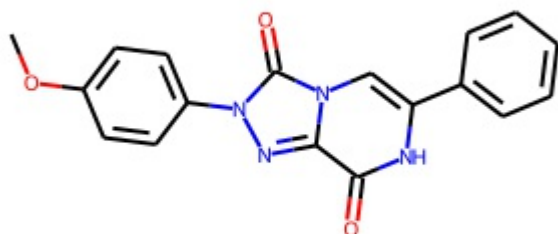
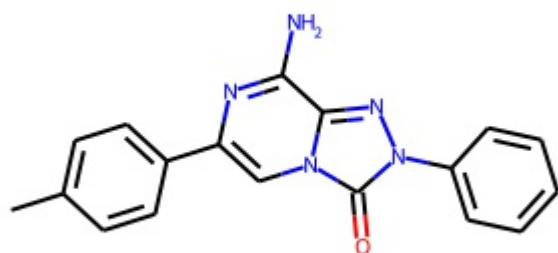


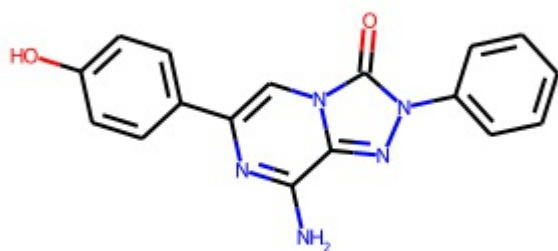
aleatoric uncertainty: [0.647]  
epistemic uncertainty: [0.376]  
p\_risky at threshold of 5: [0.007]



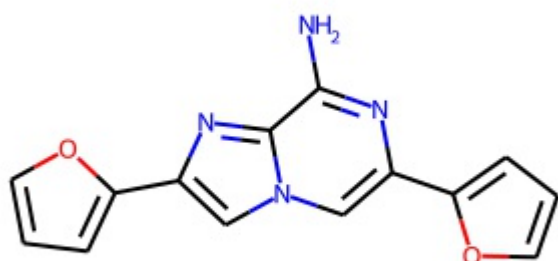
interesting mol: COc1ccc(-n2nc3c(=O)[nH]c(-c4ccccc4)cn3c2=O)cc1  
predicted mean: [5.584]  
predicted standard deviation: [0.692]  
95% CI: [4.201] - [6.968]  
aleatoric uncertainty: [0.639]  
epistemic uncertainty: [0.263]  
p\_risky at threshold of 5: [0.226]



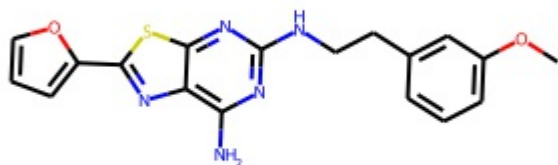
interesting mol: Cc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1  
predicted mean: [6.927]  
predicted standard deviation: [0.725]  
95% CI: [5.478] - [8.377]  
aleatoric uncertainty: [0.641]  
epistemic uncertainty: [0.305]  
p\_risky at threshold of 5: [0.002]



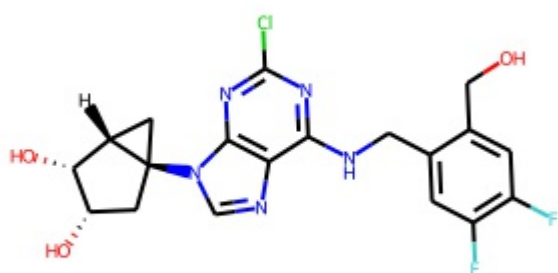
interesting mol: Nc1nc(-c2ccc(O)cc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [7.026]  
 predicted standard deviation: [0.721]  
 95% CI: [5.584] - [8.467]  
 aleatoric uncertainty: [0.639]  
 epistemic uncertainty: [0.306]  
 p\_risky at threshold of 5: [0.003]



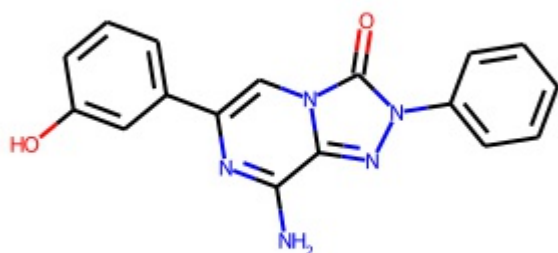
interesting mol: Nc1nc(-c2ccco2)cn2cc(-c3ccco3)nc12  
 predicted mean: [7.231]  
 predicted standard deviation: [0.7]  
 95% CI: [5.831] - [8.63]  
 aleatoric uncertainty: [0.649]  
 epistemic uncertainty: [0.235]  
 p\_risky at threshold of 5: [0.]



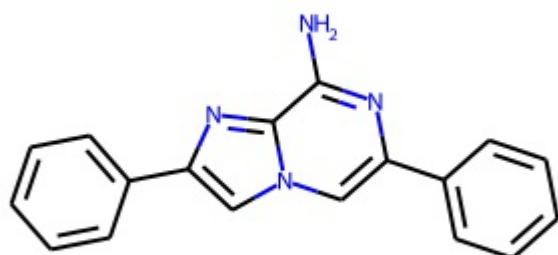
interesting mol: COc1cccc(CCNC2nc(N)c3nc(-c4ccco4)sc3n2)c1  
 predicted mean: [7.932]  
 predicted standard deviation: [0.732]  
 95% CI: [6.469] - [9.395]  
 aleatoric uncertainty: [0.648]  
 epistemic uncertainty: [0.329]  
 p\_risky at threshold of 5: [0.]



