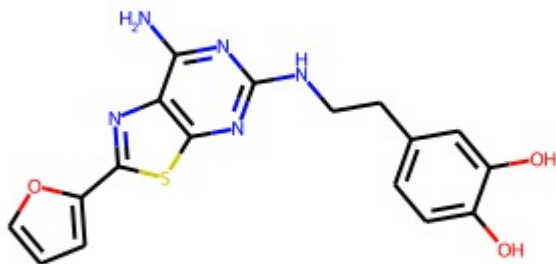


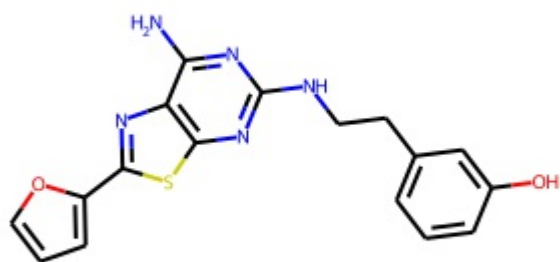
epistemic percentile: 24.2
p_risky at threshold of 5: [0.997]



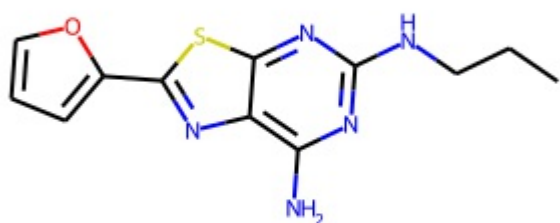
interesting mol: COC1CCCC2C(C(=O)N[C@H]3CCCC4CCCNc43)nc(N)nc12
predicted mean: [7.512]
predicted standard deviation: [0.841]
95% CI: [5.83] - [9.195]
epistemic percentile: 71.9
p_risky at threshold of 5: [0.999]



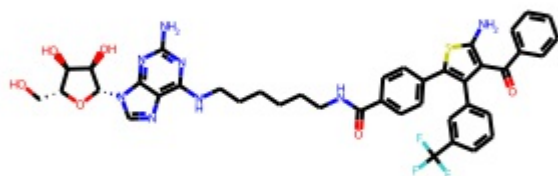
interesting mol: Nc1nc(NCCc2ccc(O)c(O)c2)nc2sc(-c3ccco3)nc12
predicted mean: [7.511]
predicted standard deviation: [0.806]
95% CI: [5.899] - [9.123]
epistemic percentile: 50.6
p_risky at threshold of 5: [0.999]



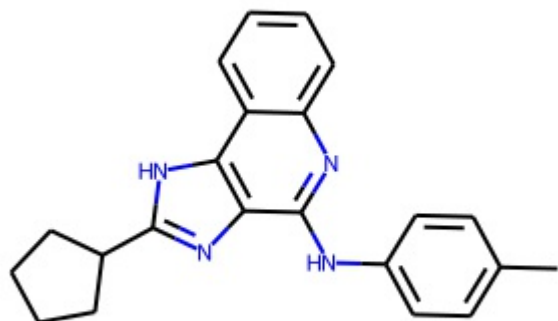
interesting mol: Nc1nc(NCCc2ccc(O)c2)nc2sc(-c3ccco3)nc12
 predicted mean: [7.683]
 predicted standard deviation: [0.845]
 95% CI: [5.994] - [9.372]
 epistemic percentile: 49.4
 p_risky at threshold of 5: [0.999]



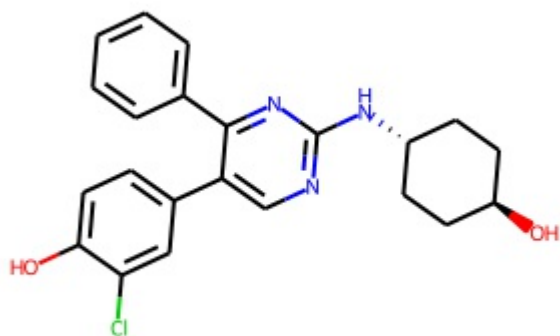
interesting mol: CCCNc1nc(N)c2nc(-c3ccco3)sc2n1
 predicted mean: [7.04]
 predicted standard deviation: [0.83]
 95% CI: [5.38] - [8.7]
 epistemic percentile: 14.9
 p_risky at threshold of 5: [0.993]



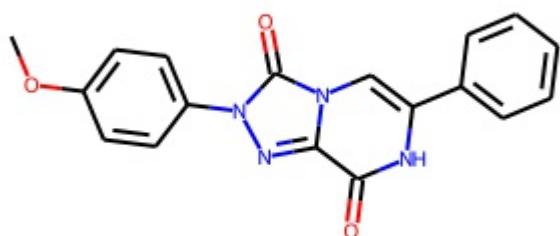
interesting mol: Nc1nc(NCCCCCNC(=O)c2ccc(-c3sc(N)c(C(=O)c4ccccc4)c3-c3cccc(C(F)(F)F)c3)cc2)c2ncn([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)c2n1
 predicted mean: [6.4]
 predicted standard deviation: [0.893]
 95% CI: [4.614] - [8.187]
 epistemic percentile: 93.3
 p_risky at threshold of 5: [0.939]



interesting mol: Cc1ccc(Nc2nc3ccccc3c3[nH]c(C4CCCC4)nc23)cc1
 predicted mean: [5.401]
 predicted standard deviation: [0.841]
 95% CI: [3.719] - [7.082]
 epistemic percentile: 81.6
 p_risky at threshold of 5: [0.675]



