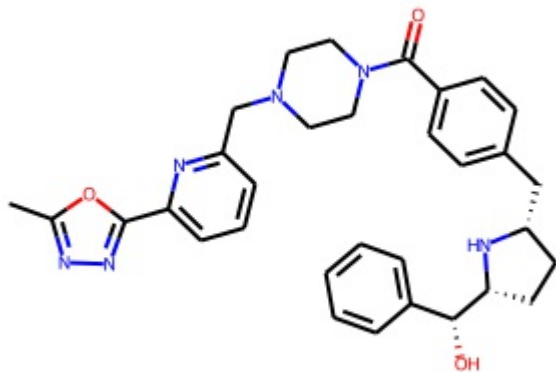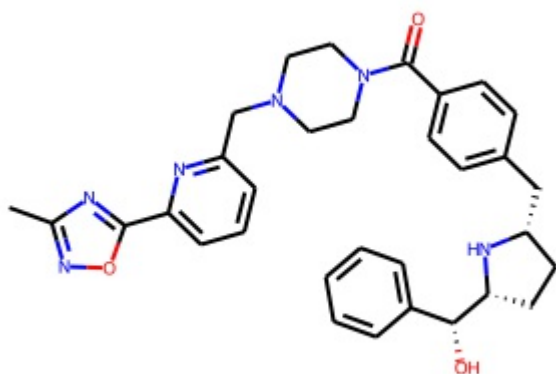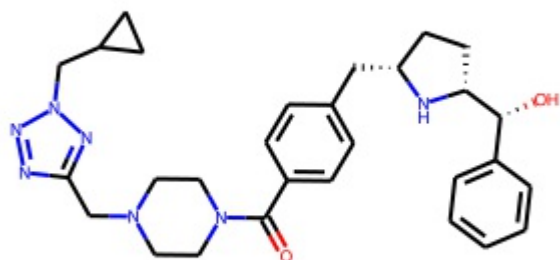aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.369]
p_risky at threshold of 5: [0.39]

interesting mol: Cc1nnc(-c2cccc(CN3CCN(C(=O)c4ccc(C[C@@H]5CC[C@H]([C@H]
(O)c6ccccc6)N5)cc4)CC3)n2)o1
predicted mean: [5.97]
predicted standard deviation: [0.857]
95% CI: [4.255] - [7.685]
aleatoric uncertainty: [0.678]
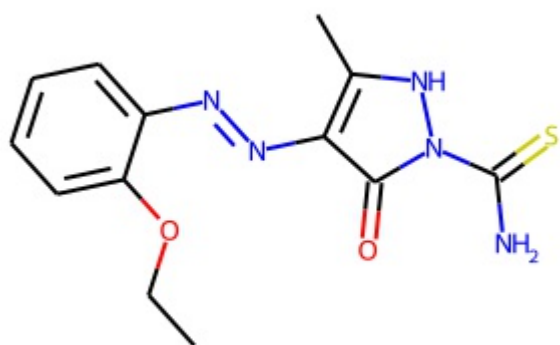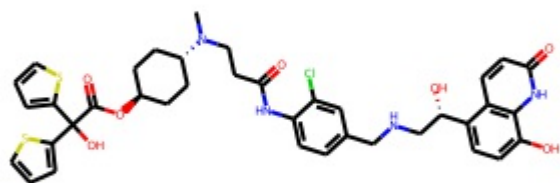epistemic uncertainty: [0.512]
p_risky at threshold of 5: [0.132]

interesting mol: Cc1noc(-c2cccc(CN3CCN(C(=O)c4ccc(C[C@@H]5CC[C@H]([C@H]
(O)c6ccccc6)N5)cc4)CC3)n2)n1
predicted mean: [5.937]
predicted standard deviation: [0.86]
95% CI: [4.217] - [7.657]
aleatoric uncertainty: [0.678]
epistemic uncertainty: [0.452]
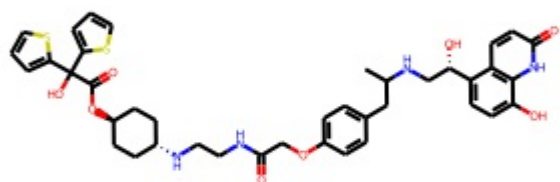p_risky at threshold of 5: [0.134]

