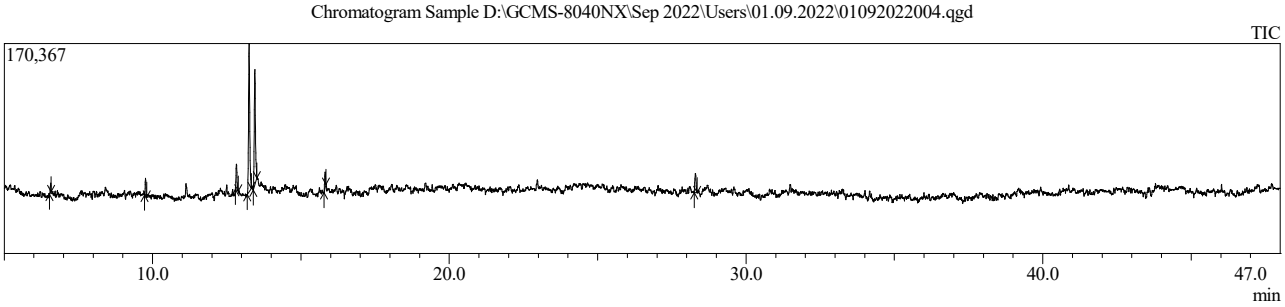
TNAU

Sample Information

Analyzed by	: Admin
Analyzed	: 01-Sep-22 8:12:49 PM
Sample Type	: Unknown
Level #	: 1
Sample Name	: Sample
Sample ID	: 1-3
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 2
Injection Volume	: 2.00
Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022004.qgd
Org Data File	: D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022004.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 10:55:36 AM

Chromatogram Sample D:\GCMS-8040NX\Sep 2022\Users\01.09.2022\01092022004.qgd



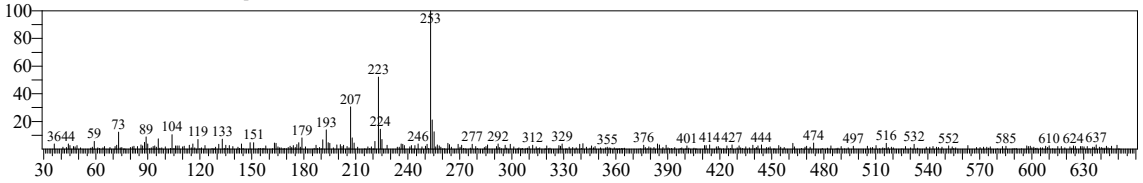
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	A/H	Similarity	Name
1	6.568	12855	1.66	7766	2.72	1.66	37	Vanillylamine-3TMS
2	9.764	27424	3.53	14387	5.04	1.91	93	Pentasiloxane, dodecamethyl-
3	12.824	50723	6.53	21179	7.43	2.39	72	1,3-Benzodioxol-5-ol
4	13.253	350172	45.09	120360	42.20	2.91	54	Methyl cis-13,16-Docosadienate
5	13.445	264201	34.02	93642	32.83	2.82	54	Methyl cis-13,16-Docosadienate
6	15.818	26638	3.43	12210	4.28	2.18	74	Malic acid 1-ethyl ester, 2TMS
7	28.294	44545	5.74	15679	5.50	2.84	89	n-Hexadecanoic acid
		776558	100.00	285223	100.00			

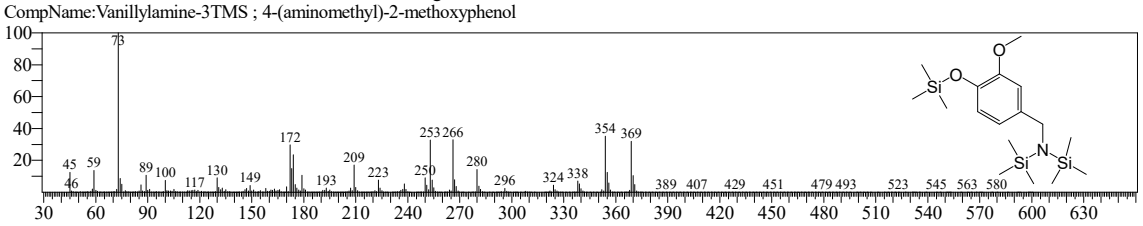
Library

TNAU

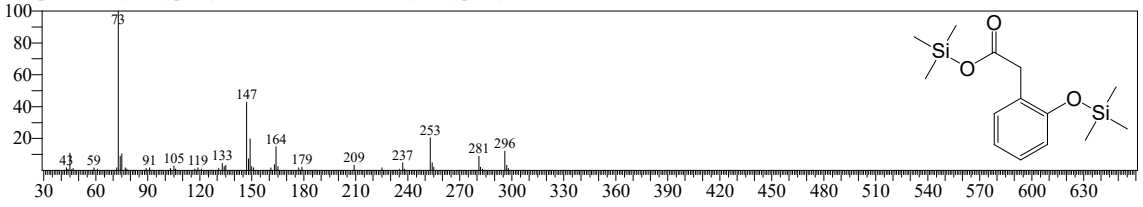
<< Target >>
Line#:1 R.Time:6.570(Scan#:315) MassPeaks:359
RawMode:Averaged 6.565-6.575(314-316) BasePeak:253.10(1080)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



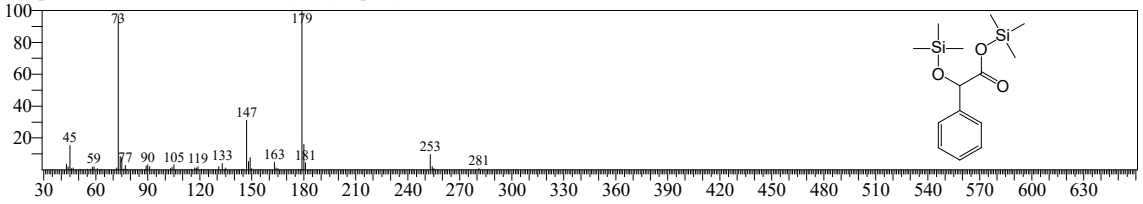
Hit#:1 Entry:368 Library:OA_TMS_DB5_67min_V3.lib
SI:37 Formula:C17H35NO2Si3 CAS:1196-92-5 MolWeight:369 RetIndex:1899
CompName:Vanillylamine-3TMS ; 4-(aminomethyl)-2-methoxyphenol



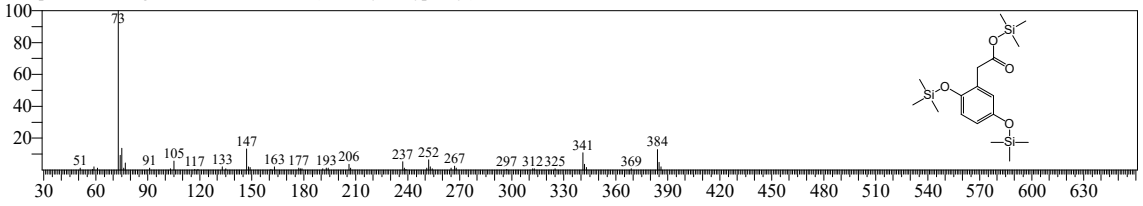
Hit#:2 Entry:184 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H24O3Si2 CAS:614-75-5 MolWeight:296 RetIndex:1579
CompName:2-Hydroxyphenylacetic acid-2TMS ; 2-(2-hydroxyphenyl)acetic acid



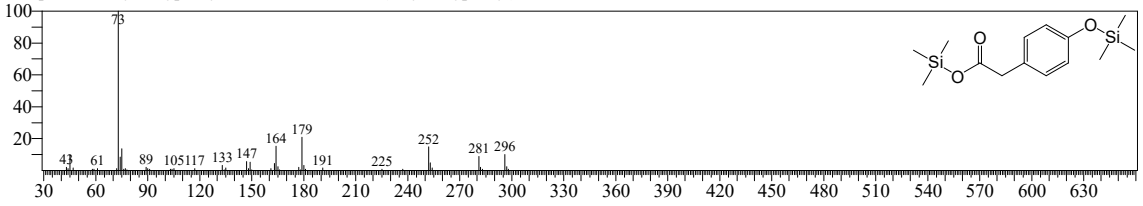
Hit#:3 Entry:138 Library:OA_TMS_DB5_67min_V3.lib
SI:36 Formula:C14H24O3Si2 CAS:90-64-2 MolWeight:296 RetIndex:1486
CompName:Mandelic acid-2TMS ; 2-hydroxy-2-phenylacetic acid



Hit#:4 Entry:332 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C17H32O4Si3 CAS:451-13-8 MolWeight:384 RetIndex:1850
CompName:Homogentisic acid-3TMS ; 2-(2,5-dihydroxyphenyl)acetic acid

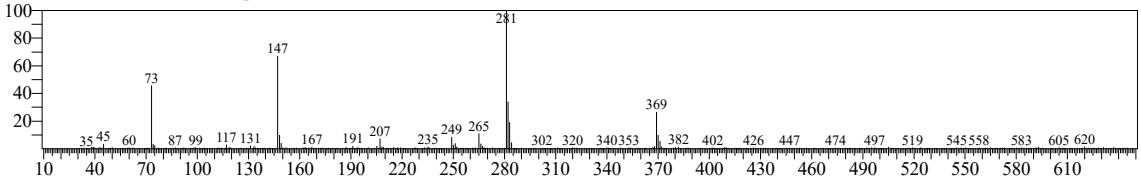


Hit#:5 Entry:220 Library:OA_TMS_DB5_67min_V3.lib
SI:34 Formula:C14H24O3Si2 CAS:156-38-7 MolWeight:296 RetIndex:1647
CompName:4-Hydroxyphenylacetic acid-2TMS ; 2-(4-hydroxyphenyl)acetic acid

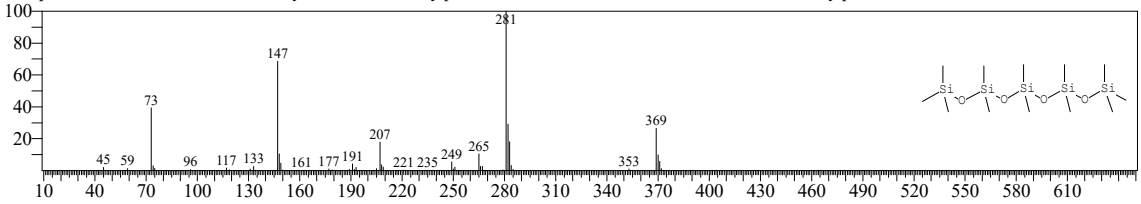


TNAU

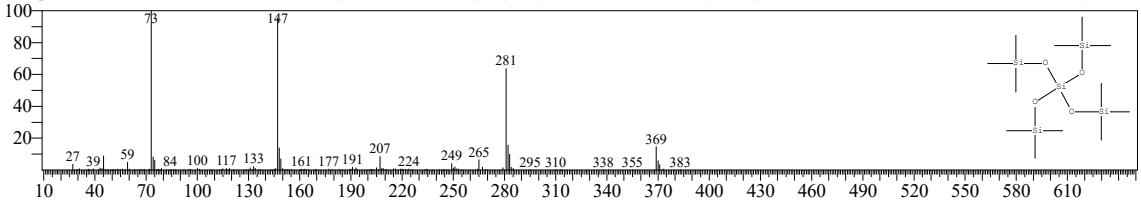
<< Target >>
Line#:2 R.Time:9.765(Scan#:954) MassPeaks:311
RawMode:Averaged 9.760-9.770(953-955) BasePeak:281.05(3530)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



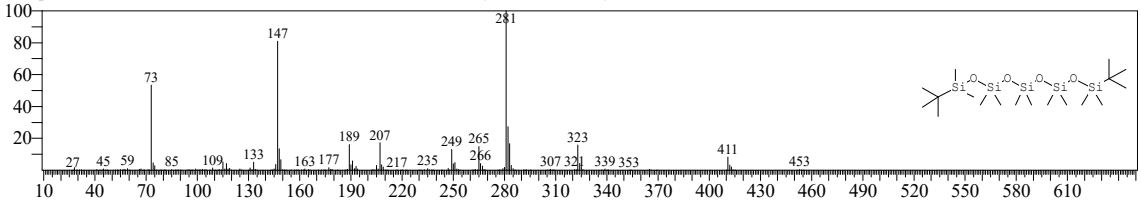
Hit#:1 Entry:40975 Library:NIST20R.lib
SI:93 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane #



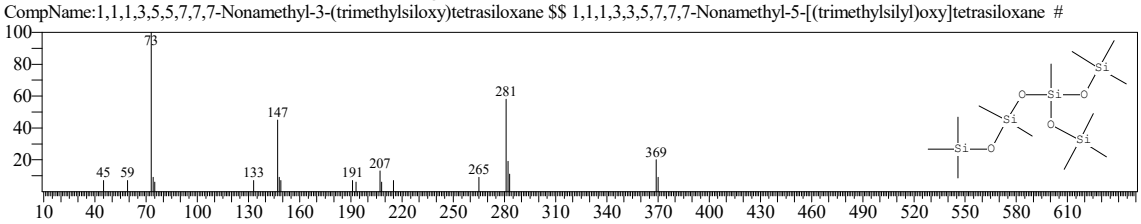
Hit#:2 Entry:249272 Library:NIST20M1.lib
SI:82 Formula:C12H36O4Si5 CAS:3555-47-3 MolWeight:384 RetIndex:1068
CompName:Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]- $$ Tetrakis(trimethylsiloxy)silane $$ Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-b



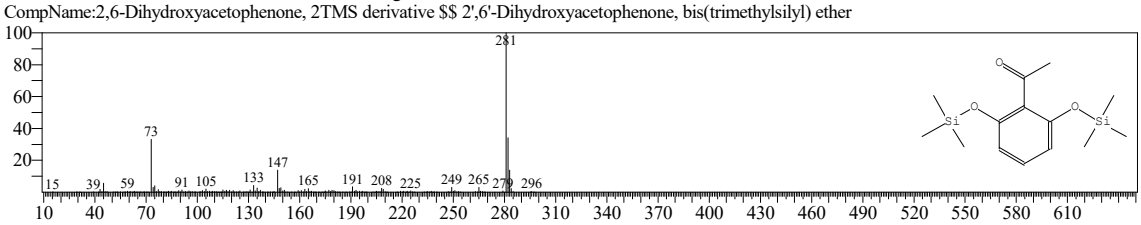
Hit#:3 Entry:27848 Library:NIST20M2.lib
SI:79 Formula:C18H48O4Si5 CAS:0-00-0 MolWeight:468 RetIndex:1495
CompName:1,3,5,7,9-Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-1,9-di(tert.butyl)-



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 #

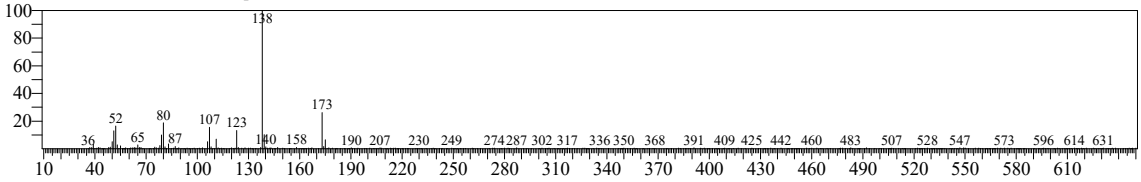


Hit#:5 Entry:158097 Library:NIST20M1.lib
SI:76 Formula:C14H24O3Si2 CAS:0-00-0 MolWeight:296 RetIndex:1625
CompName:2,6-Dihydroxyacetophenone, 2TMS derivative $$ 2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

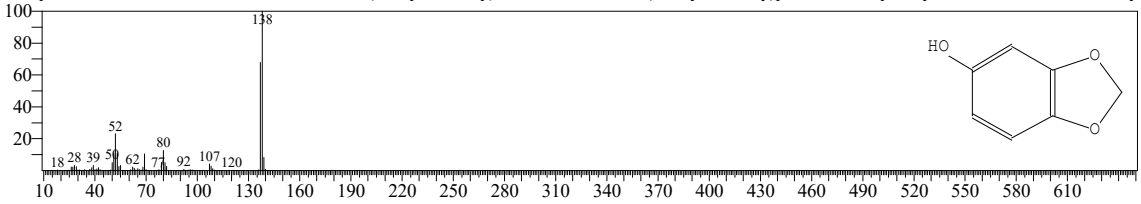


TNAU

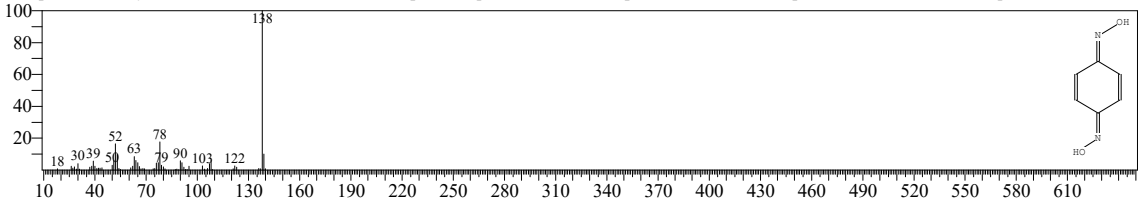
<< Target >>
Line#:3 R.Time:12.825(Scan#:1566) MassPeaks:368
RawMode:Averaged 12.820-12.830(1565-1567) BasePeak:138.10(6273)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



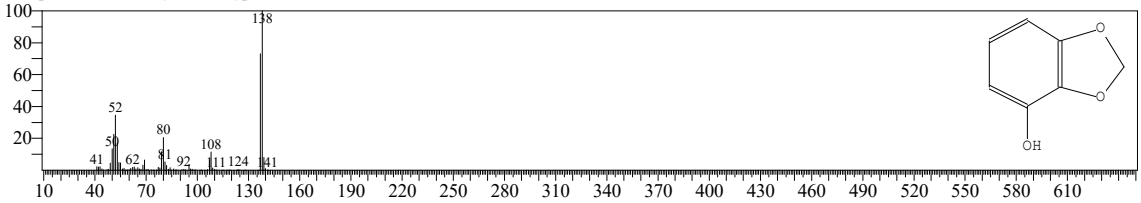
Hit#:1 Entry:11187 Library:NIST20M1.lib
SI:72 Formula:C7H6O3 CAS:533-31-3 MolWeight:138 RetIndex:1245
CompName:1,3-Benzodioxol-5-ol $$ Phenol, 3,4-(methylenedioxy)- $$ Sesamol $$ 3,4-(Methylenedioxy)phenol $$ 5-Hydroxy-1,3-benzodioxole $$ Methy



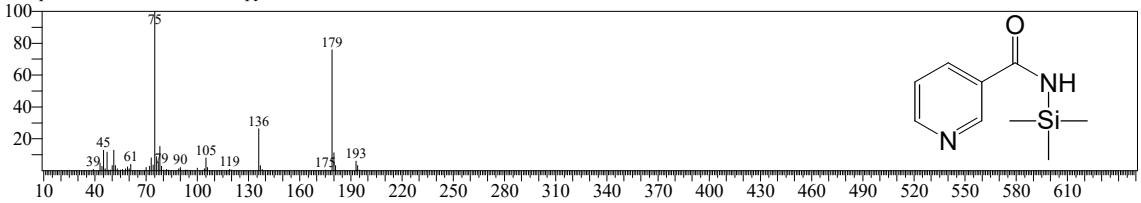
Hit#:2 Entry:8360 Library:NIST20R.lib
SI:71 Formula:C6H6N2O2 CAS:105-11-3 MolWeight:138 RetIndex:1349
CompName:2,5-Cyclohexadiene-1,4-dione, dioxime $$ p-Benzoquinone, dioxime $$ p-Quinone dioxime $$ p-Quinone oxime $$ Benzoquinone dioxime $$



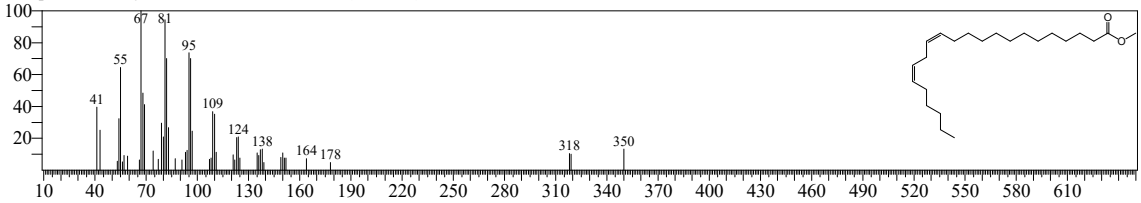
Hit#:3 Entry:11188 Library:NIST20M1.lib
SI:71 Formula:C7H6O3 CAS:69393-72-2 MolWeight:138 RetIndex:1245
CompName:2,3-Methylenedioxyphenol $$ 1,3-Benzodioxol-4-ol #



Hit#:4 Entry:137 Library:OA_TMS_DB5_67min_V3.lib
SI:33 Formula:C9H14N2OSi CAS:98-92-0 MolWeight:194 RetIndex:1486
CompName:Niacinamide-TMS ; pyridine-3-carboxamide

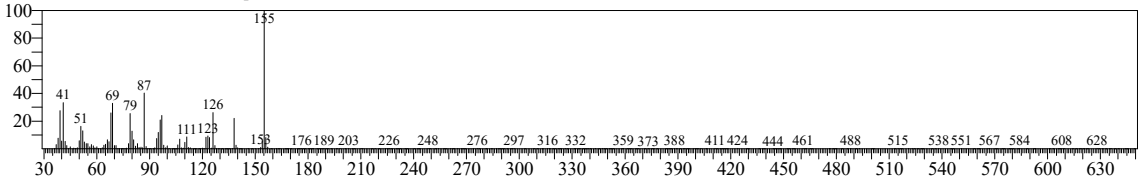


Hit#:5 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:30 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid

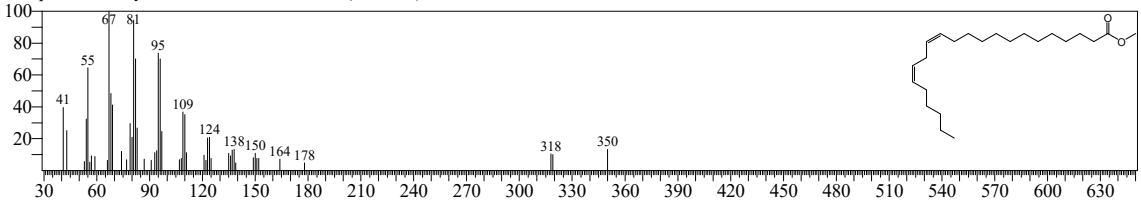


TNAU

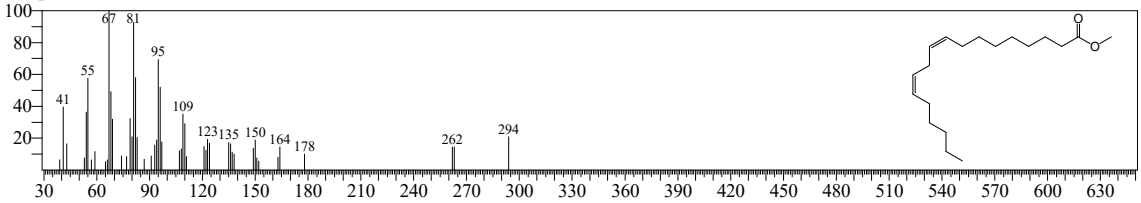
<< Target >>
Line#:4 R.Time:13.255(Scan#:1652) MassPeaks:339
RawMode:Averaged 13.250-13.260(1651-1653) BasePeak:155.05(18939)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



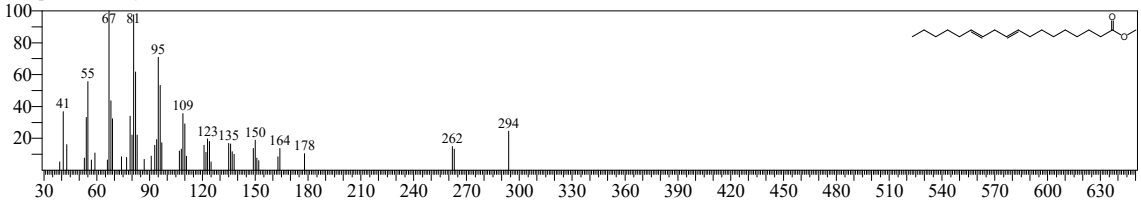
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



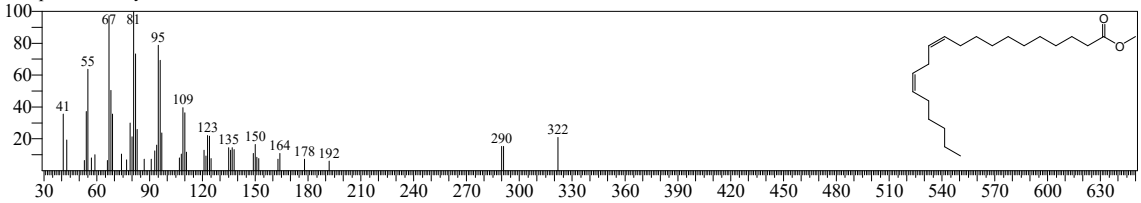
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:53 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



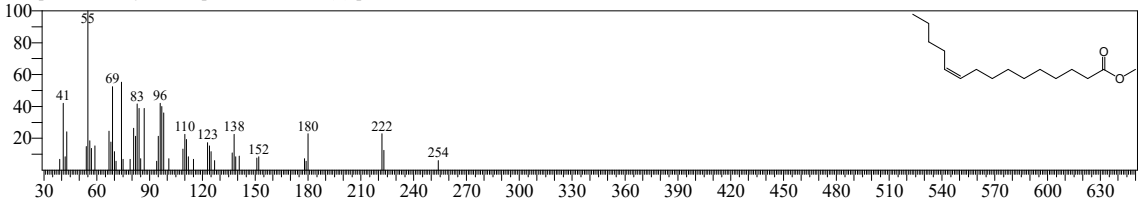
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

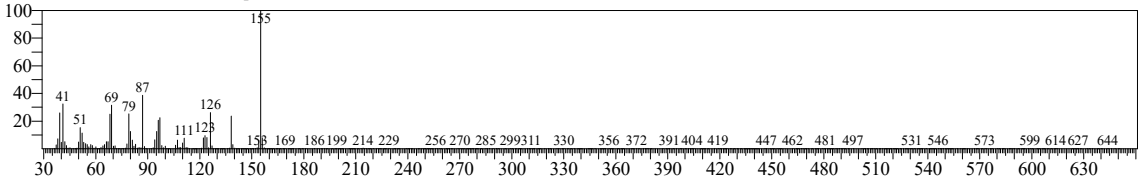


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

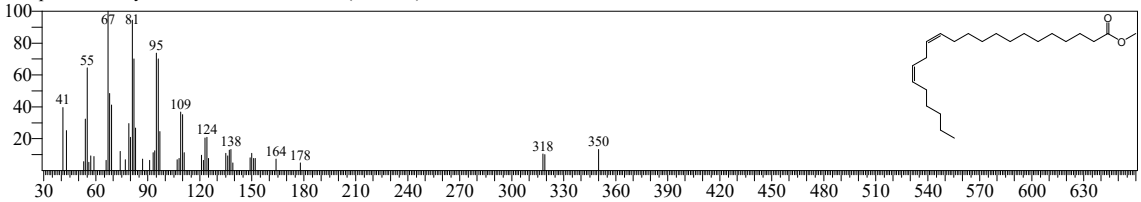


TNAU

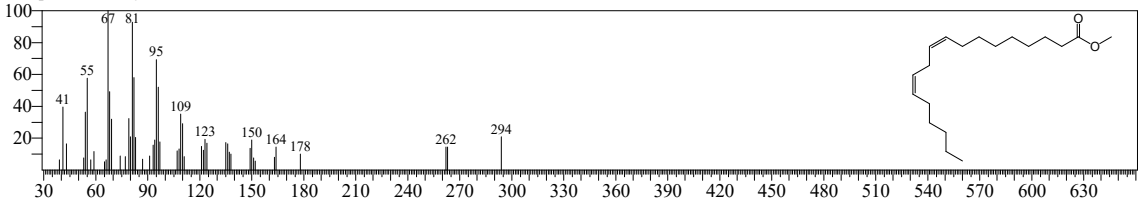
<< Target >>
Line#:5 R.Time:13.445(Scan#:1690) MassPeaks:415
RawMode:Averaged 13.440-13.450(1689-1691) BasePeak:155.10(14720)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



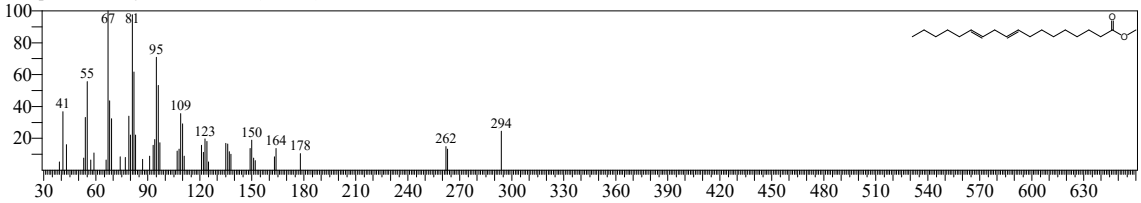
Hit#:1 Entry:34 Library:FA_ME_SP2560_EI_V3.lib
SI:54 Formula:C23H42O2 CAS:7370-49-2 MolWeight:350 RetIndex:3169
CompName:Methyl cis-13,16-Docosadienate ; (13Z,16E)-docosa-13,16-dienoic acid



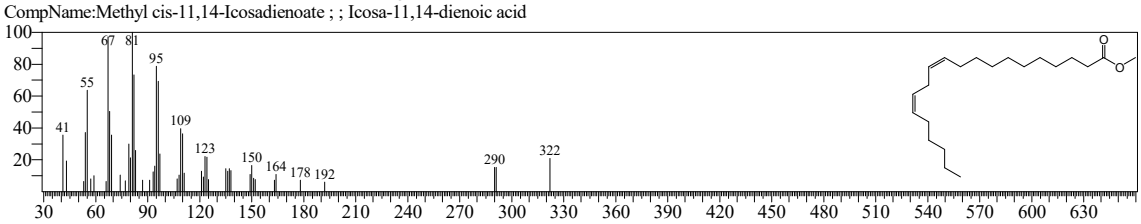
Hit#:2 Entry:21 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:60-33-3 MolWeight:294 RetIndex:2775
CompName:Methyl linoleate ; Octadeca-9,12-dienoic acid



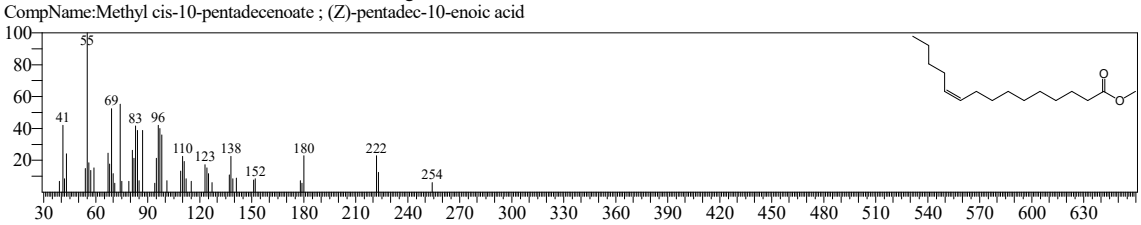
Hit#:3 Entry:20 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C19H34O2 CAS:506-21-8 MolWeight:294 RetIndex:2727
CompName:Methyl linolelaidate ; (9E,12E)-octadeca-9,12-dienoic acid



Hit#:4 Entry:27 Library:FA_ME_SP2560_EI_V3.lib
SI:52 Formula:C21H38O2 CAS:2091-39-6 MolWeight:322 RetIndex:2973
CompName:Methyl cis-11,14-Icosadienoate ; ; Icosa-11,14-dienoic acid

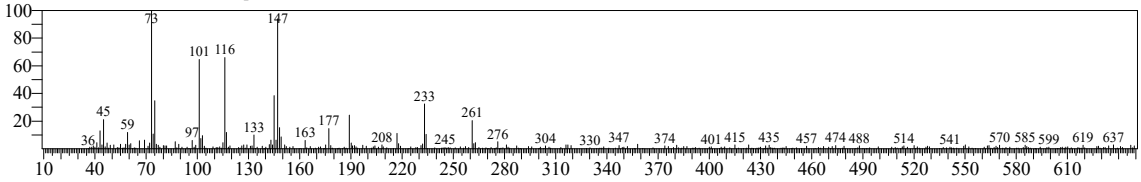


Hit#:5 Entry:11 Library:FA_ME_SP2560_EI_V3.lib
SI:51 Formula:C16H30O2 CAS:84743-29-3 MolWeight:254 RetIndex:2388
CompName:Methyl cis-10-pentadecenoate ; (Z)-pentadec-10-enoic acid

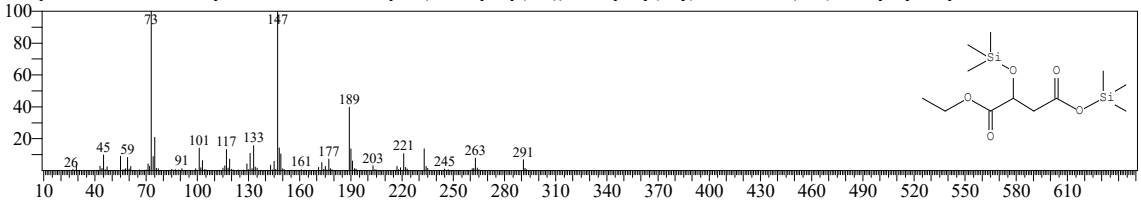


TNAU

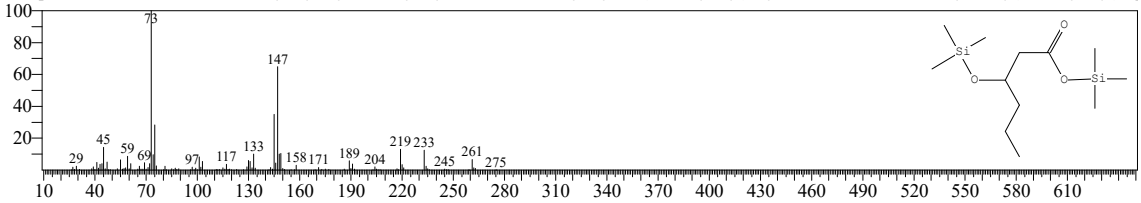
<< Target >>
Line#:6 R.Time:15.820(Scan#:2165) MassPeaks:332
RawMode:Averaged 15.815-15.825(2164-2166) BasePeak:73.05(1418)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



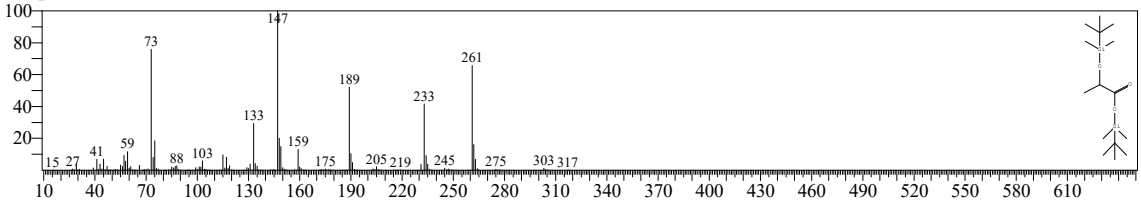
Hit#:1 Entry:169946 Library:NIST20M1.lib
SI:74 Formula:C12H26O5Si2 CAS:0-00-0 MolWeight:306 RetIndex:1380
CompName:Malic acid 1-ethyl ester, 2TMS $$ 1-Ethyl 4-(trimethylsilyl) 2-((trimethylsilyl)oxy)succinate $$ (.+/-.)-1-Ethyl hydroxybutanedioate, 2TMS $$ 1



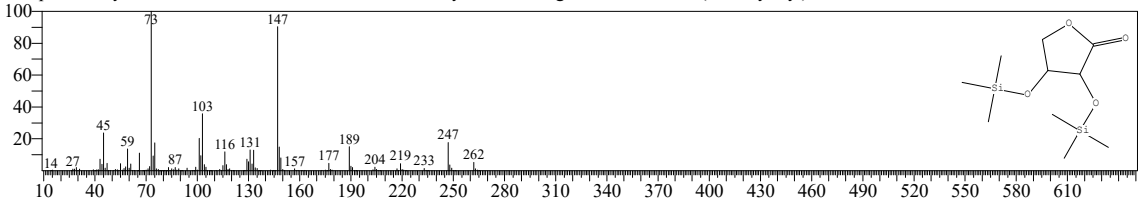
Hit#:2 Entry:33630 Library:NIST20R.lib
SI:74 Formula:C12H28O3Si2 CAS:136788-82-4 MolWeight:276 RetIndex:1213
CompName:Hexanoic acid, 3-trimethylsilyloxy, trimethylsilyl ester $$ Trimethylsilyl 3-[(trimethylsilyl)oxy]hexanoate $$ 3-Trimethylsiloxy(trimethylsilyl)ca



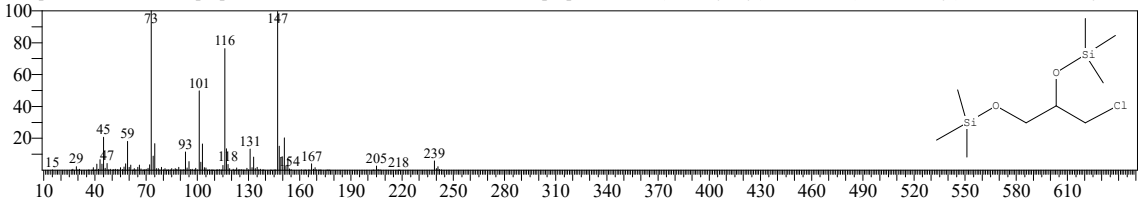
Hit#:3 Entry:184469 Library:NIST20M1.lib
SI:72 Formula:C15H34O3Si2 CAS:0-00-0 MolWeight:318 RetIndex:1342
CompName:Lactic acid, 2TBDMS derivative $$ Lactic acid ditbdms



Hit#:4 Entry:117877 Library:NIST20M1.lib
SI:72 Formula:C10H22O4Si2 CAS:0-00-0 MolWeight:262 RetIndex:1317
CompName:Erythrono-1,4-lactone, 2TMS derivative $$ D-Erythronic acid .gamma.-lactone, bis(trimethylsilyl) ether

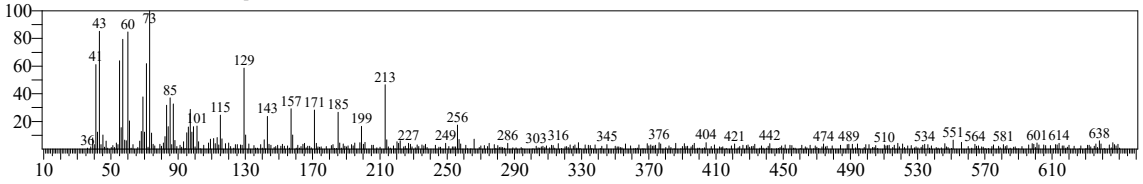


Hit#:5 Entry:108685 Library:NIST20M1.lib
SI:72 Formula:C9H23ClO2Si2 CAS:73639-52-8 MolWeight:254 RetIndex:1049
CompName:3-Chloro-1,2-propanediol, 2TMS derivative $$ 3-Chloro-1,2-propanediol, bis(trimethylsilyl) ether $$ 4-(Chloromethyl)-2,2,7,7-tetramethyl-3,6-

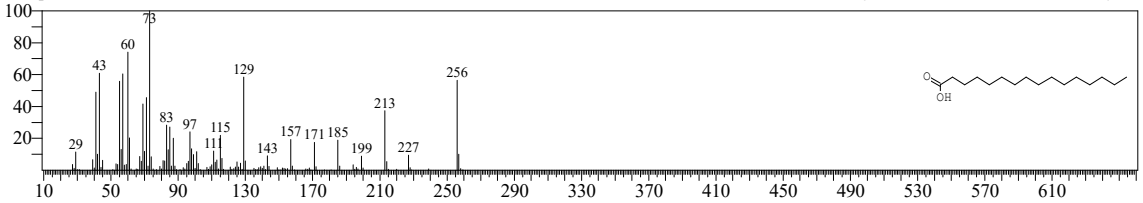


TNAU

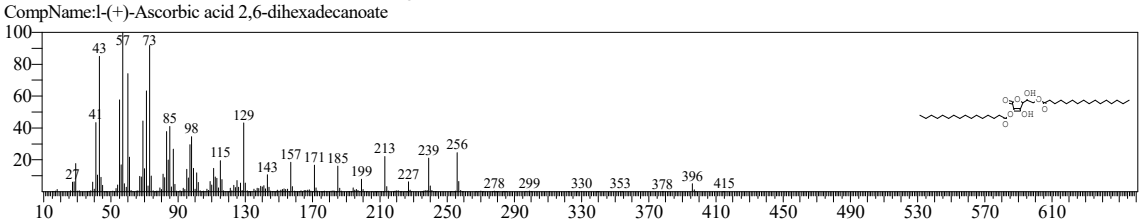
<< Target >>
Line#:7 R.Time:28.295(Scan#:4660) MassPeaks:415
RawMode:Averaged 28.290-28.300(4659-4661) BasePeak:73.05(857)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



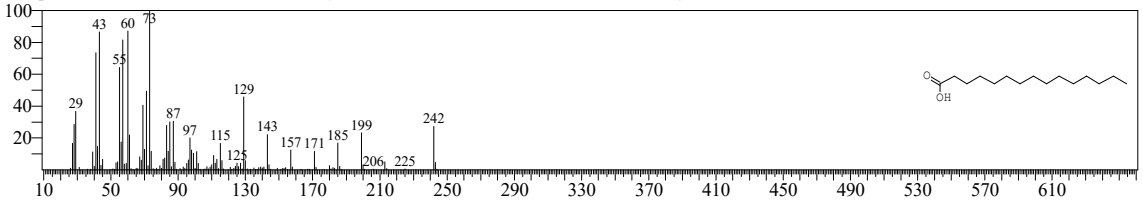
Hit#:1 Entry:31600 Library:NIST20R.lib
SI:89 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



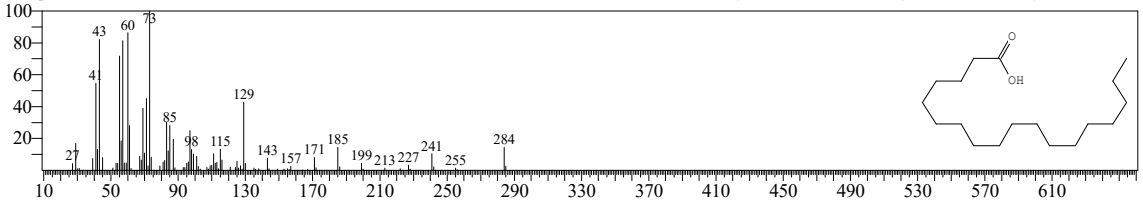
Hit#:2 Entry:44286 Library:NIST20M2.lib
SI:89 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



Hit#:3 Entry:29890 Library:NIST20R.lib
SI:89 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid



Hit#:4 Entry:144781 Library:NIST20M1.lib
SI:85 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



Hit#:5 Entry:81713 Library:NIST20M1.lib
SI:85 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