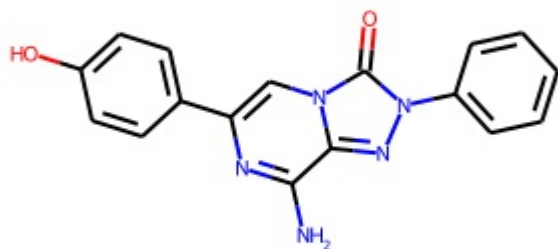
interesting mol: Oc1ccc(-c2cnc(N[C@H]3CC[C@H](O)CC3)nc2-c2ccccc2)cc1Cl
 predicted mean: [6.237]
 predicted standard deviation: [0.844]
 95% CI: [4.55] - [7.925]
 epistemic percentile: 71.9
 p_risky at threshold of 5: [0.923]



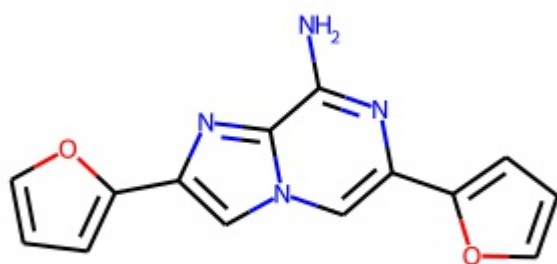
interesting mol: COc1ccc(-n2nc3c(=O)[nH]c(-c4ccccc4)cn3c2=O)cc1
 predicted mean: [5.477]
 predicted standard deviation: [0.829]
 95% CI: [3.82] - [7.135]
 epistemic percentile: 38.7
 p_risky at threshold of 5: [0.742]



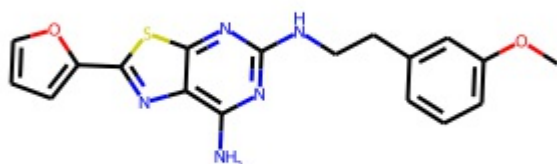
interesting mol: Cc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1
 predicted mean: [7.046]
 predicted standard deviation: [0.857]
 95% CI: [5.332] - [8.76]
 epistemic percentile: 43.4
 p_risky at threshold of 5: [0.993]



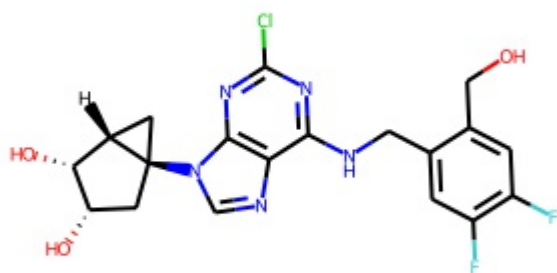
interesting mol: Nc1nc(-c2ccc(O)cc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [6.892]
 predicted standard deviation: [0.848]
 95% CI: [5.195] - [8.589]
 epistemic percentile: 51.3
 p_risky at threshold of 5: [0.988]



interesting mol: Nc1nc(-c2ccco2)cn2cc(-c3ccco3)nc12
 predicted mean: [7.101]
 predicted standard deviation: [0.838]
 95% CI: [5.425] - [8.777]
 epistemic percentile: 2.9
 p_risky at threshold of 5: [0.996]



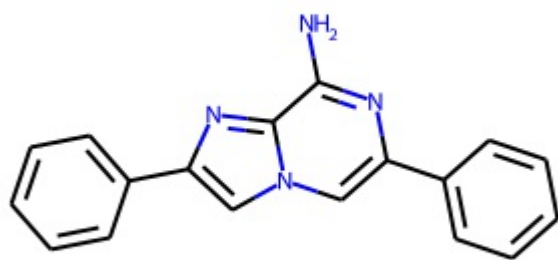
interesting mol: COc1cccc(CCNC2nc(N)c3nc(-c4ccco4)sc3n2)c1
 predicted mean: [7.656]
 predicted standard deviation: [0.849]
 95% CI: [5.959] - [9.354]
 epistemic percentile: 44.3
 p_risky at threshold of 5: [0.999]



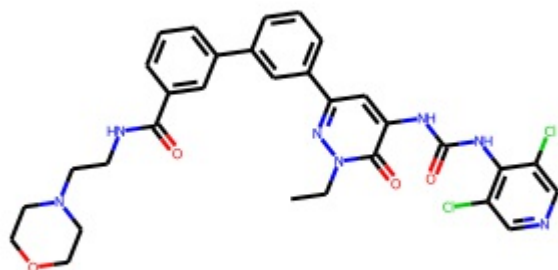
interesting mol: OCc1cc(F)c(F)cc1CNc1nc(Cl)nc2c1ncn2[C@@]12C[C@H](O)[C@H](O)[C@@H]1C2
 predicted mean: [5.757]
 predicted standard deviation: [0.812]
 95% CI: [4.133] - [7.38]
 epistemic percentile: 46.4
 p_risky at threshold of 5: [0.817]



interesting mol: Nc1nc(-c2cccc(O)c2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [7.154]
 predicted standard deviation: [0.834]
 95% CI: [5.486] - [8.823]
 epistemic percentile: 46.3
 p_risky at threshold of 5: [0.994]



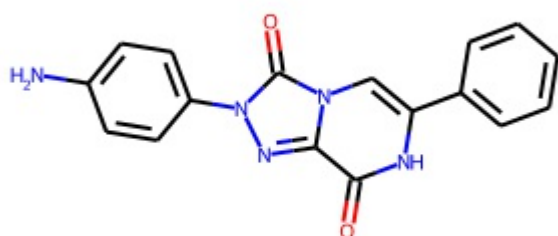
interesting mol: Nc1nc(-c2ccccc2)cn2cc(-c3ccccc3)nc12
 predicted mean: [6.379]
 predicted standard deviation: [0.789]
 95% CI: [4.801] - [7.956]
 epistemic percentile: 5.1
 p_risky at threshold of 5: [0.962]