interesting mol: O=C(c1ccc(C[C@@H]2CC[C@H]([C@H](O)c3ccccc3)N2)cc1)N1CCN(Cc2nnn(CC3CC3)n2)CC1
predicted mean: [5.098]
predicted standard deviation: [0.764]
95% CI: [3.571] - [6.626]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.398]
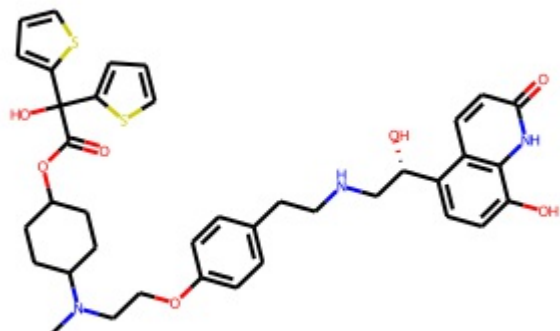p_risky at threshold of 5: [0.447]

interesting mol: CCOc1ccccc1/N=N/c1c(C)[nH]n(C(N)=S)c1=O
predicted mean: [5.365]
predicted standard deviation: [0.764]
95% CI: [3.837] - [6.893]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.336]
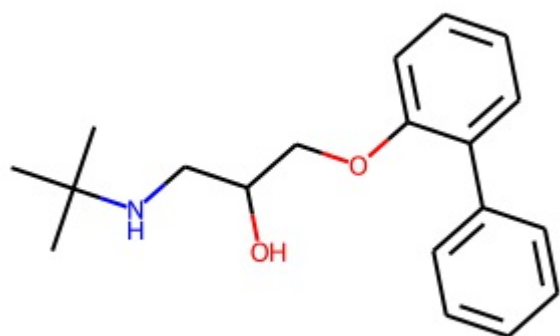p_risky at threshold of 5: [0.294]

interesting mol: CN(CCC(=O)Nc1ccc(CNC[C@H](O)c2ccc(O)c3[nH]c(=O)ccc23)cc1Cl)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [8.907]
predicted standard deviation: [0.898]
95% CI: [7.11] - [10.703]
aleatoric uncertainty: [0.687]
epistemic uncertainty: [0.594]
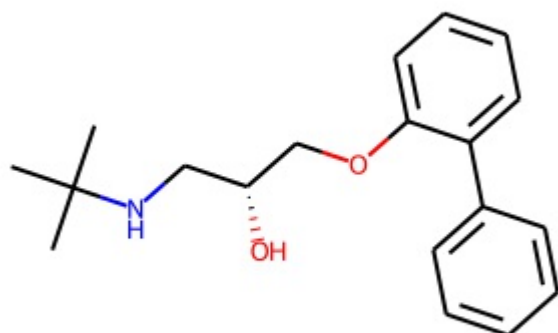p_risky at threshold of 5: [0.]

interesting mol: CC(Cc1ccc(OCC(=O)NCCN[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)cc1)NC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [10.296]
predicted standard deviation: [0.906]
95% CI: [8.484] - [12.109]
aleatoric uncertainty: [0.691]
epistemic uncertainty: [0.56]
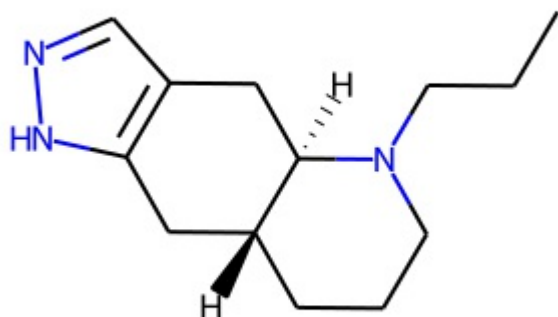p_risky at threshold of 5: [0.]

interesting mol: CN(CCOc1ccc(CCNC[C@H]
(O)c2ccc(O)c3[nH]c(=O)ccc23)cc1)C1CCC(OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [8.547]
predicted standard deviation: [0.851]
95% CI: [6.845] - [10.249]
aleatoric uncertainty: [0.686]
epistemic uncertainty: [0.523]
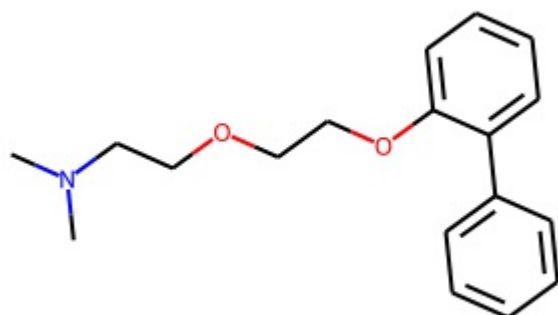p_risky at threshold of 5: [0.]