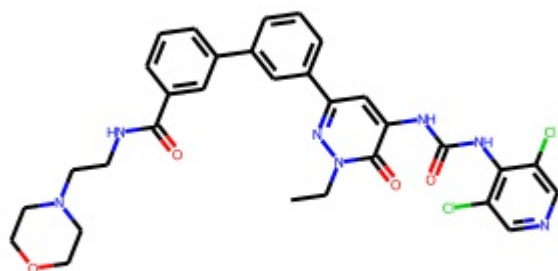
interesting mol: OCc1cc(F)c(F)cc1CNC1nc(Cl)nc2c1ncn2[C@@]12C[C@H](O)[C@H](O)[C@@H]1C2  
 predicted mean: [5.946]  
 predicted standard deviation: [0.807]  
 95% CI: [4.332] - [7.56]  
 aleatoric uncertainty: [0.646]  
 epistemic uncertainty: [0.471]  
 p\_risky at threshold of 5: [0.116]



interesting mol: Nc1nc(-c2cccc(O)c2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [7.317]  
 predicted standard deviation: [0.704]  
 95% CI: [5.91] - [8.725]  
 aleatoric uncertainty: [0.643]  
 epistemic uncertainty: [0.337]  
 p\_risky at threshold of 5: [0.001]



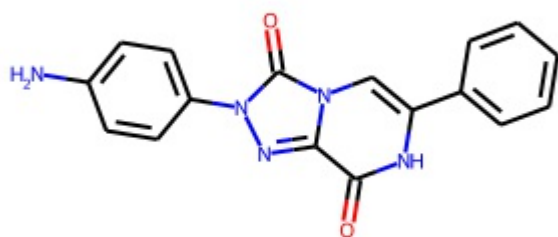
interesting mol: Nc1nc(-c2ccccc2)cn2cc(-c3ccccc3)nc12  
 predicted mean: [6.532]  
 predicted standard deviation: [0.71]  
 95% CI: [5.112] - [7.952]  
 aleatoric uncertainty: [0.646]  
 epistemic uncertainty: [0.24]  
 p\_risky at threshold of 5: [0.011]



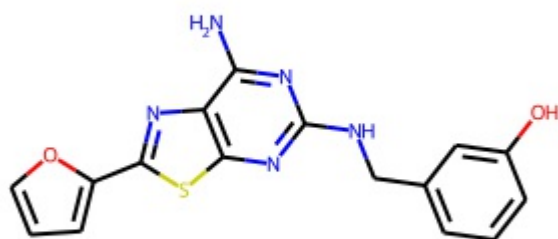
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN4CCOCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.295]  
 predicted standard deviation: [0.748]  
 95% CI: [4.799] - [7.791]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.406]  
 p\_risky at threshold of 5: [0.042]



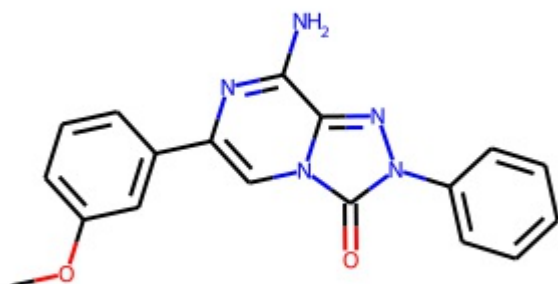
interesting mol: COc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1  
 predicted mean: [6.836]  
 predicted standard deviation: [0.719]  
 95% CI: [5.398] - [8.274]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.286]  
 p\_risky at threshold of 5: [0.006]



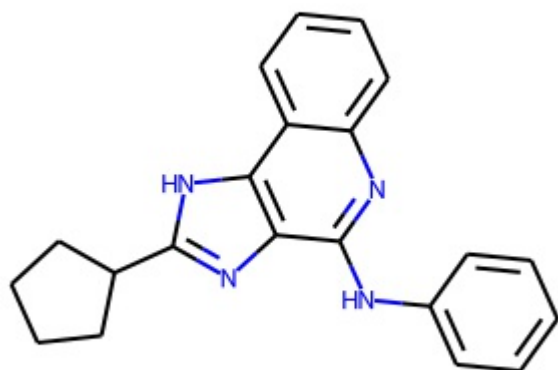
interesting mol: Nc1ccc(-n2nc3c(=O)[nH]c(-c4ccccc4)cn3c2=O)cc1  
 predicted mean: [5.908]  
 predicted standard deviation: [0.719]  
 95% CI: [4.47] - [7.346]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.346]  
 p\_risky at threshold of 5: [0.101]



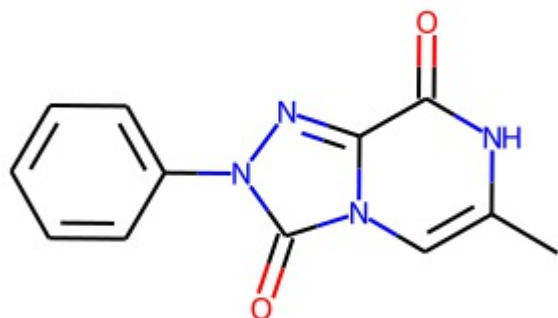
interesting mol: Nc1nc(NCc2cccc(O)c2)nc2sc(-c3ccco3)nc12  
 predicted mean: [7.376]  
 predicted standard deviation: [0.716]  
 95% CI: [5.943] - [8.809]  
 aleatoric uncertainty: [0.649]  
 epistemic uncertainty: [0.322]  
 p\_risky at threshold of 5: [0.001]