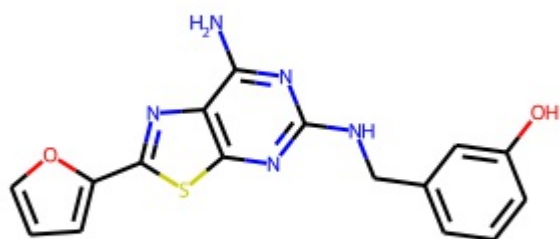
interesting mol: CCn1nc(-c2ccccc(-c3ccccc(C(=O)NCCN4CCOCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.885]
 predicted standard deviation: [0.881]
 95% CI: [4.124] - [7.647]
 epistemic percentile: 92.9
 p_risky at threshold of 5: [0.846]



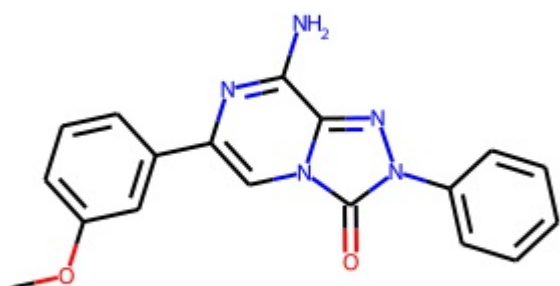
interesting mol: COc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1
 predicted mean: [6.823]
 predicted standard deviation: [0.792]
 95% CI: [5.239] - [8.407]
 epistemic percentile: 38.8
 p_risky at threshold of 5: [0.989]



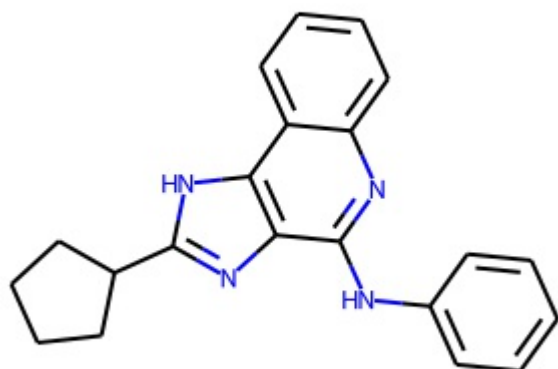
interesting mol: Nc1ccc(-n2nc3c(=O)[nH]c(-c4ccccc4)cn3c2=O)cc1
 predicted mean: [5.979]
 predicted standard deviation: [0.85]
 95% CI: [4.278] - [7.68]
 epistemic percentile: 69.4
 p_risky at threshold of 5: [0.879]



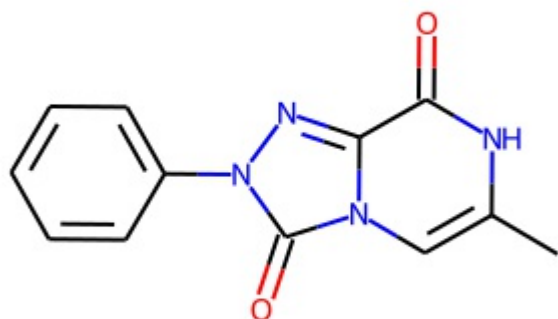
interesting mol: Nc1nc(NCc2ccc(O)c2)nc2sc(-c3ccco3)nc12
 predicted mean: [7.311]
 predicted standard deviation: [0.836]
 95% CI: [5.64] - [8.983]
 epistemic percentile: 56.9
 p_risky at threshold of 5: [0.997]



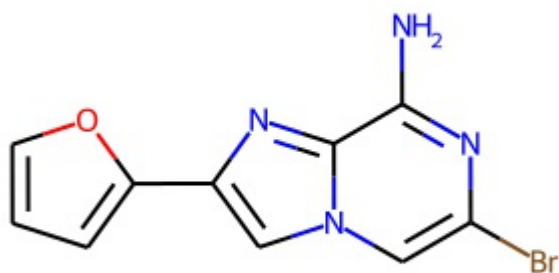
interesting mol: COc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)c1
 predicted mean: [7.298]
 predicted standard deviation: [0.814]
 95% CI: [5.67] - [8.926]
 epistemic percentile: 44.1
 p_risky at threshold of 5: [0.997]



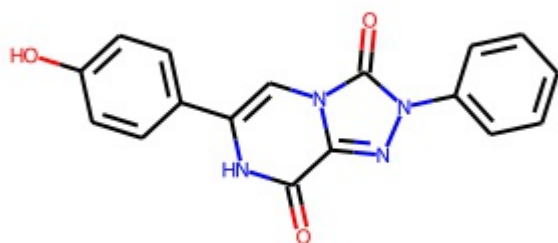
interesting mol: c1ccc(Nc2nc3ccccc3c3[nH]c(C4CCCC4)nc23)cc1
 predicted mean: [5.633]
 predicted standard deviation: [0.855]
 95% CI: [3.923] - [7.344]
 epistemic percentile: 72.2
 p_risky at threshold of 5: [0.762]



interesting mol: Cc1cn2c(=O)n(-c3ccccc3)nc2c(=O)[nH]1
 predicted mean: [5.606]
 predicted standard deviation: [0.776]
 95% CI: [4.055] - [7.157]
 epistemic percentile: 17.9
 p_risky at threshold of 5: [0.781]