interesting mol: CC(C)(C)NCC(O)COc1ccccc1-c1ccccc1
predicted mean: [7.71]
predicted standard deviation: [0.778]
95% CI: [6.153] - [9.266]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.412]
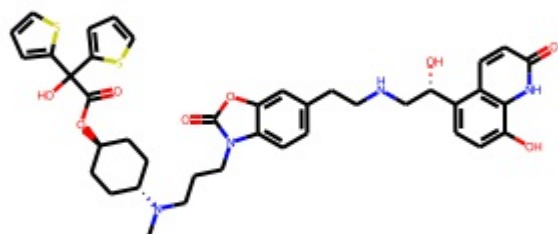p_risky at threshold of 5: [0.]

interesting mol: CC(C)(C)NC[C@@H](O)COc1ccccc1-c1ccccc1
predicted mean: [7.68]
predicted standard deviation: [0.766]
95% CI: [6.149] - [9.212]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.401]
p_risky at threshold of 5: [0.]
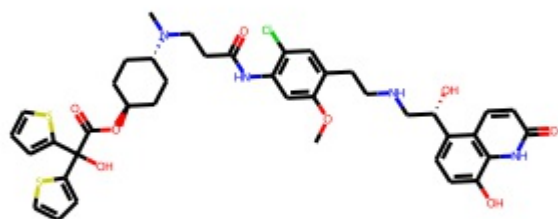

interesting mol: CCCN1CCC[C@@H]2Cc3[nH]ncc3C[C@H]21
predicted mean: [4.725]
predicted standard deviation: [0.744]
95% CI: [3.238] - [6.212]
aleatoric uncertainty: [0.675]
epistemic uncertainty: [0.357]
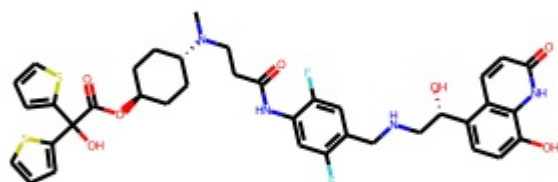p_risky at threshold of 5: [0.665]

interesting mol: CN(C)CCOCCOc1ccccc1-c1ccccc1
predicted mean: [6.097]
predicted standard deviation: [0.754]
95% CI: [4.588] - [7.605]
aleatoric uncertainty: [0.68]
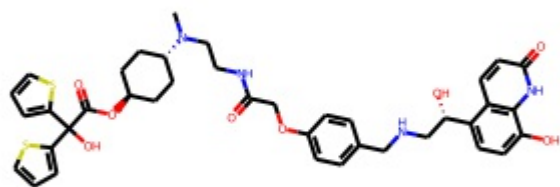epistemic uncertainty: [0.399]
p_risky at threshold of 5: [0.087]

interesting mol: CN(CCCn1c(=O)oc2cc(CCNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.846]
predicted standard deviation: [0.842]
95% CI: [6.162] - [9.53]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.559]
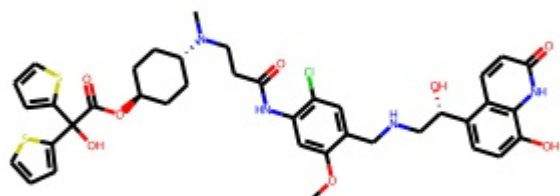p_risky at threshold of 5: [0.001]

interesting mol: COc1cc(NC(=O)CCN(C)[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(Cl)cc1CCNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [9.028]
predicted standard deviation: [0.892]
95% CI: [7.244] - [10.812]
aleatoric uncertainty: [0.687]
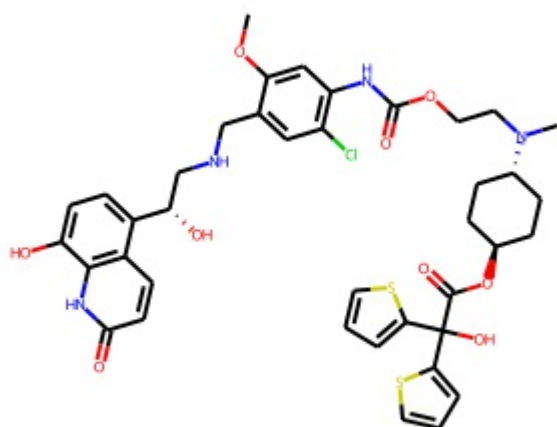epistemic uncertainty: [0.585]
p_risky at threshold of 5: [0.]

