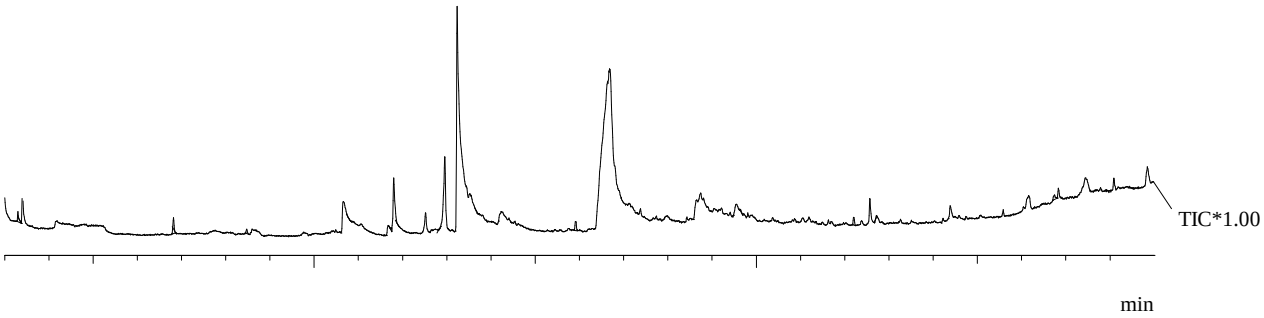
Sample Information

| | |
|---|---|
| Analyzed by | : Admin |
| Analyzed | : 2018-5-7 23:19:23 |
| Sample Type | : Unknown |
| Level # | : 1 |
| Sample Name | : 2018-5-7-4-2 |
| Sample ID | : |
| IS Amount | : [1]=1.000 |
| Sample Amount | : 1.000 |
| Dilution Factor | : 1.000 |
| Vial # | : 1 |
| Injection Volume | : 1.000 |
| Data File | : E:\陈存\GC-MS硫化物\2018-5-7-4-2.qgd |
| Org Data File | : E:\刘春宏\2018-5-7-4-2.qgd |
| Method File | : E:\刘春宏\2018-5-7-1.qgm |
| Org Method File | : E:\刘春宏\2018-5-7-1.qgm |
| Report File | : |
| Tuning File | : C:\GCMSsolution\System\Tune1\2017-3-21.qgt |
| Modified by | : Admin |
| Modified | : 2018-5-7 23:48:23 |

Chromatogram 2018-5-7-4-2 E:\陈存\GC-MS硫化物\2018-5-7-4-2.qgd

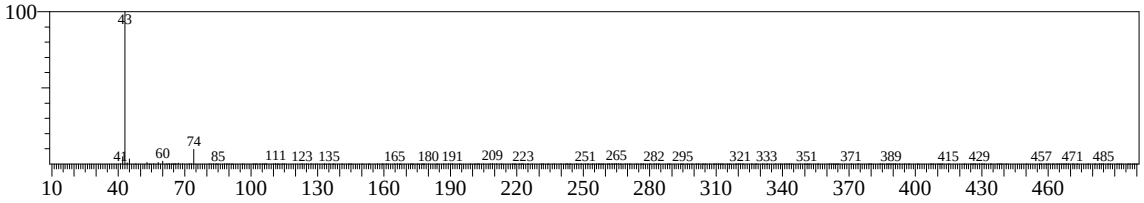



Peak Report TIC

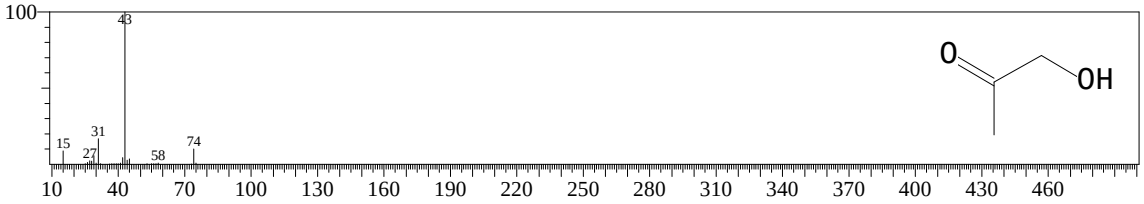
| Peak# | R.Time | I.Time | F.Time | Area | Area% | Height | Height% | A/H | Mark | Name |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.300 | 3.275 | 3.383 | 106994 | 0.37 | 55828 | 1.34 | 1.91 | | |
| 2 | 6.817 | 6.783 | 6.867 | 172277 | 0.59 | 89051 | 2.14 | 1.93 | | |
| 3 | 8.472 | 8.442 | 8.533 | 45330 | 0.16 | 24307 | 0.59 | 1.86 | | |
| 4 | 10.662 | 10.608 | 10.808 | 917429 | 3.16 | 156361 | 3.76 | 5.86 | | |
| 5 | 11.667 | 11.633 | 11.758 | 228135 | 0.79 | 50278 | 1.21 | 4.53 | | |
| 6 | 11.800 | 11.758 | 11.917 | 958915 | 3.31 | 293235 | 7.06 | 3.27 | V | |
| 7 | 12.520 | 12.467 | 12.600 | 283801 | 0.98 | 103462 | 2.49 | 2.74 | | |
| 8 | 12.954 | 12.858 | 13.017 | 1291975 | 4.46 | 397258 | 9.56 | 3.25 | | |
| 9 | 13.234 | 13.192 | 13.492 | 7765811 | 26.78 | 1248326 | 30.05 | 6.22 | | |
| 10 | 13.550 | 13.492 | 13.708 | 1013166 | 3.49 | 134574 | 3.24 | 7.52 | V | |
| 11 | 14.422 | 14.397 | 14.472 | 475092 | 1.64 | 55073 | 1.33 | 8.62 | | |
| 12 | 15.915 | 15.875 | 15.950 | 105762 | 0.36 | 51888 | 1.25 | 2.03 | | |
| 13 | 16.686 | 16.350 | 16.883 | 12993449 | 44.81 | 818285 | 19.70 | 15.87 | | |
| 14 | 18.642 | 18.575 | 18.700 | 539470 | 1.86 | 98398 | 2.37 | 5.48 | | |
| 15 | 18.741 | 18.700 | 18.792 | 582071 | 2.01 | 127829 | 3.08 | 4.55 | V | |
| 16 | 18.808 | 18.792 | 18.883 | 322597 | 1.11 | 89371 | 2.15 | 3.60 | V | |
| 17 | 18.917 | 18.883 | 18.950 | 67644 | 0.23 | 23736 | 0.57 | 2.84 | V | |
| 18 | 19.548 | 19.483 | 19.692 | 416238 | 1.44 | 61793 | 1.49 | 6.73 | | |
| 19 | 22.203 | 22.175 | 22.242 | 81481 | 0.28 | 43909 | 1.06 | 1.85 | | |
| 20 | 22.570 | 22.525 | 22.658 | 334072 | 1.15 | 139636 | 3.36 | 2.39 | | |
| 21 | 24.387 | 24.342 | 24.458 | 209896 | 0.72 | 68997 | 1.66 | 3.04 | | |
| 22 | 26.733 | 26.700 | 26.808 | 82626 | 0.28 | 22239 | 0.54 | 3.71 | | |
| | | | | 28994231 | 100.00 | 4153834 | 100.00 | | | |

Library

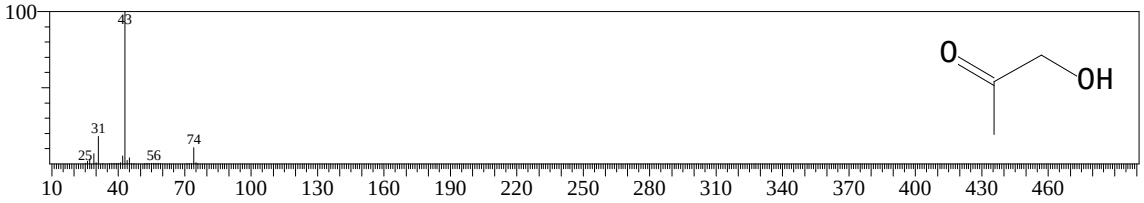
<< Target >>
Line#:1 R.Time:3.300(Scan#:37) MassPeaks:226 BasePeak:42.95(37650)
RawMode:Averaged 3.292-3.308(36-38) BG Mode:Calc. from Peak



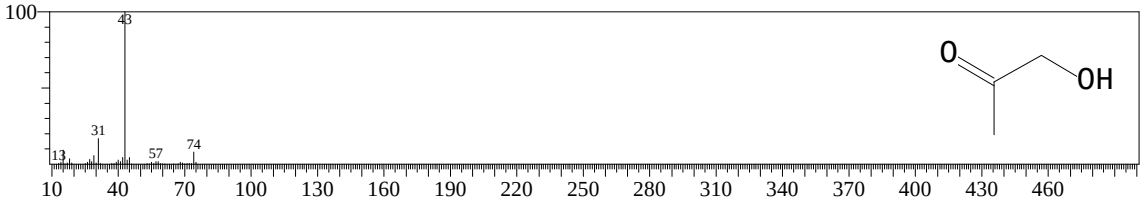

Hit#:1 Entry:368 Library:NIST05.LIB
SI:95 Formula:C3H6O2 CAS:116-9-6 MolWeight:74 RetIndex:698
CompName:2-Propanone, 1-hydroxy- $$ Acetol $$ CH3C(O)CH2OH $$ Hydroxyacetone $$ Acetone alcohol $$ Acetylcarbinol $$



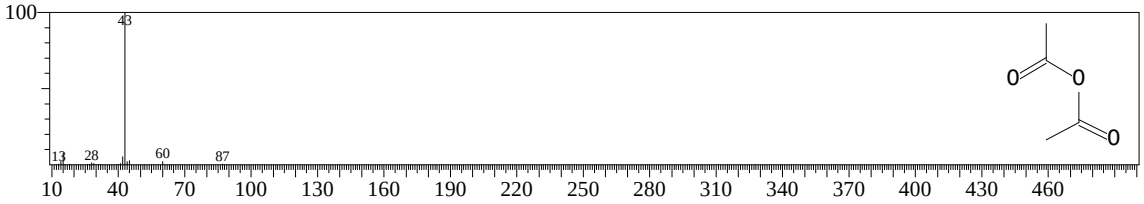

Hit#:2 Entry:415 Library:NIST05s.LIB
SI:94 Formula:C3H6O2 CAS:116-9-6 MolWeight:74 RetIndex:698
CompName:2-Propanone, 1-hydroxy- $$ Acetol $$ CH3C(O)CH2OH $$ Hydroxyacetone $$ Acetone alcohol $$ Acetylcarbinol $$



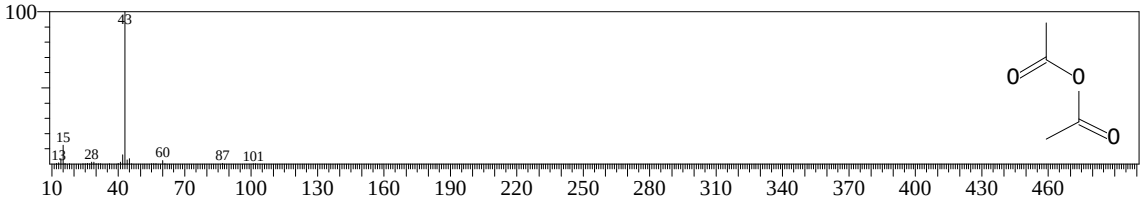

Hit#:3 Entry:414 Library:NIST05s.LIB
SI:93 Formula:C3H6O2 CAS:116-9-6 MolWeight:74 RetIndex:698
CompName:2-Propanone, 1-hydroxy- $$ Acetol $$ CH3C(O)CH2OH $$ Hydroxyacetone $$ Acetone alcohol $$ Acetylcarbinol $$



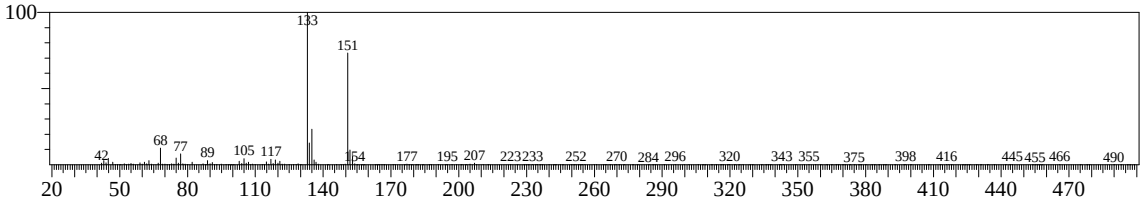

Hit#:4 Entry:1954 Library:NIST05s.LIB
SI:91 Formula:C4H6O3 CAS:108-24-7 MolWeight:102 RetIndex:722
CompName:Acetic anhydride $$ Acetic acid, anhydride $$ Acetic oxide $$ Acetyl anhydride $$ Acetyl ether $$ Acetyl oxide $$ Et



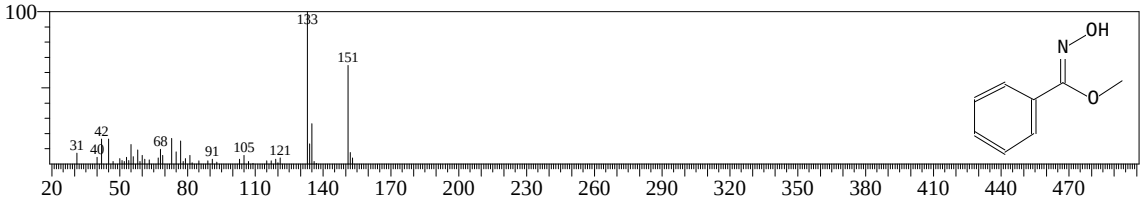

Hit#:5 Entry:1953 Library:NIST05s.LIB
SI:91 Formula:C4H6O3 CAS:108-24-7 MolWeight:102 RetIndex:722
CompName:Acetic anhydride $$ Acetic acid, anhydride $$ Acetic oxide $$ Acetyl anhydride $$ Acetyl ether $$ Acetyl oxide $$ Et



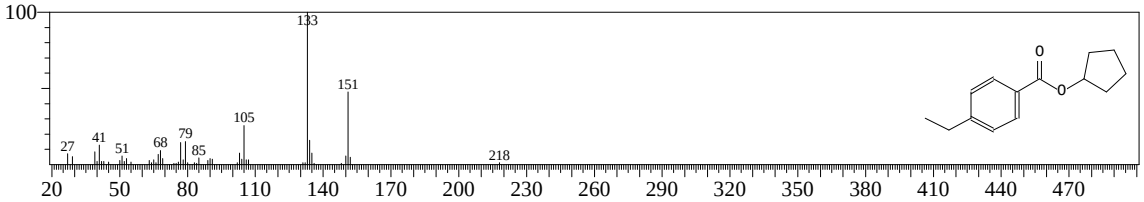
<< Target >>
Line#:2 R.Time:6.817(Scan#:459) MassPeaks:232 BasePeak:132.95(25200)
RawMode:Averaged 6.808-6.825(458-460) BG Mode:Calc. from Peak



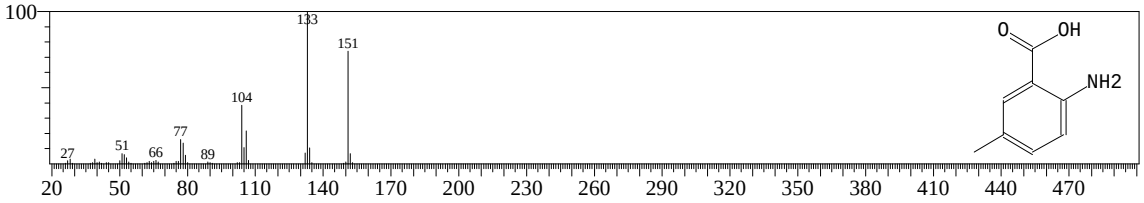

Hit#:1 Entry:15209 Library:NIST05.LIB
SI:85 Formula:C8H9NO2 CAS:0-0-0 MolWeight:151 RetIndex:1301
CompName:Oxime-, methoxy-phenyl-_



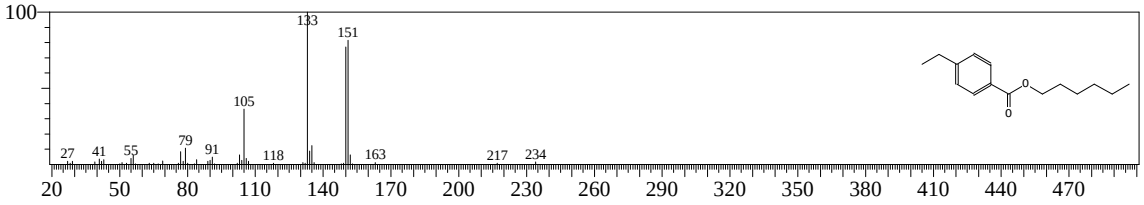

Hit#:2 Entry:51823 Library:NIST05.LIB
SI:79 Formula:C14H18O2 CAS:0-0-0 MolWeight:218 RetIndex:1714
CompName:4-Ethylbenzoic acid, cyclopentyl ester



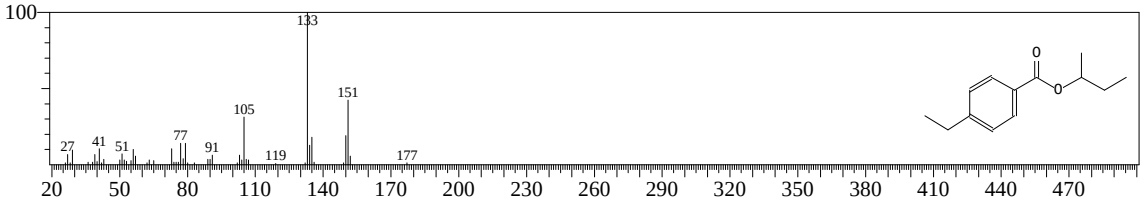

Hit#:3 Entry:15206 Library:NIST05.LIB
SI:79 Formula:C8H9NO2 CAS:2941-78-8 MolWeight:151 RetIndex:1575
CompName:2-Amino-5-methylbenzoic acid $$ 5-Methylanthranilic acid $$ Benzoic acid, 2-amino-5-methyl- $$ m-Toluic acid, 6-a



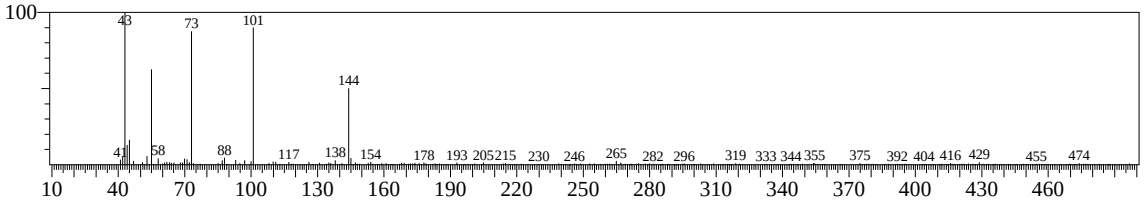

Hit#:4 Entry:61585 Library:NIST05.LIB
SI:78 Formula:C15H22O2 CAS:0-0-0 MolWeight:234 RetIndex:1770
CompName:4-Ethylbenzoic acid, hexyl ester



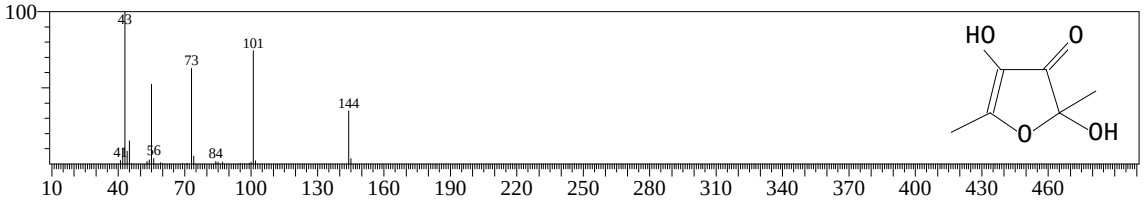

Hit#:5 Entry:44608 Library:NIST05.LIB
SI:77 Formula:C13H18O2 CAS:0-0-0 MolWeight:206 RetIndex:1507
CompName:4-Ethylbenzoic acid, 2-butyl ester



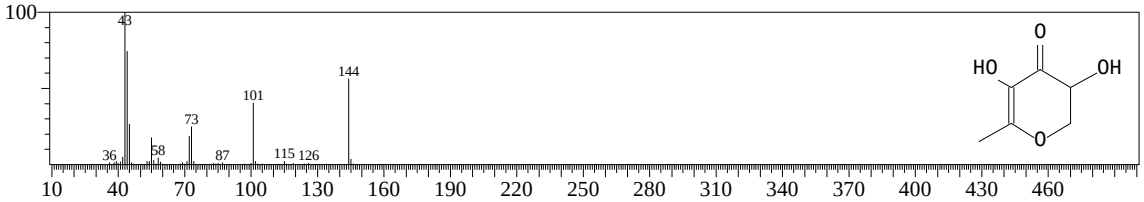
<< Target >>
Line#:3 R.Time:8.475(Scan#:658) MassPeaks:241 BasePeak:43.00(5010)
RawMode:Averaged 8.467-8.483(657-659) BG Mode:Calc. from Peak



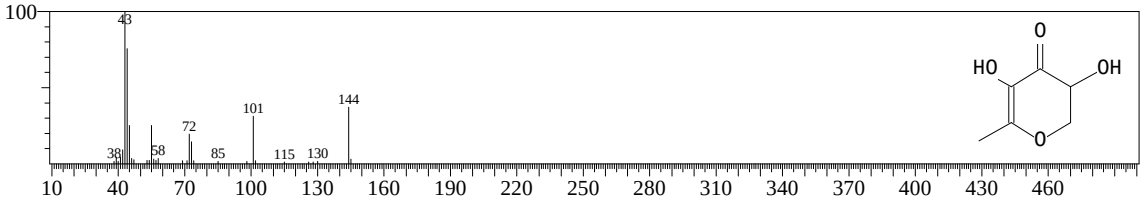

Hit#:1 Entry:12371 Library:NIST05.LIB
SI:86 Formula:C6H8O4 CAS:10230-62-3 MolWeight:144 RetIndex:1173
CompName:2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one $$ 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone # $$



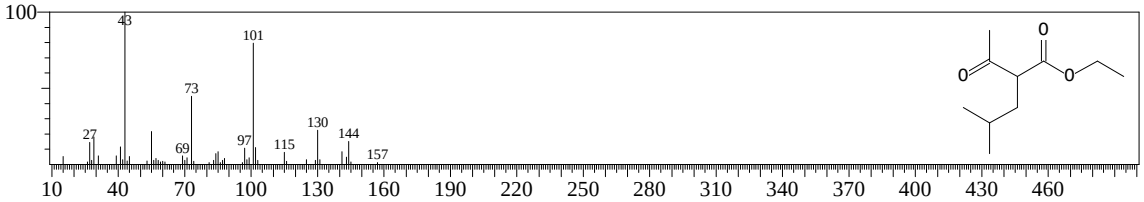

Hit#:2 Entry:7403 Library:NIST05s.LIB
SI:78 Formula:C6H8O4 CAS:28564-83-2 MolWeight:144 RetIndex:1269
CompName:4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- $$ 3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one # $$



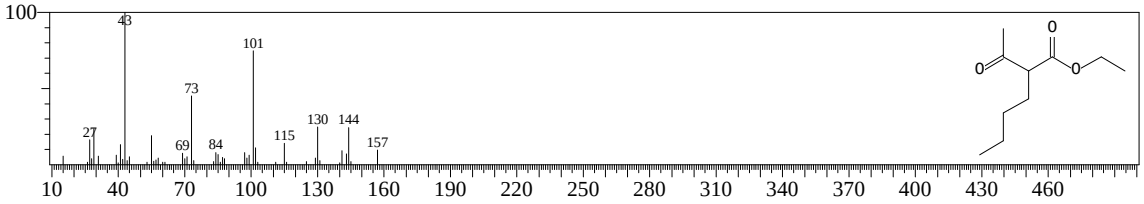

Hit#:3 Entry:12367 Library:NIST05.LIB
SI:75 Formula:C6H8O4 CAS:28564-83-2 MolWeight:144 RetIndex:1269
CompName:4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- $$ 3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one # $$



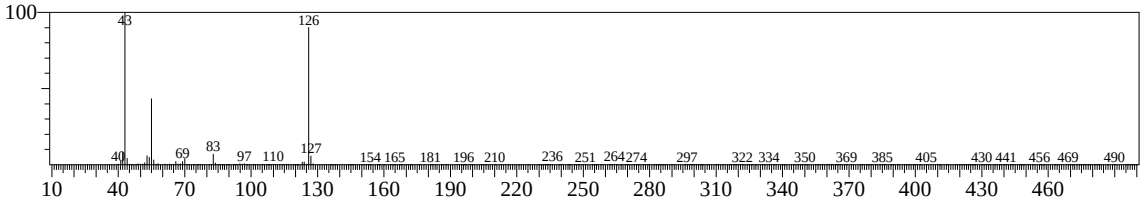

Hit#:4 Entry:33167 Library:NIST05.LIB
SI:74 Formula:C10H18O3 CAS:1522-34-5 MolWeight:186 RetIndex:1190
CompName:Pentanoic acid, 2-acetyl-4-methyl-, ethyl ester $$ Valeric acid, 2-acetyl-4-methyl-, ethyl ester $$ Ethyl 2-acetyl-4-methy



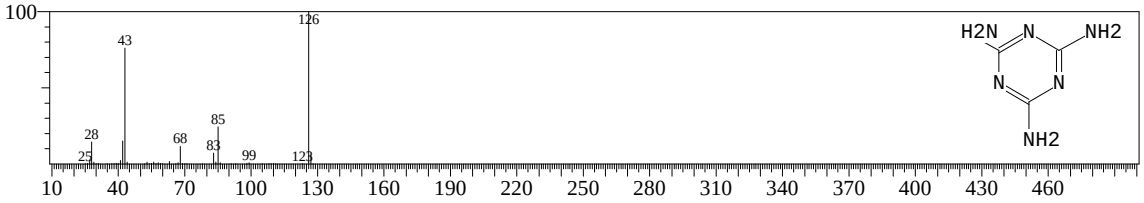

Hit#:5 Entry:33168 Library:NIST05.LIB
SI:73 Formula:C10H18O3 CAS:1540-29-0 MolWeight:186 RetIndex:1254
CompName:Hexanoic acid, 2-acetyl-, ethyl ester $$ Ethyl .alpha.-butylacetoacetate $$ Ethyl 2-acetylhexanoate $$ Ethyl 2-butylacet



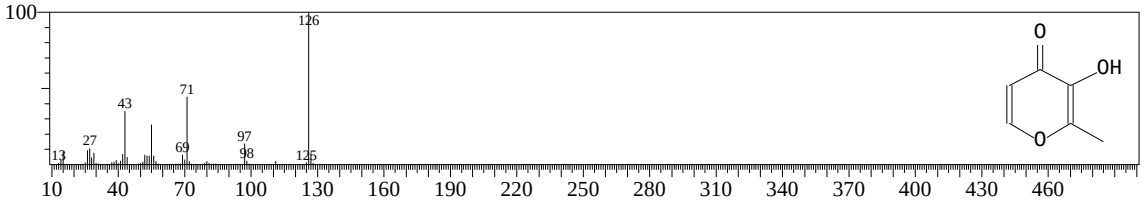
<< Target >>
Line#:4 R.Time:10.658(Scan#:920) MassPeaks:269 BasePeak:43.00(51947)
RawMode:Averaged 10.650-10.667(919-921) BG Mode:Calc. from Peak



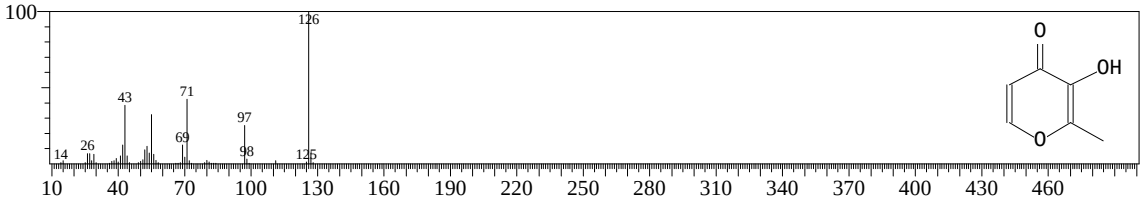

Hit#:1 Entry:4475 Library:NIST05s.LIB
SI:85 Formula:C3H6N6 CAS:108-78-1 MolWeight:126 RetIndex:1597
CompName:1,3,5-Triazine-2,4,6-triamine $$ Melamine $$ S-Triazinetriamine $$ Cyanuramide $$ Cyanurotriamide $$ Cyanurotria



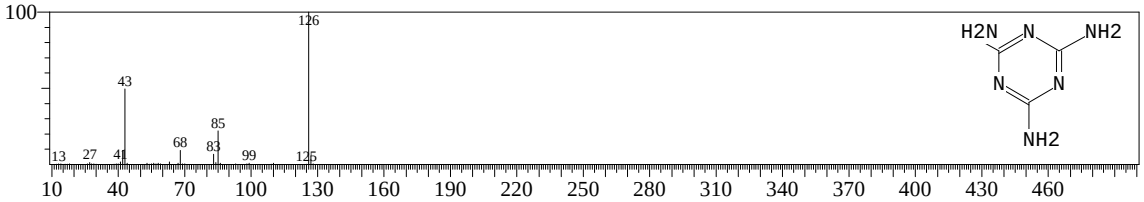

Hit#:2 Entry:6245 Library:NIST05.LIB
SI:82 Formula:C6H6O3 CAS:118-71-8 MolWeight:126 RetIndex:1063
CompName:Maltol $$ 4H-Pyran-4-one, 3-hydroxy-2-methyl- $$ Larixic acid $$ Larixinic acid $$ Palatone $$ 2-Methyl-3-hydroxyp



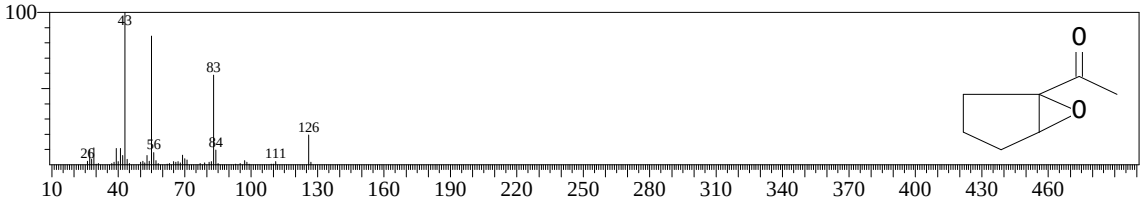

Hit#:3 Entry:4524 Library:NIST05s.LIB
SI:82 Formula:C6H6O3 CAS:118-71-8 MolWeight:126 RetIndex:1063
CompName:Maltol $$ 4H-Pyran-4-one, 3-hydroxy-2-methyl- $$ Larixic acid $$ Larixinic acid $$ Palatone $$ 2-Methyl-3-hydroxyp



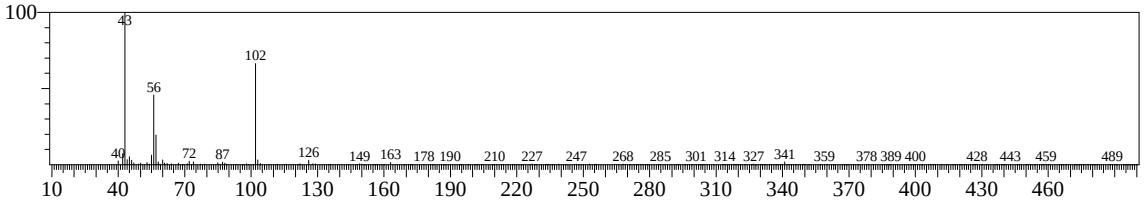

Hit#:4 Entry:6147 Library:NIST05.LIB
SI:82 Formula:C3H6N6 CAS:108-78-1 MolWeight:126 RetIndex:1597
CompName:1,3,5-Triazine-2,4,6-triamine $$ Melamine $$ S-Triazinetriamine $$ Cyanuramide $$ Cyanurotriamide $$ Cyanurotria



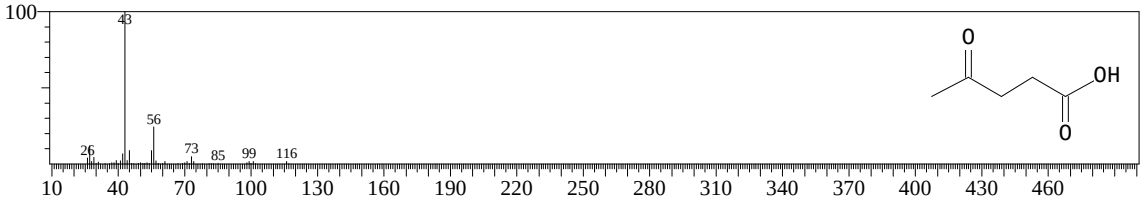

Hit#:5 Entry:6285 Library:NIST05.LIB
SI:81 Formula:C7H10O2 CAS:15121-2-5 MolWeight:126 RetIndex:920
CompName:Cyclopentane, 1-acetyl-1,2-epoxy- $$ 1-(6-Oxabicyclo[3.1.0]hex-1-yl)ethanone # $$



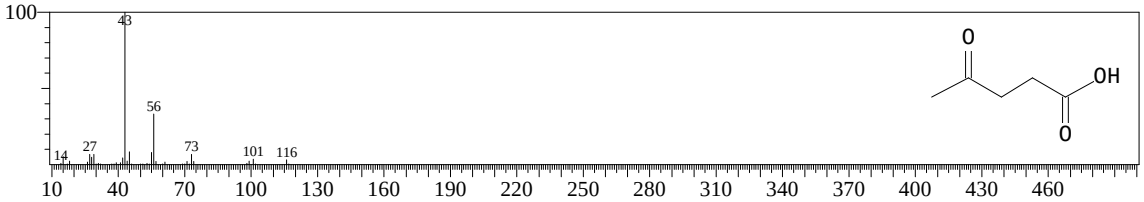
<< Target >>
Line#:5 R.Time:11.667(Scan#:1041) MassPeaks:252 BasePeak:43.00(14725)
RawMode:Averaged 11.658-11.675(1040-1042) BG Mode:Calc. from Peak



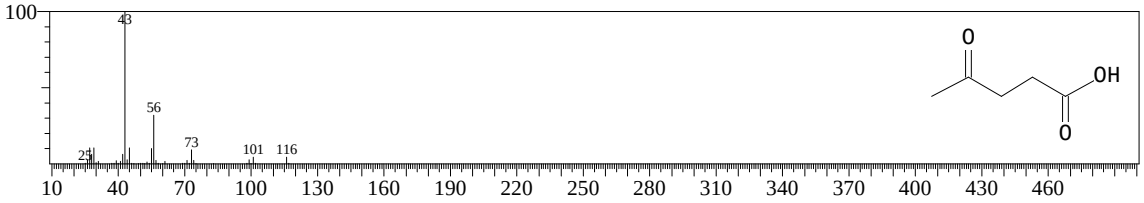

Hit#:1 Entry:3404 Library:NIST05s.LIB
SI:79 Formula:C5H8O3 CAS:123-76-2 MolWeight:116 RetIndex:1011
CompName:Pentanoic acid, 4-oxo- $$ Levulinic acid $$ .beta.-Acetylpropionic acid $$ .gamma.-Ketovaleric acid $$ Laevulinic aci



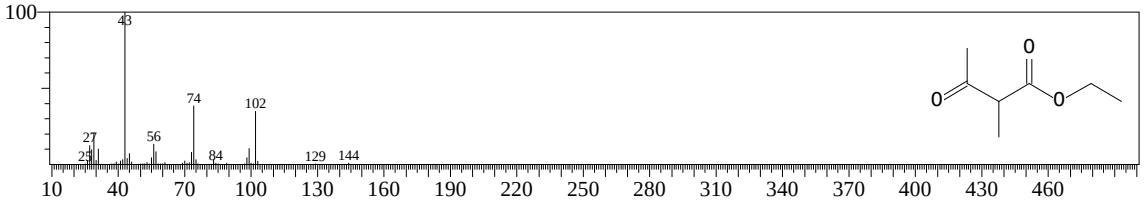

Hit#:2 Entry:4401 Library:NIST05.LIB
SI:79 Formula:C5H8O3 CAS:123-76-2 MolWeight:116 RetIndex:1011
CompName:Pentanoic acid, 4-oxo- $$ Levulinic acid $$ .beta.-Acetylpropionic acid $$ .gamma.-Ketovaleric acid $$ Laevulinic aci



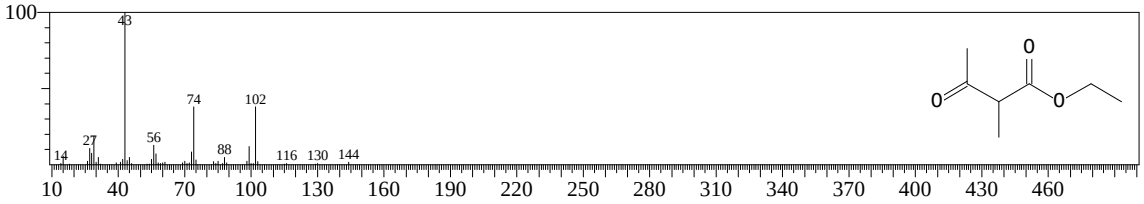

Hit#:3 Entry:3405 Library:NIST05s.LIB
SI:79 Formula:C5H8O3 CAS:123-76-2 MolWeight:116 RetIndex:1011
CompName:Pentanoic acid, 4-oxo- $$ Levulinic acid $$ .beta.-Acetylpropionic acid $$ .gamma.-Ketovaleric acid $$ Laevulinic aci



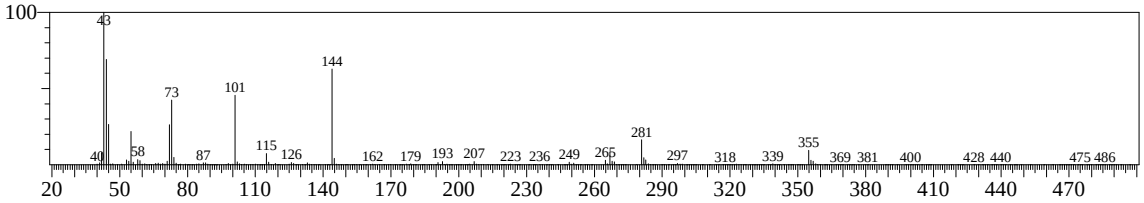

Hit#:4 Entry:7443 Library:NIST05s.LIB
SI:78 Formula:C7H12O3 CAS:609-14-3 MolWeight:144 RetIndex:956
CompName:Butanoic acid, 2-methyl-3-oxo-, ethyl ester $$ Acetoacetic acid, 2-methyl-, ethyl ester $$ .alpha.-Methylacetoacetic este



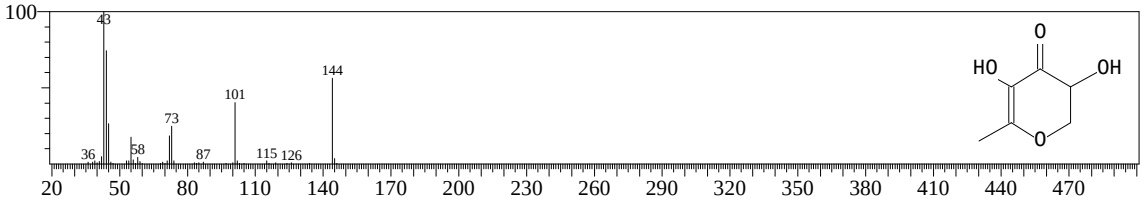

Hit#:5 Entry:7446 Library:NIST05s.LIB
SI:78 Formula:C7H12O3 CAS:609-14-3 MolWeight:144 RetIndex:956
CompName:Butanoic acid, 2-methyl-3-oxo-, ethyl ester $$ Acetoacetic acid, 2-methyl-, ethyl ester $$ .alpha.-Methylacetoacetic este



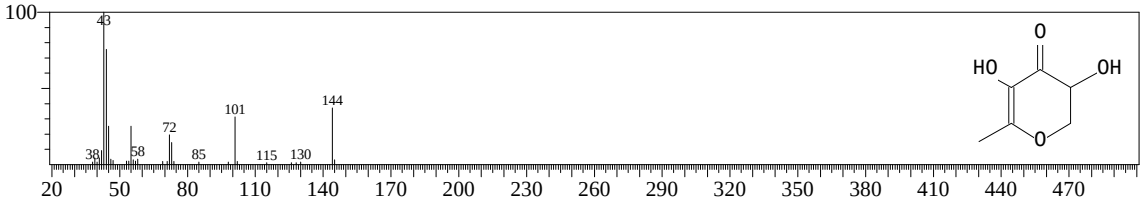
<< Target >>
Line#:6 R.Time:11.800(Scan#:1057) MassPeaks:314 BasePeak:43.00(46845)
RawMode:Averaged 11.792-11.808(1056-1058) BG Mode:Calc. from Peak



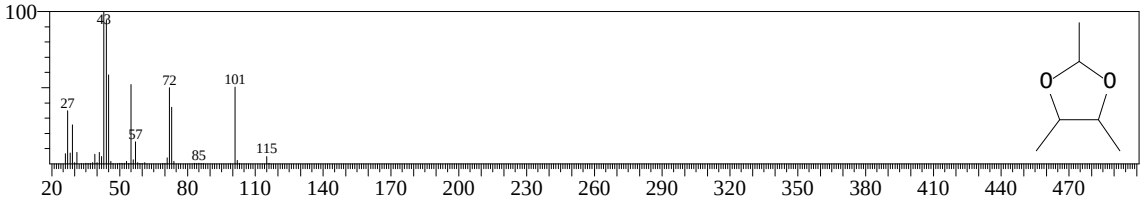

Hit#:1 Entry:7403 Library:NIST05s.LIB
SI:88 Formula:C6H8O4 CAS:28564-83-2 MolWeight:144 RetIndex:1269
CompName:4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- $$ 3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one # $$



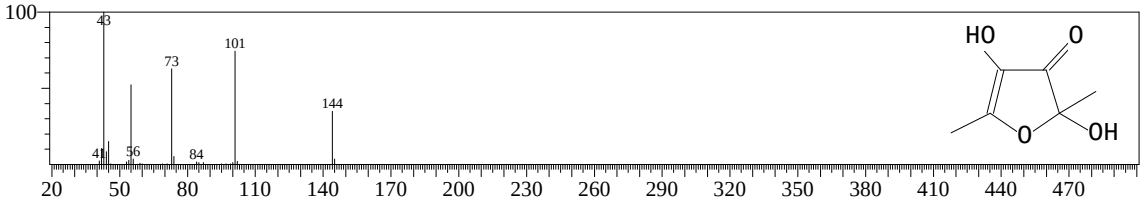

Hit#:2 Entry:12367 Library:NIST05.LIB
SI:84 Formula:C6H8O4 CAS:28564-83-2 MolWeight:144 RetIndex:1269
CompName:4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- $$ 3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one # $$



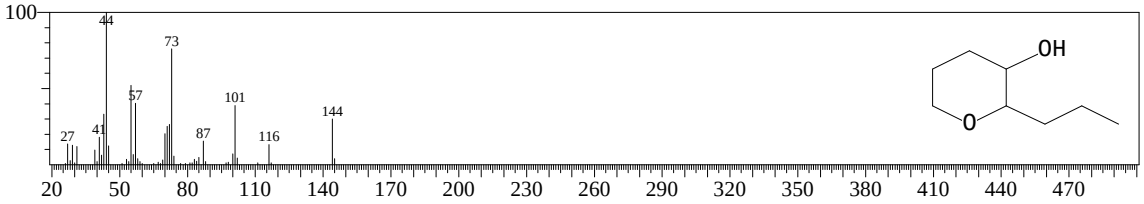

Hit#:3 Entry:4455 Library:NIST05.LIB
SI:77 Formula:C6H12O2 CAS:3299-32-9 MolWeight:116 RetIndex:761
CompName:1,3-Dioxolane, 2,4,5-trimethyl- $$ 2,4,5-Trimethyl-1,3-dioxolane # $$



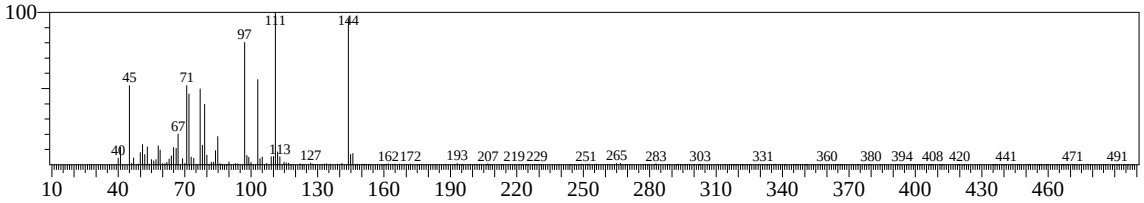

Hit#:4 Entry:12371 Library:NIST05.LIB
SI:76 Formula:C6H8O4 CAS:10230-62-3 MolWeight:144 RetIndex:1173
CompName:2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one $$ 2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone # $$



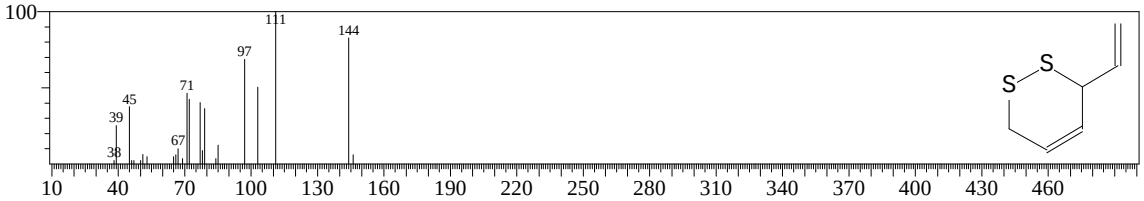

Hit#:5 Entry:12589 Library:NIST05.LIB
SI:72 Formula:C8H16O2 CAS:0-0-0 MolWeight:144 RetIndex:1156
CompName:2-Propyl-tetrahydropyran-3-ol



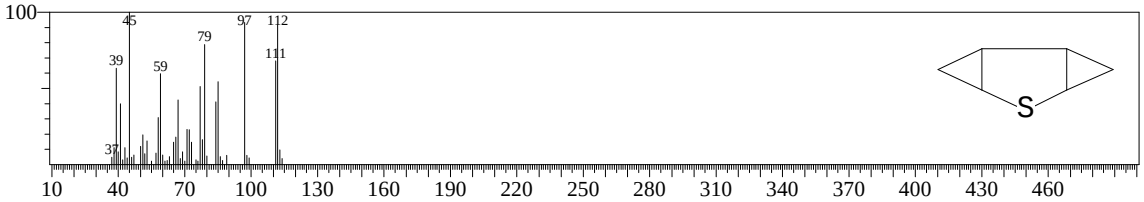
<< Target >>
Line#:7 R.Time:12.517(Scan#:1143) MassPeaks:250 BasePeak:110.95(11691)
RawMode:Averaged 12.508-12.525(1142-1144) BG Mode:Calc. from Peak



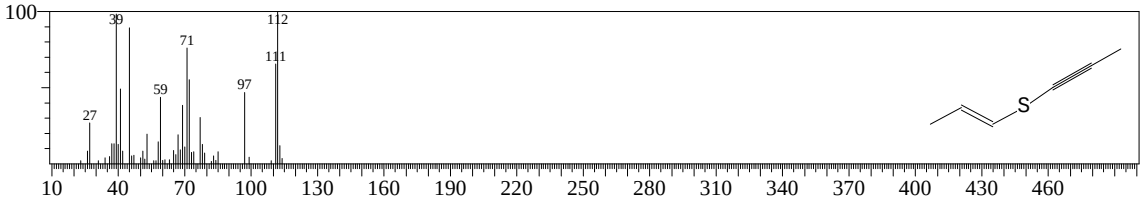

Hit#:1 Entry:12397 Library:NIST05.LIB
SI:86 Formula:C6H8S2 CAS:62488-52-2 MolWeight:144 RetIndex:1134
CompName:3-Vinyl-1,2-dithiacyclohex-4-ene $$ 3-Vinyl-3,6-dihydro-1,2-dithiine # $$



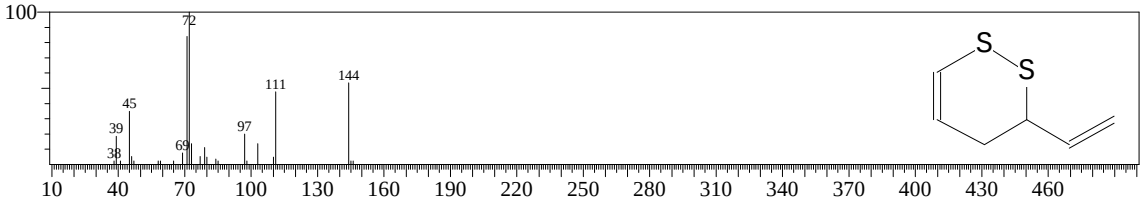

Hit#:2 Entry:3400 Library:NIST05.LIB
SI:72 Formula:C6H8S CAS:0-0-0 MolWeight:112 RetIndex:785
CompName:5-Thiatricyclo[4.1.0.0(2,4)]heptane



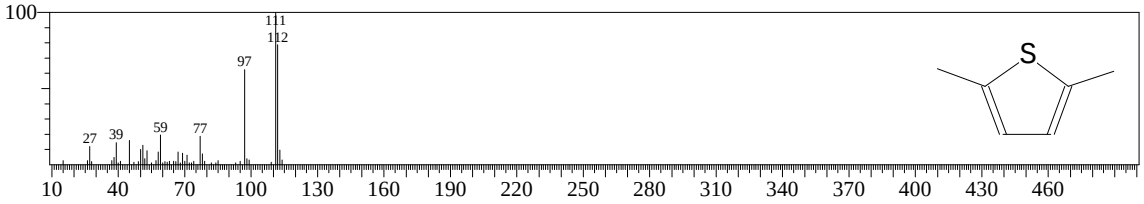

Hit#:3 Entry:3409 Library:NIST05.LIB
SI:71 Formula:C6H8S CAS:89533-93-7 MolWeight:112 RetIndex:894
CompName:Sulfide,1- propenyl 1-propynyl $$ (1E)-1-(1-Propynylsulfanyl)-1-propene # $$



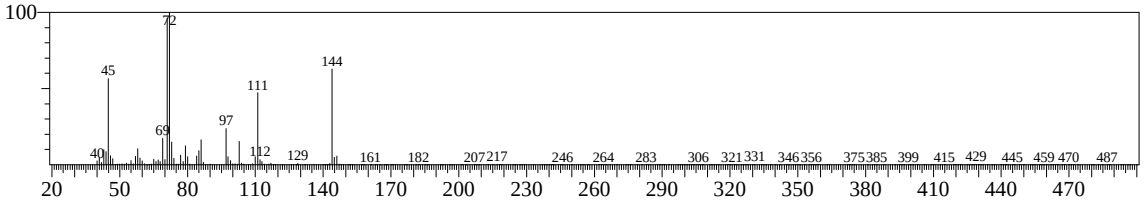

Hit#:4 Entry:12396 Library:NIST05.LIB
SI:70 Formula:C6H8S2 CAS:62488-53-3 MolWeight:144 RetIndex:1134
CompName:3-Vinyl-1,2-dithiacyclohex-5-ene $$ 3-Vinyl-3,4-dihydro-1,2-dithiine # $$



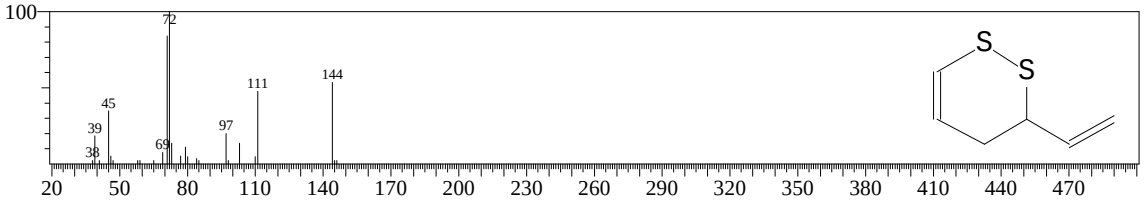

Hit#:5 Entry:3407 Library:NIST05.LIB
SI:67 Formula:C6H8S CAS:638-2-8 MolWeight:112 RetIndex:884
CompName:Thiophene, 2,5-dimethyl- $$ 2,5-Dimethylthiophene $$



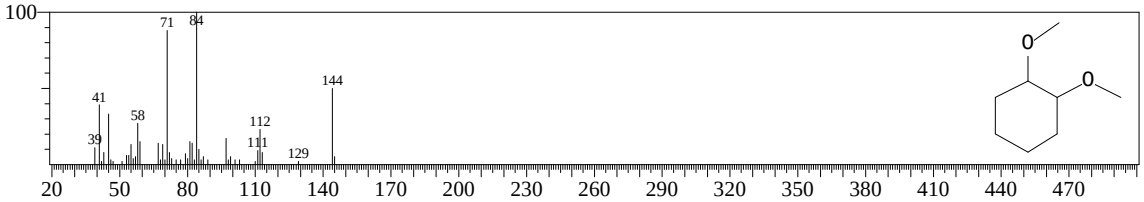
<< Target >>
Line#:8 R.Time:12.950(Scan#:1195) MassPeaks:275 BasePeak:71.95(61038)
RawMode:Averaged 12.942-12.958(1194-1196) BG Mode:Calc. from Peak



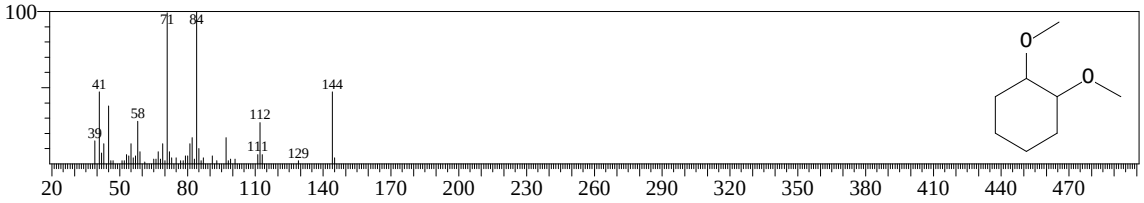

Hit#:1 Entry:12396 Library:NIST05.LIB
SI:87 Formula:C6H8S2 CAS:62488-53-3 MolWeight:144 RetIndex:1134
CompName:3-Vinyl-1,2-dithiacyclohex-5-ene $$ 3-Vinyl-3,4-dihydro-1,2-dithiine # $$



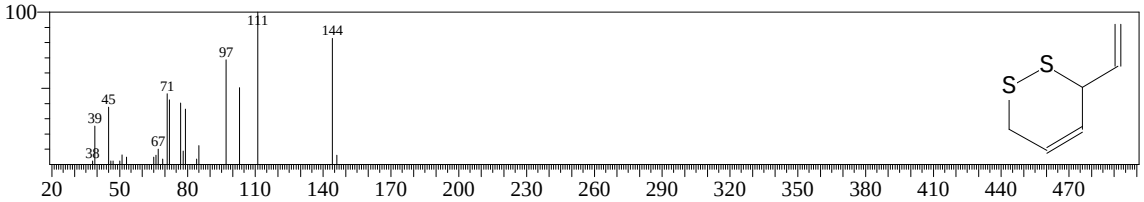

Hit#:2 Entry:12639 Library:NIST05.LIB
SI:74 Formula:C8H16O2 CAS:29887-60-3 MolWeight:144 RetIndex:993
CompName:Cyclohexane, 1,2-dimethoxy-, trans- $$ trans-1,2-Dimethoxycyclohexane $$ 1,2-Dimethoxycyclohexane # $$



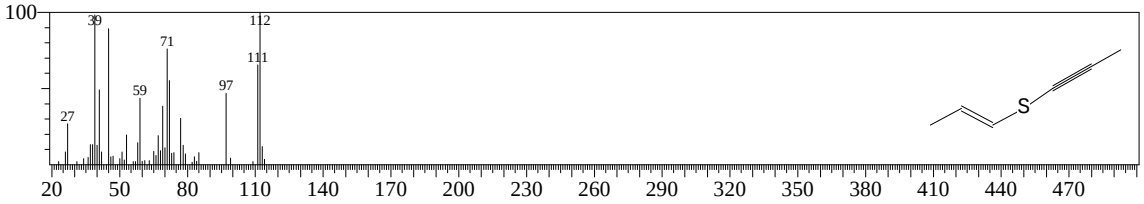

Hit#:3 Entry:12638 Library:NIST05.LIB
SI:73 Formula:C8H16O2 CAS:30363-80-5 MolWeight:144 RetIndex:993
CompName:Cyclohexane, 1,2-dimethoxy-, cis- $$ cis-1,2-Dimethoxycyclohexane $$ 1,2-Dimethoxycyclohexane # $$



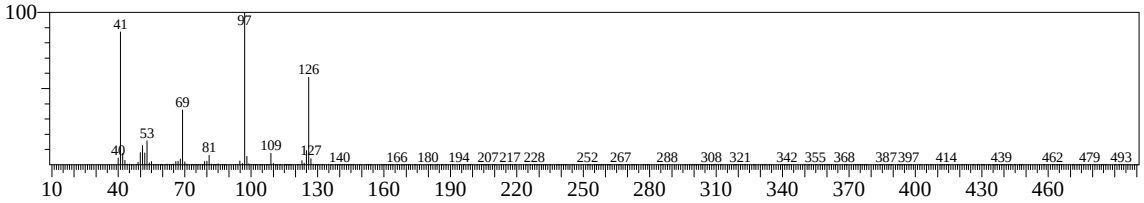

Hit#:4 Entry:12397 Library:NIST05.LIB
SI:72 Formula:C6H8S2 CAS:62488-52-2 MolWeight:144 RetIndex:1134
CompName:3-Vinyl-1,2-dithiacyclohex-4-ene $$ 3-Vinyl-3,6-dihydro-1,2-dithiine # $$



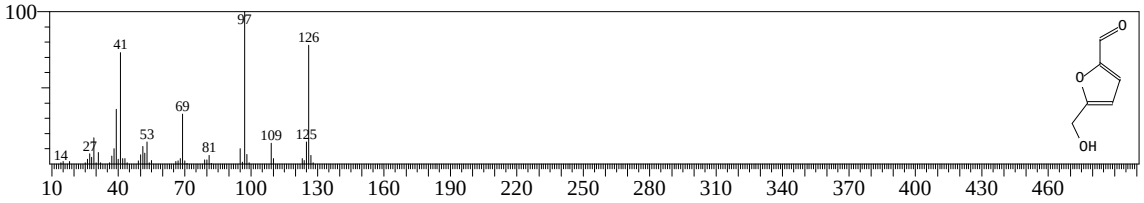

Hit#:5 Entry:3409 Library:NIST05.LIB
SI:70 Formula:C6H8S CAS:89533-93-7 MolWeight:112 RetIndex:894
CompName:Sulfide,1- propenyl 1-propynyl $$ (1E)-1-(1-Propynylsulfanyl)-1-propene # $$



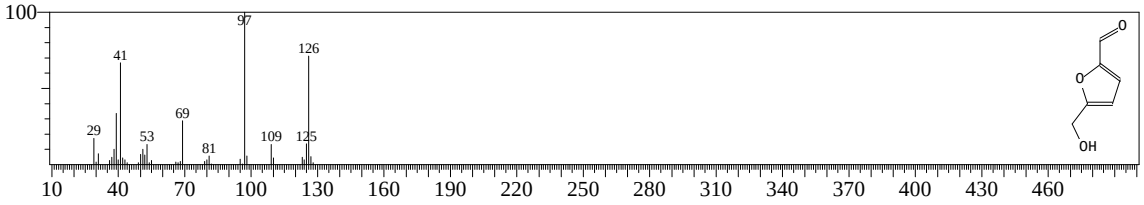
<< Target >>
Line#:9 R.Time:13.233(Scan#:1229) MassPeaks:275 BasePeak:97.00(281850)
RawMode:Averaged 13.225-13.242(1228-1230) BG Mode:Calc. from Peak



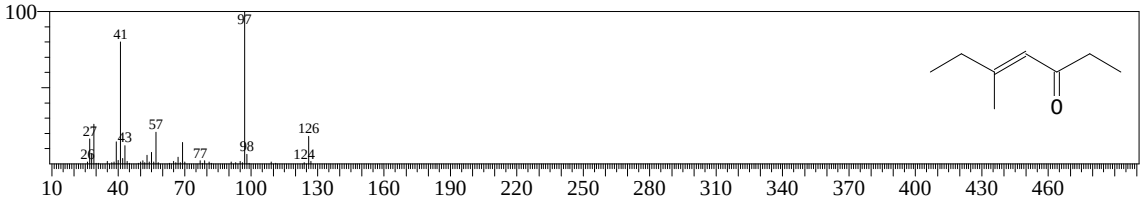
Hit#:1 Entry:6237 Library:NIST05.LIB
SI:95 Formula:C6H6O3 CAS:67-47-0 MolWeight:126 RetIndex:1163
CompName:2-Furancarboxaldehyde, 5-(hydroxymethyl)- $$ 2-Furaldehyde, 5-(hydroxymethyl)- $$ 5-Hydrxoymethylfurfural $$ Hy



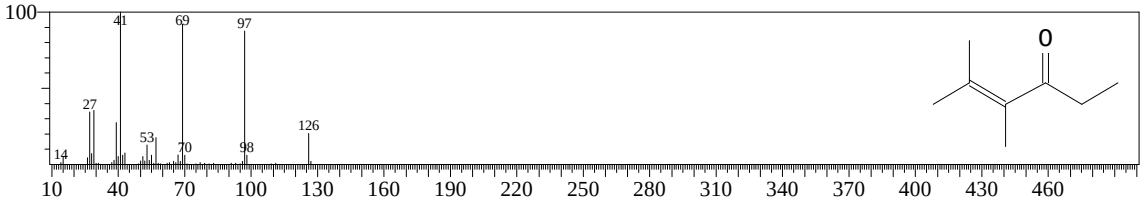
Hit#:2 Entry:4517 Library:NIST05s.LIB
SI:94 Formula:C6H6O3 CAS:67-47-0 MolWeight:126 RetIndex:1163
CompName:2-Furancarboxaldehyde, 5-(hydroxymethyl)- $$ 2-Furaldehyde, 5-(hydroxymethyl)- $$ 5-Hydrxoymethylfurfural $$ Hy



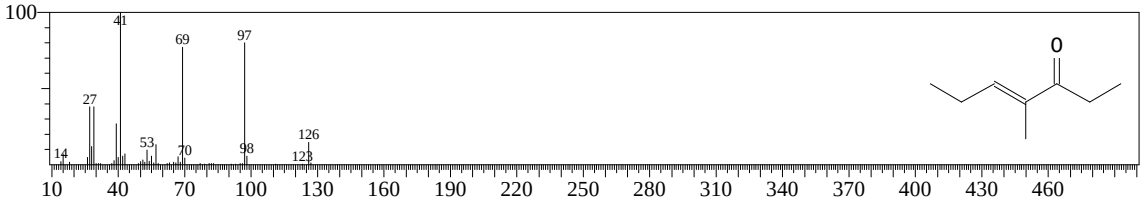
Hit#:3 Entry:6495 Library:NIST05.LIB
SI:85 Formula:C8H14O CAS:1447-26-3 MolWeight:126 RetIndex:938
CompName:4-Hepten-3-one, 5-methyl- $$ (4E)-5-Methyl-4-hepten-3-one # $$



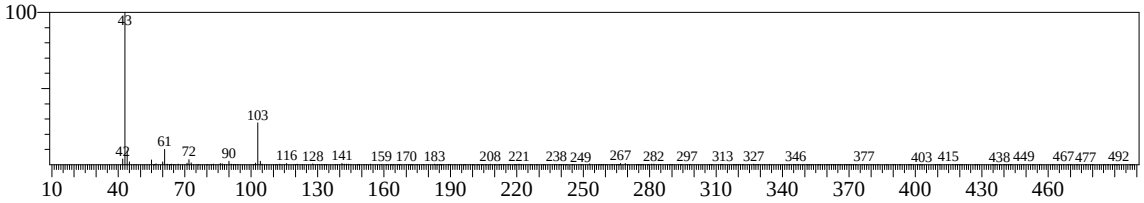
Hit#:4 Entry:6371 Library:NIST05.LIB
SI:84 Formula:C8H14O CAS:17325-90-5 MolWeight:126 RetIndex:915
CompName:4-Hexen-3-one, 4,5-dimethyl- $$ 4,5-Dimethyl-4-hexen-3-one # $$



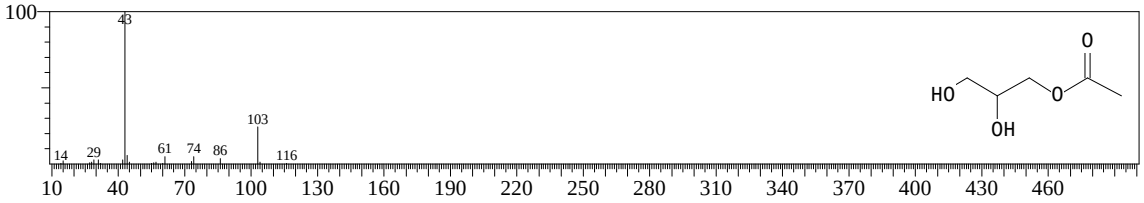
Hit#:5 Entry:6372 Library:NIST05.LIB
SI:84 Formula:C8H14O CAS:22319-31-9 MolWeight:126 RetIndex:938
CompName:4-Hepten-3-one, 4-methyl- $$ (4E)-4-Methyl-4-hepten-3-one # $$



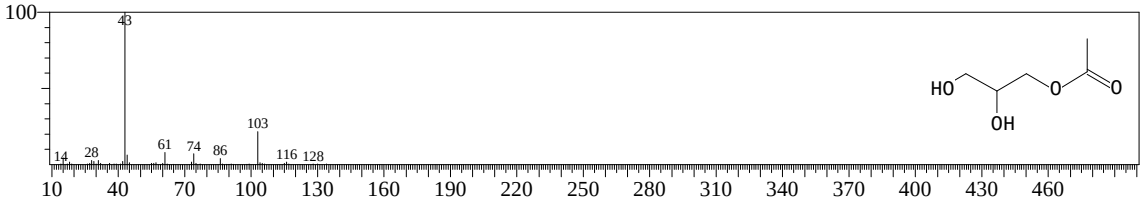
<< Target >>
Line#:10 R.Time:13.550(Scan#:1267) MassPeaks:232 BasePeak:43.00(27511)
RawMode:Averaged 13.542-13.558(1266-1268) BG Mode:Calc. from Peak



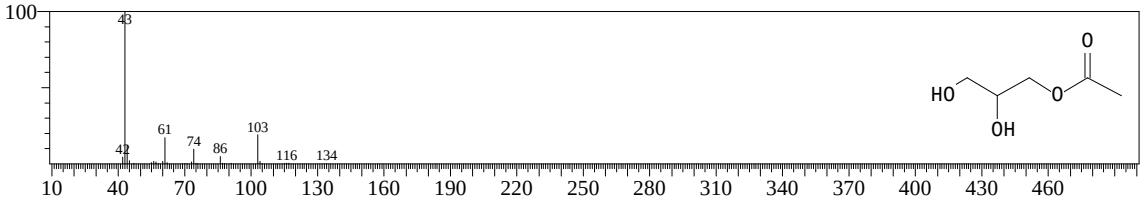

Hit#:1 Entry:5769 Library:NIST05s.LIB
SI:89 Formula:C5H10O4 CAS:26446-35-5 MolWeight:134 RetIndex:1091
CompName:1,2,3-Propanetriol, monoacetate $$ Acetin, mono- $$ Acetin $$ Acetoglyceride $$ Acetyl monoglyceride $$ Glycerin n



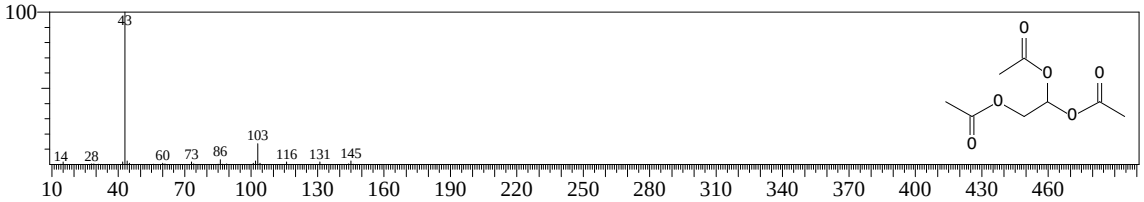

Hit#:2 Entry:8646 Library:NIST05.LIB
SI:89 Formula:C5H10O4 CAS:106-61-6 MolWeight:134 RetIndex:1091
CompName:1,2,3-Propanetriol, 1-acetate $$ Acetin, 1-mono- $$ .alpha.-Monoacetin $$ Glycerol .alpha.-monoacetate $$ 1-Monoac



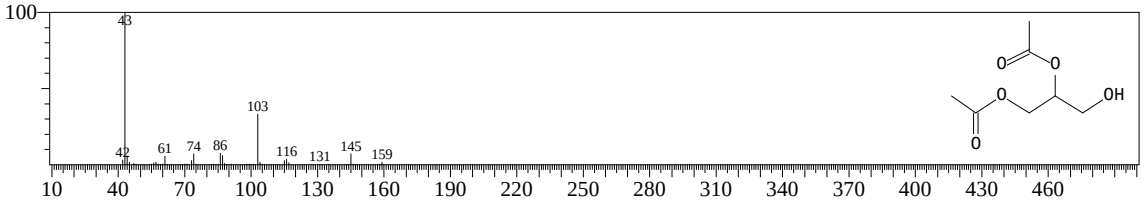

Hit#:3 Entry:8645 Library:NIST05.LIB
SI:88 Formula:C5H10O4 CAS:26446-35-5 MolWeight:134 RetIndex:1091
CompName:1,2,3-Propanetriol, monoacetate $$ Acetin, mono- $$ Acetin $$ Acetoglyceride $$ Acetyl monoglyceride $$ Glycerin n



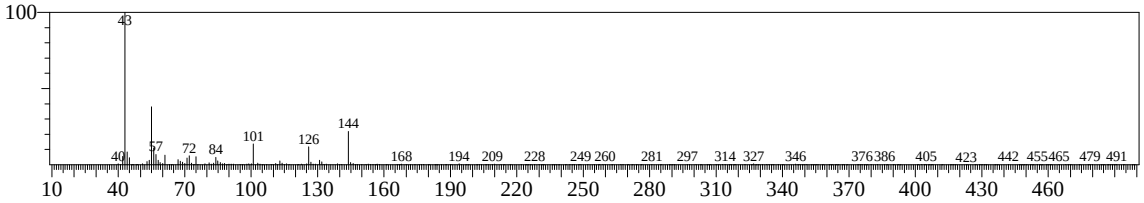

Hit#:4 Entry:42842 Library:NIST05.LIB
SI:85 Formula:C8H12O6 CAS:2983-35-9 MolWeight:204 RetIndex:1254
CompName:1,1,2-Triacetoxyethane $$ 1,1,2-Ethanetriol, triacetate $$ 1,2-Bis(acetyloxy)ethyl acetate # $$



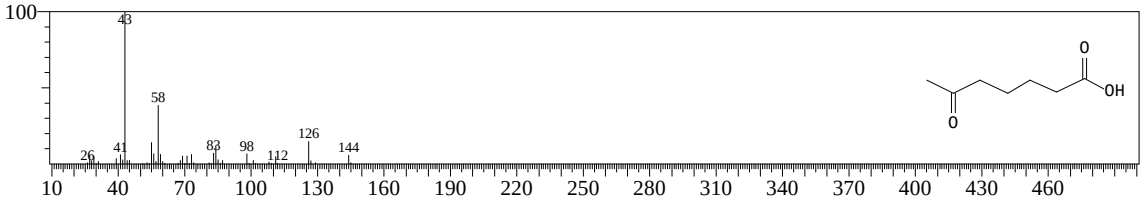

Hit#:5 Entry:12726 Library:NIST05s.LIB
SI:84 Formula:C7H12O5 CAS:25395-31-7 MolWeight:176 RetIndex:1230
CompName:1,2,3-Propanetriol, diacetate $$ Acetin, di- $$ Diacetin $$ Diacetylglycerol $$ Glycerin diacetate $$ Glycerine diacetat



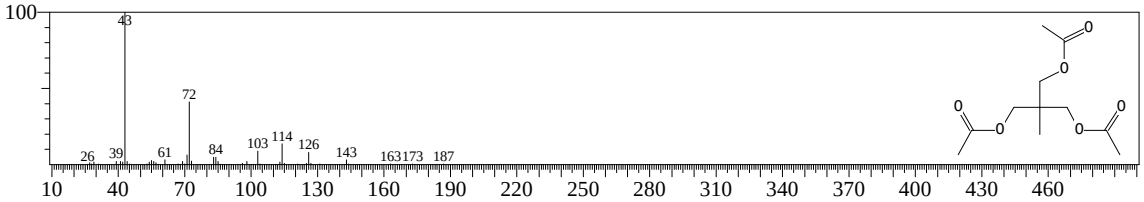
<< Target >>
Line#:11 R.Time:14.225(Scan#:1348) MassPeaks:262 BasePeak:43.00(17281)
RawMode:Averaged 14.217-14.233(1347-1349) BG Mode:Calc. from Peak



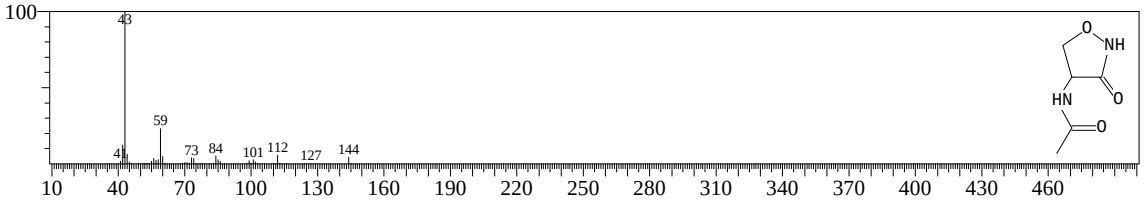

Hit#:1 Entry:12478 Library:NIST05.LIB
SI:79 Formula:C7H12O3 CAS:3128-7-2 MolWeight:144 RetIndex:1209
CompName:Heptanoic acid, 6-oxo- $$ 6-Oxoheptanoic acid # $$



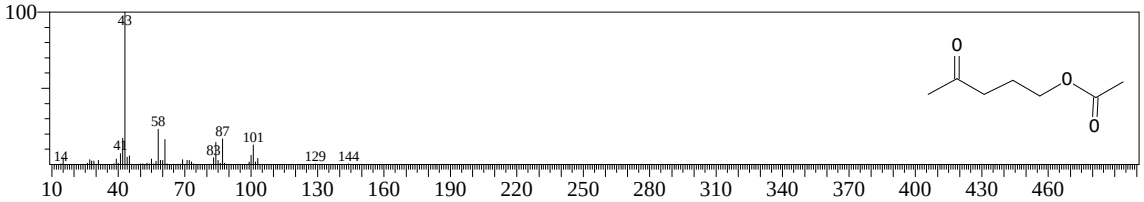

Hit#:2 Entry:68402 Library:NIST05.LIB
SI:76 Formula:C11H18O6 CAS:13431-59-9 MolWeight:246 RetIndex:1532
CompName:1,3-Propanediol, 2-hydroxymethyl-2-methyl-, triacetate $$ 3-(Acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl acetate



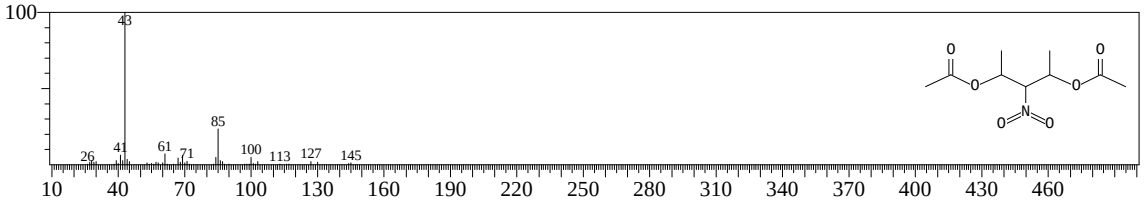

Hit#:3 Entry:12345 Library:NIST05.LIB
SI:76 Formula:C5H8N2O3 CAS:0-0-0 MolWeight:144 RetIndex:1313
CompName:N-Acetylcycloserine



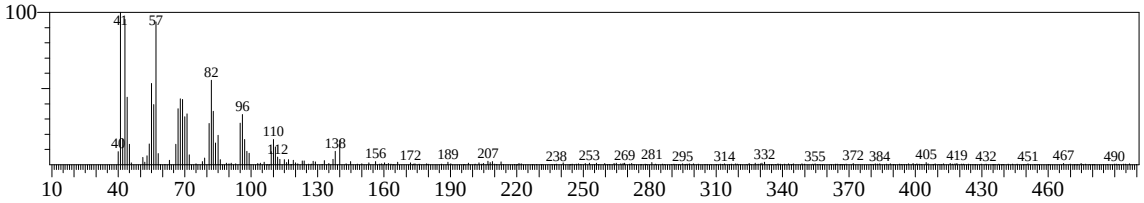

Hit#:4 Entry:12477 Library:NIST05.LIB
SI:76 Formula:C7H12O3 CAS:5185-97-7 MolWeight:144 RetIndex:1020
CompName:2-Pentanone, 5-(acetyloxy)- $$ 2-Pentanone, 5-hydroxy-, acetate $$ .gamma.-Acetylpropyl acetate $$ Acetopropyl acet



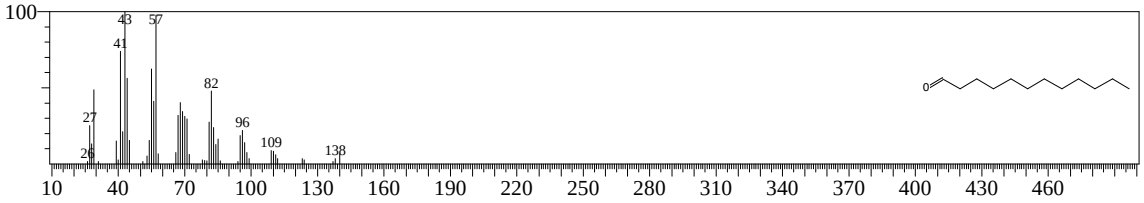

Hit#:5 Entry:60643 Library:NIST05.LIB
SI:76 Formula:C9H15NO6 CAS:78651-66-8 MolWeight:233 RetIndex:1440
CompName:2,4-Pentanediol, 3-nitro-, diacetate $$ 2,4-Di-O-acetyl-1,3,5-trideoxy-3-nitropentitol # $$



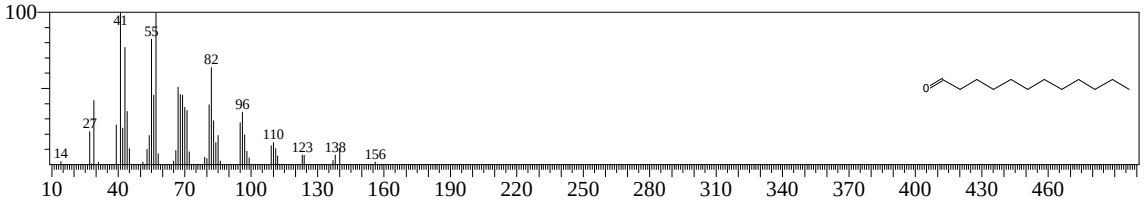
<< Target >>
Line#:12 R.Time:15.917(Scan#:1551) MassPeaks:273 BasePeak:41.00(4611)
RawMode:Averaged 15.908-15.925(1550-1552) BG Mode:Calc. from Peak



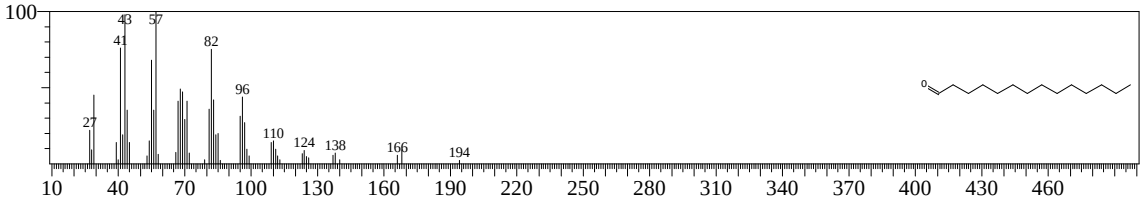

Hit#:1 Entry:14089 Library:NIST05s.LIB
SI:94 Formula:C12H24O CAS:112-54-9 MolWeight:184 RetIndex:1402
CompName:Dodecanal $$ Lauraldehyde $$ n-Dodecanal $$ n-Dodecyl aldehyde $$ n-Dodecylic aldehyde $$ n-Lauraldehyde $$ Al



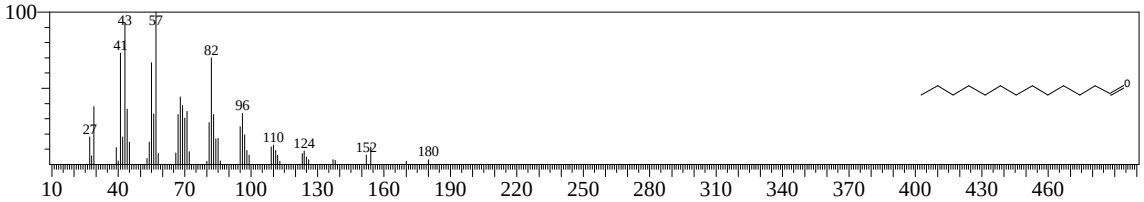

Hit#:2 Entry:14087 Library:NIST05s.LIB
SI:94 Formula:C12H24O CAS:112-54-9 MolWeight:184 RetIndex:1402
CompName:Dodecanal $$ Lauraldehyde $$ n-Dodecanal $$ n-Dodecyl aldehyde $$ n-Dodecylic aldehyde $$ n-Lauraldehyde $$ Al



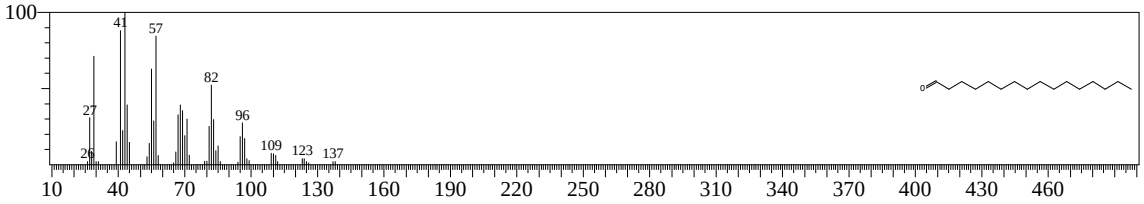

Hit#:3 Entry:17684 Library:NIST05s.LIB
SI:93 Formula:C14H28O CAS:124-25-4 MolWeight:212 RetIndex:1601
CompName:Tetradecanal $$ Myristaldehyde $$ Myristylaldehyde $$ Tetradecylaldehyde $$ n-Tetradecanal $$ Aldehyde C-14 $$ A



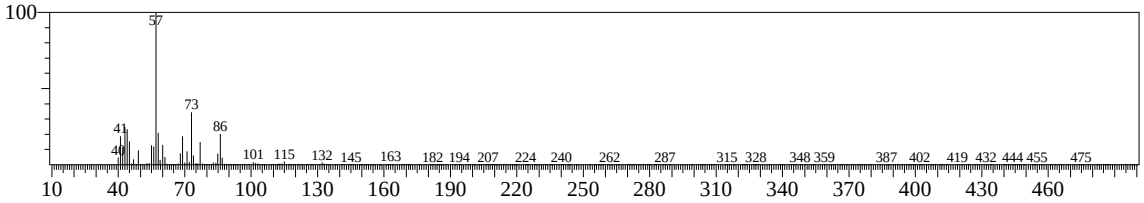

Hit#:4 Entry:40204 Library:NIST05.LIB
SI:93 Formula:C13H26O CAS:10486-19-8 MolWeight:198 RetIndex:1502
CompName:Tridecanal $$ n-Tridecylaldehyde $$ Tridecanaldehyde $$ Tridecyl aldehyde $$ 1-Tridecanal $$ Tridecane aldehyde $$



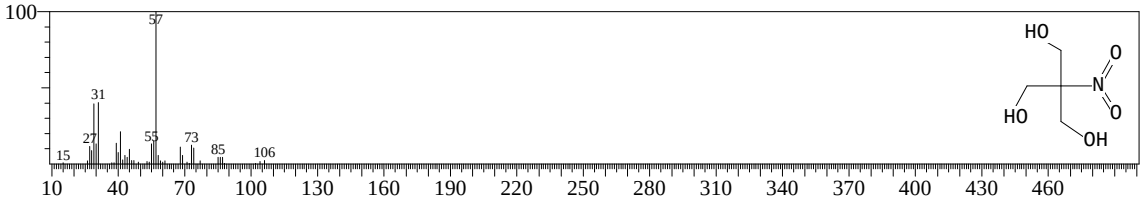

Hit#:5 Entry:65429 Library:NIST05.LIB
SI:92 Formula:C16H32O CAS:629-80-1 MolWeight:240 RetIndex:1800
CompName:Hexadecanal $$ Palmitaldehyde $$



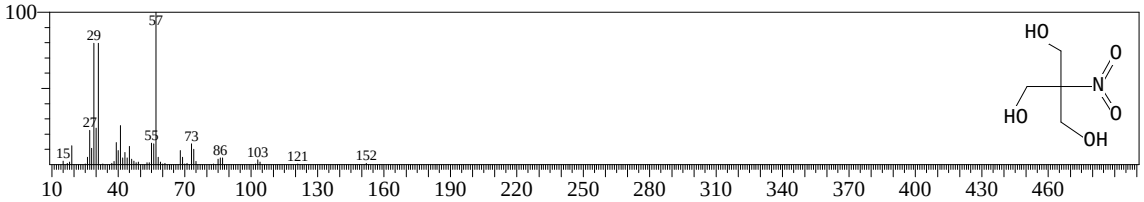
<< Target >>
Line#:13 R.Time:16.683(Scan#:1643) MassPeaks:272 BasePeak:57.00(180019)
RawMode:Averaged 16.675-16.692(1642-1644) BG Mode:Calc. from Peak



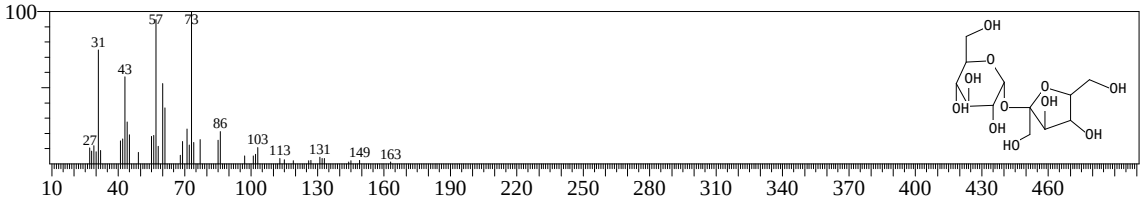
Hit#:1 Entry:8563 Library:NIST05s.LIB
SI:84 Formula:C4H9NO5 CAS:126-11-4 MolWeight:151 RetIndex:1444
CompName:1,3-Propanediol, 2-(hydroxymethyl)-2-nitro- $$ Isobutylglycerol, nitro- $$ Methane, trimethylolnitro- $$ Nitroisobutylg



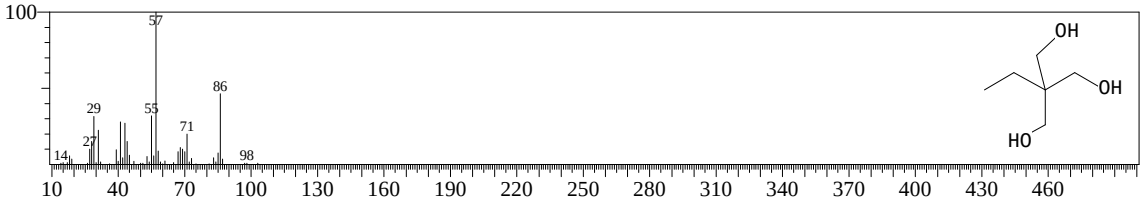
Hit#:2 Entry:15081 Library:NIST05.LIB
SI:82 Formula:C4H9NO5 CAS:126-11-4 MolWeight:151 RetIndex:1444
CompName:1,3-Propanediol, 2-(hydroxymethyl)-2-nitro- $$ Isobutylglycerol, nitro- $$ Methane, trimethylolnitro- $$ Nitroisobutylg



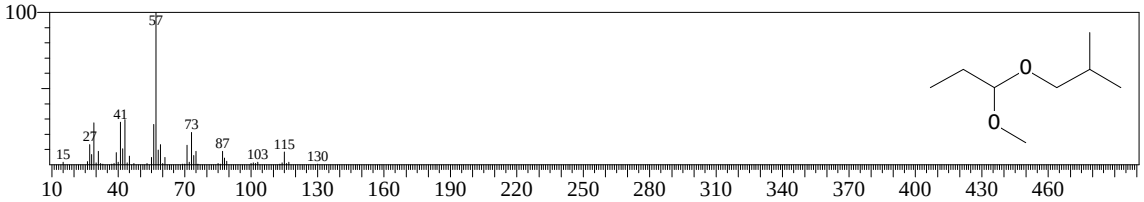
Hit#:3 Entry:123174 Library:NIST05.LIB
SI:82 Formula:C12H22O11 CAS:57-50-1 MolWeight:342 RetIndex:3139
CompName:Sucrose $$ .alpha.-D-Glucopyranoside, .beta.-D-fructofuranosyl $$ .beta.-D-Fructofuranosyl .alpha.-D-glucopyranoside



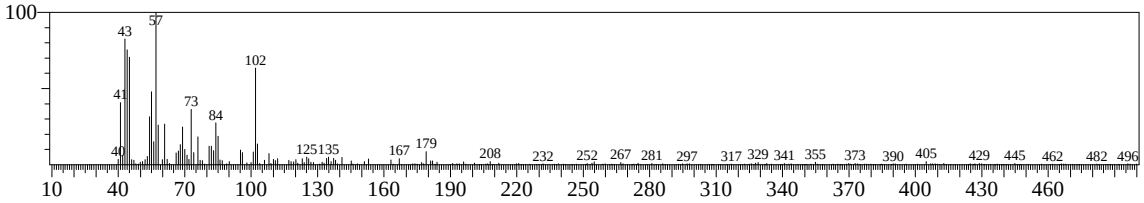
Hit#:4 Entry:5797 Library:NIST05s.LIB
SI:82 Formula:C6H14O3 CAS:77-99-6 MolWeight:134 RetIndex:1261
CompName:1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)- $$ Ethriol $$ Ethyltrimethylolmethane $$ Etriol $$ Ettriol $$ Hexaglyceri



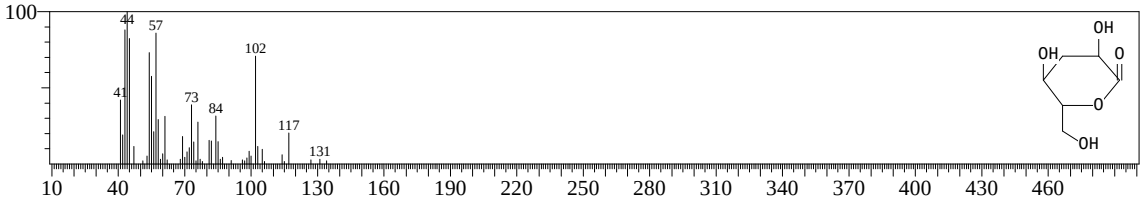
Hit#:5 Entry:13359 Library:NIST05.LIB
SI:81 Formula:C8H18O2 CAS:0-0-0 MolWeight:146 RetIndex:840
CompName:1-Isobutoxy-1-methoxypropane



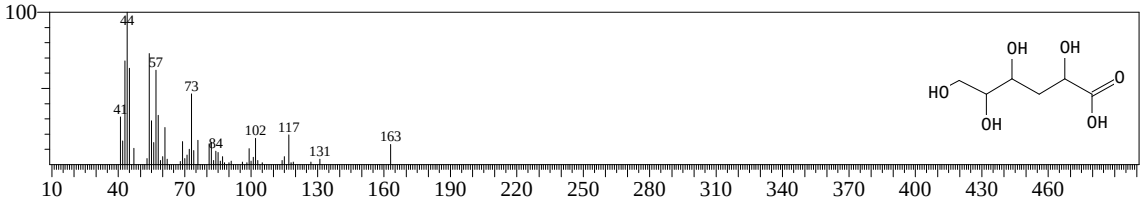
<< Target >>
Line#:14 R.Time:18.642(Scan#:1878) MassPeaks:257 BasePeak:57.00(5350)
RawMode:Averaged 18.633-18.650(1877-1879) BG Mode:Calc. from Peak



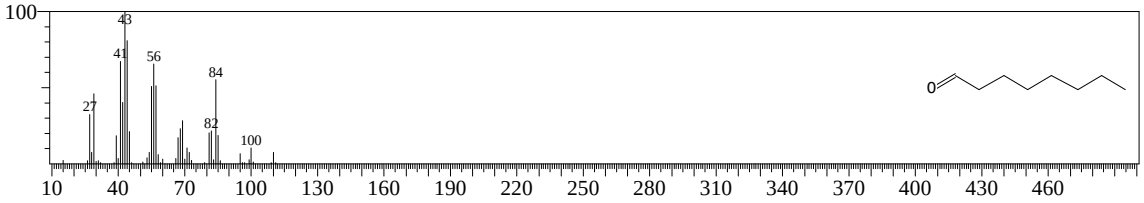
Hit#:1 Entry:20146 Library:NIST05.LIB
SI:83 Formula:C6H10O5 CAS:0-0-0 MolWeight:162 RetIndex:1625
CompName:3-Deoxy-d-mannoic lactone



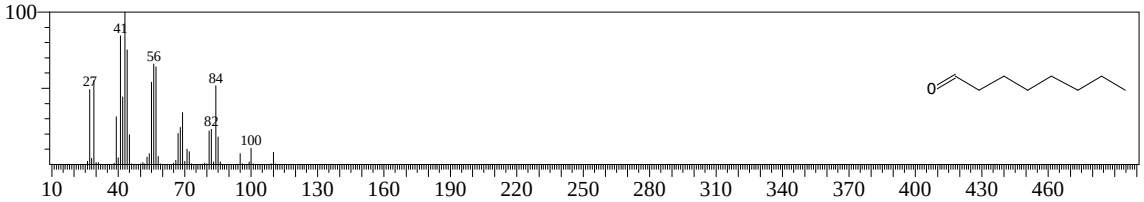
Hit#:2 Entry:29440 Library:NIST05.LIB
SI:79 Formula:C6H12O6 CAS:0-0-0 MolWeight:180 RetIndex:1704
CompName:3-Deoxy-d-mannonic acid



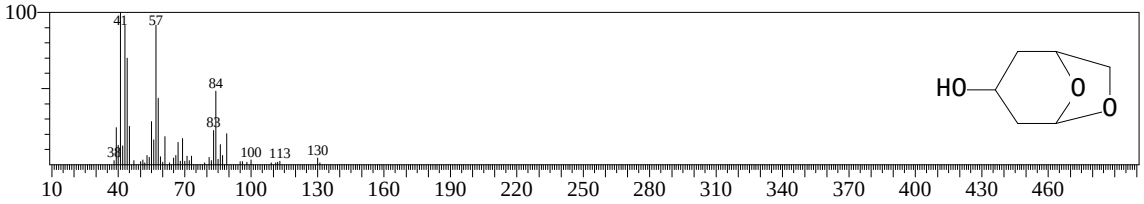
Hit#:3 Entry:7131 Library:NIST05.LIB
SI:74 Formula:C8H16O CAS:124-13-0 MolWeight:128 RetIndex:1005
CompName:Octanal $$ n-Caprylaldehyde $$ n-Octaldehyde $$ n-Octanal $$ n-Octylal $$ Antifoam-LF $$ Caprylaldehyde $$ Capı



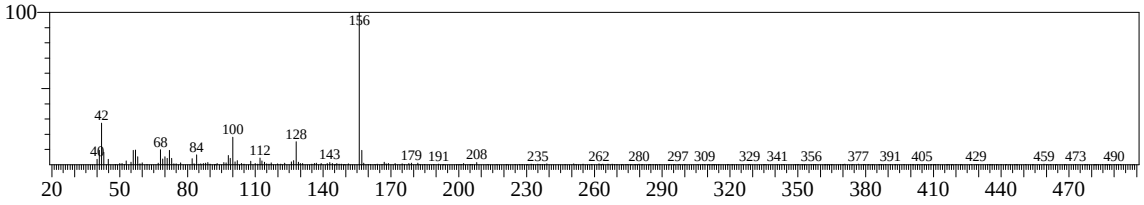
Hit#:4 Entry:4912 Library:NIST05s.LIB
SI:74 Formula:C8H16O CAS:124-13-0 MolWeight:128 RetIndex:1005
CompName:Octanal $$ n-Caprylaldehyde $$ n-Octaldehyde $$ n-Octanal $$ n-Octylal $$ Antifoam-LF $$ Caprylaldehyde $$ Capı



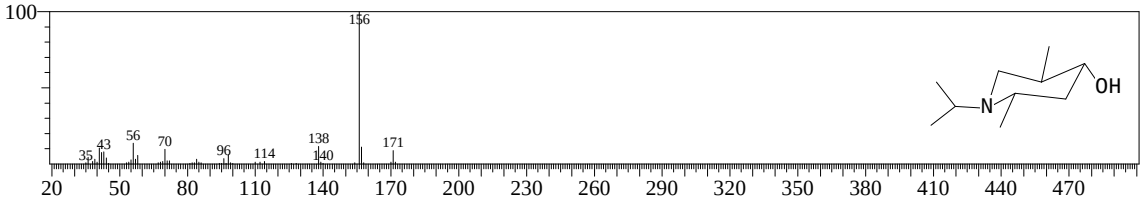
Hit#:5 Entry:7621 Library:NIST05.LIB
SI:74 Formula:C6H10O3 CAS:14241-58-8 MolWeight:130 RetIndex:1028
CompName:1,6-Anhydro-2,4-dideoxy-.beta.-D-arabo-hexopyranose



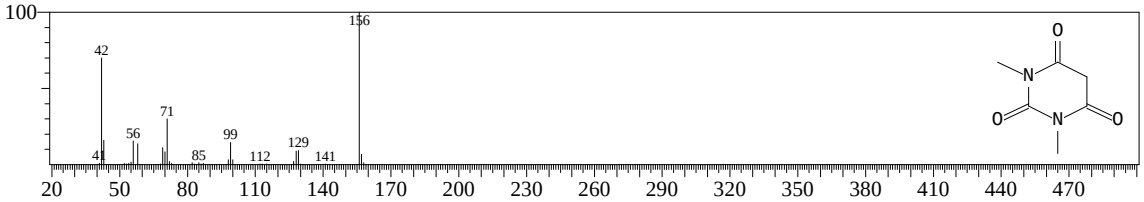
<< Target >>
Line#:15 R.Time:18.742(Scan#:1890) MassPeaks:245 BasePeak:156.00(12330)
RawMode:Averaged 18.733-18.750(1889-1891) BG Mode:Calc. from Peak



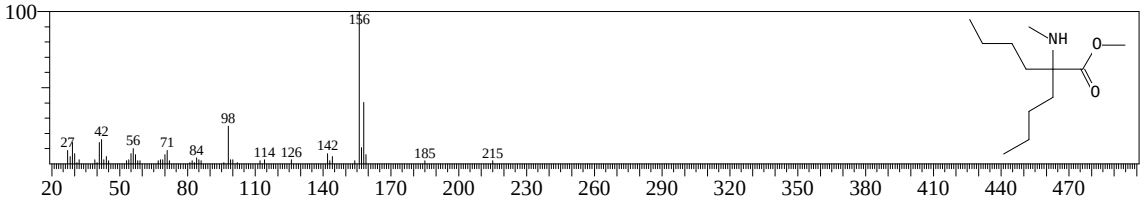

Hit#:1 Entry:25287 Library:NIST05.LIB
SI:78 Formula:C10H21NO CAS:0-0-0 MolWeight:171 RetIndex:1278
CompName:Piperidin-4-ol, 2,5-dimethyl-1-(1-methylethyl)-



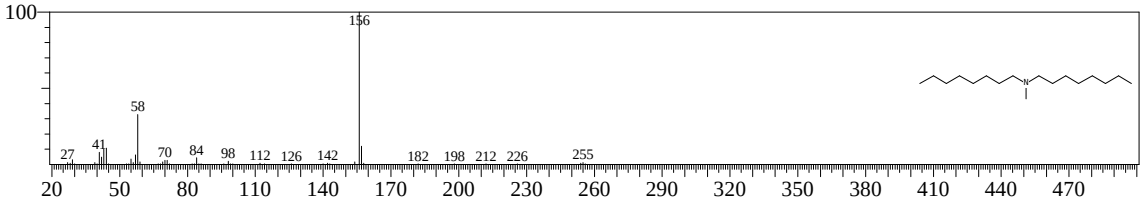

Hit#:2 Entry:9607 Library:NIST05s.LIB
SI:77 Formula:C6H8N2O3 CAS:769-42-6 MolWeight:156 RetIndex:1532
CompName:1,3-Dimethylbarbituric acid $$ 2,4,6(1H,3H,5H)-Pyrimidinetrione, 1,3-dimethyl- $$ Barbituric acid, 1,3-dimethyl- $$ I



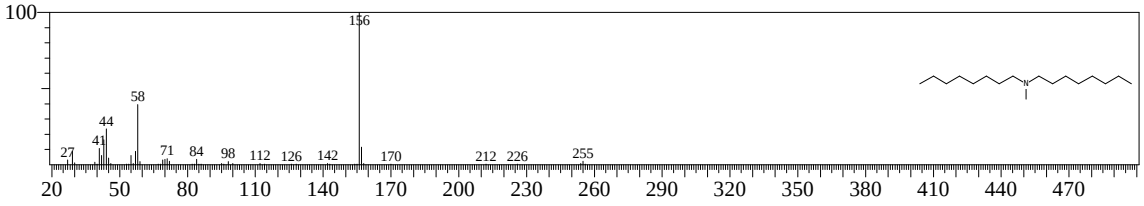

Hit#:3 Entry:49985 Library:NIST05.LIB
SI:76 Formula:C12H25NO2 CAS:6141-46-4 MolWeight:215 RetIndex:1495
CompName:Norleucine, 2-butyl-N-methyl-, methyl ester $$ Methyl 2-butyl-2-(methylamino)hexanoate # $$



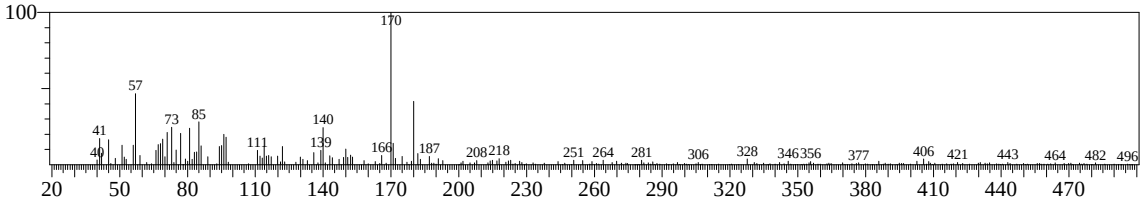

Hit#:4 Entry:21263 Library:NIST05s.LIB
SI:74 Formula:C17H37N CAS:4455-26-9 MolWeight:255 RetIndex:1760
CompName:1-Octanamine, N-methyl-N-octyl- $$ Di(octyl)methylamine $$ N-Methyldioctylamine $$ N,N-Dioctylmethylamine $$



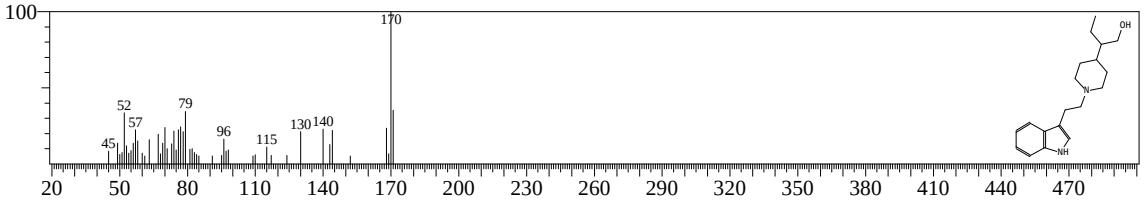

Hit#:5 Entry:21261 Library:NIST05s.LIB
SI:74 Formula:C17H37N CAS:4455-26-9 MolWeight:255 RetIndex:1760
CompName:1-Octanamine, N-methyl-N-octyl- $$ Di(octyl)methylamine $$ N-Methyldioctylamine $$ N,N-Dioctylmethylamine $$



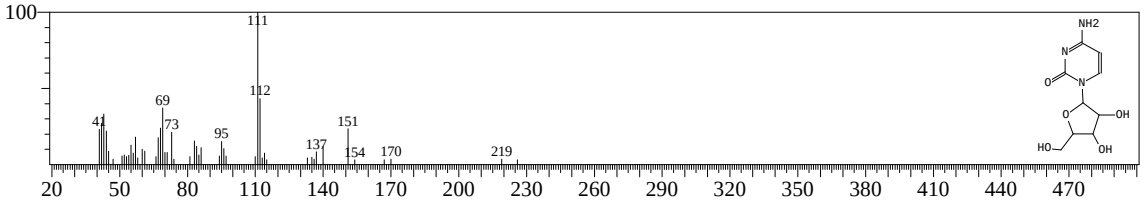
<< Target >>
Line#:16 R.Time:18.808(Scan#:1898) MassPeaks:257 BasePeak:170.05(2379)
RawMode:Averaged 18.800-18.817(1897-1899) BG Mode:Calc. from Peak



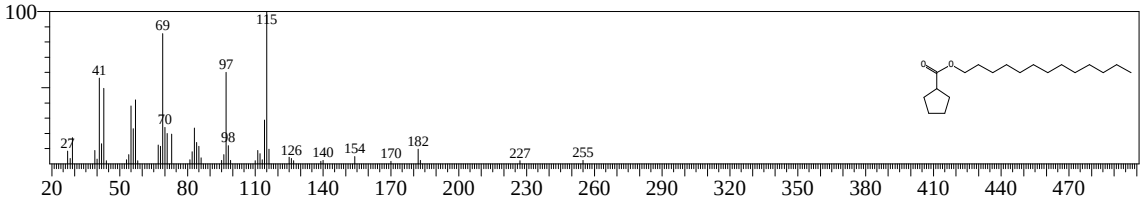

Hit#:1 Entry:101245 Library:NIST05.LIB
SI:58 Formula:C19H28N2O CAS:22311-11-1 MolWeight:300 RetIndex:2613
CompName:4-Piperidineethanol, .beta.-ethyl-1-(2-indol-3-ylethyl)- $$ 2-(1-[2-(1H-Indol-3-yl)ethyl]-4-piperidinyl)-1-butanol # $$



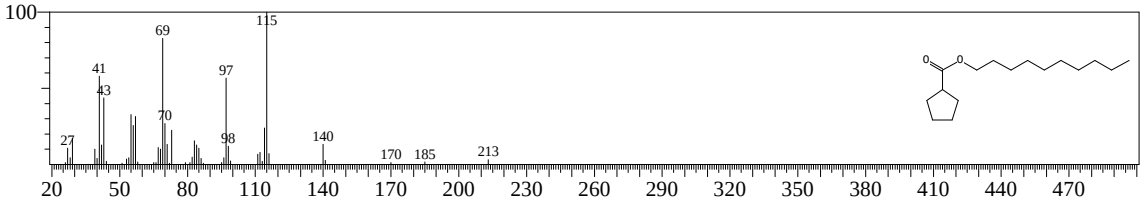

Hit#:2 Entry:66735 Library:NIST05.LIB
SI:57 Formula:C9H13N3O5 CAS:69-74-9 MolWeight:243 RetIndex:2385
CompName:Cytarabine Hydrochloride $$ 1-.beta.-D-Arabinofuranosylcytosine hydrochloride $$ Cytosine-.beta.-D-arabinofuranosi



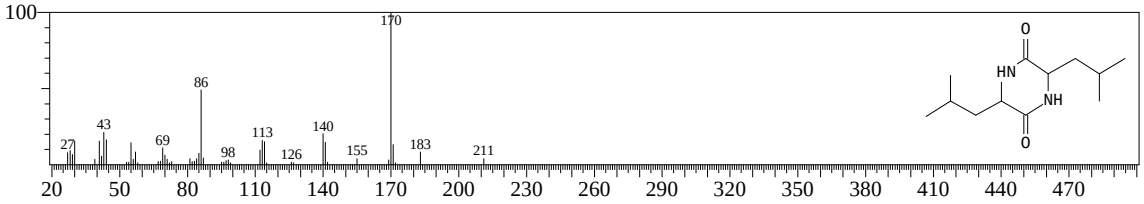

Hit#:3 Entry:98826 Library:NIST05.LIB
SI:56 Formula:C19H36O2 CAS:0-0-0 MolWeight:296 RetIndex:2120
CompName:Cyclopentanecarboxylic acid, tridecyl ester



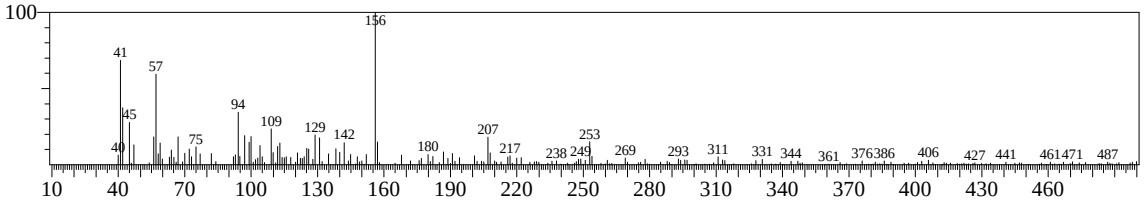

Hit#:4 Entry:73737 Library:NIST05.LIB
SI:56 Formula:C16H30O2 CAS:0-0-0 MolWeight:254 RetIndex:1822
CompName:Cyclopentanecarboxylic acid, decyl ester



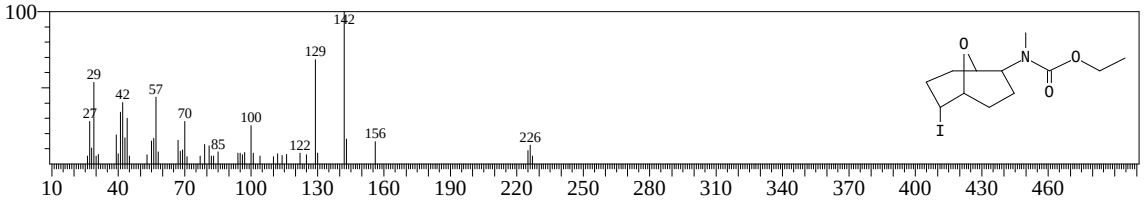

Hit#:5 Entry:56783 Library:NIST05.LIB
SI:55 Formula:C12H22N2O2 CAS:1436-27-7 MolWeight:226 RetIndex:1636
CompName:2,5-Piperazinedione, 3,6-bis(2-methylpropyl)- $$ 3,6-Diisobutyl-2,5-piperazinedione # $$



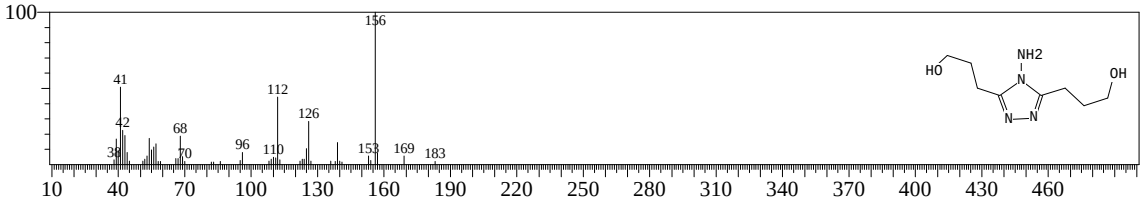
<< Target >>
Line#:17 R.Time:18.917(Scan#:1911) MassPeaks:233 BasePeak:156.00(1261)
RawMode:Averaged 18.908-18.925(1910-1912) BG Mode:Calc. from Peak



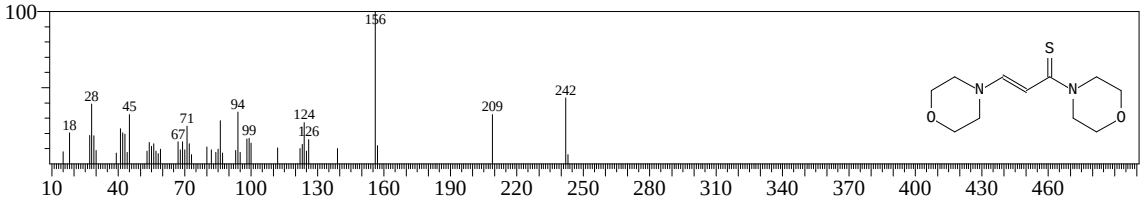
Hit#:1 Entry:128272 Library:NIST05.LIB
SI:53 Formula:C12H20INO3 CAS:0-0-0 MolWeight:353 RetIndex:1922
CompName:Carbamic acid, N-methyl-N-[6-iodo-9-oxabicyclo[3.3.1]nonan-2-yl]-, ethyl ester



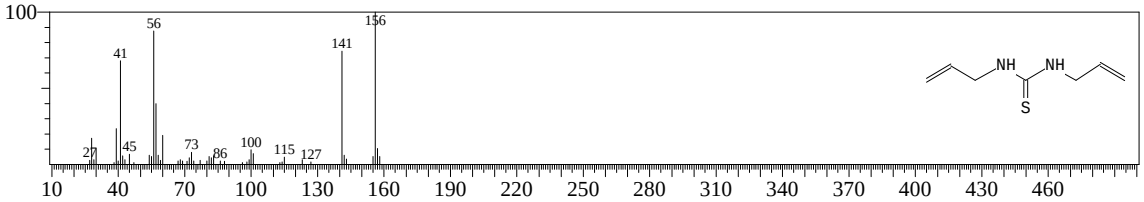
Hit#:2 Entry:40799 Library:NIST05.LIB
SI:53 Formula:C8H16N4O2 CAS:0-0-0 MolWeight:200 RetIndex:1958
CompName:1,2,4-Triazole-3,5-dipropanol, 4-amino-



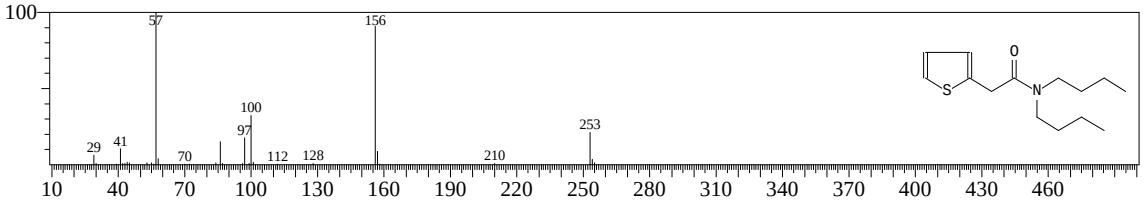
Hit#:3 Entry:66120 Library:NIST05.LIB
SI:53 Formula:C11H18N2O2S CAS:15182-54-4 MolWeight:242 RetIndex:2115
CompName:3-Morpholino-thioacrylomorpholide $$ 4-[(1E)-3-(4-Morpholinyl)-3-thioxo-1-propenyl]morpholine # $$



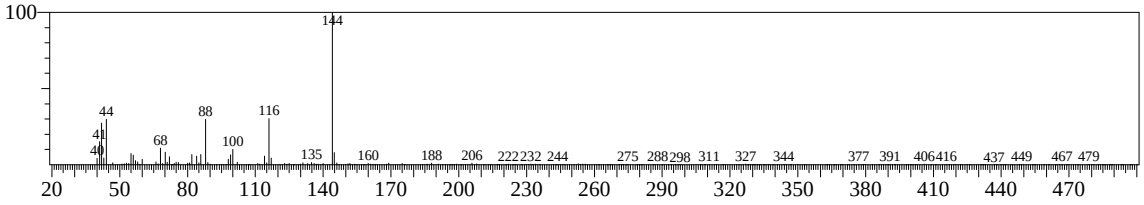
Hit#:4 Entry:17631 Library:NIST05.LIB
SI:53 Formula:C7H12N2S CAS:6601-20-3 MolWeight:156 RetIndex:1480
CompName:Thiourea, N,N'-di-2-propenyl- $$ Bisallylthiocarbamide $$ N,N'-Bis-allylthiourea $$ N,N'-Diallylthiourea $$ 1,3-Diall



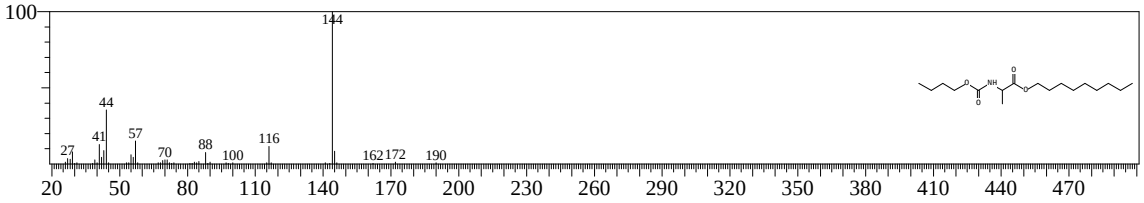
Hit#:5 Entry:72898 Library:NIST05.LIB
SI:52 Formula:C14H23NOS CAS:0-0-0 MolWeight:253 RetIndex:1890
CompName:2-Thiopheneacetamide, N,N-dibutyl-



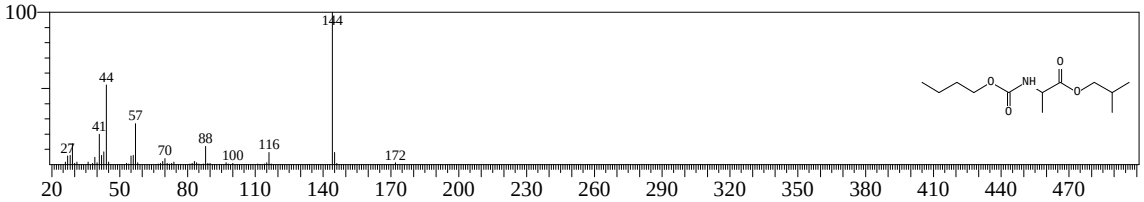
<< Target >>
Line#:18 R.Time:19.550(Scan#:1987) MassPeaks:243 BasePeak:144.00(17054)
RawMode:Averaged 19.542-19.558(1986-1988) BG Mode:Calc. from Peak



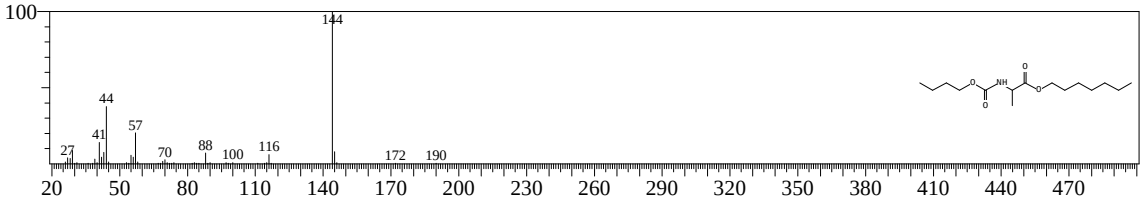

Hit#:1 Entry:109550 Library:NIST05.LIB
SI:79 Formula:C17H33NO4 CAS:0-0-0 MolWeight:315 RetIndex:2180
CompName:l-Alanine, N-butoxycarbonyl-, nonyl ester



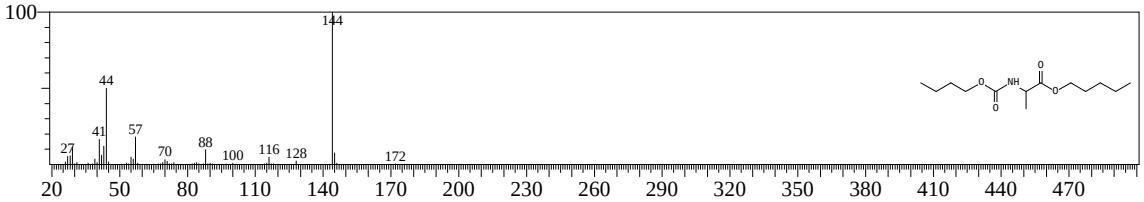

Hit#:2 Entry:67958 Library:NIST05.LIB
SI:79 Formula:C12H23NO4 CAS:0-0-0 MolWeight:245 RetIndex:1619
CompName:l-Alanine, N-butoxycarbonyl-, isobutyl ester



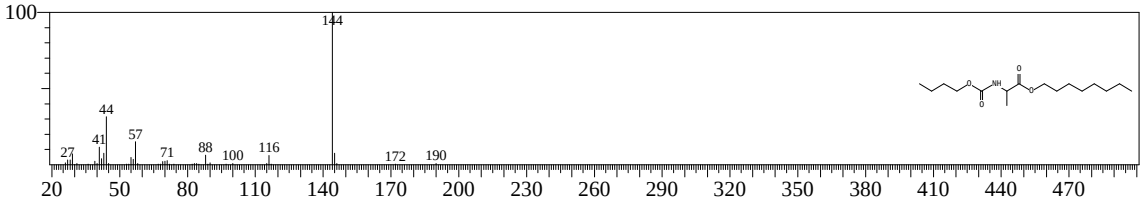

Hit#:3 Entry:93408 Library:NIST05.LIB
SI:79 Formula:C15H29NO4 CAS:0-0-0 MolWeight:287 RetIndex:1981
CompName:l-Alanine, N-butoxycarbonyl-, heptyl ester



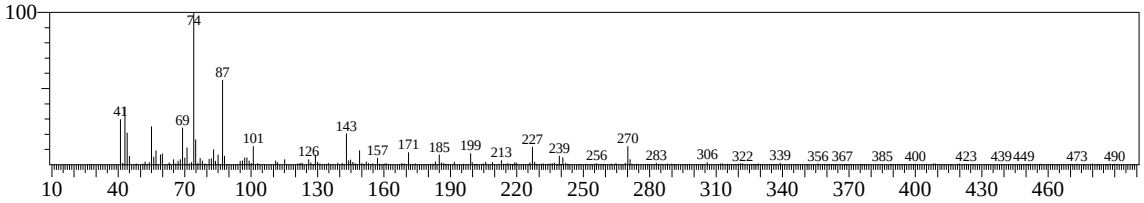

Hit#:4 Entry:76475 Library:NIST05.LIB
SI:78 Formula:C13H25NO4 CAS:0-0-0 MolWeight:259 RetIndex:1782
CompName:l-Alanine, N-butoxycarbonyl-, pentyl ester



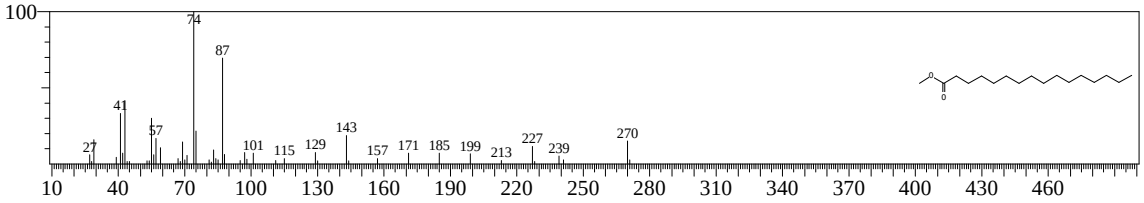

Hit#:5 Entry:101588 Library:NIST05.LIB
SI:78 Formula:C16H31NO4 CAS:0-0-0 MolWeight:301 RetIndex:2081
CompName:l-Alanine, N-butoxycarbonyl-, octyl ester



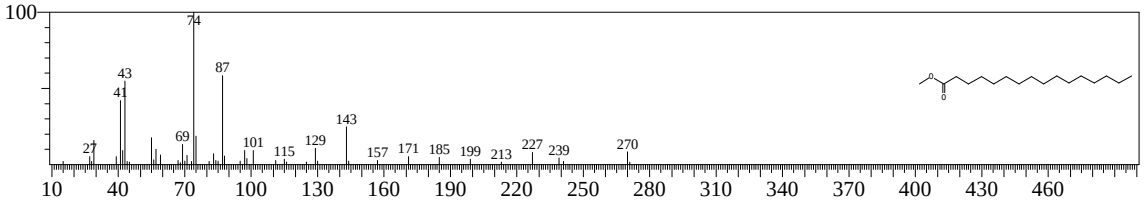
<< Target >>
Line#:19 R.Time:22.200(Scan#:2305) MassPeaks:244 BasePeak:74.00(7098)
RawMode:Averaged 22.192-22.208(2304-2306) BG Mode:Calc. from Peak



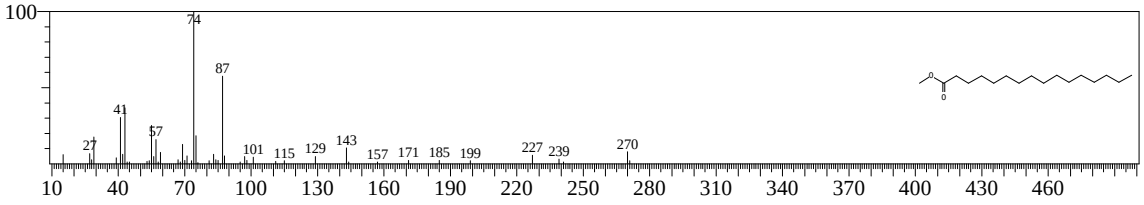
Hit#:1 Entry:83491 Library:NIST05.LIB
SI:90 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878
CompName:Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 221



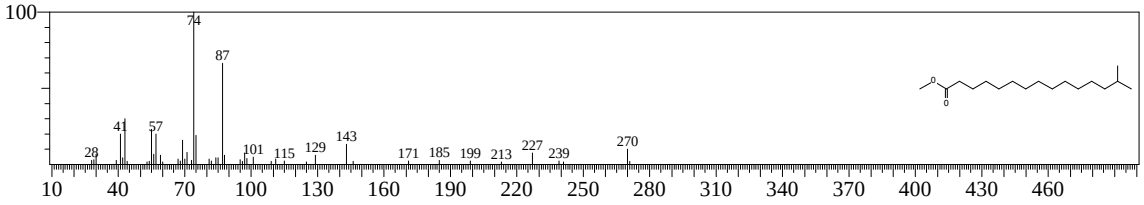
Hit#:2 Entry:22220 Library:NIST05s.LIB
SI:88 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878
CompName:Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 221



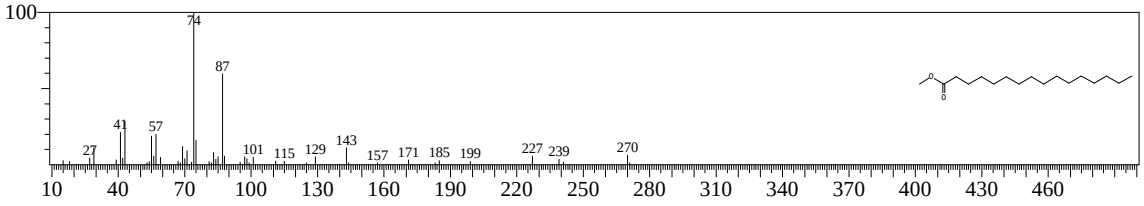
Hit#:3 Entry:22219 Library:NIST05s.LIB
SI:87 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878
CompName:Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 221



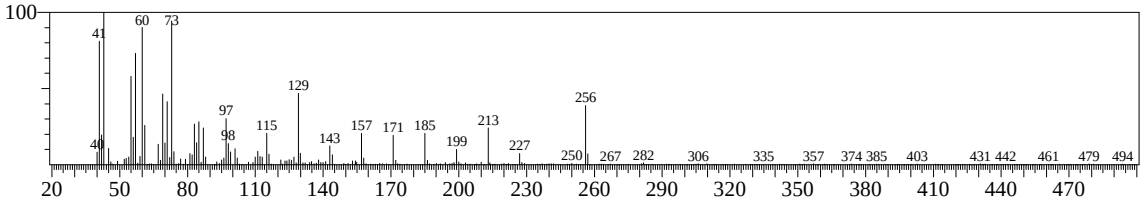
Hit#:4 Entry:22222 Library:NIST05s.LIB
SI:86 Formula:C17H34O2 CAS:5129-60-2 MolWeight:270 RetIndex:1814
CompName:Pentadecanoic acid, 14-methyl-, methyl ester $$ Methyl 14-methylpentadecanoate # $$



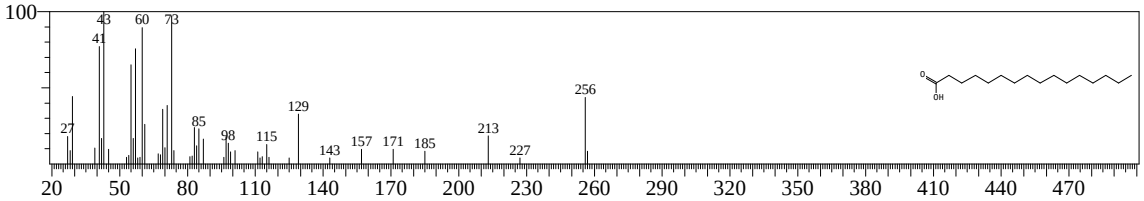
Hit#:5 Entry:22221 Library:NIST05s.LIB
SI:86 Formula:C17H34O2 CAS:112-39-0 MolWeight:270 RetIndex:1878
CompName:Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 221



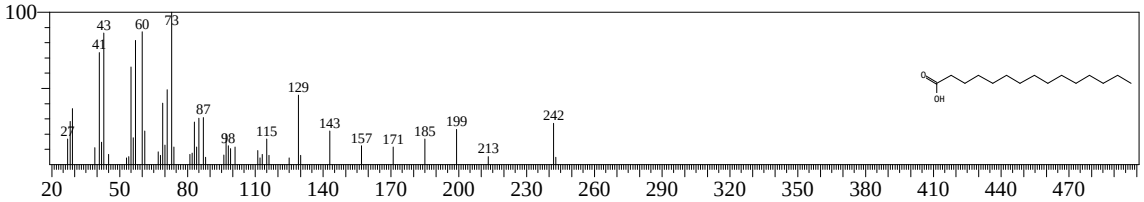
<< Target >>
Line#:20 R.Time:22.567(Scan#:2349) MassPeaks:282 BasePeak:43.00(9684)
RawMode:Averaged 22.558-22.575(2348-2350) BG Mode:Calc. from Peak



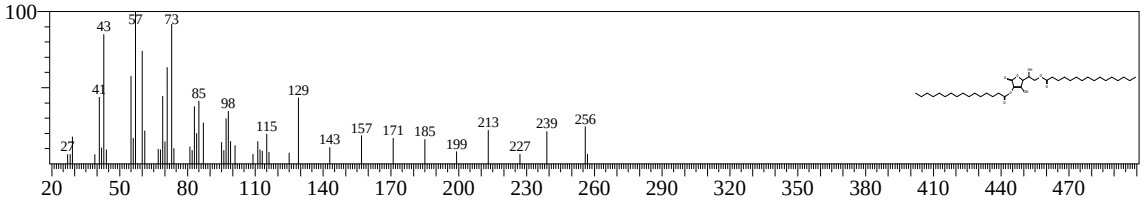
Hit#:1 Entry:21331 Library:NIST05s.LIB
SI:93 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1



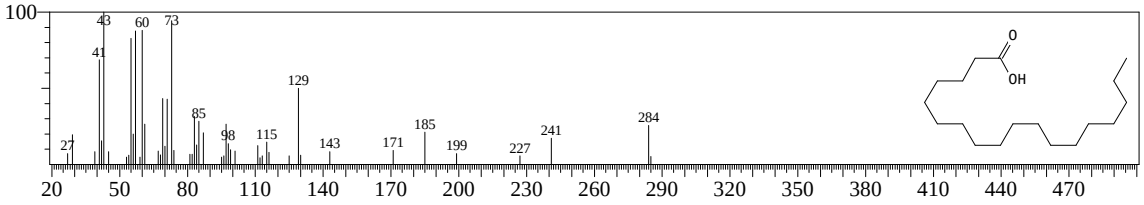
Hit#:2 Entry:20371 Library:NIST05s.LIB
SI:90 Formula:C15H30O2 CAS:1002-84-2 MolWeight:242 RetIndex:1869
CompName:Pentadecanoic acid $$ Pentadecylic acid $$ n-Pentadecanoic acid $$ n-Pentadecylic acid $$



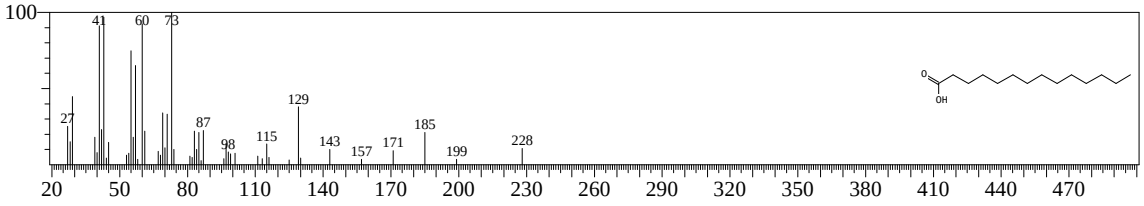
Hit#:3 Entry:161860 Library:NIST05.LIB
SI:88 Formula:C38H68O8 CAS:28474-90-0 MolWeight:652 RetIndex:4765
CompName:l-(+)-Ascorbic acid 2,6-dihexadecanoate



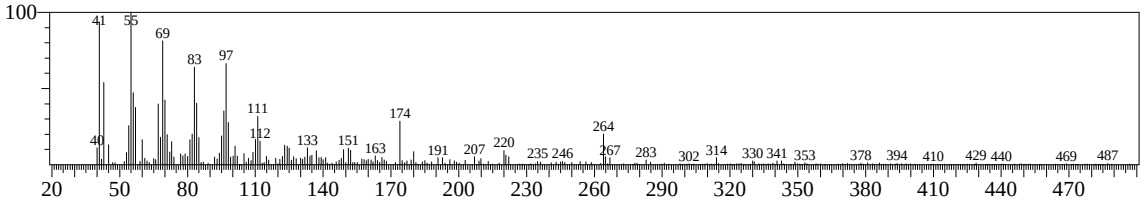
Hit#:4 Entry:22979 Library:NIST05s.LIB
SI:88 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene



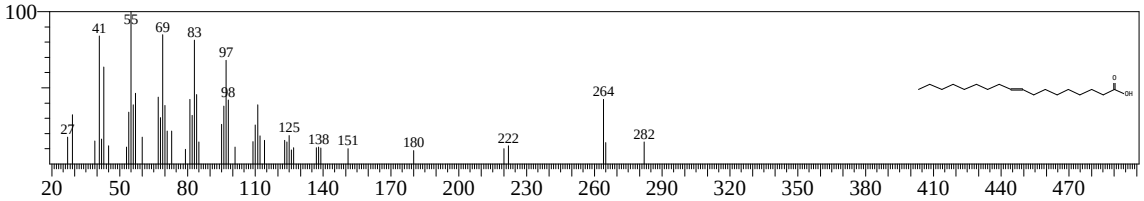
Hit#:5 Entry:19250 Library:NIST05s.LIB
SI:88 Formula:C14H28O2 CAS:544-63-8 MolWeight:228 RetIndex:1769
CompName:Tetradecanoic acid $$ Myristic acid $$ n-Tetradecanoic acid $$ n-Tetradecoic acid $$ Neo-Fat 14 $$ Univol U 316S $



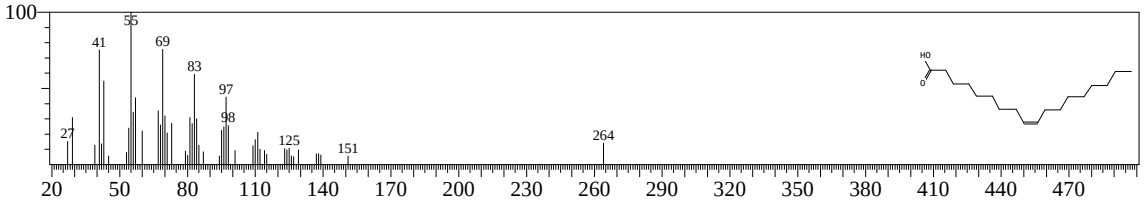
<< Target >>
Line#:21 R.Time:24.383(Scan#:2567) MassPeaks:298 BasePeak:55.00(4288)
RawMode:Averaged 24.375-24.392(2566-2568) BG Mode:Calc. from Peak



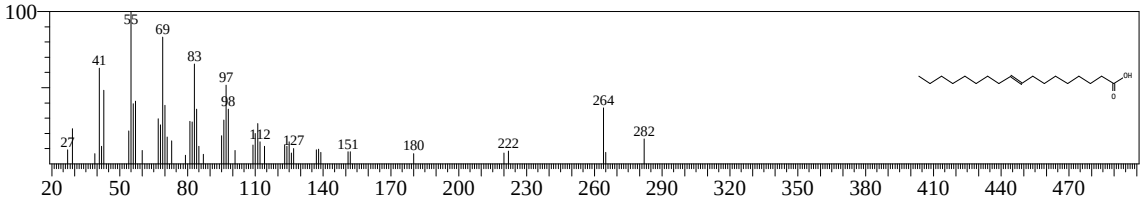

Hit#:1 Entry:90575 Library:NIST05.LIB
SI:87 Formula:C18H34O2 CAS:0-0-0 MolWeight:282 RetIndex:2175
CompName:Octadec-9-enoic acid



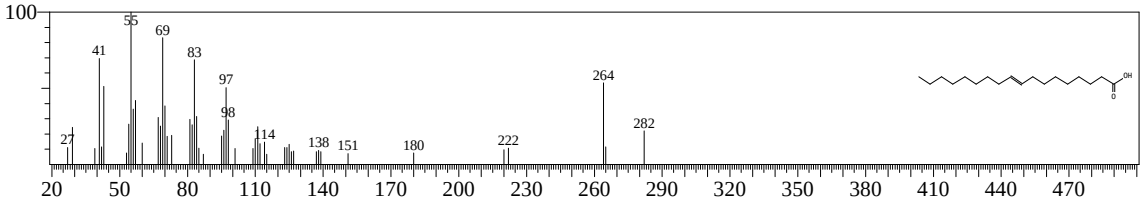

Hit#:2 Entry:90577 Library:NIST05.LIB
SI:86 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .delta.(Sup9)-cis-Oleic acid $$ cis-.delta.(Sup9)-Octadecenoic acid $$ cis-C



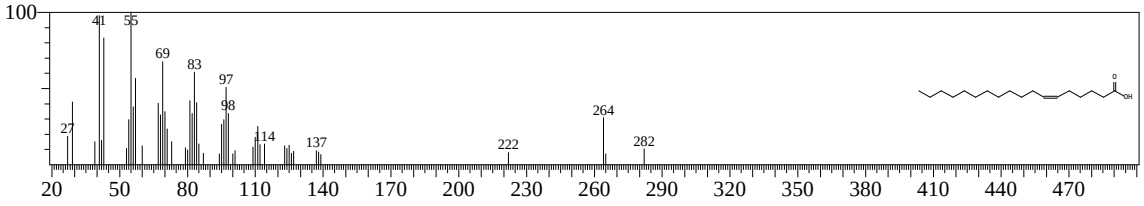

Hit#:3 Entry:22872 Library:NIST05s.LIB
SI:86 Formula:C18H34O2 CAS:112-79-8 MolWeight:282 RetIndex:2175
CompName:9-Octadecenoic acid, (E)- $$ trans-.delta.(sup 9)-Octadecenoic acid $$ trans-.delta.9-Octadecenoic acid $$ trans-Octad



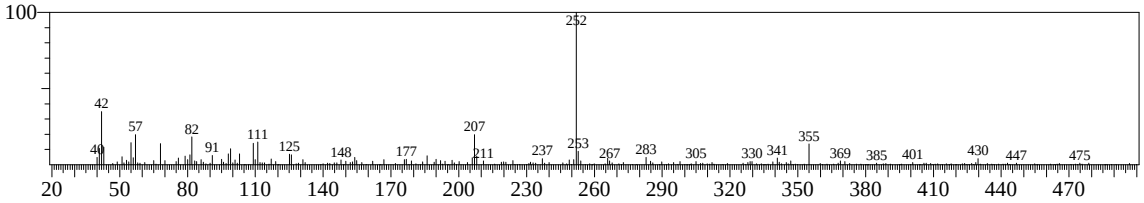

Hit#:4 Entry:90576 Library:NIST05.LIB
SI:85 Formula:C18H34O2 CAS:112-79-8 MolWeight:282 RetIndex:2175
CompName:9-Octadecenoic acid, (E)- $$ trans-.delta.(sup 9)-Octadecenoic acid $$ trans-.delta.9-Octadecenoic acid $$ trans-Octad



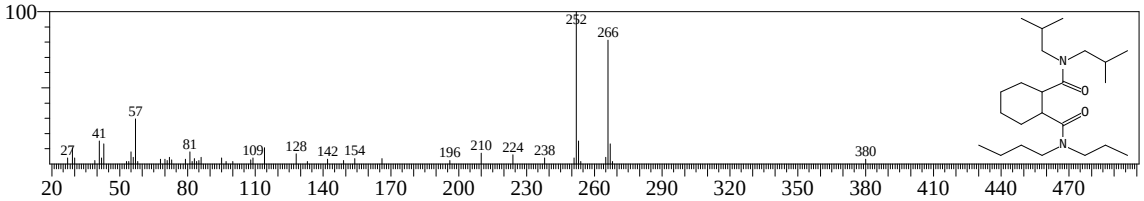

Hit#:5 Entry:90568 Library:NIST05.LIB
SI:85 Formula:C18H34O2 CAS:593-39-5 MolWeight:282 RetIndex:2175
CompName:6-Octadecenoic acid, (Z)- $$ (6Z)-6-Octadecenoic acid # $$



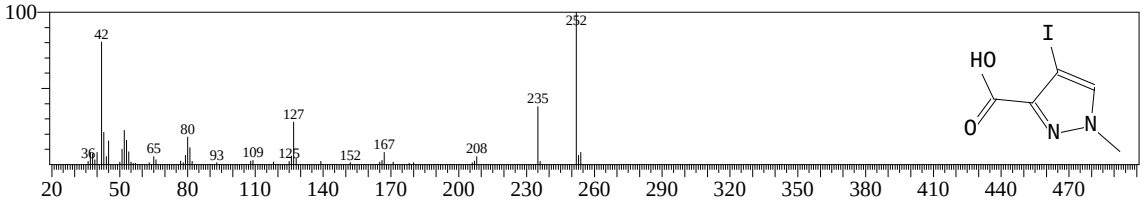
<< Target >>
Line#:22 R.Time:26.733(Scan#:2849) MassPeaks:252 BasePeak:251.95(5199)
RawMode:Averaged 26.725-26.742(2848-2850) BG Mode:Calc. from Peak



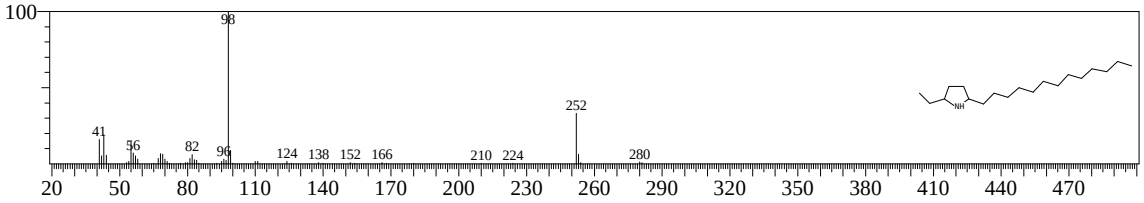
Hit#:1 Entry:139076 Library:NIST05.LIB
SI:57 Formula:C23H44N2O2 CAS:0-0-0 MolWeight:380 RetIndex:2606
CompName:Cyclohexane-1,2-dicarboxylic acid, butyl-propyl-amide) diisobutylamide



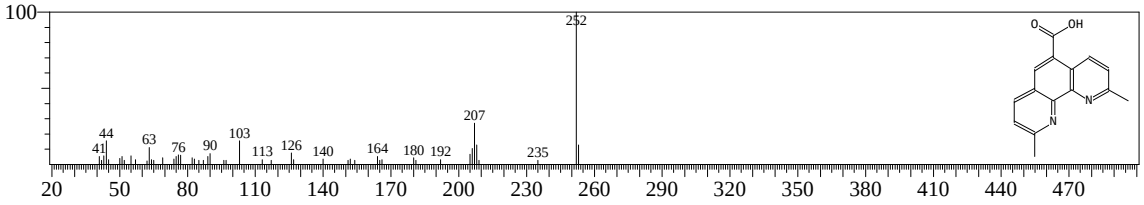
Hit#:2 Entry:71870 Library:NIST05.LIB
SI:55 Formula:C5H5IN2O2 CAS:6647-98-9 MolWeight:252 RetIndex:1565
CompName:Pyrazole-3-carboxylic acid, 4-iodo-1-methyl- $$ 4-Iodo-1-methyl-1H-pyrazole-3-carboxylic acid # $$



Hit#:3 Entry:89908 Library:NIST05.LIB
SI:54 Formula:C19H39N CAS:0-0-0 MolWeight:281 RetIndex:2160
CompName:2-Ethyl-5-tridecylpyrrolidine



Hit#:4 Entry:72354 Library:NIST05.LIB
SI:54 Formula:C15H12N2O2 CAS:0-0-0 MolWeight:252 RetIndex:2466
CompName:2,9-Dimethyl-5-carboxy-1,10-phenanthroline



Hit#:5 Entry:97931 Library:NIST05.LIB
SI:53 Formula:C15H21NO3S CAS:318466-23-8 MolWeight:295 RetIndex:2483
CompName:Quinolin-4-ol, perhydro-1-phenylsulfonyl- $$ 1-(Phenylsulfonyl)decahydro-4-quinolinol # $$