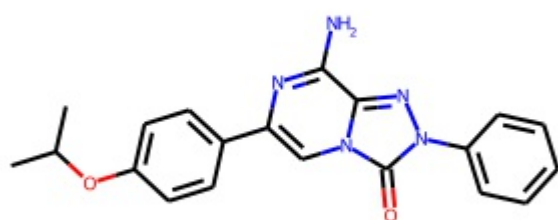
interesting mol: Nc1nc(Br)cn2cc(-c3ccco3)nc12
 predicted mean: [7.203]
 predicted standard deviation: [0.797]
 95% CI: [5.61] - [8.797]
 epistemic percentile: 10.5
 p_risky at threshold of 5: [0.997]



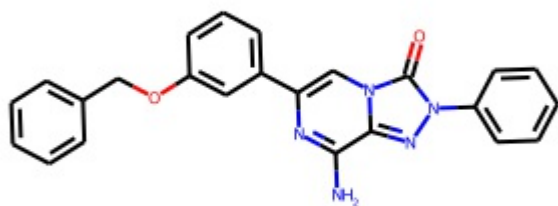
interesting mol: O=c1[nH]c(-c2ccc(O)cc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [5.742]
 predicted standard deviation: [0.812]
 95% CI: [4.119] - [7.366]
 epistemic percentile: 50.9
 p_risky at threshold of 5: [0.848]



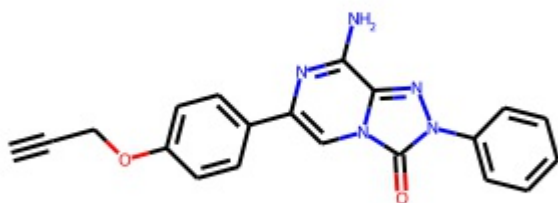
interesting mol: Nc1nc(-c2ccccc2)cn2c(=O)n(-c3ccc([N+](=O)[O-])cc3)nc12
 predicted mean: [6.667]
 predicted standard deviation: [0.84]
 95% CI: [4.986] - [8.347]
 epistemic percentile: 54.4
 p_risky at threshold of 5: [0.979]



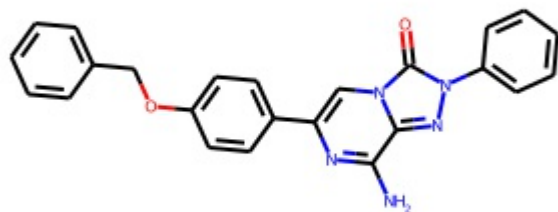
interesting mol: CC(C)Oc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1
 predicted mean: [7.058]
 predicted standard deviation: [0.847]
 95% CI: [5.364] - [8.753]
 epistemic percentile: 52.2
 p_risky at threshold of 5: [0.995]



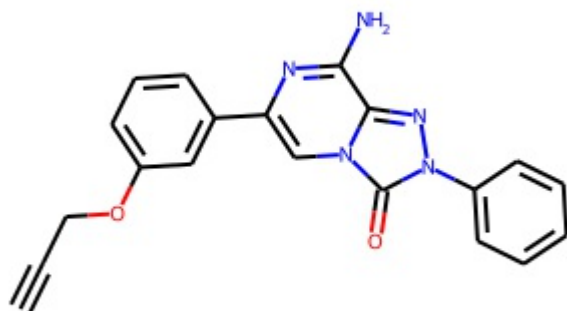
interesting mol: Nc1nc(-c2cccc(OCc3ccccc3)c2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [6.672]
 predicted standard deviation: [0.864]
 95% CI: [4.945] - [8.4]
 epistemic percentile: 78.6
 p_risky at threshold of 5: [0.975]



interesting mol: C#CCOc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1
 predicted mean: [7.429]
 predicted standard deviation: [0.842]
 95% CI: [5.746] - [9.113]
 epistemic percentile: 61.6
 p_risky at threshold of 5: [0.998]



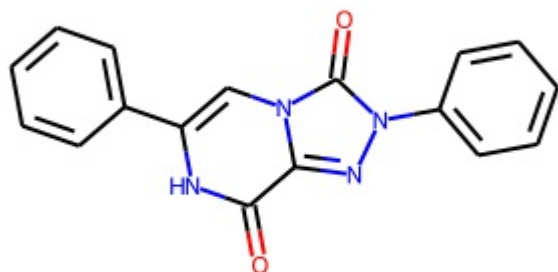
interesting mol: Nc1nc(-c2ccc(OCc3ccccc3)cc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [6.648]
 predicted standard deviation: [0.838]
 95% CI: [4.972] - [8.324]
 epistemic percentile: 75.5
 p_risky at threshold of 5: [0.976]



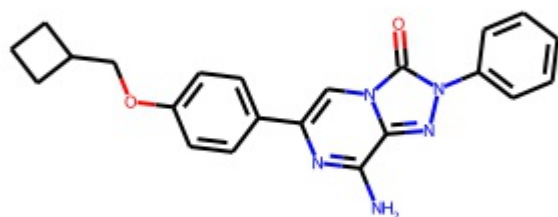
interesting mol: C#CCOc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)c1
 predicted mean: [7.518]
 predicted standard deviation: [0.838]
 95% CI: [5.842] - [9.194]
 epistemic percentile: 63.7
 p_risky at threshold of 5: [0.998]



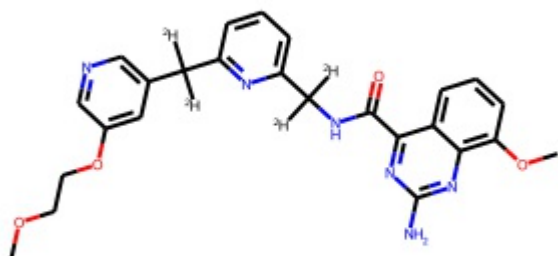
interesting mol: Nc1nc(-c2ccc(OCC3CC3)cc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [7.12]
 predicted standard deviation: [0.856]
 95% CI: [5.408] - [8.832]
 epistemic percentile: 69.9
 p_risky at threshold of 5: [0.996]