interesting mol: CN(CCC(=O)Nc1cc(F)c(CNC[C@H](O)c2ccc(O)c3[nH]c(=O)ccc23)cc1F)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [8.307]
predicted standard deviation: [0.901]
95% CI: [6.506] - [10.109]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.538]
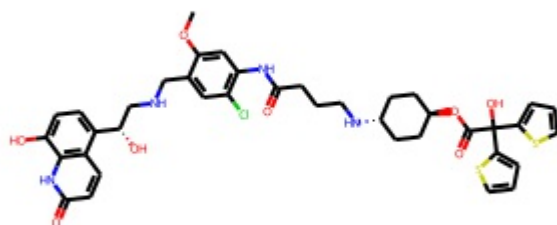p_risky at threshold of 5: [0.]

interesting mol: CN(CCNC(=O)COc1ccc(CNC[C@H](O)c2ccc(O)c3[nH]c(=O)ccc23)cc1)[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [9.085]
predicted standard deviation: [0.89]
95% CI: [7.306] - [10.865]
aleatoric uncertainty: [0.687]
epistemic uncertainty: [0.577]
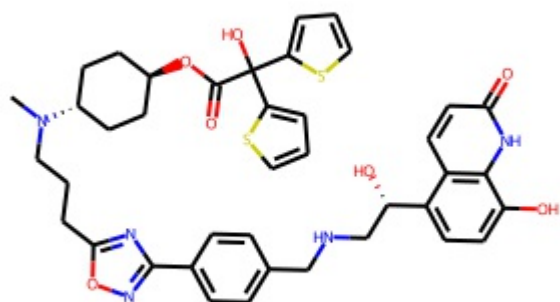p_risky at threshold of 5: [0.]

interesting mol: COc1cc(NC(=O)CCN(C)[C@H]2CC[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [8.498]
predicted standard deviation: [0.906]
95% CI: [6.687] - [10.309]
aleatoric uncertainty: [0.685]
epistemic uncertainty: [0.63]
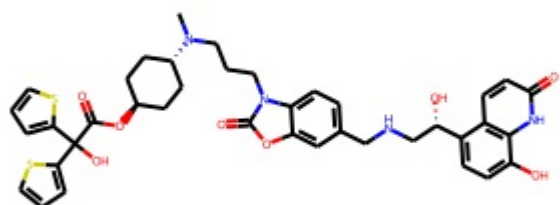p_risky at threshold of 5: [0.]

interesting mol: COc1cc(NC(=O)OCCN(C)[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [7.987]
predicted standard deviation: [0.877]
95% CI: [6.233] - [9.741]
aleatoric uncertainty: [0.683]
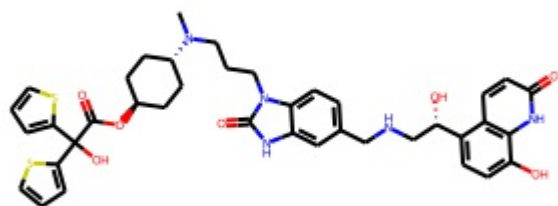epistemic uncertainty: [0.617]
p_risky at threshold of 5: [0.001]

interesting mol: COc1cc(NC(=O)CCCN[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [8.741]
predicted standard deviation: [0.929]
95% CI: [6.883] - [10.599]
aleatoric uncertainty: [0.686]
epistemic uncertainty: [0.616]
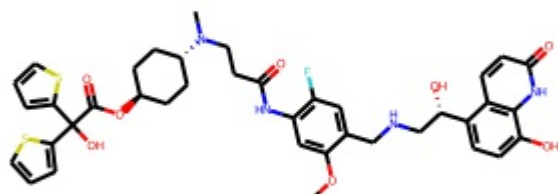p_risky at threshold of 5: [0.]

interesting mol: CN(CCCc1nc(-c2ccc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)cc2)no1)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.535]
predicted standard deviation: [0.886]
95% CI: [5.763] - [9.307]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.54]
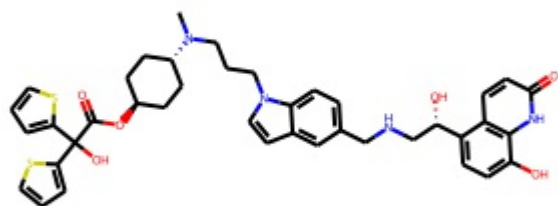p_risky at threshold of 5: [0.002]

interesting mol: CN(CCCn1c(=O)oc2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.201]
predicted standard deviation: [0.867]
95% CI: [5.467] - [8.935]
aleatoric uncertainty: [0.681]
epistemic uncertainty: [0.556]
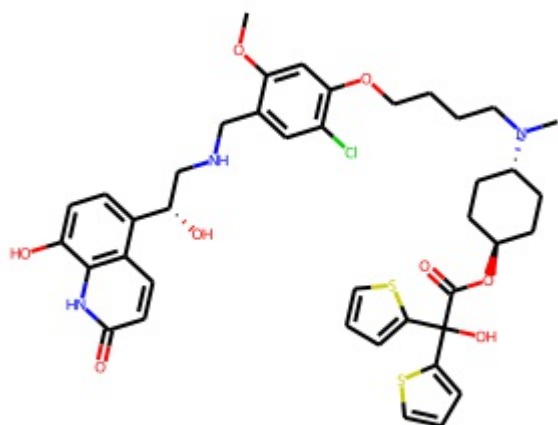p_risky at threshold of 5: [0.006]

interesting mol: CN(CCCn1c(=O)[nH]c2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.763]
predicted standard deviation: [0.915]
95% CI: [5.932] - [9.593]
aleatoric uncertainty: [0.683]
epistemic uncertainty: [0.552]
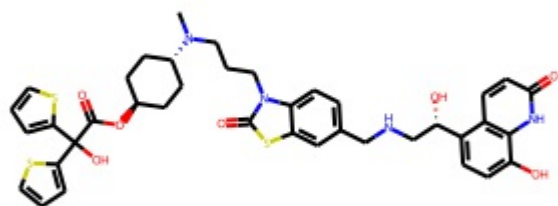p_risky at threshold of 5: [0.001]

interesting mol: COc1cc(NC(=O)CCN(C)[C@H]2CC[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)CC2)c(F)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [8.233]
predicted standard deviation: [0.909]
95% CI: [6.414] - [10.051]
aleatoric uncertainty: [0.685]
epistemic uncertainty: [0.564]
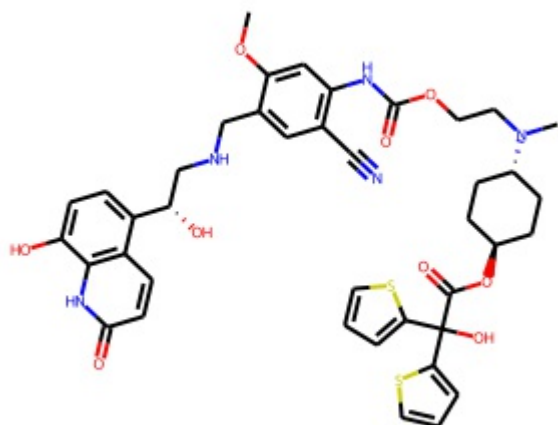p_risky at threshold of 5: [0.]

interesting mol: CN(CCCn1ccc2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.758]
predicted standard deviation: [0.98]
95% CI: [5.798] - [9.718]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.566]
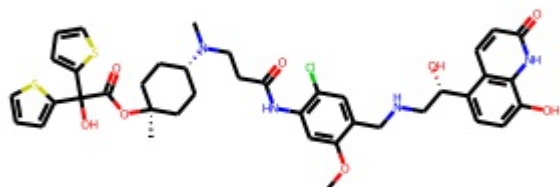p_risky at threshold of 5: [0.001]

interesting mol: COc1cc(OCCCCN(C)[C@H]2CC[C@H](OC(=O)C(O)(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [8.084]
predicted standard deviation: [0.932]
95% CI: [6.219] - [9.948]
aleatoric uncertainty: [0.683]
epistemic uncertainty: [0.61]
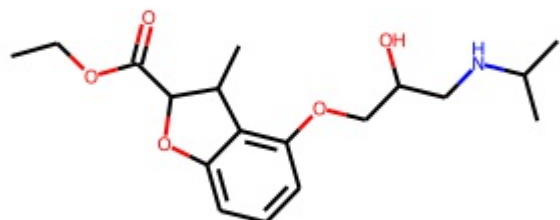p_risky at threshold of 5: [0.]

interesting mol: CN(CCCn1c(=O)sc2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)
[C@H]1CC[C@H](OC(=O)C(O)(c2cccs2)c2cccs2)CC1
predicted mean: [7.384]
predicted standard deviation: [0.897]
95% CI: [5.59] - [9.178]
aleatoric uncertainty: [0.682]
epistemic uncertainty: [0.56]
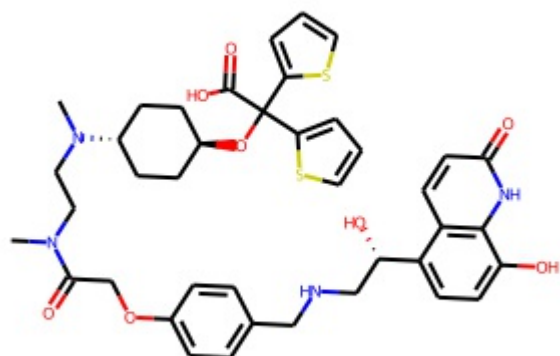p_risky at threshold of 5: [0.003]

interesting mol: COc1cc(NC(=O)OCCN(C)[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(C#N)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [6.681]
predicted standard deviation: [0.86]
95% CI: [4.961] - [8.401]
aleatoric uncertainty: [0.681]
epistemic uncertainty: [0.593]
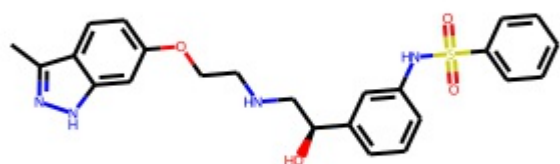p_risky at threshold of 5: [0.026]

interesting mol: COc1cc(NC(=O)CCN(C)[C@H]2CC[C@](C)(OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2[nH]c(=O)ccc12
predicted mean: [7.298]
predicted standard deviation: [0.927]
95% CI: [5.444] - [9.152]
aleatoric uncertainty: [0.681]
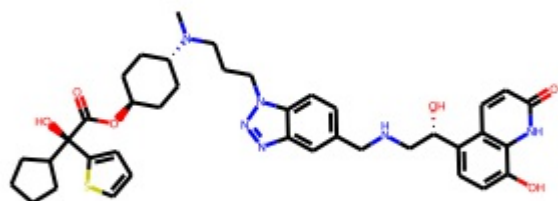epistemic uncertainty: [0.579]
p_risky at threshold of 5: [0.004]

interesting mol: CCOC(=O)C1Oc2cccc(OCC(O)CNC(C)C)c2C1C
predicted mean: [7.223]
predicted standard deviation: [0.85]
95% CI: [5.522] - [8.924]
aleatoric uncertainty: [0.682]
epistemic uncertainty: [0.422]
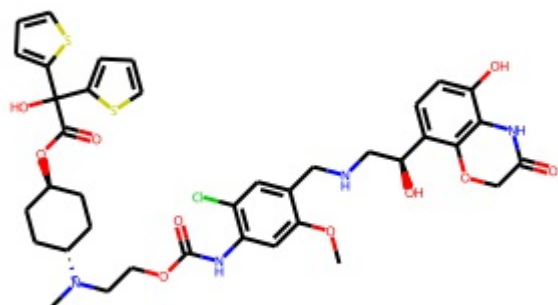p_risky at threshold of 5: [0.004]

interesting mol: CN(CCN(C)[C@H]1CC[C@H](OC(C(=O)O)
(c2cccs2)c2cccs2)CC1)C(=O)COc1ccc(CNC[C@H](O)c2ccc(O)c3[nH]c(=O)ccc23)cc1
predicted mean: [8.311]
predicted standard deviation: [0.81]
95% CI: [6.691] - [9.931]
aleatoric uncertainty: [0.686]
epistemic uncertainty: [0.503]
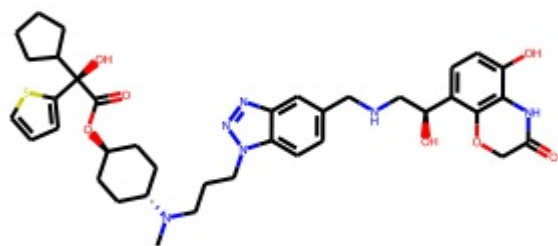p_risky at threshold of 5: [0.]

interesting mol: Cc1n[nH]c2cc(OCCNC[C@H](O)c3cccc(NS(=O)(=O)c4ccccc4)c3)ccc12
predicted mean: [5.789]
predicted standard deviation: [0.795]
95% CI: [4.199] - [7.38]
aleatoric uncertainty: [0.679]
epistemic uncertainty: [0.435]
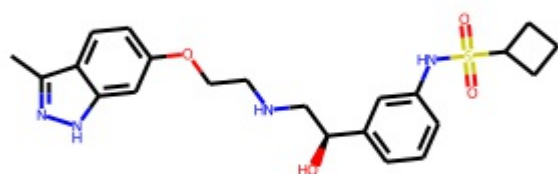p_risky at threshold of 5: [0.137]

interesting mol: CN(CCCn1nnc2cc(CNC[C@H](O)c3ccc(O)c4[nH]c(=O)ccc34)ccc21)
[C@H]1CC[C@H](OC(=O)[C@](O)(c2cccs2)C2CCCC2)CC1
predicted mean: [7.857]
predicted standard deviation: [0.872]
95% CI: [6.113] - [9.602]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.547]
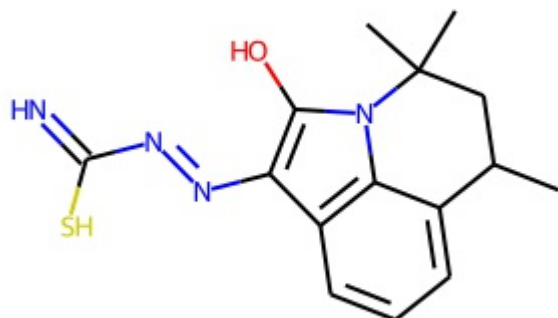p_risky at threshold of 5: [0.001]

interesting mol: COc1cc(NC(=O)OCCN(C)[C@H]2CC[C@H](OC(=O)C(O)
(c3cccs3)c3cccs3)CC2)c(Cl)cc1CNC[C@H](O)c1ccc(O)c2c1OCC(=O)N2
predicted mean: [8.676]
predicted standard deviation: [0.9]
95% CI: [6.876] - [10.475]
aleatoric uncertainty: [0.687]
epistemic uncertainty: [0.664]
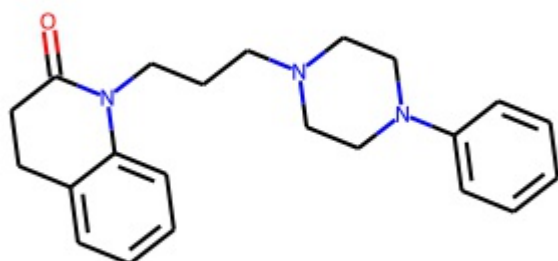p_risky at threshold of 5: [0.]

interesting mol: CN(CCCn1nnc2cc(CNC[C@H](O)c3ccc(O)c4c3OCC(=O)N4)ccc21)
[C@H]1CC[C@H](OC(=O)[C@](O)(c2cccs2)C2CCCC2)CC1
predicted mean: [8.526]
predicted standard deviation: [0.909]
95% CI: [6.708] - [10.344]
aleatoric uncertainty: [0.684]
epistemic uncertainty: [0.634]
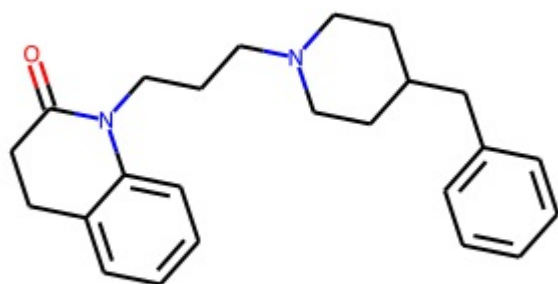p_risky at threshold of 5: [0.]