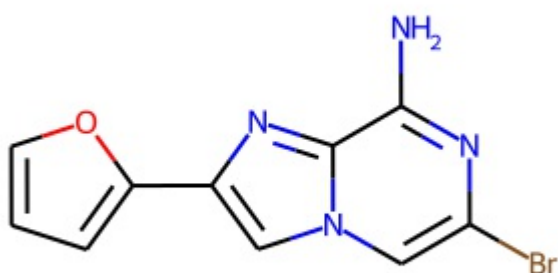
interesting mol: COc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)c1  
 predicted mean: [7.147]  
 predicted standard deviation: [0.718]  
 95% CI: [5.711] - [8.584]  
 aleatoric uncertainty: [0.645]  
 epistemic uncertainty: [0.317]  
 p\_risky at threshold of 5: [0.001]



interesting mol: c1ccc(Nc2nc3ccccc3c[nH]c(C4CCCC4)nc23)cc1  
 predicted mean: [6.338]  
 predicted standard deviation: [0.867]  
 95% CI: [4.605] - [8.072]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.595]  
 p\_risky at threshold of 5: [0.05]

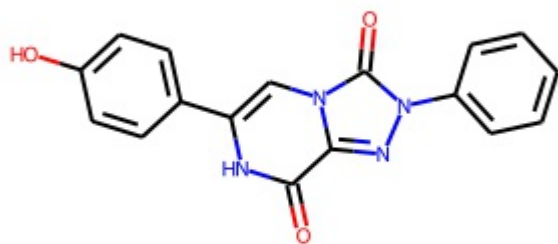


interesting mol: Cc1cn2c(=O)n(-c3ccccc3)nc2c(=O)[nH]1  
 predicted mean: [5.653]  
 predicted standard deviation: [0.676]  
 95% CI: [4.3] - [7.006]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.253]  
 p\_risky at threshold of 5: [0.173]



interesting mol: Nc1nc(Br)cn2cc(-c3ccco3)nc12  
 predicted mean: [6.965]  
 predicted standard deviation: [0.694]  
 95% CI: [5.578] - [8.353]  
 aleatoric uncertainty: [0.647]  
 epistemic uncertainty: [0.246]  
 p\_risky at threshold of 5: [0.002]

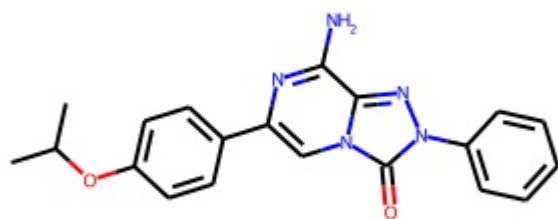




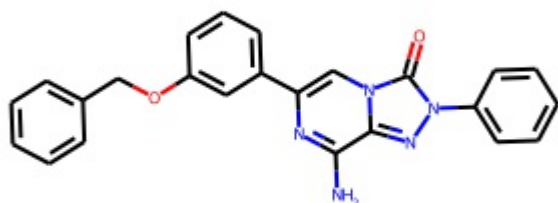
interesting mol: O=C1[nH]c(-c2ccc(O)cc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [6.014]  
 predicted standard deviation: [0.693]  
 95% CI: [4.627] - [7.401]  
 aleatoric uncertainty: [0.636]  
 epistemic uncertainty: [0.284]  
 p\_risky at threshold of 5: [0.071]



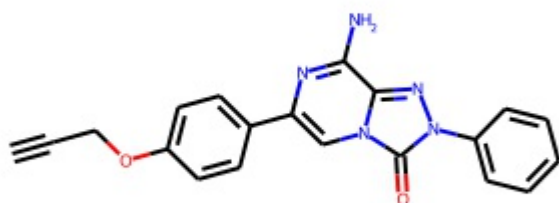
interesting mol: Nc1nc(-c2ccccc2)cn2c(=O)n(-c3ccc([N+](=O)[O-])cc3)nc12  
 predicted mean: [6.659]  
 predicted standard deviation: [0.697]  
 95% CI: [5.266] - [8.052]  
 aleatoric uncertainty: [0.642]  
 epistemic uncertainty: [0.341]  
 p\_risky at threshold of 5: [0.011]



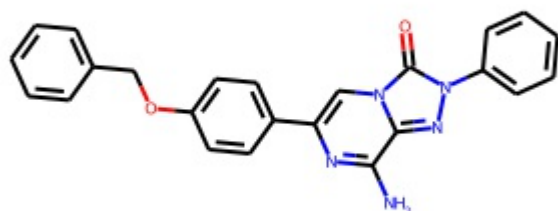
interesting mol: CC(C)Oc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1  
 predicted mean: [6.819]  
 predicted standard deviation: [0.693]  
 95% CI: [5.433] - [8.204]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.303]  
 p\_risky at threshold of 5: [0.005]



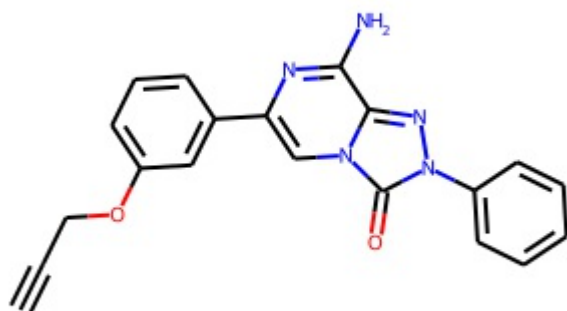
interesting mol: Nc1nc(-c2cccc(OCc3ccccc3)c2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [6.914]  
 predicted standard deviation: [0.736]  
 95% CI: [5.443] - [8.386]  
 aleatoric uncertainty: [0.645]  
 epistemic uncertainty: [0.389]  
 p\_risky at threshold of 5: [0.007]



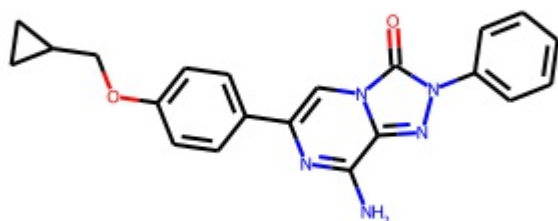
interesting mol: C#CCOc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)cc1  
 predicted mean: [7.187]  
 predicted standard deviation: [0.753]  
 95% CI: [5.681] - [8.694]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.314]  
 p\_risky at threshold of 5: [0.001]



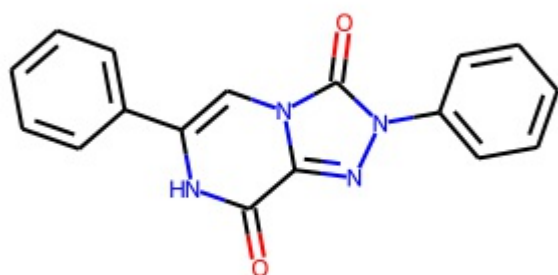
interesting mol: Nc1nc(-c2ccc(OCc3ccccc3)cc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [6.691]  
 predicted standard deviation: [0.74]  
 95% CI: [5.21] - [8.171]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.333]  
 p\_risky at threshold of 5: [0.01]



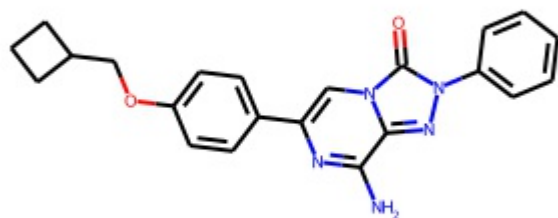
interesting mol: C#CCOc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(N)n2)c1  
 predicted mean: [7.412]  
 predicted standard deviation: [0.737]  
 95% CI: [5.938] - [8.885]  
 aleatoric uncertainty: [0.644]  
 epistemic uncertainty: [0.36]  
 p\_risky at threshold of 5: [0.001]



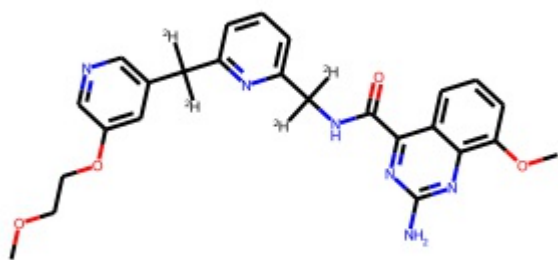
interesting mol: Nc1nc(-c2ccc(OCC3CC3)cc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [6.816]  
 predicted standard deviation: [0.73]  
 95% CI: [5.355] - [8.276]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.343]  
 p\_risky at threshold of 5: [0.006]



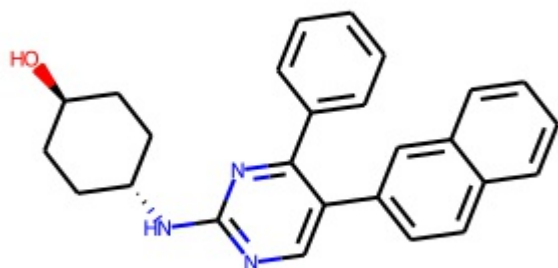
interesting mol: O=c1[nH]c(-c2ccccc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [5.938]  
 predicted standard deviation: [0.662]  
 95% CI: [4.613] - [7.262]  
 aleatoric uncertainty: [0.637]  
 epistemic uncertainty: [0.26]  
 p\_risky at threshold of 5: [0.074]



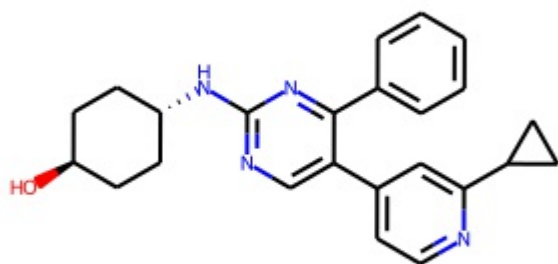
interesting mol: Nc1nc(-c2ccc(OCC3CCC3)cc2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [7.]  
 predicted standard deviation: [0.739]  
 95% CI: [5.523] - [8.478]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.357]  
 p\_risky at threshold of 5: [0.004]



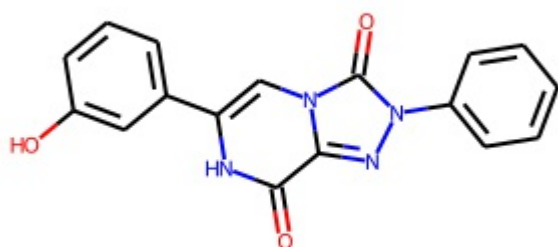
interesting mol: [2H]C([2H])(NC(=O)c1nc(N)nc2c(OC)cccc12)c1cccc(C([2H]))([2H])c2cncc(OCCOC)c2)n1  
 predicted mean: [7.621]  
 predicted standard deviation: [0.75]  
 95% CI: [6.121] - [9.122]  
 aleatoric uncertainty: [0.647]  
 epistemic uncertainty: [0.405]  
 p\_risky at threshold of 5: [0.]



interesting mol: O[C@H]1CC[C@H](Nc2ncc(-c3ccc4ccccc4c3)c(-c3ccccc3)n2)CC1  
 predicted mean: [7.109]  
 predicted standard deviation: [0.77]  
 95% CI: [5.57] - [8.648]  
 aleatoric uncertainty: [0.646]  
 epistemic uncertainty: [0.379]  
 p\_risky at threshold of 5: [0.002]



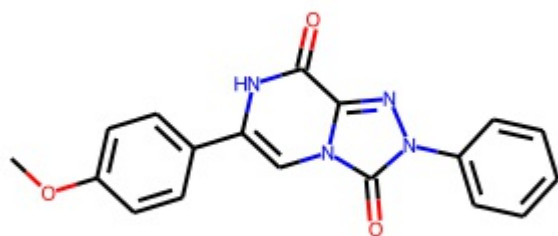
interesting mol: O[C@H]1CC[C@H](Nc2nc(-c3ccnc(C4CC4)c3)c(-c3ccccc3)n2)CC1  
 predicted mean: [6.329]  
 predicted standard deviation: [0.737]  
 95% CI: [4.855] - [7.804]  
 aleatoric uncertainty: [0.648]  
 epistemic uncertainty: [0.361]  
 p\_risky at threshold of 5: [0.037]



interesting mol: O=c1[nH]c(-c2cccc(O)c2)cn2c(=O)n(-c3ccccc3)nc12  
 predicted mean: [6.071]  
 predicted standard deviation: [0.71]  
 95% CI: [4.651] - [7.491]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.298]  
 p\_risky at threshold of 5: [0.07]

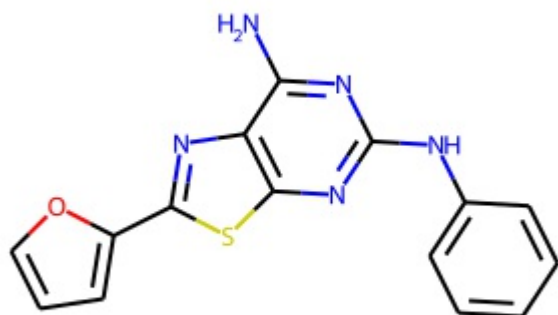


interesting mol: COc1ccccc1-n1nc2c(N)nc(-c3ccccc3)cn2c1=O  
 predicted mean: [7.021]  
 predicted standard deviation: [0.716]  
 95% CI: [5.59] - [8.453]  
 aleatoric uncertainty: [0.644]  
 epistemic uncertainty: [0.307]  
 p\_risky at threshold of 5: [0.003]

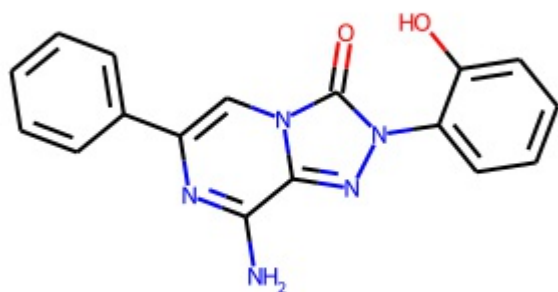


interesting mol: COc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)cc1  
 predicted mean: [5.842]  
 predicted standard deviation: [0.695]  
 95% CI: [4.451] - [7.233]  
 aleatoric uncertainty: [0.637]  
 epistemic uncertainty: [0.289]  
 p\_risky at threshold of 5: [0.097]





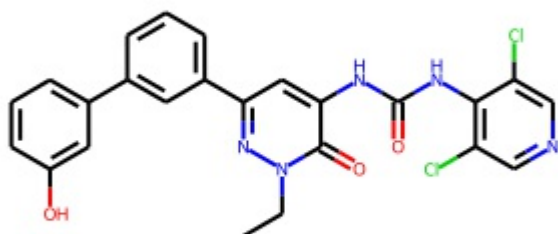
interesting mol: Nc1nc(Nc2ccccc2)nc2sc(-c3ccco3)nc12  
 predicted mean: [7.14]  
 predicted standard deviation: [0.686]  
 95% CI: [5.769] - [8.511]  
 aleatoric uncertainty: [0.649]  
 epistemic uncertainty: [0.27]  
 p\_risky at threshold of 5: [0.001]



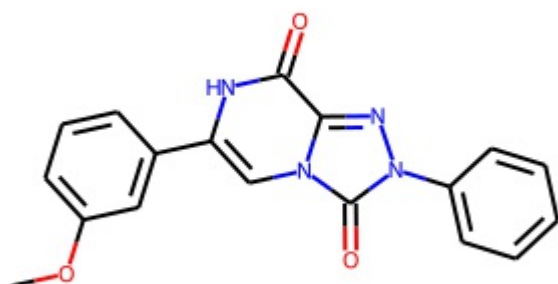
interesting mol: Nc1nc(-c2ccccc2)cn2c(=O)n(-c3ccccc3O)nc12  
 predicted mean: [6.96]  
 predicted standard deviation: [0.753]  
 95% CI: [5.453] - [8.466]  
 aleatoric uncertainty: [0.643]  
 epistemic uncertainty: [0.326]  
 p\_risky at threshold of 5: [0.003]



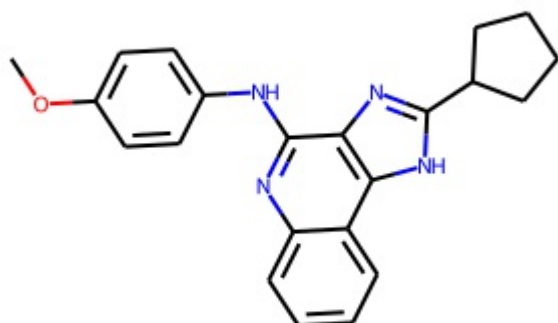
interesting mol: Cc1ccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)cc1  
 predicted mean: [5.928]  
 predicted standard deviation: [0.711]  
 95% CI: [4.506] - [7.351]  
 aleatoric uncertainty: [0.636]  
 epistemic uncertainty: [0.286]  
 p\_risky at threshold of 5: [0.102]



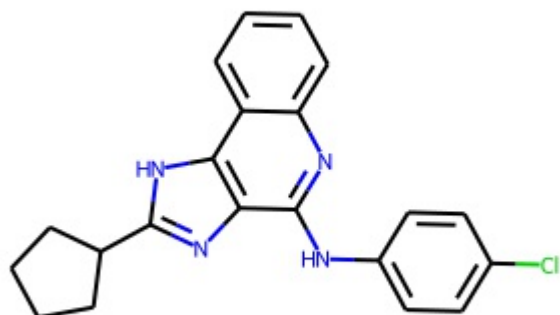
interesting mol: CCn1nc(-c2cccc(-c3cccc(O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.251]  
 predicted standard deviation: [0.733]  
 95% CI: [4.785] - [7.716]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.36]  
 p\_risky at threshold of 5: [0.045]



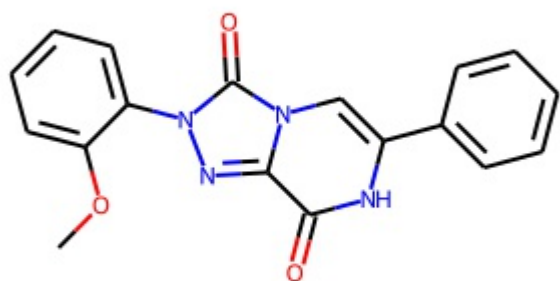
interesting mol: COc1cccc(-c2cn3c(=O)n(-c4ccccc4)nc3c(=O)[nH]2)c1  
 predicted mean: [5.81]  
 predicted standard deviation: [0.687]  
 95% CI: [4.436] - [7.184]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.288]  
 p\_risky at threshold of 5: [0.129]



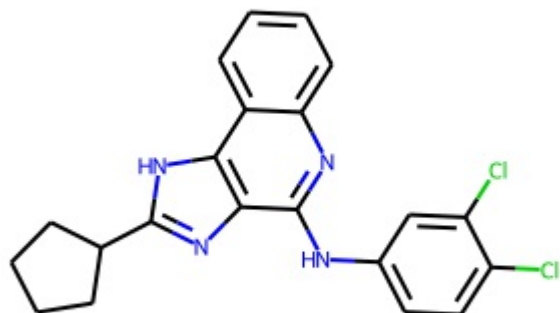
interesting mol: COc1ccc(Nc2nc3ccccc3c3[nH]c(C4CCCC4)nc23)cc1  
 predicted mean: [6.416]  
 predicted standard deviation: [0.869]  
 95% CI: [4.677] - [8.154]  
 aleatoric uncertainty: [0.635]  
 epistemic uncertainty: [0.599]  
 p\_risky at threshold of 5: [0.049]



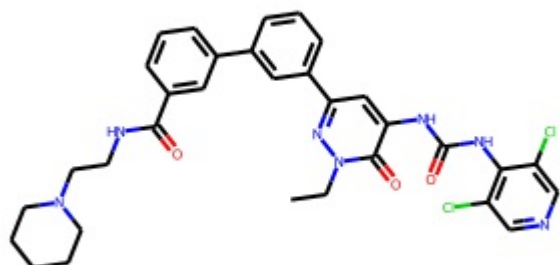
interesting mol: Clc1ccc(Nc2nc3ccccc3c[nH]c(C4CCCC4)nc23)cc1  
 predicted mean: [6.022]  
 predicted standard deviation: [0.855]  
 95% CI: [4.312] - [7.732]  
 aleatoric uncertainty: [0.636]  
 epistemic uncertainty: [0.623]  
 p\_risky at threshold of 5: [0.121]



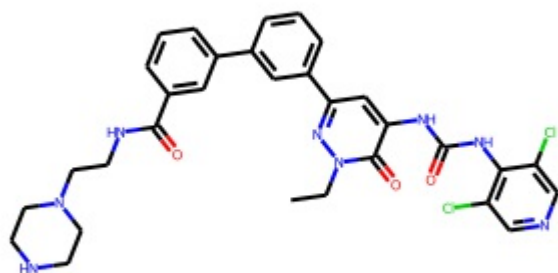
interesting mol: COc1ccccc1-n1nc2c(=O)[nH]c(-c3ccccc3)cn2c1=O  
 predicted mean: [5.754]  
 predicted standard deviation: [0.684]  
 95% CI: [4.386] - [7.121]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.288]  
 p\_risky at threshold of 5: [0.152]



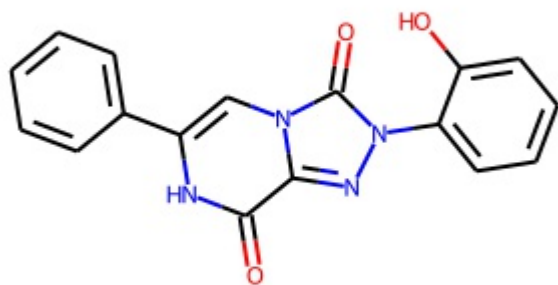
interesting mol: Clc1ccc(Nc2nc3ccccc3c[nH]c(C4CCCC4)nc23)cc1Cl  
 predicted mean: [6.461]  
 predicted standard deviation: [0.912]  
 95% CI: [4.637] - [8.285]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.667]  
 p\_risky at threshold of 5: [0.054]



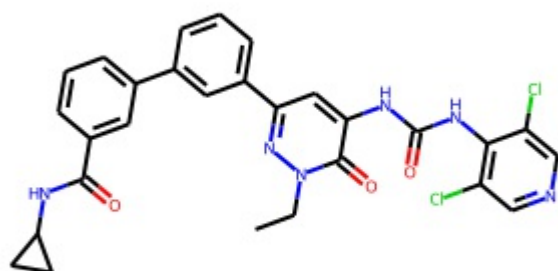
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN4CCCCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.516]  
 predicted standard deviation: [0.735]  
 95% CI: [5.047] - [7.986]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.404]  
 p\_risky at threshold of 5: [0.017]



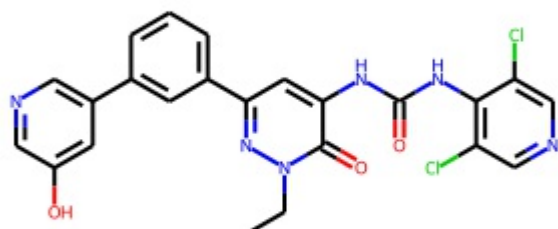
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN4CCNCC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.431]  
 predicted standard deviation: [0.744]  
 95% CI: [4.943] - [7.92]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.396]  
 p\_risky at threshold of 5: [0.025]



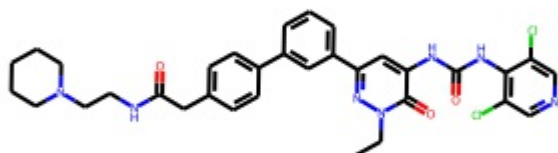
interesting mol: O=c1[nH]c(-c2cccc2)cn2c(=O)n(-c3cccc30)nc12  
 predicted mean: [5.81]  
 predicted standard deviation: [0.696]  
 95% CI: [4.418] - [7.203]  
 aleatoric uncertainty: [0.637]  
 epistemic uncertainty: [0.289]  
 p\_risky at threshold of 5: [0.126]



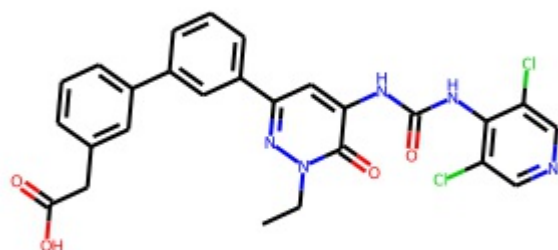
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NC4CC4)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.381]  
 predicted standard deviation: [0.748]  
 95% CI: [4.885] - [7.876]  
 aleatoric uncertainty: [0.642]  
 epistemic uncertainty: [0.43]  
 p\_risky at threshold of 5: [0.027]



interesting mol: CCn1nc(-c2cccc(-c3cncc(O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.205]  
 predicted standard deviation: [0.726]  
 95% CI: [4.752] - [7.657]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.356]  
 p\_risky at threshold of 5: [0.049]

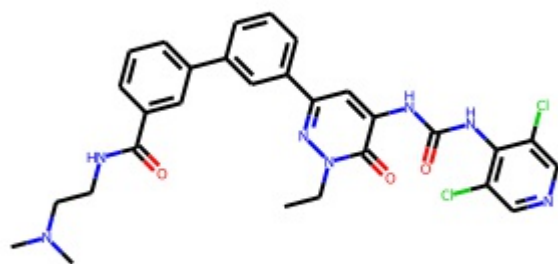


interesting mol: CCn1nc(-c2cccc(-c3ccc(CC(=O)NCCN4CCCCC4)cc3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.741]  
 predicted standard deviation: [0.806]  
 95% CI: [5.13] - [8.353]  
 aleatoric uncertainty: [0.642]  
 epistemic uncertainty: [0.485]  
 p\_risky at threshold of 5: [0.015]

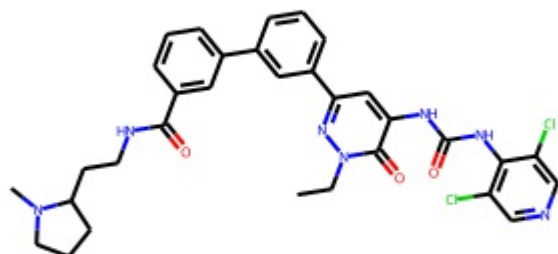


interesting mol: CCn1nc(-c2cccc(-c3cccc(CC(=O)O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [5.666]  
 predicted standard deviation: [0.742]  
 95% CI: [4.182] - [7.151]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.391]  
 p\_risky at threshold of 5: [0.173]

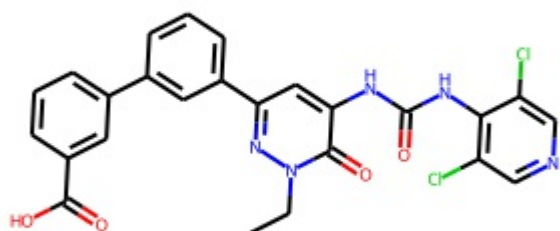




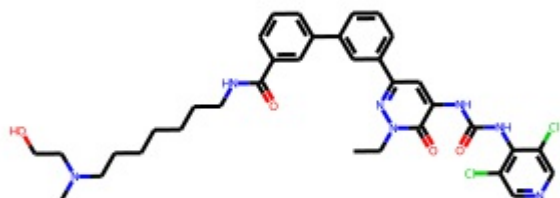
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCN(C)C)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.111]  
 predicted standard deviation: [0.752]  
 95% CI: [4.608] - [7.615]  
 aleatoric uncertainty: [0.64]  
 epistemic uncertainty: [0.38]  
 p\_risky at threshold of 5: [0.075]



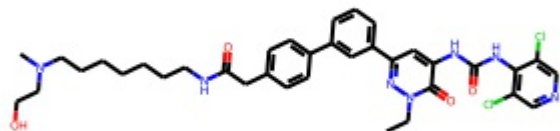
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCC4CCCN4C)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [5.976]  
 predicted standard deviation: [0.739]  
 95% CI: [4.498] - [7.455]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.405]  
 p\_risky at threshold of 5: [0.09]



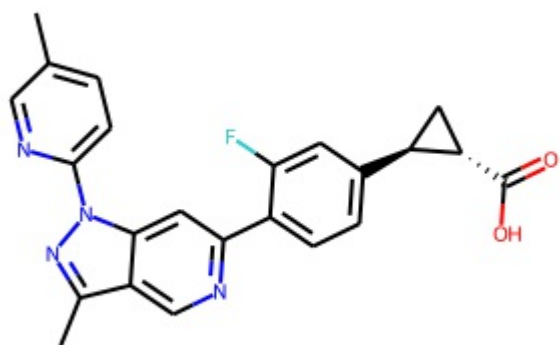
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)O)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [5.761]  
 predicted standard deviation: [0.668]  
 95% CI: [4.425] - [7.097]  
 aleatoric uncertainty: [0.637]  
 epistemic uncertainty: [0.317]  
 p\_risky at threshold of 5: [0.156]



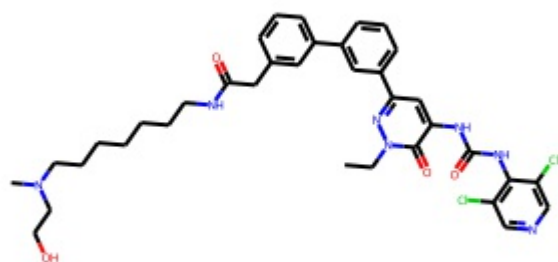
interesting mol: CCn1nc(-c2cccc(-c3cccc(C(=O)NCCCCCCCCN(C)CCO)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [5.848]  
 predicted standard deviation: [0.759]  
 95% CI: [4.33] - [7.366]  
 aleatoric uncertainty: [0.641]  
 epistemic uncertainty: [0.427]  
 p\_risky at threshold of 5: [0.152]



interesting mol: CCn1nc(-c2cccc(-c3ccc(CC(=O)NCCCCCN(C)CCO)cc3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [6.237]  
 predicted standard deviation: [0.868]  
 95% CI: [4.501] - [7.973]  
 aleatoric uncertainty: [0.642]  
 epistemic uncertainty: [0.547]  
 p\_risky at threshold of 5: [0.081]



interesting mol: Cc1ccc(-n2nc(C)c3cnc(-c4ccc([C@H]5C[C@@H]5C(=O)O)cc4F)cc32)nc1  
 predicted mean: [4.921]  
 predicted standard deviation: [0.725]  
 95% CI: [3.472] - [6.371]  
 aleatoric uncertainty: [0.638]  
 epistemic uncertainty: [0.332]  
 p\_risky at threshold of 5: [0.548]



interesting mol: CCn1nc(-c2cccc(-c3cccc(CC(=O)NCCCCCCCN(C)CCO)c3)c2)cc(NC(=O)Nc2c(Cl)cncc2Cl)c1=O  
 predicted mean: [5.971]  
 predicted standard deviation: [0.781]  
 95% CI: [4.408] - [7.534]  
 aleatoric uncertainty: [0.644]  
 epistemic uncertainty: [0.423]  
 p\_risky at threshold of 5: [0.106]

In [30]: