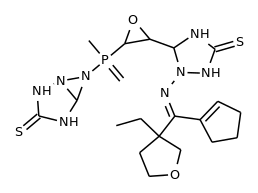
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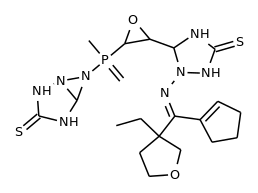


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| **Rank** | **Score** | **Template** | **Result** |
| --- | --- | --- | --- |
| 1 | 3.99050e-1 | [C:4]=[C:3]-[C:2]-[SH;D1;+0:1]>>C-C(=O)-[S;H0;D2;+0:1]-[C:2]-[C:3]=[C:4] | No Precursors |
| 2 | 1.91655e-1 |  | No Precursors |
| 3 | 1.12048e-1 | [#7:2]-[C;H0;D3;+0:1](-[C:3])=[S;H0;D1;+0]>>O=[C;H0;D3;+0:1](-[#7:2])-[C:3] | No Precursors |
| 4 | 9.88276e-2 |  | No Precursors |
| 5 | 3.50021e-2 | [#8:2]-[NH;D2;+0:1]-[C:3]>>O=[N+](-[O-])-c1:c:c:c:c:c:1-S(=O)(=O)-[N;H0;D3;+0:1](-[#8:2])-[C:3] | No Precursors |
| 6 | 2.96132e-2 | [C:2]-[CH;D2;+0:1]=[CH;D2;+0:3]-[C:4]>>C=[CH;D2;+0:1]-[C:2].C=[CH;D2;+0:3]-[C:4] | No Precursors |
| 7 | 1.71594e-2 | [C:2]-[OH;D1;+0:1]>>C-[Si](-C)(-C)-[O;H0;D2;+0:1]-[C:2] | No Precursors |
| 8 | 1.41288e-2 | [#7:2]-[C;H0;D3;+0:1](-[C:3])=[N;H0;D2;+0]-[O;H1;D1;+0]>>S=[C;H0;D3;+0:1](-[#7:2])-[C:3] | No Precursors |
| 9 | 1.40860e-2 |  | No Precursors |
| 10 | 1.20749e-2 | [C:2]=[NH;D1;+0:1]>>O=[N+](-[O-])/[N;H0;D2;+0:1]=[C:2] | No Precursors |
| 11 | 6.94014e-3 |  | No Precursors |
| 12 | 6.32136e-3 | [C:4]-[CH;D2;+0:3]=[CH;D2;+0:1]-[C:2]>>C=[CH;D2;+0:1]-[C:2].C=[CH;D2;+0:3]-[C:4] | No Precursors |
| 13 | 5.26887e-3 | [#7:2]/[C;H0;D3;+0:1](-[C:3])=[N;H0;D2;+0]\[O;H1;D1;+0]>>S=[C;H0;D3;+0:1](-[#7:2])-[C:3] | No Precursors |
| 14 | 3.17057e-3 |  | No Precursors |
| 15 | 2.88022e-3 |  | No Precursors |
| 16 | 2.42529e-3 | [C:2]-[OH;D1;+0:1]>>C-C(=O)-[O;H0;D2;+0:1]-[C:2] | No Precursors |
| 17 | 2.40508e-3 | [C:2]-[OH;D1;+0:1]>>C-C-[Si](-C-C)(-C-C)-[O;H0;D2;+0:1]-[C:2] | No Precursors |

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Page 2 of 15

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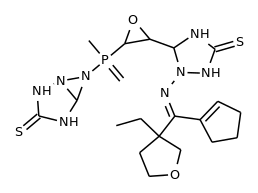
| **Rank** | **Score** | **Template** | **Result** |
| --- | --- | --- | --- |
| 21 | 1.99351e-3 |  | Apply Template |
| 22 | 1.95263e-3 |  | Apply Template |
| 23 | 1.88982e-3 | [C:2]-[NH;D2;+0:1]-[C:3]>>O=C(-O-C-c1:c:c:c:c:c:1)-[N;H0;D3;+0:1](-[C:2])-[C:3] | https://askcos.mit.edu/api/v2/draw/?&smiles=C%3DP(C)(C1OC1C1NC(%3DS)NN1%2FN%3DC(%5CC1%3DCCCC1)C1(CC)CCOC1)N1C2N(C(%3DO)OCc3ccccc3)C(%3DS)NN21 |
| 24 | 1.48799e-3 |  | No Precursors |
| 25 | 1.17679e-3 |  | No Precursors |
| 26 | 1.16084e-3 | [C:2]-[OH;D1;+0:1]>>C-C(-C)(-C)-[Si](-C)(-C)-[O;H0;D2;+0:1]-[C:2] | No Precursors |
| 27 | 1.15122e-3 |  | No Precursors |
| 28 | 1.14229e-3 | [C:4]=[C:3]-[C:2]-[OH;D1;+0:1]>>C-C(=O)-[O;H0;D2;+0:1]-[C:2]-[C:3]=[C:4] | No Precursors |
| 29 | 9.86053e-4 | [#7:2]-[C;H0;D3;+0:1](=[S;H0;D1;+0])-[C:3]-[#7:4]>>O=[C;H0;D3;+0:1](-[#7:2])-[C:3]-[#7:4] | No Precursors |
| 30 | 9.80621e-4 | [C:3]=[#7:2]-[OH;D1;+0:1]>>C-[Si](-C)(-C)-[O;H0;D2;+0:1]-[#7:2]=[C:3] | No Precursors |
| 31 | 9.34389e-4 |  | No Precursors |
| 32 | 8.90984e-4 |  | No Precursors |
| 33 | 8.81831e-4 |  | https://askcos.mit.edu/api/v2/draw/?&smiles=C%3DP(C)(C1OC1C1NC(%3DS)NN1N)N1C2NC(%3DS)NN21.CCC1(C(%3DO)C2%3DCCCC2)CCOC1 |
| 34 | 7.05558e-4 | [#8:2]-[C;H0;D3;+0:1](-[C:3])=[S;H0;D1;+0]>>O=[C;H0;D3;+0:1](-[#8:2])-[C:3] | No Precursors |
| 35 | 6.62252e-4 | [#7:2]-[C;H0;D3;+0:1](=[S;H0;D1;+0])-[C:3]-[#8:4]>>O=[C;H0;D3;+0:1](-[#7:2])-[C:3]-[#8:4] | No Precursors |
| 36 | 6.54742e-4 | [C:2]-[CH2;D2;+0:1]-[CH;D2;+0:4]=[C:3]>>C=C-[CH2;D2;+0:1]-[C:2].[C:3]=[CH2;D1;+0:4] | https://askcos.mit.edu/api/v2/draw/?&smiles=C%3DCCCCC(%3DC)%2FC(%3DN%5CN1NC(%3DS)NC1C1OC1P(%3DC)(C)N1C2NC(%3DS)NN21)C1(CC)CCOC1 |
| 37 | 6.33137e-4 | [C:3]-[O;H0;D2;+0:4]-[CH2;D2;+0:1]-[c:2]>>Br-[CH2;D2;+0:1]-[c:2].[C:3]-[OH;D1;+0:4] | No Precursors |
| 38 | 6.21339e-4 |  | No Precursors |
| 39 | 4.96049e-4 | [C:2]-[N;H0;D2;+0:3]=[CH2;D1;+0:1]>>O=[CH2;D1;+0:1].[C:2]-[NH2;D1;+0:3] | No Precursors |
| 40 | 4.90347e-4 | [C:1]=[C:2]-[C:3]-[OH;D1;+0:4]>>[C:1]=[C:2]-[C:3]-[O;H0;D2;+0:4]-C1-C-C-C-C-O-1 | No Precursors |