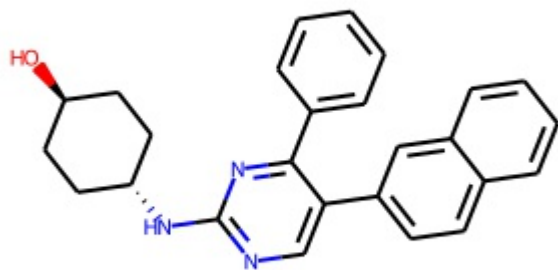
interesting mol: O=c1[nH]c(-c2ccccc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [5.907]
 predicted standard deviation: [0.797]
 95% CI: [4.313] - [7.502]
 epistemic percentile: 26.3
 p_risky at threshold of 5: [0.884]



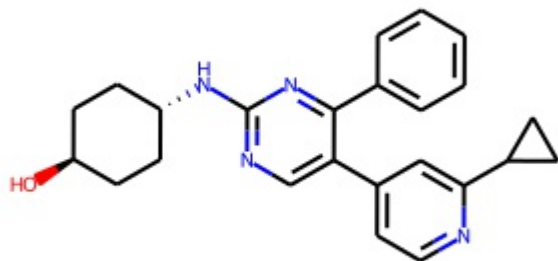
interesting mol: Nc1nc(-c2ccc(OCC3CCC3)cc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [7.061]
 predicted standard deviation: [0.865]
 95% CI: [5.33] - [8.791]
 epistemic percentile: 70.9
 p_risky at threshold of 5: [0.991]



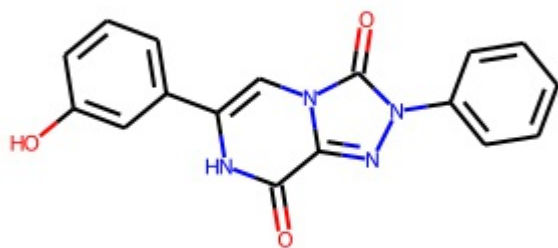
interesting mol: [2H]C([2H])(NC(=O)c1nc(N)nc2c(OC)cccc12)c1cccc(C([2H])([2H])c2cncc(OCCOC)c2)n1
 predicted mean: [7.66]
 predicted standard deviation: [0.846]
 95% CI: [5.968] - [9.353]
 epistemic percentile: 82.8
 p_risky at threshold of 5: [0.999]



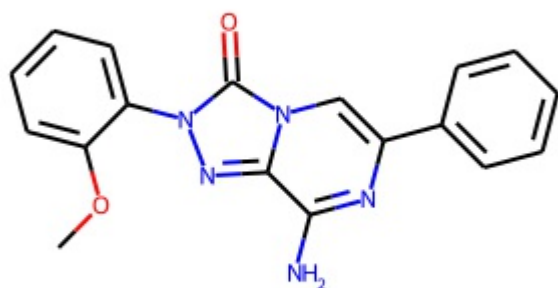
interesting mol: O[C@H]1CC[C@H](Nc2ncc(-c3ccc4ccccc4c3)c(-c3ccccc3)n2)CC1
 predicted mean: [6.306]
 predicted standard deviation: [0.86]
 95% CI: [4.586] - [8.027]
 epistemic percentile: 49.8
 p_risky at threshold of 5: [0.937]



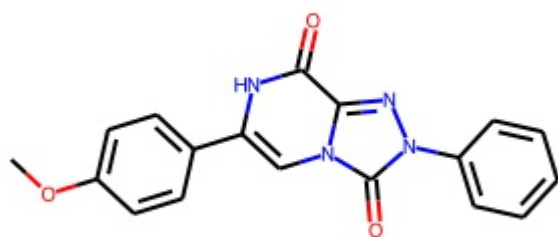
interesting mol: O[C@H]1CC[C@H](Nc2ncc(-c3ccnc(C4CC4)c3)c(-c3ccccc3)n2)CC1
 predicted mean: [6.165]
 predicted standard deviation: [0.804]
 95% CI: [4.558] - [7.772]
 epistemic percentile: 46.3
 p_risky at threshold of 5: [0.905]



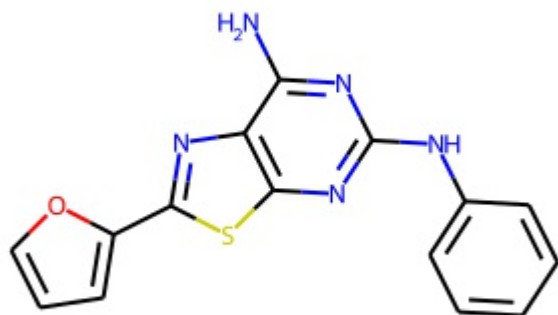
interesting mol: O=c1[nH]c(-c2cccc(O)c2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [5.941]
 predicted standard deviation: [0.797]
 95% CI: [4.347] - [7.535]
 epistemic percentile: 36.2
 p_risky at threshold of 5: [0.872]



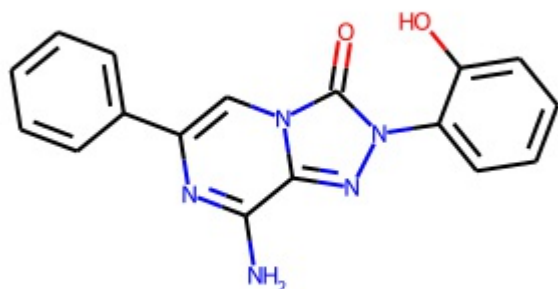
interesting mol: COc1ccccc1-n1nc2c(N)nc(-c3ccccc3)cn2c1=O
 predicted mean: [6.878]
 predicted standard deviation: [0.824]
 95% CI: [5.23] - [8.525]
 epistemic percentile: 45.6
 p_risky at threshold of 5: [0.99]



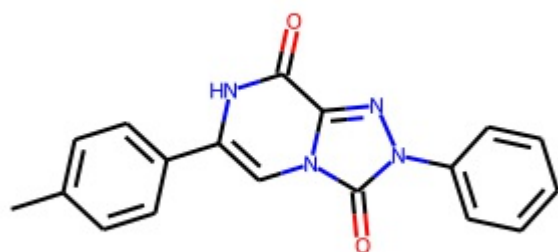
interesting mol: COc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)cc1
 predicted mean: [5.756]
 predicted standard deviation: [0.785]
 95% CI: [4.187] - [7.325]
 epistemic percentile: 26.3
 p_risky at threshold of 5: [0.827]



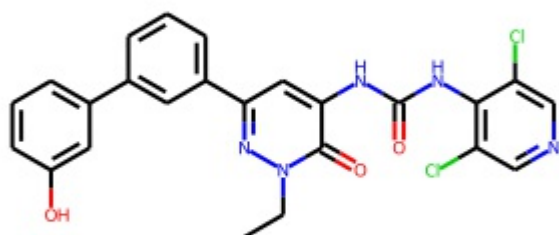
interesting mol: Nc1nc(Nc2ccccc2)nc2sc(-c3ccco3)nc12
 predicted mean: [6.631]
 predicted standard deviation: [0.792]
 95% CI: [5.048] - [8.215]
 epistemic percentile: 21.0
 p_risky at threshold of 5: [0.975]



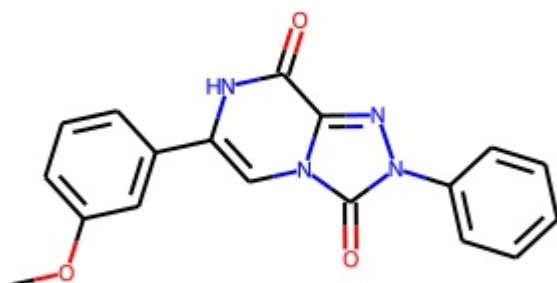
interesting mol: Nc1nc(-c2ccccc2)cn2c(=O)n(-c3ccccc3)nc12
 predicted mean: [6.84]
 predicted standard deviation: [0.833]
 95% CI: [5.175] - [8.505]
 epistemic percentile: 42.5
 p_risky at threshold of 5: [0.989]



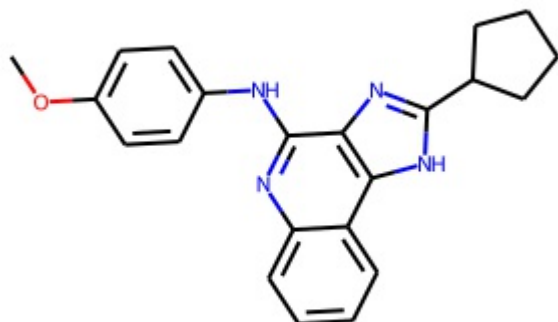
interesting mol: Cc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)cc1
 predicted mean: [5.839]
 predicted standard deviation: [0.834]
 95% CI: [4.172] - [7.507]
 epistemic percentile: 30.3
 p_risky at threshold of 5: [0.856]



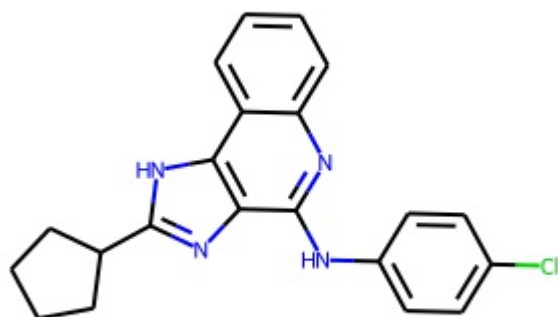
interesting mol: CCn1nc(-c2ccc(-c3ccc(O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.823]
 predicted standard deviation: [0.84]
 95% CI: [4.143] - [7.504]
 epistemic percentile: 76.3
 p_risky at threshold of 5: [0.839]



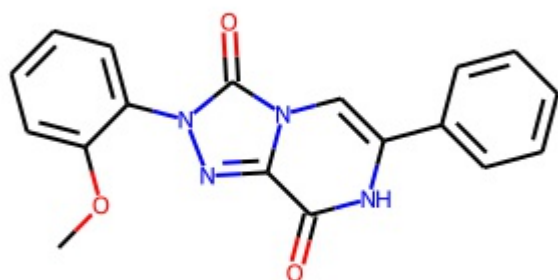
interesting mol: COc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)c1
 predicted mean: [6.119]
 predicted standard deviation: [0.815]
 95% CI: [4.49] - [7.749]
 epistemic percentile: 35.0
 p_risky at threshold of 5: [0.914]



