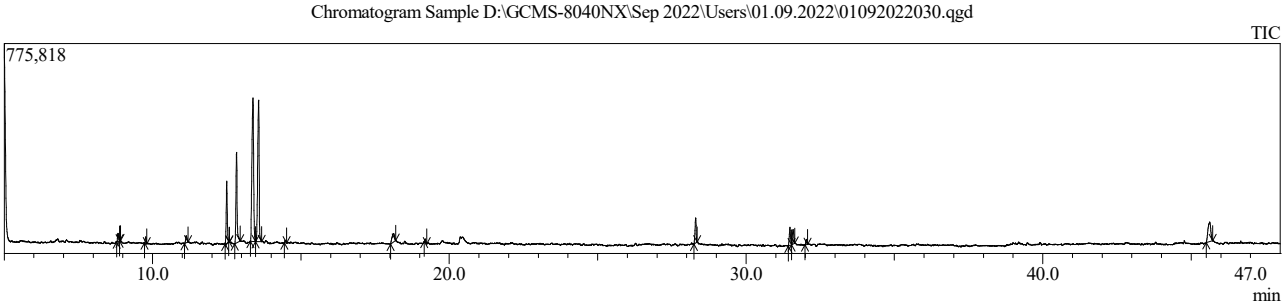
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 7:05:08 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 10-2
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 11
Injection Volume	: 5.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022030.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022030.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 11:10:11 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022030.qgd



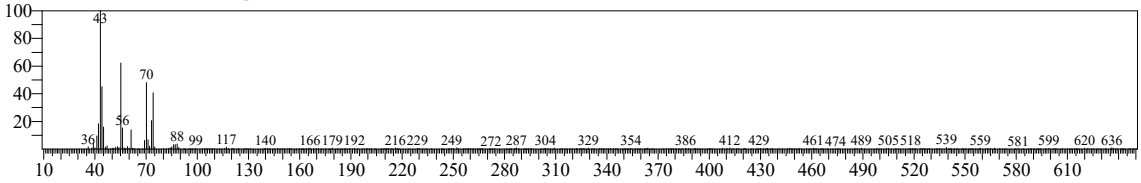
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.836	91525	1.30	30516	1.47	3.00	85	1-Butanol, 3-methyl-, acetate
2	8.895	8497	0.12	7901	0.38	1.08	19	Caffeine
3	9.771	50996	0.73	24524	1.19	2.08	95	Pentasiloxane, dodecamethyl-
4	11.137	84951	1.21	25682	1.24	3.31	42	Methyl myristoleate
5	12.499	594786	8.48	230832	11.16	2.58	73	2,5-Cyclohexadiene-1,4-dione, dioxime
6	12.575	185	0.00	1681	0.08	0.11	14	Dimethylglycine-TMS
7	12.829	925171	13.19	334850	16.18	2.76	74	1,3-Benzodioxol-5-ol
8	13.382	2109301	30.06	530228	25.63	3.98	53	Methyl cis-13,16-Docosadienate
9	13.573	1776467	25.32	523024	25.28	3.40	53	Methyl cis-13,16-Docosadienate
10	14.472	24659	0.35	10004	0.48	2.46	75	5-(4-Methylbenzyl)-1,3,4-thiadiazol-2-amine
11	18.125	187083	2.67	31176	1.51	6.00	94	D-Allose
12	19.190	28558	0.41	12911	0.62	2.21	84	2,4-Di-tert-butylphenoxytrimethylsilane
13	28.301	244108	3.48	92967	4.49	2.63	95	n-Hexadecanoic acid
14	31.479	195899	2.79	66998	3.24	2.92	95	10E,12Z-Octadecadienoic acid
15	31.585	165408	2.36	54056	2.61	3.06	88	cis-9-Hexadecenal
16	32.032	50697	0.72	19693	0.95	2.57	91	Octadecanoic acid
17	45.623	478058	6.81	72111	3.49	6.63	90	Diosgenin
		7016349	100.00	2069154	100.00			

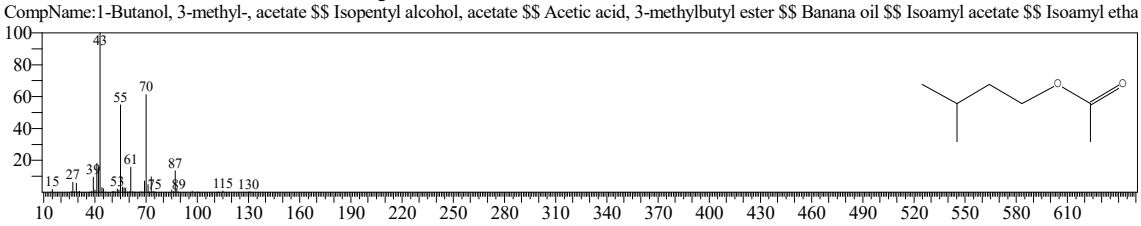
Library

TNAU

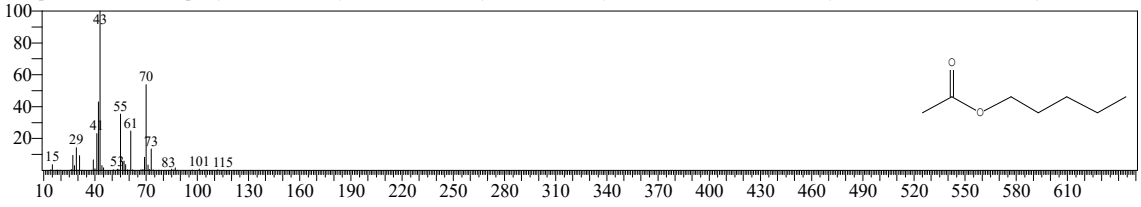
<< Target >>
Line#:1 R.Time:8.835(Scan#:768) MassPeaks:340
RawMode:Averaged 8.830-8.840(767-769) BasePeak:43.05(5526)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



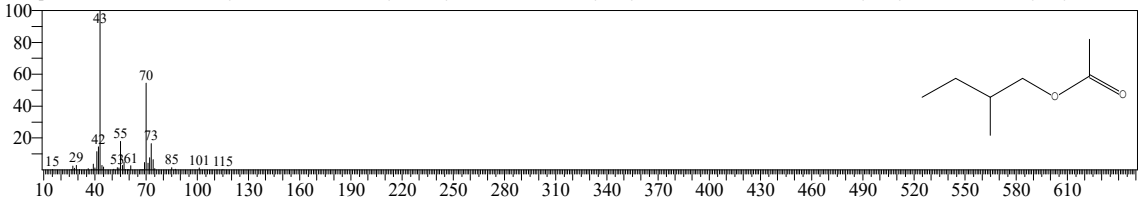
Hit#:1 Entry:6784 Library:NIST20R.lib
SI:85 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



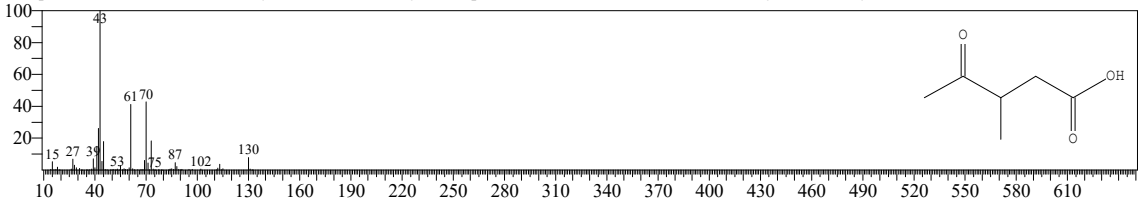
Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:82 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ An



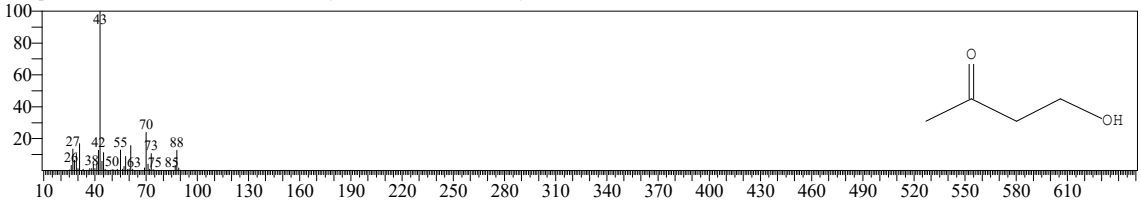
Hit#:3 Entry:6819 Library:NIST20R.lib
SI:82 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:8539 Library:NIST20M1.lib
SI:80 Formula:C6H10O3 CAS:6628-79-1 MolWeight:130 RetIndex:1046
CompName:Pentanoic acid, 3-methyl-4-oxo- $$ 3-Methyl-4-oxopentanoic acid $$ Levulinic acid, 3-methyl $$ 3-Methyllevulinic acid

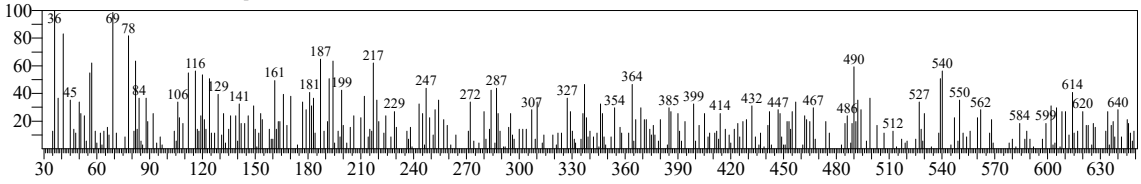


Hit#:5 Entry:1220 Library:NIST20R.lib
SI:80 Formula:C4H8O2 CAS:590-90-9 MolWeight:88 RetIndex:798
CompName:CH3C(O)CH2CH2OH $$ Methylolacetone $$ Monomethylolacetone $$ 3-Ketobutan-1-ol $$ 3-Oxo-1-butanol $$ 3-Oxobutanol $$ 4-Butanol-

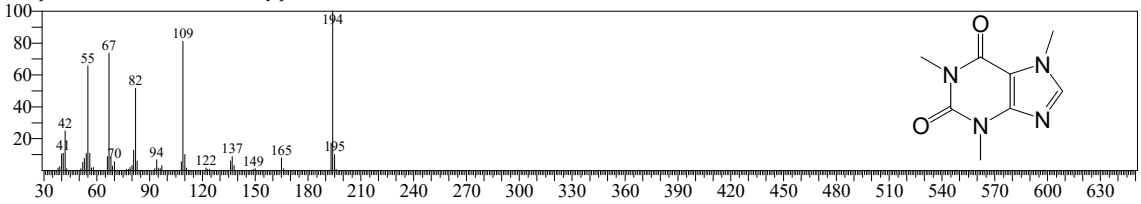


TNAU

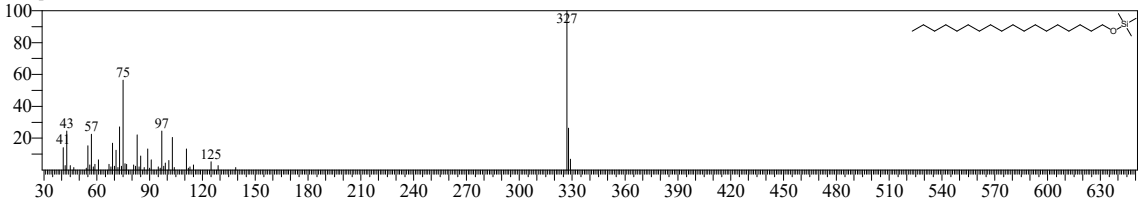
<< Target >>
Line#:2 R.Time:8.895(Scan#:780) MassPeaks:324
RawMode:Averaged 8.890-8.900(779-781) BasePeak:36.00(71)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



