Sample Information

Method

```
: Admin
: 7/29/2015 10:11:08 AM
Analyzed by
Analyzed
Sample Type
                     : Unknown
Level #
Sample Name
                     : ECB
Sample ID
IS Amount
Sample Amount
Dilution Factor
                     : 1
Vial #
Injection Volume
                     : 4.00
Data File
                     : C:\GCMSsolution\Data - PREVIOUS\nurain\ECB FILE.qgd
Org Data File
                     : C:\GCMSsolution\Data - PREVIOUS\nurain\ECB FILE.qgd
Method File
                     Org Method File
                     Report File
                     : C:\GCMSsolution\System\Tune1\EI Tune 4-17-2015.qgt
Tuning File
Modified by
                     : Admin
Modified
                     : 7/29/2015 2:09:52 PM
[Comment]
==== Analytical Line 1 =====
[AOC-20i+s]
# of Rinses with Presolvent
# of Rinses with Solvent(post)
                                     :3
# of Rinses with Sample
                                     :Middle
Plunger Speed(Suction)
Viscosity Comp. Time
Plunger Speed(Injection)
Syringe Insertion Speed
                                     ·0.2 sec
                                     :Middle
                                     :High
Injection Mode
                                     :Normal
Pumping Times
                                     :0.3 sec
Inj. Port Dwell Time
Terminal Air Gap
                                     :No
Plunger Washing Speed
                                     :High
Washing Volume
                                     :8uL
Syringe Suction Position
                                     :0.0 mm
Syringe Injection Position
                                     :0.0 mm
                                     :All A,B,C
Solvent Selection
[GC-2010]
Column Oven Temp.
                           :60.0 °C
Injection Temp.
                            :200.00 °C
Injection Mode
                            :Splitless
Sampling Time
                            :0.50 min
Flow Control Mode
                           :Linear Velocity
                           :54.9 kPa
:100.9 mL/min
Pressure
Total Flow
Column Flow
                           :0.97 mL/min
Linear Velocity
                            :35.9 cm/sec
Purge Flow
                            :3.0 mL/min
Split Ratio
                           :100.0
High Pressure Injection
                           :OFF
Carrier Gas Saver
                           ·OFF
Oven Temp. Program
 Rate
                           Temperature(^{\circ}C)
                                                       Hold Time(min)
 40.00
                           325.0
                                                       10.00
< Ready Check Heat Unit >
   Column Oven
                           : Yes
   SPL1
                           : Yes
                            : Yes
< Ready Check Detector(FTD/BID) >
< Ready Check Baseline Drift >
< Ready Check Injection Flow >
SPL1 Carrier : You
SPL1 Purge
< Ready Check APC Flow >
                           : Yes
< Ready Check Detector APC Flow >
External Wait
Equilibrium Time
                           :1.0 min
[GC Program]
[GCMS-QP2010]
IonSourceTemp
                       :200.00 °C
Interface Temp.
                       :250.00 °C
Solvent Cut Time
                       :2.50 min
                       :Relative to the Tuning Result :+0.00 kV
Detector Gain Mode
Detector Gain
                       :20
Threshold
```

[MS Table]

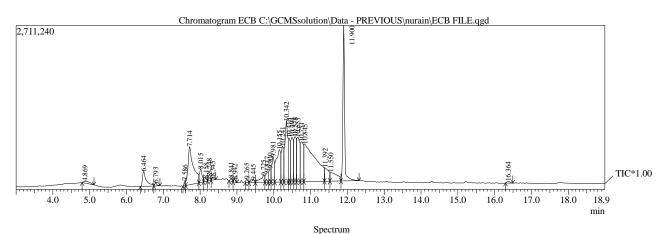
--Group 1 - Event 1--

Start Time :3.00min End Time :19.00min ACQ Mode :Scan Event Time :0.50sec Scan Speed : 769 :35.00 Start m/z :400.00 End m/z

Sample Inlet Unit :GC

[MS Program]

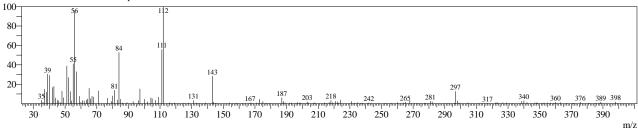
Use MS Program :OFF



Line#:1 R.Time:4.9(Scan#:225)

MassPeaks:213

RawMode:Averaged 4.9-4.9(224-226) BasePeak:112(3796) BG Mode:Calc. from Peak Group 1 - Event 1

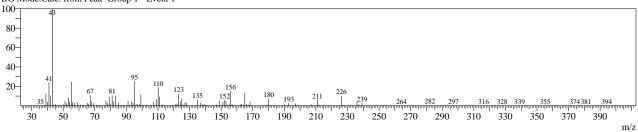


Line#:2 R.Time:6.5(Scan#:417)

MassPeaks:255

RawMode: Averaged 6.5-6.5(416-418) BasePeak: 43(46480)

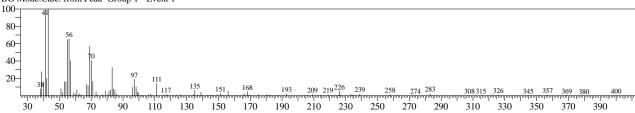
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:3 R.Time:6.8(Scan#:456)

MassPeaks:213

RawMode:Averaged 6.8-6.8(455-457) BasePeak:43(8536) BG Mode:Calc. from Peak Group 1 - Event 1

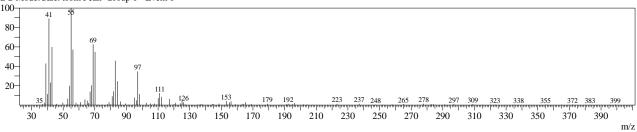


Line#:4 R.Time:7.6(Scan#:551)

MassPeaks:202

RawMode:Averaged 7.6-7.6(550-552) BasePeak:55(11780)

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

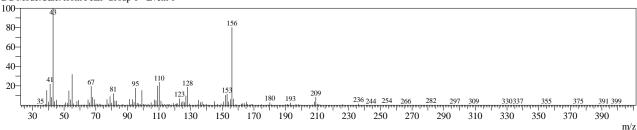


Line#:5 R.Time:7.7(Scan#:567)

MassPeaks:251

RawMode: Averaged 7.7-7.7(566-568) BasePeak: 43(86734)

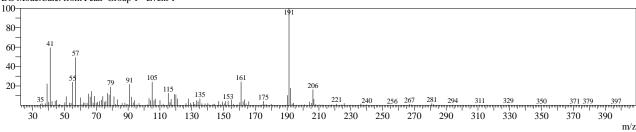
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:6 R.Time:8.0(Scan#:603)

MassPeaks:220

RawMode:Averaged 8.0-8.0(602-604) BasePeak:191(23913) BG Mode:Calc. from Peak Group 1 - Event 1

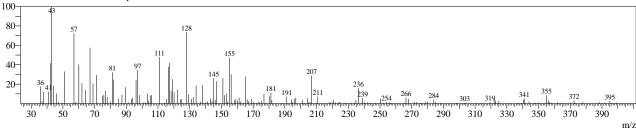


Line#:7 R.Time:8.2(Scan#:620)

MassPeaks:206

RawMode: Averaged 8.2-8.2(619-621) BasePeak: 43(2552)

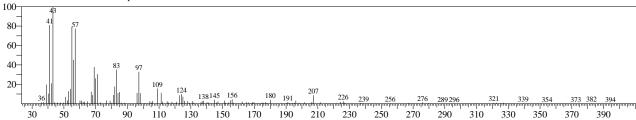
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:8 R.Time:8.3(Scan#:631)

MassPeaks:204

RawMode: Averaged 8.2-8.3(630-632) BasePeak: 43(14868) BG Mode: Calc. from Peak Group 1 - Event 1

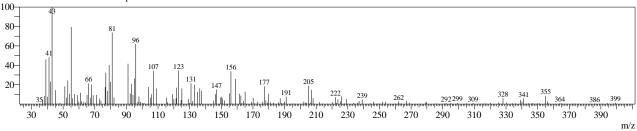


Line#:9 R.Time:8.3(Scan#:642)

MassPeaks:221

RawMode: Averaged 8.3-8.3(641-643) BasePeak: 43(4834)

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

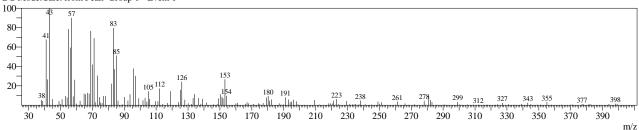


Line#:10 R.Time:8.8(Scan#:702)

MassPeaks:208

RawMode: Averaged 8.8-8.8(701-703) BasePeak: 43(5036)

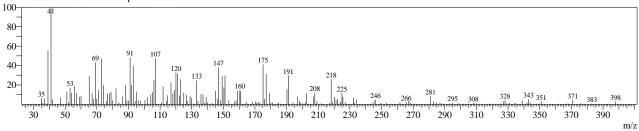
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:11 R.Time:8.9(Scan#:714)

MassPeaks:220

RawMode:Averaged 8.9-8.9(713-715) BasePeak:41(3323) BG Mode:Calc. from Peak Group 1 - Event 1

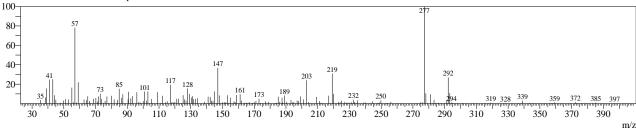


Line#:12 R.Time:9.3(Scan#:753)

MassPeaks:239

RawMode:Averaged 9.3-9.3(752-754) BasePeak:277(8310)

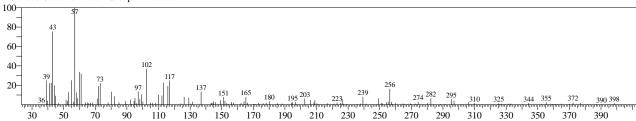
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:13 R.Time:9.4(Scan#:774)

MassPeaks:203

RawMode:Averaged 9.4-9.4(773-775) BasePeak:57(5135) BG Mode:Calc. from Peak Group 1 - Event 1

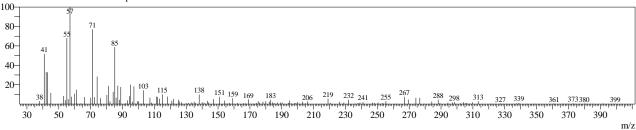


Line#:14 R.Time:9.7(Scan#:808)

MassPeaks:197

RawMode: Averaged 9.7-9.7(807-809) BasePeak: 57(6620)

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

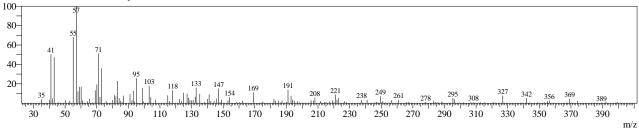


Line#:15 R.Time:9.8(Scan#:819)

MassPeaks:193

RawMode:Averaged 9.8-9.8(818-820) BasePeak:57(7062)

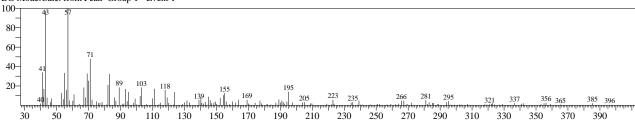
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:16 R.Time:9.9(Scan#:829)

MassPeaks:208

RawMode:Averaged 9.9-9.9(828-830) BasePeak:57(6968) BG Mode:Calc. from Peak Group 1 - Event 1

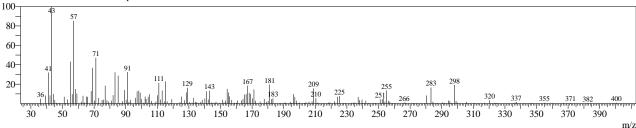


Line#:17 R.Time:10.0(Scan#:839)

MassPeaks:252

RawMode:Averaged 10.0-10.0(838-840) BasePeak:43(15696)

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

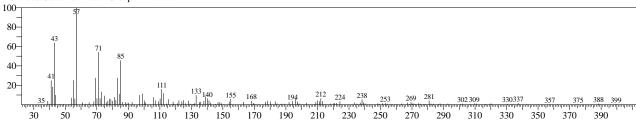


Line#:18 R.Time:10.2(Scan#:860)

MassPeaks:238

RawMode: Averaged 10.2-10.2(859-861) BasePeak: 57(20465)

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

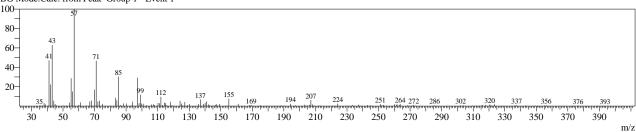


Line#:19 R.Time:10.2(Scan#:870)

MassPeaks:195

RawMode: Averaged 10.2-10.3(869-871) BasePeak: 57(25952)

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

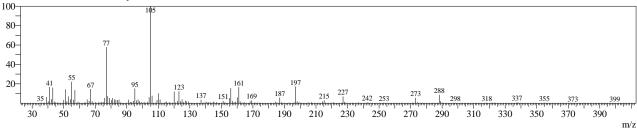


Line#:20 R.Time:10.3(Scan#:882)

MassPeaks:251

RawMode:Averaged 10.3-10.4(881-883) BasePeak:105(94060)

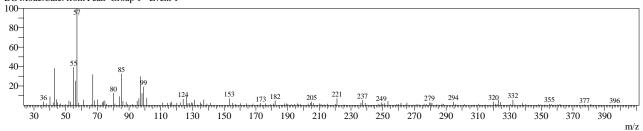
 $BG\ Mode: Calc.\ from\ Peak\ \ Group\ 1$ - Event 1



Line#:21 R.Time:10.4(Scan#:890)

MassPeaks:215

RawMode: Averaged 10.4-10.4(889-891) BasePeak: 57(16456) BG Mode: Calc. from Peak Group 1 - Event 1

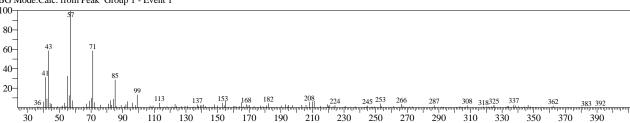


Line#:22 R.Time:10.5(Scan#:900)

MassPeaks:218

RawMode:Averaged 10.5-10.5(899-901) BasePeak:57(23047)

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

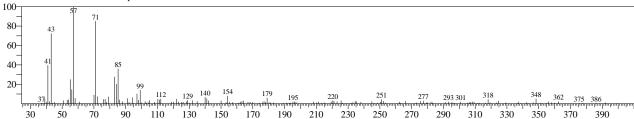


Line#:23 R.Time:10.6(Scan#:910)

MassPeaks:209

RawMode: Averaged 10.6-10.6(909-911) BasePeak: 57(17651)

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

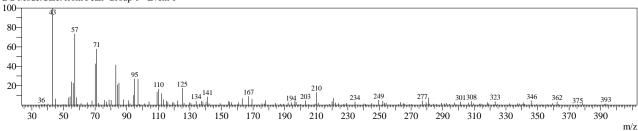


Line#:24 R.Time:10.7(Scan#:919)

MassPeaks:197

RawMode: Averaged 10.6-10.7(918-920) BasePeak: 43(14239)

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

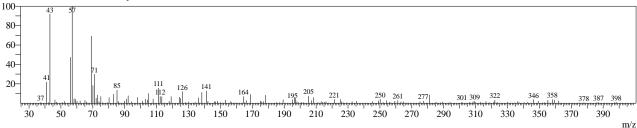


Line#:25 R.Time:10.8(Scan#:931)

MassPeaks:188

RawMode:Averaged 10.7-10.8(930-932) BasePeak:57(12822)

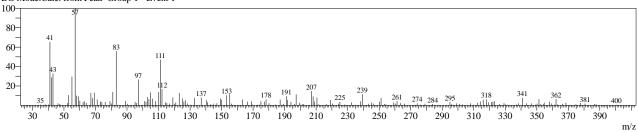
 $BG\ Mode: Calc.\ from\ Peak\ \ Group\ 1$ - Event 1



Line#:26 R.Time:10.8(Scan#:942)

MassPeaks:216

RawMode:Averaged 10.8-10.9(941-943) BasePeak:57(9905) BG Mode:Calc. from Peak Group 1 - Event 1

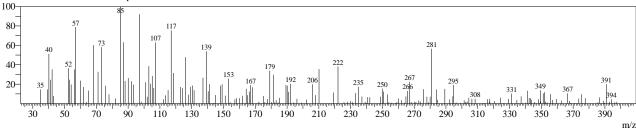


Line#:27 R.Time:11.4(Scan#:1008)

MassPeaks:195

RawMode:Averaged 11.4-11.4(1007-1009) BasePeak:85(2312)

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

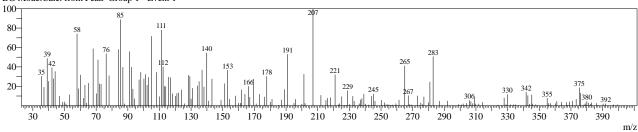


Line#:28 R.Time:11.6(Scan#:1027)

MassPeaks:197

RawMode: Averaged 11.5-11.6(1026-1028) BasePeak: 207(1512)

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

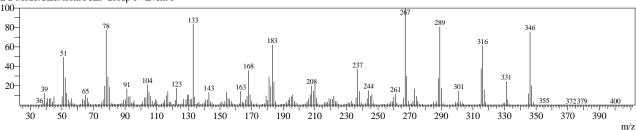


Line#:29 R.Time:11.9(Scan#:1069)

MassPeaks:330

RawMode:Averaged 11.9-11.9(1068-1070) BasePeak:267(187703)

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

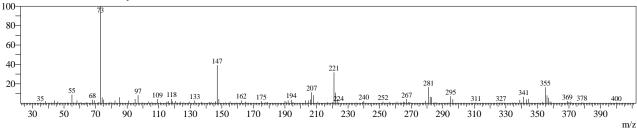


Line#:30 R.Time:16.4(Scan#:1605)

MassPeaks:199

RawMode:Averaged 16.4-16.4(1604-1606) BasePeak:73(10103)

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



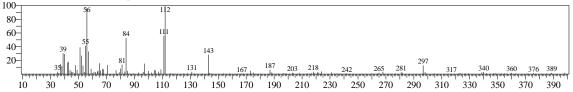
Library

<< Target >>

Line#:1 R.Time:4.867(Scan#:225) MassPeaks:213

RawMode: Averaged 4.858-4.875(224-226) BasePeak: 112.00(3796)

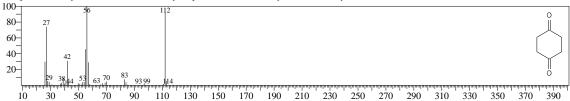
BG Mode:Calc. from Peak Group 1 - Event 1



Hit#:1 Entry:3437 Library:NIST11.lib

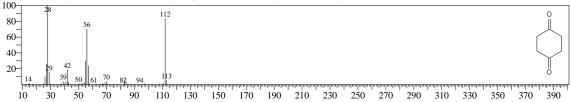
SI:70 Formula:C6H8O2 CAS:637-88-7 MolWeight:112 RetIndex:1062

CompName:1,4-Cyclohexanedione \$\$ Tetrahydroquinone \$\$ 1,4-Dioxocyclohexane \$\$ Cyclohexane-1,4-dione \$\$

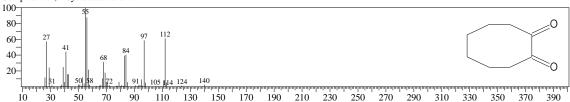


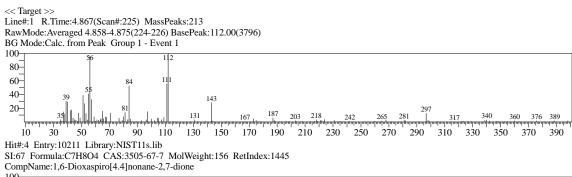
Hit#:2 Entry:2880 Library:NIST11s.lib SI:68 Formula:C6H8O2 CAS:637-88-7 MolWeight:112 RetIndex:1062

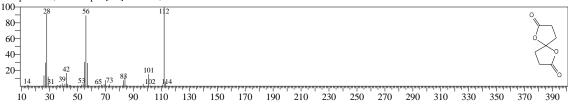
CompName:1,4-Cyclohexanedione \$\$ Tetrahydroquinone \$\$ 1,4-Dioxocyclohexane \$\$ Cyclohexane-1,4-dione \$\$



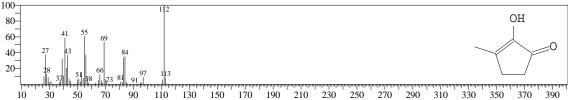
Hit#:3 Entry:11088 Library:NIST11.lib SI:68 Formula:C8H12O2 CAS:3008-37-5 MolWeight:140 RetIndex:1302 CompName:1,2-Cyclooctanedione

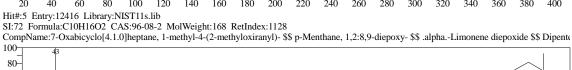




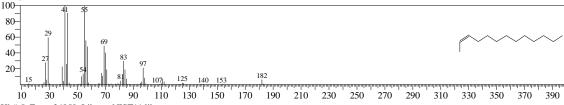


Hit#:5 Entry:2906 Library:NIST11s.lib SI:67 Formula:C6H8O2 CAS:80-71-7 MolWeight:112 RetIndex:972 CompName:2-Cyclopenten-1-one, 2-hydroxy-3-methyl-\$\$ Corylon \$\$ Cycloten \$\$ Cycloten \$\$ 2-Hydroxy-1-methylcyclopenten-3-one



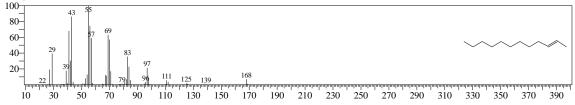


60-40-20-



Hit#:5 Entry:24850 Library:NIST11.lib SI:87 Formula:C12H24 CAS:7206-13-5 MolWeight:168 RetIndex:1222

CompName:2-Dodecene, (E)- \$\$ (2E)-2-Dodecene \$\$ 2-Dodecene, trans- \$\$ (E)-2-Dodecene \$\$ trans-2-Dodecene \$\$



CompName:Hydrazinedicarboxylic acid, 1-(2-isopropenylcyclopropyl)-, diisopropyl ester \$\$ Diisopropyl 1-(2-isopropenylcyclopropyl)-1,2-hydrazine

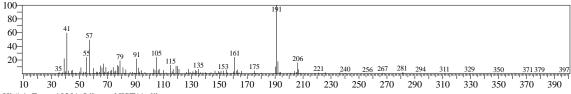
Hit#:5 Entry:105592 Library:NIST11.lib

80-60-40-20-

SI:69 Formula:C14H24N2O4 CAS:0-00-0 MolWeight:284 RetIndex:1798

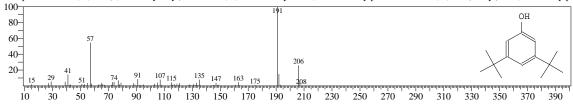
Line#:6 R.Time:8.017(Scan#:603) MassPeaks:220 RawMode:Averaged 8.008-8.025(602-604) BasePeak:191.15(23913)

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



Hit#:1 Entry:18381 Library:NIST11s.lib

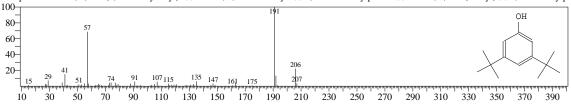
Si:72 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- \$\$ Phenol, 3,5-di-tert-butyl- \$\$ 3,5-Di-tert-butylphenol \$\$ Phenol, 3,5-bis(t-butyl) \$\$ 3,5-Di-tert-butylphenol



Hit#:2 Entry:18383 Library:NIST11s.lib

SI:71 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555

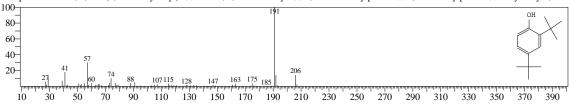
CompName:Phenol, 3,5-bis(1,1-dimethylethyl)- \$\$ Phenol, 3,5-di-tert-butyl- \$\$ 3,5-Di-tert-butylphenol \$\$ Phenol, 3,5-bis(t-butyl) \$\$ 3,5-Di-t-butylp



Hit#:3 Entry:18377 Library:NIST11s.lib

SI:71 Formula:C14H22O CAS:96-76-4 MolWeight:206 RetIndex:1555

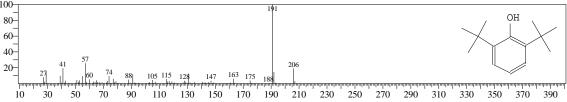
CompName:Phenol, 2,4-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,4-di-tert-butyl- \$\$ 2,4-Di-tert-butylphenol \$\$ 2,4-di-t-Butylphenol \$\$ 1-Hydroxy-2,4-di-



Hit#:4 Entry:18376 Library:NIST11s.lib

SI:71 Formula:C14H22O CAS:128-39-2 MolWeight:206 RetIndex:1555

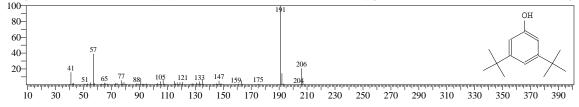
CompName:Phenol, 2,6-bis(1,1-dimethylethyl)- \$\$ Phenol, 2,6-di-tert-butyl- \$\$ 2,6-Bis(tert-butyl)phenol \$\$ 2,6-Bis(1,1-dimethylethyl)phenol \$\$ 2,6-



Hit#:5 Entry:18382 Library:NIST11s.lib

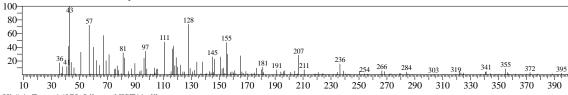
SI:70 Formula:C14H22O CAS:1138-52-9 MolWeight:206 RetIndex:1555

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

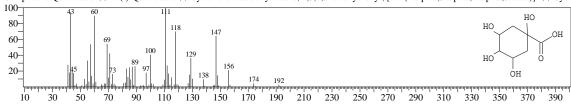


Line#:7 R.Time:8.158(Scan#:620) MassPeaks:206 RawMode:Averaged 8.150-8.167(619-621) BasePeak:43.00(2552)

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



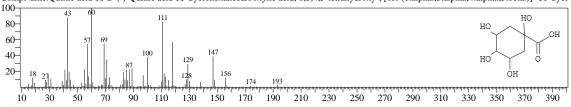
Hit#:1 Entry:16078 Library:NIST11s.lib SI:50 Formula:C7H12O6 CAS:77-95-2 MolWeight:192 RetIndex:1852 CompName:Quinic acid \$\$ D-(-)-Quinic acid \$\$ Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]- \$\$ Cycl



Hit#:2 Entry:38096 Library:NIST11.lib

SI:50 Formula:C7H12O6 CAS:77-95-2 MolWeight:192 RetIndex:1852

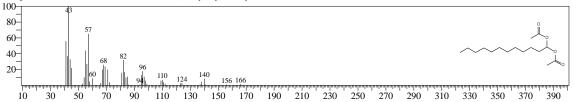
CompName:Quinic acid \$\$ D-(-)-Quinic acid \$\$ Cyclohexanecarboxylic acid, 1,3,4,5-tetrahydroxy-, [1R-(1.alpha.,3.alpha.,4.alpha.,5.beta.)]- \$\$ Cycl



Hit#:3 Entry:107436 Library:NIST11.lib

SI:49 Formula:C16H30O4 CAS:56438-07-4 MolWeight:286 RetIndex:1882

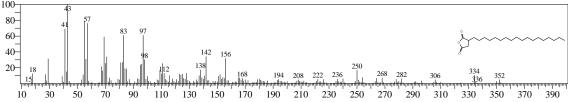
CompName:1,1-Dodecanediol, diacetate \$\$ 1-(Acetyloxy)dodecyl acetate #\$\$



Hit#:4 Entry:157026 Library:NIST11.lib

SI:49 Formula:C22H40O3 CAS:47458-32-2 MolWeight:352 RetIndex:2747

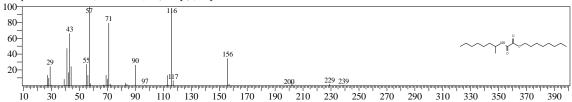
CompName: 2,5-Furandione, dihydro-3-octadecyl- \$\$ n-Octadecylsuccinic anhydride \$\$ 2-Octadecylsuccinic anhydride \$\$ Octadecylsuccinic anhydride

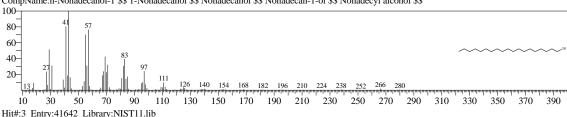


Hit#:5 Entry:128744 Library:NIST11.lib

SI:49 Formula:C18H35NO3 CAS:0-00-0 MolWeight:313 RetIndex:2314

CompName:Oxalic acid, monoamide, N-(2-octyl)-, octyl ester





250

250

270

290

310

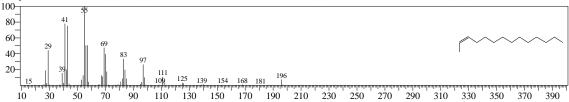
330

350

370

SI:87 Formula:C14H28 CAS:35953-54-9 MolWeight:196 RetIndex:1421

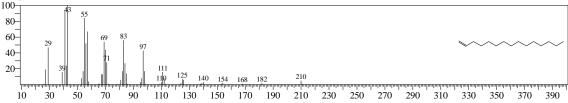
CompName: 2-Tetradecene, (E)- \$\$ (2E)-2-Tetradecene \$\$ trans-2-Tetradecene \$\$ (E)-2-Tetradecene, (2E)- \$\$ 2-Tetradecene, trans-



Hit#:4 Entry:18888 Library:NIST11s.lib

SI:87 Formula:C15H30 CAS:13360-61-7 MolWeight:210 RetIndex:1502

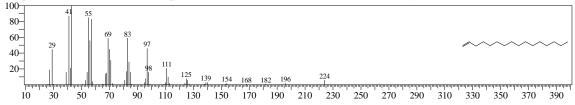
CompName: 1-Pentadecene \$\$ Pentadecene, 1- \$\$ Pentadec-1-ene \$\$



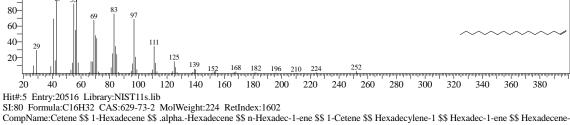
Hit#:5 Entry:60964 Library:NIST11.lib

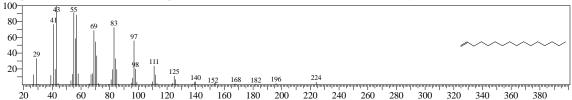
SI:87 Formula:C16H32 CAS:629-73-2 MolWeight:224 RetIndex:1602

CompName:Cetene \$\$ 1-Hexadecene \$\$.alpha.-Hexadecene \$\$ n-Hexadec-1-ene \$\$ 1-Cetene \$\$ Hexadecylene-1 \$\$ Hexadec-1-ene \$\$ Hexadecylene-1



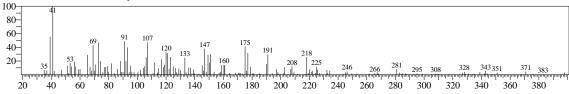
60-40-20-



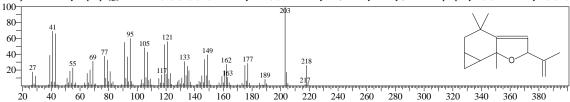


Line#:11 R.Time:8.942(Scan#:714) MassPeaks:220 RawMode:Averaged 8.933-8.950(713-715) BasePeak:41.05(3323)

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



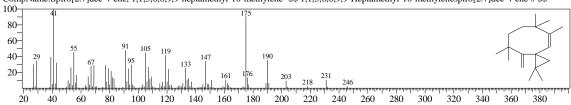
Hit#:1 Entry:56368 Library:NIST11.lib SI:64 Formula:C15H22O CAS:102681-49-2 MolWeight:218 RetIndex:1438 CompName:2H-Cyclopropa[g]benzofuran, 4,5,5a,6,6a,6b-hexahydro-4,4,6b-trimethyl-2-(1-methylethenyl)- \$\$ 2-Isopropenyl-4,4,6b-trimethyl-4,5,5a,



Hit#:2 Entry:76877 Library:NIST11.lib

SI:64 Formula:C18H30 CAS:0-00-0 MolWeight:246 RetIndex:1656

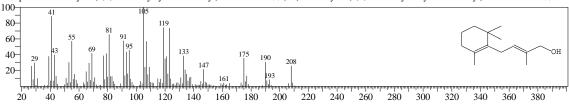
CompName:Spiro[2.7]dec-4-ene, 1,1,5,6,6,9,9-heptamethyl-10-methylene- \$\$ 1,1,5,6,6,9,9-Heptamethyl-10-methylenespiro[2.7]dec-4-ene #\$\$



Hit#:3 Entry:49581 Library:NIST11.lib

SI:62 Formula:C14H24O CAS:62924-17-8 MolWeight:208 RetIndex:1641

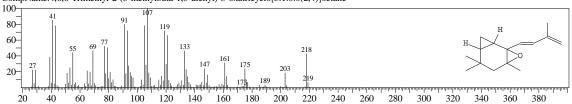
CompName: 2-Methyl-4-(2,6,6-trimethylcyclohex-1-enyl)but-2-en-1-ol \$\$ (2E)-2-Methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-buten-1-ol #\$\$



Hit#:4 Entry:56331 Library:NIST11.lib

SI:61 Formula:C15H22O CAS:0-00-0 MolWeight:218 RetIndex:1407

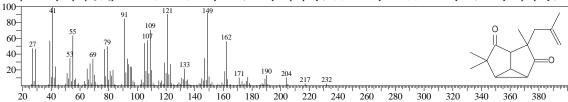
CompName: 4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane



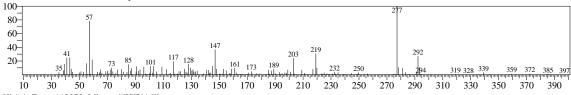
Hit#:5 Entry:66525 Library:NIST11.lib

SI:61 Formula:C15H20O2 CAS:94609-18-4 MolWeight:232 RetIndex:1518

CompName:Cyclopropa[c,d]pentalene-1,3-dione, hexahydro-4-(2-methyl-2-propenyl)-2,2,4-trimethyl- \$\$ 2,2,4-Trimethyl-4-(2-methyl-2-propenyl)hexahydro-4-(2-methyl-2-pro



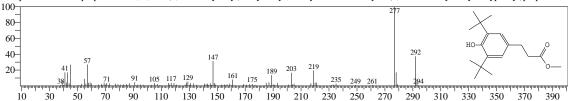
BG Mode:Calc. from Peak Group 1 - Event 1



Hit#:1 Entry:112373 Library:NIST11.lib

SI:69 Formula:C18H28O3 CAS:6386-38-5 MolWeight:292 RetIndex:2134

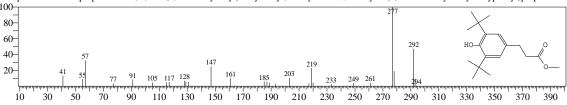
CompName:Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester \$\$ Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate \$



Hit#:2 Entry:25692 Library:NIST11s.lib

SI:64 Formula:C18H28O3 CAS:6386-38-5 MolWeight:292 RetIndex:2134

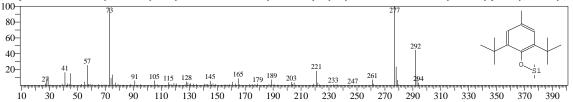
CompName:Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester \$\$ Methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate \$



Hit#:3 Entry:112386 Library:NIST11.lib

SI:56 Formula:C18H32OSi CAS:18510-49-1 MolWeight:292 RetIndex:1745

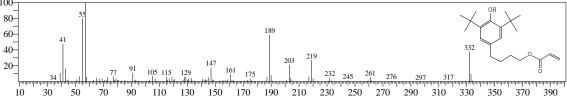
CompName:3,5-Di-tert-butyl-4-trimethylsiloxytoluene \$\$ 3,5-Di-t-butyl-4-trimethylsilyloxytoluene \$\$ (2,6-Ditert-butyl-4-methylphenoxy)(trimethyl):



Hit#:4 Entry:143271 Library:NIST11.lib

SI:55 Formula:C21H32O3 CAS:87033-84-9 MolWeight:332 RetIndex:2422

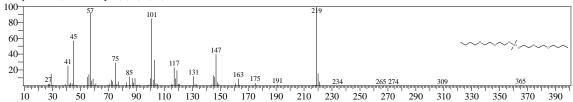
CompName:4-(3,5-Di-tert-butyl-4-hydroxyphenyl)butyl acrylate



Hit#:5 Entry:173012 Library:NIST11.lib

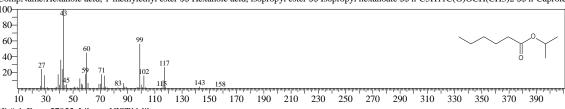
SI:52 Formula:C18H40O6Si CAS:0-00-0 MolWeight:380 RetIndex:2176

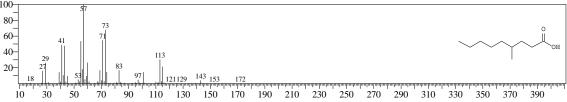
CompName: 12,12-Dimethyl-5,8,11,13,16,19-hexaoxa-12-silatricosane



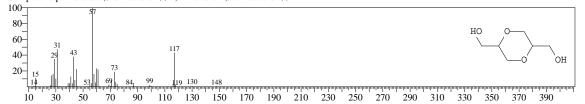
370

390



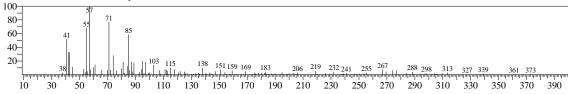


Hit#:5 Entry:14316 Library:NIST11.lib SI:64 Formula:C6H12O4 CAS:14236-12-5 MolWeight:148 RetIndex:1305 CompName:p-Dioxane-2,5-dimethanol \$\$ 1,4-Dioxane-2,5-dimethanol \$\$



Line#14 R.Time:9.725(Scan#:808) MassPeaks:197 RawMode:Averaged 9.717-9.733(807-809) BasePeak:57.05(6620)

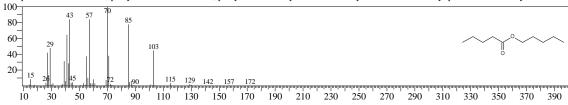
BG Mode:Calc. from Peak Group 1 - Event 1



Hit#:1 Entry:13093 Library:NIST11s.lib

SE:70 Formula:C10H2002 CAS:2173-56-0 MolWeight:172 RetIndex:1183

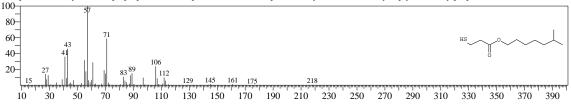
CompName:Pentanoic acid, pentyl ester \$\$ Valeric acid, pentyl ester \$\$ Amyl valerianate \$\$ Pentyl pentanoate \$\$ Pentyl valerate \$\$



Hit#:2 Entry:55950 Library:NIST11.lib

SI:68 Formula:C11H22O2S CAS:30374-01-7 MolWeight:218 RetIndex:1521

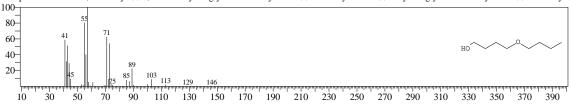
CompName:Isooctyl 3-mercaptopropionate \$\$ Propanoic acid, 3-mercapto-, isooctyl ester \$\$ 6-Methylheptyl 3-sulfanylpropanoate #\$\$



Hit#:3 Entry:8240 Library:NIST11s.lib

SI:68 Formula:C8H18O2 CAS:4161-24-4 MolWeight:146 RetIndex:1135

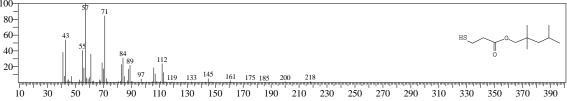
CompName: 1-Butanol, 4-butoxy- \$\$ 1,4-Tetrabutyleneglycol monobutyl ether \$\$ 4-Butoxybutanol \$\$ Butylene glycol monobutyl ether \$\$ 4-Butoxy-



Hit#:4 Entry:55949 Library:NIST11.lib

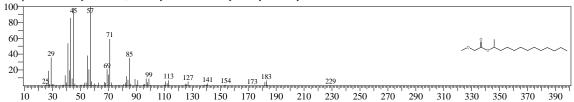
SI:68 Formula:C11H22O2S CAS:77916-53-1 MolWeight:218 RetIndex:1437

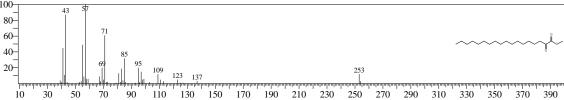
CompName:Propionic acid, 3-mercapto-, isooctyl ester \$\$ 2,2,4-Trimethylpentyl 3-sulfanylpropanoate #\$\$



Hit#:5 Entry:96802 Library:NIST11.lib SI:68 Formula:C16H32O3 CAS:0-00-0 MolWeight:272 RetIndex:1791

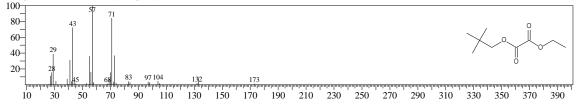
CompName:Methoxyacetic acid, 2-tridecyl ester \$\$ 1-Methyldodecyl methoxyacetate # \$\$

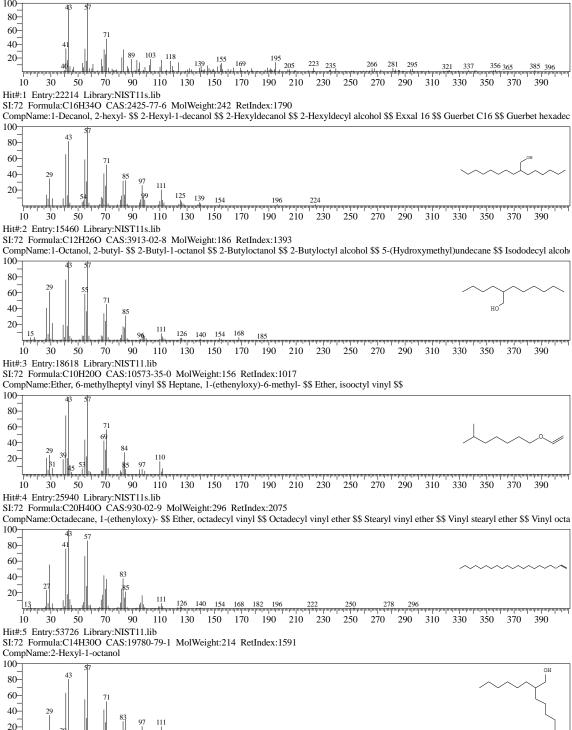




Hit#:5 Entry:35968 Library:NIST11.lib SI:66 Formula:C9H16O4 CAS:0-00-0 MolWeight:188 RetIndex:1166

CompName:Oxalic acid, ethyl neopentyl ester





 310 340

280

130 160

100

10 40

190

220 250

370 400

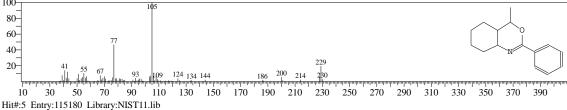
430

460

490

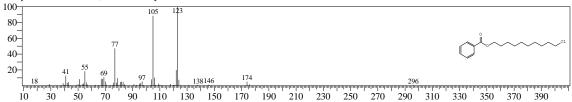
520

550 580



SI:70 Formula:C17H25ClO2 CAS:0-00-0 MolWeight:296 RetIndex:2180

CompName:Benzoic acid, 10-chlorodecyl ester



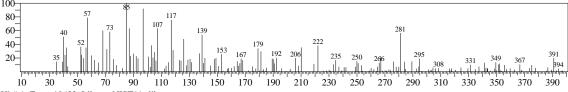
190 210

150 170

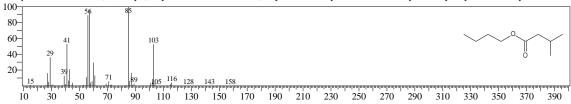
60-40-20-

Line#:27 R.Time:11.392(Scan#:1008) MassPeaks:195 RawMode:Averaged 11.383-11.400(1007-1009) BasePeak:85.20(2312)

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



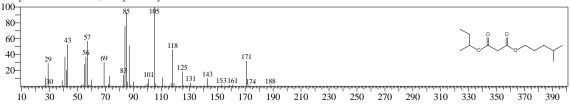
Hit#:1 Entry:10632 Library:NIST11s.lib SI:43 Formula:C9H18O2 CAS:109-19-3 MolWeight:158 RetIndex:1019 CompName:Butanoic acid, 3-methyl-, butyl ester \$\$ Isovaleria caid, butyl ester \$\$ Butyl isovalerate \$\$ Butyl 3-methylbutyrate \$\$ 1-Butyl isovalerate



Hit#:2 Entry:74977 Library:NIST11.lib

SI:42 Formula:C13H24O4 CAS:0-00-0 MolWeight:244 RetIndex:1520

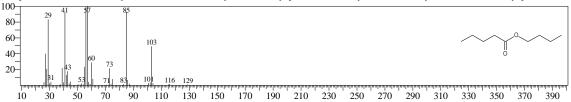
CompName:Malonic acid, 2-butyl isohexyl ester



Hit#:3 Entry:10607 Library:NIST11s.lib

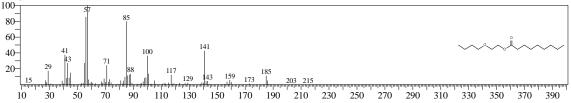
SI:42 Formula:C9H18O2 CAS:591-68-4 MolWeight:158 RetIndex:1083

CompName:Pentanoic acid, butyl ester \$\$ Valeric acid, butyl ester \$\$ Butyl pentanoate \$\$ Butyl valerate \$\$ Butyl valerianate \$\$ n-Butyl pentanoate \$\$



Hit#:4 Entry:85829 Library:NIST11.lib SI:41 Formula:C15H30O3 CAS:0-00-0 MolWeight:258 RetIndex:1755

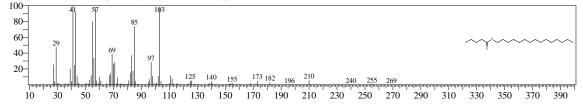
CompName:2-Butoxyethyl nonanoate



Hit#:5 Entry:128146 Library:NIST11.lib

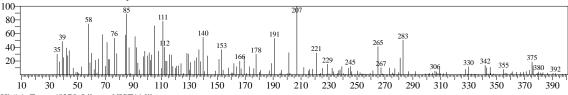
SI:41 Formula:C20H40O2 CAS:125164-53-6 MolWeight:312 RetIndex:2177

CompName: Valeric acid, pentadecyl ester \$\$ Pentadecyl pentanoate # \$\$



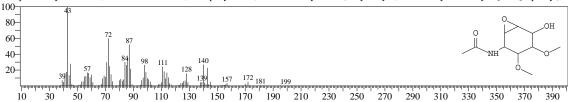
Line#:28 R.Time:11.550(Scan#:1027) MassPeaks:197 RawMode:Averaged 11.542-11.558(1026-1028) BasePeak:207.00(1512)

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



Hit#:1 Entry:65375 Library:NIST11.lib

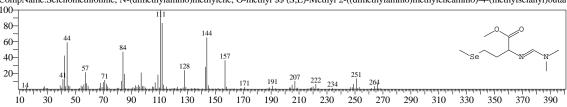
Si:42 Formula:C10H17NO5 CAS:0-00-0 MolWeight:231 RetIndex:1753
CompName:Cyclohexanol, 1R-4cis-acetamido-5,6cis-epoxy-2trans,3cis-dimethoxy- \$\$ N-(5-Hydroxy-3,4-dimethoxy-7-oxabicyclo[4.1.0]hept-2-yl)ac



Hit#:2 Entry:91117 Library:NIST11.lib

SI:41 Formula:C9H18N2O2Se CAS:0-00-0 MolWeight:266 RetIndex:0

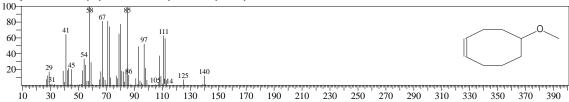
CompName: Selenomethionine, N-(dimethylamino)methylene, O-methyl \$\$ (S,E)-Methyl 2-((dimethylamino)methyleneamino)-4-(methylselanyl)butar



Hit#:3 Entry:11271 Library:NIST11.lib

SI:41 Formula:C9H16O CAS:32160-45-5 MolWeight:140 RetIndex:1078

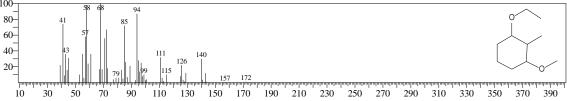
CompName:5-Methoxy-cyclooctene \$\$ 4-Cycloocten-1-yl methyl ether # \$\$



Hit#:4 Entry:27069 Library:NIST11.lib

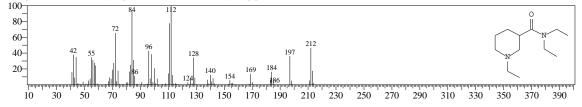
SI:41 Formula:C10H20O2 CAS:59014-00-5 MolWeight:172 RetIndex:1154

CompName:1R-Ethoxy-3-cis-methoxy-2-cis-methylcyclohexane \$\$ 1-Ethoxy-3-methoxy-2-methylcyclohexane #\$\$



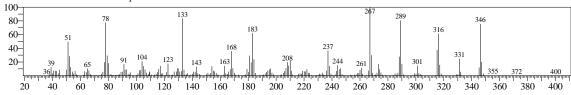
Hit#:5 Entry:52143 Library:NIST11.lib

SI:41 Formula:C12H24N2O CAS:3367-94-0 MolWeight:212 RetIndex:1592 CompName:N,N,N'-Triethylnipecotamide \$\$ N,N,1-Triethyl-3-piperidinecarboxamide #\$\$

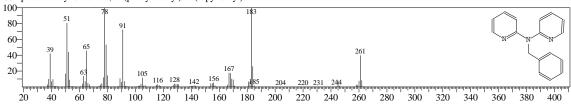


Line#:29 R.Time:11.900(Scan#:1069) MassPeaks:330 RawMode:Averaged 11.892-11.908(1068-1070) BasePeak:267.15(187703)

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

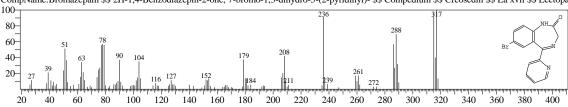


Hit#:1 Entry:88042 Library:NIST11.lib SI:47 Formula:C17H15N3 CAS:0-00-0 MolWeight:261 RetIndex:2176 CompName:2-Pyridinamine, N-(phenylmethyl)-N-(2-pyridinyl)-



Hit#:2 Entry:129976 Library:NIST11.lib

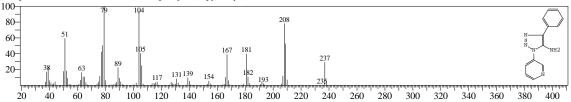
SI:46 Formula:C14H10BrN3O CAS:1812-30-2 MolWeight:315 RetIndex:2446 CompName:Bromazepam \$\$ 2H-1,4-Benzodiazepin-2-one, 7-bromo-1,3-dihydro-5-(2-pyridinyl)- \$\$ Compedium \$\$ Creosedin \$\$ La xvii \$\$ Lectopa



Hit#:3 Entry:69754 Library:NIST11.lib

SI:44 Formula:C13H11N5 CAS:0-00-0 MolWeight:237 RetIndex:0

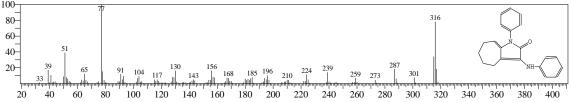
CompName: 1H-1,2,3-Triazol-5-amine, 4-phenyl-1-(3-pyridinyl)-



Hit#:4 Entry:131270 Library:NIST11.lib

SI:43 Formula:C21H20N2O CAS:0-00-0 MolWeight:316 RetIndex:2878

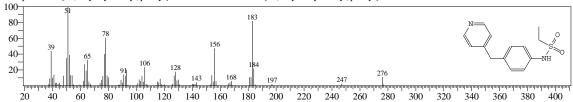
CompName:Cyclohepta[b]pyrrol-2(1H)-one, 4,5,6,7-tetrahydro-1-phenyl-3-(phenylamino)-



Hit#:5 Entry:99496 Library:NIST11.lib

SI:42 Formula:C14H16N2O2S CAS:333352-34-4 MolWeight:276 RetIndex:2378

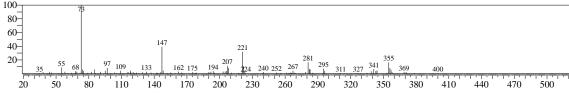
CompName:N-[4-(4-Pyridylmethyl)phenyl]ethanesulfonamide \$\$ N-[4-(4-Pyridinylmethyl)phenyl]ethanesulfonamide #\$\$



Line#:30 R.Time:16.367(Scan#:1605) MassPeaks:199

RawMode: Averaged 16.358-16.375(1604-1606) BasePeak: 73.05(10103)

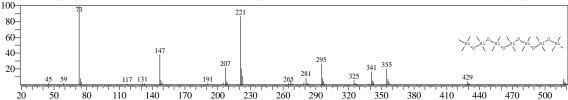
BG Mode:Calc. from Peak Group 1 - Event 1



Hit#:1 Entry:207275 Library:NIST11.lib

SI:74 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437

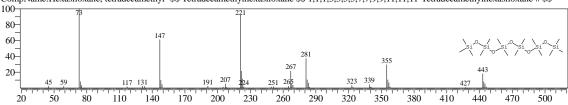
CompName:Heptasiloxane, hexadecamethyl- \$\$ Hexadecamethylheptasiloxane \$\$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane



Hit#:2 Entry:198359 Library:NIST11.lib

SI:70 Formula:C14H42O5Si6 CAS:107-52-8 MolWeight:458 RetIndex:1252

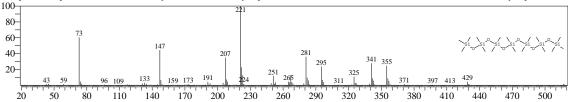
CompName:Hexasiloxane, tetradecamethyl- \$\$ Tetradecamethylhexasiloxane \$\$ 1,1,1,3,3,5,5,7,9,9,11,11,11-Tetradecamethylhexasiloxane #\$\$



Hit#:3 Entry:30665 Library:NIST11s.lib

SI:69 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437

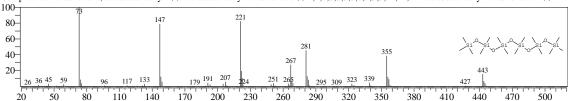
CompName:Heptasiloxane, hexadecamethyl- \$\$ Hexadecamethylheptasiloxane \$\$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane



Hit#:4 Entry:30338 Library:NIST11s.lib

SI:68 Formula:C14H42O5Si6 CAS:107-52-8 MolWeight:458 RetIndex:1252

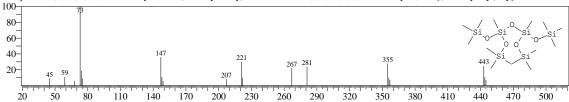
CompName:Hexasiloxane, tetradecamethyl-\$\$ Tetradecamethylhexasiloxane \$\$ 1,1,1,3,3,5,5,7,7,9,9,11,11.11-Tetradecamethylhexasiloxane #\$\$



Hit#:5 Entry:198358 Library:NIST11.lib

SI:68 Formula:C14H42O5Si6 CAS:2003-92-1 MolWeight:458 RetIndex:1252

CompName:1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane \$\$ 1,1,1,3,5,7,7,7-Octamethyl-3,5-bis[(trimethylsilyl)oxy]tetrasiloxane #



					Peak R	eport TIC				
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	4.869	4.792	5.117	385493	0.53	27858	0.23	13.84		1,4-Cyclohexanedione
2	6.464	6.375	6.742	1825700	2.51	247061	2.08	7.39		3-Buten-2-ol, 2-methyl-4-(1,3,3-trimetl
3	6.793	6.742	6.908	201829	0.28	48856	0.41	4.13	V	1-Dodecene
4	7.586	7.533	7.608	226390	0.31	82915	0.70	2.73		Cyclodecane
5	7.714	7.608	7.967	6310110	8.66	627513	5.27	10.06	V	4-Hexenoic acid, 2-acetyl-2-methyl-, et
6	8.015	7.967	8.092	1075395	1.48	224045	1.88	4.80	V	Phenol, 3,5-bis(1,1-dimethylethyl)-
7	8.158	8.092	8.200	334882	0.46	49014	0.41	6.83	V	Quinic acid
8	8.248	8.200	8.300	389857	0.54	106118	0.89	3.67	V	n-Tetracosanol-1
9	8.345	8.300	8.425	197569	0.27	51504	0.43	3.84	V	Isoaromadendrene epoxide
10	8.841	8.783	8.892	201545	0.28	52996	0.45	3.80		1-Hexadecanol
11	8.942	8.892	9.000	147234	0.20	38504	0.32	3.82	V	2H-Cyclopropa[g]benzofuran, 4,5,5a,6
12	9.265	9.225	9.325	228182	0.31	61534	0.52	3.71	V	Benzenepropanoic acid, 3,5-bis(1,1-dir
13	9.445	9.325	9.500	318223	0.44	41656	0.35	7.64	V	Hexanoic acid, propyl ester
14	9.725	9.500	9.758	970907	1.33	113025	0.95	8.59	V	Pentanoic acid, pentyl ester
15	9.817	9.758	9.850	818223	1.12	165925	1.39	4.93	V	4-Methylnonanoic acid
16	9.900	9.850	9.925	925055	1.27	221538	1.86	4.18	V	1-Decanol, 2-hexyl-
17	9.981	9.925	10.025	2061704	2.83	411934	3.46	5.00	V	Behenyl chloride
18	10.155	10.025	10.192	4379897	6.01	534605	4.49	8.19	V	Sulfurous acid, pentadecyl 2-propyl est
19	10.241	10.192	10.275	2764954	3.80	592148	4.98	4.67	V	Nonadecane, 2-methyl-
20	10.342	10.275	10.392	5485851	7.53	1003930	8.44	5.46	V	2,N-Dibenzoyl-6-hexanelactam
21	10.410	10.392	10.450	2466683	3.39	728873	6.12	3.38	V	Hexane, 1-(hexyloxy)-5-methyl-
22	10.494	10.450	10.533	3548425	4.87	735810	6.18	4.82	V	Heptadecane, 2,6,10,14-tetramethyl-
23	10.578	10.533	10.617	3626499	4.98	745627	6.26	4.86	V	Decane, 5-propyl-
24	10.653	10.617	10.717	4203746	5.77	738117	6.20	5.70	V	4-Methyldocosane
25	10.751	10.717	10.817	3838938	5.27	659313	5.54	5.82	V	Decane, 3,4-dimethyl-
26	10.845	10.817	11.375	13729167	18.85	623003	5.23	22.04	V	Decane, 5,6-bis(2,2-dimethylpropylide
27	11.392	11.375	11.525	1683029	2.31	221450	1.86	7.60	V	Butanoic acid, 3-methyl-, butyl ester
28	11.550	11.525	11.825	1949882	2.68	147607	1.24	13.21	V	Cyclohexanol, 1R-4cis-acetamido-5,6c
29	11.900	11.825	12.317	8390406	11.52	2569219	21.59	3.27	SV	2-Pyridinamine, N-(phenylmethyl)-N-(
30	16.364	16.292	16.492	166111	0.23	29996	0.25	5.54		Heptasiloxane, hexadecamethyl-
				72851886	100.00	11901694	100.00			- ·