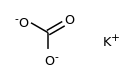


Reagents:



Solvent:

CCCCO

Τέλος φόρμας

| **Rank** | **Product** | **Probability** | **Max. Score** | **Molecular Weight** | **Predict impurities** | **Predict regio-selectivities** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | NN1NC(=S)NC1C1CO1 | 0.6748 | -69.916 | 160.2 |  |  |
| 2 | CCCCOC1=NC(C(O)CCl)N(N)N1 | 0.0981 | -71.845 | 236.7 |  |  |
| 3 | CCCCOCC(O)C1NC(=S)NN1N | 0.0732 | -72.137 | 234.3 |  |  |
| 4 | CCCCOC1=NN(N)C(C(O)CCl)N1 | 0.0509 | -72.501 | 236.7 |  |  |
| 5 | NN1NC2=NC1C(CCl)O2 | 0.0243 | -73.240 | 162.6 |  |  |
| 6 | NN1NCNC1C(O)CCl | 0.0141 | -73.782 | 166.6 |  |  |
| 7 | NN1N=C2NC1C(CCl)O2 | 0.0117 | -73.967 | 162.6 |  |  |
| 8 | NN1NC=NC1C(O)CCl | 0.0085 | -74.285 | 164.6 |  |  |
| 9 | NN1N=CNC1C(O)CCl | 0.0066 | -74.549 | 164.6 |  |  |
| 10 | OC(CCl)C1N=C2NN1N2 | 0.0063 | -74.590 | 162.6 |  |  |
| 11 | NN1NCNC1C(O)CS | 0.0048 | -74.853 | 164.2 |  |  |
| 12 | CCCCOC1NC(C(O)CCl)N(N)N1 | 0.0048 | -74.868 | 238.7 |  |  |
| 13 | CC(O)C1NC(=S)NN1N | 0.0039 | -75.058 | 162.2 |  |  |
| 14 | OC(CCl)C1Nc2nn1[nH]2 | 0.0029 | -75.355 | 162.6 |  |  |
| 15 | CCCCOC1=NC(C(O)CS)N(N)N1 | 0.0025 | -75.527 | 234.3 |  |  |
| 16 | NN1NC2NC1C(CCl)O2 | 0.0022 | -75.631 | 164.6 |  |  |
| 17 | CCCCOC1OC1C1NC(=S)NN1N | 0.0014 | -76.077 | 232.3 |  |  |
| 18 | NN1N=C=NC1C(O)CCl | 0.0012 | -76.272 | 162.6 |  |  |
| 19 | CCCCOC1=NN(N)C(C(O)CS)N1 | 0.0012 | -76.287 | 234.3 |  |  |
| 20 | OC(CCl)C1NNC(=S)N1 | 0.0010 | -76.438 | 181.6 |  |  |
| 21 | NN1NC(S)=NC1C(O)CCl | 0.0009 | -76.592 | 196.7 |  |  |
| 22 | NC1=NC(C(O)CCl)NN1 | 0.0005 | -77.068 | 164.6 |  |  |
| 23 | NN1N=C(S)NC1C(O)CCl | 0.0005 | -77.094 | 196.7 |  |  |
| 24 | CCCCOC(O)(CCl)C1NC(=S)NN1N | 0.0004 | -77.231 | 268.8 |  |  |
| 25 | NN1NC=NC1C(O)CS | 0.0004 | -77.324 | 162.2 |  |  |
| 26 | NN1NC2=NC1C(O)CS2 | 0.0004 | -77.378 | 160.2 |  |  |
| 27 | CC(O)C1N=C(Cl)NN1N | 0.0003 | -77.577 | 164.6 |  |  |
| 28 | NN1NC2=NC1C(CS)O2 | 0.0002 | -77.983 | 160.2 |  |  |
| 29 | NN1N=C2NC1C(O)CS2 | 0.0002 | -78.059 | 160.2 |  |  |
| 30 | NN1N=CNC1C(O)CS | 0.0002 | -78.215 | 162.2 |  |  |
| 31 | OC(CS)C1N=C2NN1N2 | 0.0002 | -78.294 | 160.2 |  |  |
| 32 | CC(O)C1NC(Cl)=NN1N | 0.0001 | -78.384 | 164.6 |  |  |
| 33 | NN1NC(Cl)=NC1C1CO1 | 0.0001 | -78.422 | 162.6 |  |  |
| 34 | CCCCOC1NC(C(O)CS)N(N)N1 | 0.0001 | -78.471 | 236.3 |  |  |
| 35 | CCCCOCOCC1NC(=S)NN1N | 0.0001 | -78.481 | 234.3 |  |  |
| 36 | CCCCOC12NC(C(CCl)O1)N(N)N2 | 0.0001 | -78.484 | 236.7 |  |  |
| 37 | NN1N=C2NC1C(CS)O2 | 0.0001 | -78.708 | 160.2 |  |  |
| 38 | COCC1NC(=S)NN1N | 0.0001 | -78.780 | 162.2 |  |  |
| 39 | OC(CS)C1Nc2nn1[nH]2 | 0.0001 | -79.180 | 160.2 |  |  |
| 40 | NN1NC(=S)NC1CO | 0.0001 | -79.329 | 148.2 |  |  |
| 41 | NN1N=C(Cl)NC1C1CO1 | 0.0001 | -79.381 | 162.6 |  |  |
| 42 | NC1=NNC(C(O)CCl)N1 | 0.0000 | -79.489 | 164.6 |  |  |
| 43 | NN1NC(=S)NC1C1OC1Cl | 0.0000 | -79.528 | 194.6 |  |  |
| 44 | NN1N=C=NC1C(O)CS | 0.0000 | -79.812 | 160.2 |  |  |
| 45 | CCCC(O)OC(CCl)C1NC(=S)NN1N | 0.0000 | -80.031 | 268.8 |  |  |
| 46 | CCCCOC(O)C1NC(=S)NN1N | 0.0000 | -80.136 | 220.3 |  |  |
| 47 | NN1NC2NC1C(CS)O2 | 0.0000 | -80.336 | 162.2 |  |  |
| 48 | NN1NC(Cl)NC1C1CO1 | 0.0000 | -80.861 | 164.6 |  |  |
| 49 | CCCCOCC(O)C1N=C(Cl)NN1N | 0.0000 | -80.985 | 236.7 |  |  |
| 50 | CC(O)C1NC(Cl)NN1N | 0.0000 | -81.214 | 166.6 |  |  |
| 51 | CCCCOC(Cl)C(O)C1NC(=S)NN1N | 0.0000 | -81.371 | 268.8 |  |  |
| 52 | CCCCOC(OC)C1NC(=S)NN1N | 0.0000 | -81.424 | 234.3 |  |  |
| 53 | CCCCOCC(O)C1NC(Cl)=NN1N | 0.0000 | -81.748 | 236.7 |  |  |
| 54 | NN1NCNC1C1OC1S | 0.0000 | -81.771 | 162.2 |  |  |
| 55 | CCCCOC12NC(C(CS)O1)N(N)N2 | 0.0000 | -81.973 | 234.3 |  |  |
| 56 | NN1NC(=S)NC1COCCl | 0.0000 | -82.442 | 196.7 |  |  |
| 57 | CCCCOCC(O)C1NC(Cl)NN1N | 0.0000 | -83.222 | 238.7 |  |  |
| 58 | NN1NC=NC1C1OC1S | 0.0000 | -84.122 | 160.2 |  |  |
| 59 | CCCCOC(S)C(O)C1NCNN1N | 0.0000 | -84.202 | 236.3 |  |  |
| 60 | NN1NC2=NC1C1OC1S2 | 0.0000 | -84.399 | 158.2 |  |  |
| 61 | NN1NC(Cl)=NC1C(O)CS | 0.0000 | -84.408 | 196.7 |  |  |
| 62 | CSC1=NC(CO)N(N)N1 | 0.0000 | -84.877 | 162.2 |  |  |
| 63 | NN1N=CNC1C1OC1S | 0.0000 | -84.957 | 160.2 |  |  |
| 64 | NN1NCNC1C(O)C(S)Cl | 0.0000 | -85.075 | 198.7 |  |  |
| 65 | NN1N=C(Cl)NC1C(O)CS | 0.0000 | -85.213 | 196.7 |  |  |
| 66 | CSC1=NN(N)C(CO)N1 | 0.0000 | -85.215 | 162.2 |  |  |
| 67 | NN1NC2NC1C(O)CS2 | 0.0000 | -85.391 | 162.2 |  |  |
| 68 | NN1N=C2NC1C1OC1S2 | 0.0000 | -85.602 | 158.2 |  |  |
| 69 | CCCCOC1(Cl)NC(C2CO2)N(N)N1 | 0.0000 | -85.629 | 236.7 |  |  |
| 70 | CCCCOC1NC(C2OC2S)N(N)N1 | 0.0000 | -85.634 | 234.3 |  |  |
| 71 | CCCCOC1NC(CO)N(N)N1 | 0.0000 | -86.097 | 190.2 |  |  |
| 72 | CCCCOC(S)C(O)C1N=CNN1N | 0.0000 | -86.341 | 234.3 |  |  |
| 73 | CCCCOC1SC2=NC(C1O)N(N)N2 | 0.0000 | -86.378 | 232.3 |  |  |
| 74 | CCCCOC1(Cl)NC(C(C)O)N(N)N1 | 0.0000 | -86.588 | 238.7 |  |  |
| 75 | NN1NC2NC1CO2 | 0.0000 | -87.032 | 116.1 |  |  |
| 76 | NN1NC(Cl)=NC1CO | 0.0000 | -87.120 | 150.6 |  |  |
| 77 | NN1NC=NC1C(O)C(S)Cl | 0.0000 | -87.203 | 196.7 |  |  |
| 78 | NN1NC(Cl)NC1C(O)CS | 0.0000 | -87.243 | 198.7 |  |  |
| 79 | CCCCOC1=NC(C(O)C(S)Cl)N(N)N1 | 0.0000 | -87.278 | 268.8 |  |  |
| 80 | CCCCOC(S)C(O)C1NC=NN1N | 0.0000 | -87.330 | 234.3 |  |  |
| 81 | CCCCOC1OC1C1NC(Cl)NN1N | 0.0000 | -87.520 | 236.7 |  |  |
| 82 | CCCCOC1SC2=NN(N)C(N2)C1O | 0.0000 | -87.572 | 232.3 |  |  |
| 83 | CCCCOC(OCCl)C1NC(=S)NN1N | 0.0000 | -87.727 | 268.8 |  |  |
| 84 | CCCCOC(O)C1NCNN1N | 0.0000 | -88.043 | 190.2 |  |  |
| 85 | NN1N=CNC1C(O)C(S)Cl | 0.0000 | -88.096 | 196.7 |  |  |
| 86 | CCCCOC1=NN(N)C(C(O)C(S)Cl)N1 | 0.0000 | -88.204 | 268.8 |  |  |
| 87 | NN1NCNC1COCS | 0.0000 | -88.294 | 164.2 |  |  |
| 88 | NN1N=C(Cl)NC1CO | 0.0000 | -88.565 | 150.6 |  |  |
| 89 | CCCCOC1NC(C(O)C(S)Cl)N(N)N1 | 0.0000 | -88.624 | 270.8 |  |  |
| 90 | NN1NCNC1CO | 0.0000 | -88.869 | 118.1 |  |  |
| 91 | CCCCOCC1OC2(Cl)NC1N(N)N2 | 0.0000 | -89.087 | 236.7 |  |  |
| 92 | NN1NC2=NC1C(O)C(Cl)S2 | 0.0000 | -89.098 | 194.6 |  |  |
| 93 | CCCCOC1=NC(CO)N(N)N1 | 0.0000 | -89.191 | 188.2 |  |  |
| 94 | CC1OC2(Cl)NC1N(N)N2 | 0.0000 | -89.282 | 164.6 |  |  |
| 95 | OC(C(S)Cl)C1N=C2NN1N2 | 0.0000 | -89.457 | 194.6 |  |  |
| 96 | CCCCOC(S)C1OC2NC1N(N)N2 | 0.0000 | -89.635 | 234.3 |  |  |