TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022026.qgd

TIC

490,722

Peak Report TIC

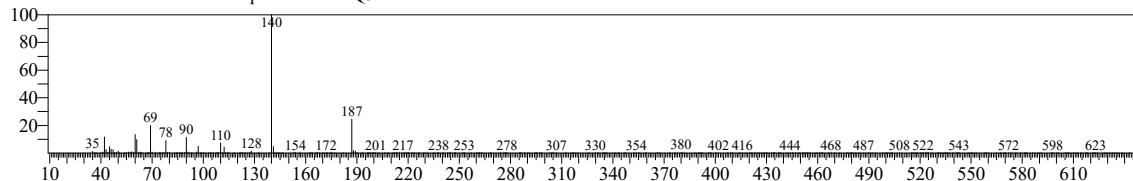| Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	5.393	73967	2.39	33068	3.51	2.24	80	(2-Chloroethyl)(methyl)amine, N-trifluoroacet
2	5.587	64079	2.07	15447	1.64	4.15	93	L-Lactic acid
3	8.827	61487	1.98	20229	2.15	3.04	84	1-Butanol, 3-methyl-, acetate
4	9.775	46682	1.51	19335	2.05	2.41	93	Pentasiloxane, dodecamethyl-
5	11.146	29367	0.95	10536	1.12	2.79	41	Fendiline
6	12.500	200347	6.47	76484	8.13	2.62	74	1,3-Benzodioxol-5-ol
7	12.828	293758	9.48	114887	12.21	2.56	73	2,5-Cyclohexadiene-1,4-dione, dioxime
8	13.367	744160	24.01	194498	20.67	3.83	51	Methyl cis-13,16-Docosadienate
9	13.554	580275	18.73	161161	17.13	3.60	53	Methyl cis-13,16-Docosadienate
10	13.817	18405	0.59	8219	0.87	2.24	72	Trisiloxane, octamethyl-
11	18.084	50563	1.63	14956	1.59	3.38	88	.beta.-D-Glucopyranose, 1,6-anhydro-
12	19.200	31439	1.01	13609	1.45	2.31	85	2,4-Di-tert-butylphenoxytrimethylsilane
13	28.306	255944	8.26	98543	10.47	2.60	95	n-Hexadecanoic acid
14	31.482	169608	5.47	57128	6.07	2.97	94	9,12-Octadecadienoic acid (Z,Z)-
15	31.592	189688	6.12	55536	5.90	3.42	89	cis-9-Hexadecenal
16	45.637	286454	9.24	41582	4.42	6.89	89	Diosgenin
17	45.715	2552	0.08	5832	0.62	0.44	16	2-Deoxy-glucose-4TMS(1)
		3098775	100.00	941050	100.00			

Library

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<< Target >>
Line#:1 R.Time:5.390(Scan#:79) MassPeaks:310
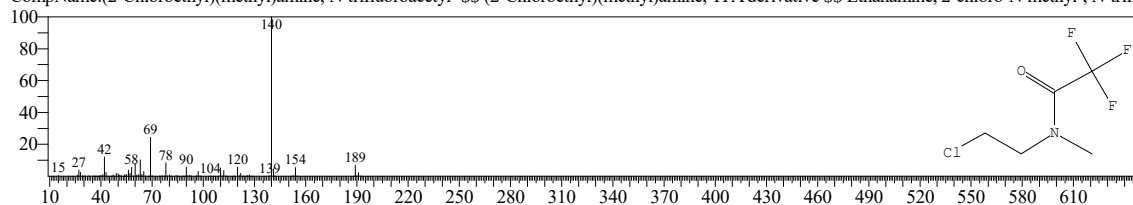RawMode:Averaged 5.385-5.395(78-80) BasePeak:140.00(12817)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:43299 Library:NIST20M1.lib
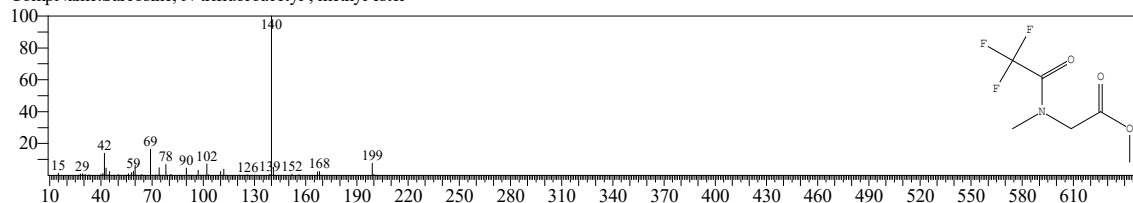SI:80 Formula:C5H7ClF3NO CAS:18060-05-4 MolWeight:189 RetIndex:779
CompName:(2-Chloroethyl)(methyl)amine, N-trifluoroacetyl- $$ (2-Chloroethyl)(methyl)amine, TFA derivative $$ Ethanamine, 2-chloro-N-methyl-, N-triflu

Hit#:2 Entry:52064 Library:NIST20M1.lib
SI:80 Formula:C6H8F3NO3 CAS:0-00-0 MolWeight:199 RetIndex:820
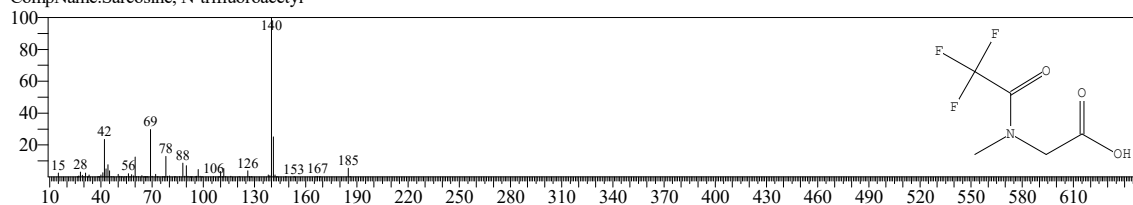CompName:Sarcosine, N-trifluoroacetyl-, methyl ester

Hit#:3 Entry:40334 Library:NIST20M1.lib
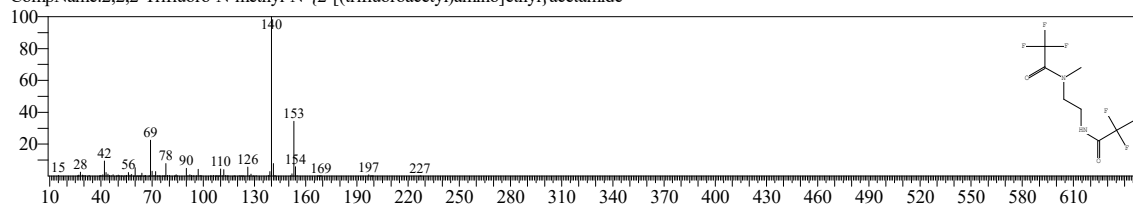SI:80 Formula:C5H6F3NO3 CAS:0-00-0 MolWeight:185 RetIndex:910
CompName:Sarcosine, N-trifluoroacetyl-

Hit#:4 Entry:122117 Library:NIST20M1.lib
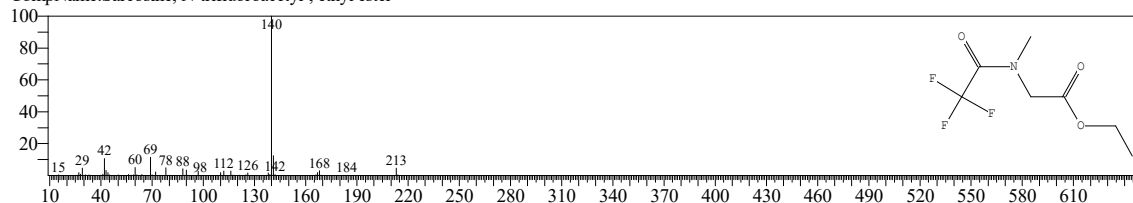SI:78 Formula:C7H8F6N2O2 CAS:0-00-0 MolWeight:266 RetIndex:987
CompName:2,2,2-Trifluoro-N-methyl-N-{2-[(trifluoroacetyl)amino]ethyl}acetamide

Hit#:5 Entry:65348 Library:NIST20M1.lib
SI:78 Formula:C7H10F3NO3 CAS:0-00-0 MolWeight:213 RetIndex:919
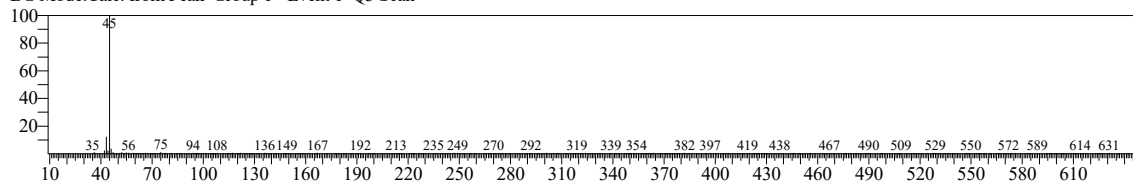CompName:Sarcosine, N-trifluoroacetyl-, ethyl ester

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<< Target >>
Line#:2 R.Time:5.585(Scan#:118) MassPeaks:349
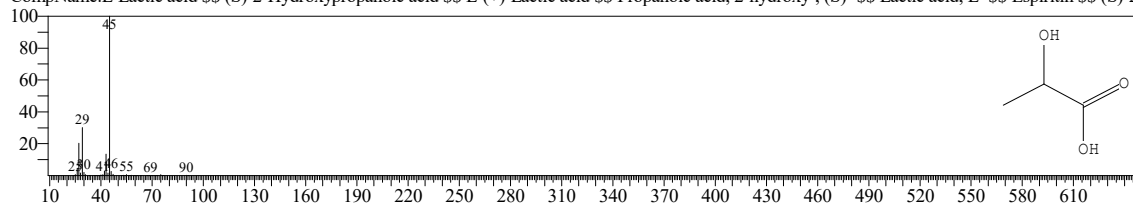RawMode:Averaged 5.580-5.590(117-119) BasePeak:45.05(10707)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:1162 Library:NIST20M1.lib
SI:93 Formula:C3H6O3 CAS:79-33-4 MolWeight:90 RetIndex:838
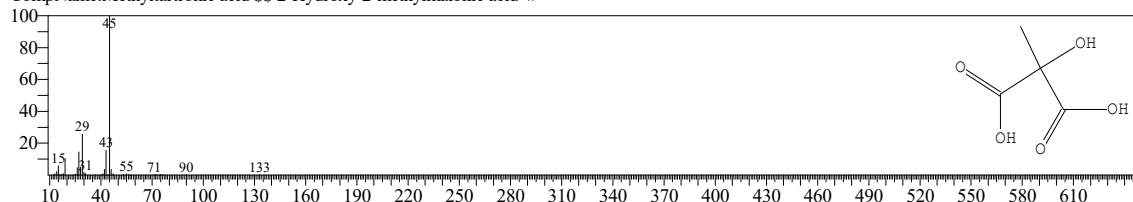CompName:L-Lactic acid $$ (S)-2-Hydroxypropanoic acid $$ L-(+)-Lactic acid $$ Propanoic acid, 2-hydroxy-, (S)- $$ Lactic acid, L- $$ Espiritin $$ (S)-2-

Hit#:2 Entry:9648 Library:NIST20M1.lib
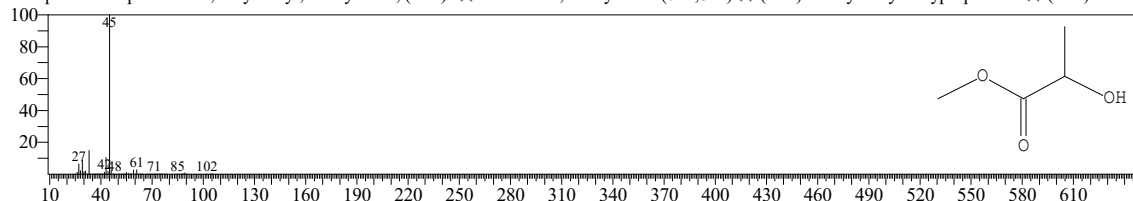SI:92 Formula:C4H6O5 CAS:595-98-2 MolWeight:134 RetIndex:1223
CompName:Methyltartronic acid $$ 2-Hydroxy-2-methylmalonic acid #

Hit#:3 Entry:2686 Library:NIST20R.lib
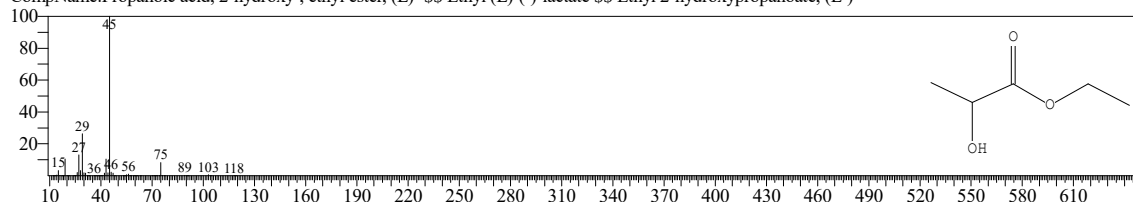SI:92 Formula:C4H8O3 CAS:547-64-8 MolWeight:104 RetIndex:748
CompName:Propanoic acid, 2-hydroxy-, methyl ester, (.+/-.)- $$ Lactic acid, methyl ester (7CI,8CI) $$ (.+/-.)-Methyl 2-hydroxypropanoate $$ (.+/-.)-Methyl

Hit#:4 Entry:5294 Library:NIST20M1.lib
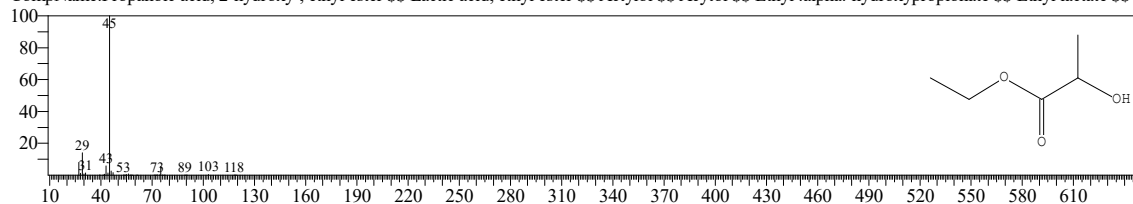SI:91 Formula:C5H10O3 CAS:687-47-8 MolWeight:118 RetIndex:848
CompName:Propanoic acid, 2-hydroxy-, ethyl ester, (L)- $$ Ethyl (L)-(-)-lactate $$ Ethyl 2-hydroxypropanoate, (L-)-

Hit#:5 Entry:4651 Library:NIST20R.lib
SI:91 Formula:C5H10O3 CAS:97-64-3 MolWeight:118 RetIndex:848
CompName:Propanoic acid, 2-hydroxy-, ethyl ester $$ Lactic acid, ethyl ester $$ Actylol $$ Acytol $$ Ethyl .alpha.-hydroxypropionate $$ Ethyl lactate $$ S

<< Target >>
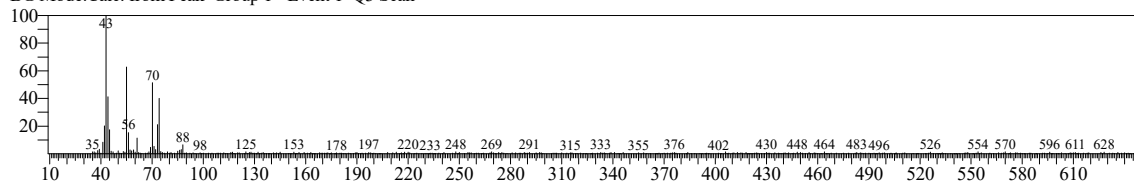Line#:3 R.Time:8.825(Scan#:766) MassPeaks:388
RawMode:Averaged 8.820-8.830(765-767) BasePeak:43.00(3675)
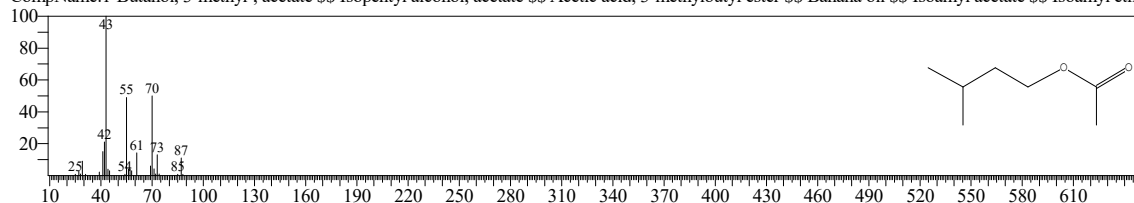BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:6783 Library:NIST20R.lib
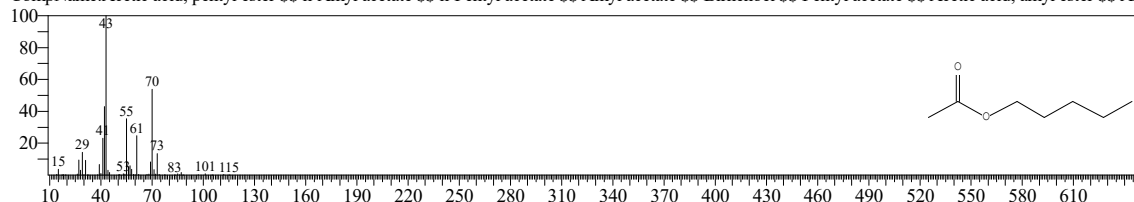SI:84 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha

Hit#:2 Entry:8685 Library:NIST20M1.lib
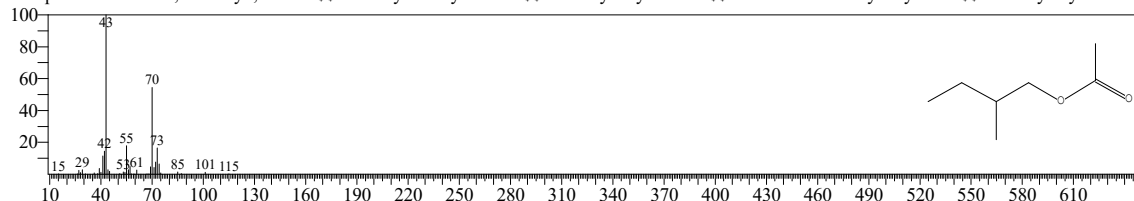SI:82 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ Am

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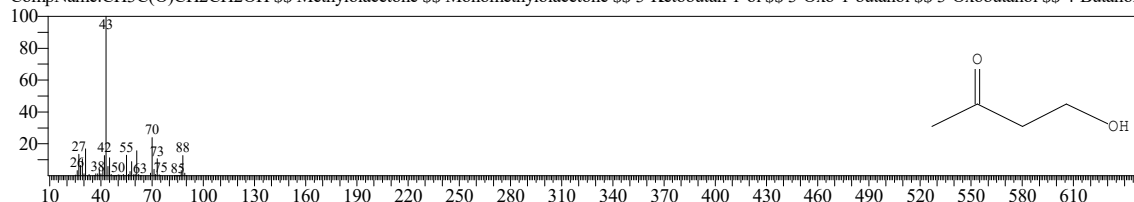SI:82 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate

Hit#:4 Entry:1220 Library:NIST20R.lib
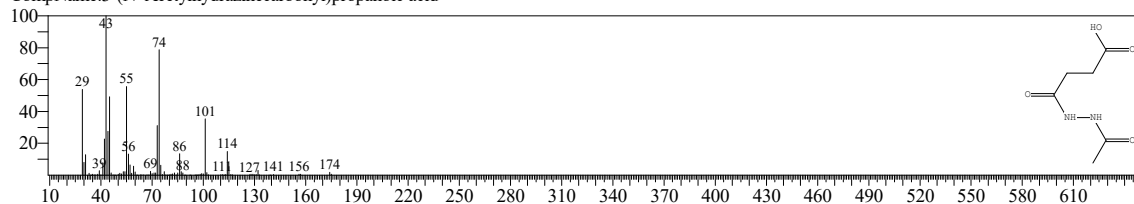SI:80 Formula:C4H8O2 CAS:590-90-9 MolWeight:88 RetIndex:798
CompName:CH3C(O)CH2CH2OH $$ Methylolacetone $$ Monomethylolacetone $$ 3-Ketobutan-1-ol $$ 3-Oxo-1-butanol $$ 3-Oxobutanol $$ 4-Butanol-

Hit#:5 Entry:32045 Library:NIST20M1.lib
SI:79 Formula:C6H10N2O4 CAS:0-00-0 MolWeight:174 RetIndex:1774
CompName:3-(N'-Acetylhydrazinecarbonyl)propanoic acid
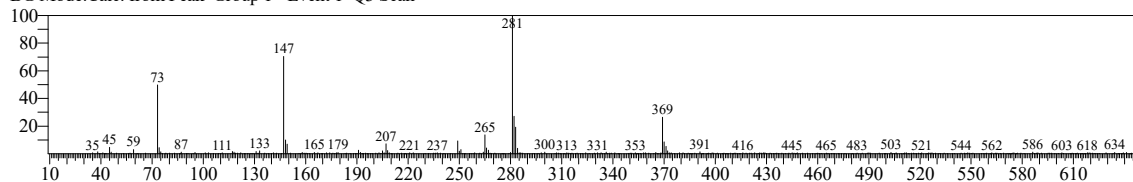
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<< Target >>
Line#:4 R.Time:9.775(Scan#:956) MassPeaks:362
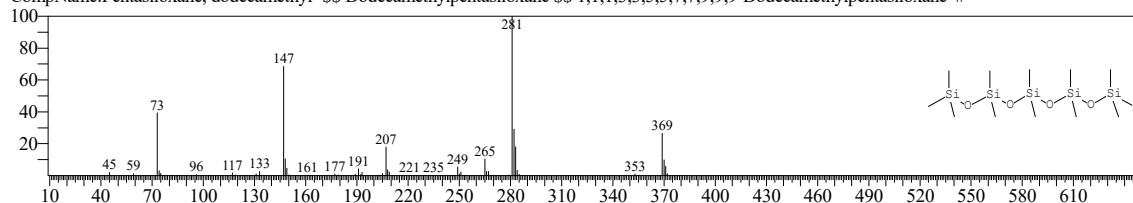RawMode:Averaged 9.770-9.780(955-957) BasePeak:281.05(4115)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:40975 Library:NIST20R.lib
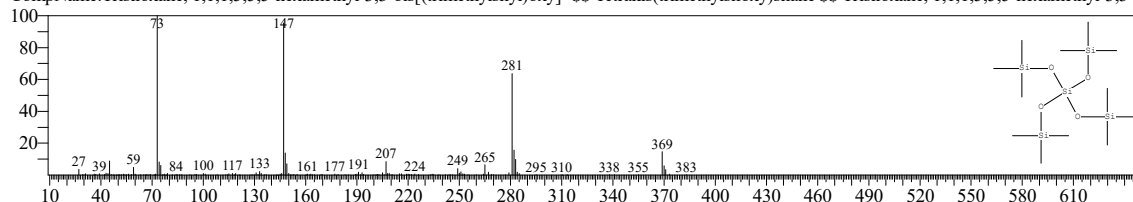SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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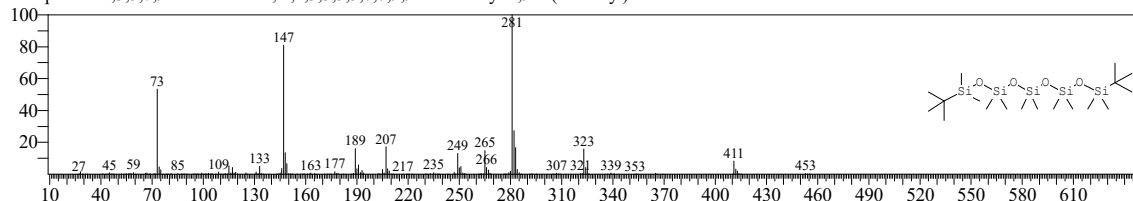SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b

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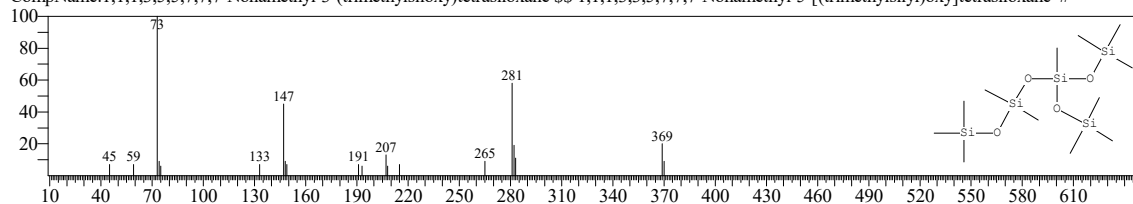SI:80 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

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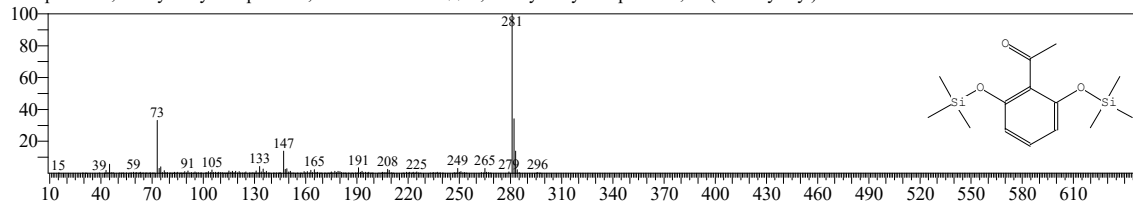CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:75 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
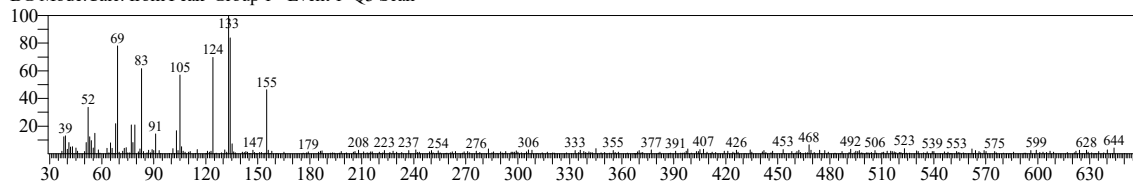CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

<< Target >>
Line#:5 R.Time:11.145(Scan#:1230) MassPeaks:326
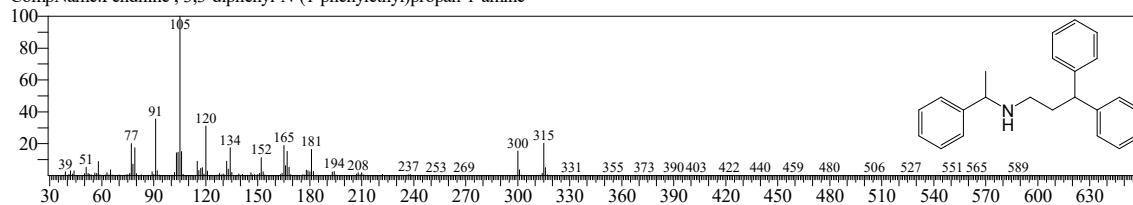RawMode:Averaged 11.140-11.150(1229-1231) BasePeak:133.05(1181)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:530 Library:OA_TMS_DB5_67min_V3.lib
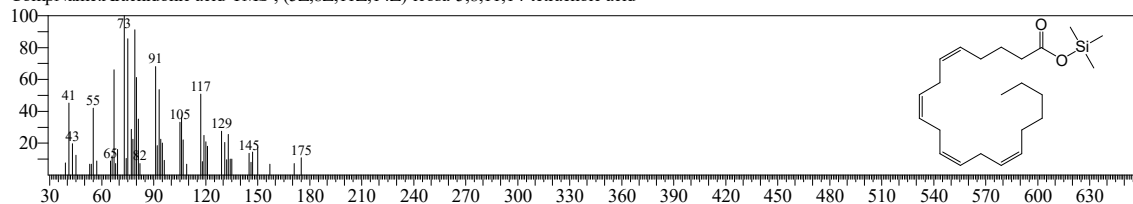SI:41 Formula:C23H25N CAS:13042-18-7 MolWeight:315 RetIndex:2545
CompName:Fendiline ; 3,3-diphenyl-N-(1-phenylethyl)propan-1-amine

Hit#:2 Entry:508 Library:OA_TMS_DB5_67min_V3.lib
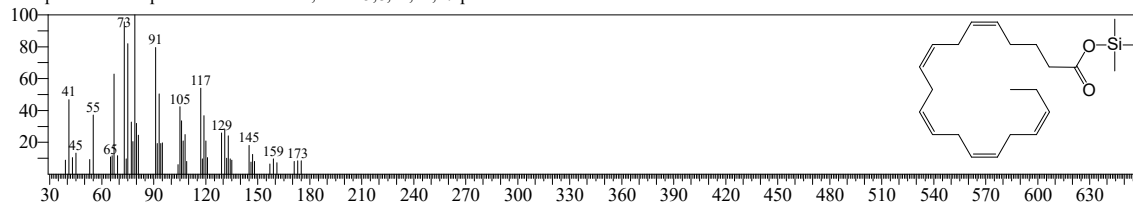SI:38 Formula:C23H40O2Si CAS:506-32-1 MolWeight:376 RetIndex:2381
CompName:Arachidonic acid-TMS ; (5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid

Hit#:3 Entry:509 Library:OA_TMS_DB5_67min_V3.lib
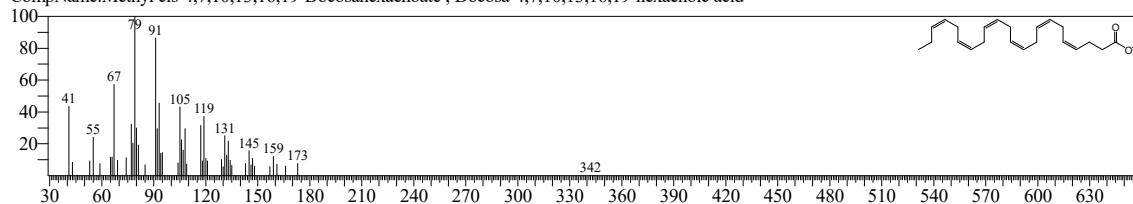SI:37 Formula:C23H38O2Si CAS:10417-94-4 MolWeight:374 RetIndex:2389
CompName:Eicosapentaenoic acid-TMS ; icosa-5,8,11,14,17-pentaenoic acid

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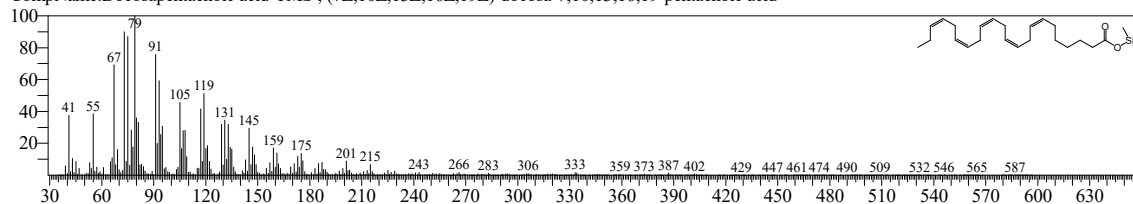CompName:Methyl cis-4,7,10,13,16,19-Docosahexaenoate ; Docosa-4,7,10,13,16,19-hexaenoic acid

Hit#:5 Entry:534 Library:OA_TMS_DB5_67min_V3.lib
SI:35 Formula:C25H42O2Si CAS:24880-45-3 MolWeight:402 RetIndex:2591
CompName:Docosapentaenoic acid-TMS ; (7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoic acid
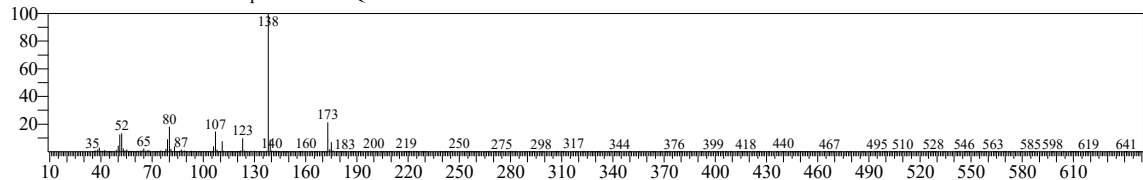
TNAU

<< Target >>
Line#:6 R.Time:12.500(Scan#:1501) MassPeaks:327
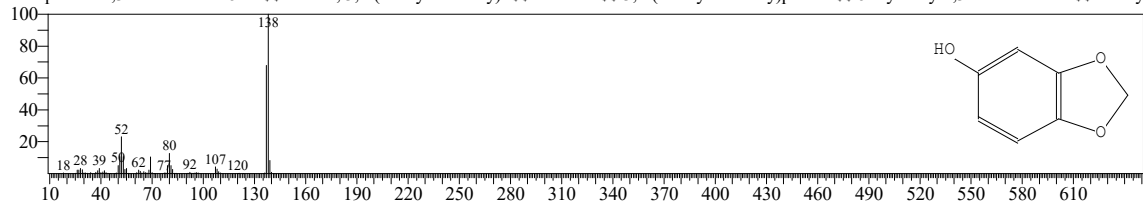RawMode:Averaged 12.495-12.505(1500-1502) BasePeak:138.05(27306)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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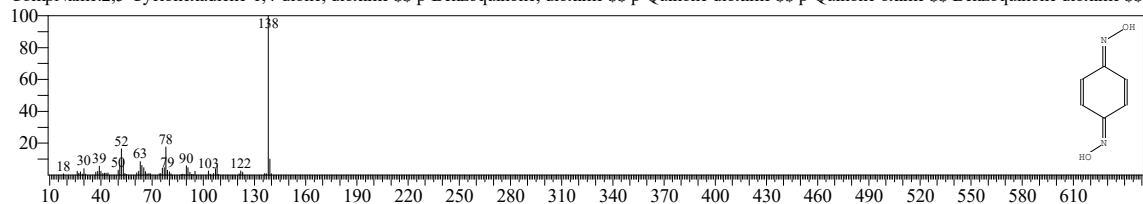SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy

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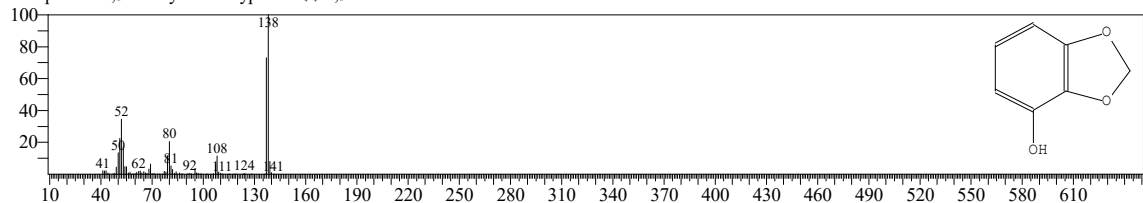SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

Hit#:3 Entry:11188 Library:NIST20M1.lib
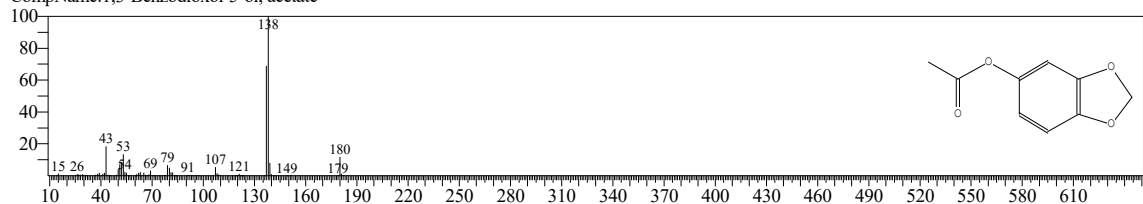SI:73 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #

Hit#:4 Entry:36491 Library:NIST20M1.lib
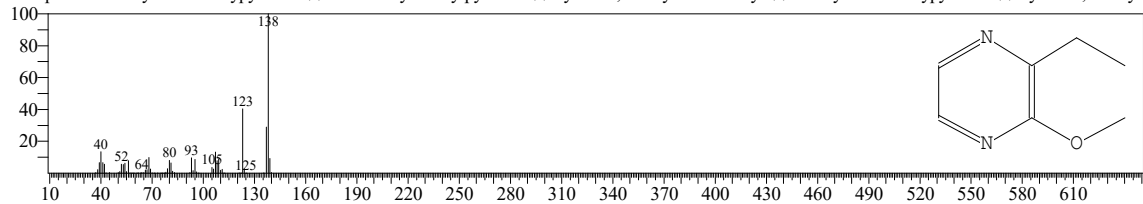SI:71 Formula:C9H8O4 CAS:326-58-9 MolWeight:180 RetIndex:1404
CompName:1,3-Benzodioxol-5-ol, acetate

Hit#:5 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-
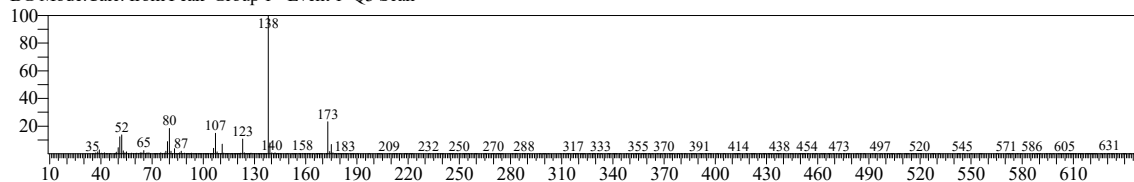
TNAU

<< Target >>
Line#:7 R.Time:12.830(Scan#:1567) MassPeaks:346
RawMode:Averaged 12.825-12.835(1566-1568) BasePeak:138.05(40451)
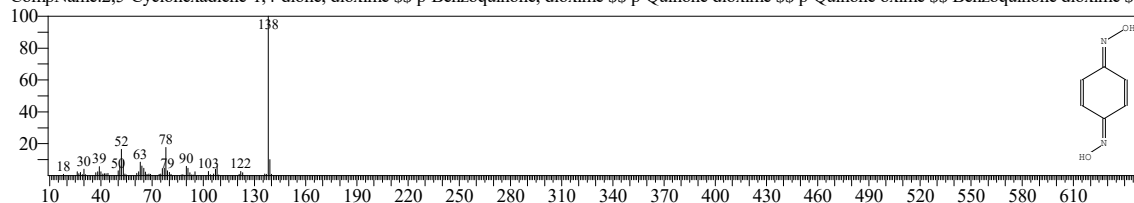BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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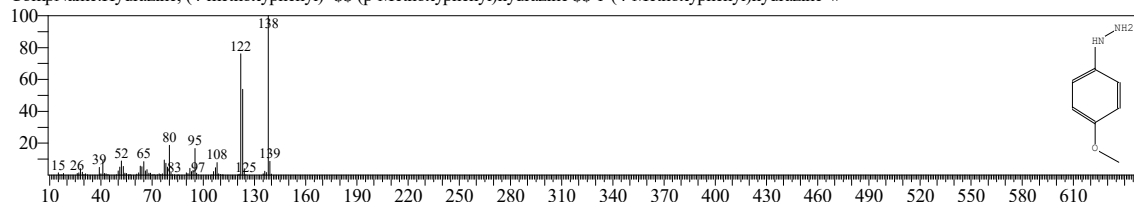SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

Hit#:2 Entry:11222 Library:NIST20M1.lib
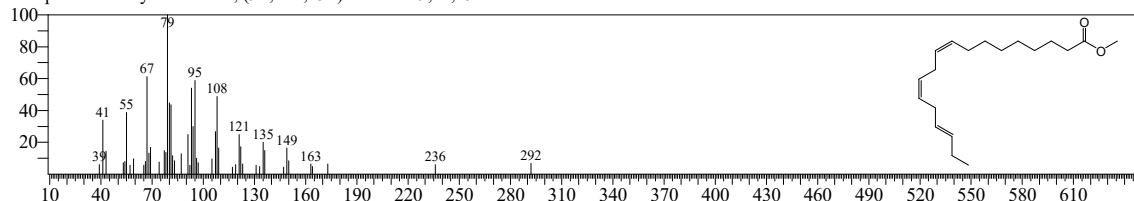SI:71 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

Hit#:3 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
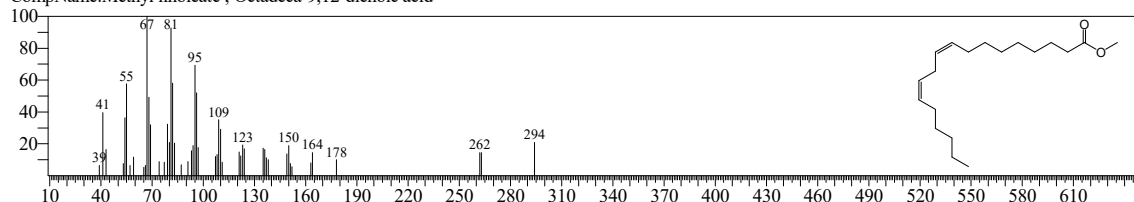SI:34 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

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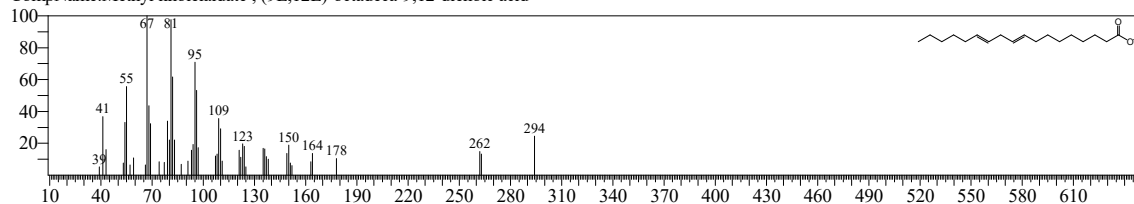SI:33 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

Hit#:5 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:32 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid
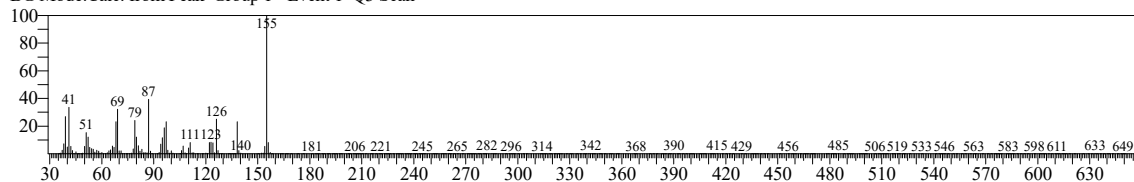
TNAU

<< Target >>
Line#:8 R.Time:13.365(Scan#:1674) MassPeaks:357
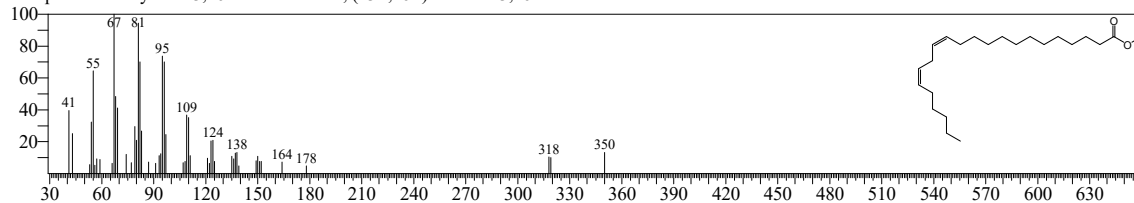RawMode:Averaged 13.360-13.370(1673-1675) BasePeak:155.05(32082)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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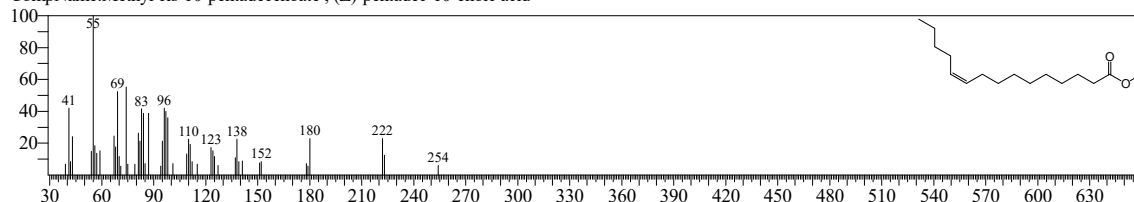SI:51 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

Hit#:2 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
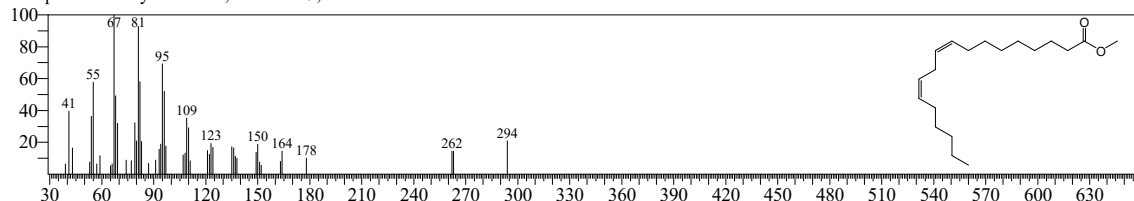SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

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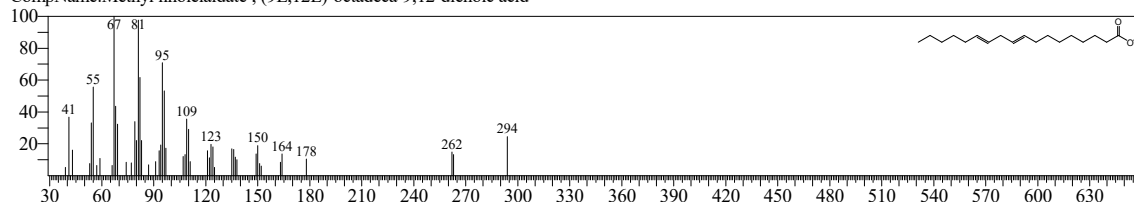SI:50 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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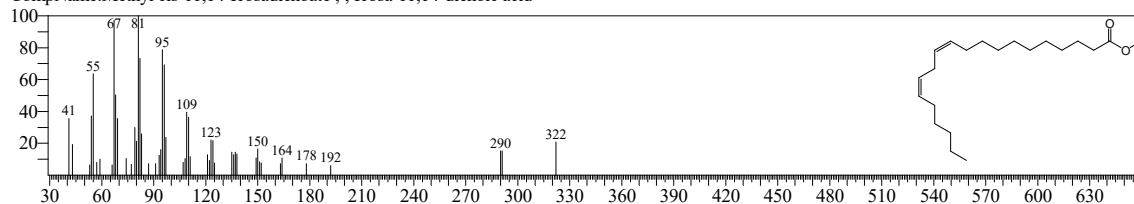SI:50 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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
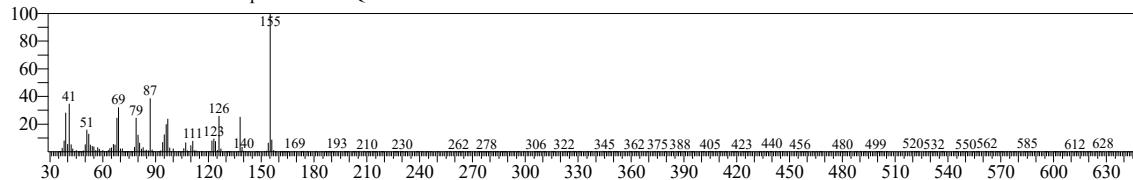
TNAU