Re-evaluateClose

Αρχή φόρμας

Target

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Page 3 of 15

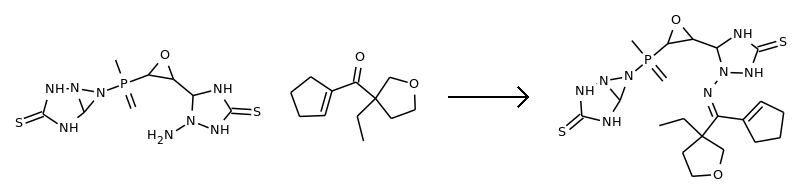
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| **Rank** | **Score** | **Template** | **Result** |
| --- | --- | --- | --- |
| 41 | 4.53042e-4 |  | Apply Template |
| 42 | 4.51558e-4 | [C:2]-[SH;D1;+0:1]>>C-C(=O)-[S;H0;D2;+0:1]-[C:2] | Apply Template |
| 43 | 4.44915e-4 |  | Apply Template |
| 44 | 4.44842e-4 |  | Apply Template |
| 45 | 4.40899e-4 | [C:3]-[N;H0;D2;+0:2]=[C;H0;D1;+0:1]>>O=[CH;D2;+0:1]-[NH;D2;+0:2]-[C:3] | Apply Template |
| 46 | 4.23178e-4 | [C:1]-[NH;D2;+0:2]-[C:3]>>[C:1]-[N;H0;D3;+0:2](-[C:3])-C-c1:c:c:c:c:c:1 | https://askcos.mit.edu/api/v2/draw/?&smiles=C%3DP(C)(C1OC1C1NC(%3DS)NN1%2FN%3DC(%5CC1%3DCCCC1)C1(CC)CCOC1)N1C2N(Cc3ccccc3)C(%3DS)NN21 |
| 47 | 3.74529e-4 | [C:2]=[NH;D1;+0:1]>>O/[N;H0;D2;+0:1]=[C:2] | Apply Template |
| 48 | 3.62433e-4 | [C:2]-[NH;D2;+0:1]-[c:3]>>C-C(-C)(-C)-O-C(=O)-[N;H0;D3;+0:1](-[C:2])-[c:3] | Apply Template |
| 49 | 3.53575e-4 |  | Apply Template |
| 50 | 3.52690e-4 | [C:1]-[CH;D3;+0:2](-[C:3])-[OH;D1;+0:4]>>[C:1]-[C;H0;D3;+0:2](-[C:3])=[O;H0;D1;+0:4] | Apply Template |
| 51 | 3.21906e-4 | [C:2]-[NH;D2;+0:1]-[C:3]-[C:4]=[C:5]>>C-C(-C)(-C)-O-C(=O)-[N;H0;D3;+0:1](-[C:2])-[C:3]-[C:4]=[C:5] | Apply Template |
| 52 | 3.11386e-4 | [C:1]-[SH;D1;+0:2]>>[C:1]-[S;H0;D2;+0:2]-C-c1:c:c:c:c:c:1 | Apply Template |
| 53 | 2.94558e-4 | [C:1]-[CH;D2;+0:2]=[CH2;D1;+0:3]>>[C:1]-[C;H0;D2;+0:2]#[CH;D1;+0:3] | Apply Template |
| 54 | 2.89095e-4 | [C:2]-[OH;D1;+0:1]>>O=C(-[O;H0;D2;+0:1]-[C:2])-c1:c:c:c:c:c:1 | Apply Template |
| 55 | 2.87045e-4 | [C:1]-[CH;D3;+0:2](-[OH;D1;+0:3])-[c:4]>>[C:1]-[C;H0;D3;+0:2](=[O;H0;D1;+0:3])-[c:4] | Apply Template |



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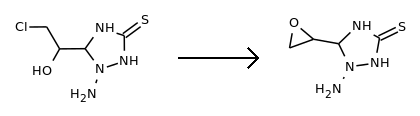
Solvent:



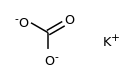
Τέλος φόρμας

| **Rank** | **Product** | **Probability** | **Max. Score** | **Molecular Weight** | **Predict impurities** | **Predict regio-selectivities** |
| --- | --- | --- | --- | --- | --- | --- |
| 1 | C=P(C)(C1OC1C1NNC(=S)N1)N1C2NC(=S)NN21 | 0.7623 | -78.137 | 319.4 |  |  |
| 2 | CCC1(C(=O)C2=C(C=P(C)(C3OC3C3NC(=S)NN3N)N3C4NC(=S)NN43)CCC2)CCOC1 | 0.0581 | -80.712 | 526.6 |  |  |
| 3 | CCC1(CC2=CCCC2)CCOC1 | 0.0476 | -80.911 | 180.3 |  |  |
| 4 | CCC1(C(=O)C2CCCC2)CCOC1 | 0.0347 | -81.227 | 196.3 |  |  |
| 5 | C=P(C)(C1OC1C(NN)NC(N)=S)N1C2NC(=S)NN21 | 0.0139 | -82.145 | 336.4 |  |  |
| 6 | C=P(C)(C1OC1C1NC(=S)NN1N)N1C2NCNN21 | 0.0138 | -82.147 | 304.3 |  |  |
| 7 | C=P(C)(C1OC1C1NC(=S)NN1N)N1C2NC=NN21 | 0.0134 | -82.181 | 302.3 |  |  |
| 8 | C[P+](C)(C1OC1C1NC(=S)NN1N)N1C2NC(=S)NN21 | 0.0109 | -82.381 | 335.4 |  |  |
| 9 | C=P(C)(C1OC1C1NCNN1N)N1C2NC(=S)NN21 | 0.0098 | -82.490 | 304.3 |  |  |
| 10 | C=P(C)(C1OC1C1N=CNN1N)N1C2NC(=S)NN21 | 0.0073 | -82.783 | 302.3 |  |  |
| 11 | C=P(C)(C1OC1C(N)NC(N)=S)N1C2NC(=S)NN21 | 0.0048 | -83.205 | 321.4 |  |  |
| 12 | O=C(C1=CCCC1)C1CCOC1 | 0.0044 | -83.290 | 166.2 |  |  |
| 13 | C=P(C)(C1OC1C1NC=NN1N)N1C2NC(=S)NN21 | 0.0031 | -83.655 | 302.3 |  |  |
| 14 | CCC1(C(=O)C2CCCC2C=P(C)(C2OC2C2NC(=S)NN2N)N2C3NC(=S)NN32)CCOC1 | 0.0027 | -83.767 | 528.6 |  |  |
| 15 | CCCCCC(=O)C1(CC)CCOC1 | 0.0026 | -83.811 | 198.3 |  |  |
| 16 | C=P(C)(C1OC1C1NC(=S)NN1N)N1C2N=CNN21 | 0.0024 | -83.889 | 302.3 |  |  |
| 17 | CCC1(C(=O)C2=C(C[P+](C)(C3OC3C3NC(=S)NN3N)N3C4NC(=S)NN43)CCC2)CCOC1 | 0.0022 | -83.965 | 527.6 |  |  |
| 18 | C=P(C)(C1OC1C1NC(=S)NN1N)N1C2N=C=NN21 | 0.0020 | -84.090 | 300.3 |  |  |
| 19 | CCC1(C(=O)CCCCCC=P(C)(C2OC2C2NC(=S)NN2N)N2C3NC(=S)NN32)CCOC1 | 0.0016 | -84.307 | 530.7 |  |  |
| 20 | C=P(C)(C1OC1C1N=C=NN1N)N1C2NC(=S)NN21 | 0.0013 | -84.526 | 300.3 |  |  |
| 21 | CCC1(C=O)CCOC1 | 0.0005 | -85.442 | 128.2 |  |  |
| 22 | CCC(CC)(CO)C(=O)C1=CCCC1 | 0.0005 | -85.565 | 196.3 |  |  |
| 23 | CCC1(C(=O)C2CCCC2C[P+](C)(C2OC2C2NC(=S)NN2N)N2C3NC(=S)NN32)CCOC1 | 0.0001 | -87.311 | 529.7 |  |  |
| 24 | CCC1(C(=O)CCCCCC[P+](C)(C2OC2C2NC(=S)NN2N)N2C3NC(=S)NN32)CCOC1 | 0.0000 | -87.801 | 531.7 |  |  |
| 25 | C=P(C)(C1OC1C(NN)NC=N)N1C2NC(=S)NN21 | 0.0000 | -88.094 | 304.3 |  |  |
| 26 | C=P(C)(C1OC1C(N=C=N)NN)N1C2NC(=S)NN21 | 0.0000 | -88.633 | 302.3 |  |  |
| 27 | CP(=CC1CCCC1)(C1OC1C1NC(=S)NN1N)N1C2NC(=S)NN21 | 0.0000 | -89.314 | 402.5 |  |  |
| 28 | C=P(C)(C1OC1C(N)NC=N)N1C2NC(=S)NN21 | 0.0000 | -89.583 | 289.3 |  |  |
| 29 | C=P(C)(C1OC1C(N)N=C=N)N1C2NC(=S)NN21 | 0.0000 | -90.675 | 287.3 |  |  |
| 30 | CCCCCC=P(C)(C1OC1C1NC(=S)NN1N)N1C2NC(=S)NN21 | 0.0000 | -90.688 | 404.5 |  |  |
| 31 | CCC1(C)CCOC1 | 0.0000 | -90.773 | 114.2 |  |  |
| 32 | C[P+](CC1CCCC1)(C1OC1C1NC(=S)NN1N)N1C2NC(=S)NN21 | 0.0000 | -92.448 | 403.5 |  |  |
| 33 | CCCCCC[P+](C)(C1OC1C1NC(=S)NN1N)N1C2NC(=S)NN21 | 0.0000 | -93.574 | 405.5 |  |  |

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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 |  |  |