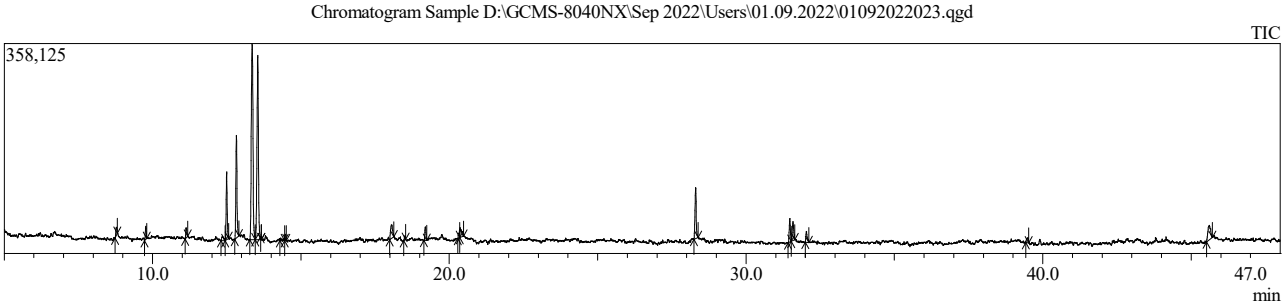
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 02-Sep-22 12:55:30 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 8-1
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 9
Injection Volume	: 5.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022023.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022023.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 11:05:56 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022023.qgd



Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	8.781	39165	0.91	14160	1.09	2.77	83	1-Butanol, 3-methyl-, acetate
2	9.773	46517	1.08	22381	1.72	2.08	94	Pentasiloxane, dodecamethyl-
3	11.132	43377	1.01	17303	1.33	2.51	41	Methyl myristoleate
4	12.335	32310	0.75	5526	0.42	5.85	19	Methyl butanoate
5	12.496	283885	6.60	115607	8.87	2.46	75	1,3-Benzodioxol-5-ol
6	12.824	456603	10.61	175366	13.45	2.60	74	1,3-Benzodioxol-5-ol
7	13.356	1290996	30.01	334453	25.66	3.86	53	Methyl cis-13,16-Docosadienate
8	13.546	1080258	25.11	314703	24.14	3.43	53	Methyl cis-13,16-Docosadienate
9	13.655	1137	0.03	2772	0.21	0.41	12	Kynurenic acid-2TMS
10	14.310	16283	0.38	3140	0.24	5.19	20	Methyl butanoate
11	14.472	22495	0.52	10937	0.84	2.06	74	5-(4-Methylbenzyl)-1,3,4-thiadiazol-2-amine
12	18.063	107362	2.50	22717	1.74	4.73	93	.beta.-D-Glucopyranose, 1,6-anhydro-
13	18.504	14339	0.33	6509	0.50	2.20	84	Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphen
14	19.194	56718	1.32	22639	1.74	2.51	91	2,4-Di-tert-butylphenoxytrimethylsilane
15	20.305	29399	0.68	7697	0.59	3.82	44	Isovalerylglycine-TMS
16	20.363	71159	1.65	16958	1.30	4.20	42	2-Ketoisocaproic acid-meto-TMS(1)
17	28.301	245655	5.71	86914	6.67	2.83	95	n-Hexadecanoic acid
18	31.476	114137	2.65	40059	3.07	2.85	95	10E,12Z-Octadecadienoic acid
19	31.583	103252	2.40	32151	2.47	3.21	88	cis-9-Hexadecenal
20	32.031	60261	1.40	18770	1.44	3.21	91	Octadecanoic acid
21	39.494	28573	0.66	8370	0.64	3.41	56	Methyl erucate
22	45.613	157765	3.67	24332	1.87	6.48	89	Diosgenin
		4301646	100.00	1303464	100.00			

TNAU

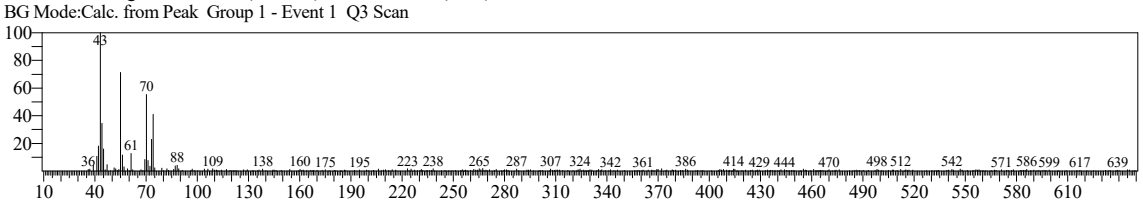
Library

<< Target >>

Line#:1 R.Time:8.780(Scan#:757) MassPeaks:338

RawMode:Averaged 8.775-8.785(756-758) BasePeak:43.05(2769)

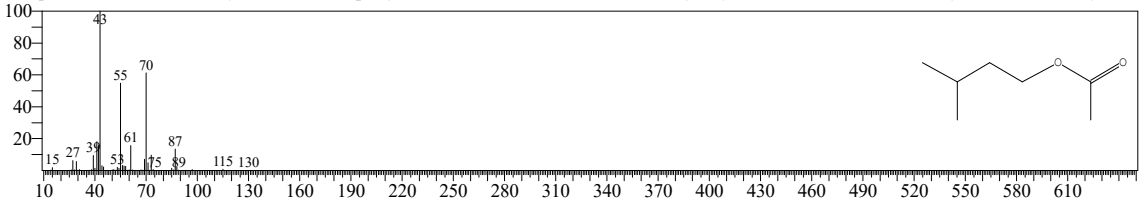
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



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

SI:83 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820

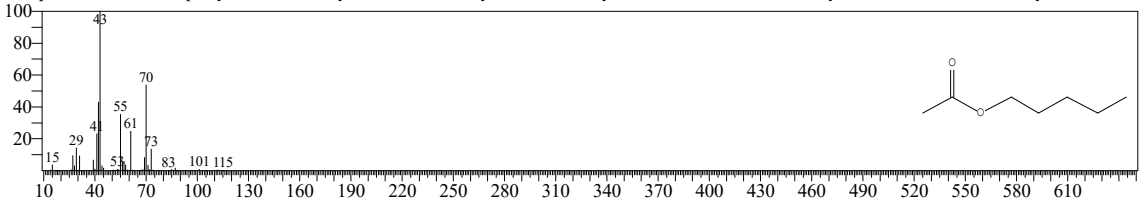
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha



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

SI:80 Formula:C7H14O2 CAS:628-63-7 MolWeight:130 RetIndex:884

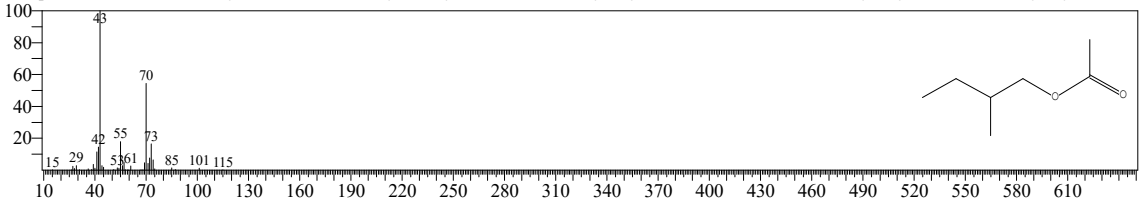
CompName:Acetic acid, pentyl ester $$ n-Amyl acetate $$ n-Pentyl acetate $$ Amyl acetate $$ Birnenoel $$ Pentyl acetate $$ Acetic acid, amyl ester $$ Am



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

SI:80 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820

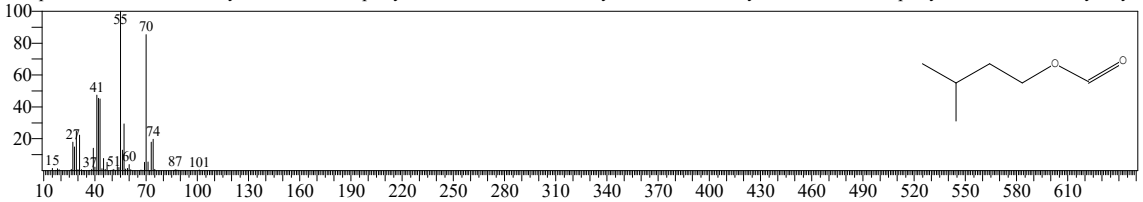
CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate



Hit#:4 Entry:4411 Library:NIST20R.lib

SI:78 Formula:C6H12O2 CAS:110-45-2 MolWeight:116 RetIndex:818

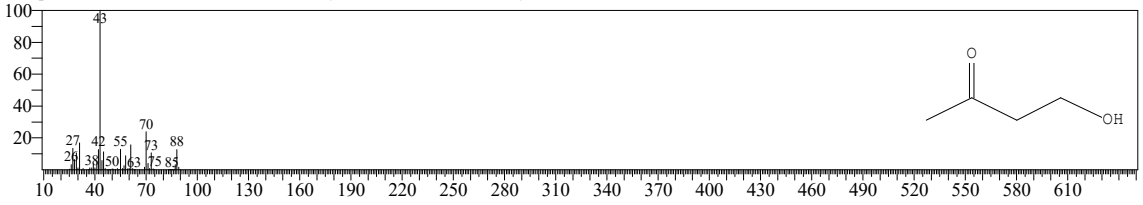
CompName:1-Butanol, 3-methyl-, formate $$ Isopentyl alcohol, formate $$ Isoamyl formate $$ Isoamyl methanoate $$ Isopentyl formate $$ 3-Methylbutyl



Hit#:5 Entry:1220 Library:NIST20R.lib

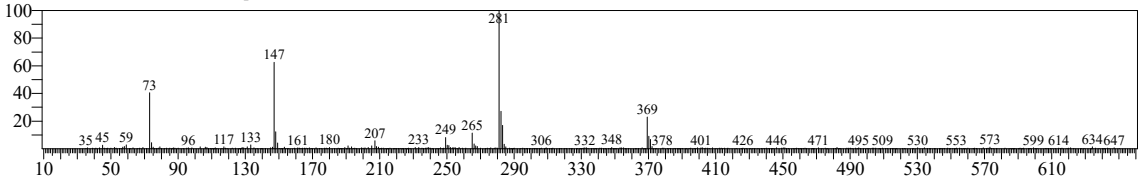
SI:77 Formula:C4H8O2 CAS:590-90-9 MolWeight:88 RetIndex:798

CompName:CH3C(O)CH2CH2OH $$ Methylolacetone $$ Monomethylolacetone $$ 3-Ketobutan-1-ol $$ 3-Oxo-1-butanol $$ 3-Oxobutanol $$ 4-Butanol-

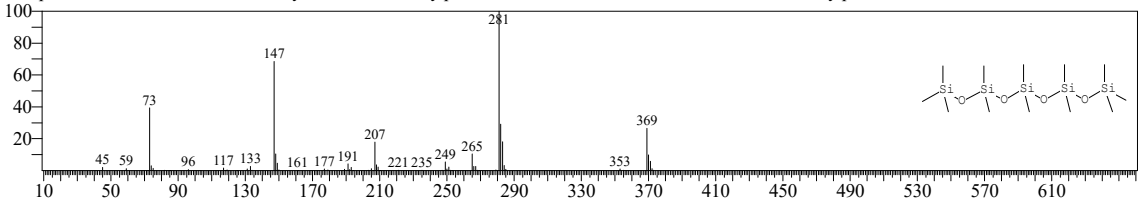


TNAU

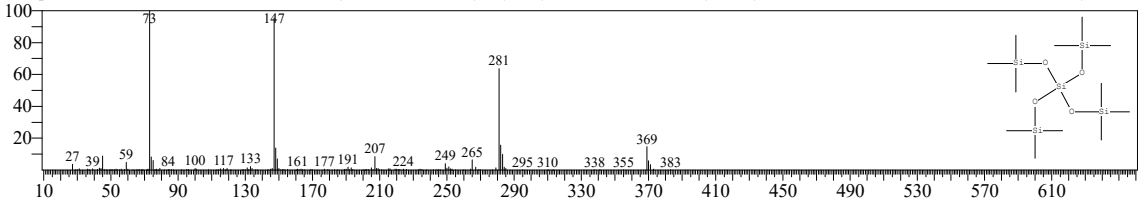
<< Target >>
Line#:2 R.Time:9.770(Scan#:955) MassPeaks:410
RawMode:Averaged 9.765-9.775(954-956) BasePeak:281.05(4664)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



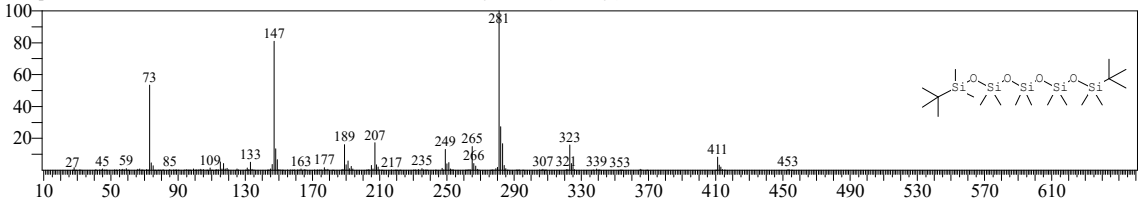
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:94 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



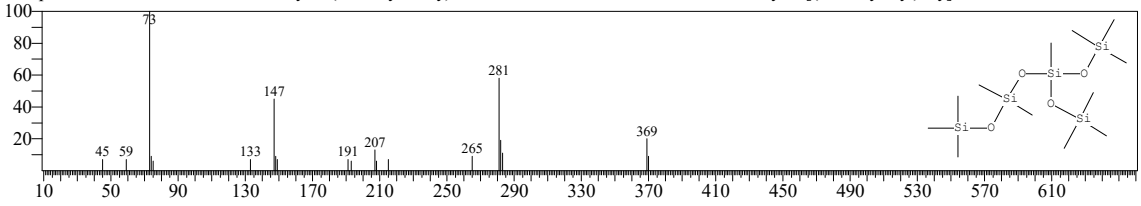
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:83 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



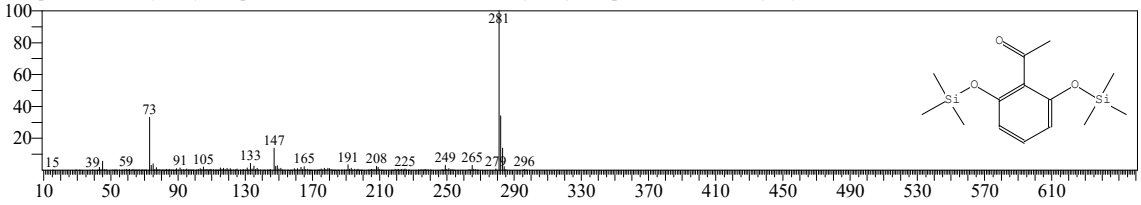
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:81 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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

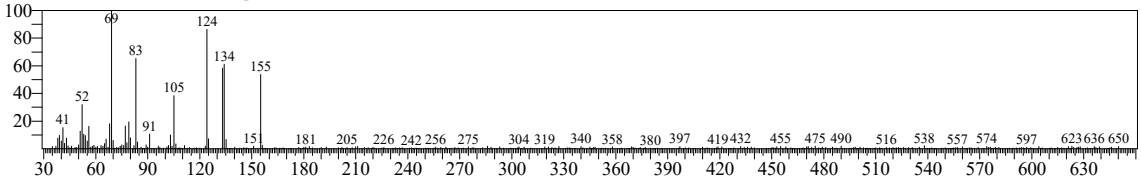


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

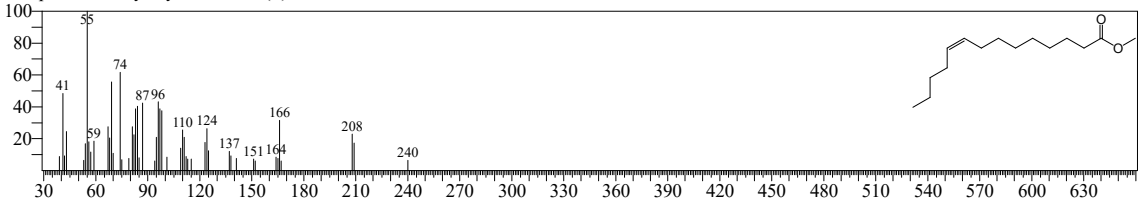


TNAU

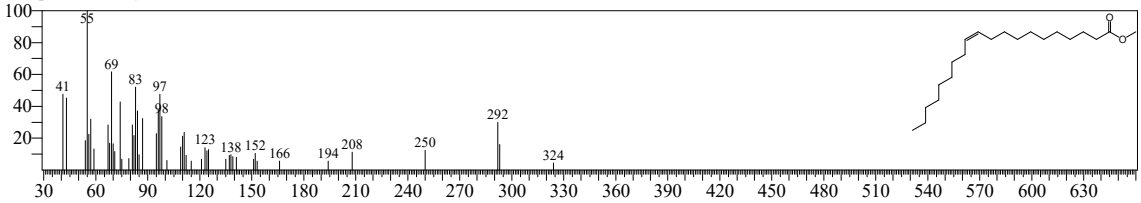
<< Target >>
Line#:3 R.Time:11.130(Scan#:1227) MassPeaks:359
RawMode:Averaged 11.125-11.135(1226-1228) BasePeak:69.05(2046)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



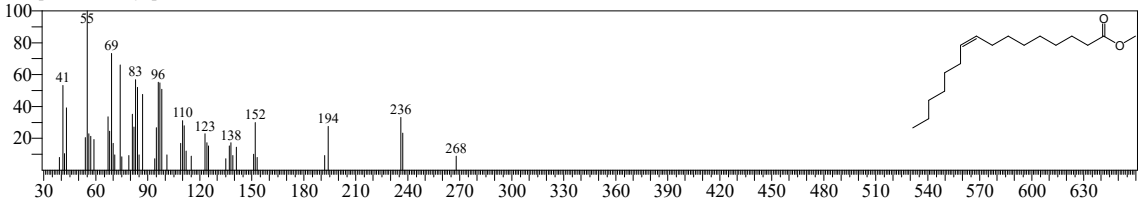
Hit#:1 Entry:9 Library:FA_ME_SP2560_EI_V3.lib
SI:41 Formula:C15H28O2 CAS:544-64-9 MolWeight:240 RetIndex:2283
CompName:Methyl myristoleate ; ; (Z)-tetradec-9-enoic acid



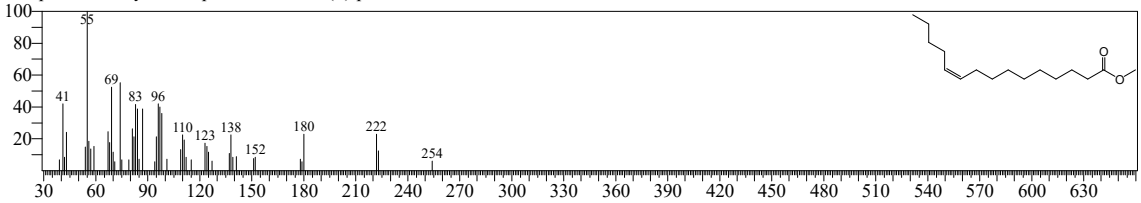
Hit#:2 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:39 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid



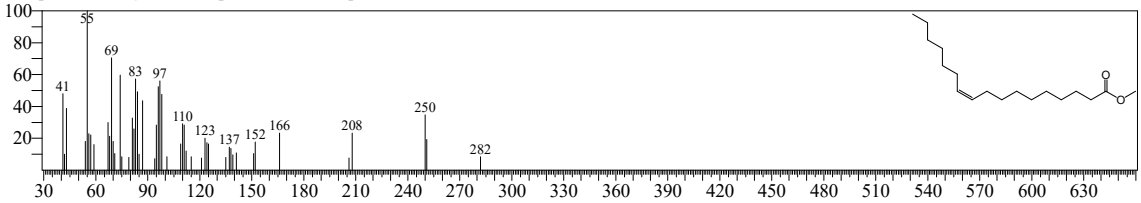
Hit#:3 Entry:13 Library:FA_ME_SP2560_EI_V3.lib
SI:39 Formula:C17H32O2 CAS:373-49-9 MolWeight:268 RetIndex:2478
CompName:Methyl palmitoleate ; Hexadec-9-enoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:39 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

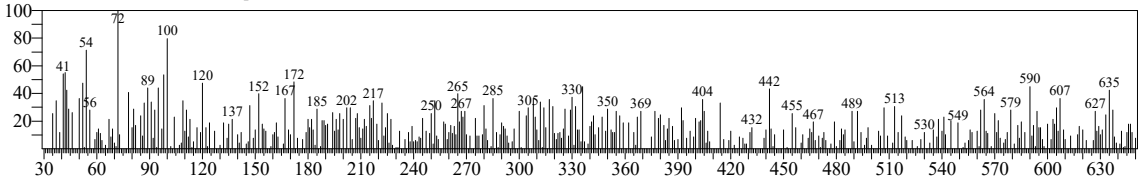


Hit#:5 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:39 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

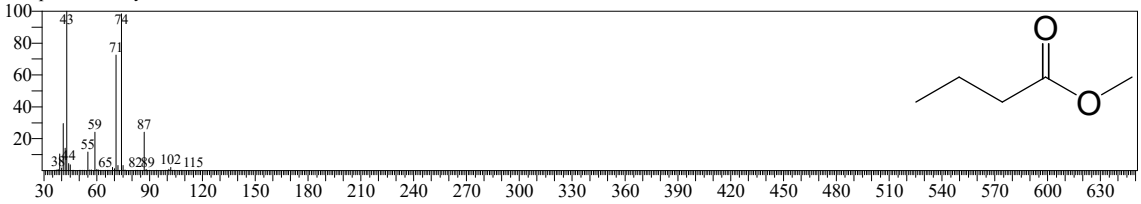


TNAU

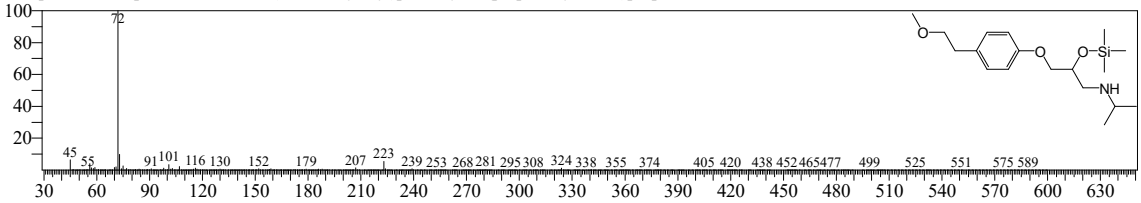
<< Target >>
Line#:4 R.Time:12.335(Scan#:1468) MassPeaks:397
RawMode:Averaged 12.330-12.340(1467-1469) BasePeak:72.00(118)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



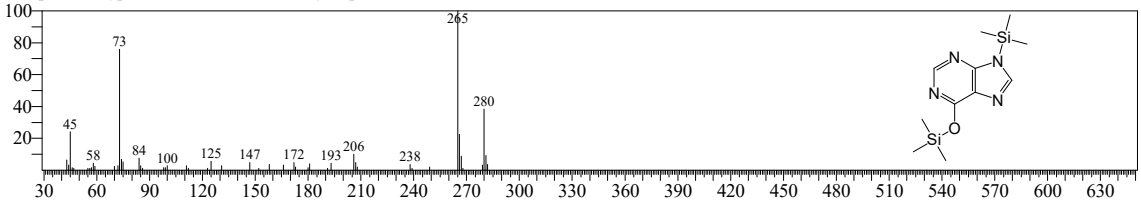
Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:19 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



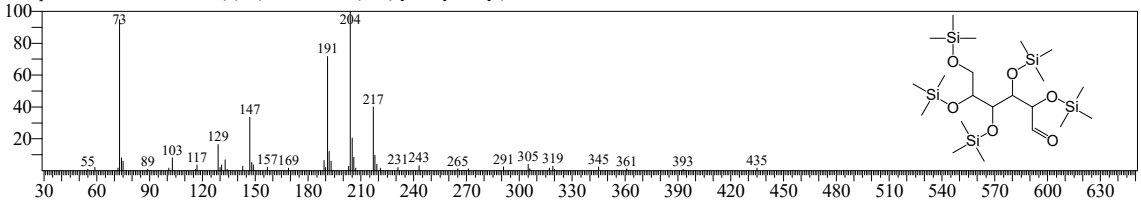
Hit#:2 Entry:456 Library:OA_TMS_DB5_67min_V3.lib
SI:18 Formula:C18H33NO3Si CAS:37350-58-6 MolWeight:339 RetIndex:2094
CompName:Metoprolol-TMS ; 1-[4-(2-methoxyethyl)phenoxy]-3-(propan-2-ylamino)propan-2-ol



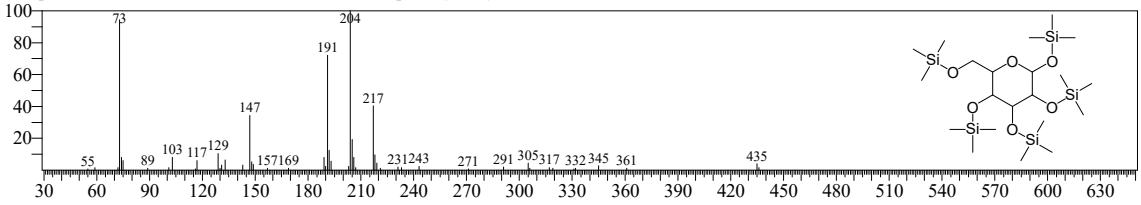
Hit#:3 Entry:310 Library:OA_TMS_DB5_67min_V3.lib
SI:17 Formula:C11H20N4OSi2 CAS:68-94-0 MolWeight:280 RetIndex:1822
CompName:Hypoxanthine-2TMS ; 3,7-dihydropurin-6-one



Hit#:4 Entry:345 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C21H52O6Si5 CAS:59-23-4 MolWeight:540 RetIndex:1868
CompName:Galactose-5TMS(2) ; (3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol

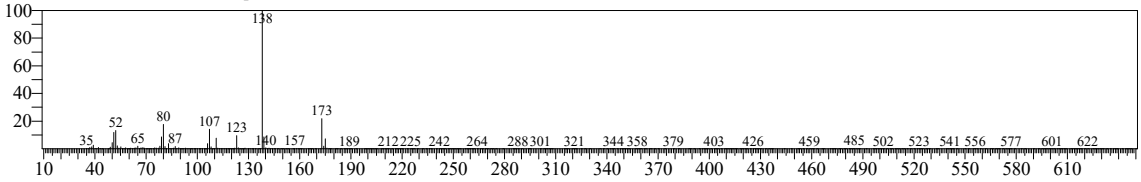


Hit#:5 Entry:349 Library:OA_TMS_DB5_67min_V3.lib
SI:15 Formula:C21H52O6Si5 CAS:2595-97-3 MolWeight:540 RetIndex:1874
CompName:Allose-5TMS ; (2R,3R,4R,5R)-2,3,4,5,6-pentahydroxyhexanal

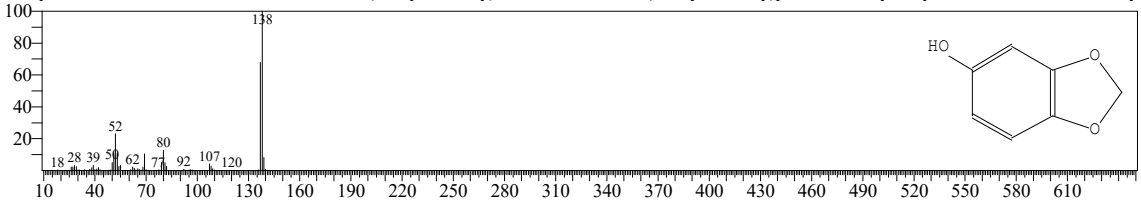


TNAU

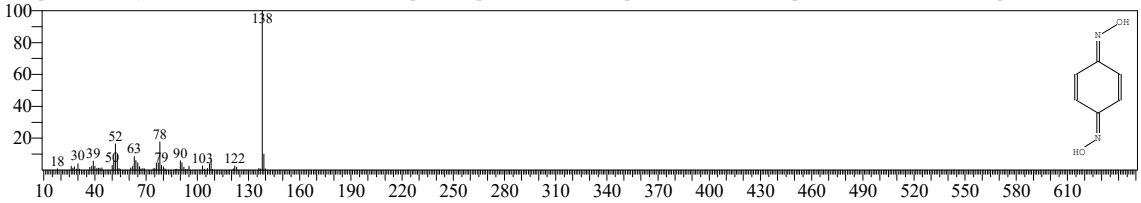
<< Target >>
Line#:5 R.Time:12.495(Scan#:1500) MassPeaks:402
RawMode:Averaged 12.490-12.500(1499-1501) BasePeak:138.05(40091)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



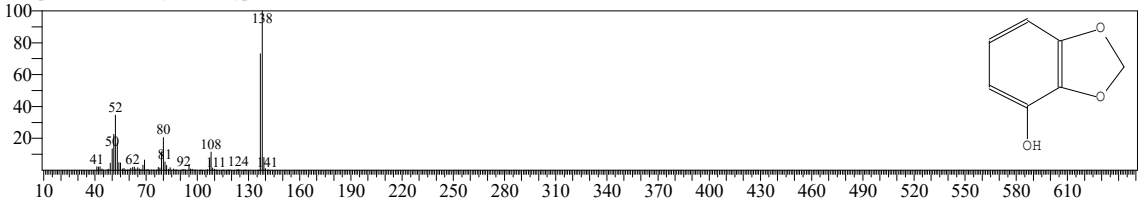
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:75 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



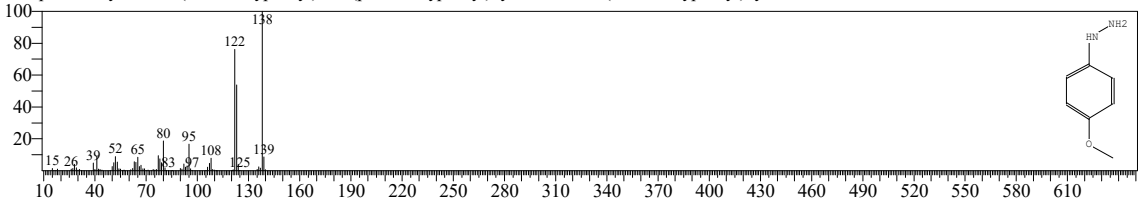
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



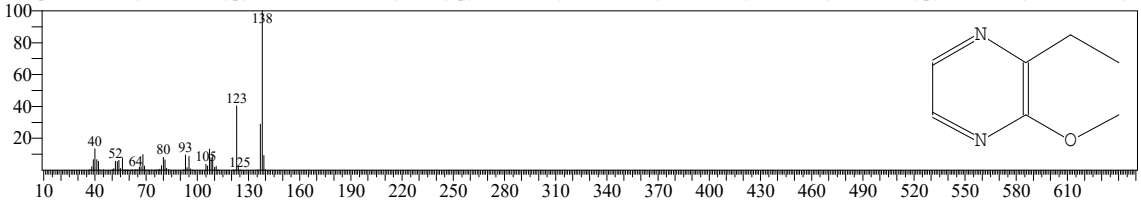
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:73 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



Hit#:4 Entry: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 #

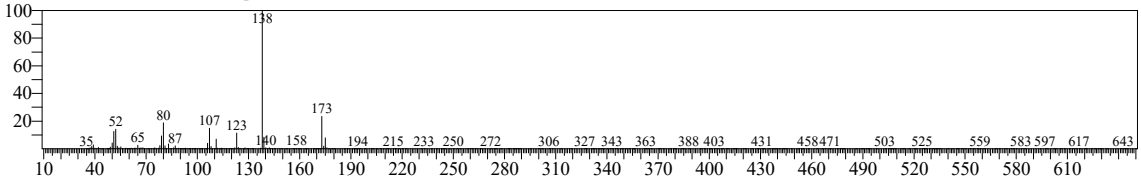


Hit#:5 Entry:8422 Library:NIST20R.lib
SI:71 Formula:C7H10N2O CAS:25680-58-4 MolWeight:138 RetIndex:1070
CompName:2-Ethyl-3-methoxypyrazine $$ 2-Methoxy-3-ethylpyrazine $$ Pyrazine, 2-ethyl-3-methoxy- $$ 3-Ethyl-2-methoxypyrazine $$ Pyrazine, 3-ethyl·

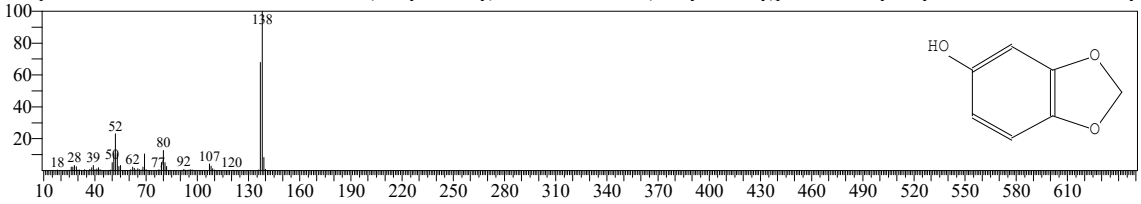


TNAU

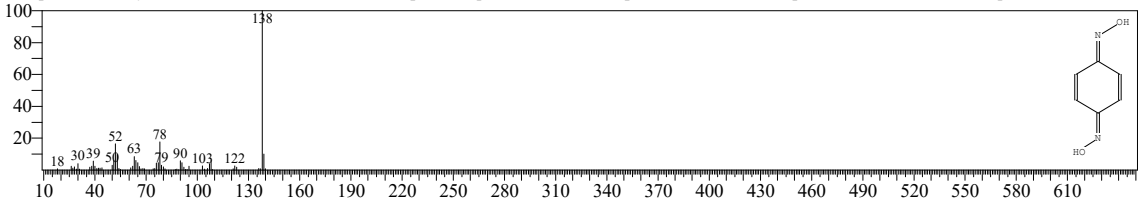
<< Target >>
Line#:6 R.Time:12.825(Scan#:1566) MassPeaks:320
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.05(60785)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



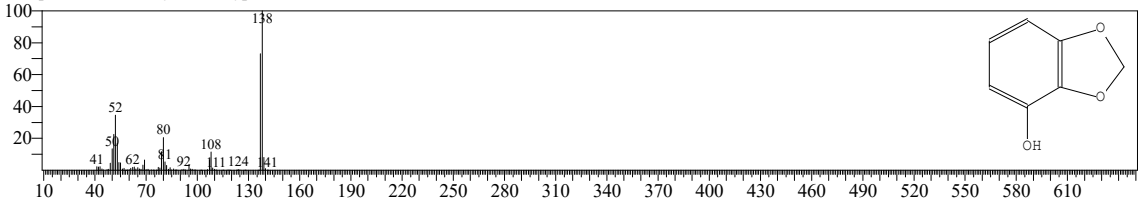
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



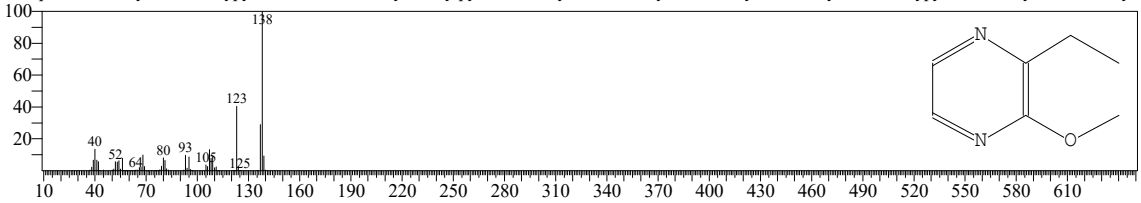
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



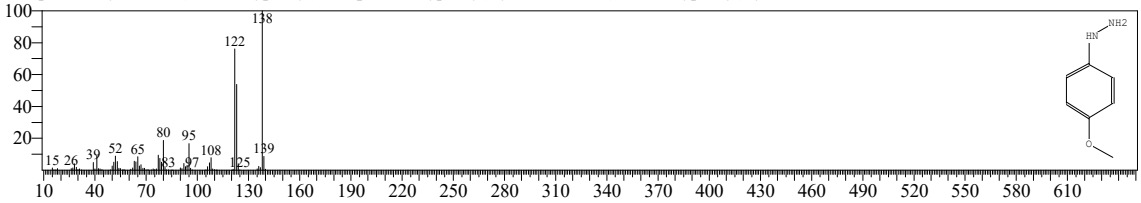
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:72 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



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

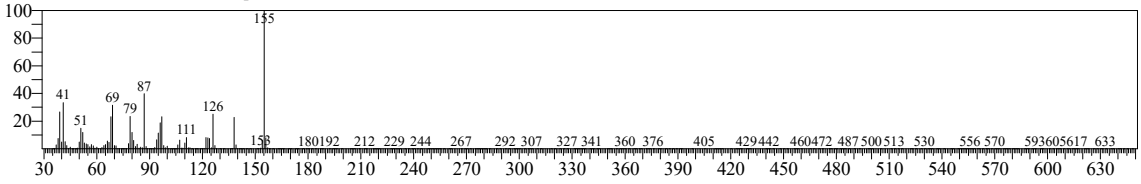


Hit#:5 Entry:11222 Library:NIST20M1.lib
SI:70 Formula:C7H10N2O CAS:3471-32-7 MolWeight:138 RetIndex:1325
CompName:Hydrazine, (4-methoxyphenyl)- $$ (p-Methoxyphenyl)hydrazine $$ 1-(4-Methoxyphenyl)hydrazine #

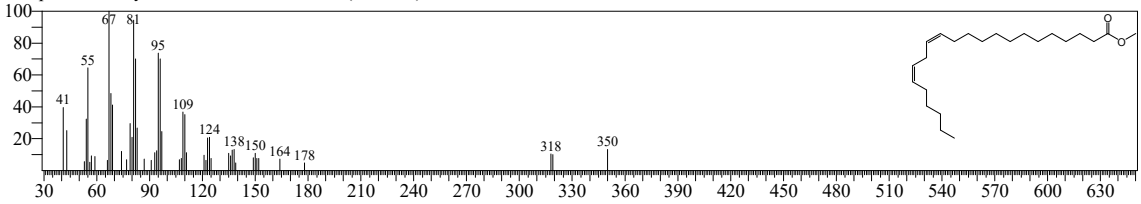


TNAU

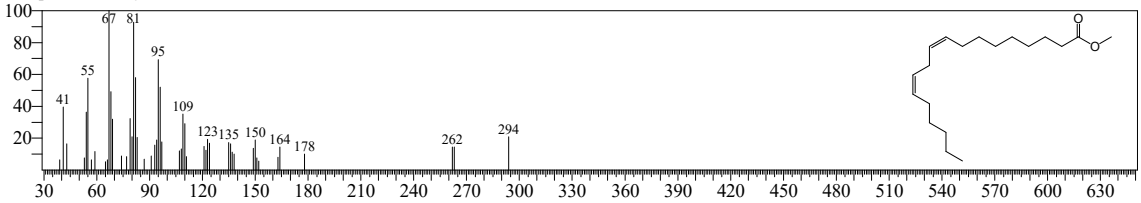
<< Target >>
Line#:7 R.Time:13.355(Scan#:1672) MassPeaks:358
RawMode:Averaged 13.350-13.360(1671-1673) BasePeak:155.05(55664)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



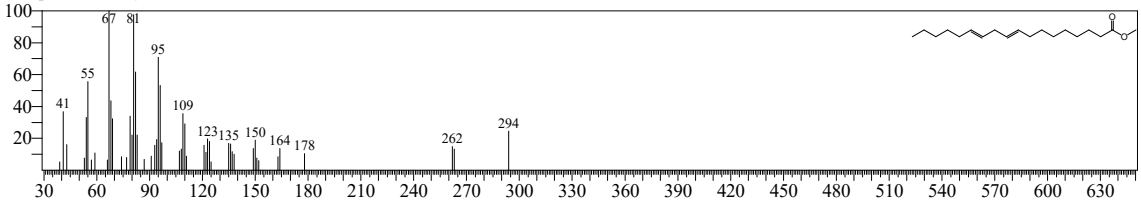
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



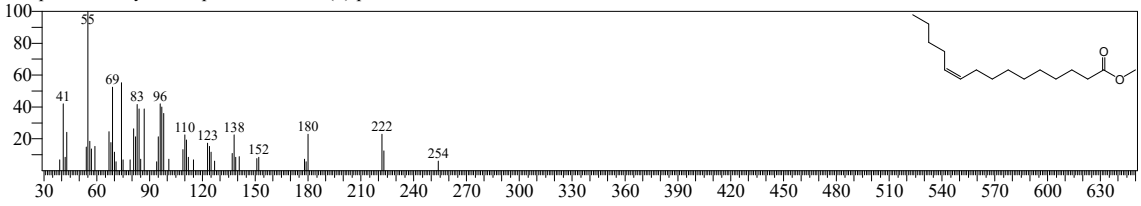
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



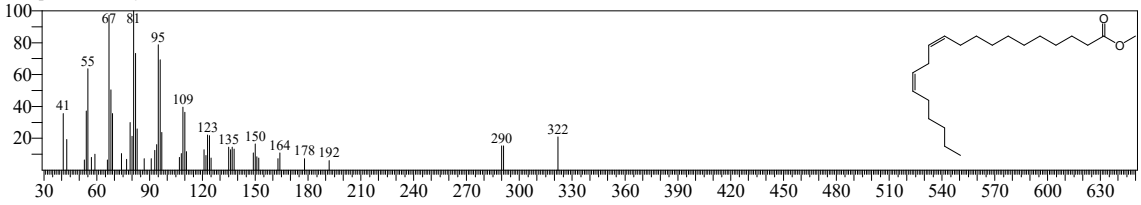
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

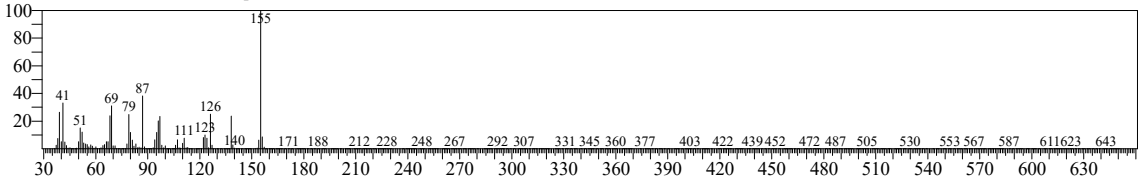


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

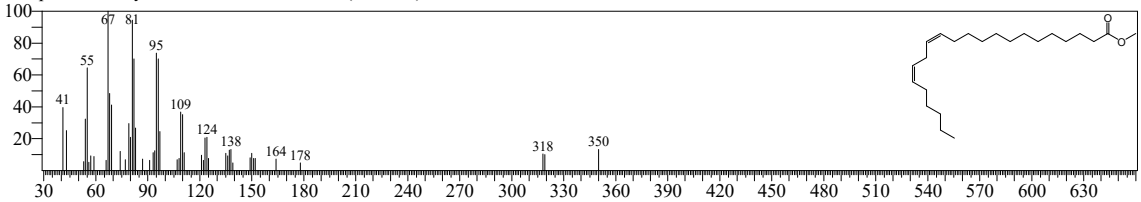


TNAU

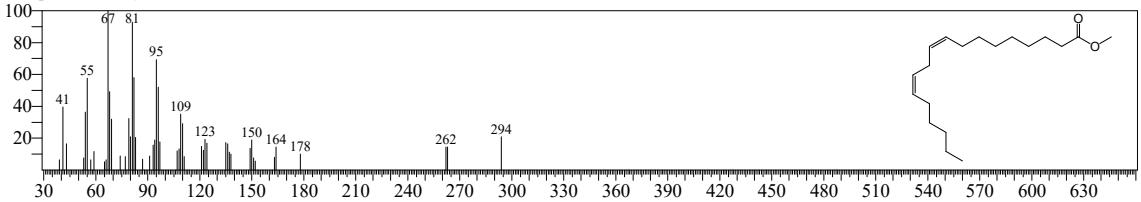
<< Target >>
Line#:8 R.Time:13.545(Scan#:1710) MassPeaks:434
RawMode:Averaged 13.540-13.550(1709-1711) BasePeak:155.05(50959)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



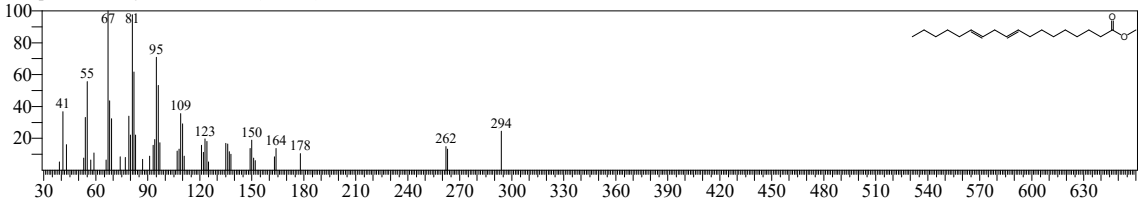
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



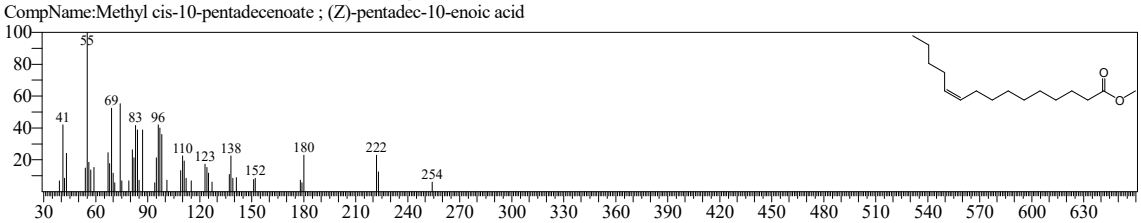
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



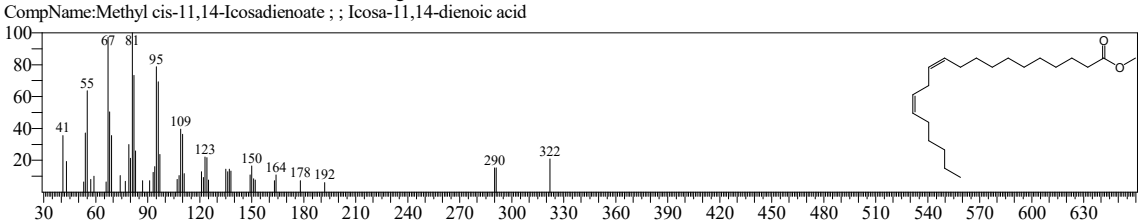
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

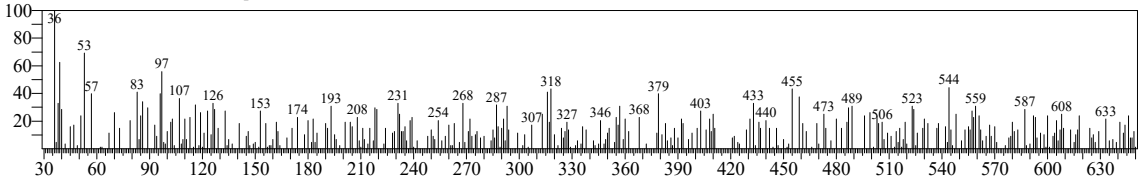


Hit#:5 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

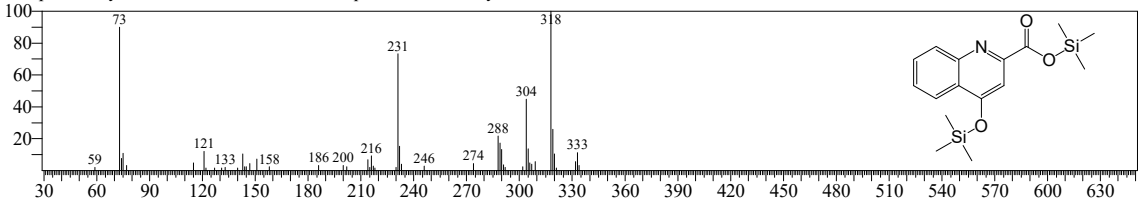


TNAU

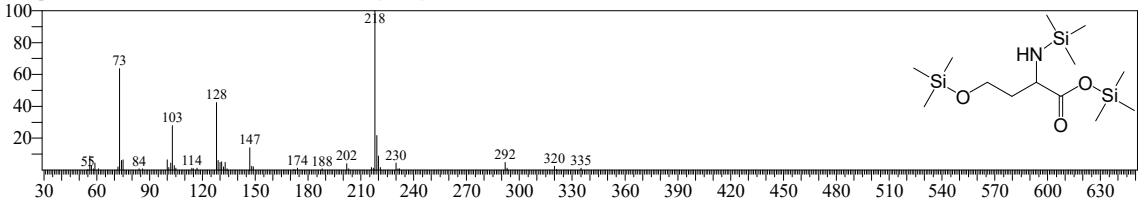
<< Target >>
Line#:9 R.Time:13.655(Scan#:1732) MassPeaks:329
RawMode:Averaged 13.650-13.660(1731-1733) BasePeak:36.00(88)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



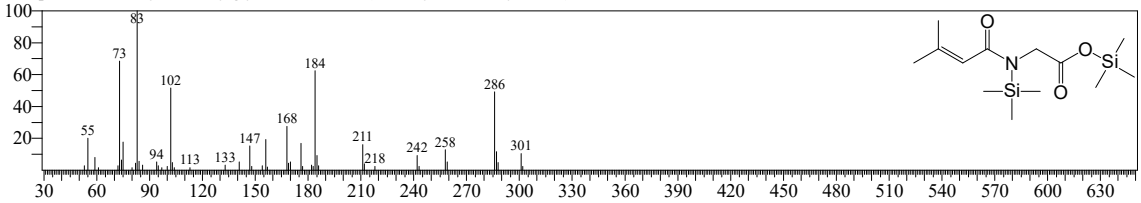
Hit#:1 Entry:454 Library:OA_TMS_DB5_67min_V3.lib
SI:12 Formula:C16H23NO3Si2 CAS:492-27-3 MolWeight:333 RetIndex:2089
CompName:Kynurenic acid-2TMS ; 4-oxo-1H-quinoline-2-carboxylic acid



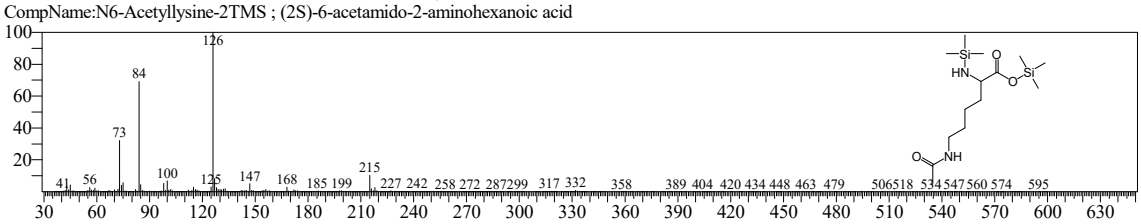
Hit#:2 Entry:130 Library:OA_TMS_DB5_67min_V3.lib
SI:12 Formula:C13H33NO3Si3 CAS:672-15-1 MolWeight:335 RetIndex:1458
CompName:Homoserine-3TMS ; (2S)-2-amino-4-hydroxybutanoic acid



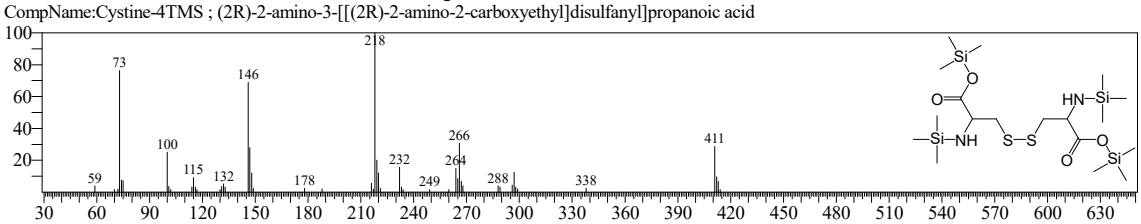
Hit#:3 Entry:183 Library:OA_TMS_DB5_67min_V3.lib
SI:12 Formula:C13H27NO3Si2 CAS:33008-07-0 MolWeight:301 RetIndex:1578
CompName:3-Methylcrotonoylglycine-2TMS ; 2-(3-methylbut-2-enoylamino)acetic acid



Hit#:4 Entry:409 Library:OA_TMS_DB5_67min_V3.lib
SI:11 Formula:C14H32N2O3Si2 CAS:692-04-6 MolWeight:332 RetIndex:1951
CompName:N6-Acetyllysine-2TMS ; (2S)-6-acetamido-2-aminohexanoic acid

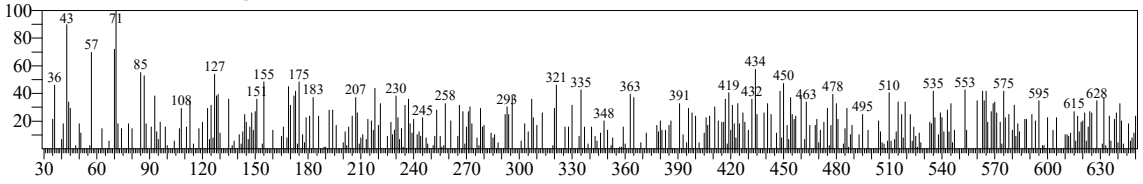


Hit#:5 Entry:500 Library:OA_TMS_DB5_67min_V3.lib
SI:11 Formula:C18H44N2O4S2Si4 CAS:56-89-3 MolWeight:528 RetIndex:2322
CompName:Cystine-4TMS ; (2R)-2-amino-3-[[(2R)-2-amino-2-carboxyethyl]disulfanyl]propanoic acid

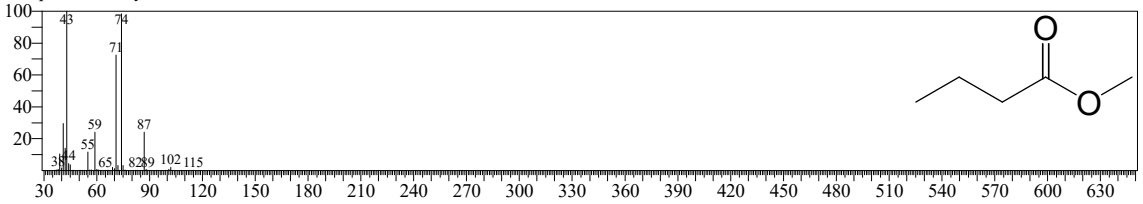


TNAU

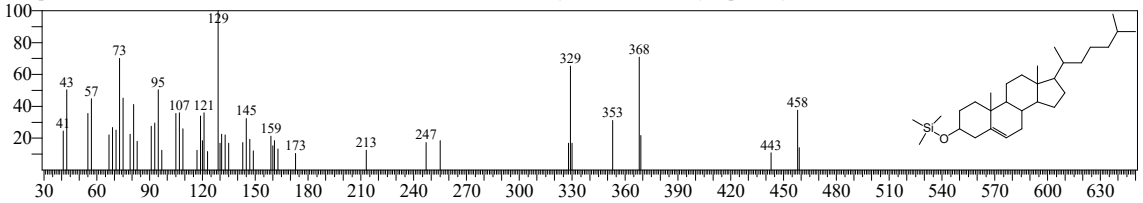
<< Target >>
Line#:10 R.Time:14.310(Scan#:1863) MassPeaks:352
RawMode:Averaged 14.305-14.315(1862-1864) BasePeak:71.00(89)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



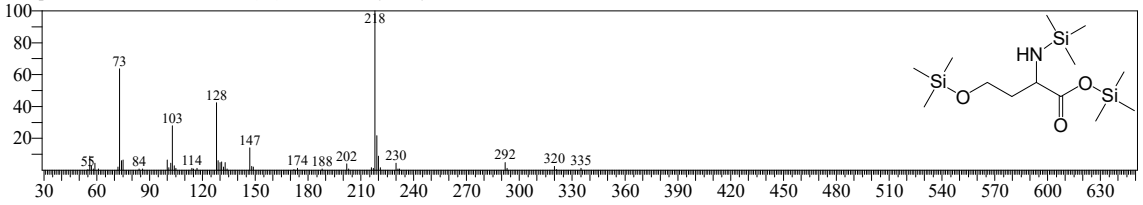
Hit#:1 Entry:1 Library:FA_ME_SP2560_EI_V3.lib
SI:20 Formula:C5H10O2 CAS:107-92-6 MolWeight:102 RetIndex:1113
CompName:Methyl butanoate ; Butanoic acid



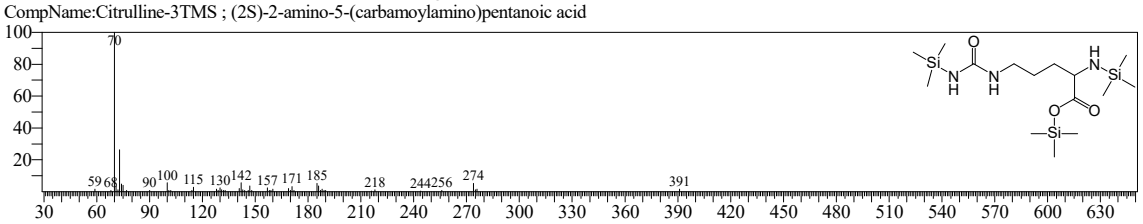
Hit#:2 Entry:567 Library:OA_TMS_DB5_67min_V3.lib
SI:16 Formula:C30H54OSi CAS:57-88-5 MolWeight:458 RetIndex:3221
CompName:Cholesterol-TMS ; (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R)-6-methylheptan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodec



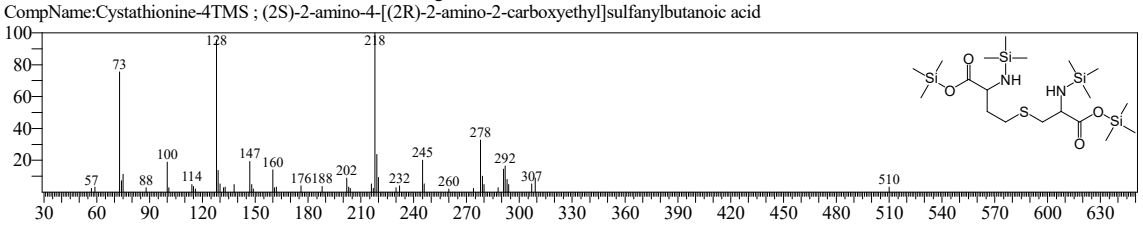
Hit#:3 Entry:130 Library:OA_TMS_DB5_67min_V3.lib
SI:14 Formula:C13H33NO3Si3 CAS:672-15-1 MolWeight:335 RetIndex:1458
CompName:Homoserine-3TMS ; (2S)-2-amino-4-hydroxybutanoic acid



Hit#:4 Entry:459 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C15H37N3O3Si3 CAS:372-75-8 MolWeight:391 RetIndex:2112
CompName:Citrulline-3TMS ; (2S)-2-amino-5-(carbamoylamino)pentanoic acid

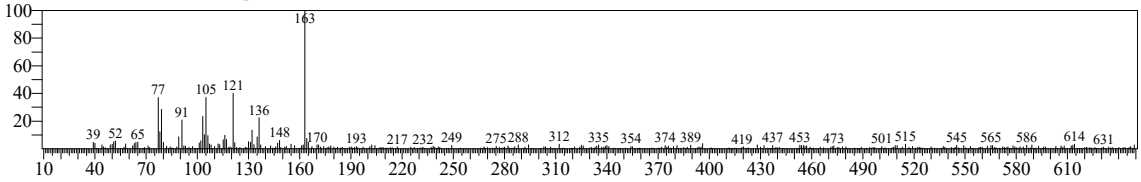


Hit#:5 Entry:489 Library:OA_TMS_DB5_67min_V3.lib
SI:13 Formula:C19H46N2O4SSi4 CAS:56-88-2 MolWeight:510 RetIndex:2233
CompName:Cystathionine-4TMS ; (2S)-2-amino-4-[(2R)-2-amino-2-carboxyethyl]sulfanylbutanoic acid

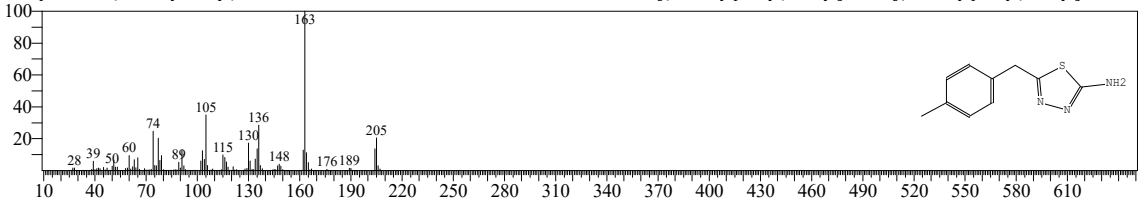


TNAU

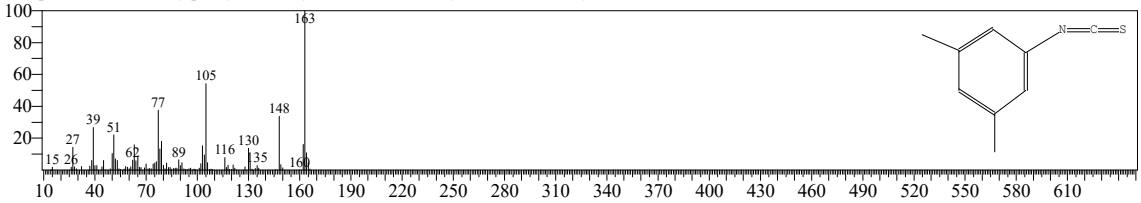
<< Target >>
Line#:11 R.Time:14.470(Scan#:1895) MassPeaks:354
RawMode:Averaged 14.465-14.475(1894-1896) BasePeak:163.05(1213)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



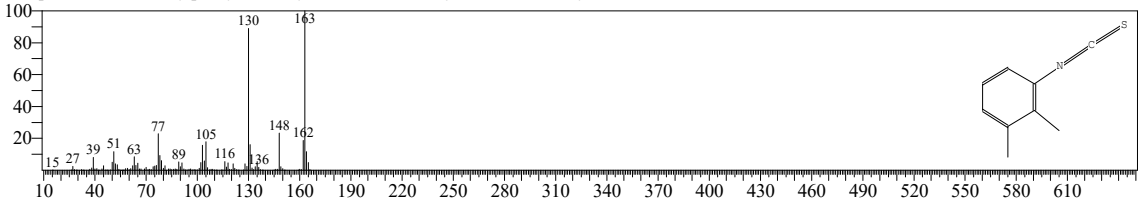
Hit#:1 Entry:57597 Library:NIST20M1.lib
SI:74 Formula:C10H11N3S CAS:39181-45-8 MolWeight:205 RetIndex:1890
CompName:5-(4-Methylbenzyl)-1,3,4-thiadiazol-2-amine $$ 1,3,4-Thiadiazol-2-amine, 5-[(4-methylphenyl)methyl]- $$ 5-[(4-Methylphenyl)methyl]-1,3,4-tl



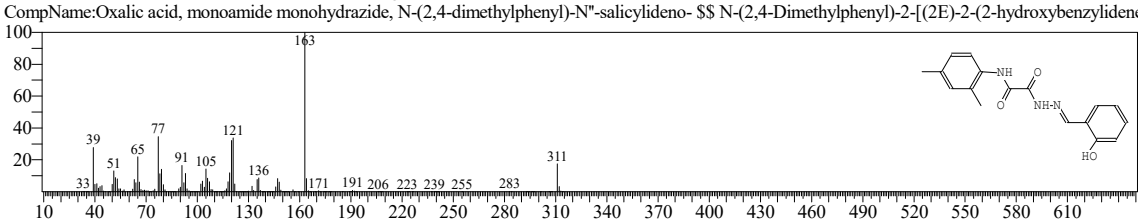
Hit#:2 Entry:24672 Library:NIST20M1.lib
SI:74 Formula:C9H9NS CAS:40046-30-8 MolWeight:163 RetIndex:0
CompName:3,5-Dimethylphenyl isothiocyanate $$ 1-Isothiocyanato-3,5-dimethylbenzene #



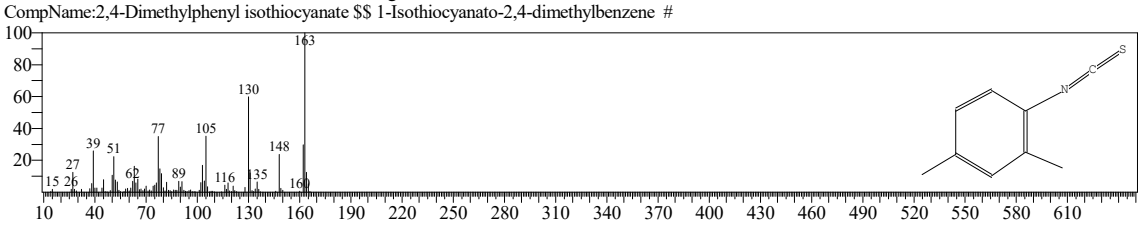
Hit#:3 Entry:14264 Library:NIST20R.lib
SI:73 Formula:C9H9NS CAS:1539-20-4 MolWeight:163 RetIndex:0
CompName:2,3-Dimethylphenylisothiocyanate $$ 1-Isothiocyanato-2,3-dimethylbenzene #



Hit#:4 Entry:176186 Library:NIST20M1.lib
SI:72 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-hydroxybenzylidene

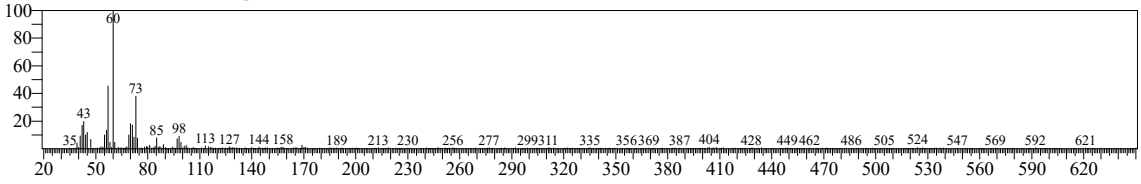


Hit#:5 Entry:24676 Library:NIST20M1.lib
SI:72 Formula:C9H9NS CAS:39842-01-8 MolWeight:163 RetIndex:0
CompName:2,4-Dimethylphenyl isothiocyanate $$ 1-Isothiocyanato-2,4-dimethylbenzene #

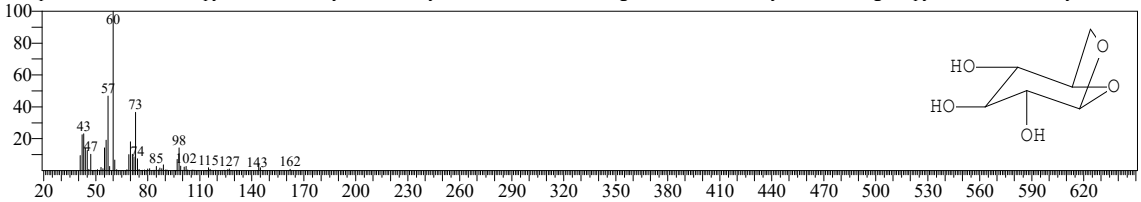


TNAU

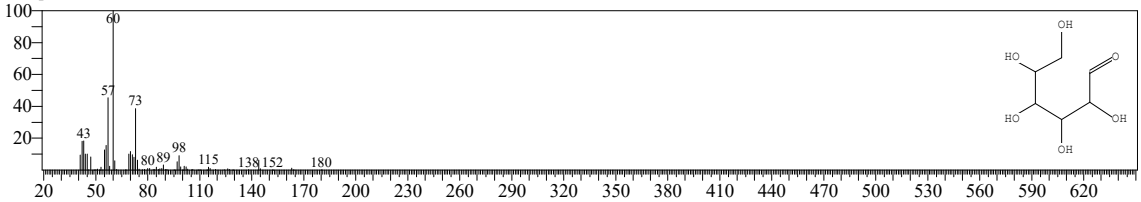
<< Target >>
Line#:12 R.Time:18.065(Scan#:2614) MassPeaks:352
RawMode:Averaged 18.060-18.070(2613-2615) BasePeak:60.00(4801)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



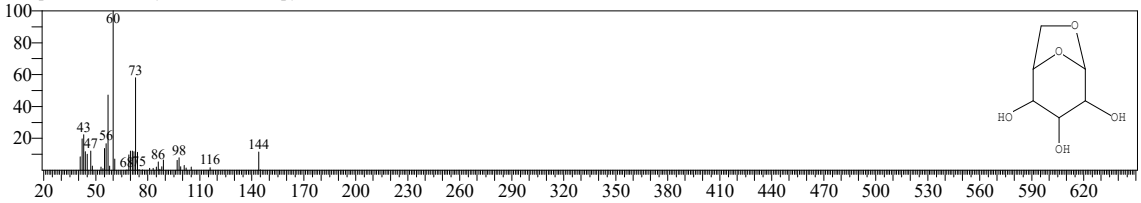
Hit#:1 Entry:13905 Library:NIST20R.lib
SI:93 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-



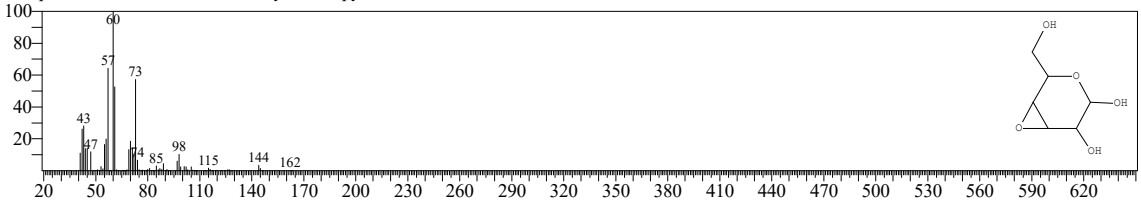
Hit#:2 Entry:36240 Library:NIST20M1.lib
SI:93 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #



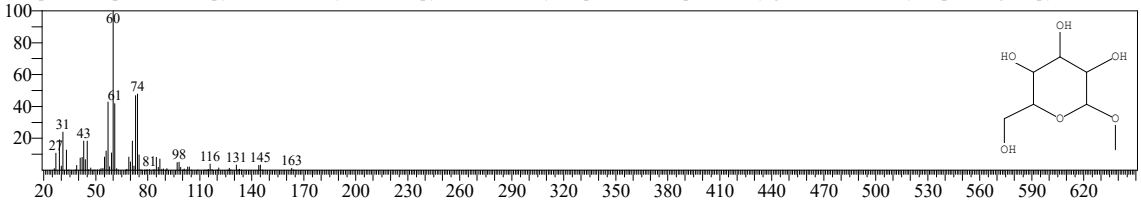
Hit#:3 Entry:23812 Library:NIST20M1.lib
SI:90 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-d-talopyranose



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 #

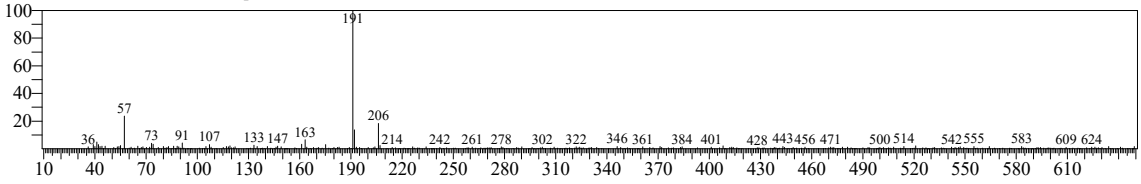


Hit#:5 Entry:21209 Library:NIST20R.lib
SI:84 Formula:C7H14O6 CAS:97-30-3 MolWeight:194 RetIndex:1714
CompName:.alpha.-D-Glucopyranoside, methyl $$ Glucopyranoside, methyl, .alpha.-D- $$ .alpha.-Methylglucoside $$ Methyl .alpha.-D-glucopyranoside $$

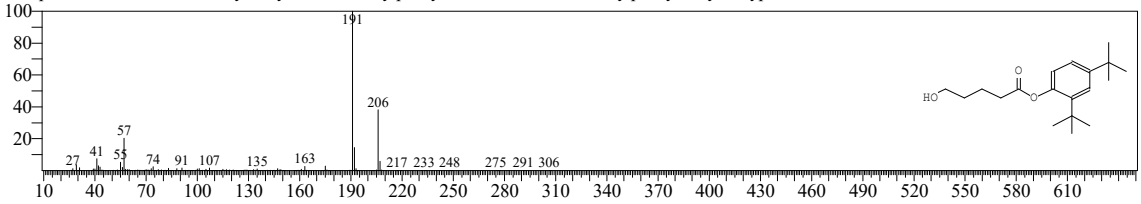


TNAU

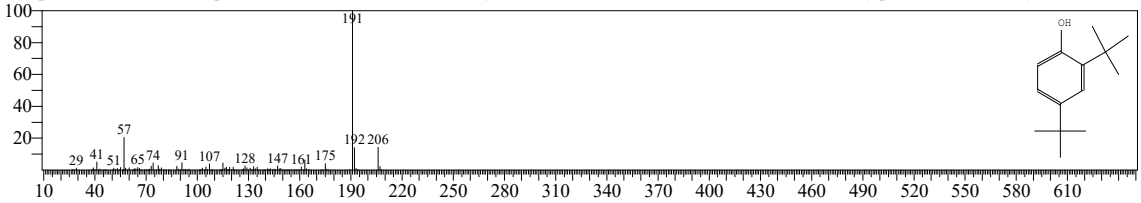
<< Target >>
Line#:13 R.Time:18.505(Scan#:2702) MassPeaks:330
RawMode:Averaged 18.500-18.510(2701-2703) BasePeak:191.10(2311)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



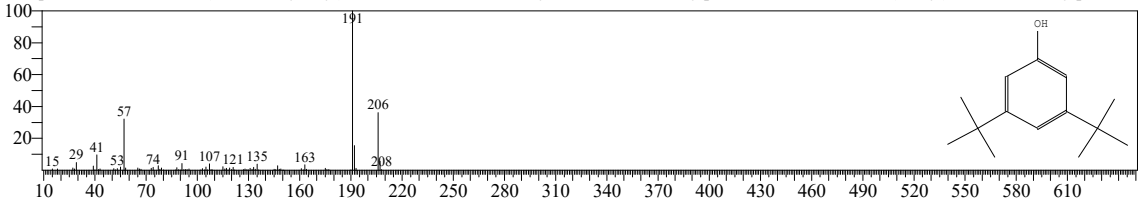
Hit#:1 Entry:170993 Library:NIST20M1.lib
SI:84 Formula:C19H30O3 CAS:166273-38-7 MolWeight:306 RetIndex:2255
CompName:Pentanoic acid, 5-hydroxy-, 2,4-di-t-butylphenyl esters $$ 2,4-Ditert-butylphenyl 5-hydroxypentanoate #



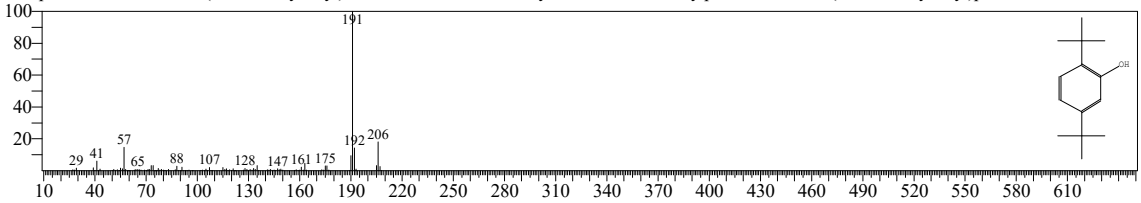
Hit#:2 Entry:24088 Library:NIST20R.lib
SI:83 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu



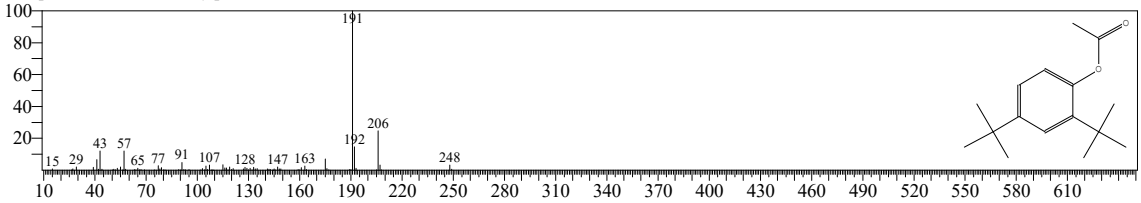
Hit#:3 Entry:24110 Library:NIST20R.lib
SI:82 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $



Hit#:4 Entry:59059 Library:NIST20M1.lib
SI:82 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol

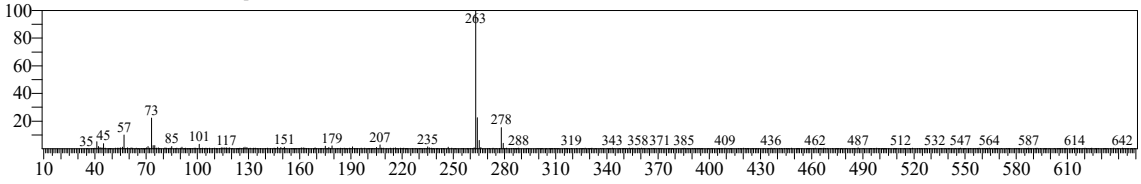


Hit#:5 Entry:103047 Library:NIST20M1.lib
SI:80 Formula:C16H24O2 CAS:104316-22-5 MolWeight:248 RetIndex:1714
CompName:2,4-Di-tert-butylphenol, acetate

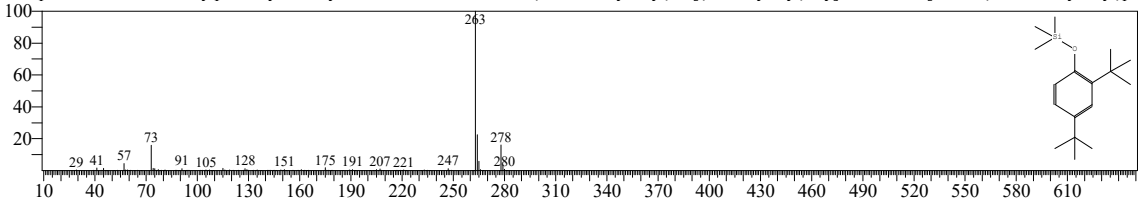


TNAU

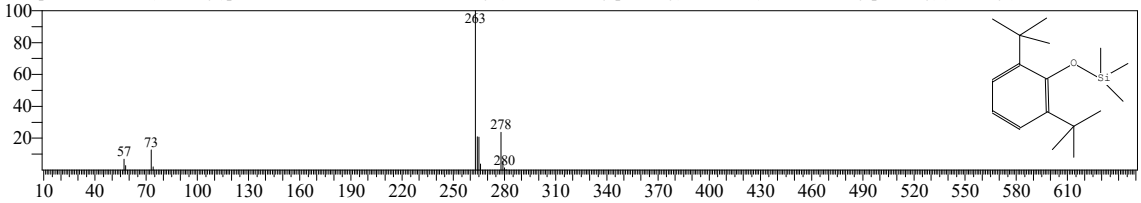
<< Target >>
Line#:14 R.Time:19.195(Scan#:2840) MassPeaks:409
RawMode:Averaged 19.190-19.200(2839-2841) BasePeak:263.15(7670)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



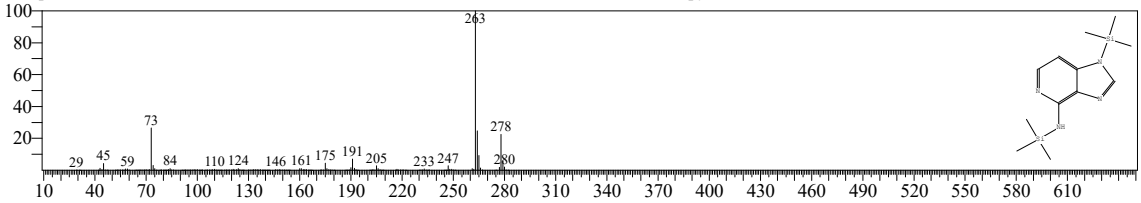
Hit#:1 Entry:33874 Library:NIST20R.lib
SI:91 Formula:C17H30OSi CAS:53925-65-8 MolWeight:278 RetIndex:1632
CompName:2,4-Di-tert-butylphenoxytrimethylsilane $$ Benzene, 2,4-bis(1,1-dimethylethyl)-1-[(trimethylsilyl)oxy]- $$ Silane, [2,4-bis(1,1-dimethylethyl)ph



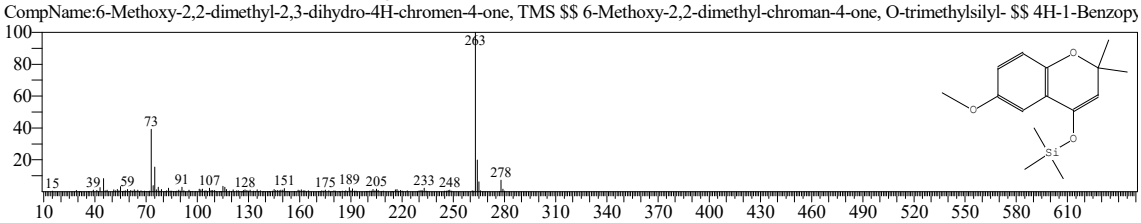
Hit#:2 Entry:33871 Library:NIST20R.lib
SI:82 Formula:C17H30OSi CAS:10416-73-6 MolWeight:278 RetIndex:1632
CompName:2,6-Bis(tert-butyl)phenol, TMS derivative $$ Trimethyl(2,6 ditert.-butylphenoxy)silane $$ (2,6-Ditert-butylphenoxy)(trimethyl)silane #



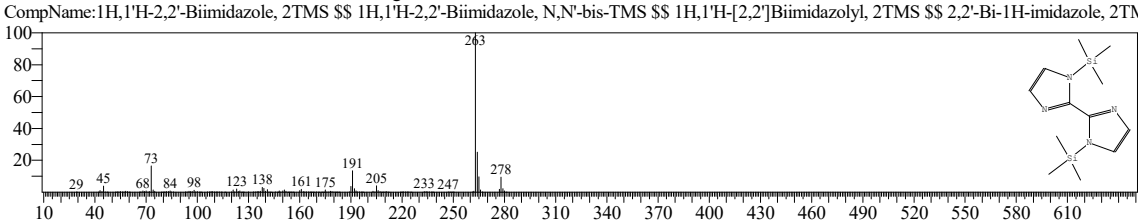
Hit#:3 Entry:136557 Library:NIST20M1.lib
SI:82 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1703
CompName:3-Deazaadenine, 2TMS $$ 3-Deazaadenine, N,N'-bis-TMS $$ 1H-Imidazo[4,5-c]pyridin-4-amine, N,N'-bis-TMS



Hit#:4 Entry:137020 Library:NIST20M1.lib
SI:79 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

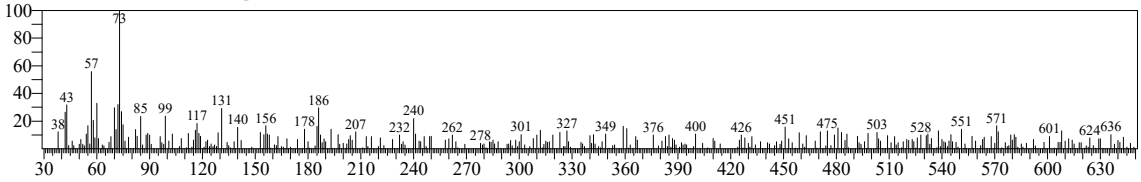


Hit#:5 Entry:136556 Library:NIST20M1.lib
SI:78 Formula:C12H22N4Si2 CAS:0-00-0 MolWeight:278 RetIndex:1606
CompName:1H,1'H-2,2'-Biimidazole, 2TMS $$ 1H,1'H-2,2'-Biimidazole, N,N'-bis-TMS $$ 1H,1'H-[2,2']Biimidazolyl, 2TMS $$ 2,2'-Bi-1H-imidazole, 2TM

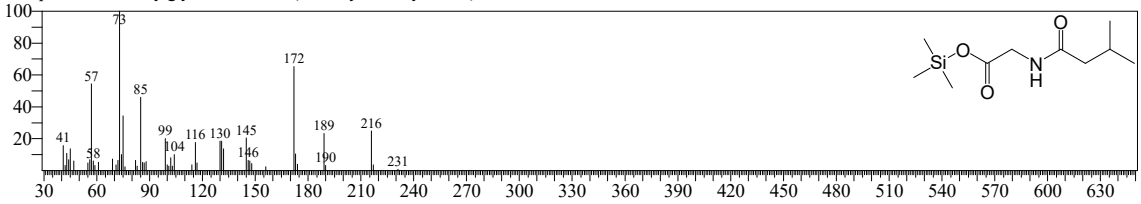


TNAU

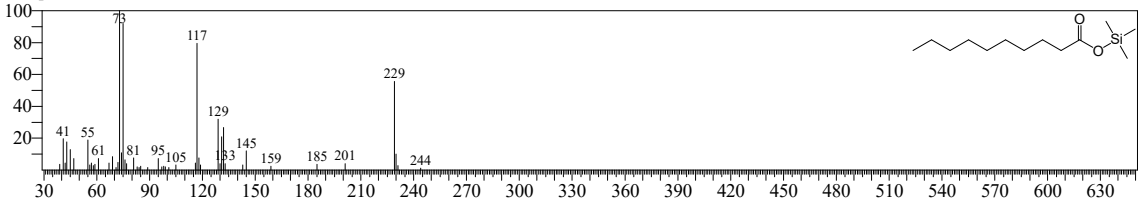
<< Target >>
Line#:15 R.Time:20.305(Scan#:3062) MassPeaks:333
RawMode:Averaged 20.300-20.310(3061-3063) BasePeak:73.00(253)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



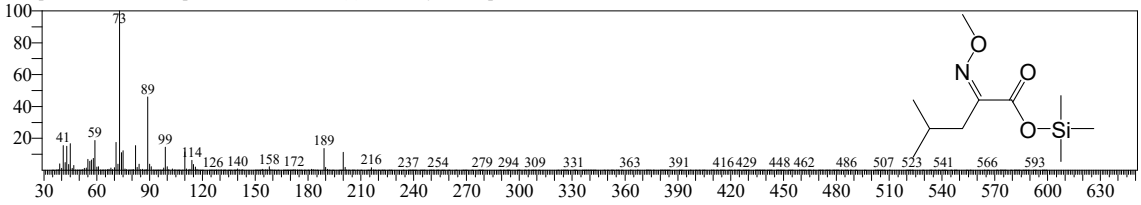
Hit#:1 Entry:139 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C10H21NO3Si CAS:16284-60-9 MolWeight:231 RetIndex:1487
CompName:Isovalerylglycine-TMS ; 2-(3-methylbutanoylamino)acetic acid



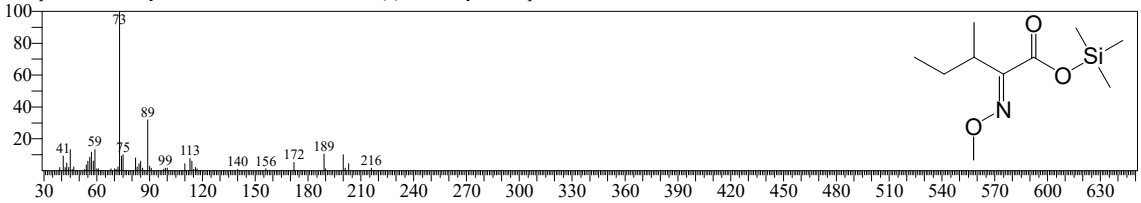
Hit#:2 Entry:129 Library:OA_TMS_DB5_67min_V3.lib
SI:44 Formula:C13H28O2Si CAS:334-48-5 MolWeight:244 RetIndex:1457
CompName:Decanoic acid-TMS ; decanoic acid



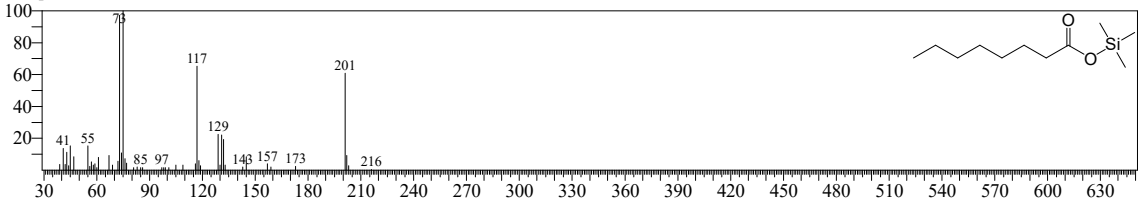
Hit#:3 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid



Hit#:4 Entry:40 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C10H21NO3Si CAS:1460-34-0 MolWeight:231 RetIndex:1184
CompName:3-Methyl-2-oxovaleric acid-meto-TMS(1) ; 3-methyl-2-oxopentanoic acid

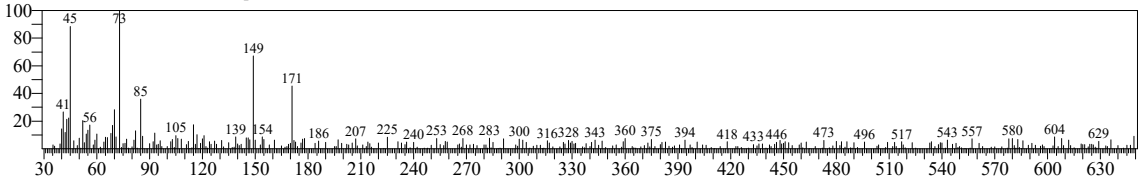


Hit#:5 Entry:70 Library:OA_TMS_DB5_67min_V3.lib
SI:43 Formula:C11H24O2Si CAS:124-07-2 MolWeight:216 RetIndex:1263
CompName:Octanoic acid-TMS ; octanoic acid

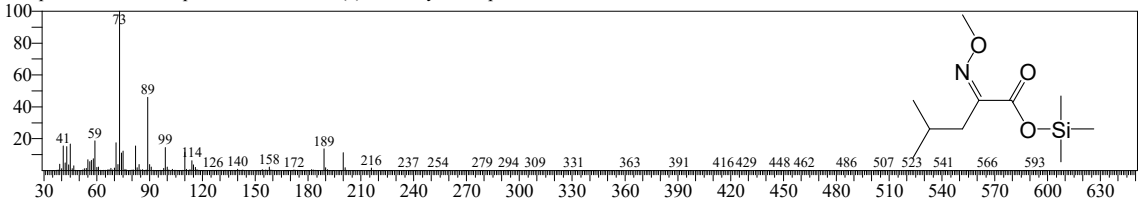


TNAU

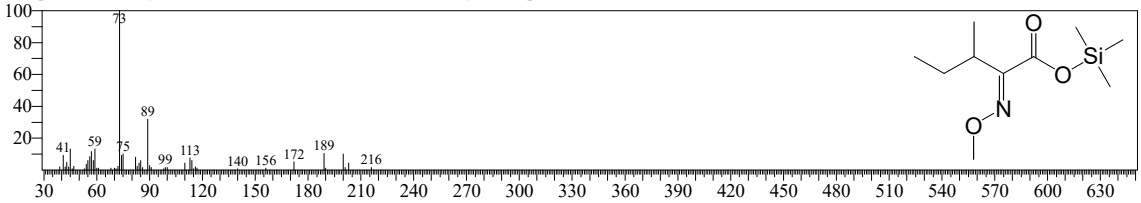
<< Target >>
Line#:16 R.Time:20.365(Scan#:3074) MassPeaks:333
RawMode:Averaged 20.360-20.370(3073-3075) BasePeak:73.05(521)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



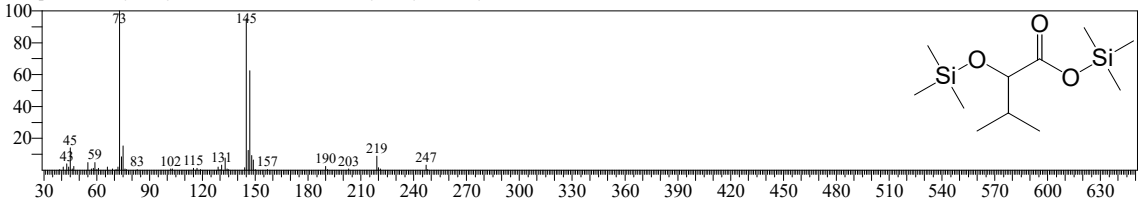
Hit#:1 Entry:39 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C10H21NO3Si CAS:816-66-0 MolWeight:231 RetIndex:1181
CompName:2-Ketoisocaproic acid-meto-TMS(1) ; 4-methyl-2-oxopentanoic acid



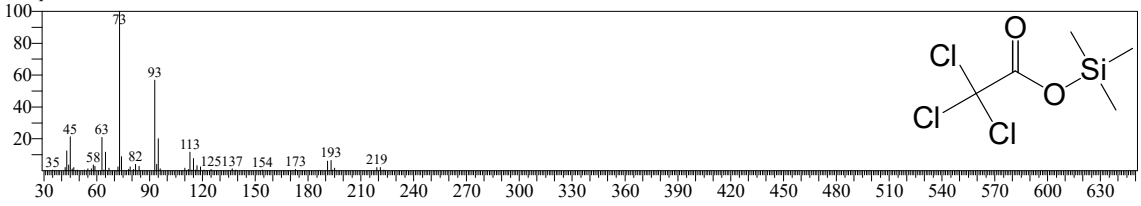
Hit#:2 Entry:40 Library:OA_TMS_DB5_67min_V3.lib
SI:42 Formula:C10H21NO3Si CAS:1460-34-0 MolWeight:231 RetIndex:1184
CompName:3-Methyl-2-oxovaleric acid-meto-TMS(1) ; 3-methyl-2-oxopentanoic acid



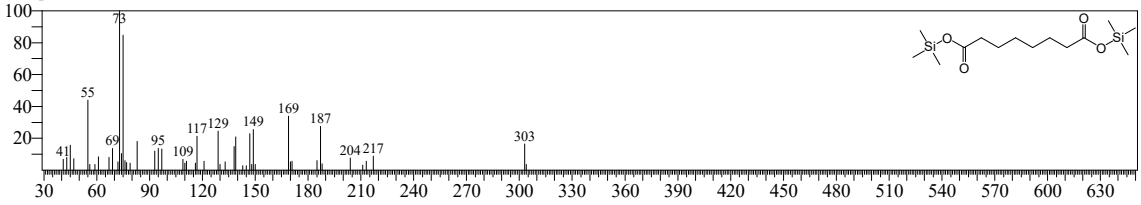
Hit#:3 Entry:37 Library:OA_TMS_DB5_67min_V3.lib
SI:40 Formula:C11H26O3Si2 CAS:4026-18-0 MolWeight:262 RetIndex:1169
CompName:2-Hydroxyisovaleric acid-2TMS ; 2-hydroxy-3-methylbutanoic acid



Hit#:4 Entry:6 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C5H9Cl3O2Si CAS:76-03-9 MolWeight:234 RetIndex:1059
CompName:Trichloroacetic acid-TMS ; 2,2,2-trichloroacetic acid

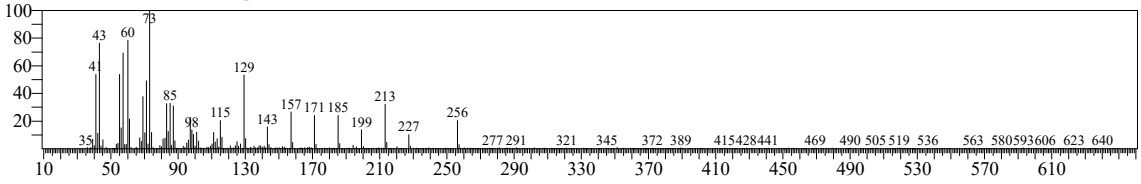


Hit#:5 Entry:258 Library:OA_TMS_DB5_67min_V3.lib
SI:39 Formula:C14H30O4Si2 CAS:505-48-6 MolWeight:318 RetIndex:1700
CompName:Suberic acid-2TMS ; octanedioic acid

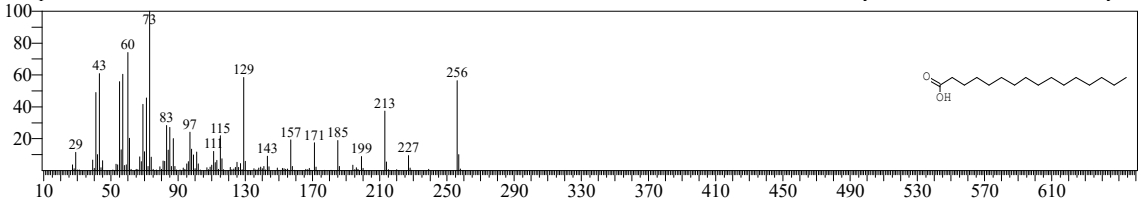


TNAU

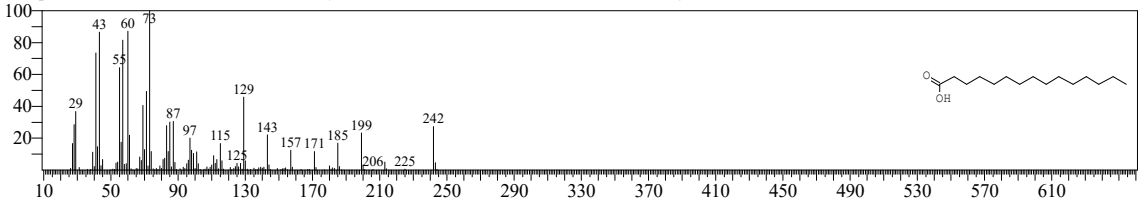
<< Target >>
Line#:17 R.Time:28.300(Scan#:4661) MassPeaks:406
RawMode:Averaged 28.295-28.305(4660-4662) BasePeak:73.05(6787)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



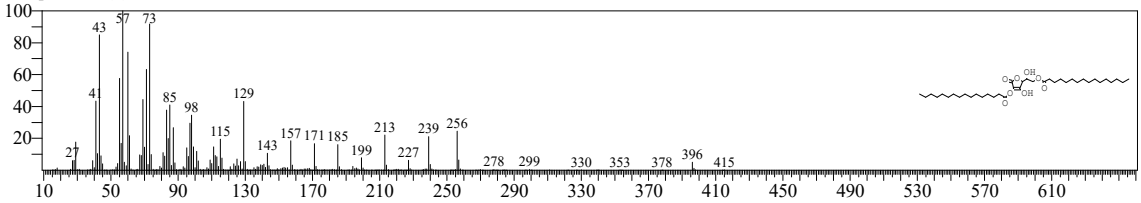
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



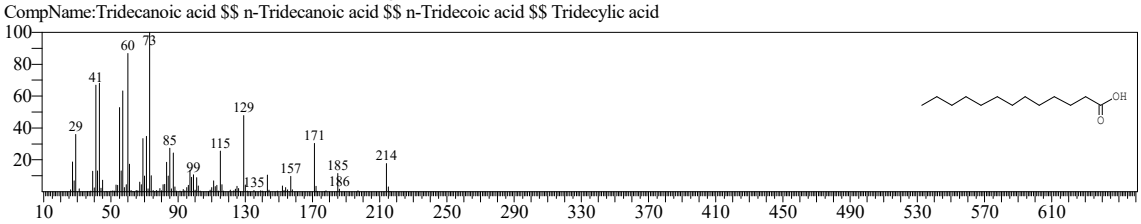
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



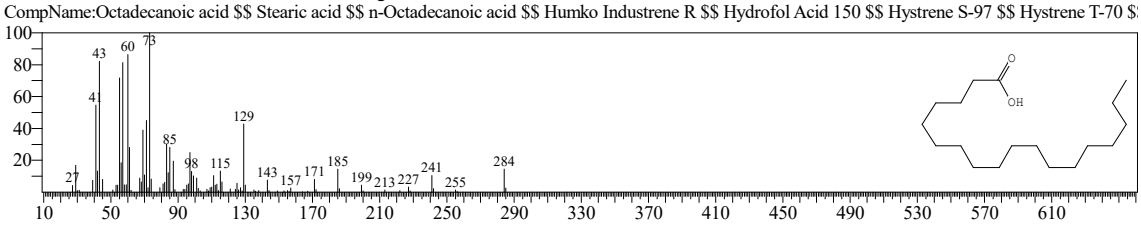
Hit#:3 Entry:44286 Library:NIST20M2.lib
SI:91 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



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

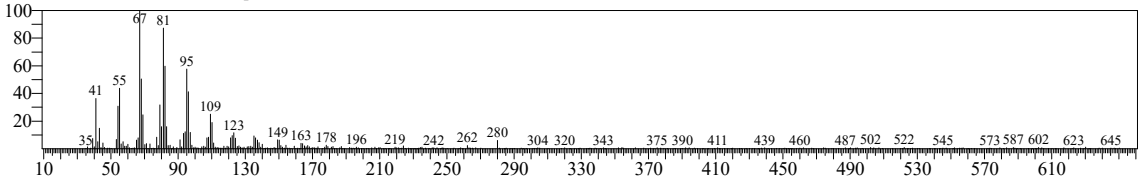


Hit#:5 Entry:144781 Library:NIST20M1.lib
SI:89 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $

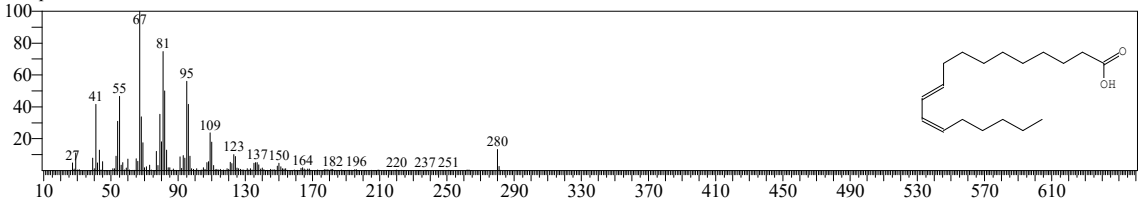


TNAU

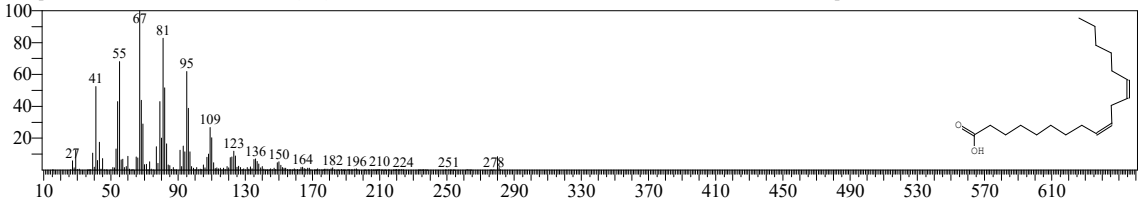
<< Target >>
Line#:18 R.Time:31.475(Scan#:5296) MassPeaks:351
RawMode:Averaged 31.470-31.480(5295-5297) BasePeak:67.05(3855)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



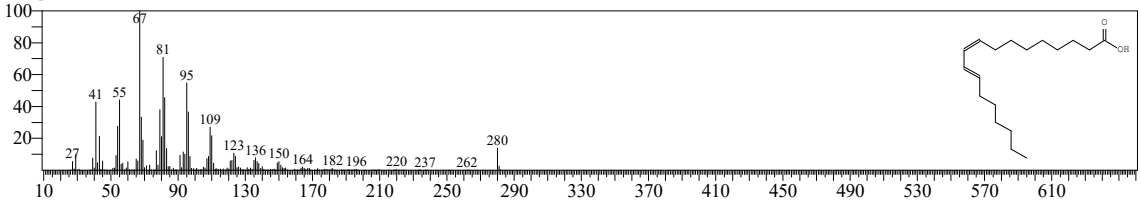
Hit#:1 Entry:139646 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid



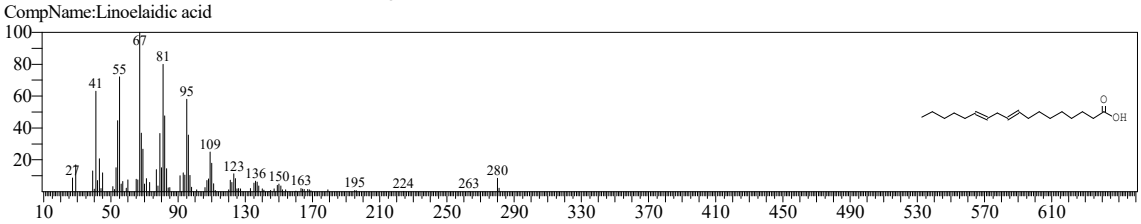
Hit#:2 Entry:34035 Library:NIST20R.lib
SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$



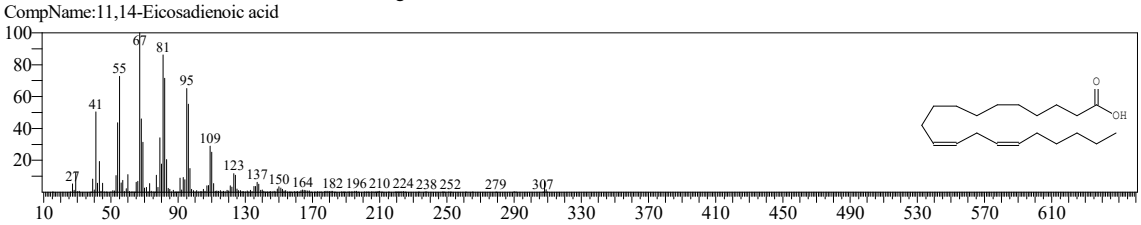
Hit#:3 Entry:139651 Library:NIST20M1.lib
SI:95 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid



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

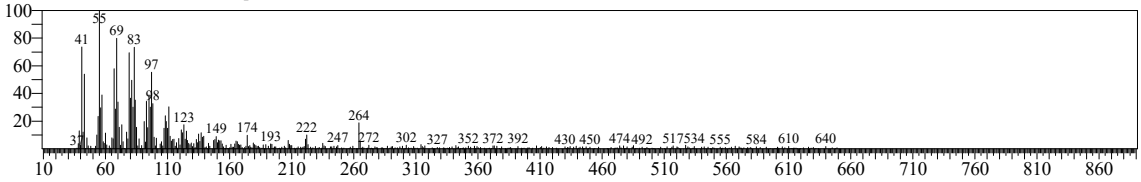


Hit#:5 Entry:173215 Library:NIST20M1.lib
SI:93 Formula:C20H36O2 CAS:2091-39-6 MolWeight:308 RetIndex:2382
CompName:11,14-Eicosadienoic acid

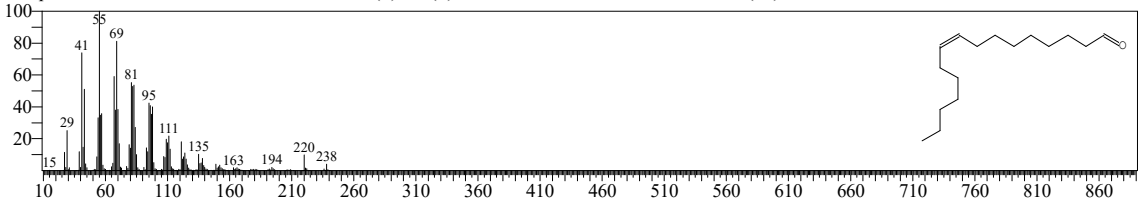


TNAU

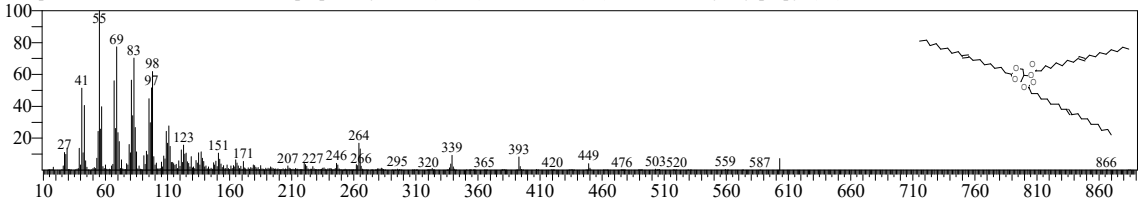
<< Target >>
Line#:19 R.Time:31.585(Scan#:5318) MassPeaks:383
RawMode:Averaged 31.580-31.590(5317-5319) BasePeak:55.10(1609)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



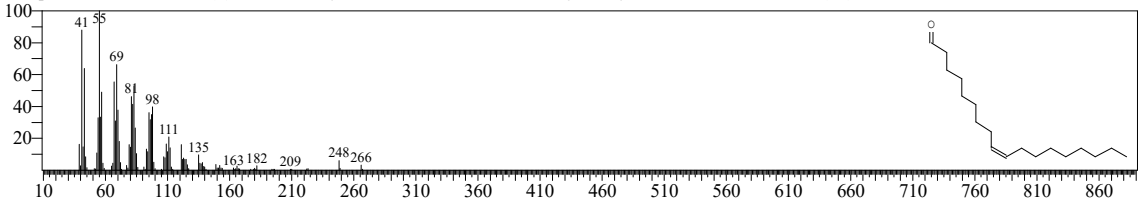
Hit#:1 Entry:92244 Library:NIST20M1.lib
SI:88 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #



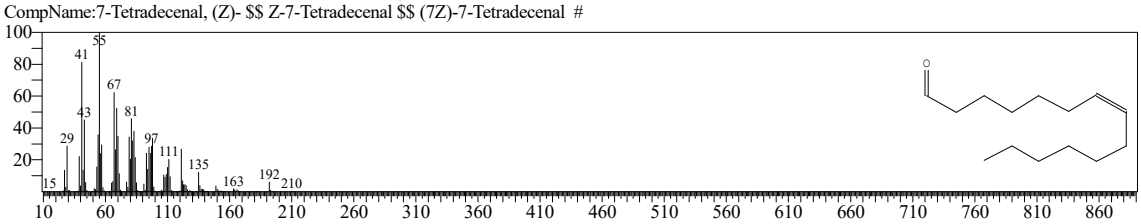
Hit#:2 Entry:46357 Library:NIST20M2.lib
SI:88 Formula:C57H104O6 CAS:537-39-3 MolWeight:884 RetIndex:6149
CompName:9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)- $$ 2,3-Bis[(9E)-9-octadecenoyloxy]propyl (9E)-9-octadecenoate #



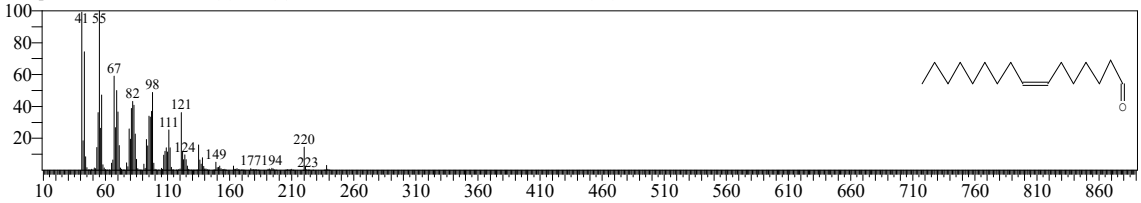
Hit#:3 Entry:123421 Library:NIST20M1.lib
SI:88 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal #



Hit#:4 Entry:63176 Library:NIST20M1.lib
SI:87 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #

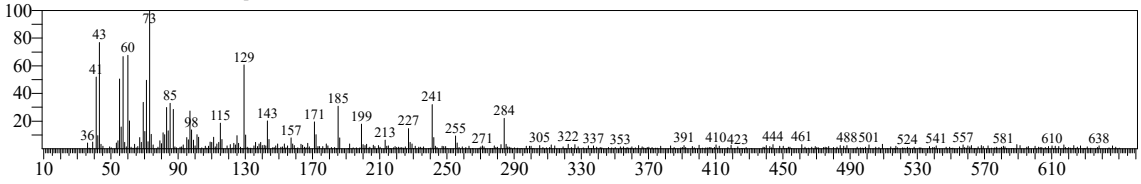


Hit#:5 Entry:92227 Library:NIST20M1.lib
SI:87 Formula:C16H30O CAS:56797-40-1 MolWeight:238 RetIndex:1808
CompName:7-Hexadecenal, (Z)- $$ (Z)-7-Hexadecenal $$ Z-7-Hexadecenal $$ (7Z)-7-Hexadecenal #

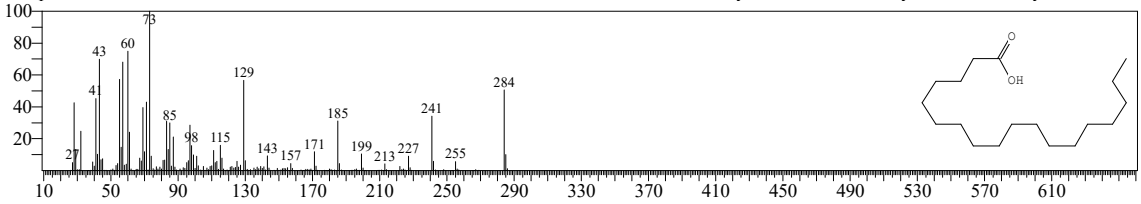


TNAU

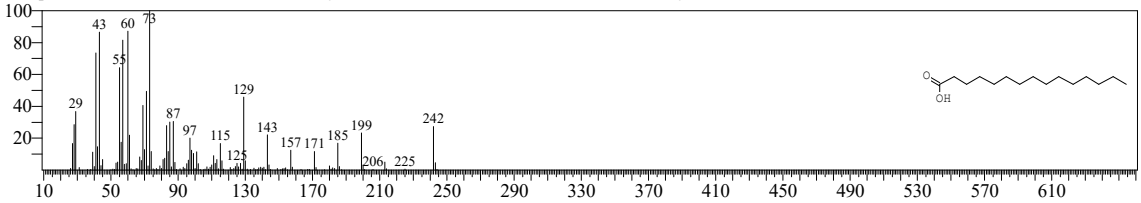
<< Target >>
Line#:20 R.Time:32.030(Scan#:5407) MassPeaks:383
RawMode:Averaged 32.025-32.035(5406-5408) BasePeak:73.05(1287)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



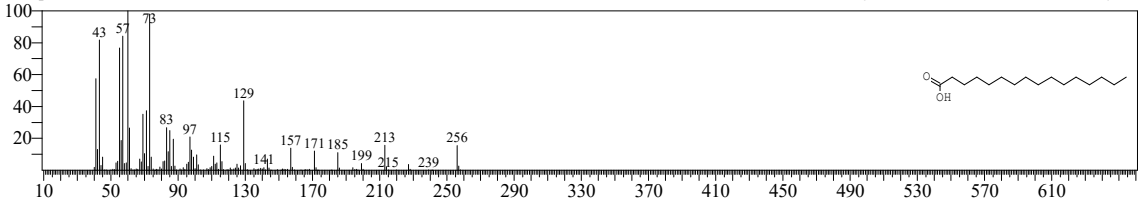
Hit#:1 Entry:34463 Library:NIST20R.lib
SI:91 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



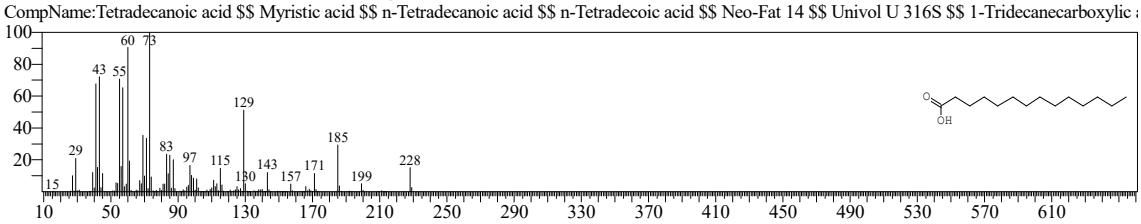
Hit#:2 Entry:29890 Library:NIST20R.lib
SI:88 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



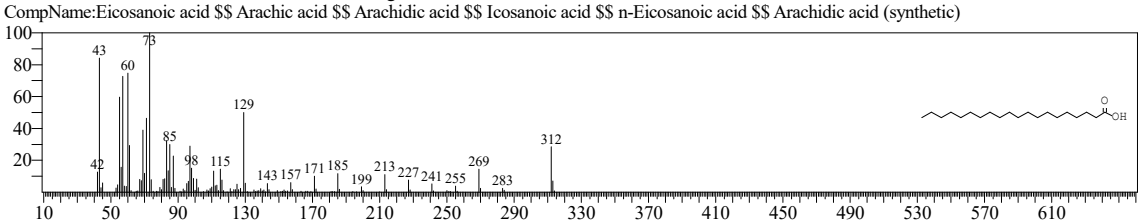
Hit#:3 Entry:31599 Library:NIST20R.lib
SI:86 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



Hit#:4 Entry:81713 Library:NIST20M1.lib
SI:86 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

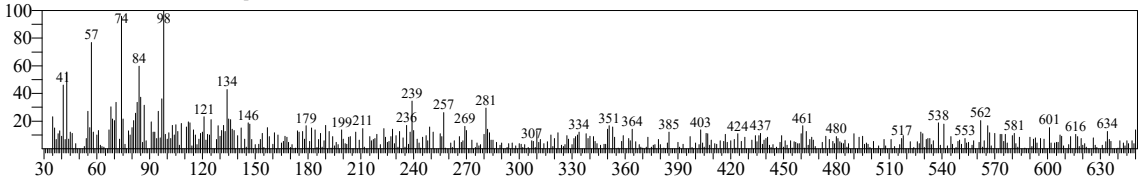


Hit#:5 Entry:178153 Library:NIST20M1.lib
SI:85 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)

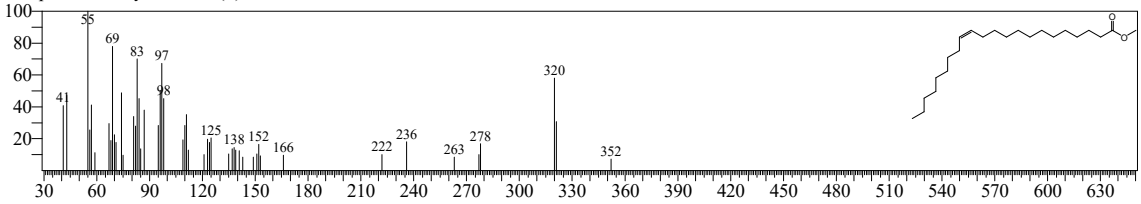


TNAU

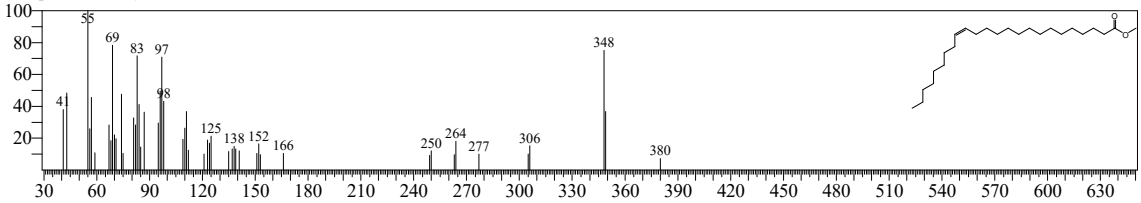
<< Target >>
Line#:21 R.Time:39.495(Scan#:6900) MassPeaks:441
RawMode:Averaged 39.490-39.500(6899-6901) BasePeak:98.00(241)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



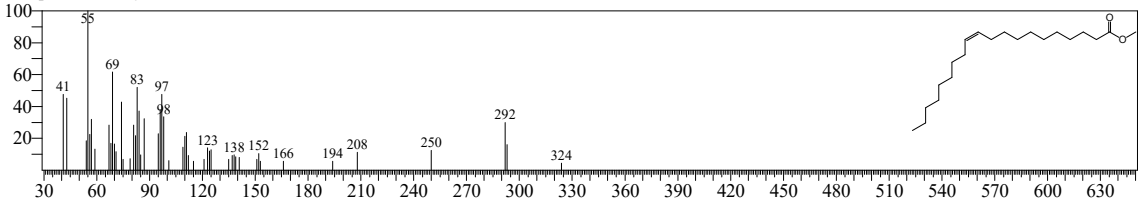
Hit#:1 Entry:30 Library:FA_ME_SP2560_EI_V3.lib
SI:56 Formula:C23H44O2 CAS:112-86-7 MolWeight:352 RetIndex:3070
CompName:Methyl erucate ; (Z)-docos-13-enoic acid



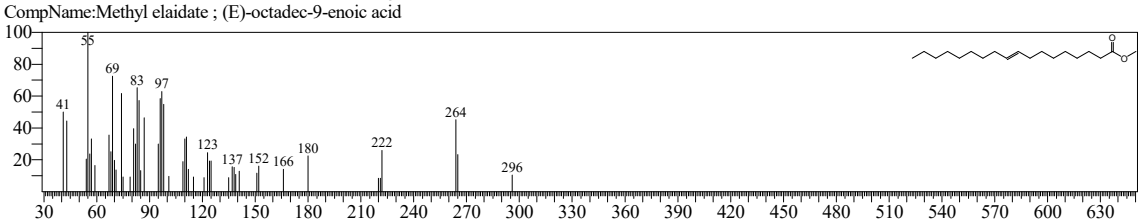
Hit#:2 Entry:37 Library:FA_ME_SP2560_EI_V3.lib
SI:55 Formula:C25H48O2 CAS:506-37-6 MolWeight:380 RetIndex:3263
CompName:Methyl nervonate ; Tetracos-15-enoic acid



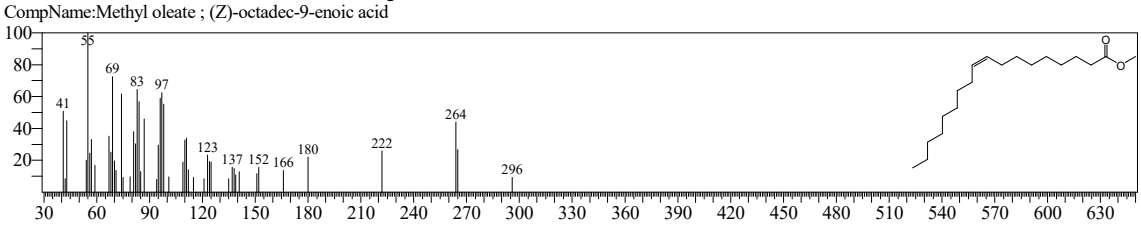
Hit#:3 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
SI:55 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid



Hit#:4 Entry:17 Library:FA_ME_SP2560_EI_V3.lib
SI:55 Formula:C19H36O2 CAS:112-79-8 MolWeight:296 RetIndex:2653
CompName:Methyl elaidate ; (E)-octadec-9-enoic acid

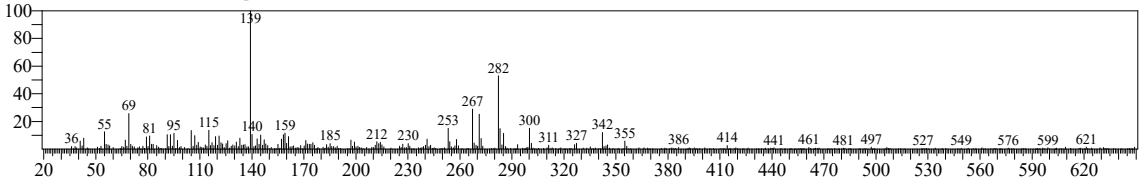


Hit#:5 Entry:18 Library:FA_ME_SP2560_EI_V3.lib
SI:55 Formula:C19H36O2 CAS:112-80-1 MolWeight:296 RetIndex:2675
CompName:Methyl oleate ; (Z)-octadec-9-enoic acid

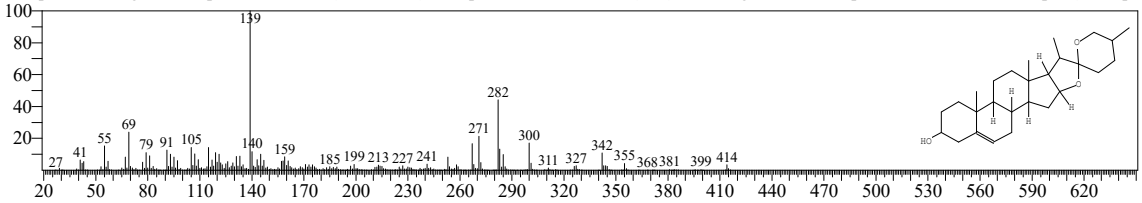


TNAU

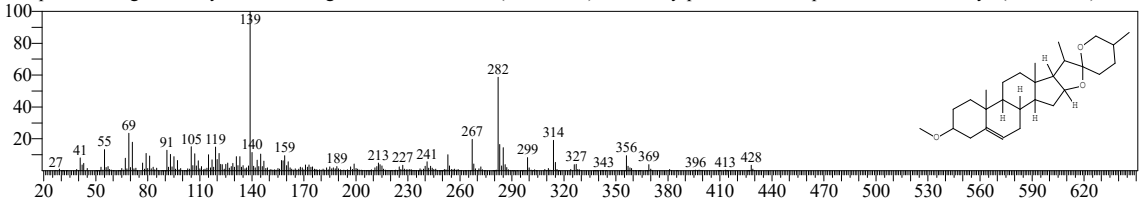
<< Target >>
Line#:22 R.Time:45.615(Scan#:8124) MassPeaks:390
RawMode:Averaged 45.610-45.620(8123-8125) BasePeak:139.10(2681)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



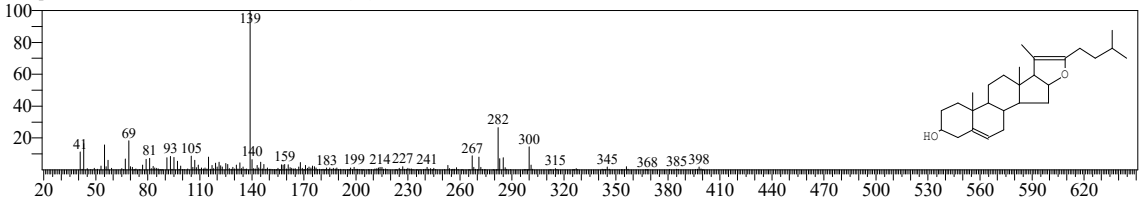
Hit#:1 Entry:8297 Library:NIST20M2.lib
SI:89 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-napl



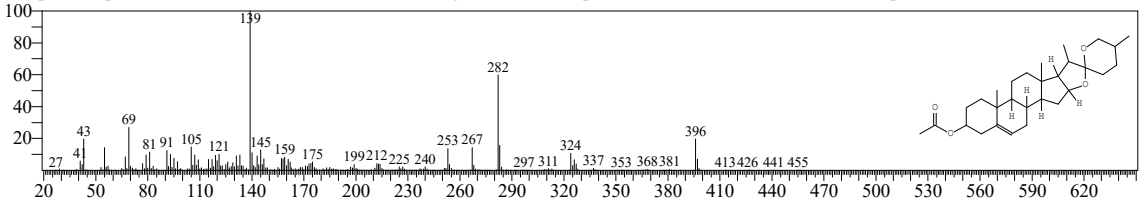
Hit#:2 Entry:14852 Library:NIST20M2.lib
SI:81 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-



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



Hit#:4 Entry:24878 Library:NIST20M2.lib
SI:80 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (2



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