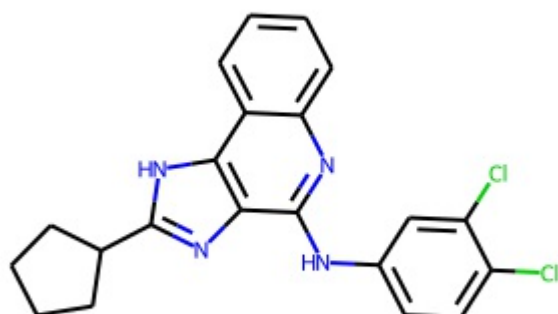
interesting mol: COc1ccc(Nc2nc3ccccc3c[nH]c(C4CCCC4)nc23)cc1
 predicted mean: [5.345]
 predicted standard deviation: [0.843]
 95% CI: [3.66] - [7.03]
 epistemic percentile: 58.8
 p_risky at threshold of 5: [0.635]



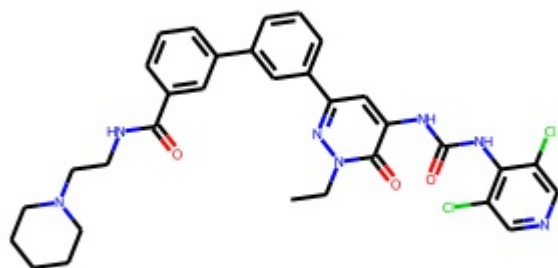
interesting mol: Clc1ccc(Nc2nc3ccccc3c[nH]c(C4CCCC4)nc23)cc1
 predicted mean: [5.339]
 predicted standard deviation: [0.809]
 95% CI: [3.722] - [6.956]
 epistemic percentile: 79.7
 p_risky at threshold of 5: [0.67]



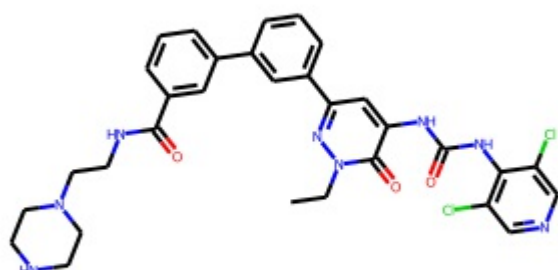
interesting mol: COc1ccccc1-n1nc2c(=O)[nH]c(-c3ccccc3)cn2c1=O
 predicted mean: [5.791]
 predicted standard deviation: [0.829]
 95% CI: [4.134] - [7.449]
 epistemic percentile: 37.9
 p_risky at threshold of 5: [0.828]



interesting mol: Clc1ccc(Nc2nc3ccccc3c3[nH]c(C4CCCC4)nc23)cc1Cl
 predicted mean: [5.872]
 predicted standard deviation: [0.912]
 95% CI: [4.049] - [7.696]
 epistemic percentile: 93.2
 p_risky at threshold of 5: [0.843]



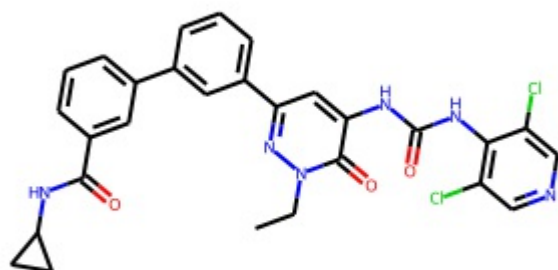
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN4CCCCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.837]
 predicted standard deviation: [0.899]
 95% CI: [4.04] - [7.635]
 epistemic percentile: 91.7
 p_risky at threshold of 5: [0.841]



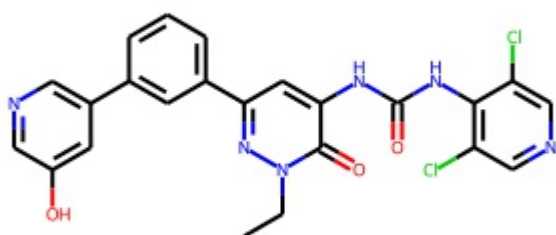
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN4CCNCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.995]
 predicted standard deviation: [0.88]
 95% CI: [4.234] - [7.756]
 epistemic percentile: 92.3
 p_risky at threshold of 5: [0.867]



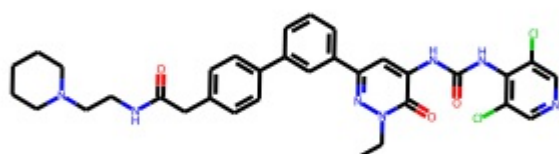
interesting mol: O=C1[nH]c(-c2ccccc2)cn2c(=O)n(-c3ccccc3O)nc12
 predicted mean: [5.767]
 predicted standard deviation: [0.796]
 95% CI: [4.176] - [7.359]
 epistemic percentile: 36.0
 p_risky at threshold of 5: [0.807]



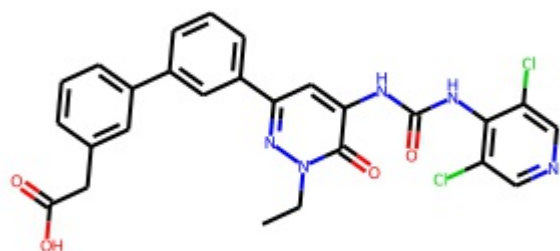
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NC4CC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.748]
 predicted standard deviation: [0.853]
 95% CI: [4.041] - [7.455]
 epistemic percentile: 83.0
 p_risky at threshold of 5: [0.815]



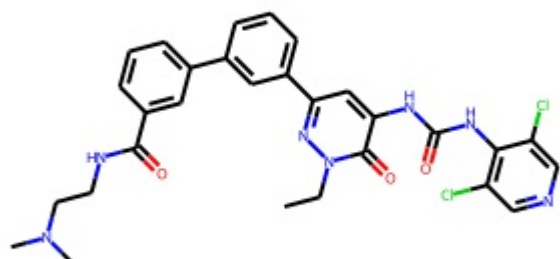
interesting mol: CCn1nc(-c2cccc(-c3cncc(O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.867]
 predicted standard deviation: [0.811]
 95% CI: [4.244] - [7.489]
 epistemic percentile: 69.1
 p_risky at threshold of 5: [0.838]



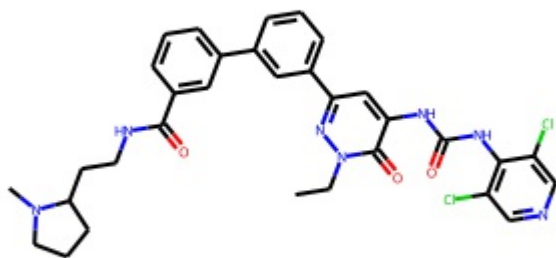
interesting mol: CCn1nc(-c2cccc(-c3ccc(CC(=O)NCCN4CCCCC4)cc3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [6.138]
 predicted standard deviation: [0.863]
 95% CI: [4.412] - [7.863]
 epistemic percentile: 94.5
 p_risky at threshold of 5: [0.899]



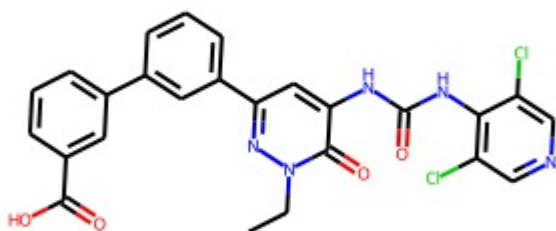
interesting mol: CCn1nc(-c2cccc(-c3cccc(CC(=O)O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.234]
 predicted standard deviation: [0.843]
 95% CI: [3.549] - [6.919]
 epistemic percentile: 78.6
 p_risky at threshold of 5: [0.64]



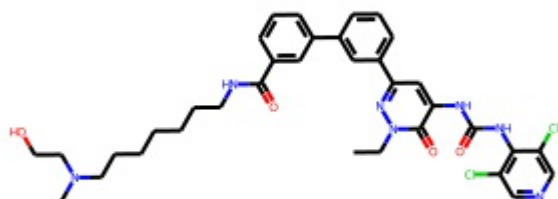
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN(C)C)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.837]
 predicted standard deviation: [0.879]
 95% CI: [4.079] - [7.595]
 epistemic percentile: 93.6
 p_risky at threshold of 5: [0.824]



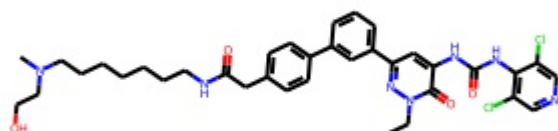
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCC4CCCN4C)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.795]
 predicted standard deviation: [0.891]
 95% CI: [4.013] - [7.576]
 epistemic percentile: 91.6
 p_risky at threshold of 5: [0.798]



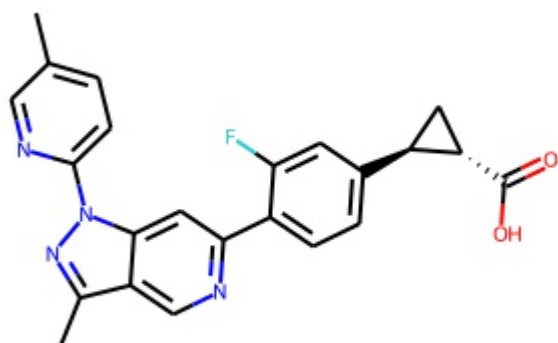
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [4.735]
 predicted standard deviation: [0.841]
 95% CI: [3.053] - [6.417]
 epistemic percentile: 56.8
 p_risky at threshold of 5: [0.379]



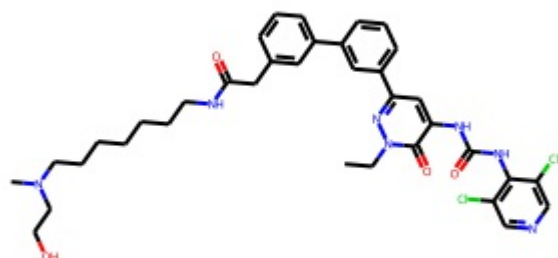
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCCCCCCN(C)CCO)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [5.913]
 predicted standard deviation: [0.861]
 95% CI: [4.192] - [7.634]
 epistemic percentile: 95.0
 p_risky at threshold of 5: [0.846]



interesting mol: CCn1nc(-c2cccc(-c3ccc(CC(=O)NCCCCCCCN(C)CCO)cc3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [6.169]
 predicted standard deviation: [0.896]
 95% CI: [4.377] - [7.96]
 epistemic percentile: 97.6
 p_risky at threshold of 5: [0.899]



interesting mol: Cc1ccc(-n2nc(C)c3cnc(-c4ccc([C@H]5C[C@@H]5C(=O)O)cc4F)cc32)nc1
 predicted mean: [4.915]
 predicted standard deviation: [0.815]
 95% CI: [3.285] - [6.546]
 epistemic percentile: 47.4
 p_risky at threshold of 5: [0.452]



interesting mol: CCn1nc(-c2cccc(-c3cccc(CC(=O)NCCCCCCCNC(C)CCO)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O
 predicted mean: [6.176]
 predicted standard deviation: [0.876]
 95% CI: [4.425] - [7.928]
 epistemic percentile: 93.0
 p_risky at threshold of 5: [0.895]

In [5]: