TNAU

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022036.qgd

Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	5.143	1466244	28.96	250900	19.46	5.84	98	Pyridine
2	8.927	51171	1.01	18493	1.43	2.77	81	1-Butanol, 3-methyl-, acetate
3	9.766	40390	0.80	18038	1.40	2.24	94	Pentasiloxane, dodecamethyl-
4	12.492	278234	5.49	110000	8.53	2.53	73	2,5-Cyclohexadiene-1,4-dione, dioxime
5	12.820	429474	8.48	162798	12.63	2.64	74	1,3-Benzodioxol-5-ol
6	13.387	900538	17.78	191786	14.88	4.70	53	Methyl cis-13,16-Docosadienate
7	13.568	689915	13.62	152594	11.84	4.52	53	Methyl cis-13,16-Docosadienate
8	13.670	1405	0.03	2745	0.21	0.51	21	Methyl palmitoleate
9	18.113	58179	1.15	13934	1.08	4.18	92	D-Allose
10	18.495	30629	0.60	11310	0.88	2.71	90	2,4-Di-tert-butylphenol
11	20.371	51590	1.02	12518	0.97	4.12	80	1,6-Anhydro-.alpha.-d-galactofuranose
12	28.294	213955	4.23	82508	6.40	2.59	95	n-Hexadecanoic acid
13	31.473	126405	2.50	45409	3.52	2.78	95	9,12-Octadecadienoic acid (Z,Z)-
14	31.581	103547	2.04	33741	2.62	3.07	88	cis-9-Hexadecenal
15	32.028	45661	0.90	16742	1.30	2.73	94	Octadecanoic acid
16	41.588	35853	0.71	11604	0.90	3.09	84	Tetracosamethyl-cyclododecasiloxane
17	43.793	20879	0.41	8755	0.68	2.38	80	Tetracosamethyl-cyclododecasiloxane
18	44.163	16512	0.33	8032	0.62	2.06	81	13-Docosenamide, (Z)-
19	45.585	237265	4.69	67202	5.21	3.53	82	Diosgenin
20	45.615	223803	4.42	57963	4.50	3.86	27	Urocanic acid-2TMS
21	45.768	42176	0.83	12097	0.94	3.49	81	Tetracosamethyl-cyclododecasiloxane
		5063825	100.00	1289169	100.00			

TNAU
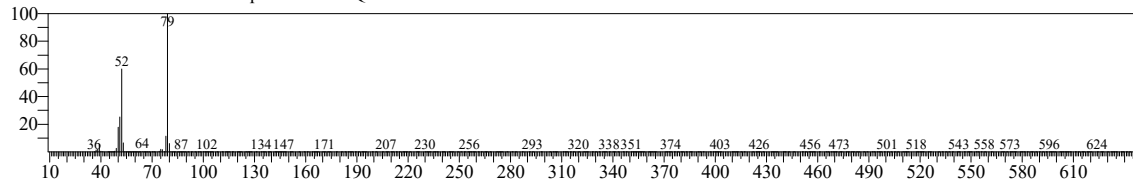
<< Target >>
Line#:1   R.Time:5.145(Scan#:30)   MassPeaks:346
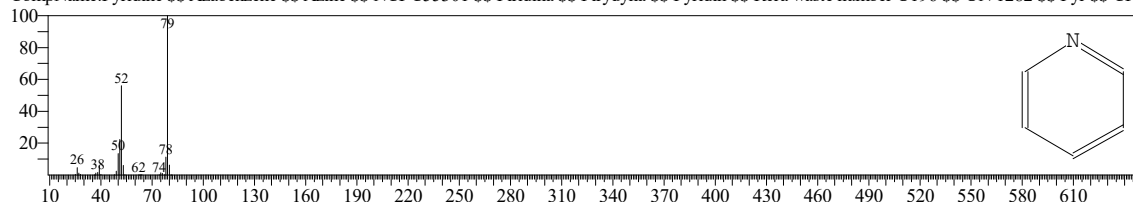RawMode:Averaged 5.140-5.150(29-31) BasePeak:79.05(104995)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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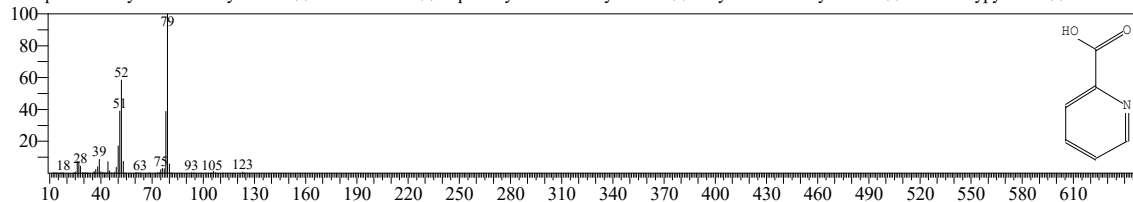SI:98 Formula:C5H5N CAS:110-86-1 MolWeight:79 RetIndex:674
CompName:Pyridine $$ Azabenzene $$ Azine $$ NCI-C55301 $$ Piridina $$ Pirydyna $$ Pyridin $$ Rcra waste number U196 $$ UN 1282 $$ Pyr $$ CP

Hit#:2   Entry:6149 Library:NIST20M1.lib
SI:93 Formula:C6H5NO2 CAS:98-98-6 MolWeight:123 RetIndex:1144
CompName:2-Pyridinecarboxylic acid $$ Picolinic acid $$ .alpha.-Pyridinecarboxylic acid $$ o-Pyridinecarboxylic acid $$ 2-Carboxypyridine $$ 2-Picolini

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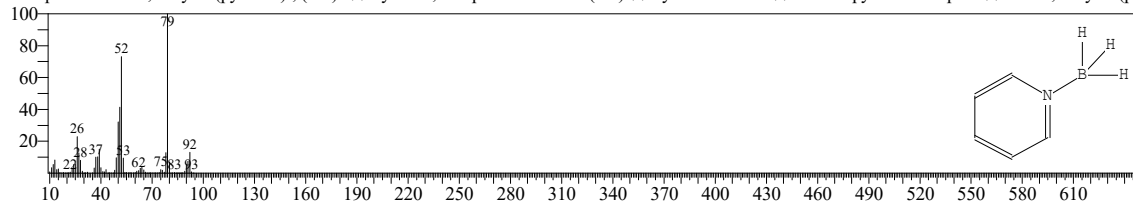SI:91 Formula:C6H5NO CAS:1121-60-4 MolWeight:107 RetIndex:976
CompName:2-Pyridinecarboxaldehyde $$ Picolinaldehyde $$ 2-Pyridinealdehyde $$ Pyridine-2-carboxaldehyde $$ Pyridine-2-aldehyde $$ 2-Pyridylaldehy

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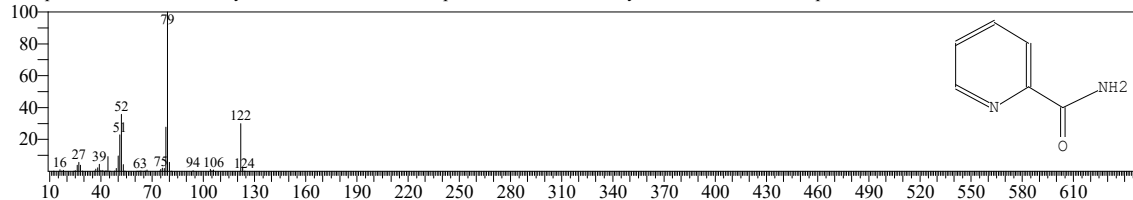SI:86 Formula:C5H8BN CAS:110-51-0 MolWeight:93 RetIndex:0
CompName:Boron, trihydro(pyridine)-, (T-4)- $$ Pyridine, compd. with borane (1:1) $$ Pyridine borane $$ Borane-pyridine complex $$ Boron, trihydro(py

Hit#:5   Entry:5194 Library:NIST20R.lib
SI:86 Formula:C6H6N2O CAS:1452-77-3 MolWeight:122 RetIndex:1197
CompName:Picolinamide $$ Pyridine-2-carboxamide $$ .alpha.-Picolinamide $$ 2-Pyridinecarboxamide $$ .alpha.-Picolinic acid amide $$ Picolinic acid an

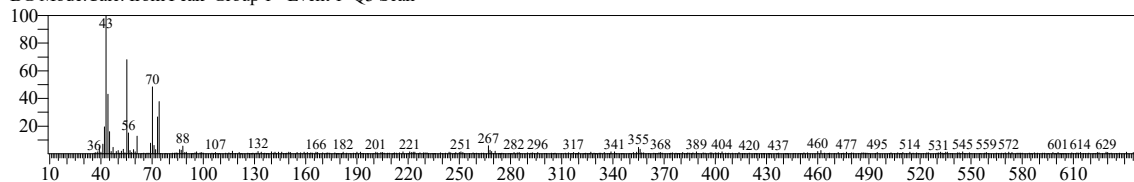# TNAU

<< Target >>
Line#:2 R.Time:8.925(Scan#:786) MassPeaks:383
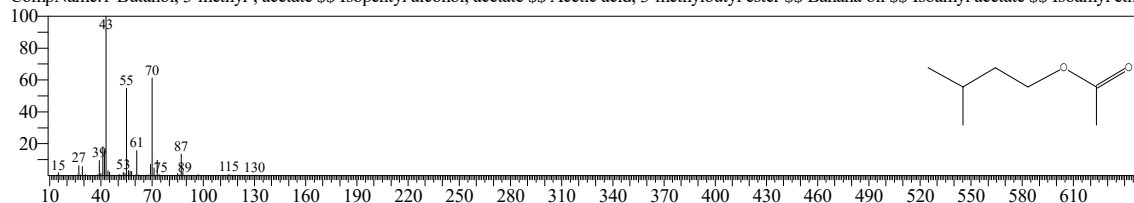RawMode:Averaged 8.920-8.930(785-787) BasePeak:43.00(3049)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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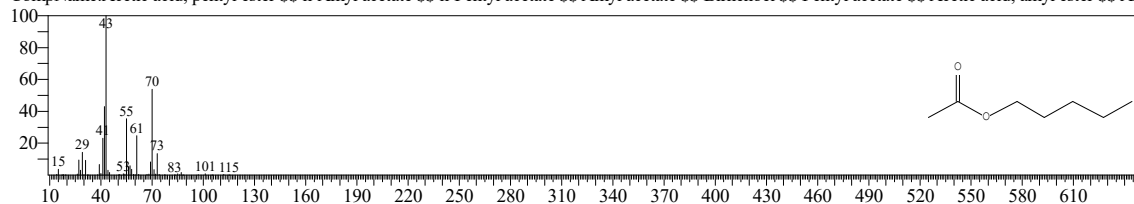SI:81 Formula:C7H14O2 CAS:123-92-2 MolWeight:130 RetIndex:820
CompName:1-Butanol, 3-methyl-, acetate $$ Isopentyl alcohol, acetate $$ Acetic acid, 3-methylbutyl ester $$ Banana oil $$ Isoamyl acetate $$ Isoamyl etha

Hit#:2 Entry:8685 Library:NIST20M1.lib
SI:79 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:5225 Library:NIST20M1.lib
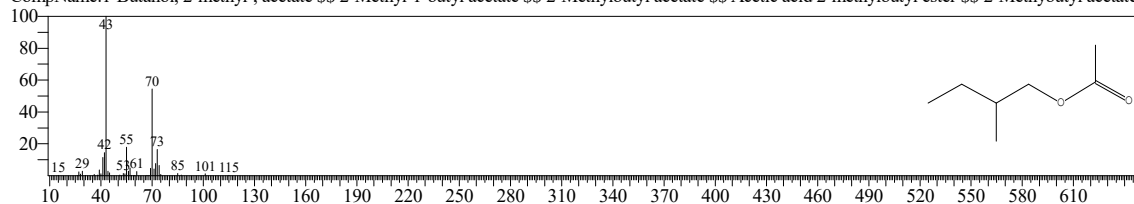SI:78 Formula:C4H6O4 CAS:17675-99-9 MolWeight:118 RetIndex:1201
CompName:2-Furanone, 3,4-dihydroxytetrahydro $$ 3,4-Dihydroxydihydro-2(3H)-furanone #

Hit#:4 Entry:6819 Library:NIST20R.lib
SI:77 Formula:C7H14O2 CAS:624-41-9 MolWeight:130 RetIndex:820
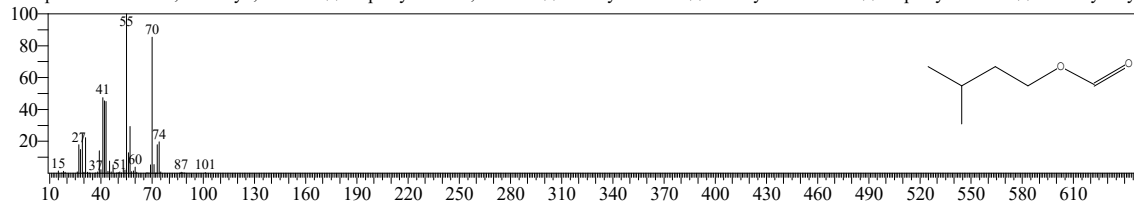CompName:1-Butanol, 2-methyl-, acetate $$ 2-Methyl-1-butyl acetate $$ 2-Methylbutyl acetate $$ Acetic acid 2-methylbutyl ester $$ 2-Methybutyl acetate

Hit#:5 Entry:4411 Library:NIST20R.lib
SI:77 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
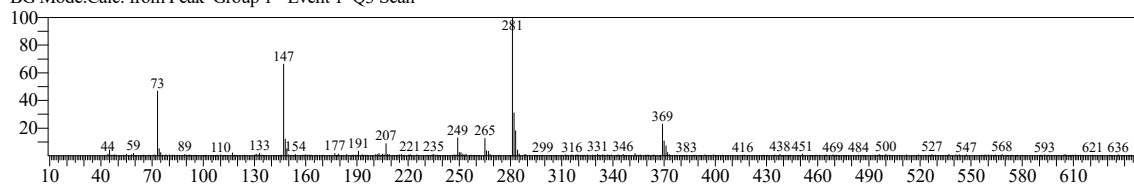
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<< Target >>
Line#:3   R.Time:9.765(Scan#:954) MassPeaks:337
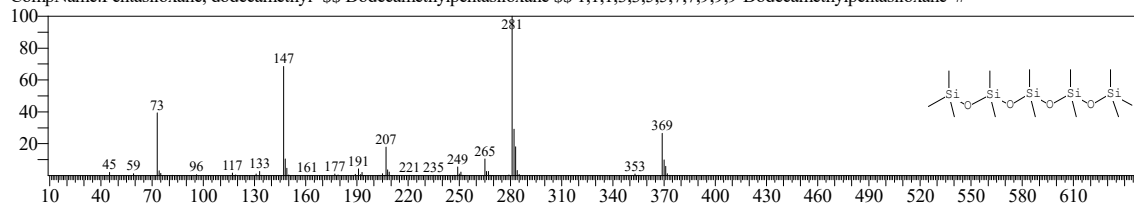RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(3905)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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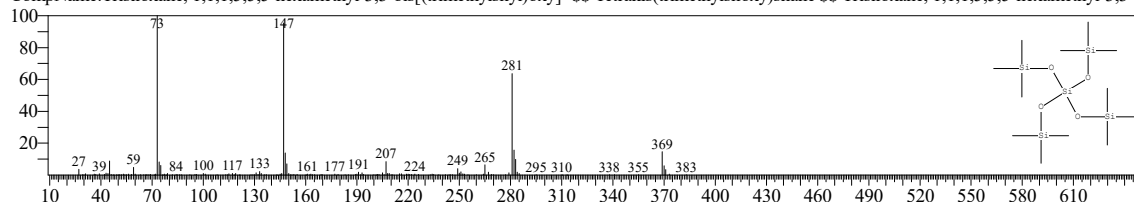SI:94 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #

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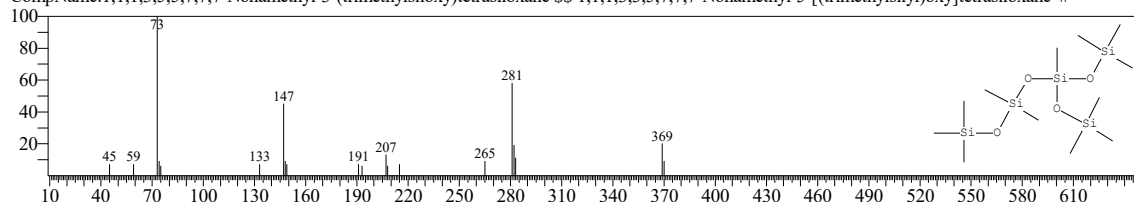SI:81 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-

Hit#:4 Entry:249271 Library:NIST20M1.lib
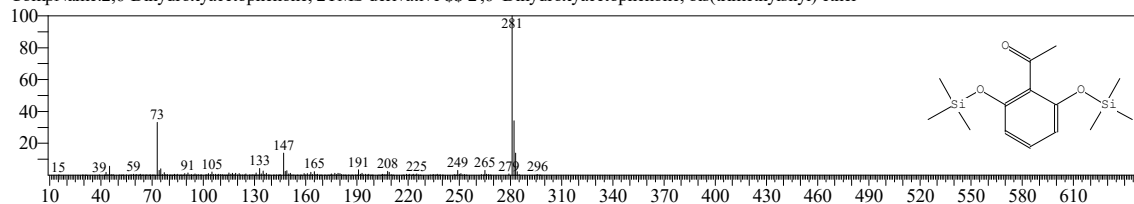SI:78 Formula:C12H36O4Si5 CAS:38146-99-5 MolWeight:384 RetIndex:1068
CompName:1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane $$ 1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

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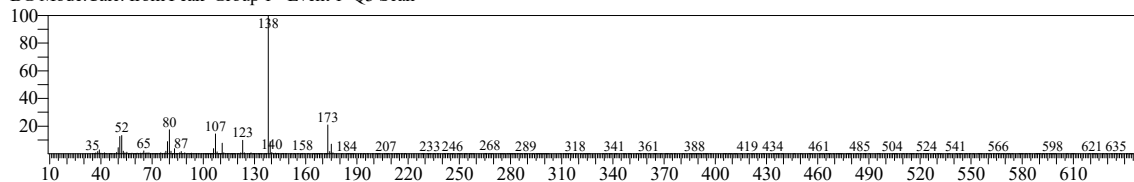
TNAU

<< Target >>
Line#:4 R.Time:12.490(Scan#:1499) MassPeaks:347
RawMode:Averaged 12.485-12.495(1498-1500) BasePeak:138.05(39195)
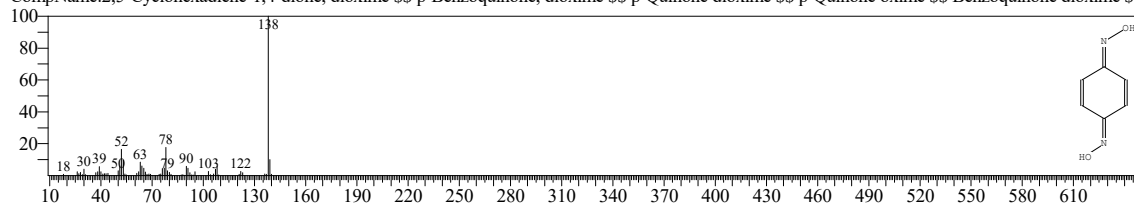BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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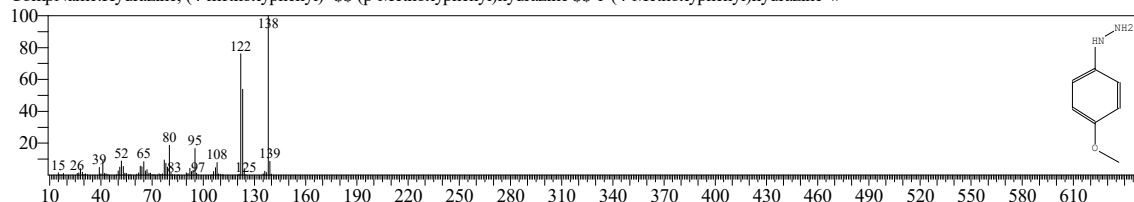CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

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

Hit#:3 Entry:25 Library:FA_ME_SP2560_EI_V3.lib
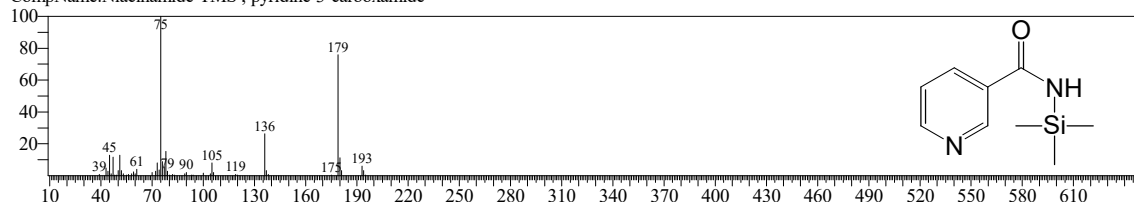SI:33 Formula:C19H32O2 CAS:463-40-1 MolWeight:292 RetIndex:2892
CompName:Methyl linolenate ; (9Z,12Z,15Z)-octadeca-9,12,15-trienoic acid

Hit#:4 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:32 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
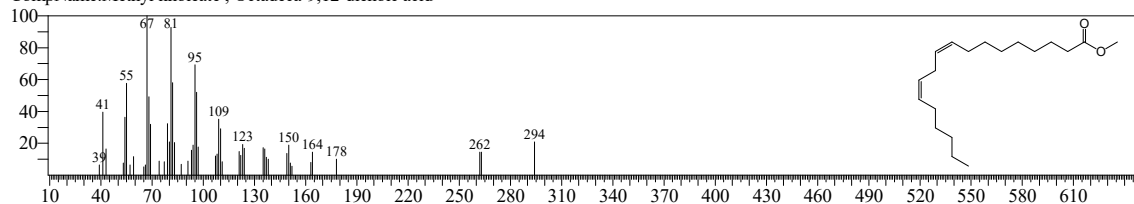CompName:Niacinamide-TMS ; pyridine-3-carboxamide

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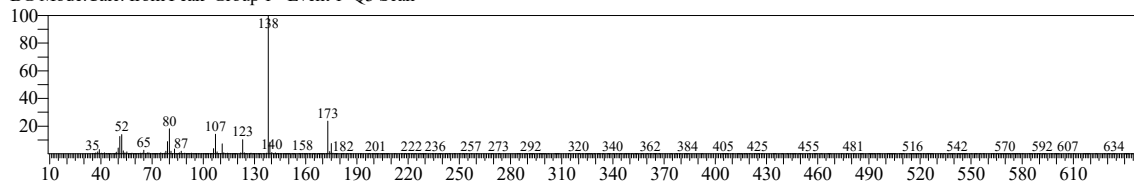CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

TNAU

<< Target >>
Line#:5   R.Time:12.820(Scan#:1565) MassPeaks:339
RawMode:Averaged 12.815-12.825(1564-1566) BasePeak:138.05(56897)
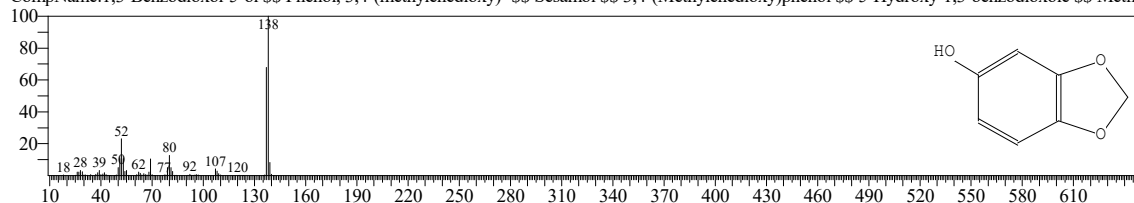BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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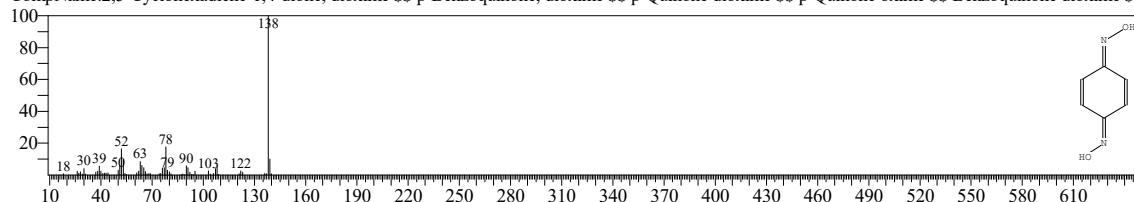SI:74 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy

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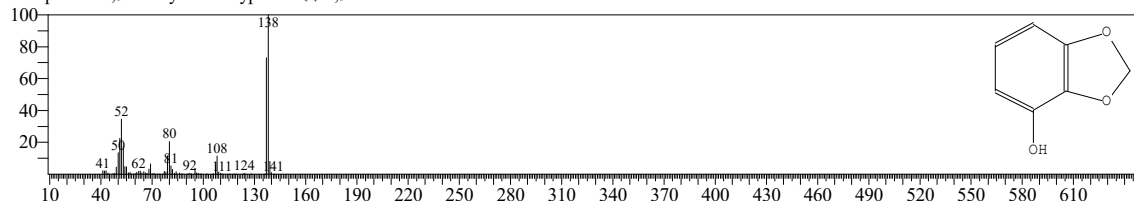SI:73 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$

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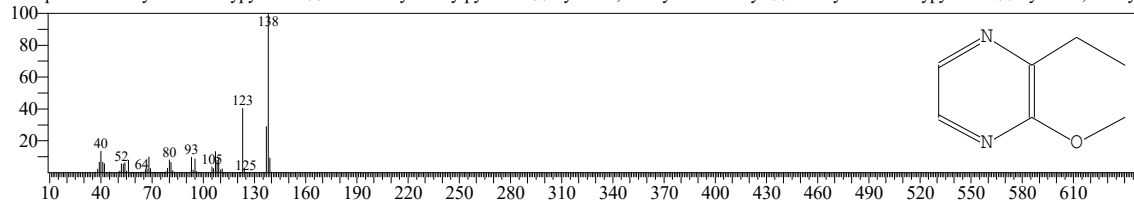SI:72 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #

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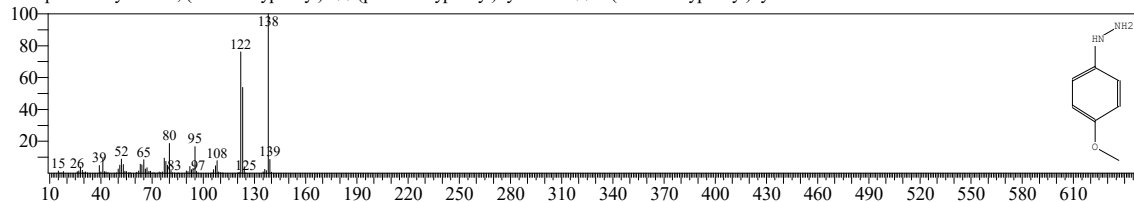SI:71 Formula:C7H10N2O CAS:25680-58-4 MolWeight:138 RetIndex:1070
CompName:2-Ethyl-3-methoxypyrazine $$ 2-Methoxy-3-ethylpyrazine $$ Pyrazine, 2-ethyl-3-methoxy- $$ 3-Ethyl-2-methoxypyrazine $$ Pyrazine, 3-ethyl-

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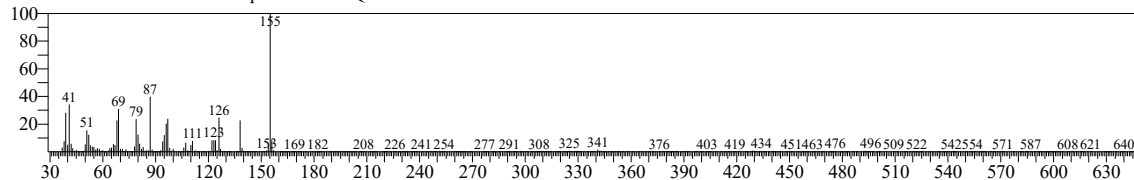
TNAU

<< Target >>
Line#:6　R.Time:13.385(Scan#:1678)　MassPeaks:389
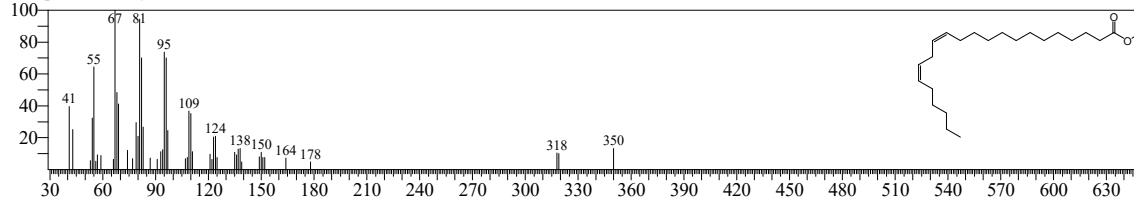RawMode:Averaged 13.380-13.390(1677-1679) BasePeak:155.05(31673)
BG Mode:Calc. from Peak　Group 1 - Event 1　Q3 Scan

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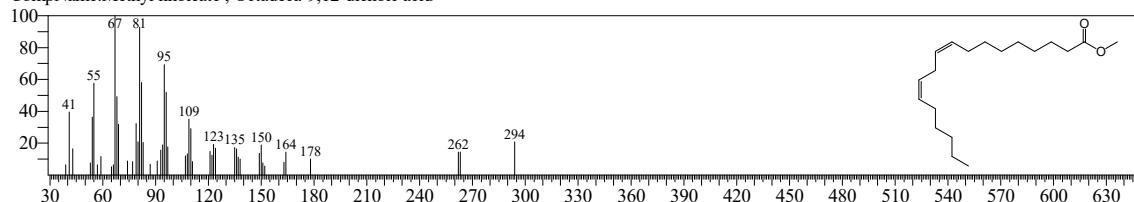SI:53　Formula:C23H42O2　CAS:7370-49-2　MolWeight:350　RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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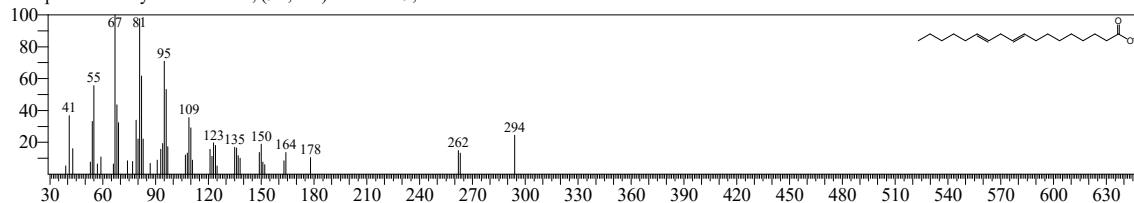SI:52　Formula:C19H34O2　CAS:60-33-3　MolWeight:294　RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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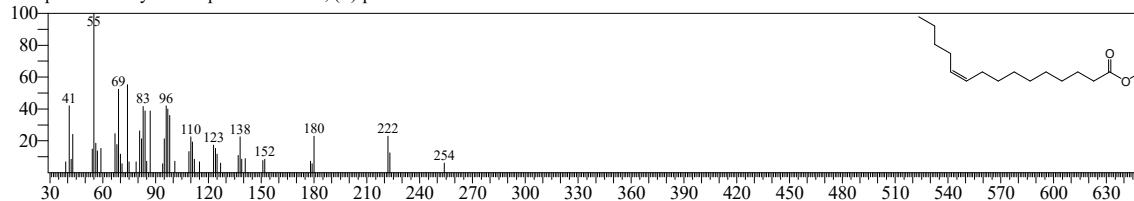SI:51　Formula:C19H34O2　CAS:506-21-8　MolWeight:294　RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

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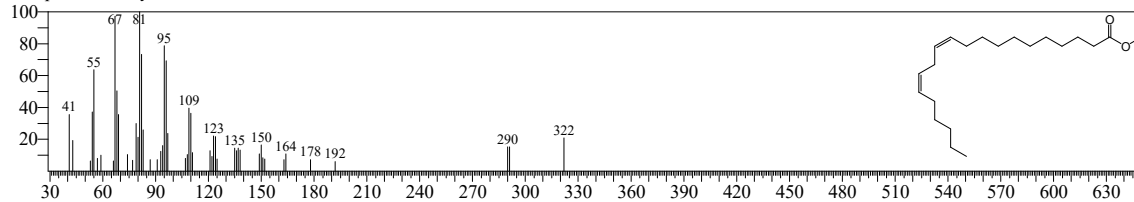SI:51　Formula:C16H30O2　CAS:84743-29-3　MolWeight:254　RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

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
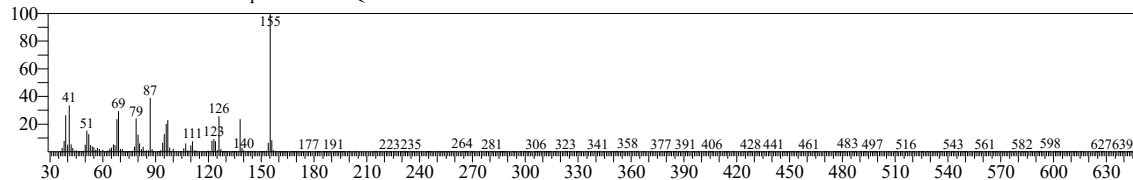
TNAU

<< Target >>
Line#:7 R.Time:13.570(Scan#:1715) MassPeaks:367
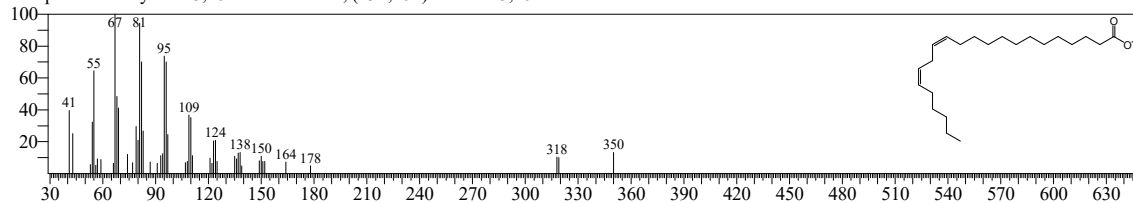RawMode:Averaged 13.565-13.575(1714-1716) BasePeak:155.05(25684)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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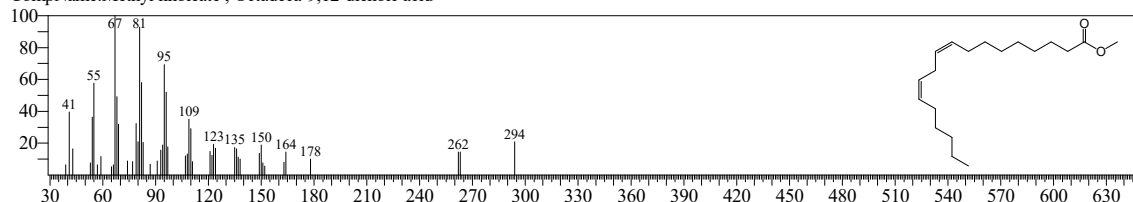SI:53 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

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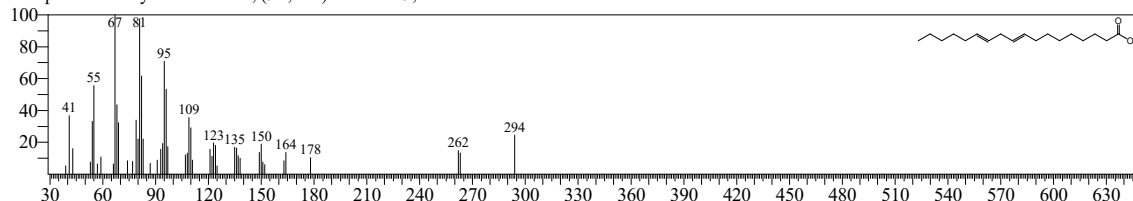SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid

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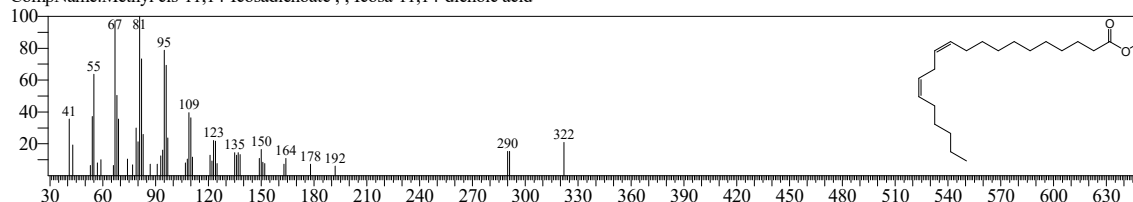CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid

Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
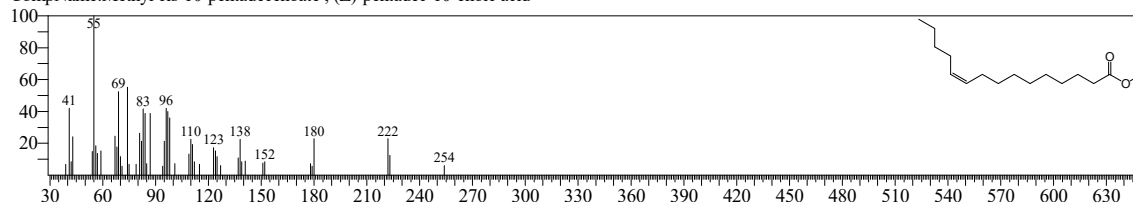SI:51 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

Hit#:5 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
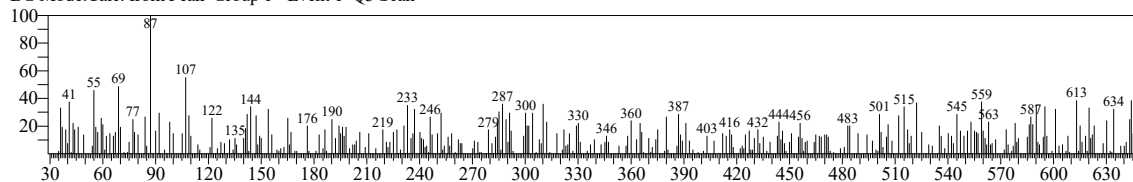
TNAU

<< Target >>
Line#:8 R.Time:13.670(Scan#:1735) MassPeaks:333
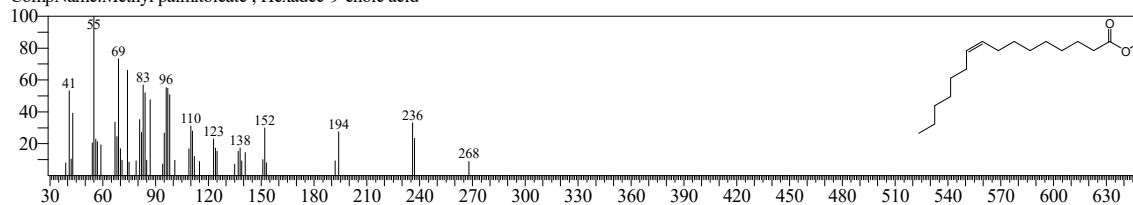RawMode:Averaged 13.665-13.675(1734-1736) BasePeak:87.10(109)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:13 Library:FA_ME_SP2560_EI_V3.lib
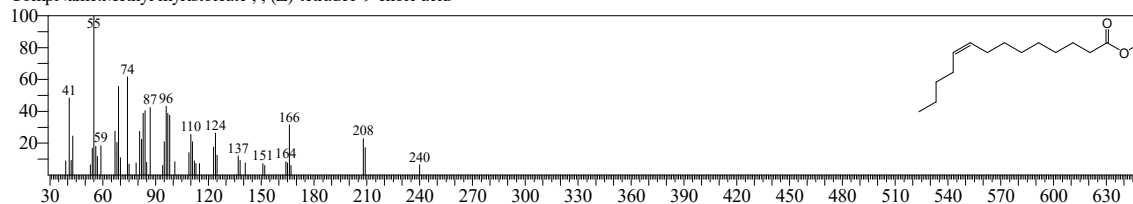SI:21 Formula:C17H32O2 CAS:373-49-9 MolWeight:268 RetIndex:2478
CompName:Methyl palmitoleate ; Hexadec-9-enoic acid

Hit#:2 Entry:9 Library:FA_ME_SP2560_EI_V3.lib
SI:21 Formula:C15H28O2 CAS:544-64-9 MolWeight:240 RetIndex:2283
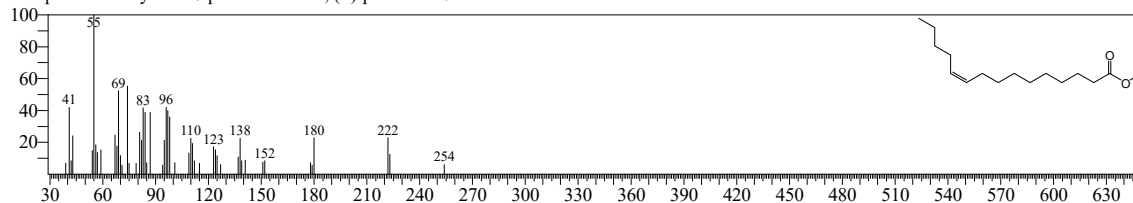CompName:Methyl myristoleate ; ; (Z)-tetradec-9-enoic acid

Hit#:3 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:20 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
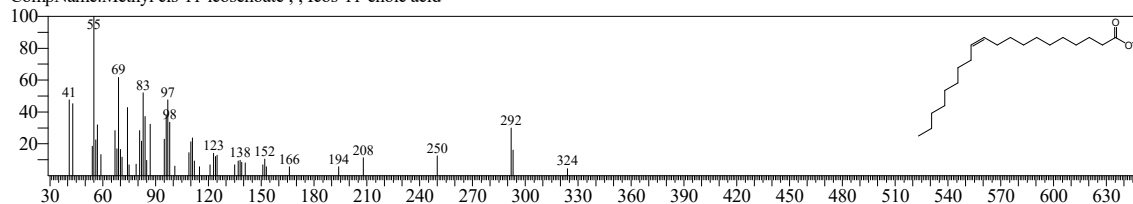CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

Hit#:4 Entry:24 Library:FA_ME_SP2560_EI_V3.lib
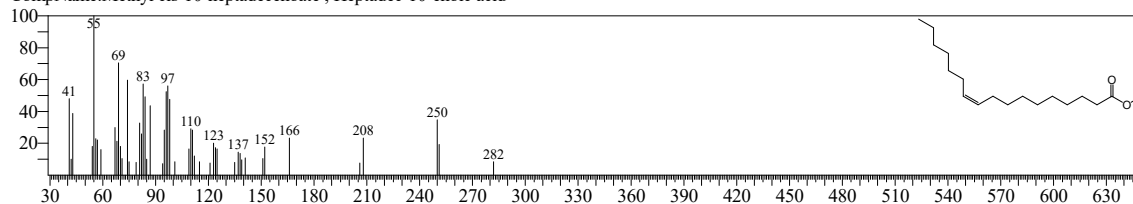SI:20 Formula:C21H40O2 CAS:5561-99-9 MolWeight:324 RetIndex:2874
CompName:Methyl cis-11-icosenoate ; ; Icos-11-enoic acid

Hit#:5 Entry:15 Library:FA_ME_SP2560_EI_V3.lib
SI:19 Formula:C18H34O2 CAS:29743-97-3 MolWeight:282 RetIndex:2581
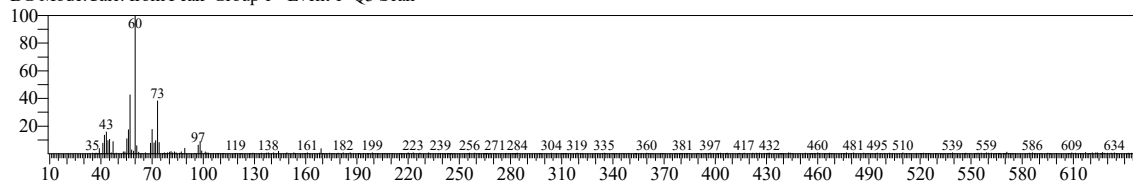CompName:Methyl cis-10-heptadecenoate ; Heptadec-10-enoic acid

TNAU

<< Target >>
Line#:9 R.Time:18.115(Scan#:2624) MassPeaks:283
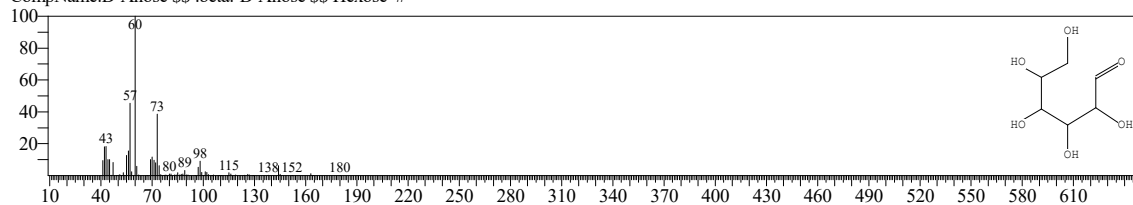RawMode:Averaged 18.110-18.120(2623-2625) BasePeak:60.05(4083)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:36240 Library:NIST20M1.lib
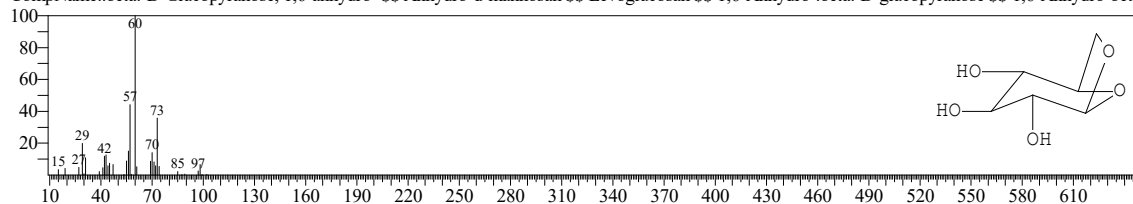SI:92 Formula:C6H12O6 CAS:2595-97-3 MolWeight:180 RetIndex:1698
CompName:D-Allose $$ .beta.-D-Allose $$ Hexose #

Hit#:2 Entry:23811 Library:NIST20M1.lib
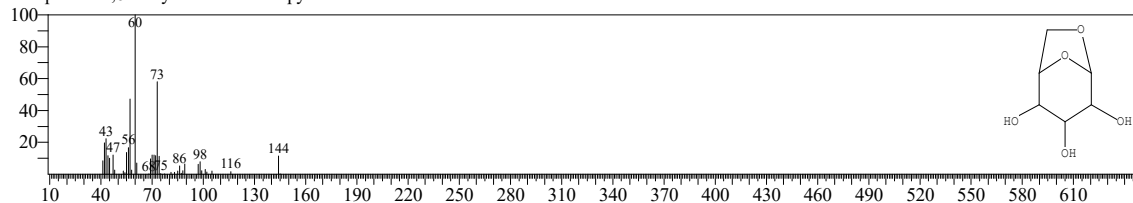SI:92 Formula:C6H10O5 CAS:498-07-7 MolWeight:162 RetIndex:1404
CompName:.beta.-D-Glucopyranose, 1,6-anhydro- $$ Anhydro-d-mannosan $$ Levoglucosan $$ 1,6-Anhydro-.beta.-D-glucopyranose $$ 1,6-Anhydro-beta-

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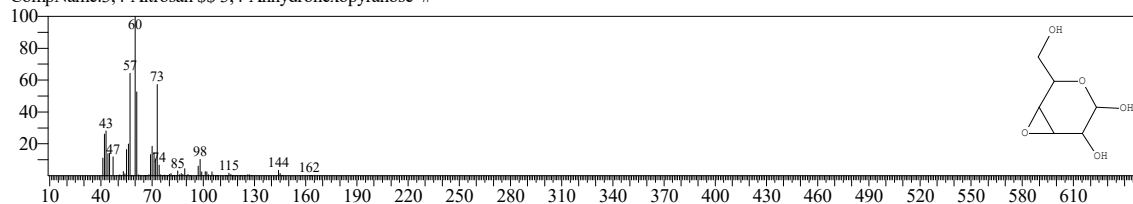CompName:1,6-Anhydro-.beta.-d-talopyranose

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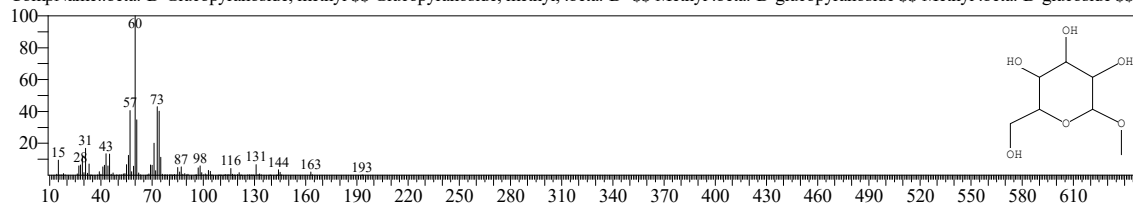SI:87 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1400
CompName:3,4-Altrosan $$ 3,4-Anhydrohexopyranose #

Hit#:5 Entry:47352 Library:NIST20M1.lib
SI:83 Formula:C7H14O6 CAS:709-50-2 MolWeight:194 RetIndex:1714
CompName:.beta.-D-Glucopyranoside, methyl $$ Glucopyranoside, methyl, .beta.-D- $$ Methyl .beta.-D-glucopyranoside $$ Methyl .beta.-D-glucoside $$ 1
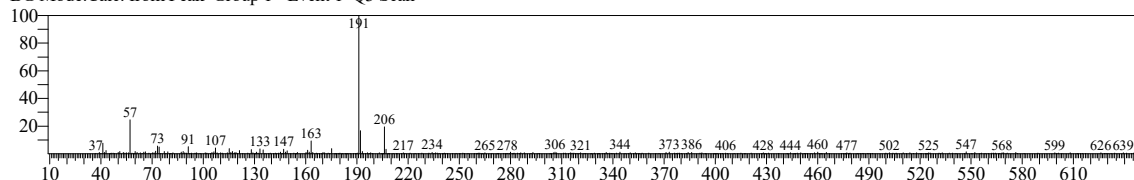
TNAU

<< Target >>
Line#:10 R.Time:18.495(Scan#:2700) MassPeaks:342
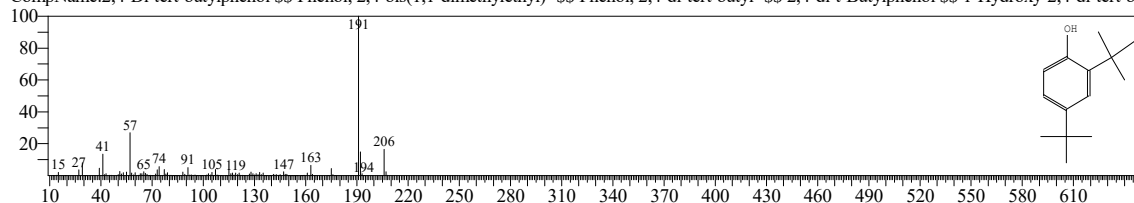RawMode:Averaged 18.490-18.500(2699-2701) BasePeak:191.15(3795)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:24086 Library:NIST20R.lib
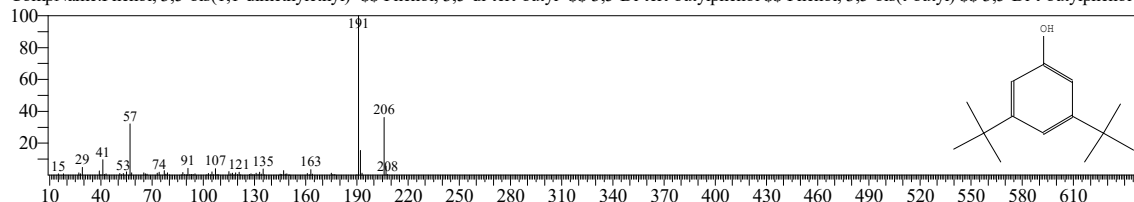SI:90 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555
CompName:2,4-Di-tert-butylphenol $$ Phenol, 2,4-bis(1,1-dimethylethyl)- $$ Phenol, 2,4-di-tert-butyl- $$ 2,4-di-t-Butylphenol $$ 1-Hydroxy-2,4-di-tert-bu

Hit#:2 Entry:24110 Library:NIST20R.lib
SI:88 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
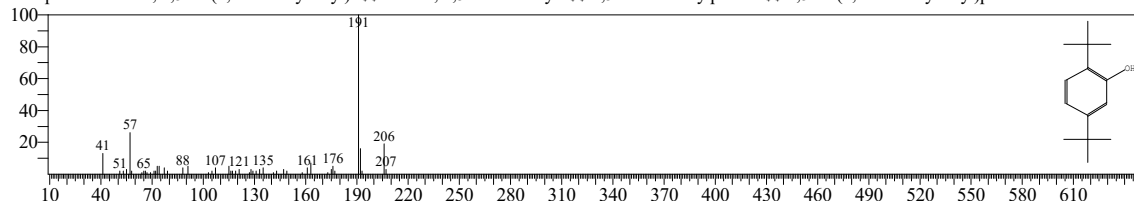CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- $$ Phenol, 3,5-di-tert-butyl- $$ 3,5-Di-tert-butylphenol $$ Phenol, 3,5-bis(t-butyl) $$ 3,5-Di-t-butylphenol $

Hit#:3 Entry:24098 Library:NIST20R.lib
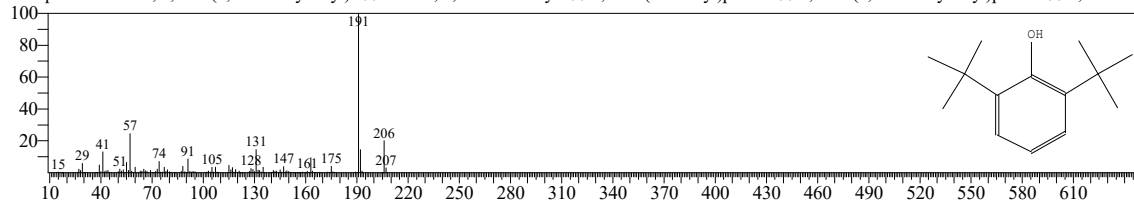SI:88 Formula:C14H22O CAS:5875-45-6 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,5-bis(1,1-dimethylethyl)- $$ Phenol, 2,5-di-tert-butyl- $$ 2,5-Di-tert-butylphenol $$ 2,5-bis(1,1-Dimethylethyl)phenol

Hit#:4 Entry:59031 Library:NIST20M1.lib
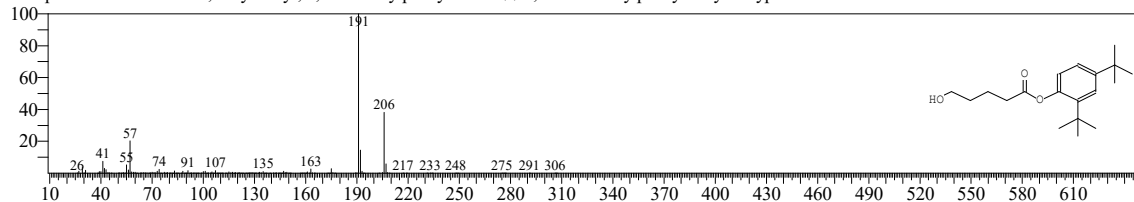SI:87 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- $$ Phenol, 2,6-di-tert-butyl- $$ 2,6-Bis(tert-butyl)phenol $$ 2,6-Bis(1,1-dimethylethyl)phenol $$ 2,6-Di-tert

Hit#:5 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 #
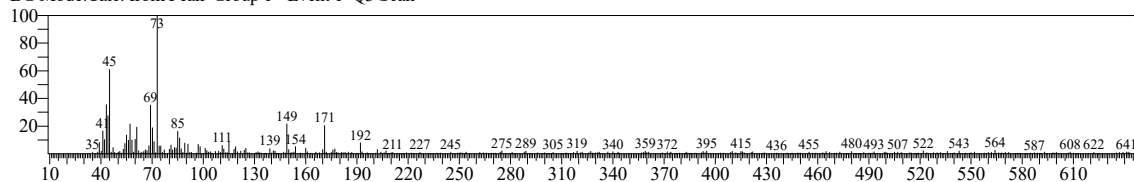
TNAU

<< Target >>
Line#:11 R.Time:20.370(Scan#:3075) MassPeaks:329
RawMode:Averaged 20.365-20.375(3074-3076) BasePeak:73.00(1903)
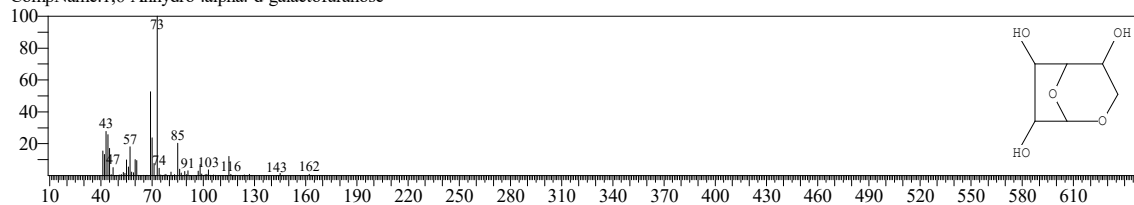BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:23805 Library:NIST20M1.lib
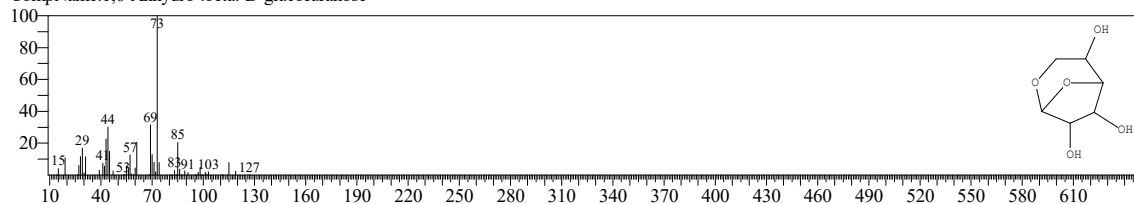SI:80 Formula:C6H10O5 CAS:0-00-0 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.alpha.-d-galactofuranose

Hit#:2 Entry:23804 Library:NIST20M1.lib
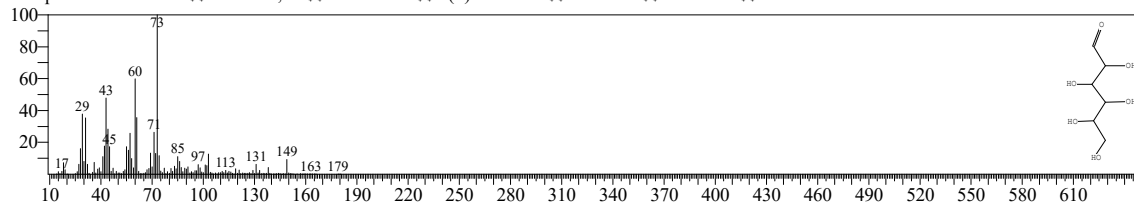SI:79 Formula:C6H10O5 CAS:7425-74-3 MolWeight:162 RetIndex:1404
CompName:1,6-Anhydro-.beta.-D-glucofuranose

Hit#:3 Entry:36239 Library:NIST20M1.lib
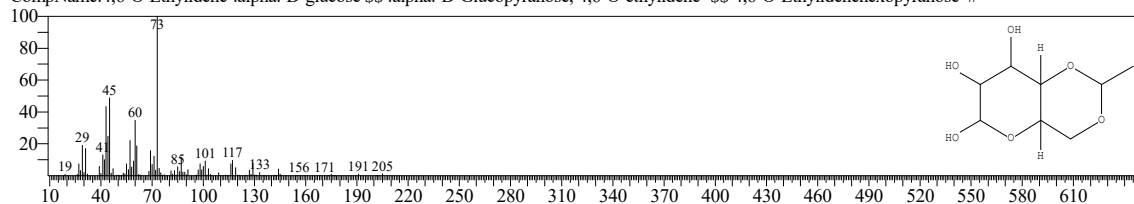SI:77 Formula:C6H12O6 CAS:3458-28-4 MolWeight:180 RetIndex:1698
CompName:d-Mannose $$ Mannose, d- $$ Carubinose $$ d(+)-Mannose $$ Mannose $$ Seminose $$ Hexose #

Hit#:4 Entry:58194 Library:NIST20M1.lib
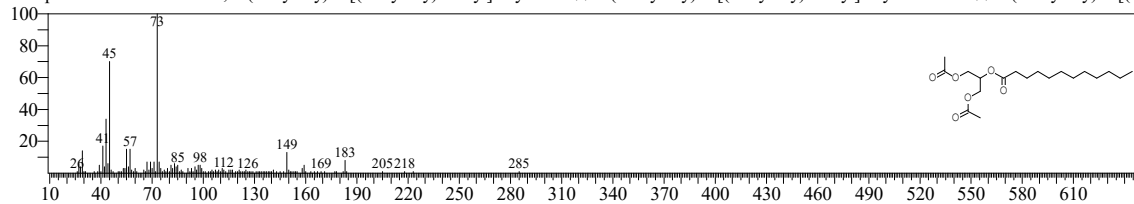SI:77 Formula:C8H14O6 CAS:13224-99-2 MolWeight:206 RetIndex:1694
CompName:4,6-O-Ethylidene-.alpha.-D-glucose $$ .alpha.-D-Glucopyranose, 4,6-O-ethylidene- $$ 4,6-O-Ethylidenehexopyranose #

Hit#:5 Entry:227937 Library:NIST20M1.lib
SI:76 Formula:C19H34O6 CAS:55191-43-0 MolWeight:358 RetIndex:2348
CompName:Dodecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl]ethyl ester $$ 2-(Acetyloxy)-1-[(acetyloxy)methyl]ethyl laurate # $$ 2-(Acetyloxy)-1-[(ac
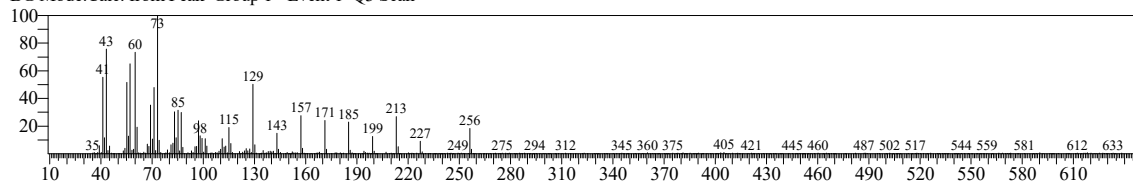
TNAU

<< Target >>
Line#:12 R.Time:28.295(Scan#:4660) MassPeaks:387
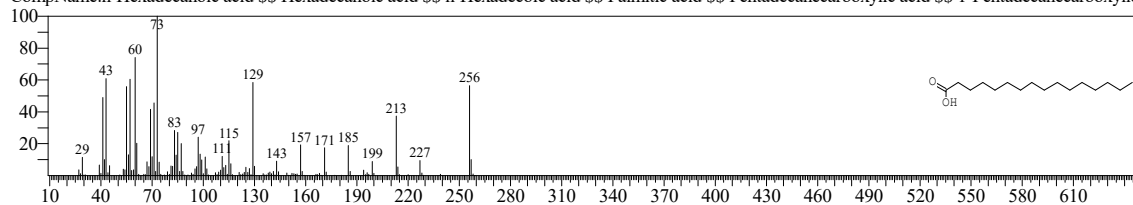RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.05(6780)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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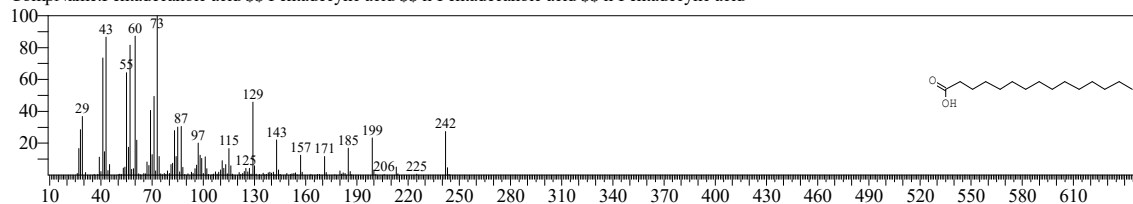SI:95 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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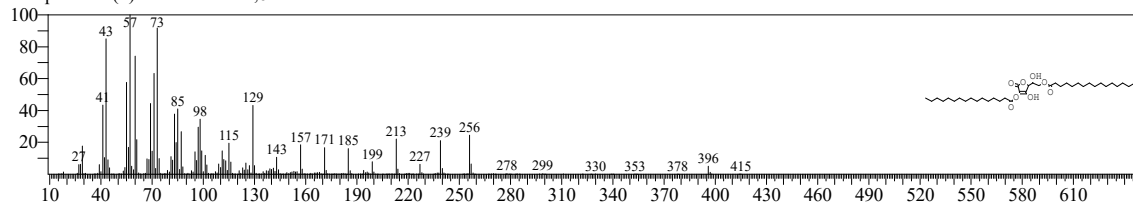SI:92 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

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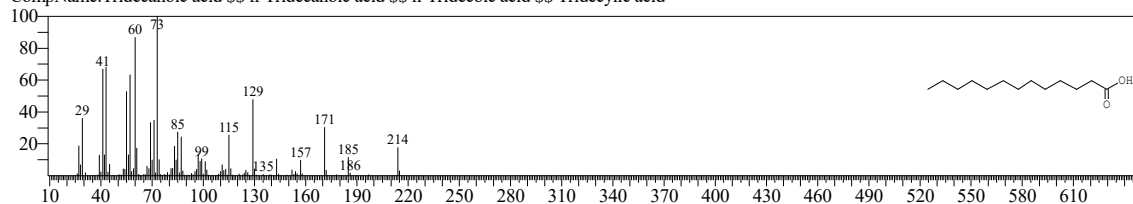CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

Hit#:4 Entry:25643 Library:NIST20R.lib
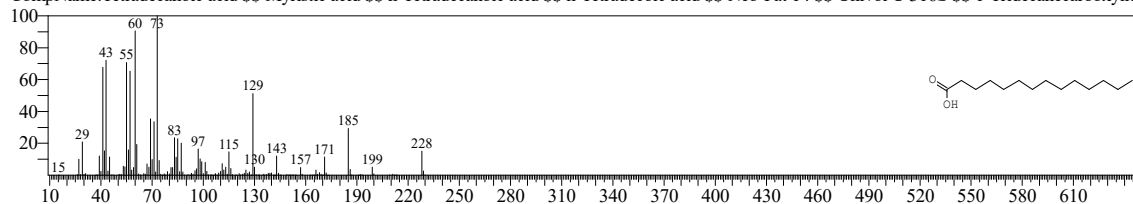SI:91 Formula:C13H26O2 CAS:638-53-9 MolWeight:214 RetIndex:1670
CompName:Tridecanoic acid $$ n-Tridecanoic acid $$ n-Tridecoic acid $$ Tridecylic acid

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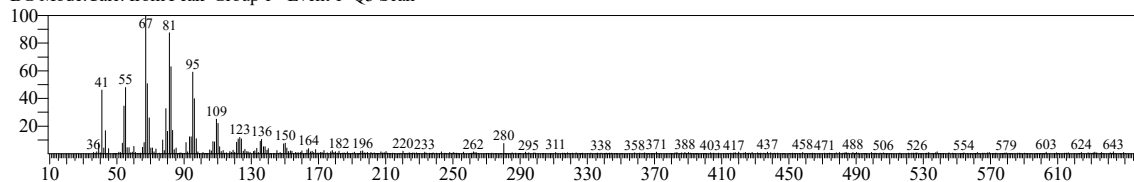
TNAU

<< Target >>
Line#:13 R.Time:31.475(Scan#:5296) MassPeaks:416
RawMode:Averaged 31.470-31.480(5295-5297) BasePeak:67.05(3848)
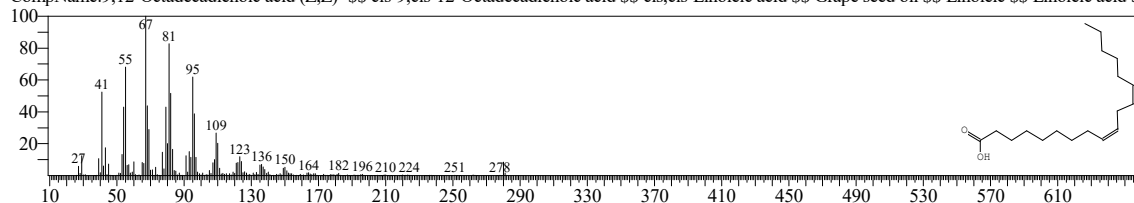BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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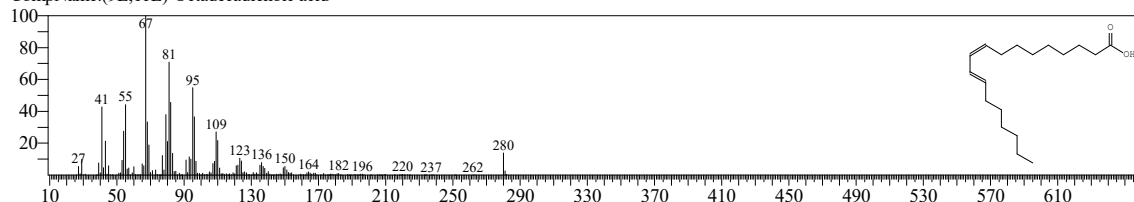SI:95 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $$

Hit#:2 Entry:139651 Library:NIST20M1.lib
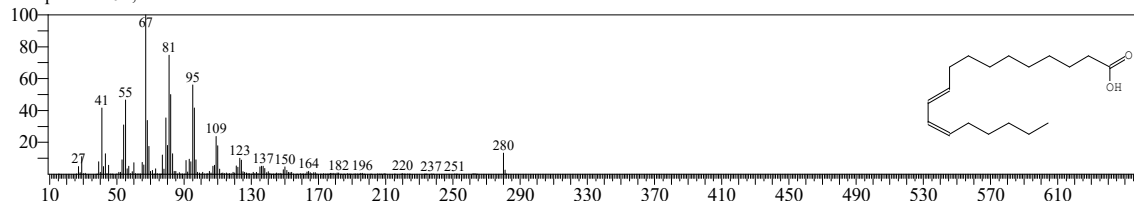SI:95 Formula:C18H32O2 CAS:544-71-8 MolWeight:280 RetIndex:2183
CompName:(9E,11E)-Octadecadienoic acid

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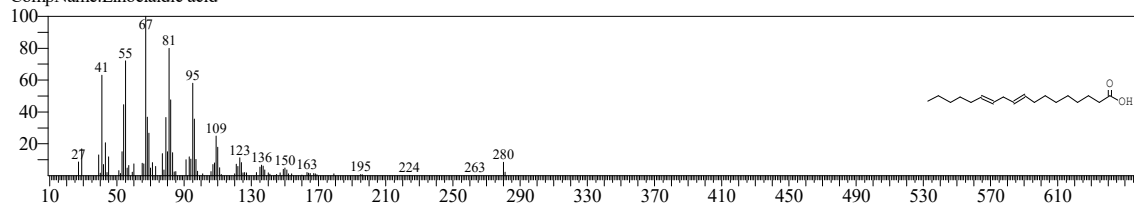SI:94 Formula:C18H32O2 CAS:2420-56-6 MolWeight:280 RetIndex:2183
CompName:10E,12Z-Octadecadienoic acid

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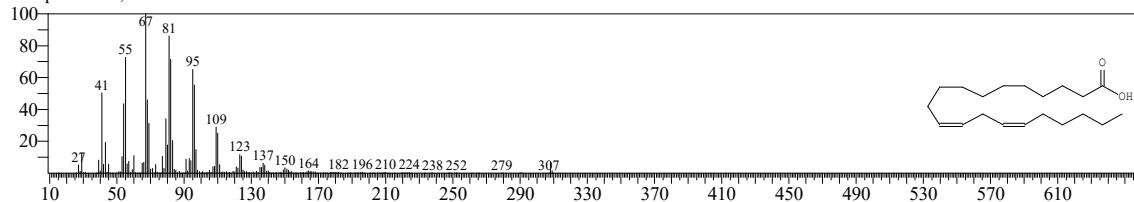SI:94 Formula:C18H32O2 CAS:506-21-8 MolWeight:280 RetIndex:2183
CompName:Linoelaidic acid

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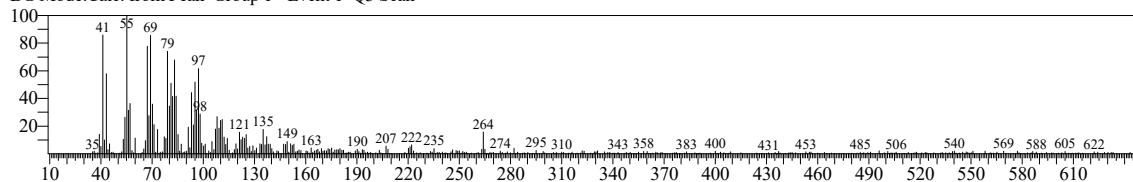CompName:11,14-Eicosadienoic acid

TNAU

<< Target >>
Line#:14 R.Time:31.580(Scan#:5317) MassPeaks:384
RawMode:Averaged 31.575-31.585(5316-5318) BasePeak:55.05(1664)
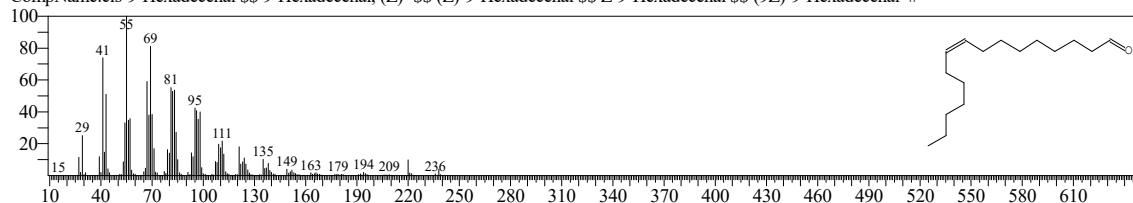BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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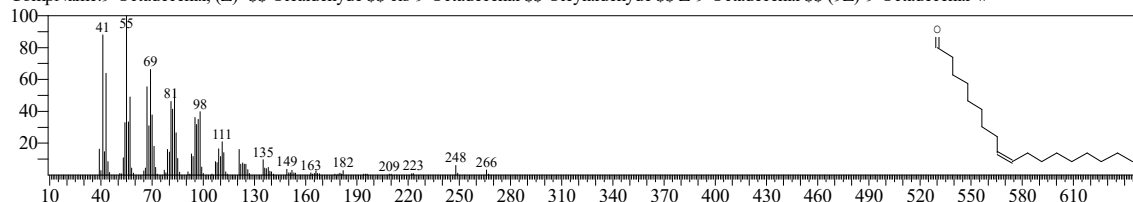SI:88 Formula:C16H30O CAS:56219-04-6 MolWeight:238 RetIndex:1808
CompName:cis-9-Hexadecenal $$ 9-Hexadecenal, (Z)- $$ (Z)-9-Hexadecenal $$ Z-9-Hexadecenal $$ (9Z)-9-Hexadecenal #

Hit#:2 Entry:123421 Library:NIST20M1.lib
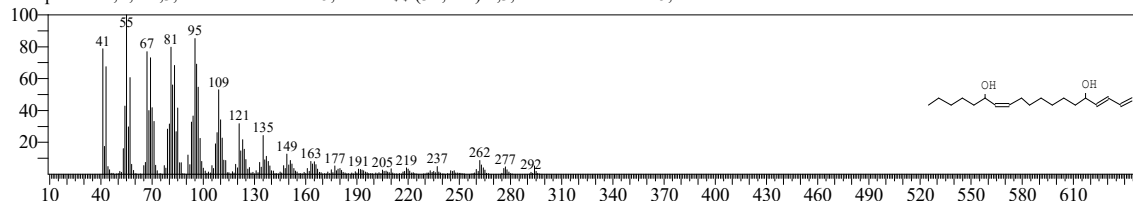SI:87 Formula:C18H34O CAS:2423-10-1 MolWeight:266 RetIndex:2007
CompName:9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal $$ (9Z)-9-Octadecenal #

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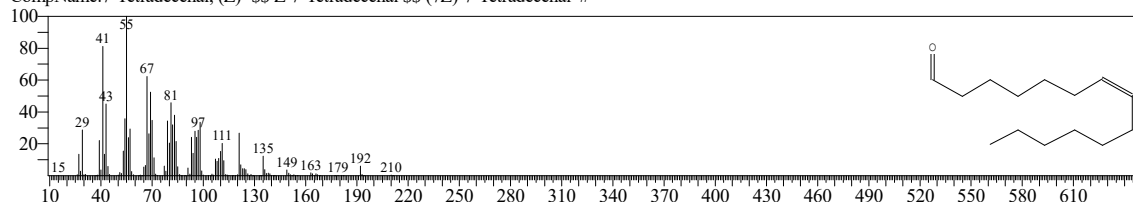SI:87 Formula:C19H34O2 CAS:0-00-0 MolWeight:294 RetIndex:2241
CompName:E,E,Z-1,3,12-Nonadecatriene-5,14-diol $$ (3E,12Z)-1,3,12-Nonadecatriene-5,14-diol #

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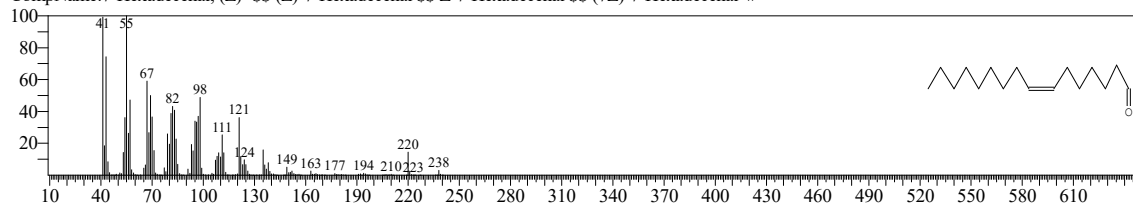SI:87 Formula:C14H26O CAS:65128-96-3 MolWeight:210 RetIndex:1609
CompName:7-Tetradecenal, (Z)- $$ Z-7-Tetradecenal $$ (7Z)-7-Tetradecenal #

Hit#:5 Entry:92227 Library:NIST20M1.lib
SI:86 Formula:C16H30O CAS:56797-40-1 MolWeight:238 RetIndex:1808
CompName:7-Hexadecenal, (Z)- $$ (Z)-7-Hexadecenal $$ Z-7-Hexadecenal $$ (7Z)-7-Hexadecenal #
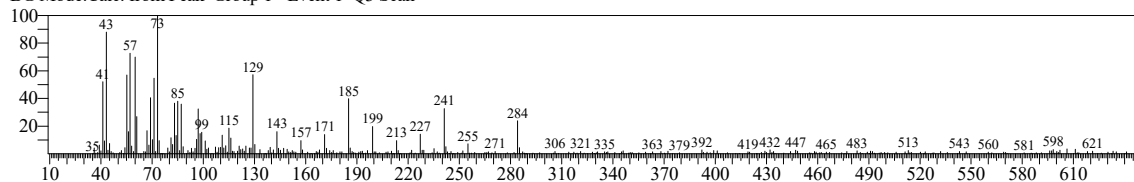
TNAU

<< Target >>
Line#:15 R.Time:32.030(Scan#:5407) MassPeaks:300
RawMode:Averaged 32.025-32.035(5406-5408) BasePeak:73.05(1316)
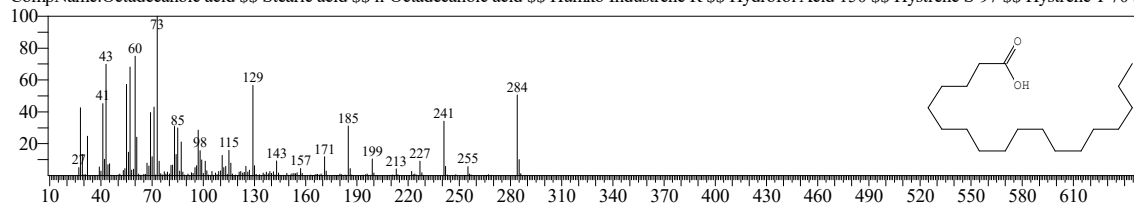BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:34463 Library:NIST20R.lib
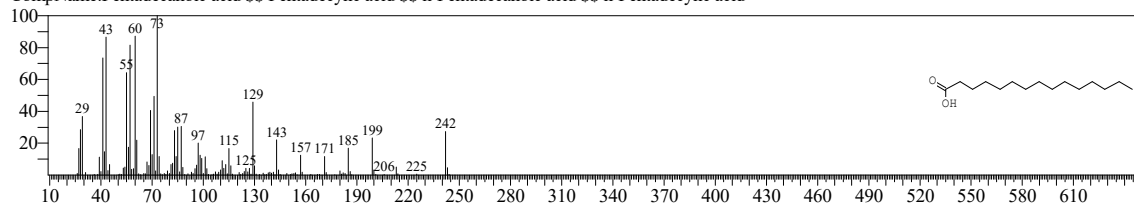SI:94 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $$

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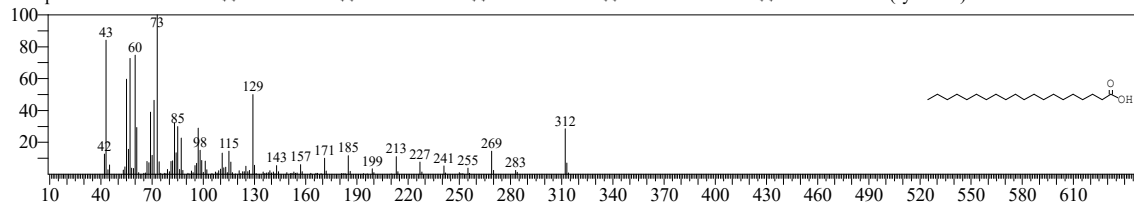SI:90 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid

Hit#:3 Entry:178153 Library:NIST20M1.lib
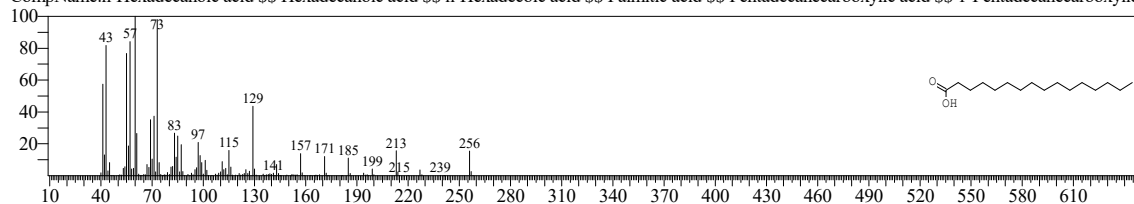SI:88 Formula:C20H40O2 CAS:506-30-9 MolWeight:312 RetIndex:2366
CompName:Eicosanoic acid $$ Arachic acid $$ Arachidic acid $$ Icosanoic acid $$ n-Eicosanoic acid $$ Arachidic acid (synthetic)

Hit#:4 Entry:31599 Library:NIST20R.lib
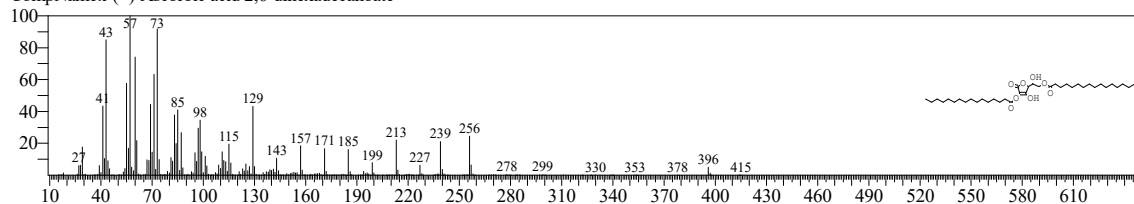SI:87 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic

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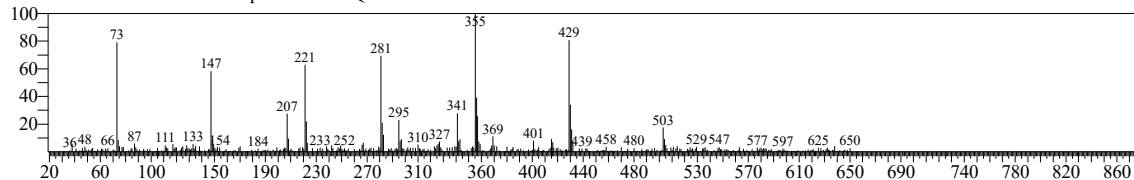CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate

TNAU

<< Target >>
Line#:16 R.Time:41.590(Scan#:7319) MassPeaks:409
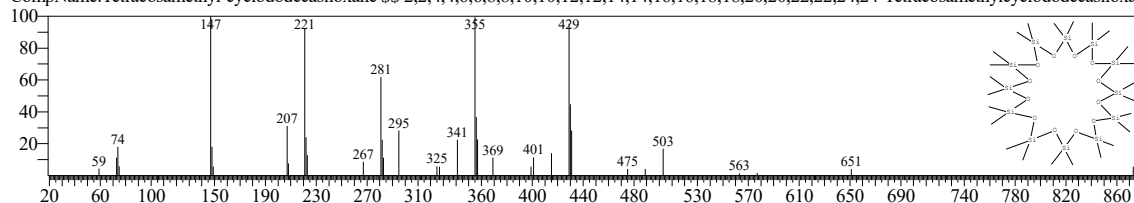RawMode:Averaged 41.585-41.595(7318-7320) BasePeak:355.10(910)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
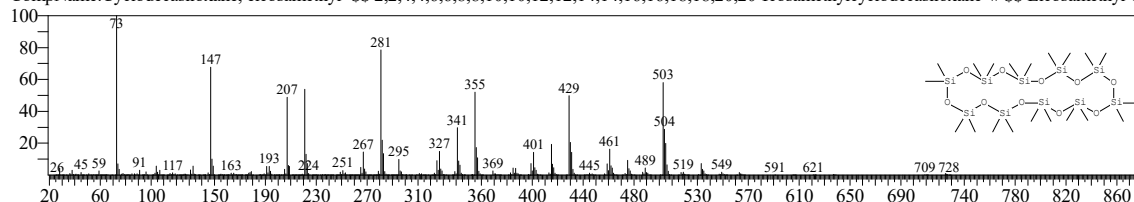SI:84 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

Hit#:2 Entry:45685 Library:NIST20M2.lib
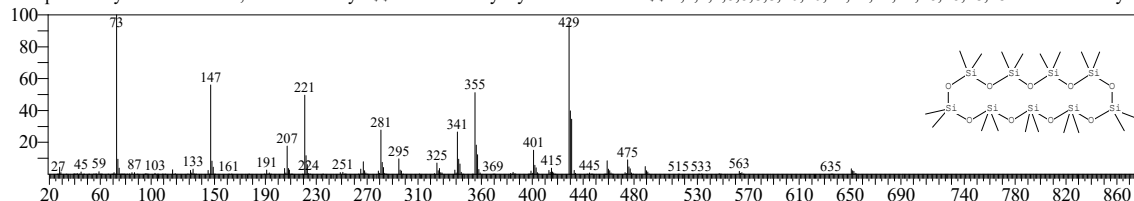SI:80 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:80 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
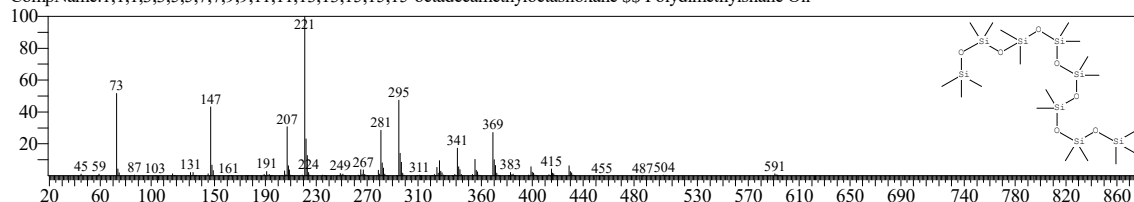CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
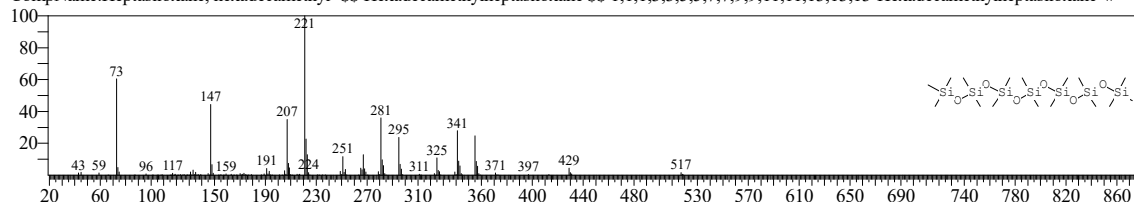SI:73 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:73 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #
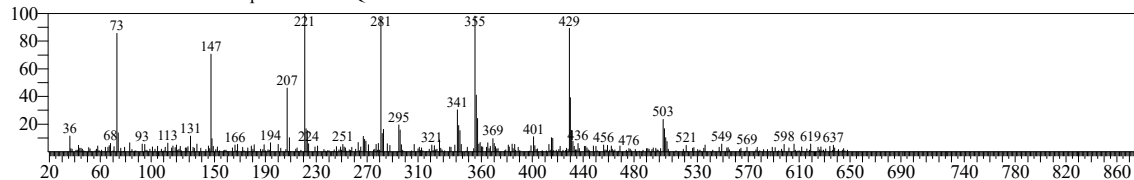
TNAU

<< Target >>
Line#:17 R.Time:43.795(Scan#:7760) MassPeaks:343
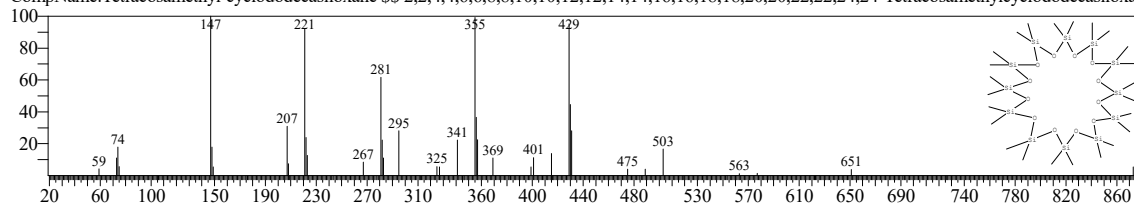RawMode:Averaged 43.790-43.800(7759-7761) BasePeak:221.00(671)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:46368 Library:NIST20M2.lib
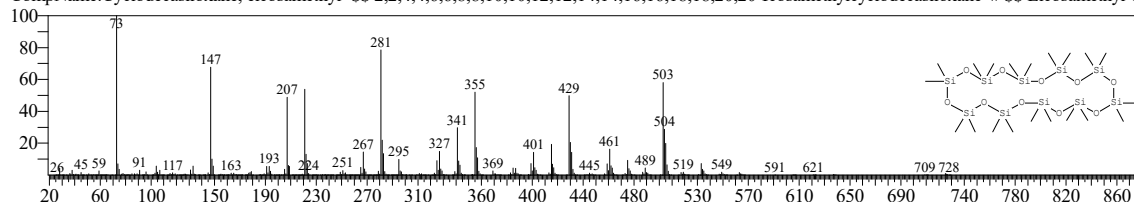SI:80 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

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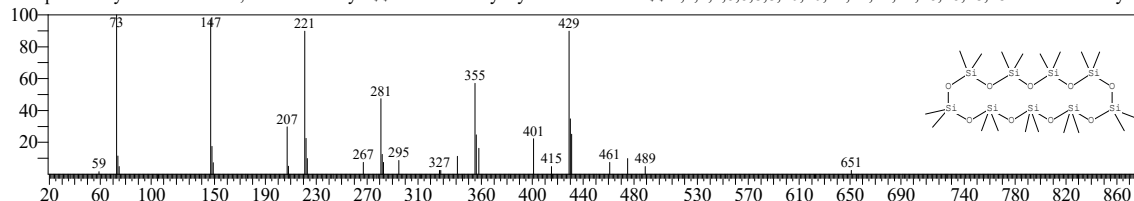SI:78 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:43658 Library:NIST20R.lib
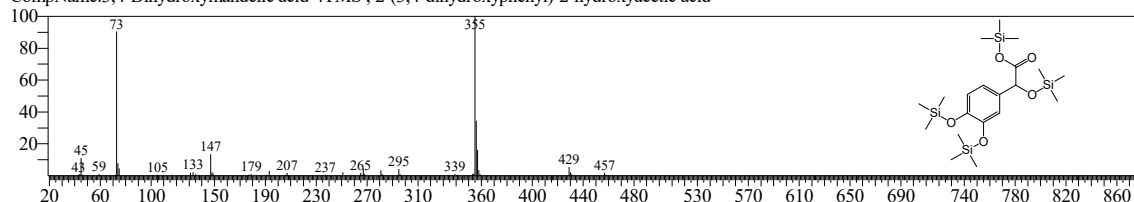SI:75 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:402 Library:OA_TMS_DB5_67min_V3.lib
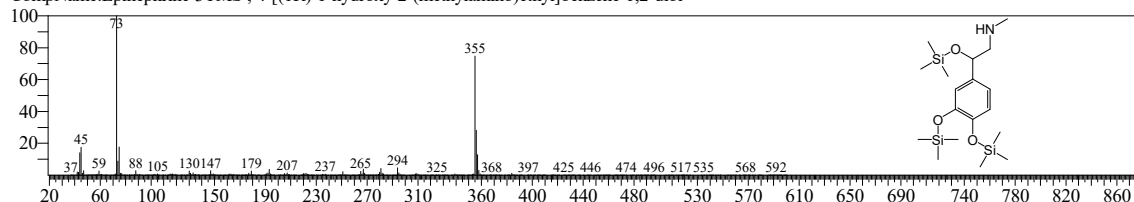SI:55 Formula:C20H42O4Si4 CAS:775-01-9 MolWeight:458 RetIndex:1942
CompName:3,4-Dihydroxymandelic acid-4TMS ; 2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid

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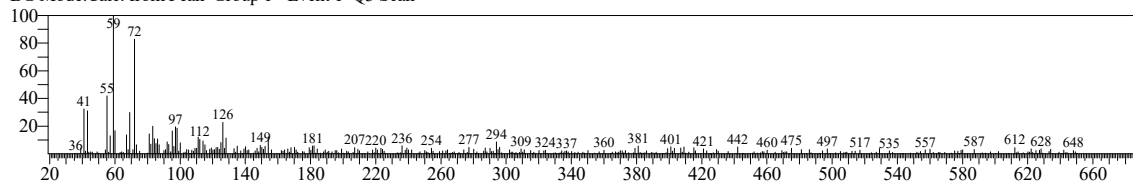
TNAU

<< Target >>
Line#:18 R.Time:44.165(Scan#:7834) MassPeaks:337
RawMode:Averaged 44.160-44.170(7833-7835) BasePeak:59.05(934)
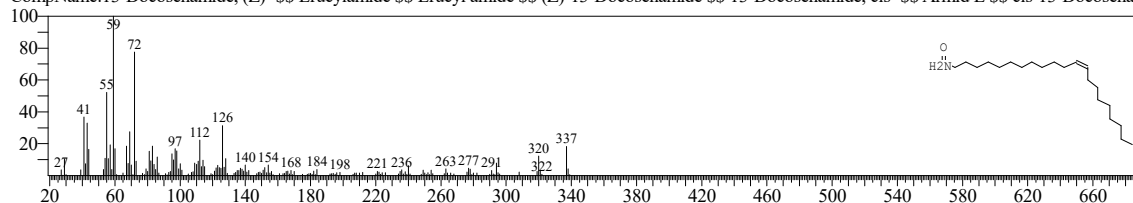BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:206446 Library:NIST20M1.lib
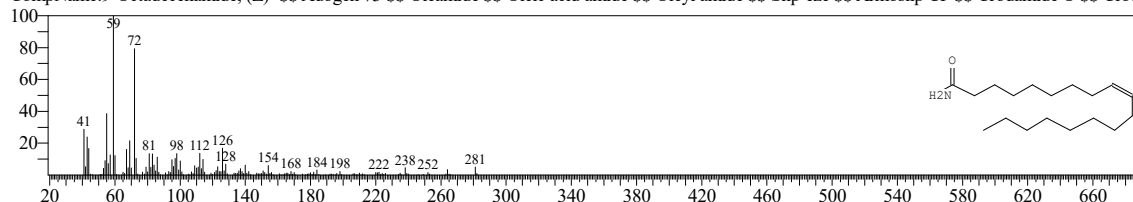SI:81 Formula:C22H43NO CAS:112-84-5 MolWeight:337 RetIndex:2625
CompName:13-Docosenamide, (Z)- $$ Erucylamide $$ Erucyl amide $$ (Z)-13-Docosenamide $$ 13-Docosenamide, cis- $$ Armid E $$ cis-13-Docosenam

Hit#:2 Entry:34121 Library:NIST20R.lib
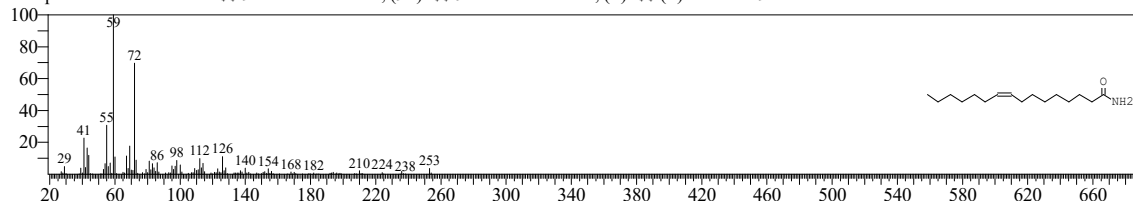SI:79 Formula:C18H35NO CAS:301-02-0 MolWeight:281 RetIndex:2228
CompName:9-Octadecenamide, (Z)- $$ Adogen 73 $$ Oleamide $$ Oleic acid amide $$ Oleyl amide $$ Slip-eze $$ Armoslip CP $$ Crodamide O $$ Croda

Hit#:3 Entry:108453 Library:NIST20M1.lib
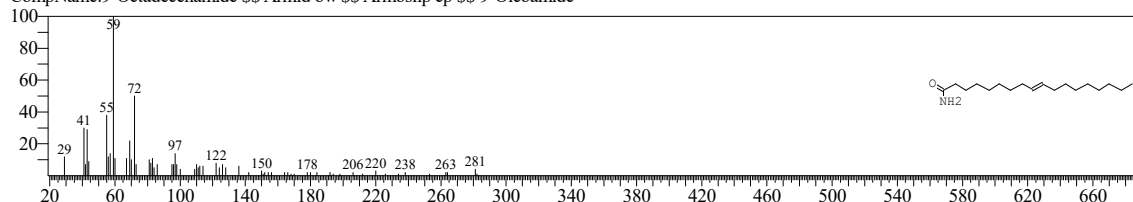SI:76 Formula:C16H31NO CAS:106010-22-4 MolWeight:253 RetIndex:2029
CompName:Palmitoleamide $$ 9-Hexadecenamide, (9Z)- $$ 9-Hexadecenamide, (Z)- $$ (Z)-Hexadec-9-enamide

Hit#:4 Entry:140706 Library:NIST20M1.lib
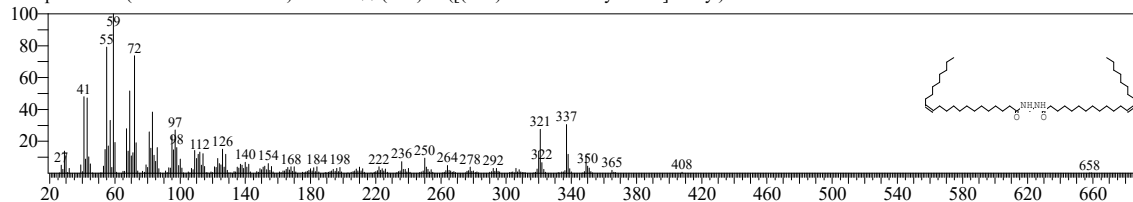SI:75 Formula:C18H35NO CAS:3322-62-1 MolWeight:281 RetIndex:2228
CompName:9-Octadecenamide $$ Armid ow $$ Armoslip cp $$ 9-Oleoamide

Hit#:5 Entry:44970 Library:NIST20M2.lib
SI:73 Formula:C45H86N2O2 CAS:10436-19-8 MolWeight:686 RetIndex:5311
CompName:Bis(cis-13-docosenamido)methane $$ (13Z)-N-([(13Z)-13-Docosenoylamino]methyl)-13-docosenamide #
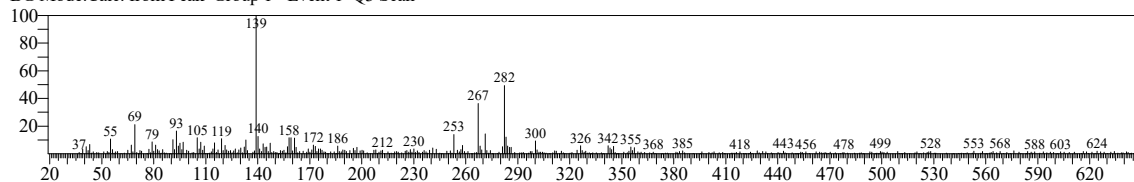
TNAU

<< Target >>
Line#:19 R.Time:45.585(Scan#:8118) MassPeaks:415
RawMode:Averaged 45.580-45.590(8117-8119) BasePeak:139.10(2093)
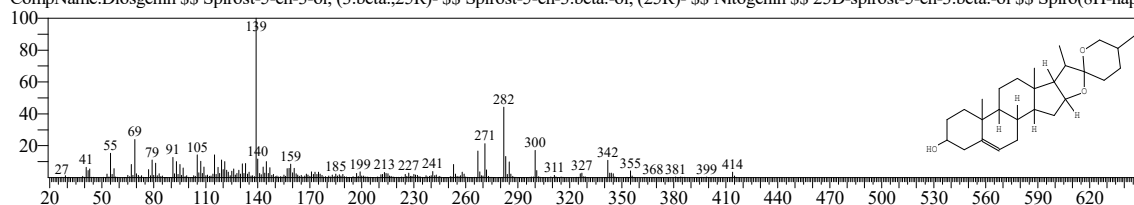BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:8297 Library:NIST20M2.lib
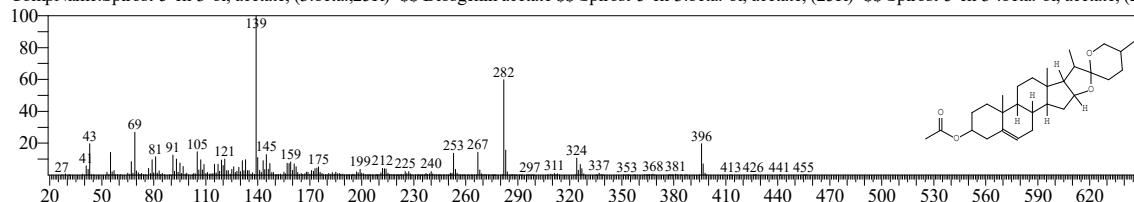SI:82 Formula:C27H42O3 CAS:512-04-9 MolWeight:414 RetIndex:2844
CompName:Diosgenin $$ Spirost-5-en-3-ol, (3.beta.,25R)- $$ Spirost-5-en-3.beta.-ol, (25R)- $$ Nitogenin $$ 25D-spirost-5-en-3.beta.-ol $$ Spiro(8H-naph

Hit#:2 Entry:24878 Library:NIST20M2.lib
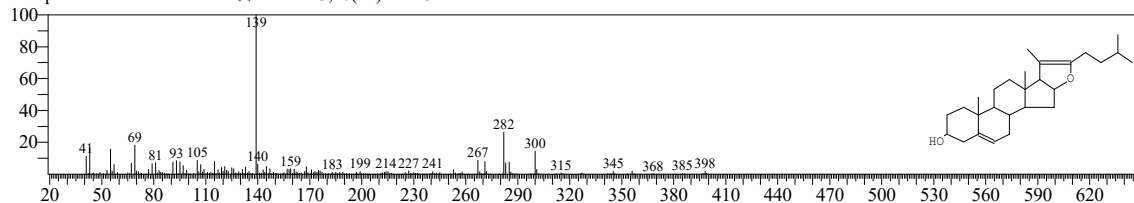SI:78 Formula:C29H44O4 CAS:1061-54-7 MolWeight:456 RetIndex:2984
CompName:Spirost-5-en-3-ol, acetate, (3.beta.,25R)- $$ Diosgenin acetate $$ Spirost-5-en-3.beta.-ol, acetate, (25R)- $$ Spirost-5-en-3-.beta.-ol, acetate, (25

Hit#:3 Entry:41561 Library:NIST20R.lib
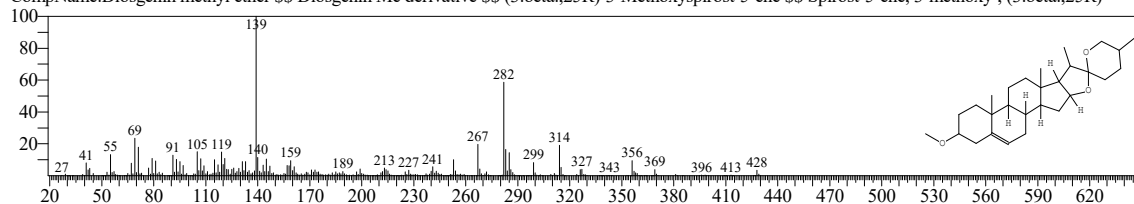SI:77 Formula:C27H42O2 CAS:32277-73-9 MolWeight:398 RetIndex:2713
CompName:Des-N-solasodine $$ Furosta-5,20(22)-dien-3-ol #

Hit#:4 Entry:14852 Library:NIST20M2.lib
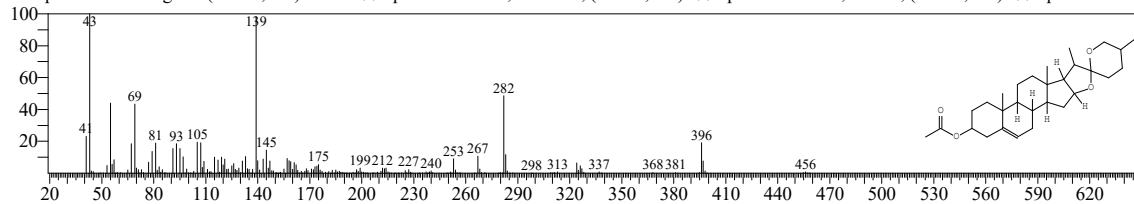SI:76 Formula:C28H44O3 CAS:116292-24-1 MolWeight:428 RetIndex:2793
CompName:Diosgenin methyl ether $$ Diosgenin Me derivative $$ (3.beta.,25R)-3-Methoxyspirost-5-ene $$ Spirost-5-ene, 3-methoxy-, (3.beta.,25R)-

Hit#:5 Entry:42677 Library:NIST20R.lib
SI:73 Formula:C29H44O4 CAS:1180-12-7 MolWeight:456 RetIndex:2984
CompName:Neodiosgenin (3.beta.,25S) acetate $$ Spirost-5-en-3-ol, 3-acetate, (3.beta.,25S)- $$ Spirost-5-en-3-ol, acetate, (3.beta.,25S)- $$ Spirost-5-en-3.
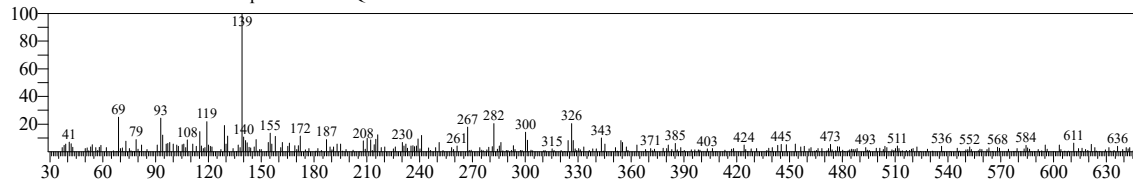
TNAU

<< Target >>
Line#:20 R.Time:45.615(Scan#:8124) MassPeaks:332
RawMode:Averaged 45.610-45.620(8123-8125) BasePeak:139.10(586)
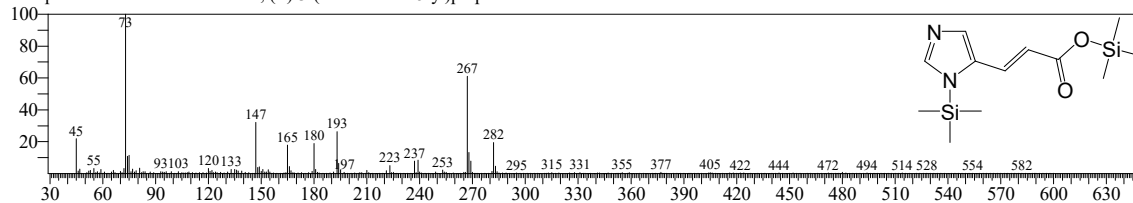BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

Hit#:1 Entry:438 Library:OA_TMS_DB5_67min_V3.lib
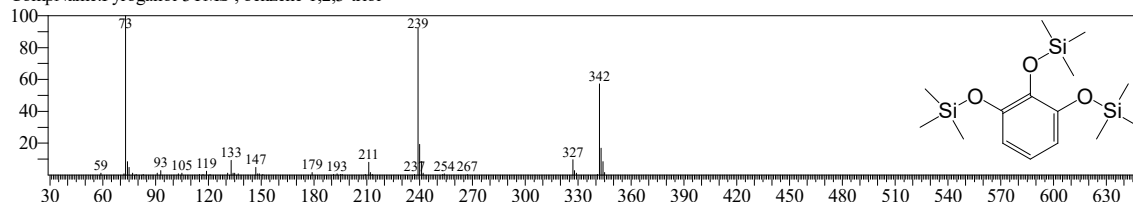SI:27 Formula:C12H22N2O2Si2 CAS:104-98-3 MolWeight:282 RetIndex:2014
CompName:Urocanic acid-2TMS ; (E)-3-(1H-imidazol-5-yl)prop-2-enoic acid

Hit#:2 Entry:173 Library:OA_TMS_DB5_67min_V3.lib
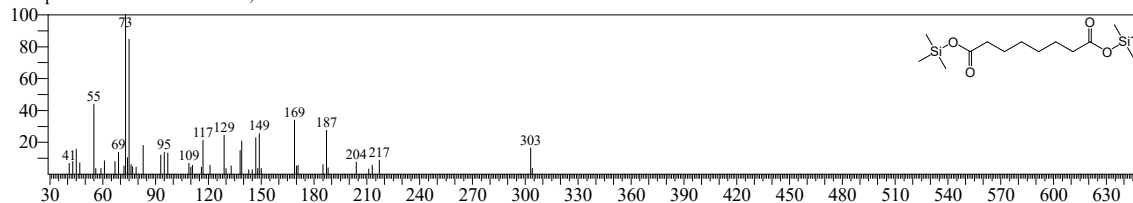SI:27 Formula:C15H30O3Si3 CAS:87-66-1 MolWeight:342 RetIndex:1559
CompName:Pyrogallol-3TMS ; benzene-1,2,3-triol

Hit#:3 Entry:258 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C14H30O4Si2 CAS:505-48-6 MolWeight:318 RetIndex:1700
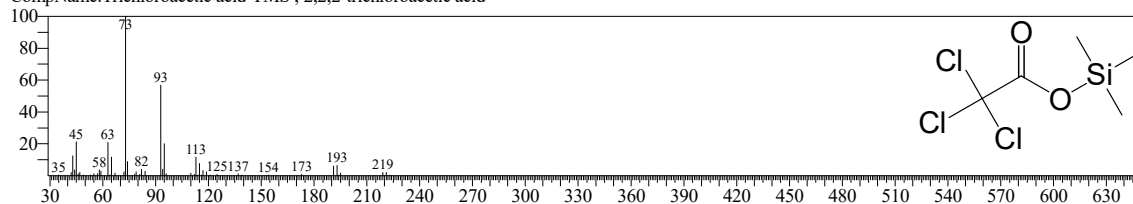CompName:Suberic acid-2TMS ; octanedioic acid

Hit#:4 Entry:6 Library:OA_TMS_DB5_67min_V3.lib
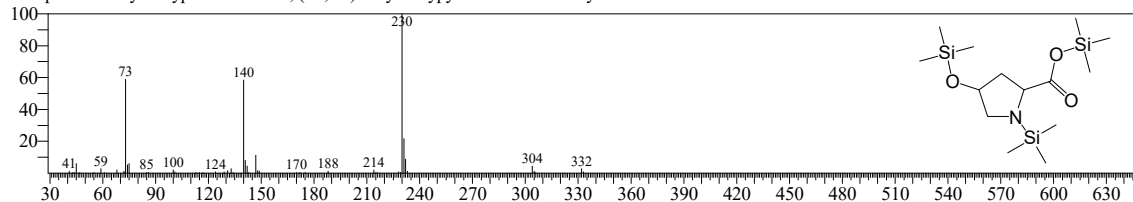SI:26 Formula:C5H9Cl3O2Si CAS:76-03-9 MolWeight:234 RetIndex:1059
CompName:Trichloroacetic acid-TMS ; 2,2,2-trichloroacetic acid

Hit#:5 Entry:164 Library:OA_TMS_DB5_67min_V3.lib
SI:26 Formula:C14H33NO3Si3 CAS:51-35-4 MolWeight:347 RetIndex:1538
CompName:4-Hydroxyproline-3TMS ; (2S,4R)-4-hydroxypyrrolidine-2-carboxylic acid
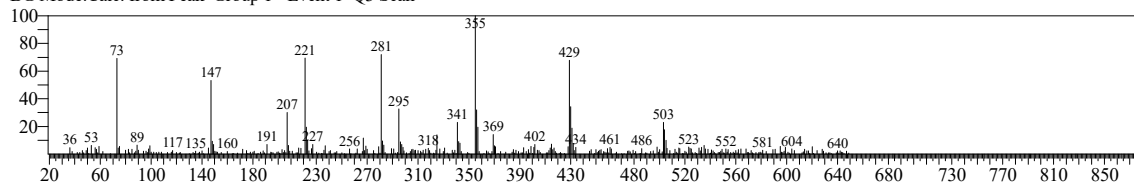
TNAU

<< Target >>
Line#:21 R.Time:45.770(Scan#:8155) MassPeaks:359
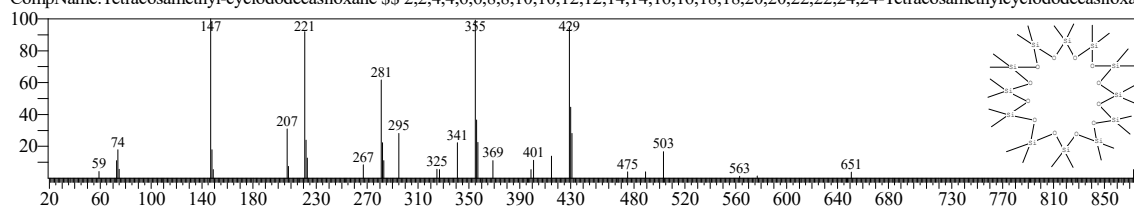RawMode:Averaged 45.765-45.775(8154-8156) BasePeak:355.05(798)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

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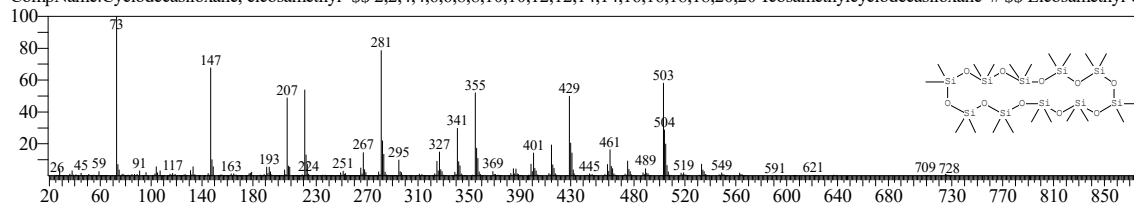SI:81 Formula:C24H72O12Si12 CAS:18919-94-3 MolWeight:888 RetIndex:2480
CompName:Tetracosamethyl-cyclododecasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20,22,22,24,24-Tetracosamethylcyclododecasiloxan

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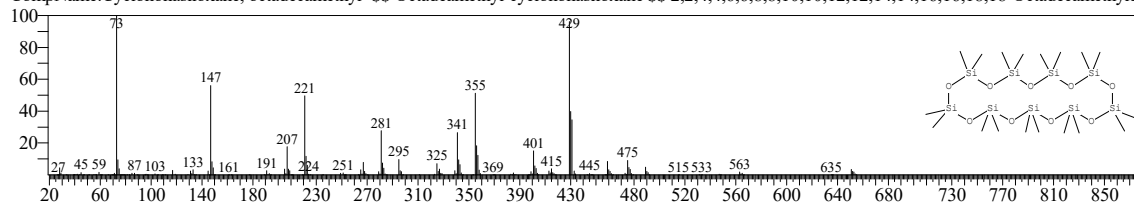SI:77 Formula:C20H60O10Si10 CAS:18772-36-6 MolWeight:740 RetIndex:2067
CompName:Cyclodecasiloxane, eicosamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane # $$ Eicosamethyl-cy

Hit#:3 Entry:44570 Library:NIST20M2.lib
SI:75 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
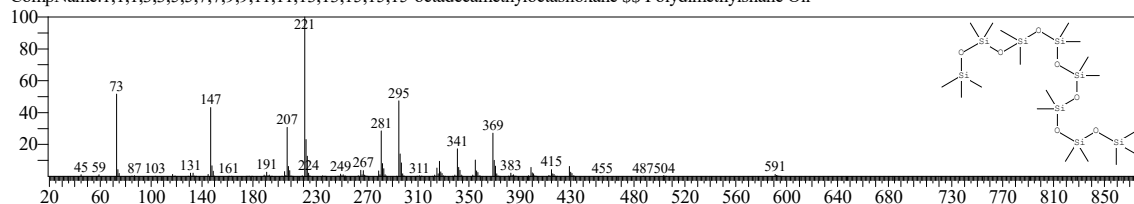CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy

Hit#:4 Entry:42942 Library:NIST20M2.lib
SI:73 Formula:C18H54O7Si8 CAS:556-69-4 MolWeight:606 RetIndex:1622
CompName:1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15,15-octadecamethyloctasiloxane $$ Polydimethylsilane Oil

Hit#:5 Entry:43312 Library:NIST20R.lib
SI:72 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane #