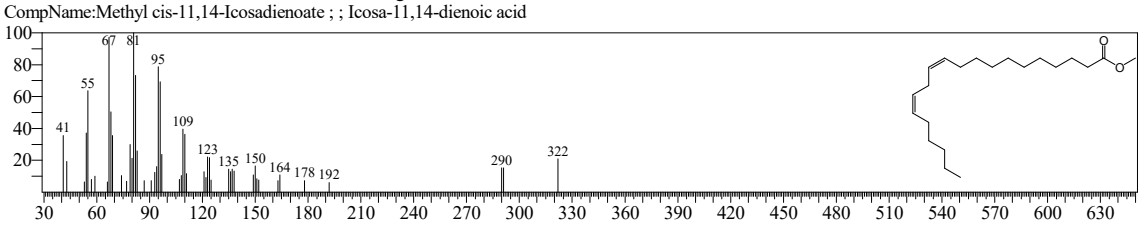
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

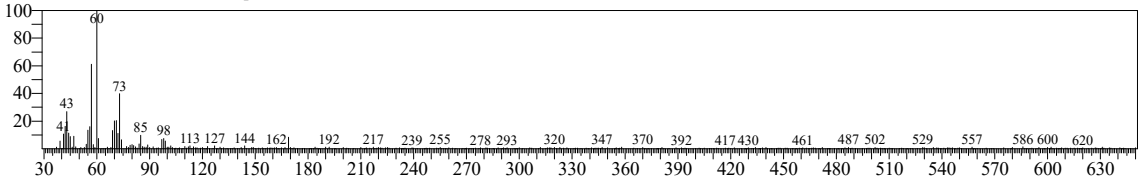


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

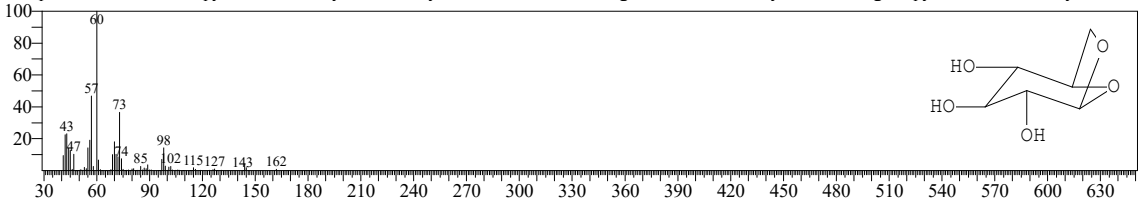


TNAU

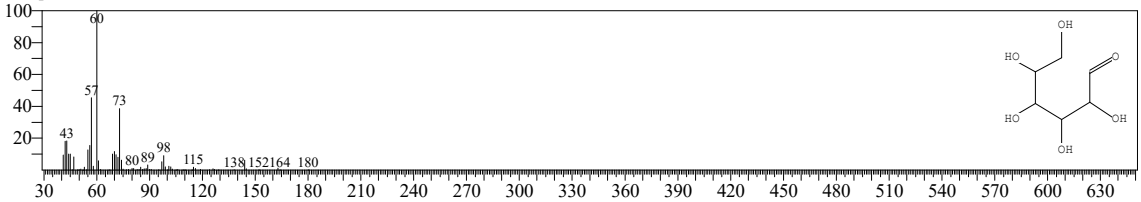
<< Target >>
Line#:9 R.Time:18.090(Scan#:2619) MassPeaks:375
RawMode:Averaged 18.085-18.095(2618-2620) BasePeak:60.00(2954)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



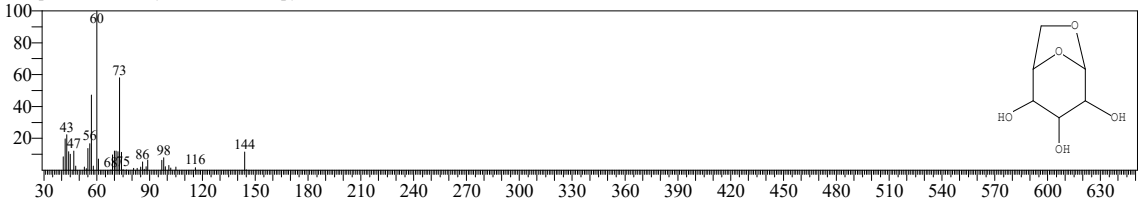
Hit#:1 Entry:13905 Library:NIST20R.lib
SI:90 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-



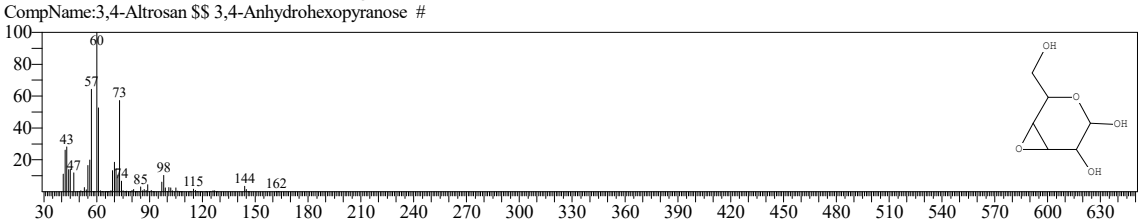
Hit#:2 Entry:36240 Library:NIST20M1.lib
SI:89 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #



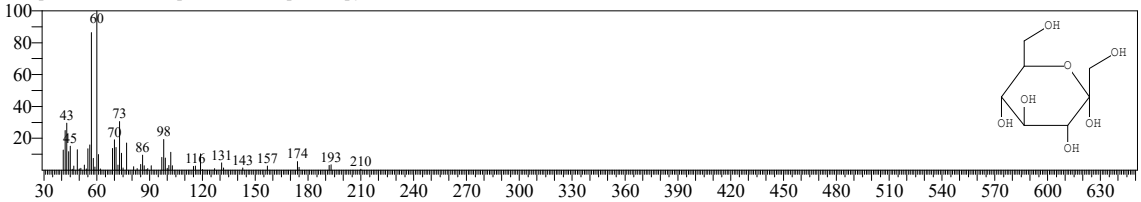
Hit#:3 Entry:23812 Library:NIST20M1.lib
SI:88 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose



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

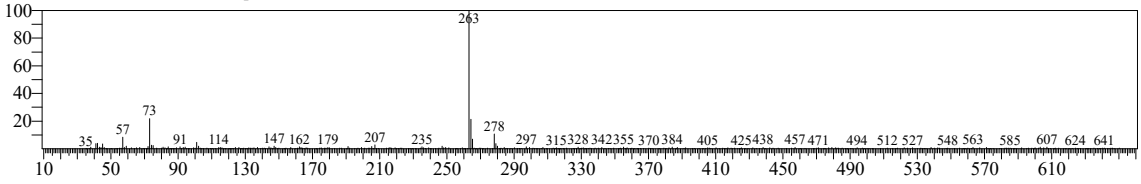


Hit#:5 Entry:62131 Library:NIST20M1.lib
SI:83 Formula:C7H14O7 CAS:0-00-0 MolWeight:210 RetIndex:2031
CompName:d-Gluco-heptulosan $$ Hept-2-ulopyranose #

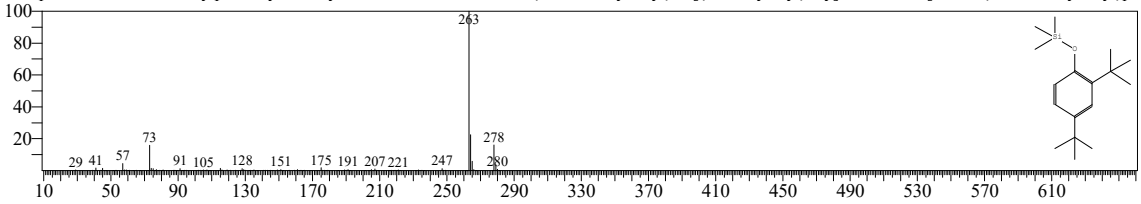


TNAU

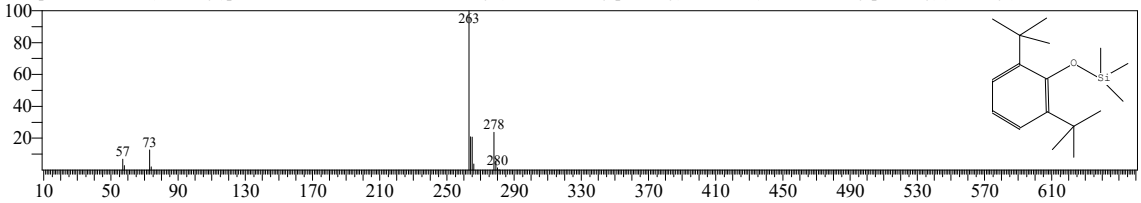
<< Target >>
Line#:10 R.Time:19.195(Scan#:2840) MassPeaks:374
RawMode:Averaged 19.190-19.200(2839-2841) BasePeak:263.15(4028)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



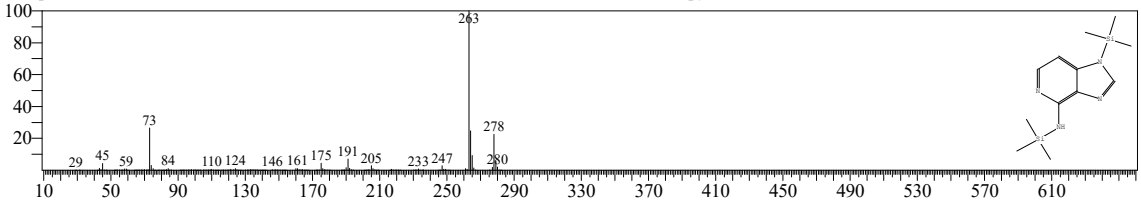
Hit#:1 Entry:33874 Library:NIST20R.lib
SI:84 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph



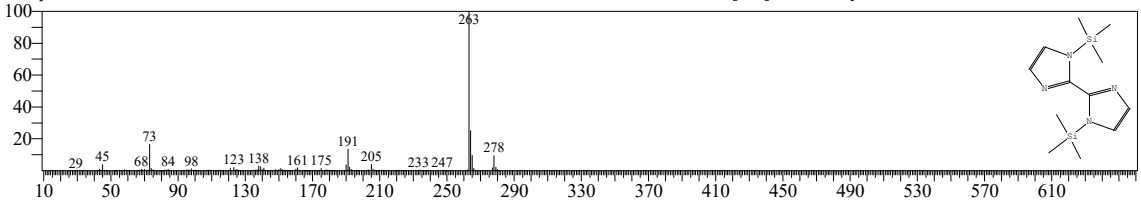
Hit#:2 Entry:33871 Library:NIST20R.lib
SI:79 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #



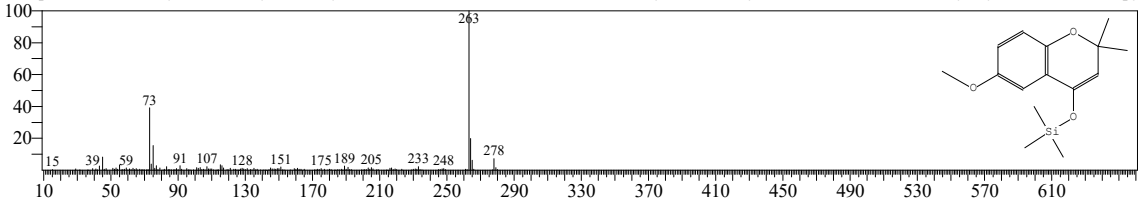
Hit#:3 Entry:136557 Library:NIST20M1.lib
SI:79 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



Hit#:4 Entry:136556 Library:NIST20M1.lib
SI:76 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM

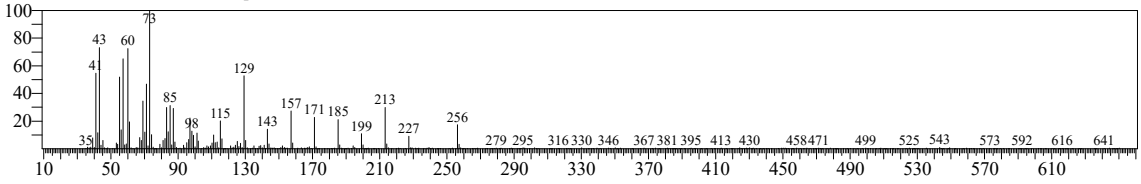


Hit#:5 Entry:137020 Library:NIST20M1.lib
SI:73 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy

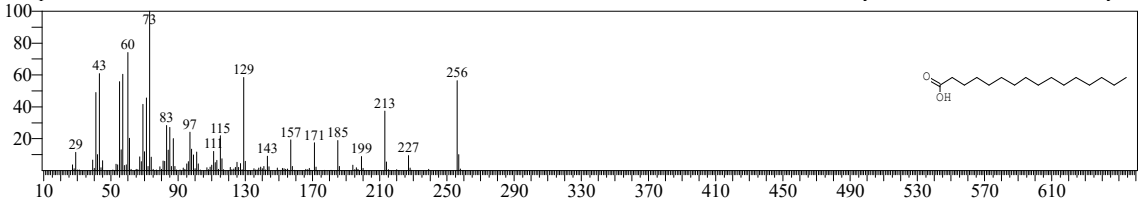


TNAU

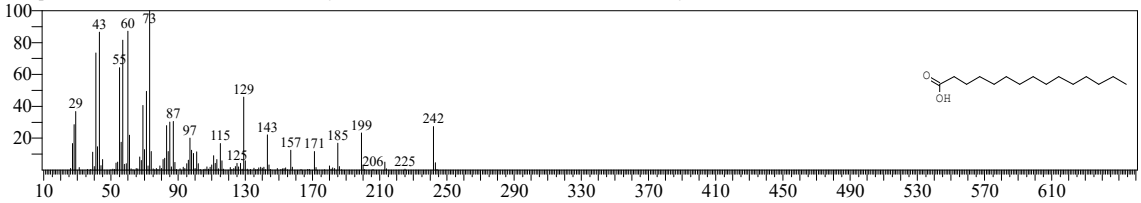
<< Target >>
Line#:11 R.Time:28.295(Scan#:4660) MassPeaks:363
RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.05(6044)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



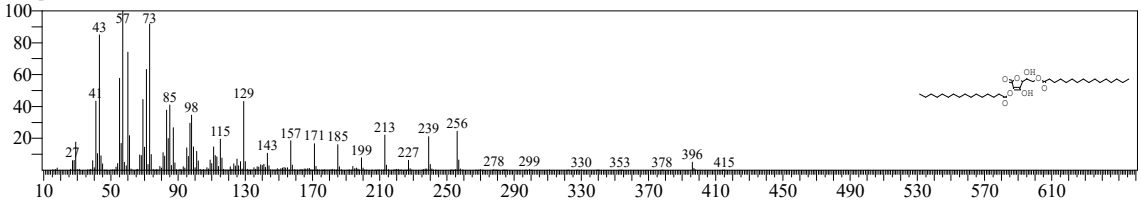
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



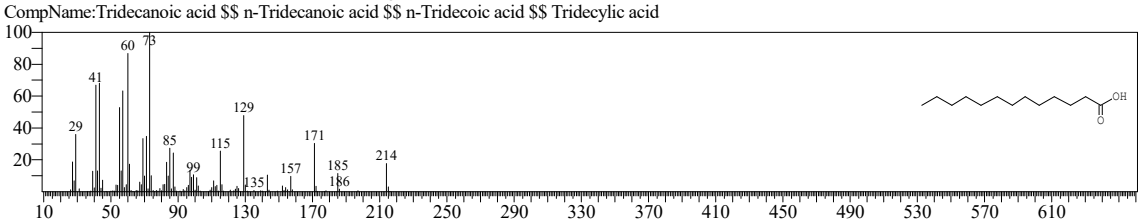
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



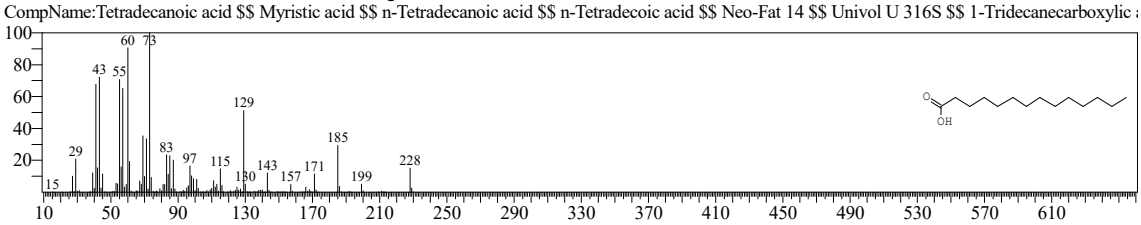
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



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

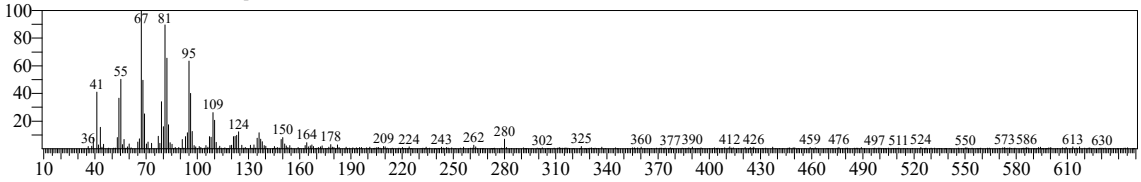


Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:90 Formula:C14H28O2 CAS:544-63-8 MolWeight:228 RetIndex:1769
CompName:Tetradecanoic acid $$ Myristic acid $$ n-Tetradecanoic acid $$ n-Tetradecoic acid $$ Neo-Fat 14 $$ Univol U 316S $$ 1-Tridecanecarboxylic

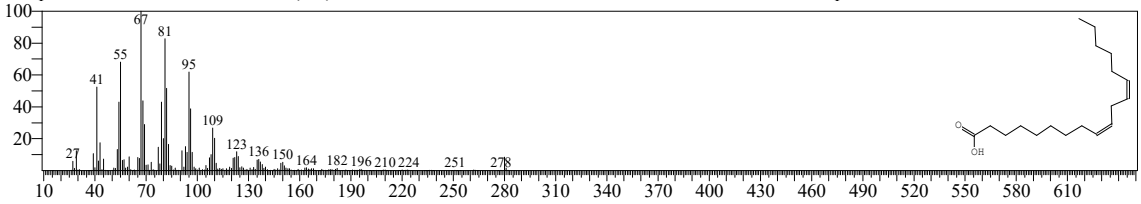


TNAU

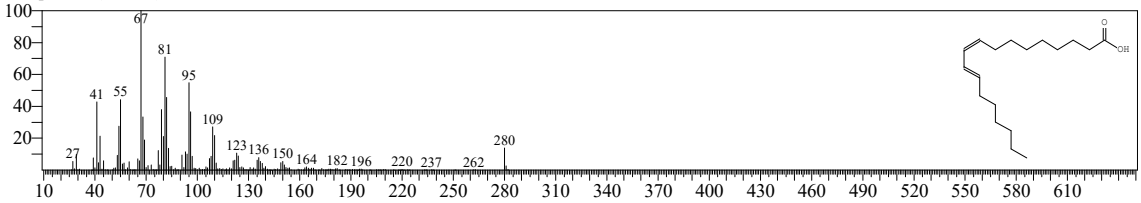
<< Target >>
Line#:12 R.Time:31.465(Scan#:5294) MassPeaks:380
RawMode:Averaged 31.460-31.470(5293-5295) BasePeak:67.05(3294)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



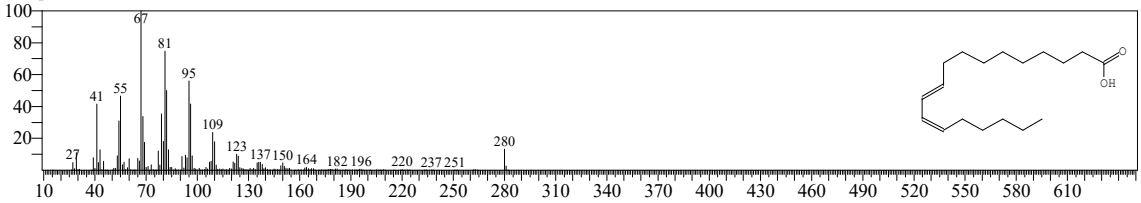
Hit#:1 Entry:34035 Library:NIST20R.lib
SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



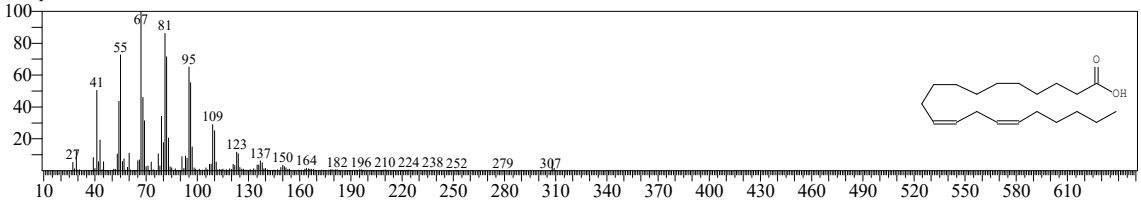
Hit#:2 Entry:139651 Library:NIST20M1.lib
SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



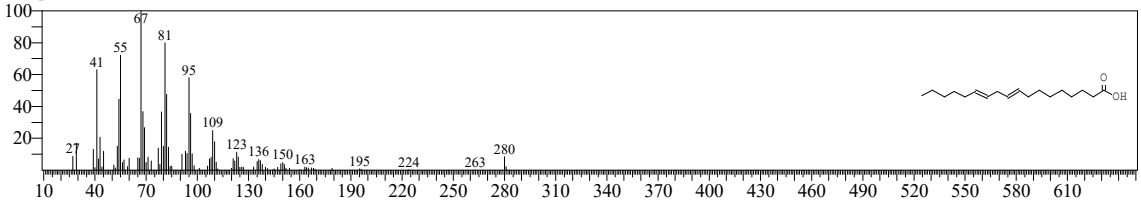
Hit#:3 Entry:139646 Library:NIST20M1.lib
SI:94 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid



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

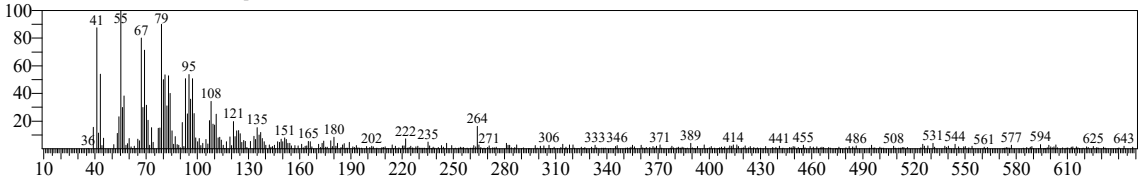


Hit#:5 Entry:139661 Library:NIST20M1.lib
SI:93 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

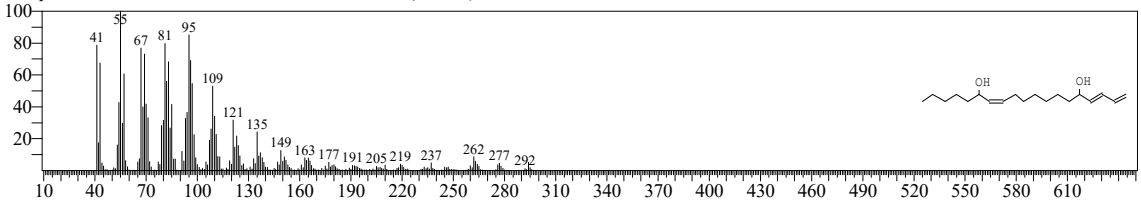


TNAU

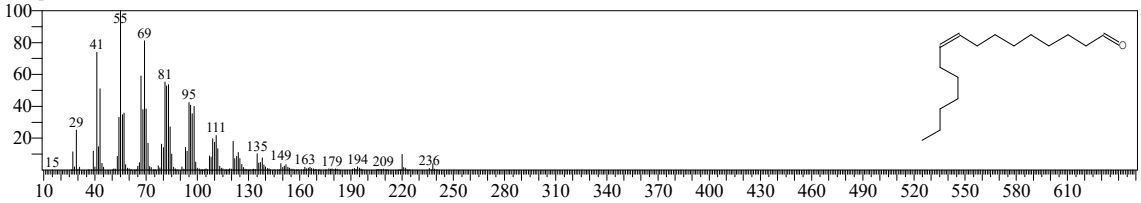
<< Target >>
Line#:13 R.Time:31.575(Scan#:5316) MassPeaks:391
RawMode:Averaged 31.570-31.580(5315-5317) BasePeak:55.10(1315)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



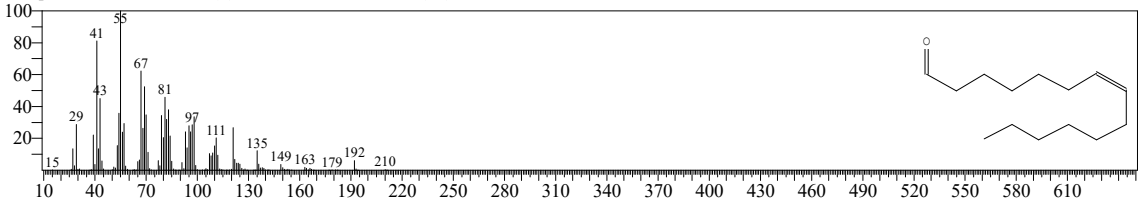
Hit#:1 Entry:156549 Library:NIST20M1.lib
SI:87 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #



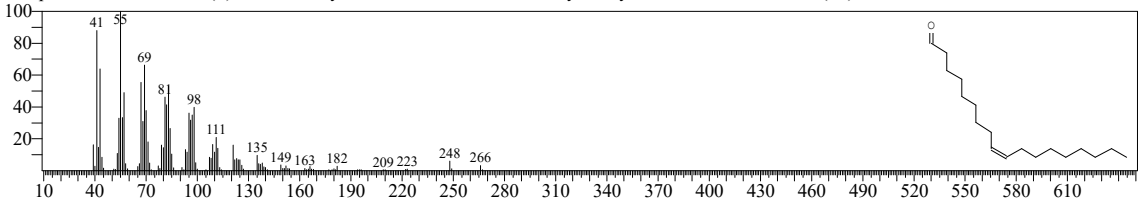
Hit#:2 Entry:92244 Library:NIST20M1.lib
SI:86 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #



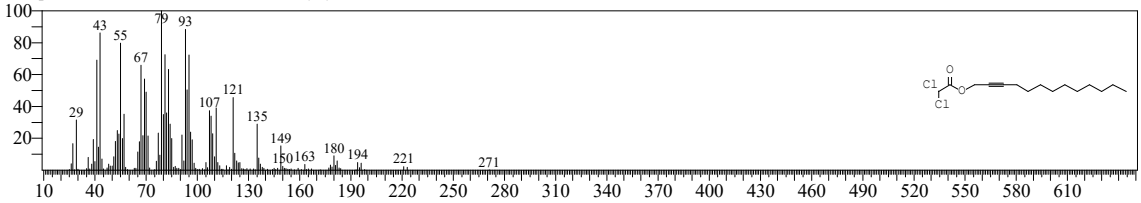
Hit#:3 Entry:63176 Library:NIST20M1.lib
SI:86 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #



Hit#: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 #

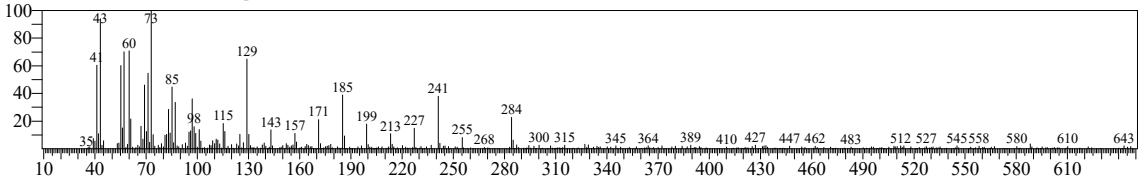


Hit#:5 Entry:170238 Library:NIST20M1.lib
SI:86 Formula:C15H24Cl2O2 CAS:0-00-0 MolWeight:306 RetIndex:2042
CompName:Dichloroacetic acid, tridec-2-ynyl ester

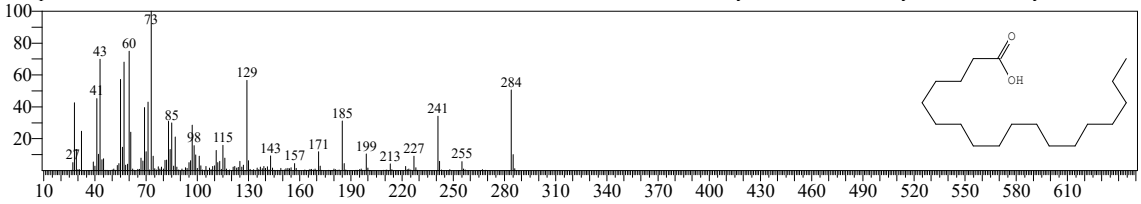


TNAU

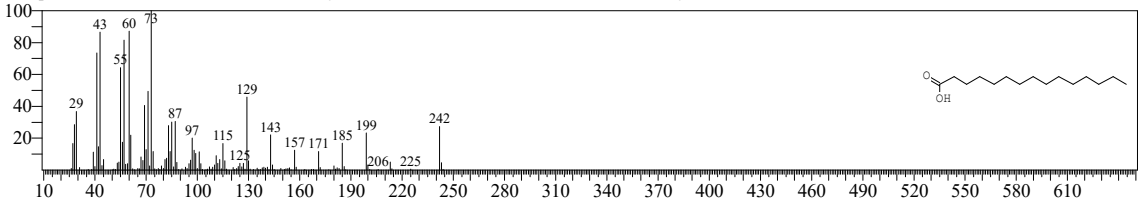
<< Target >>
Line#:14 R.Time:32.025(Scan#:5406) MassPeaks:362
RawMode:Averaged 32.020-32.030(5405-5407) BasePeak:73.00(1466)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



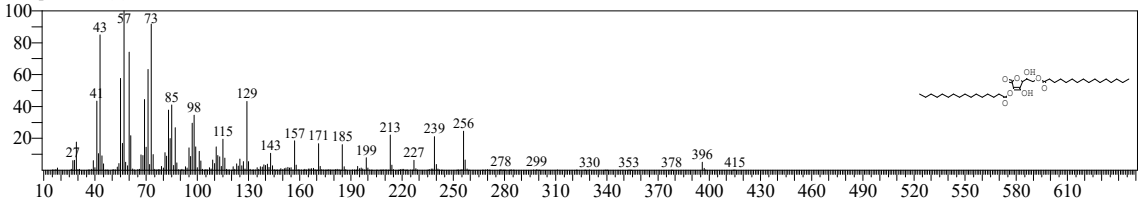
Hit#:1 Entry:34463 Library:NIST20R.lib
SI:91 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



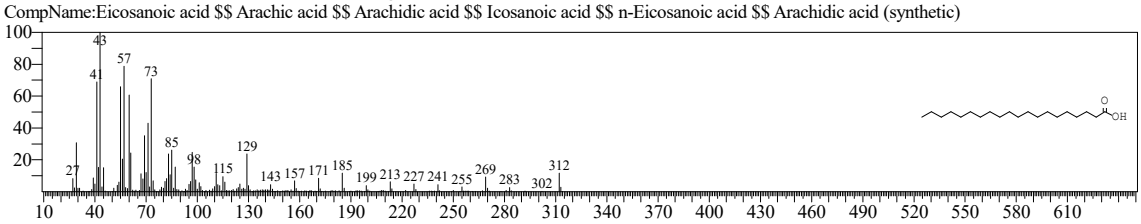
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:88 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



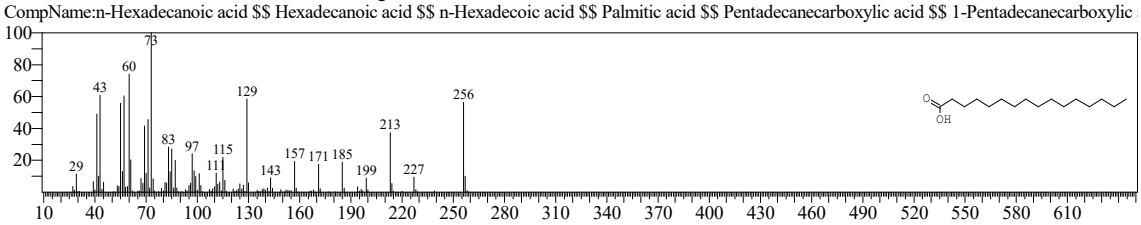
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:87 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:4 Entry:36903 Library:NIST20R.lib
SI:87 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)

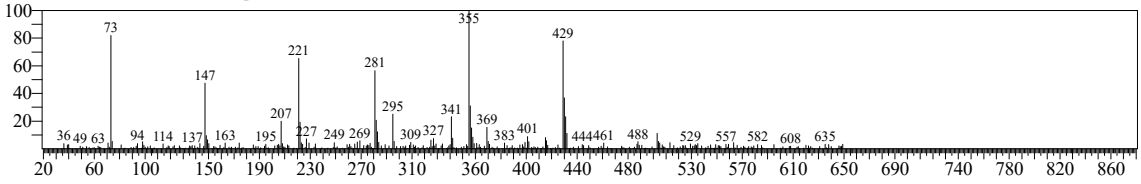


Hit#:5 Entry:31600 Library:NIST20R.lib
SI:86 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

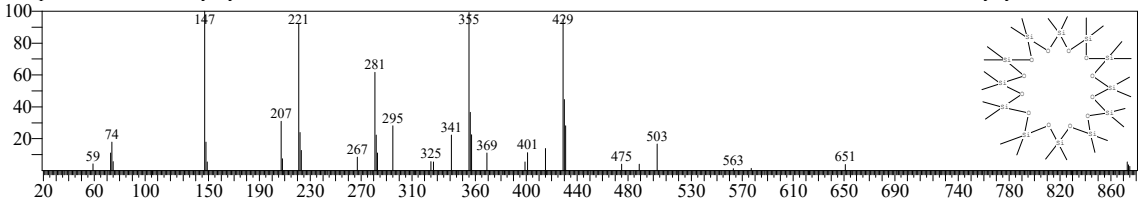


TNAU

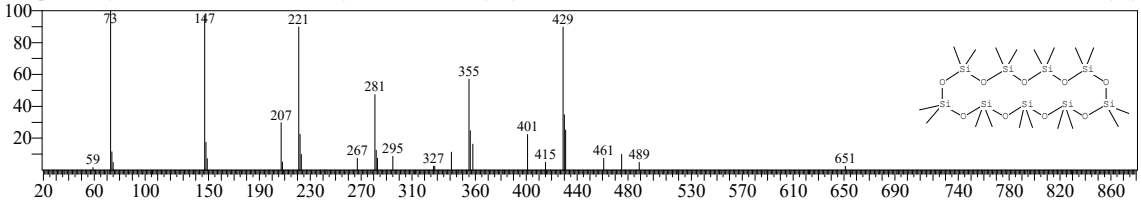
<< Target >>
Line#:15 R.Time:41.595(Scan#:7320) MassPeaks:328
RawMode:Averaged 41.590-41.600(7319-7321) BasePeak:355.05(888)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



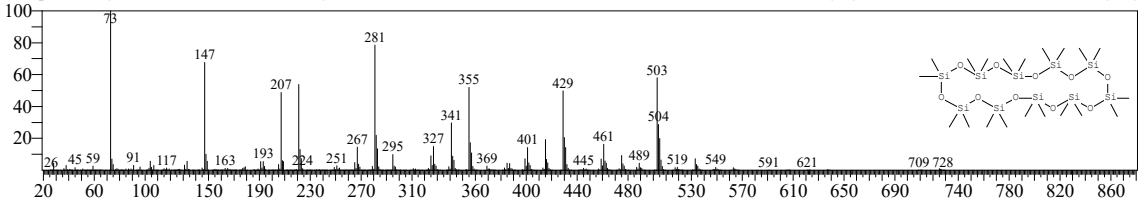
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:83 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



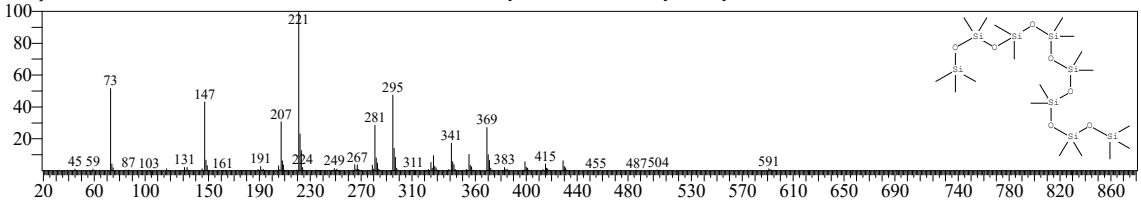
Hit#:2 Entry:43658 Library:NIST20R.lib
SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



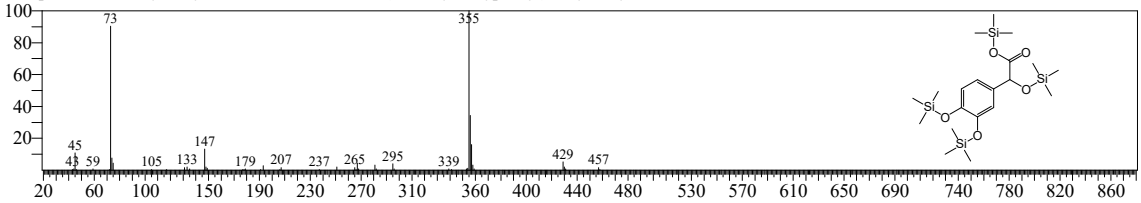
Hit#:3 Entry:45685 Library:NIST20M2.lib
SI:78 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



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

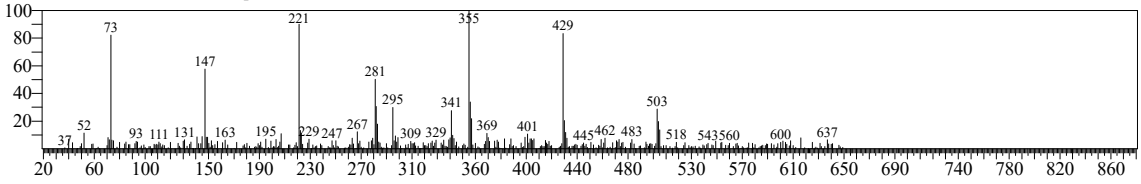


Hit#:5 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:61 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

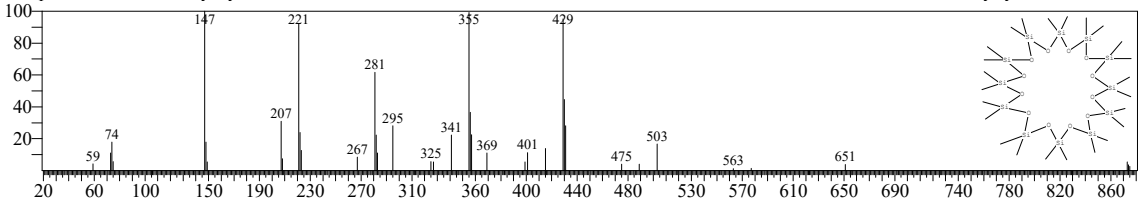


TNAU

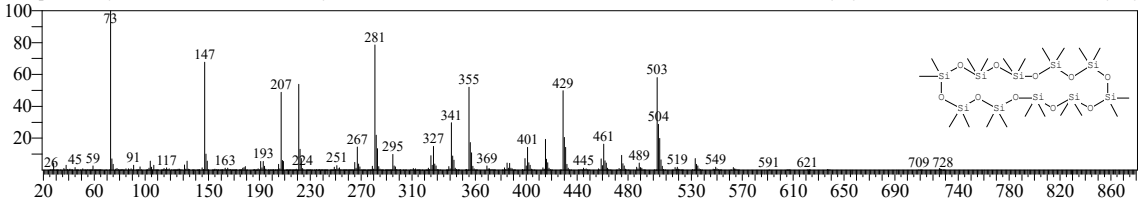
<< Target >>
Line#:16 R.Time:43.795(Scan#:7760) MassPeaks:387
RawMode:Averaged 43.790-43.800(7759-7761) BasePeak:355.05(664)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



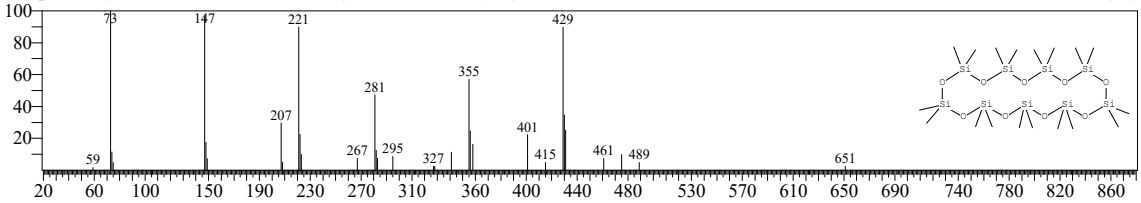
Hit#:1 Entry:46368 Library:NIST20M2.lib
SI:77 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan



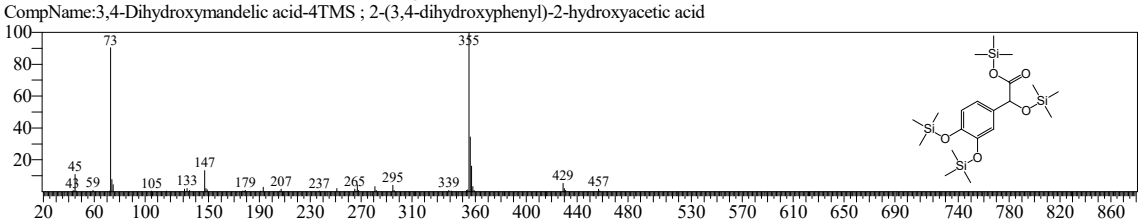
Hit#:2 Entry:45685 Library:NIST20M2.lib
SI:74 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy



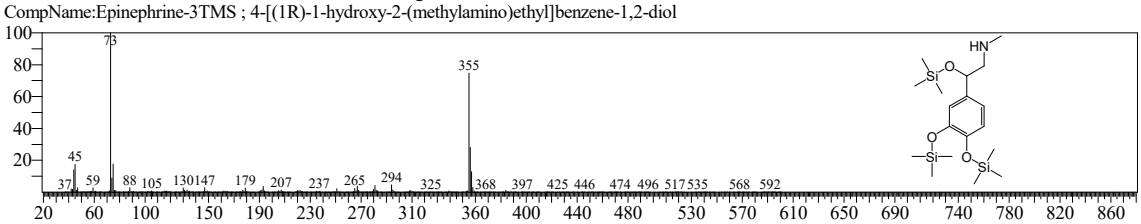
Hit#:3 Entry:43658 Library:NIST20R.lib
SI:72 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:53 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

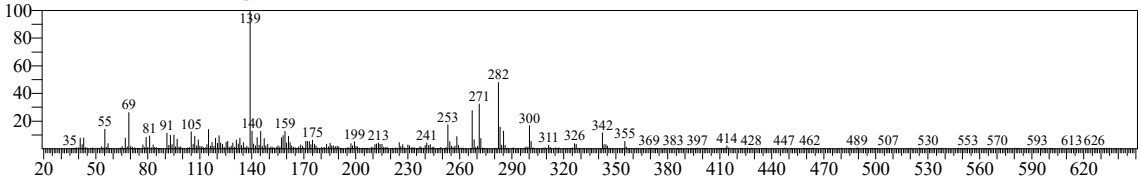


Hit#:5 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:41 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol

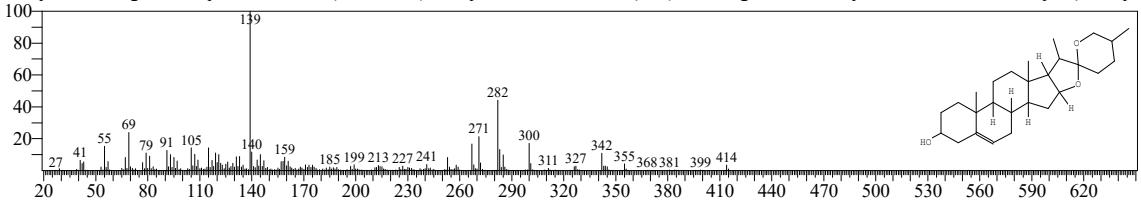


TNAU

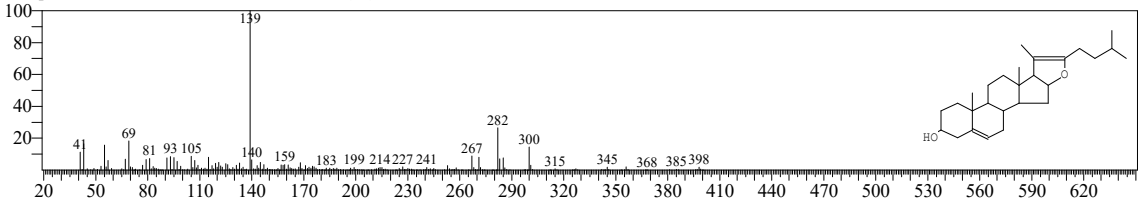
<< Target >>
Line#:17 R.Time:45.615(Scan#:8124) MassPeaks:382
RawMode:Averaged 45.610-45.620(8123-8125) BasePeak:139.10(6661)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



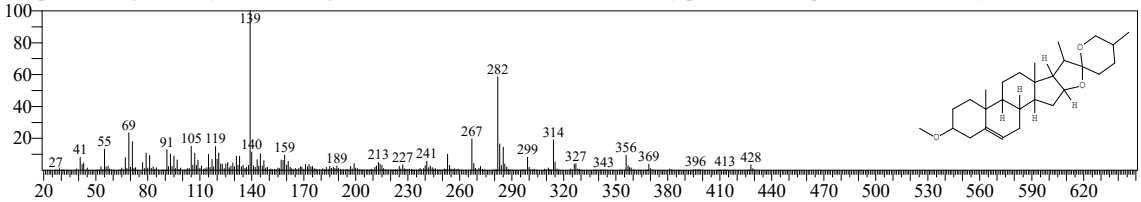
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:90 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



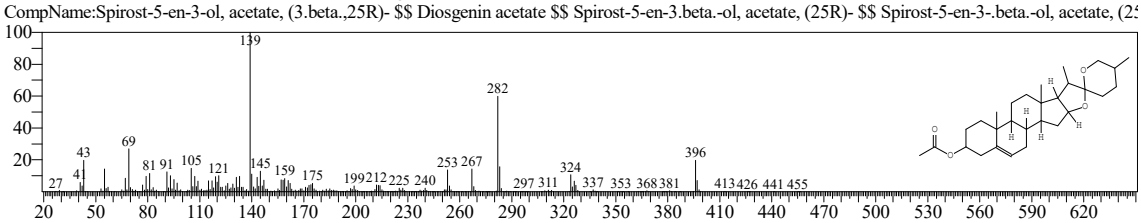
Hit#:2 Entry:41561 Library:NIST20R.lib
SI:81 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #



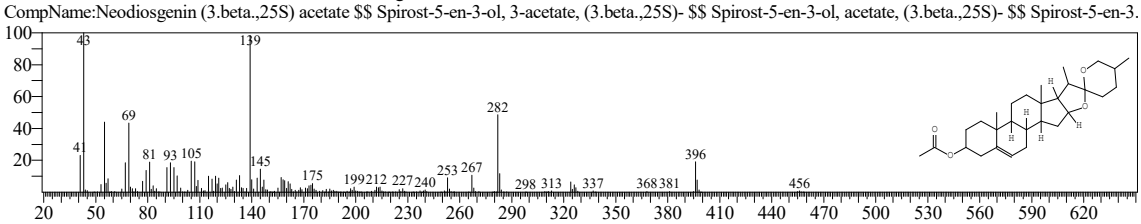
Hit#:3 Entry:14852 Library:NIST20M2.lib
SI:80 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#: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

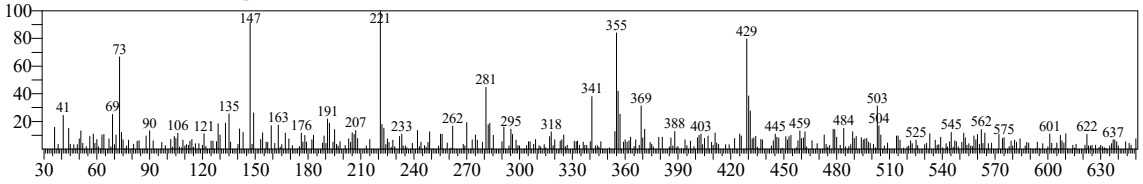


Hit#:5 Entry:42677 Library:NIST20R.lib
SI:75 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.

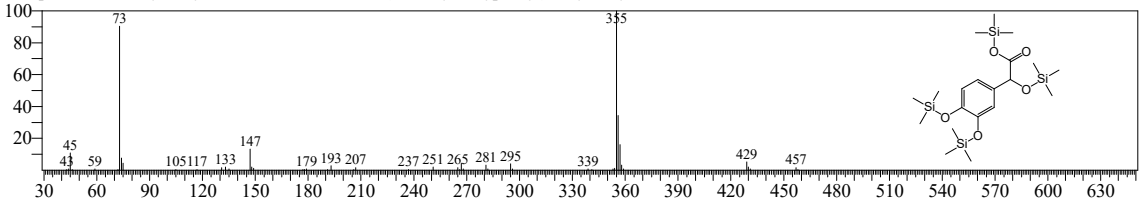


TNAU

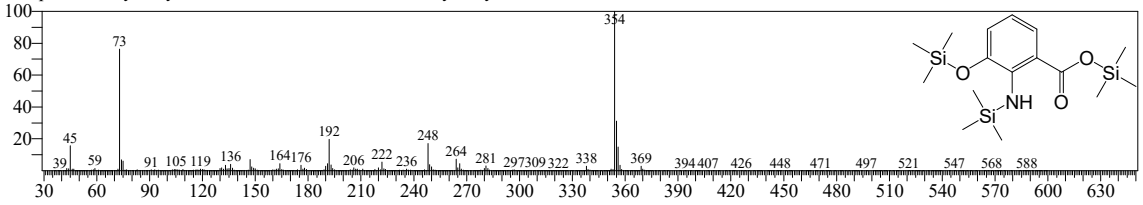
<< Target >>
Line#:18 R.Time:45.790(Scan#:8159) MassPeaks:390
RawMode:Averaged 45.785-45.795(8158-8160) BasePeak:221.00(313)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



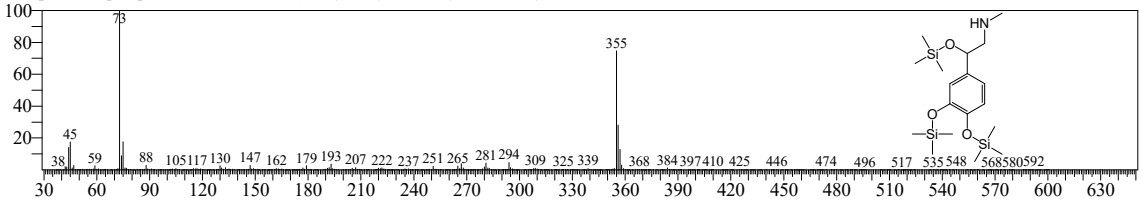
Hit#:1 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid



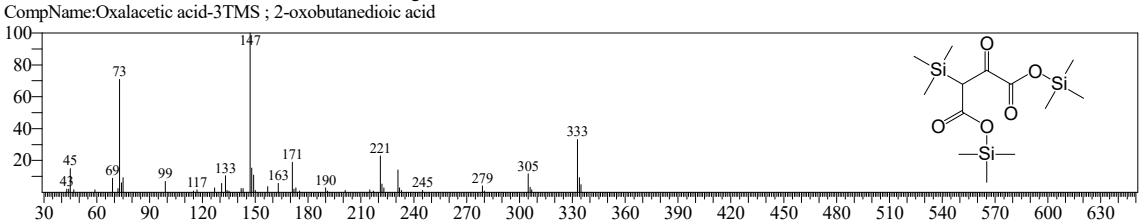
Hit#:2 Entry:354 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C16H31NO3Si3 CAS:548-93-6 MolWeight:369 RetIndex:1886
CompName:3-Hydroxyanthranilic acid-3TMS ; 2-amino-3-hydroxybenzoic acid



Hit#:3 Entry:343 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C18H37NO3Si3 CAS:51-43-4 MolWeight:399 RetIndex:1868
CompName:Epinephrine-3TMS ; 4-[(1R)-1-hydroxy-2-(methylamino)ethyl]benzene-1,2-diol



Hit#:4 Entry:174 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C13H28O5Si3 CAS:328-42-7 MolWeight:348 RetIndex:1560
CompName:Oxalacetic acid-3TMS ; 2-oxobutanedioic acid



Hit#:5 Entry:24 Library:OA_TMS_DB5_67min_V3.lib
SI:30 Formula: CAS:0-00-0 MolWeight:236 RetIndex:1130
CompName:Oxalic acid-13C2-2TMS ;