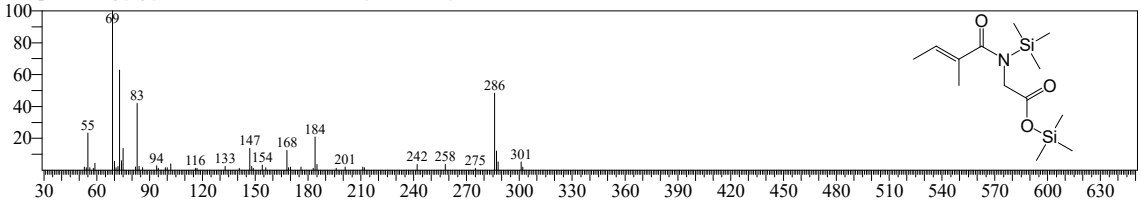
Hit#:1 Entry:342 Library:OA_TMS_DB5_67min_V3.lib
SI:19 Formula:C8H10N4O2 CAS:58-08-2 MolWeight:194 RetIndex:1867
CompName:Caffeine ; 1,3,7-trimethylpurine-2,6-dione



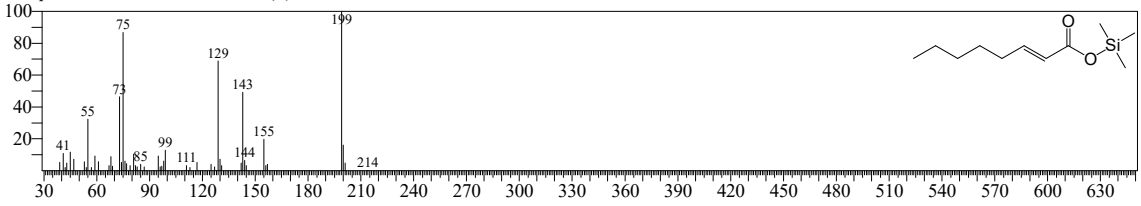
Hit#:2 Entry:477 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C21H46OSi CAS:112-92-5 MolWeight:342 RetIndex:2156
CompName:Octadecanol-TMS ; octadecan-1-ol



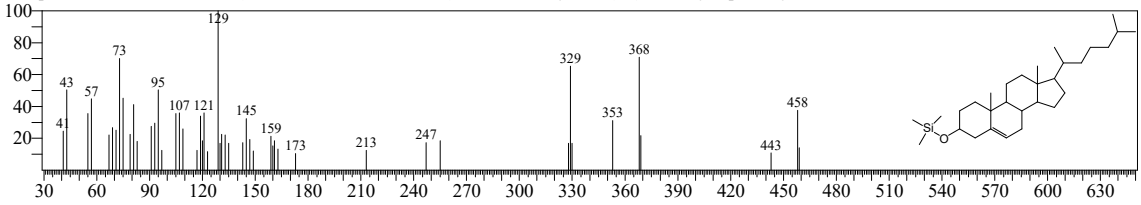
Hit#:3 Entry:176 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C13H27NO3Si2 CAS:35842-45-6 MolWeight:301 RetIndex:1564
CompName:Tiglylglycine-2TMS ; 2-[[(E)-2-methylbut-2-enoyl]amino]acetic acid



Hit#:4 Entry:91 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C11H22O2Si CAS:1871-67-6 MolWeight:214 RetIndex:1313
CompName:2-Octenoic acid-TMS ; (E)-oct-2-enoic acid

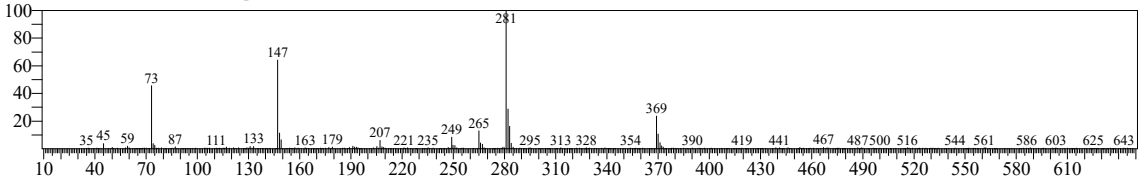


Hit#:5 Entry:567 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C30H54OSi CAS:57-88-5 MolWeight:458 RetIndex:3221
CompName:Cholesterol-TMS ; (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R)-6-methylheptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodec

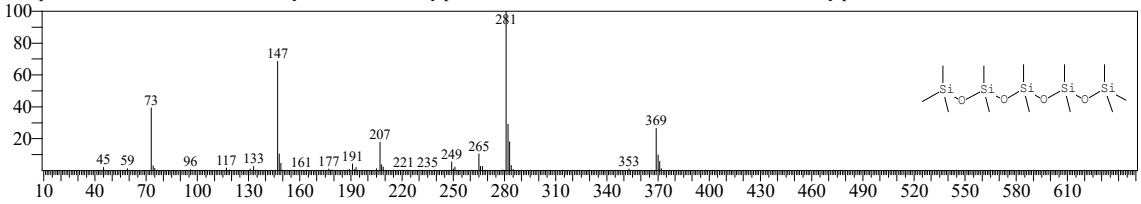


TNAU

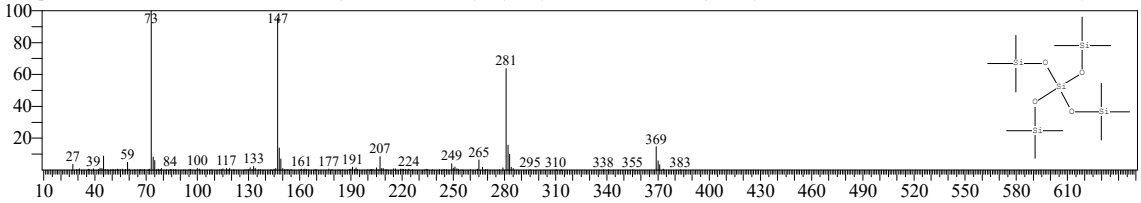
<< Target >>
Line#:3 R.Time:9.770(Scan#:955) MassPeaks:365
RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.00(5472)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



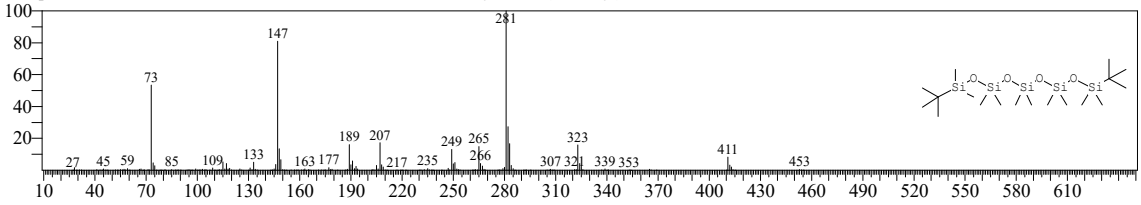
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:95 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



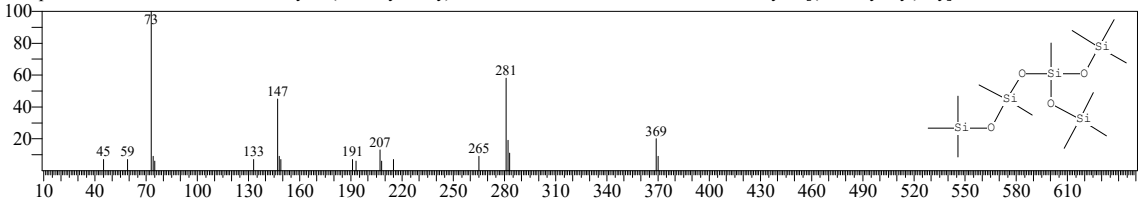
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:84 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



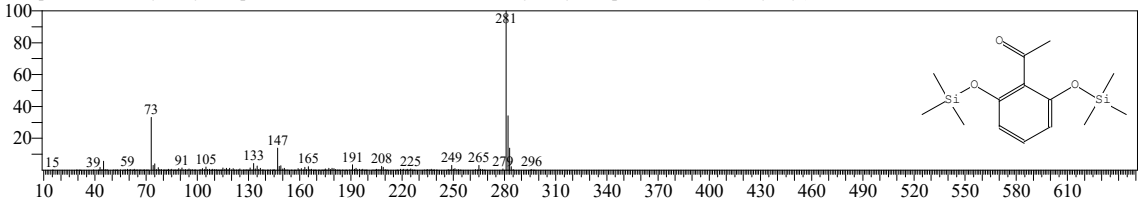
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:82 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



Hit#:4 Entry:249271 Library:NIST20M1.lib
SI:80 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

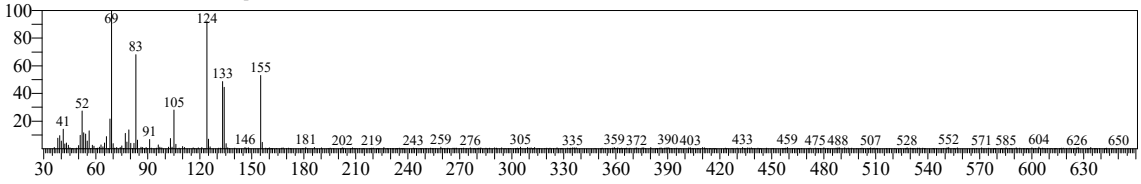


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:77 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

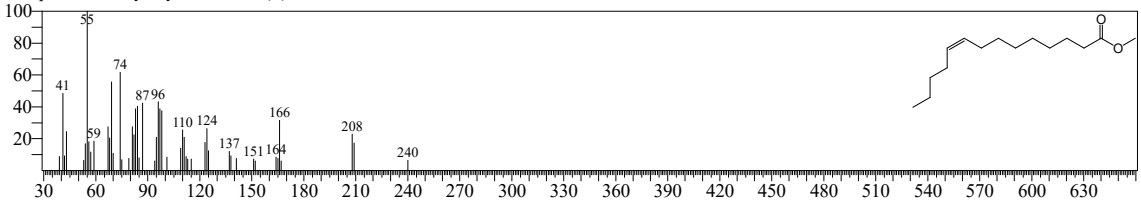


TNAU

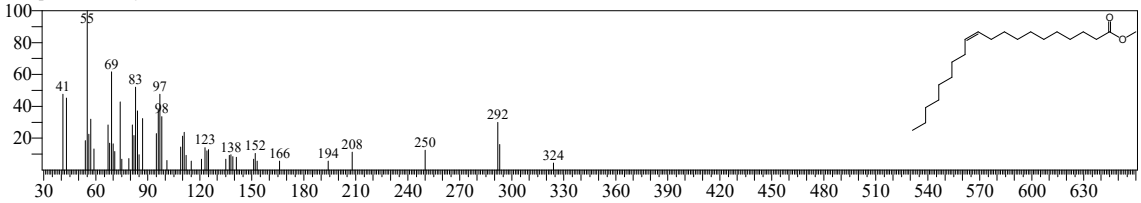
<< Target >>
Line#:4 R.Time:11.135(Scan#:1228) MassPeaks:338
RawMode:Averaged 11.130-11.140(1227-1229) BasePeak:69.05(3558)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



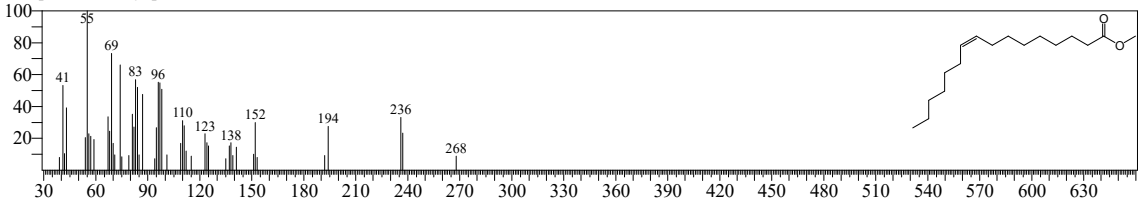
Hit#:1 Entry:9 Library:FA_ME_SP2560_EI_V3.lib
SI:42 Formula:C15H28O2 CAS:544-64-9 MolWeight:240 RetIndex:2283
CompName:Methyl myristoleate ; ; (Z)-tetradec-9-enoic acid



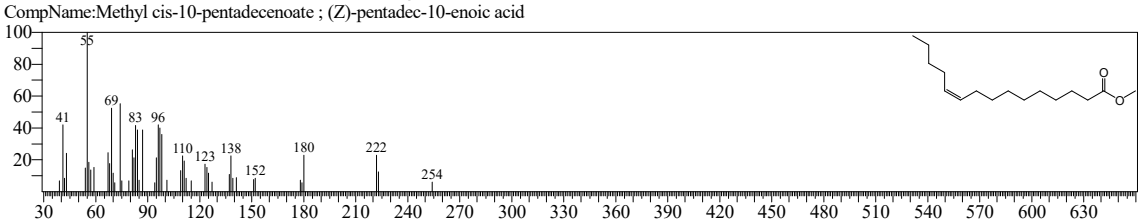
Hit#:2 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid



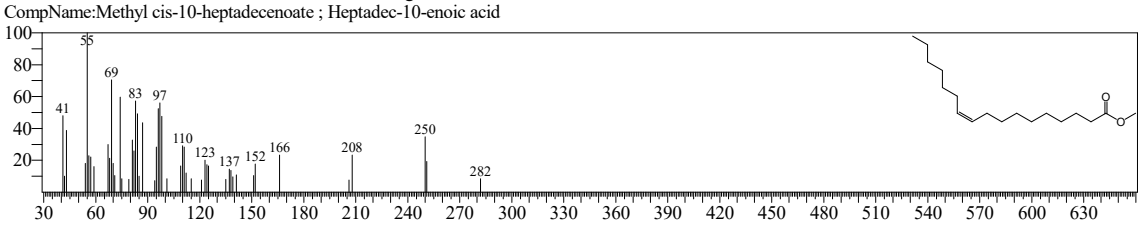
Hit#:3 Entry:13 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C17H32O2 CAS:373-49-9 MolWeight:268 RetIndex:2478
CompName:Methyl palmitoleate ; Hexadec-9-enoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

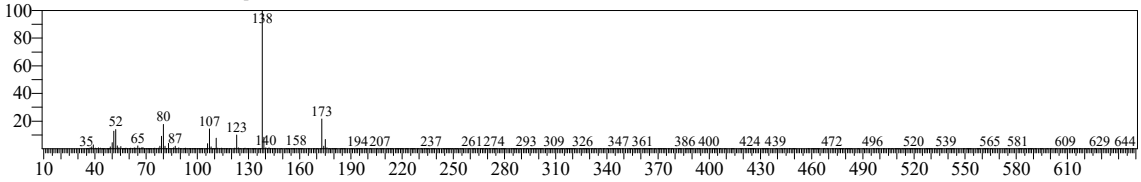


Hit#:5 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:40 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

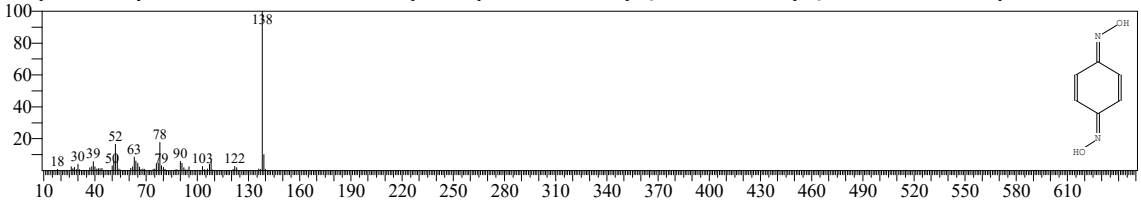


TNAU

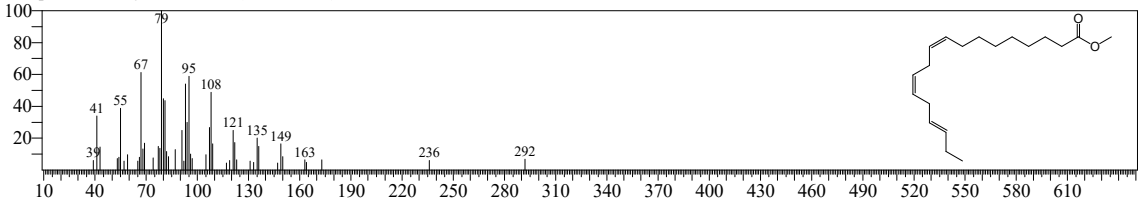
<< Target >>
Line#:5 R.Time:12.500(Scan#:1501) MassPeaks:389
RawMode:Averaged 12.495-12.505(1500-1502) BasePeak:138.05(80440)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



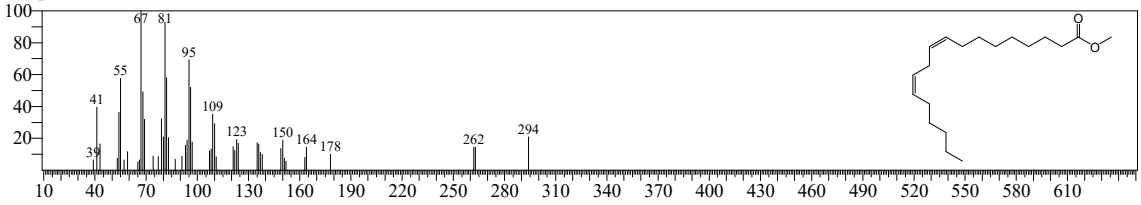
Hit#:1 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



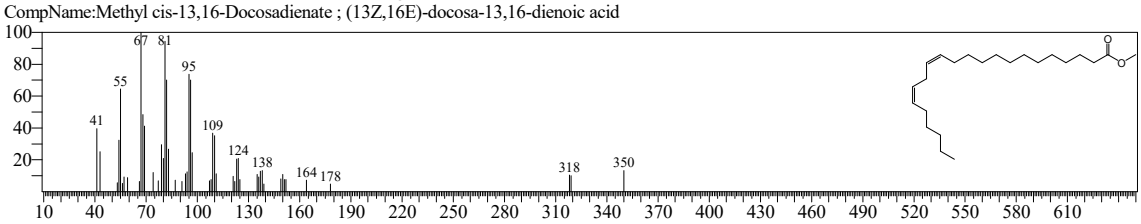
Hit#:2 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
SI:34 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid



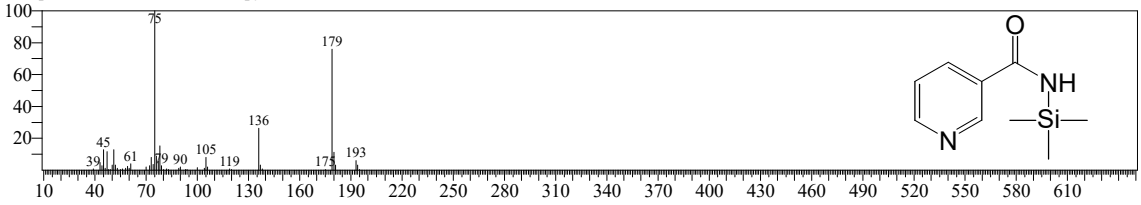
Hit#:3 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



Hit#:4 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:33 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

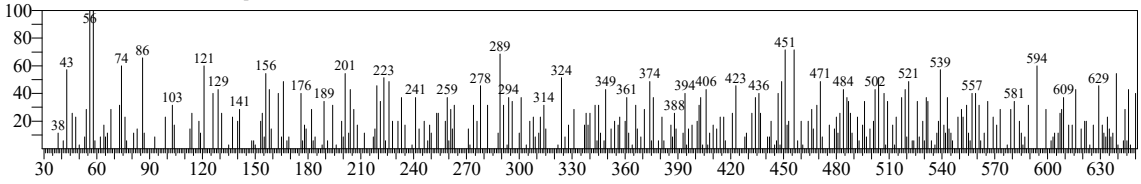


Hit#:5 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide

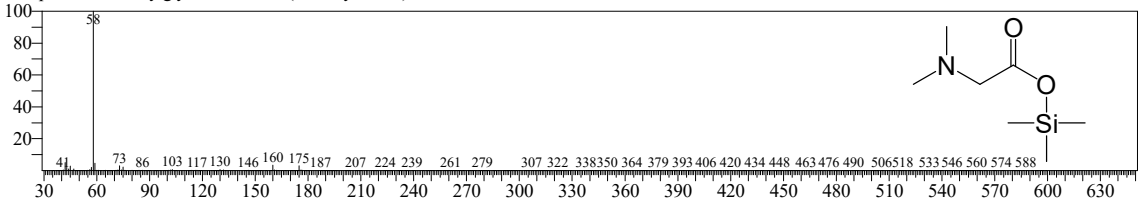


TNAU

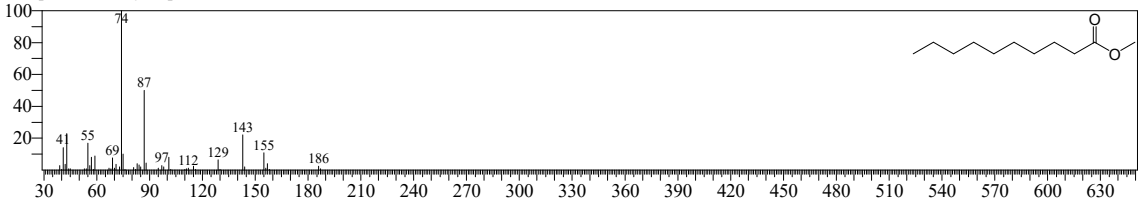
<< Target >>
Line#:6 R.Time:12.575(Scan#:1516) MassPeaks:309
RawMode:Averaged 12.570-12.580(1515-1517) BasePeak:56.00(35)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



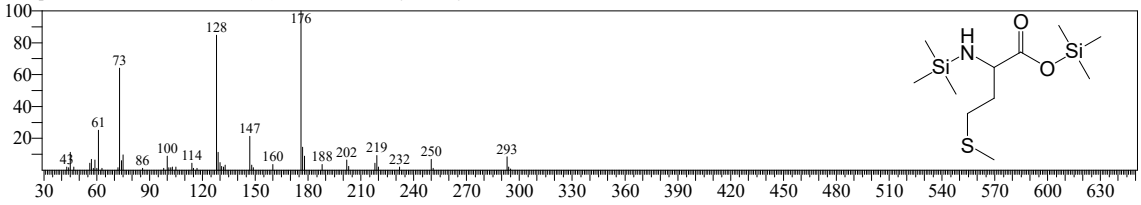
Hit#:1 Entry:1 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C7H17NO2Si CAS:1118-68-9 MolWeight:175 RetIndex:990
CompName:Dimethylglycine-TMS ; 2-(dimethylamino)acetic acid



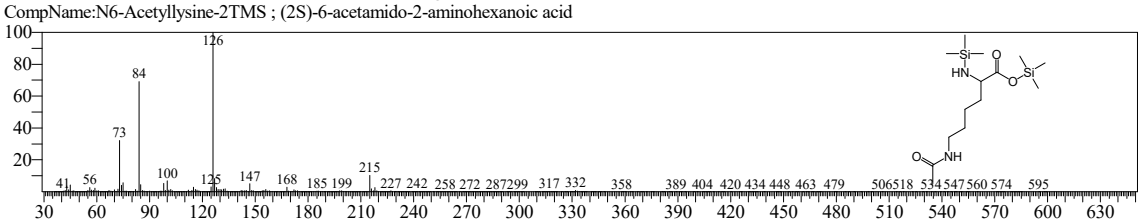
Hit#:2 Entry:4 Library:FA_ME_SP2560_EI_V3.lib
SI:14 Formula:C11H22O2 CAS:334-48-5 MolWeight:186 RetIndex:1767
CompName:Methyl caprate ; Decanoic acid



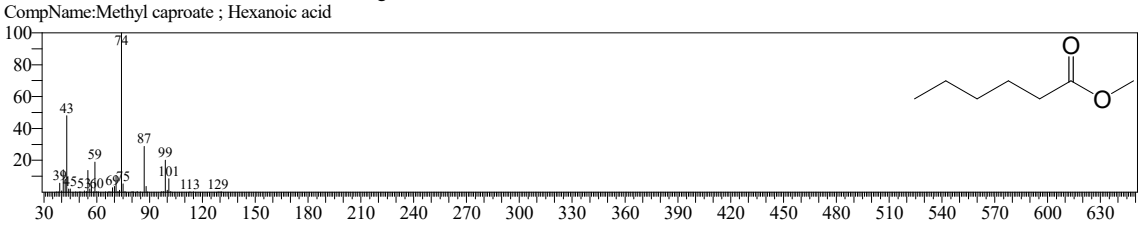
Hit#:3 Entry:160 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C11H27NO2SSi2 CAS:63-68-3 MolWeight:293 RetIndex:1530
CompName:Methionine-2TMS ; (2S)-2-amino-4-methylsulfanylbutanoic acid



Hit#:4 Entry:409 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C14H32N2O3Si2 CAS:692-04-6 MolWeight:332 RetIndex:1951
CompName:N6-Acetyllysine-2TMS ; (2S)-6-acetamido-2-aminohexanoic acid

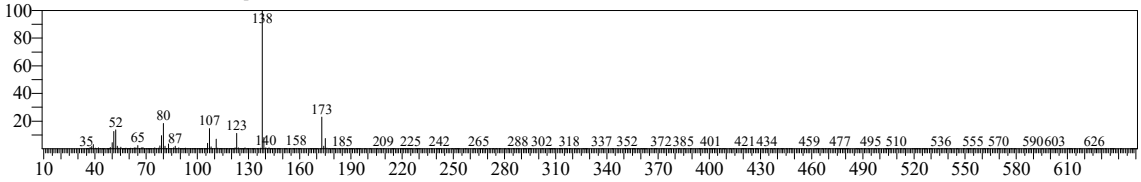


Hit#:5 Entry:2 Library:FA_ME_SP2560_EI_V3.lib
SI:13 Formula:C7H14O2 CAS:142-62-1 MolWeight:130 RetIndex:1332
CompName:Methyl caproate ; Hexanoic acid

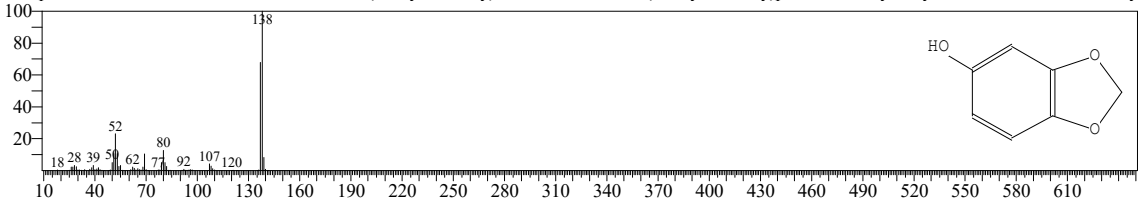


TNAU

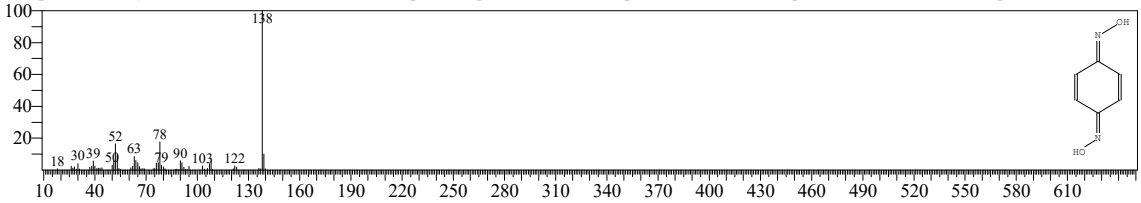
<< Target >>
Line#:7 R.Time:12.830(Scan#:1567) MassPeaks:345
RawMode:Averaged 12.825-12.835(1566-1568) BasePeak:138.05(116433)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



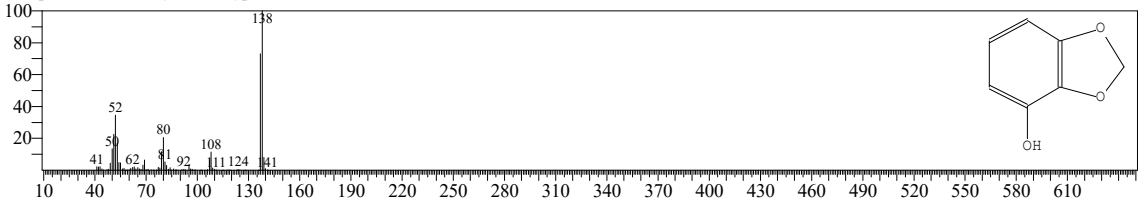
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



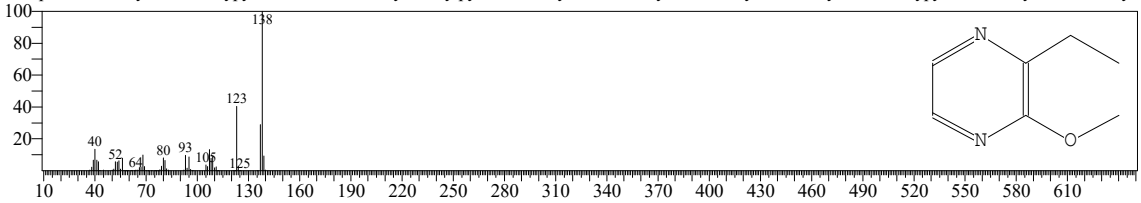
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



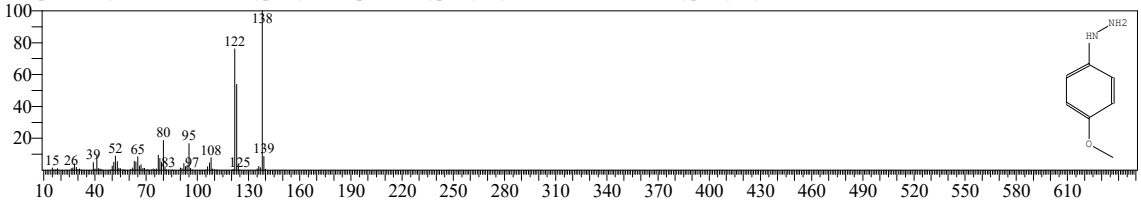
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:72 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



Hit#:4 Entry:8422 Library:NIST20R.lib
SI:72 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·

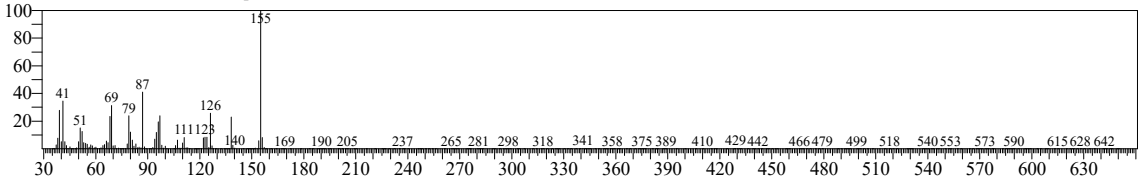


Hit#:5 Entry:11222 Library:NIST20M1.lib
SI:71 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

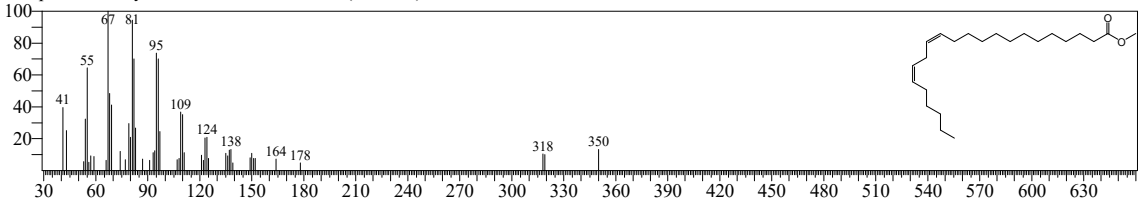


TNAU

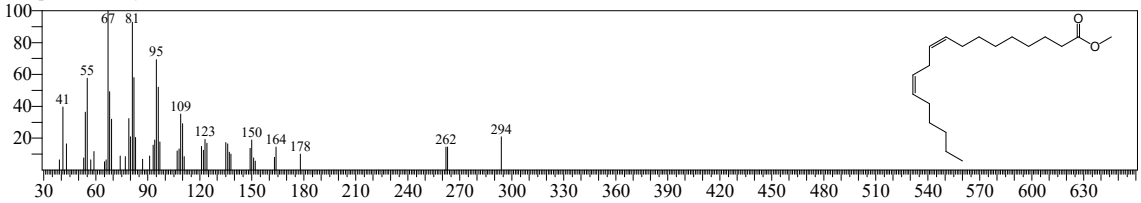
<< Target >>
Line#:8 R.Time:13.380(Scan#:1677) MassPeaks:329
RawMode:Averaged 13.375-13.385(1676-1678) BasePeak:155.05(87513)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



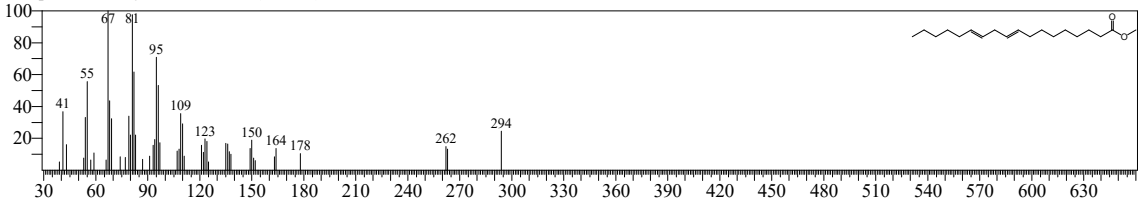
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



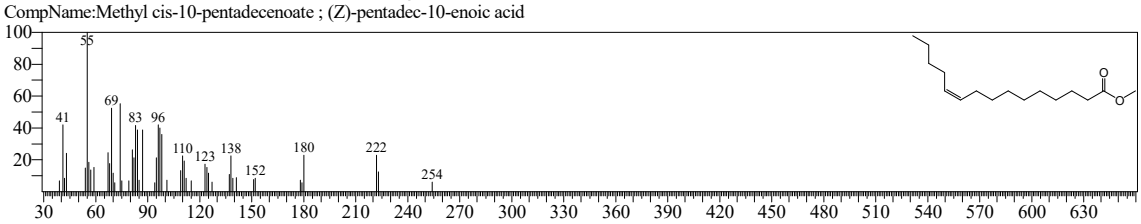
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



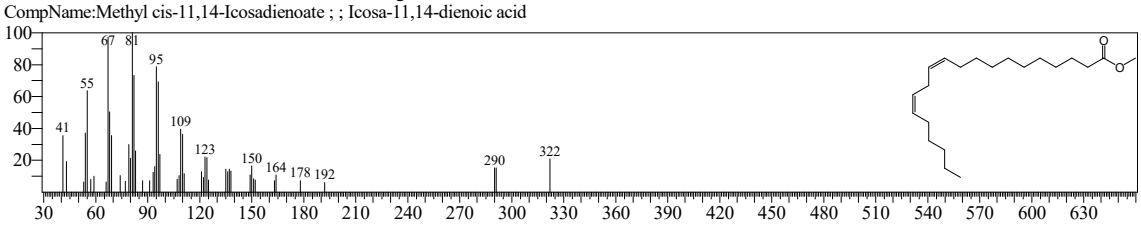
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

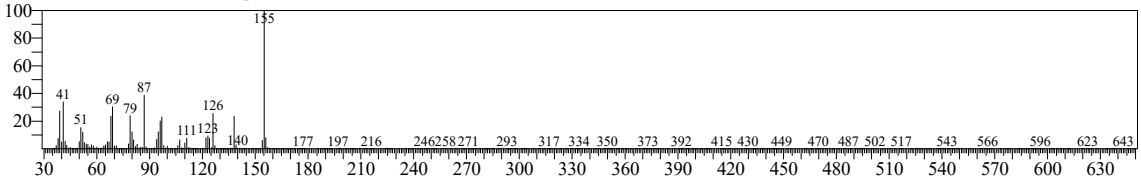


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

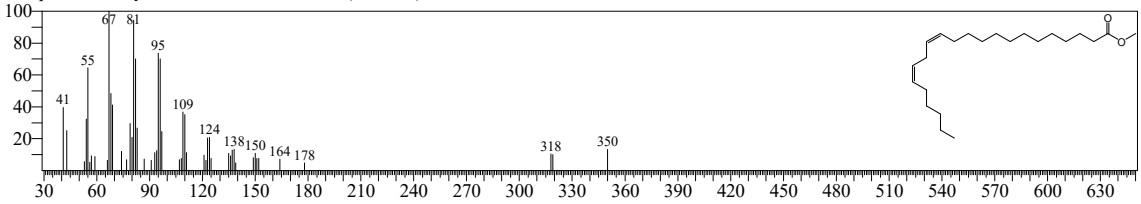


TNAU

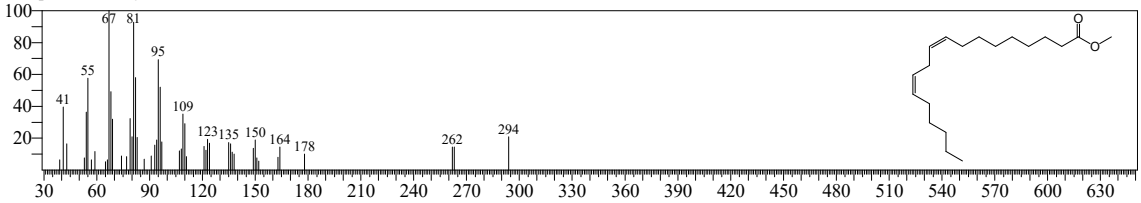
<< Target >>
Line#:9 R.Time:13.575(Scan#:1716) MassPeaks:373
RawMode:Averaged 13.570-13.580(1715-1717) BasePeak:155.05(85854)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



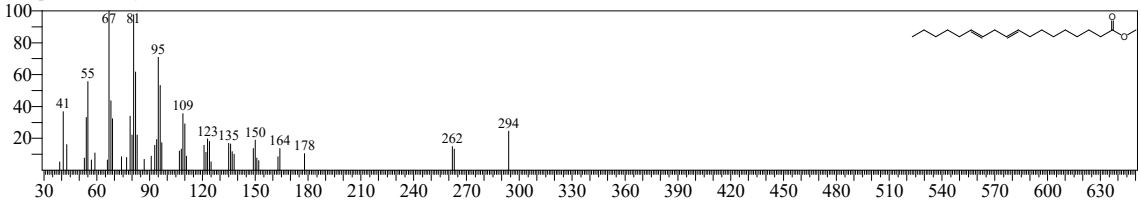
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



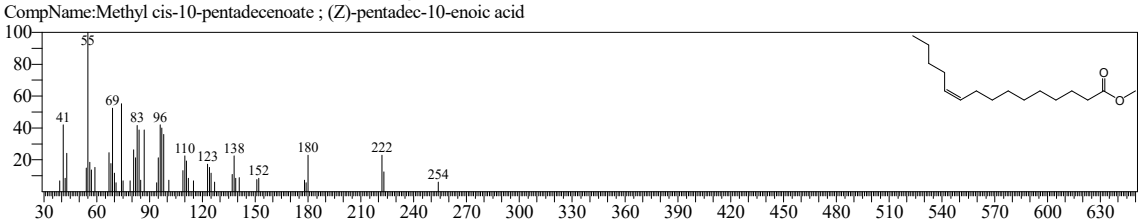
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



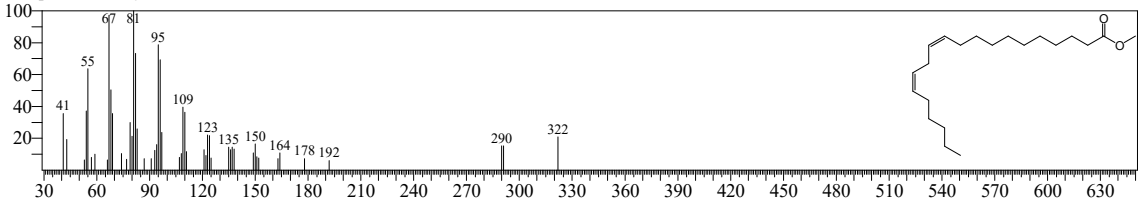
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



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

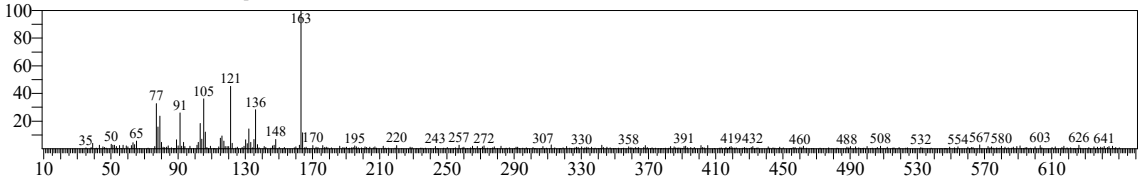


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

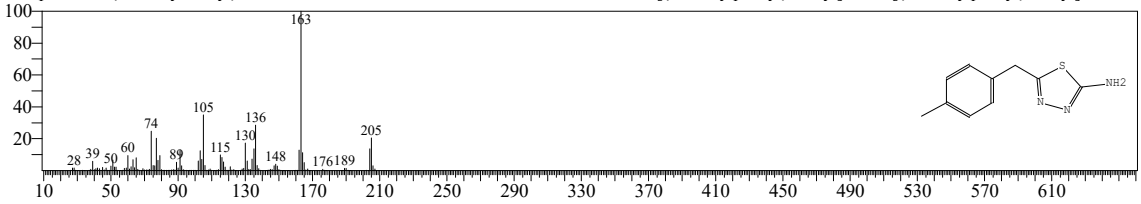


TNAU

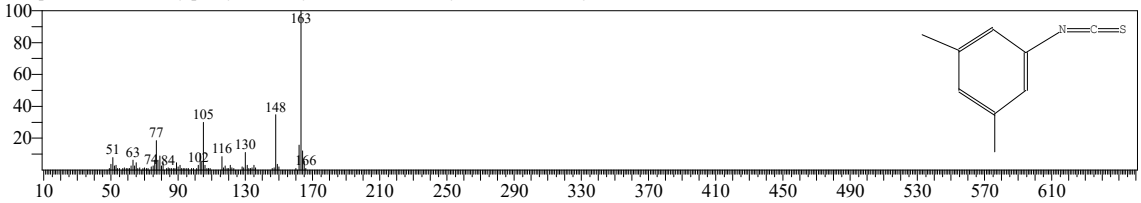
<< Target >>
Line#:10 R.Time:14.470(Scan#:1895) MassPeaks:357
RawMode:Averaged 14.465-14.475(1894-1896) BasePeak:163.10(1680)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



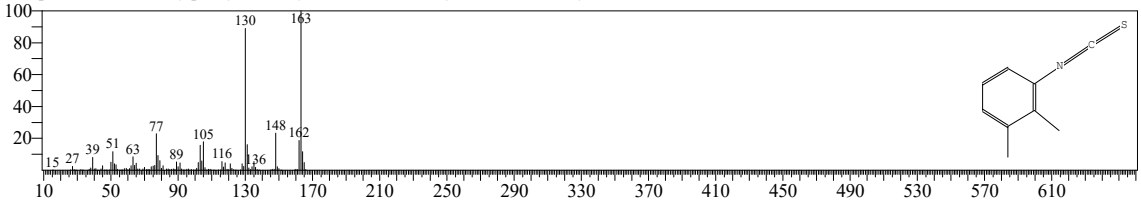
Hit#:1 Entry:57597 Library:NIST20M1.lib
SI:75 Formula:C10H11N3S CAS:39181-45-8 MolWeight:205 RetIndex:1890
CompName:5-(4-Methylbenzyl)-1,3,4-thiadiazol-2-amine $$ 1,3,4-Thiadiazol-2-amine, 5-[(4-methylphenyl)methyl]- $$ 5-[(4-Methylphenyl)methyl]-1,3,4-tl



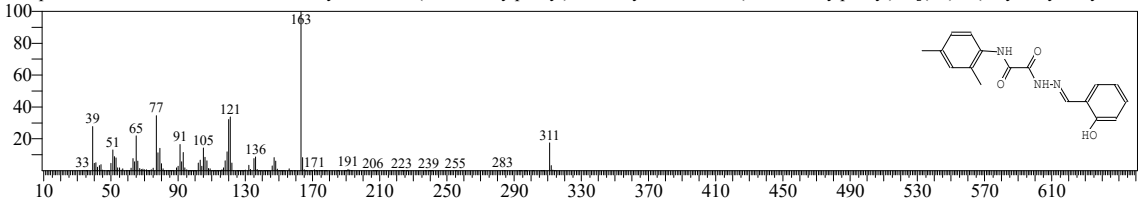
Hit#:2 Entry:14259 Library:NIST20R.lib
SI:74 Formula:C9H9NS CAS:40046-30-8 MolWeight:163 RetIndex:0
CompName:3,5-Dimethylphenyl isothiocyanate $$ 1-Isothiocyanato-3,5-dimethylbenzene #



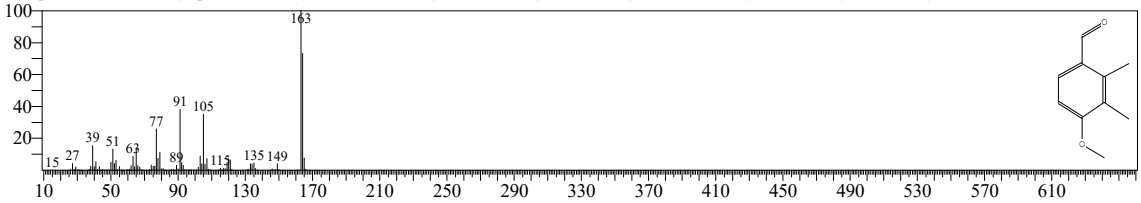
Hit#:3 Entry:14264 Library:NIST20R.lib
SI:73 Formula:C9H9NS CAS:1539-20-4 MolWeight:163 RetIndex:0
CompName:2,3-Dimethylphenylisothiocyanate $$ 1-Isothiocyanato-2,3-dimethylbenzene #



Hit#:4 Entry:176186 Library:NIST20M1.lib
SI:73 Formula:C17H17N3O3 CAS:0-00-0 MolWeight:311 RetIndex:3129
CompName:Oxalic acid, monoamide monohydrazide, N-(2,4-dimethylphenyl)-N"-salicylideno- $$ N-(2,4-Dimethylphenyl)-2-[(2E)-2-(2-hydroxybenzyliden

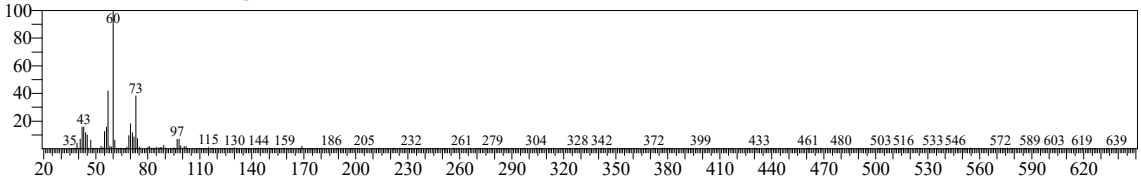


Hit#:5 Entry:25351 Library:NIST20M1.lib
SI:72 Formula:C10H12O2 CAS:38998-17-3 MolWeight:164 RetIndex:1398
CompName:2,3-Dimethyl-para-anisaldehyde $$ Benzaldehyde, 4-methoxy-2,3-dimethyl- $$ 4-Methoxy-2,3-dimethylbenzaldehyde #

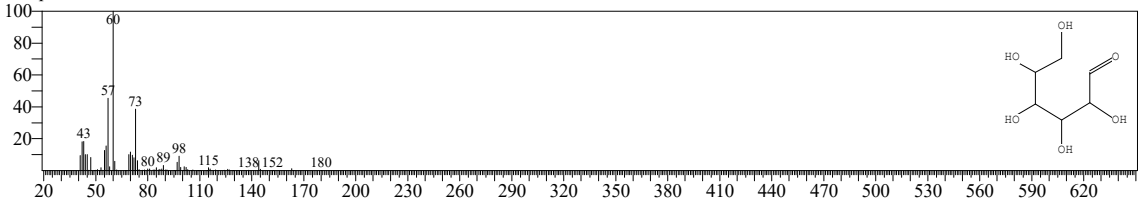


TNAU

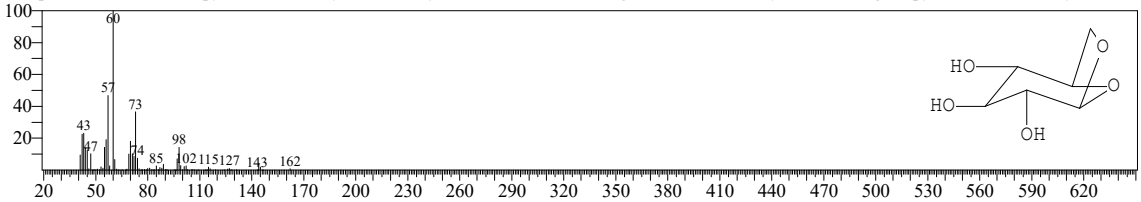
<< Target >>
Line#:11 R.Time:18.125(Scan#:2626) MassPeaks:342
RawMode:Averaged 18.120-18.130(2625-2627) BasePeak:60.00(7814)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



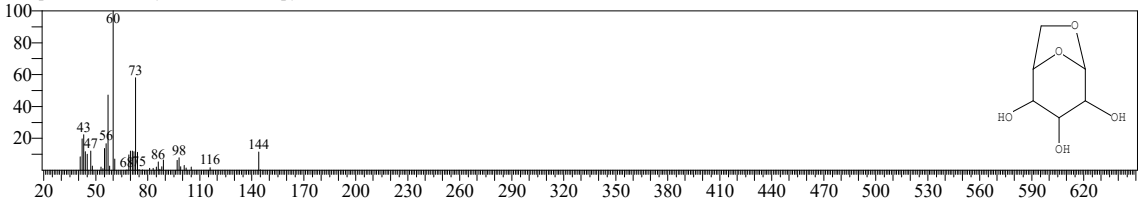
Hit#:1 Entry:36240 Library:NIST20M1.lib
SI:94 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #



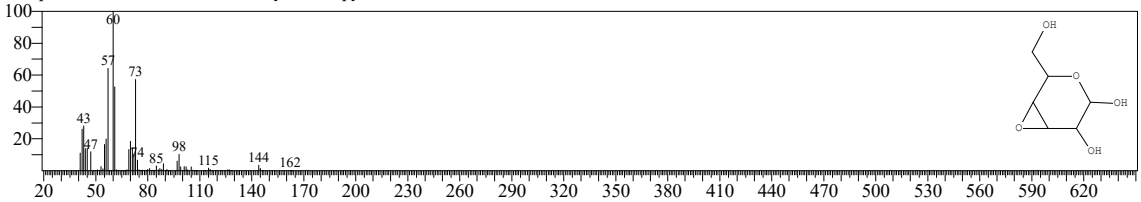
Hit#:2 Entry:13905 Library:NIST20R.lib
SI:94 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-



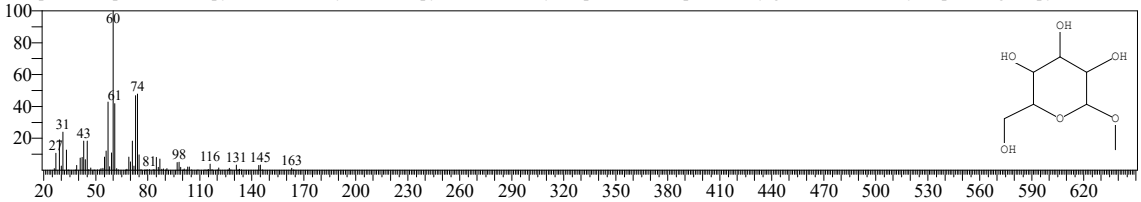
Hit#:3 Entry:23812 Library:NIST20M1.lib
SI:92 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose



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 #

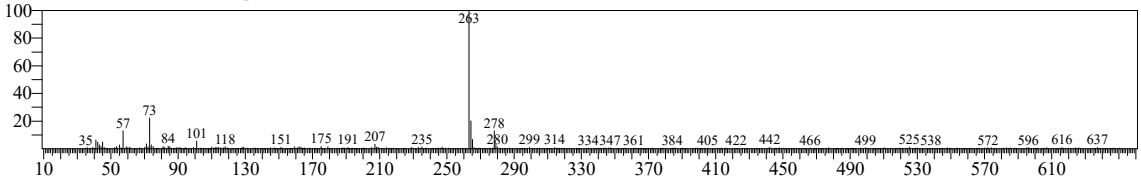


Hit#:5 Entry:21209 Library:NIST20R.lib
SI:85 Formula:C7H14O6 CAS:97-30-3 MolWeight:194 RetIndex:1714
CompName:.alpha.-D-Glucopyranoside, methyl $$ Glucopyranoside, methyl, .alpha.-D- $$ .alpha.-Methylglucoside $$ Methyl .alpha.-D-glucopyranoside $$

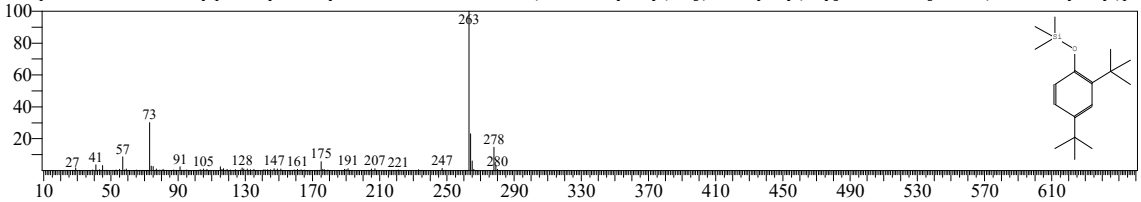


TNAU

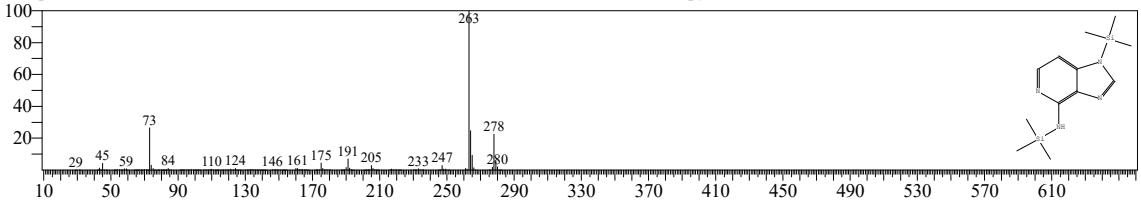
<< Target >>
Line#:12 R.Time:19.190(Scan#:2839) MassPeaks:365
RawMode:Averaged 19.185-19.195(2838-2840) BasePeak:263.15(4479)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



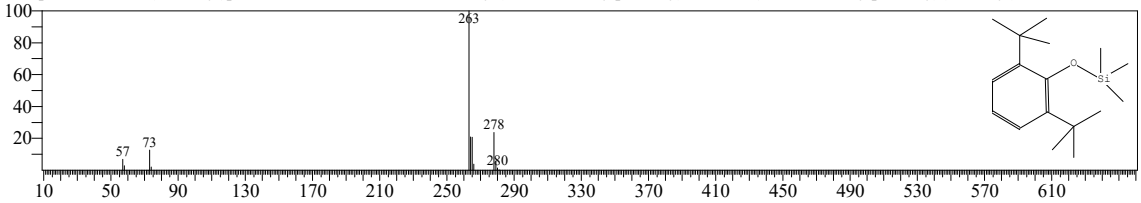
Hit#:1 Entry:137399 Library:NIST20M1.lib
SI:84 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph



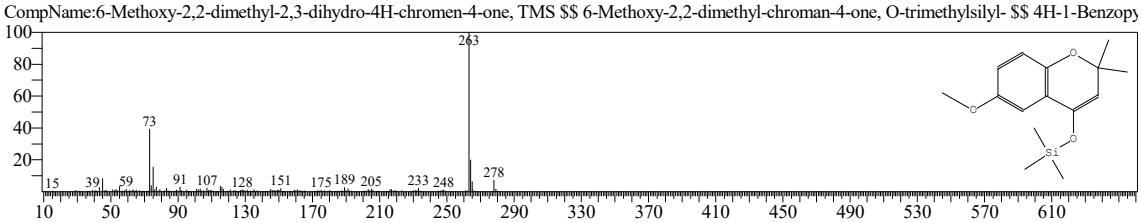
Hit#:2 Entry:136557 Library:NIST20M1.lib
SI:78 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



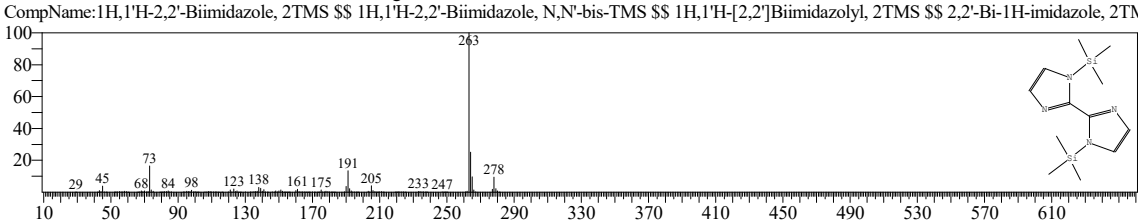
Hit#:3 Entry:33871 Library:NIST20R.lib
SI:77 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #



Hit#:4 Entry:137020 Library:NIST20M1.lib
SI:75 Formula:C15H22O3Si CAS:0-00-0 MolWeight:278 RetIndex:1736
CompName:6-Methoxy-2,2-dimethyl-2,3-dihydro-4H-chromen-4-one, TMS $$ 6-Methoxy-2,2-dimethyl-chroman-4-one, O-trimethylsilyl- $$ 4H-1-Benzopy

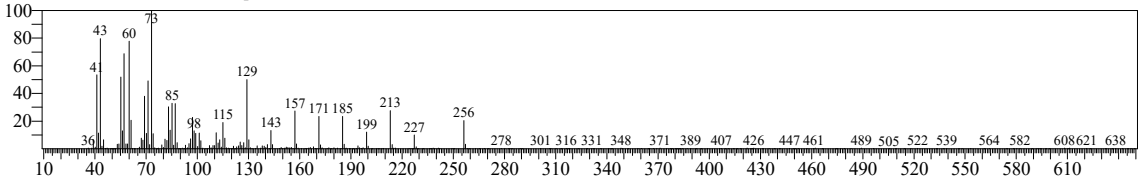


Hit#:5 Entry:136556 Library:NIST20M1.lib
SI:75 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM

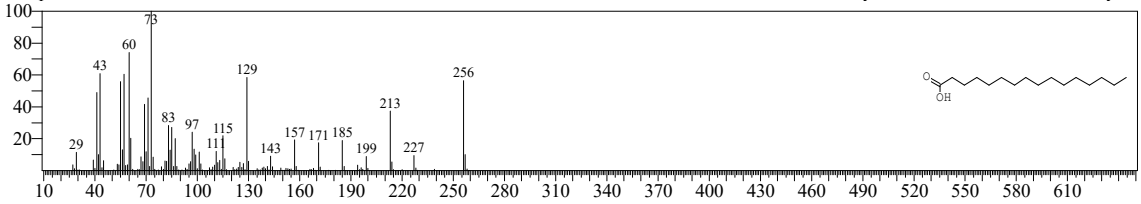


TNAU

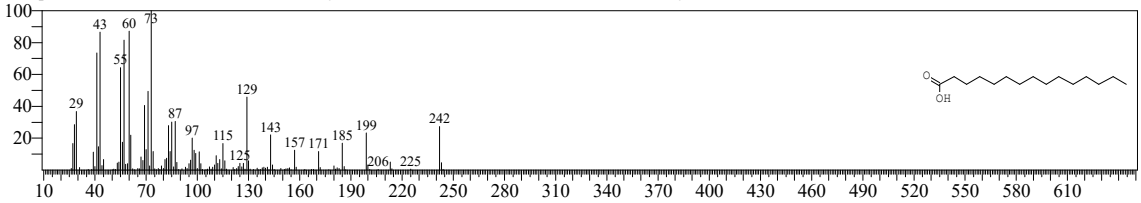
<< Target >>
Line#:13 R.Time:28.300(Scan#:4661) MassPeaks:286
RawMode:Averaged 28.295-28.305(4660-4662) BasePeak:73.05(7874)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



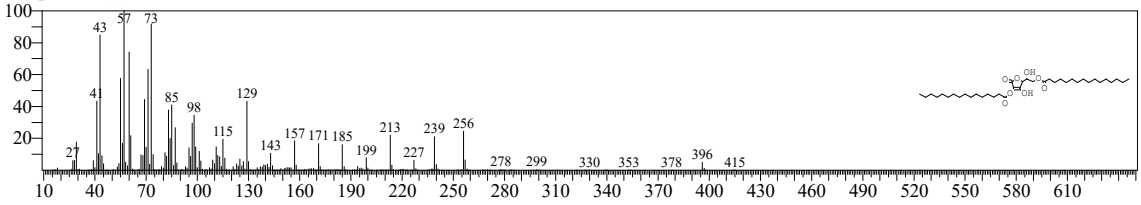
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



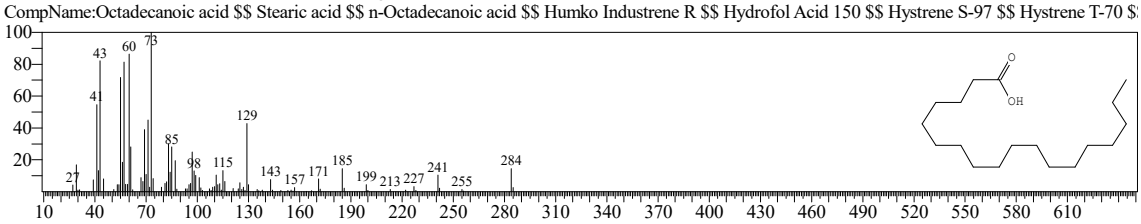
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



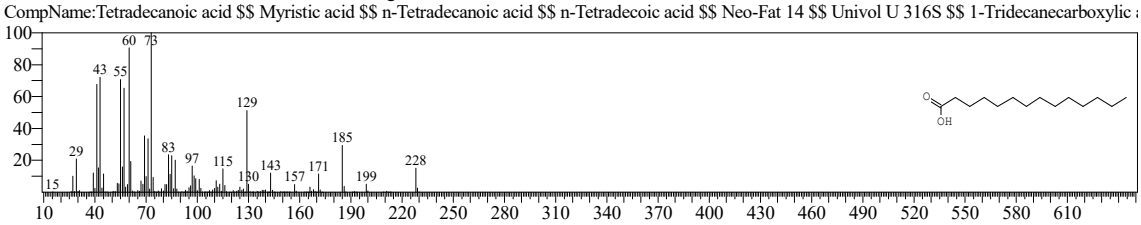
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:4 Entry: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 $

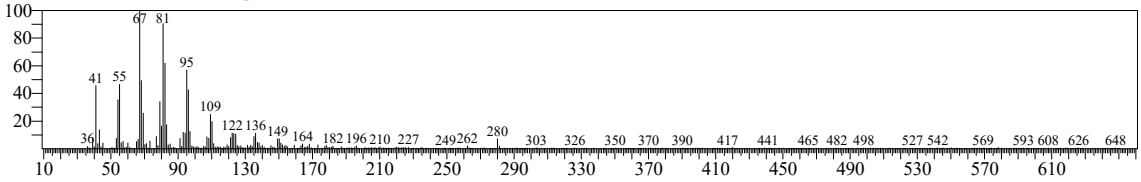


Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:90 Formula:C14H28O2 CAS:544-63-8 MolWeight:228 RetIndex:1769
CompName:Tetradecanoic acid $$ Myristic acid $$ n-Tetradecanoic acid $$ n-Tetradecoic acid $$ Neo-Fat 14 $$ Univol U 316S $$ 1-Tridecanecarboxylic

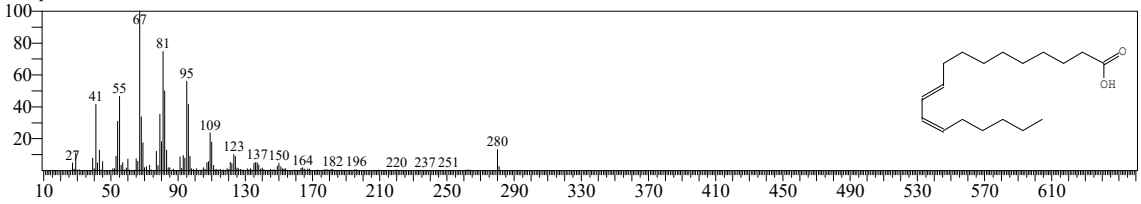


TNAU

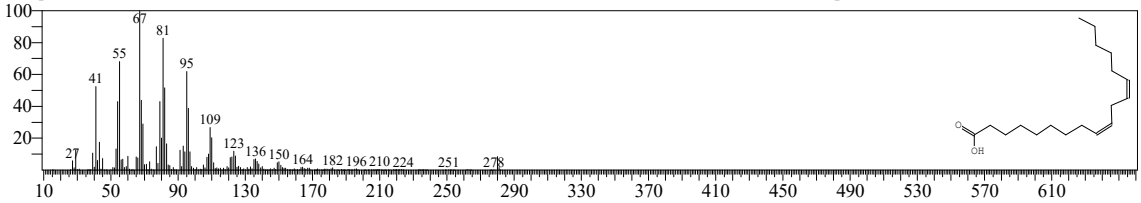
<< Target >>
Line#:14 R.Time:31.480(Scan#:5297) MassPeaks:428
RawMode:Averaged 31.475-31.485(5296-5298) BasePeak:67.05(5758)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



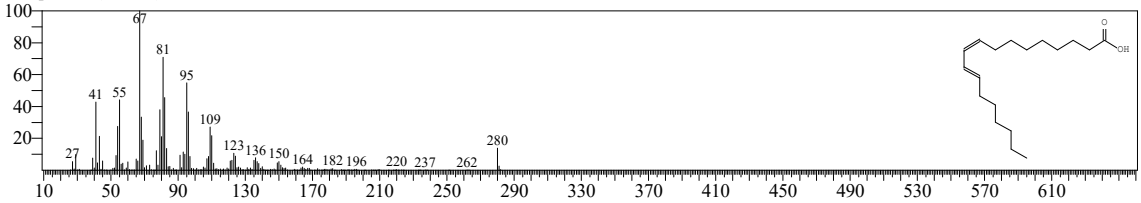
Hit#:1 Entry:139646 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid



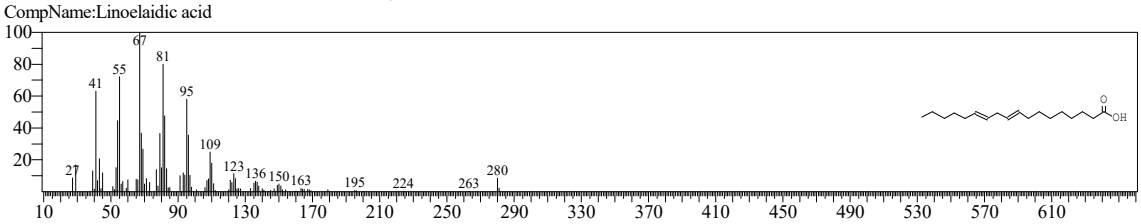
Hit#:2 Entry:34035 Library:NIST20R.lib
SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



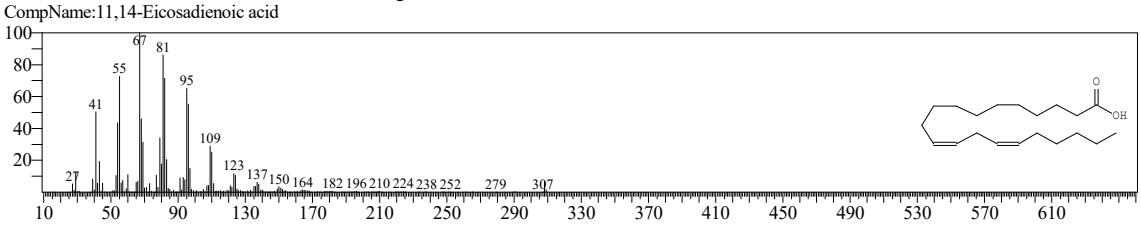
Hit#:3 Entry:139651 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



Hit#:4 Entry:139661 Library:NIST20M1.lib
SI:94 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

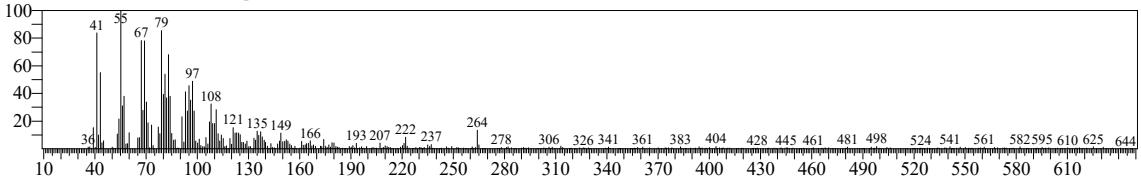


Hit#:5 Entry:173215 Library:NIST20M1.lib
SI:93 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382
CompName:11,14-Eicosadienoic acid

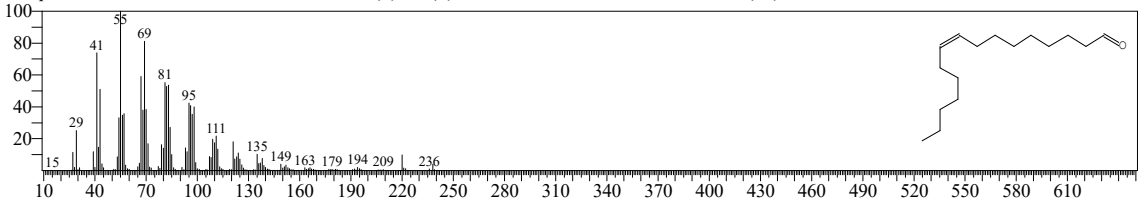


TNAU

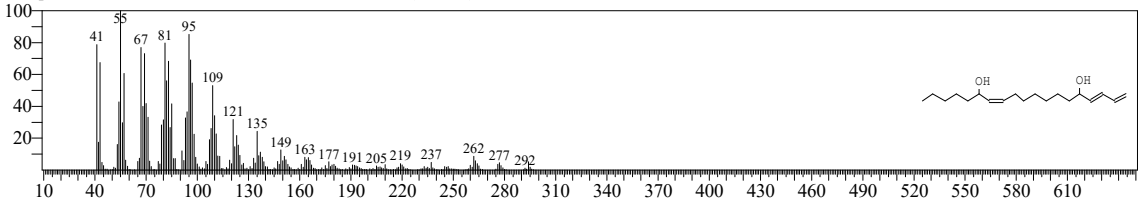
<< Target >>
Line#:15 R.Time:31.585(Scan#:5318) MassPeaks:373
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:55.10(2679)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



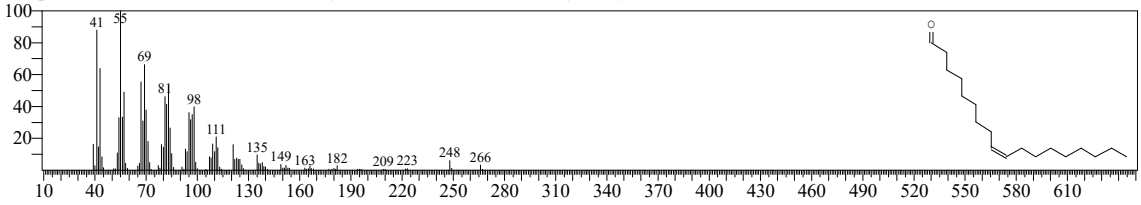
Hit#:1 Entry:92244 Library:NIST20M1.lib
SI:88 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #



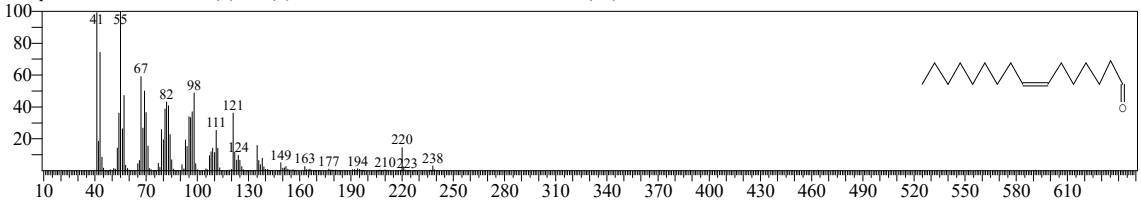
Hit#:2 Entry:156549 Library:NIST20M1.lib
SI:88 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #



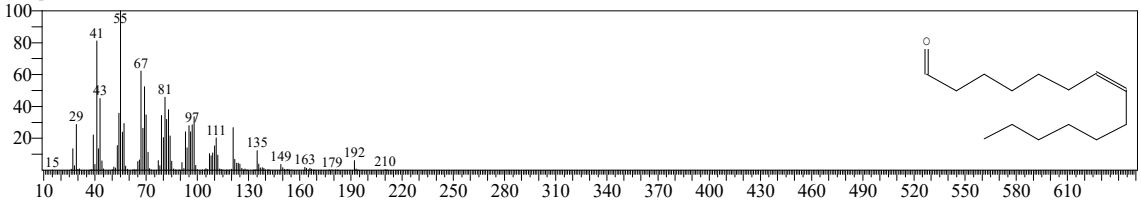
Hit#:3 Entry:123421 Library:NIST20M1.lib
SI:87 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal #



Hit#:4 Entry:92227 Library:NIST20M1.lib
SI:87 Formula:C16H30O CAS:56797-40-1 MolWeight:238 RetIndex:1808
CompName:7-Hexadecenal, (Z)- $$ (Z)-7-Hexadecenal $$ Z-7-Hexadecenal $$ (7Z)-7-Hexadecenal #

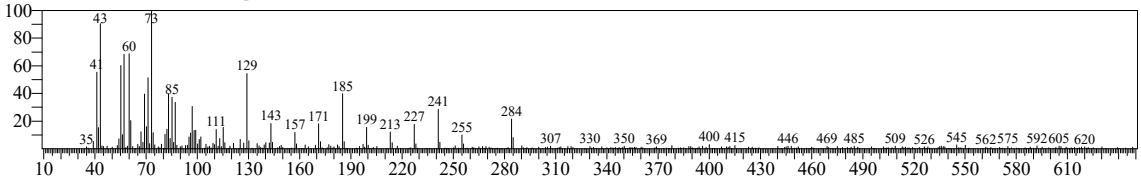


Hit#:5 Entry:63176 Library:NIST20M1.lib
SI:87 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #

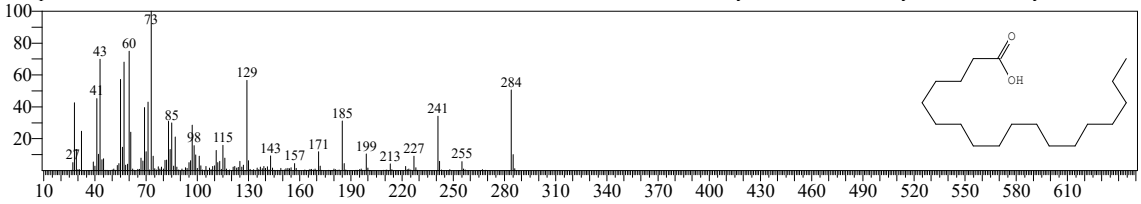


TNAU

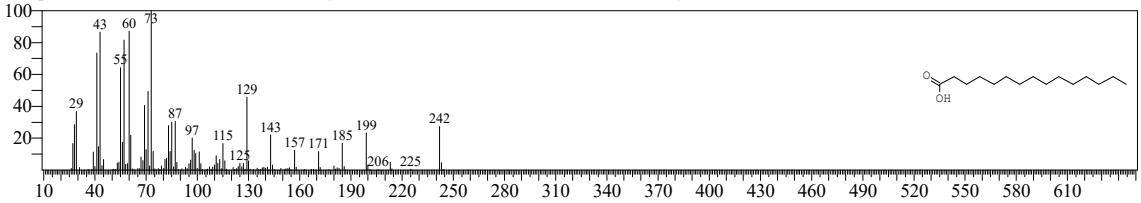
<< Target >>
Line#:16 R.Time:32.030(Scan#:5407) MassPeaks:346
RawMode:Averaged 32.025-32.035(5406-5408) BasePeak:73.05(1458)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



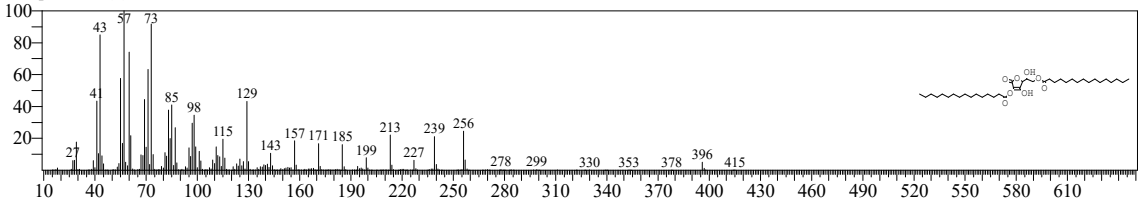
Hit#:1 Entry:34463 Library:NIST20R.lib
SI:91 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



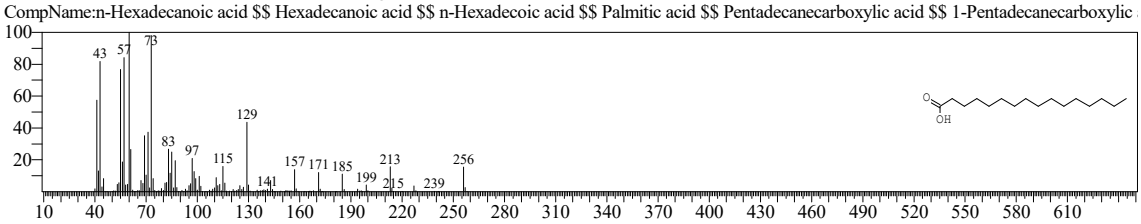
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:88 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



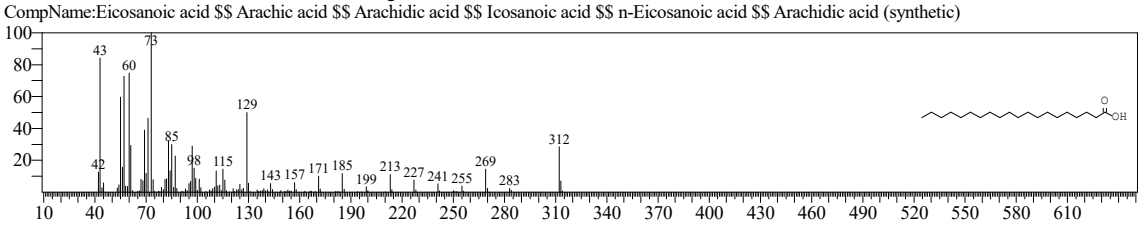
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:87 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:4 Entry:31599 Library:NIST20R.lib
SI:87 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

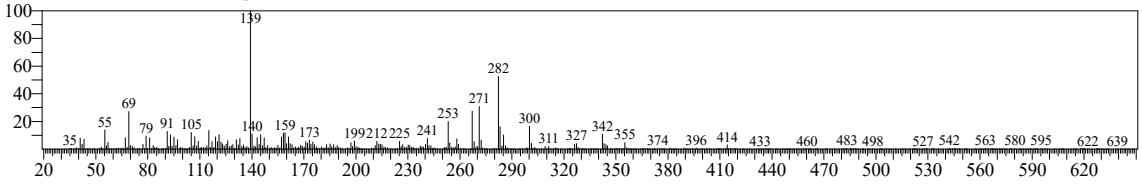


Hit#:5 Entry:178153 Library:NIST20M1.lib
SI:86 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)

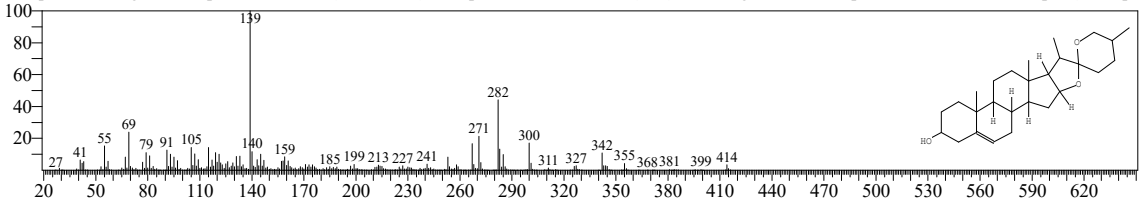


TNAU

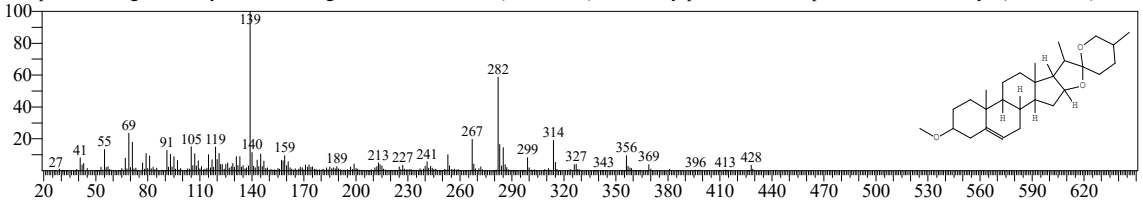
<< Target >>
Line#:17 R.Time:45.625(Scan#:8126) MassPeaks:430
RawMode:Averaged 45.620-45.630(8125-8127) BasePeak:139.10(7505)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



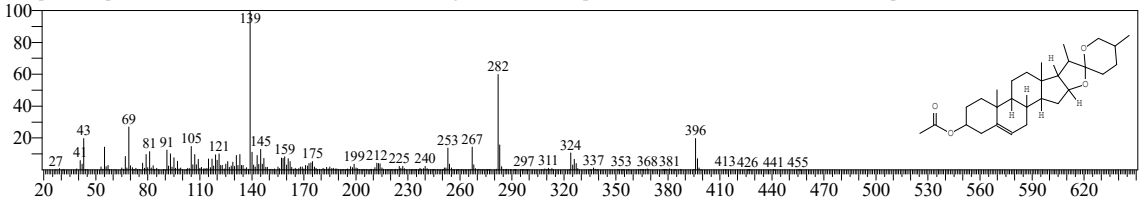
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:90 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



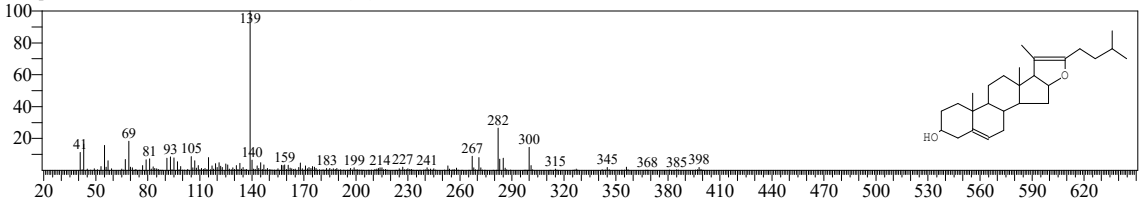
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:82 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



Hit#:3 Entry:24878 Library:NIST20M2.lib
SI:81 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#:4 Entry:41561 Library:NIST20R.lib
SI:80 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #



Hit#: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.