<< Target >>
Line#:9 R.Time:13.555(Scan#:1712) MassPeaks:348
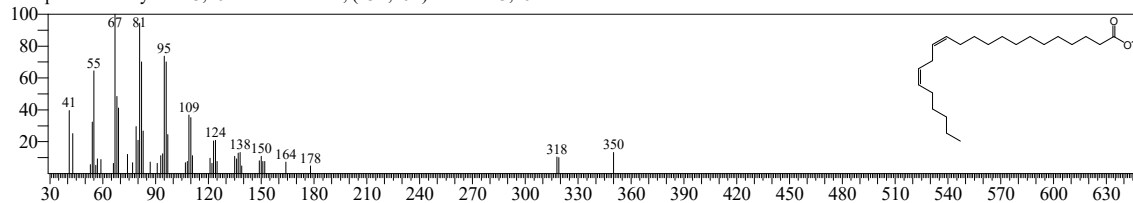RawMode:Averaged 13.550-13.560(1711-1713) BasePeak:155.05(26021)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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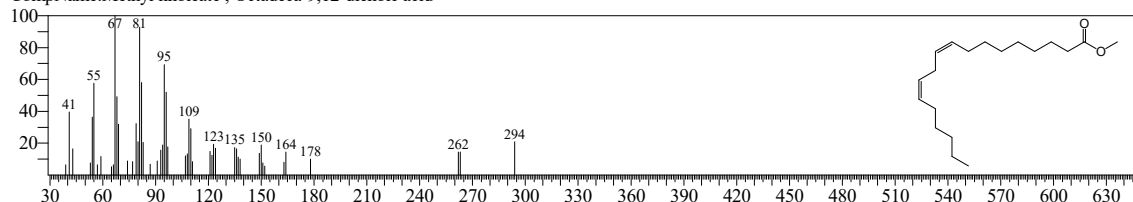SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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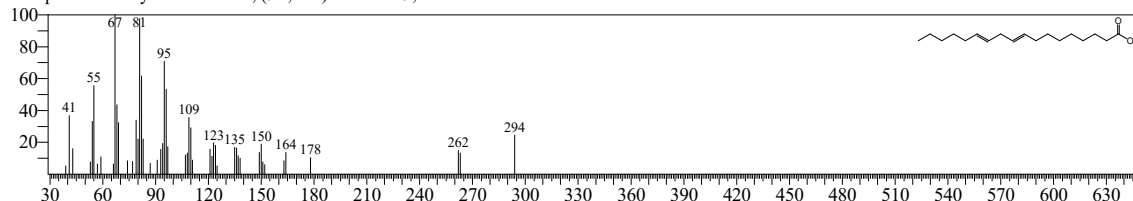SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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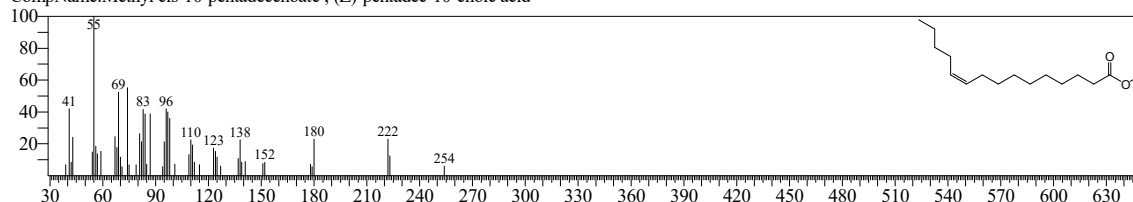CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
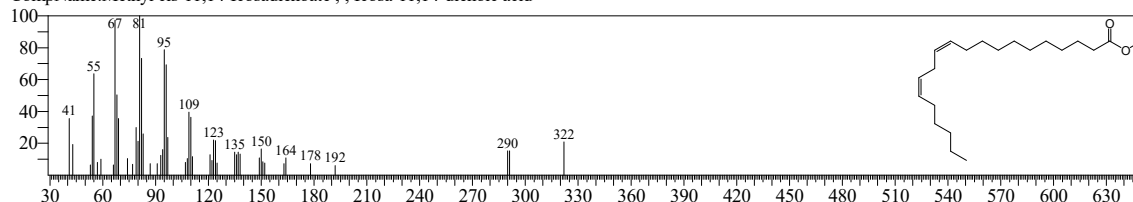SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

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
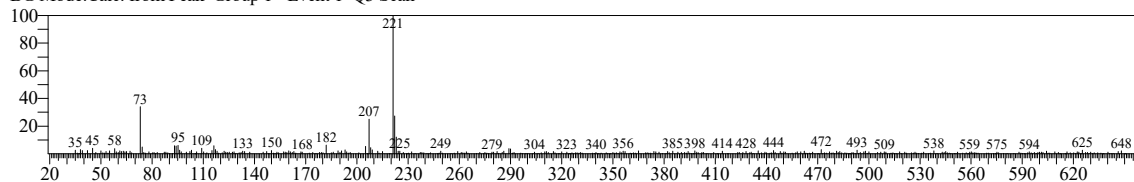
TNAU

<< Target >>
Line#:10 R.Time:13.815(Scan#:1764) MassPeaks:384
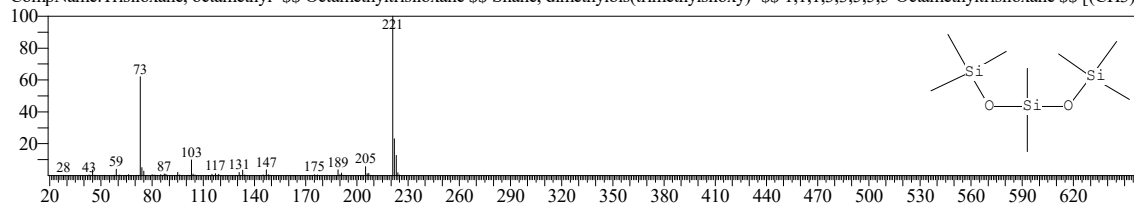RawMode:Averaged 13.810-13.820(1763-1765) BasePeak:221.10(1807)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:28950 Library:NIST20R.lib
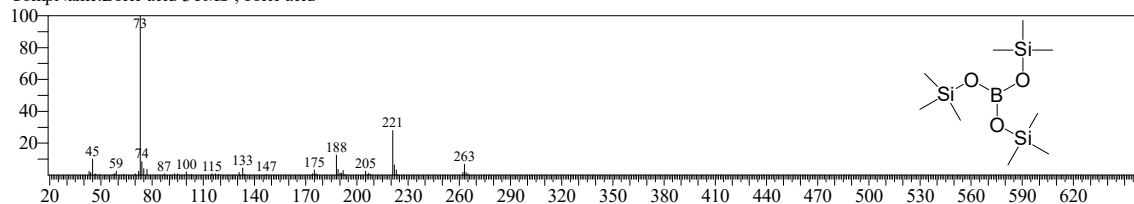SI:72 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3

Hit#:2 Entry:3 Library:OA_TMS_DB5_67min_V3.lib
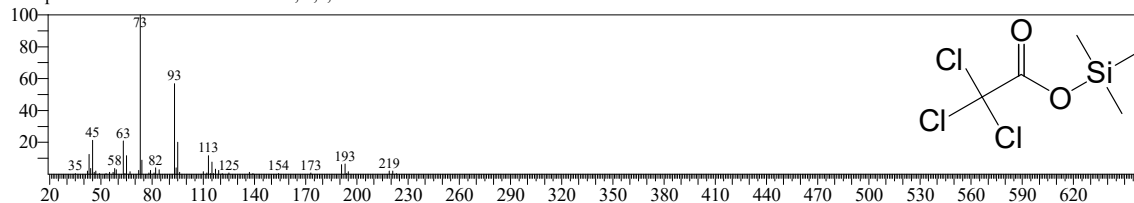SI:53 Formula:C9H27BO3Si3 CAS:10043-35-3 MolWeight:278 RetIndex:992
CompName:Boric acid-3TMS ; boric acid

Hit#:3 Entry:6 Library:OA_TMS_DB5_67min_V3.lib
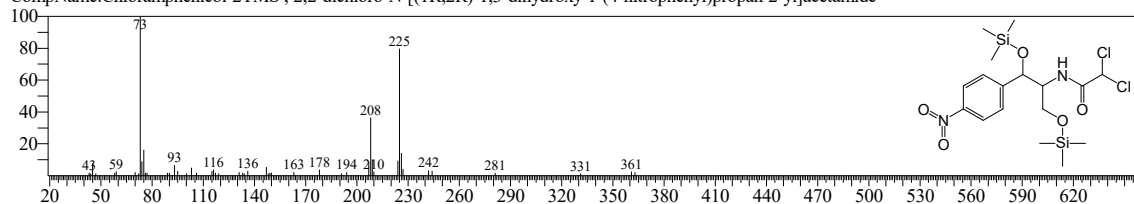SI:45 Formula:C5H9Cl3O2Si CAS:76-03-9 MolWeight:234 RetIndex:1059
CompName:Trichloroacetic acid-TMS ; 2,2,2-trichloroacetic acid

Hit#:4 Entry:528 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C17H28Cl2N2O5Si2 CAS:56-75-7 MolWeight:466 RetIndex:2508
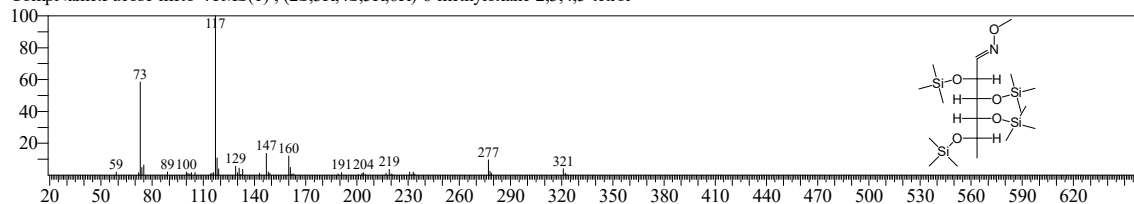CompName:Chloramphenicol-2TMS ; 2,2-dichloro-N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide

Hit#:5 Entry:283 Library:OA_TMS_DB5_67min_V3.lib
SI:38 Formula:C19H47NO5Si4 CAS:3615-37-0 MolWeight:481 RetIndex:1754
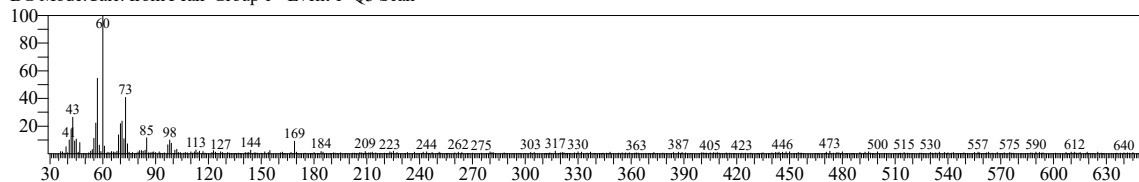CompName:Fucose-meto-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

TNAU

<< Target >>
Line#:11 R.Time:18.085(Scan#:2618) MassPeaks:356
RawMode:Averaged 18.080-18.090(2617-2619) BasePeak:60.00(2594)
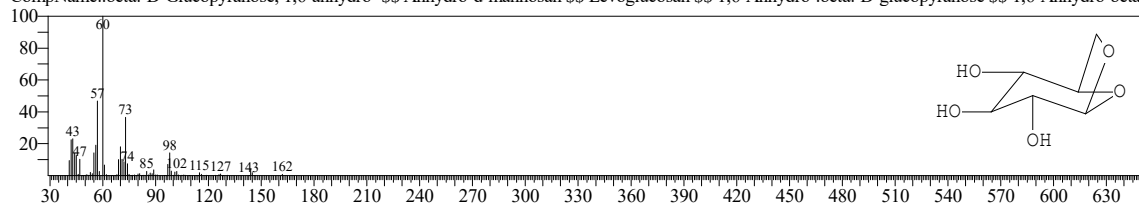BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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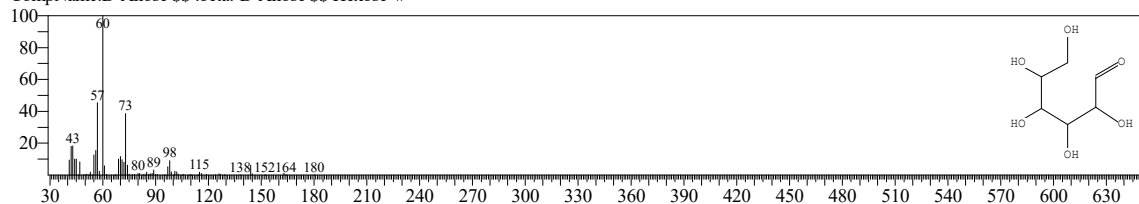SI:88 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-

Hit#:2 Entry:36240 Library:NIST20M1.lib
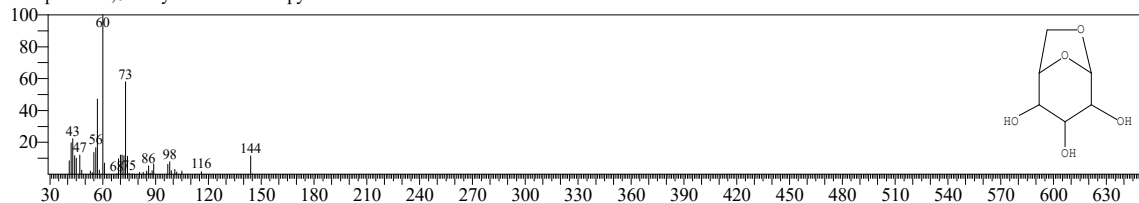SI:88 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #

Hit#:3 Entry:23812 Library:NIST20M1.lib
SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
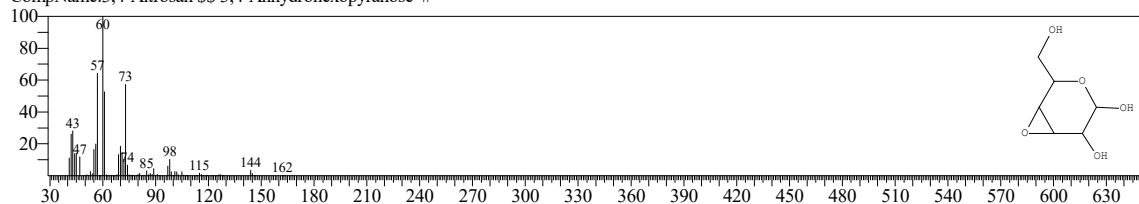CompName:1,6-Anhydro-.beta.-d-talopyranose

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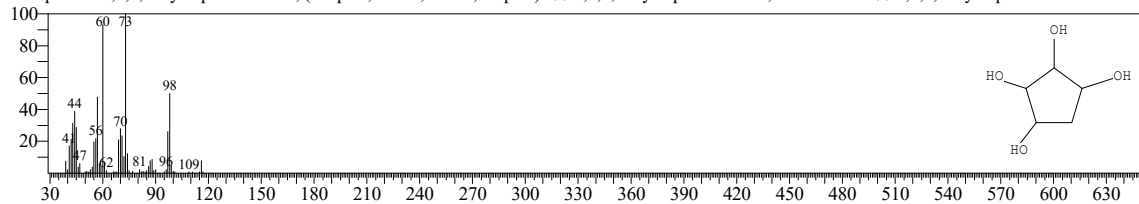SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1400
CompName:3,4-Altrosan $$ 3,4-Anhydrohexopyranose #

Hit#:5 Entry:9697 Library:NIST20M1.lib
SI:81 Formula:C5H10O4 CAS:14003-71-5 MolWeight:134 RetIndex:1352
CompName:1,2,3,4-Cyclopentanetetrol, (1.alpha.,2.beta.,3.beta.,4.alpha.)- $$ 1,2,3,4-Cyclopentanetetrol, stereoisomer $$ 1,2,3,4-Cyclopentanetetrol #
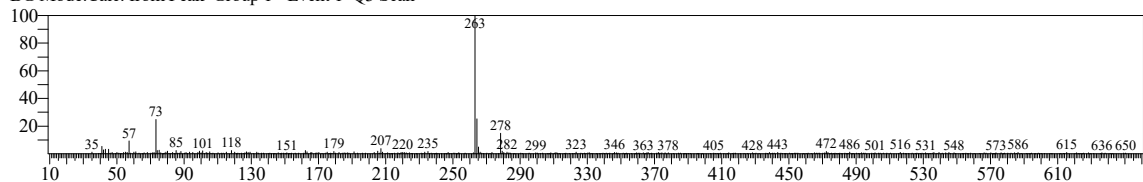
TNAU

<< Target >>
Line#:12 R.Time:19.200(Scan#:2841) MassPeaks:410
RawMode:Averaged 19.195-19.205(2840-2842) BasePeak:263.15(3940)
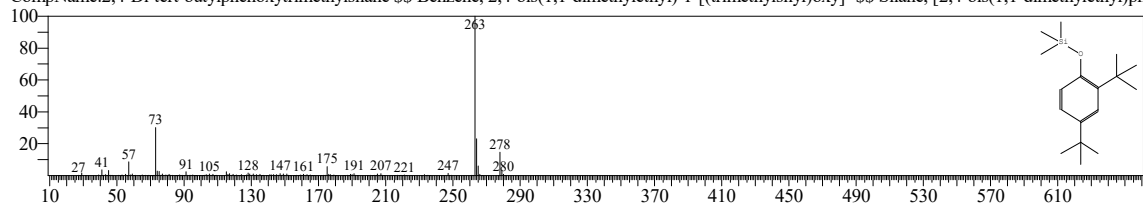BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:137399 Library:NIST20M1.lib
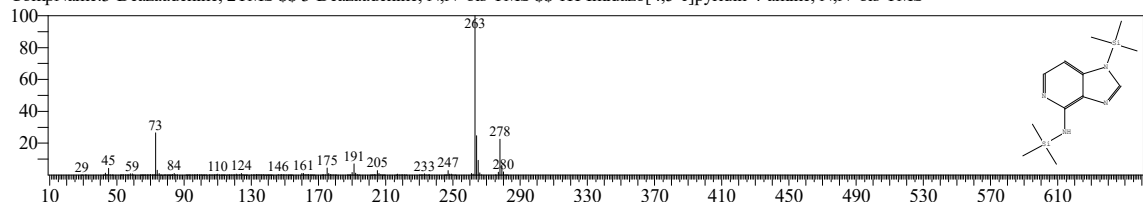SI:85 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph

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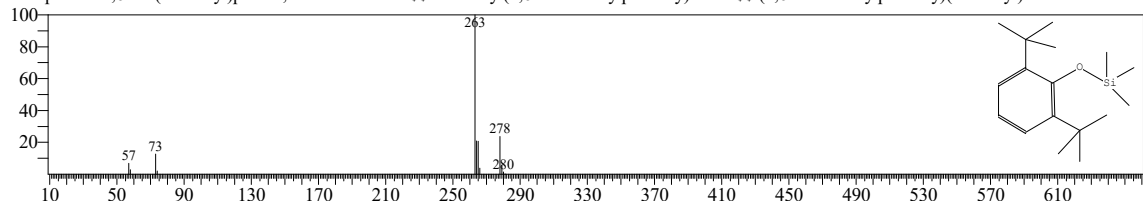SI:78 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS

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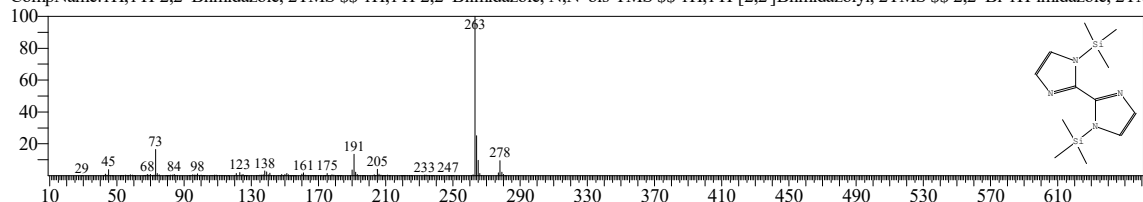SI:78 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #

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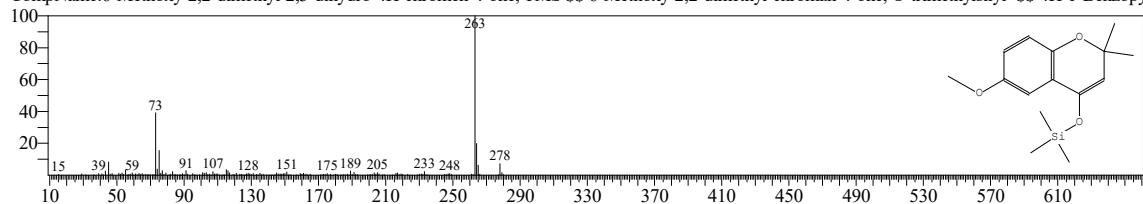SI:75 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM

Hit#:5 Entry:137020 Library:NIST20M1.lib
SI:74 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
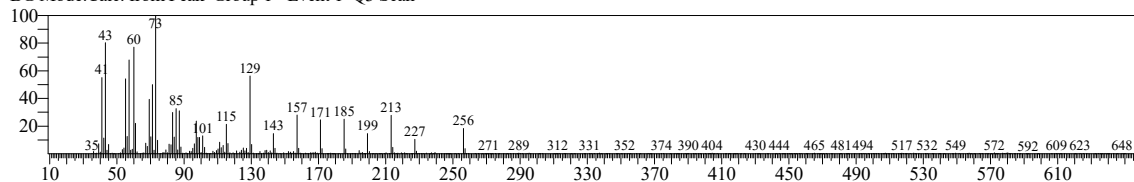
TNAU

<< Target >>
Line#:13 R.Time:28.305(Scan#:4662) MassPeaks:381
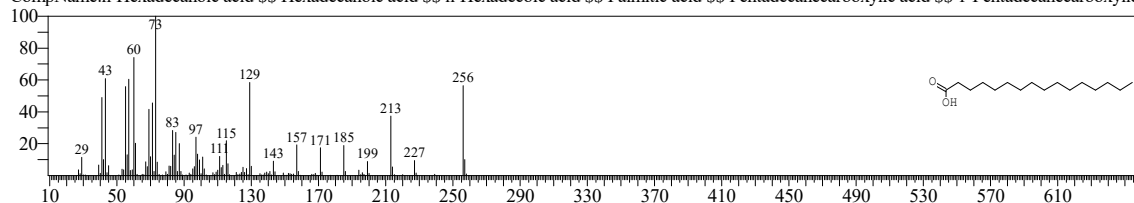RawMode:Averaged 28.300-28.310(4661-4663) BasePeak:73.05(7724)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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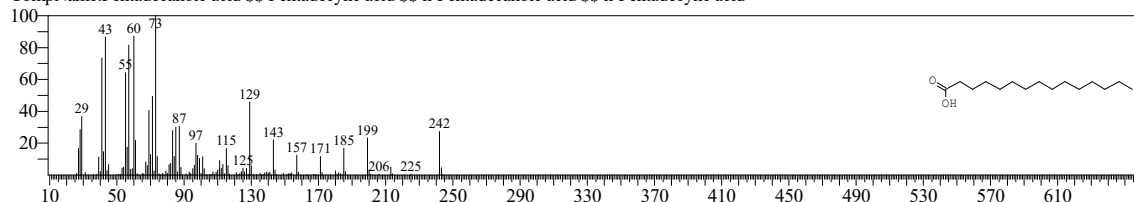SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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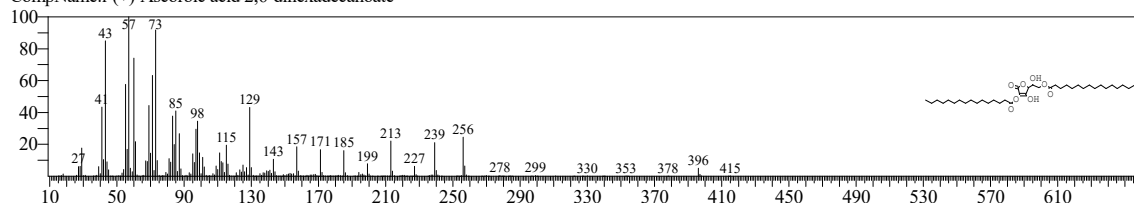SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

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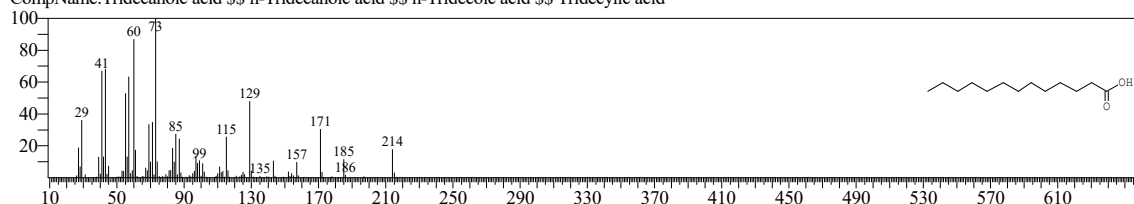SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

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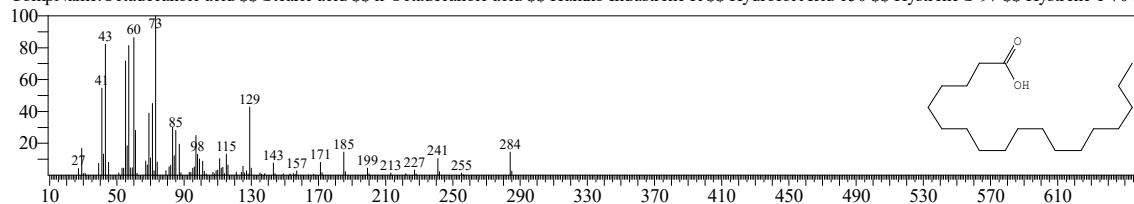SI:90 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

Hit#:5 Entry:144781 Library:NIST20M1.lib
SI:90 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $$
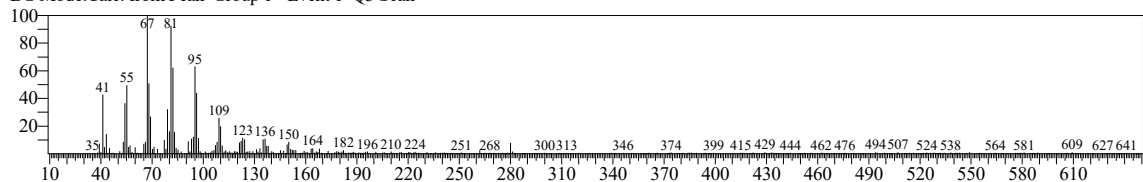
TNAU

<< Target >>
Line#:14 R.Time:31.480(Scan#:5297) MassPeaks:377
RawMode:Averaged 31.475-31.485(5296-5298) BasePeak:67.10(5024)
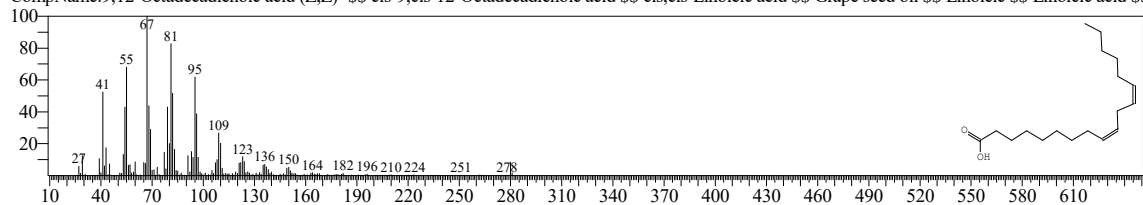BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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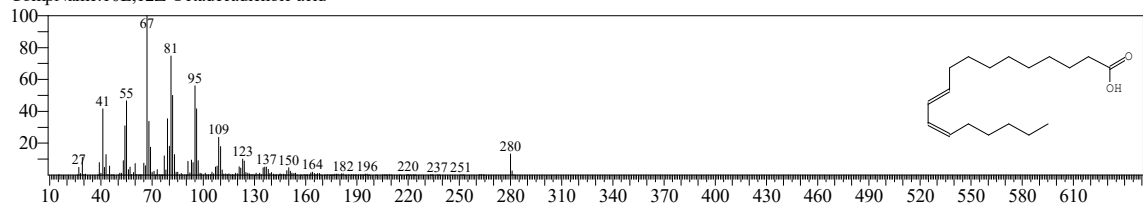SI:94 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $

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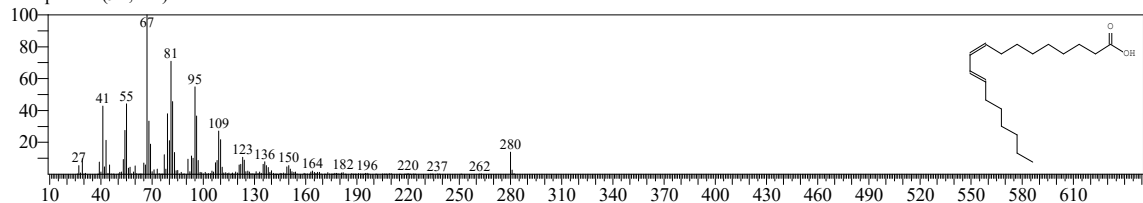CompName:10E,12Z-Octadecadienoic acid

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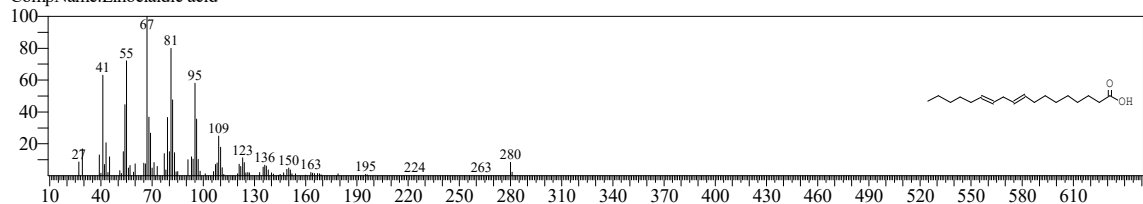SI:94 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid

Hit#:4 Entry:139661 Library:NIST20M1.lib
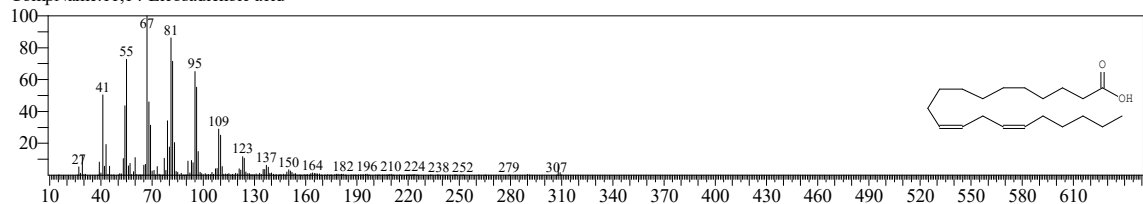SI:93 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

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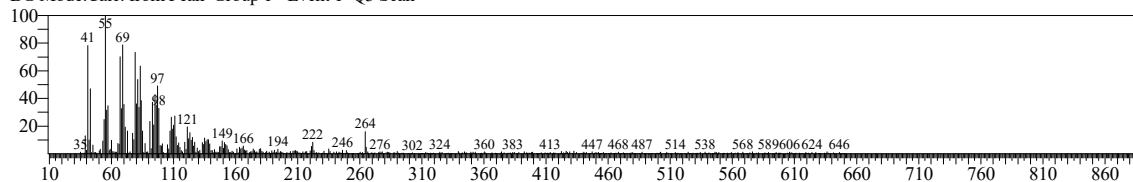CompName:11,14-Eicosadienoic acid

TNAU

<< Target >>
Line#:15 R.Time:31.590(Scan#:5319) MassPeaks:425
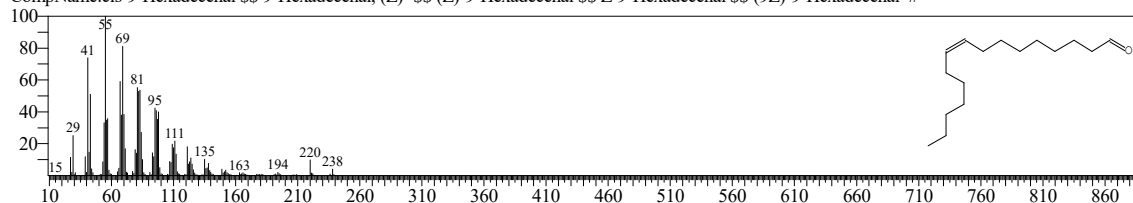RawMode:Averaged 31.585-31.595(5318-5320) BasePeak:55.05(2649)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:92244 Library:NIST20M1.lib
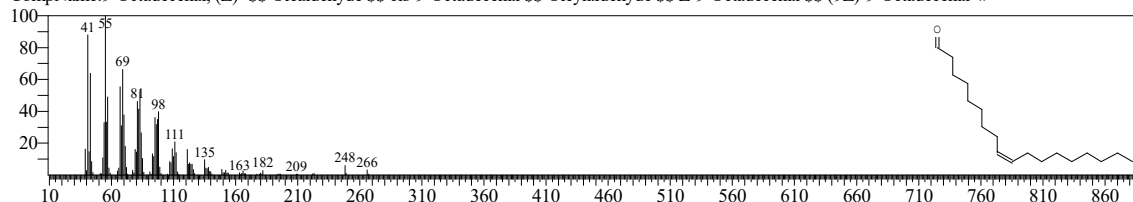SI:89 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #

Hit#:2 Entry:123421 Library:NIST20M1.lib
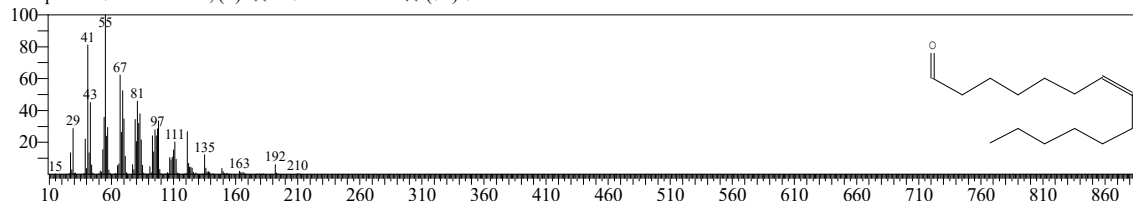SI:88 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal #

Hit#:3 Entry:63176 Library:NIST20M1.lib
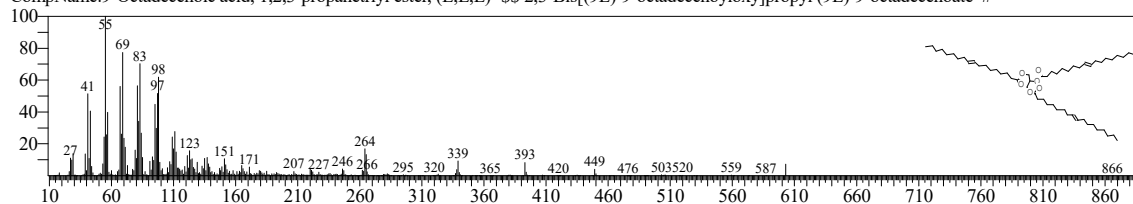SI:88 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #

Hit#:4 Entry:46357 Library:NIST20M2.lib
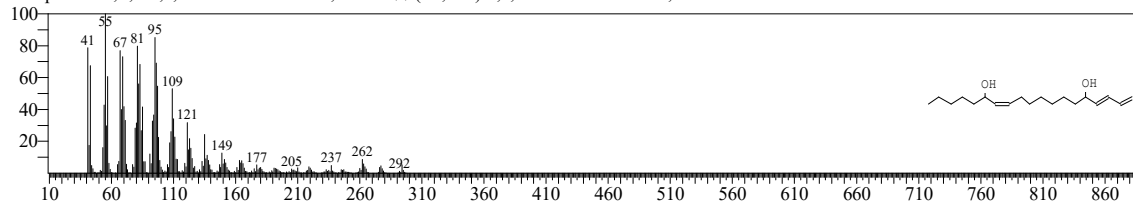SI:88 Formula:C57H104O6 CAS:537-39-3 MolWeight:884 RetIndex:6149
CompName:9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)- $$ 2,3-Bis[(9E)-9-octadecenoyloxy]propyl (9E)-9-octadecenoate #

Hit#:5 Entry:156549 Library:NIST20M1.lib
SI:88 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
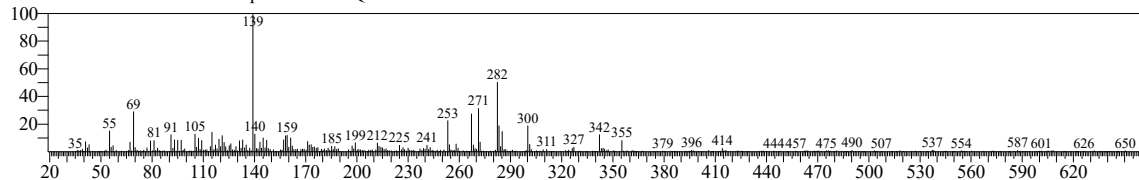CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #

<< Target >>
Line#:16 R.Time:45.635(Scan#:8128) MassPeaks:396
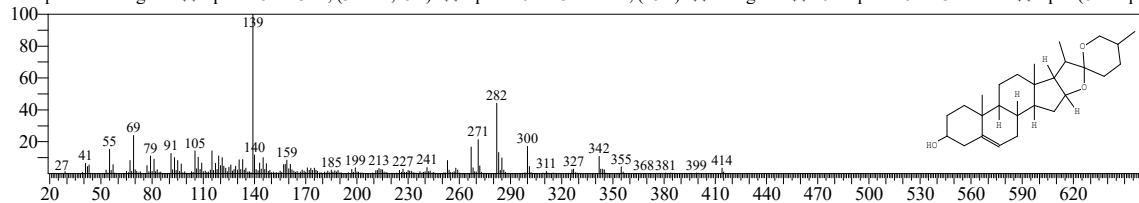RawMode:Averaged 45.630-45.640(8127-8129) BasePeak:139.10(3965)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:89 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
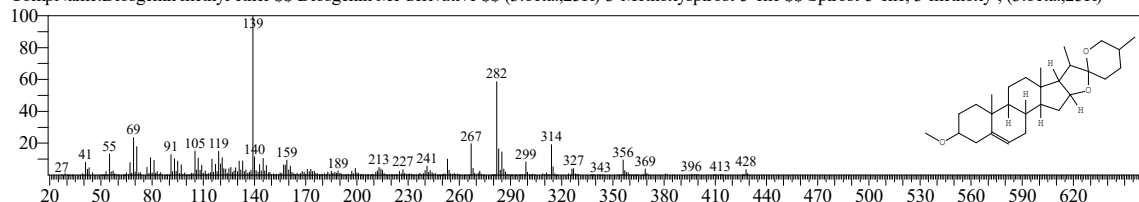CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

Hit#:2 Entry:14852 Library:NIST20M2.lib
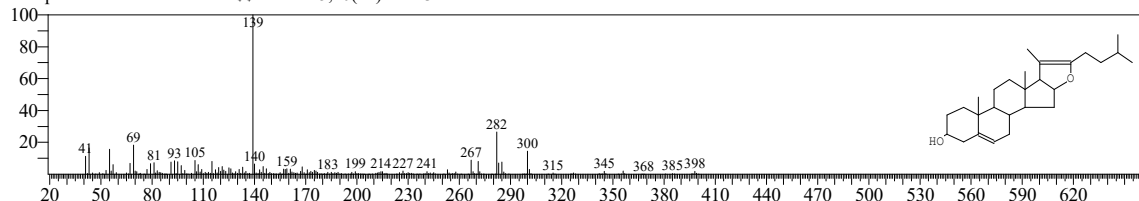SI:79 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:3 Entry:41561 Library:NIST20R.lib
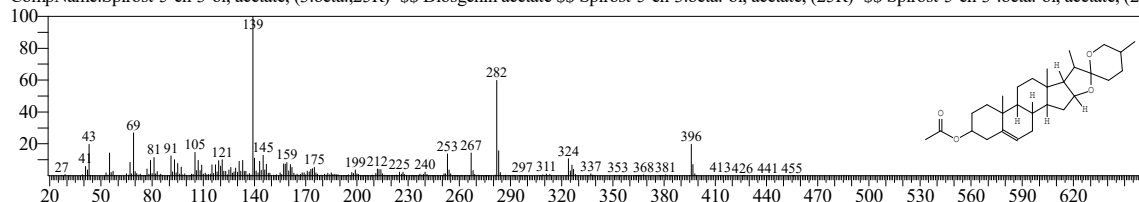SI:79 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #

Hit#:4 Entry:24878 Library:NIST20M2.lib
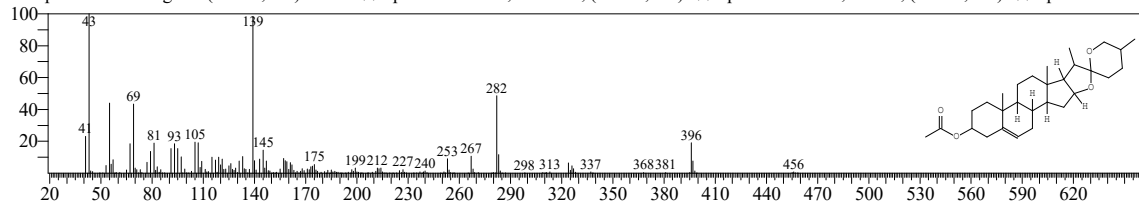SI:77 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (25

Hit#:5 Entry:42677 Library:NIST20R.lib
SI:72 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.
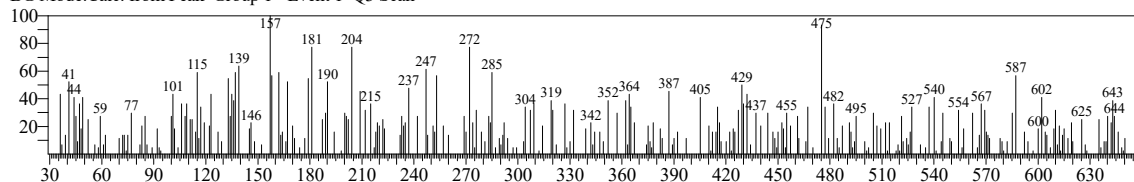
TNAU

<< Target >>
Line#:17 R.Time:45.715(Scan#:8144) MassPeaks:283
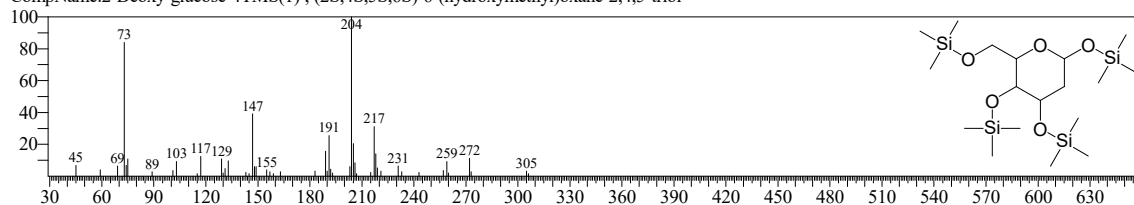RawMode:Averaged 45.710-45.720(8143-8145) BasePeak:157.10(44)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:276 Library:OA_TMS_DB5_67min_V3.lib
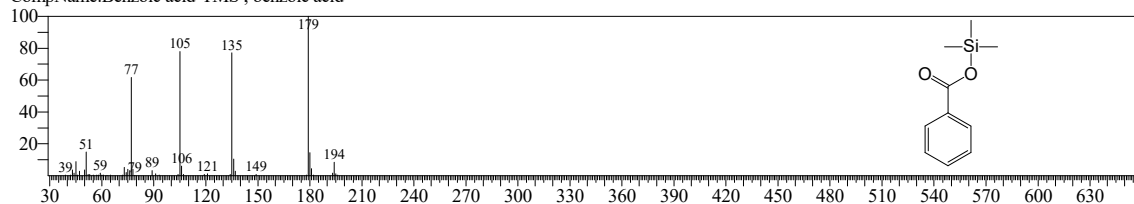SI:16 Formula:C18H44O5Si4 CAS:154-17-6 MolWeight:452 RetIndex:1745
CompName:2-Deoxy-glucose-4TMS(1) ; (2S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,4,5-triol

Hit#:2 Entry:66 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C10H14O2Si CAS:65-85-0 MolWeight:194 RetIndex:1252
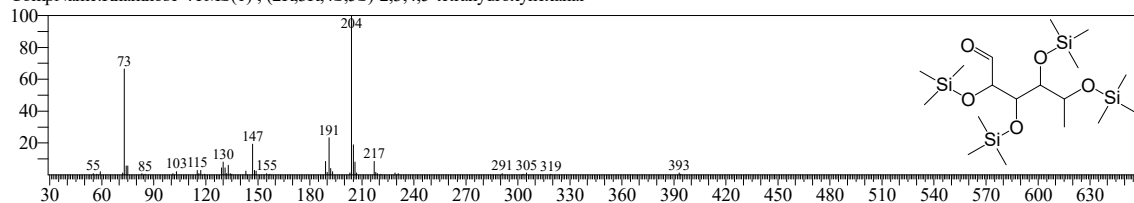CompName:Benzoic acid-TMS ; benzoic acid

Hit#:3 Entry:219 Library:OA_TMS_DB5_67min_V3.lib
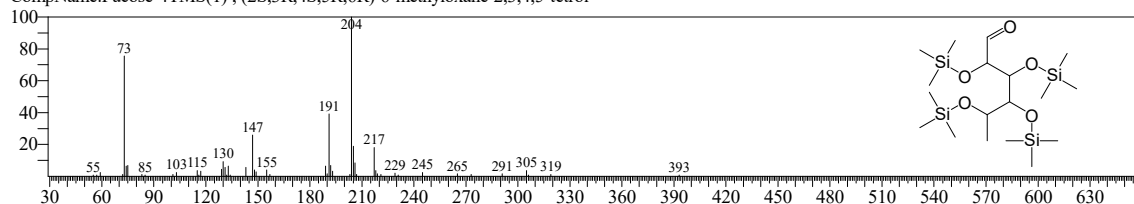SI:14 Formula:C18H44O5Si4 CAS:10485-94-6 MolWeight:452 RetIndex:1646
CompName:Rhamnose-4TMS(1) ; (2R,3R,4S,5S)-2,3,4,5-tetrahydroxyhexanal

Hit#:4 Entry:252 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C18H44O5Si4 CAS:3615-37-0 MolWeight:452 RetIndex:1695
CompName:Fucose-4TMS(1) ; (2S,3R,4S,5R,6R)-6-methyloxane-2,3,4,5-tetrol

Hit#:5 Entry:395 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C10H16N4O2Si CAS:58-55-9 MolWeight:252 RetIndex:1936
CompName:Theophylline-TMS ; 1,3-dimethyl-7H-purine-2,6-dione