interesting mol: Cc1n[nH]c2cc(OCCNC[C@H](O)c3cccc(NS(=O)(=O)C4CCC4)c3)ccc12
predicted mean: [5.998]
predicted standard deviation: [0.789]
95% CI: [4.42] - [7.577]
aleatoric uncertainty: [0.679]
epistemic uncertainty: [0.427]
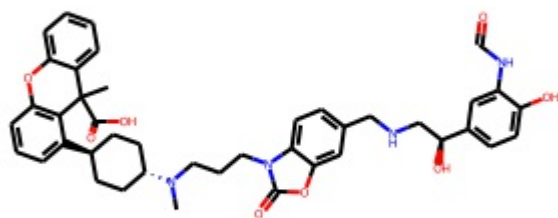p_risky at threshold of 5: [0.072]

interesting mol: CC1CC(C)(C)n2c(O)c(/N=N/C(=N)S)c3cccc1c32
predicted mean: [5.088]
predicted standard deviation: [0.794]
95% CI: [3.501] - [6.675]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.418]
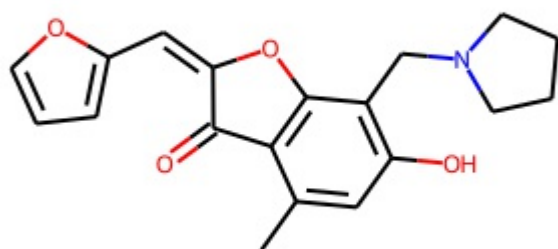p_risky at threshold of 5: [0.47]

interesting mol: O=C1CCc2ccccc2N1CCCN1CCN(c2ccccc2)CC1
predicted mean: [4.625]
predicted standard deviation: [0.725]
95% CI: [3.175] - [6.076]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.351]
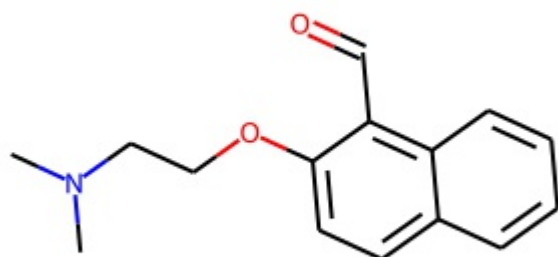p_risky at threshold of 5: [0.625]

interesting mol: O=C1CCc2ccccc2N1CCCN1CCC(Cc2ccccc2)CC1
predicted mean: [5.281]
predicted standard deviation: [0.799]
95% CI: [3.683] - [6.879]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.339]
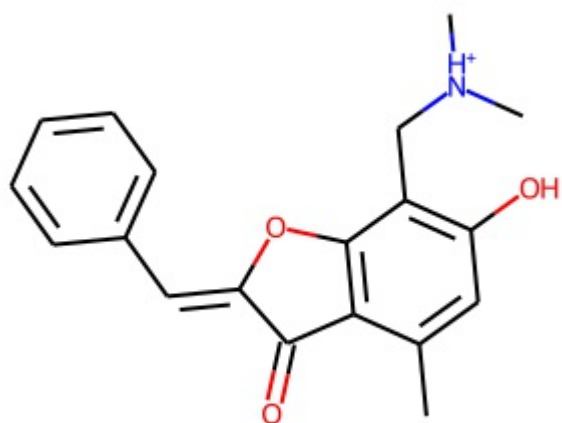p_risky at threshold of 5: [0.338]

interesting mol: CN(CCCn1c(=O)oc2cc(CNC[C@H](O)c3ccc(O)c(NC=O)c3)ccc21)
[C@H]1CC[C@H](c2cccc3c2C(C)(C(=O)O)c2ccccc2O3)CC1
predicted mean: [6.284]
predicted standard deviation: [0.88]
95% CI: [4.525] - [8.043]
aleatoric uncertainty: [0.678]
epistemic uncertainty: [0.574]
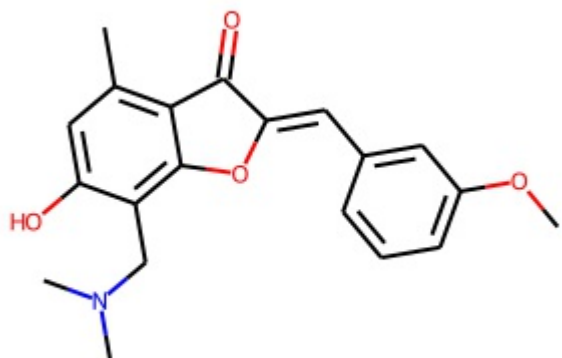p_risky at threshold of 5: [0.071]

interesting mol: Cc1cc(O)c(CN2CCCC2)c2c1C(=O)/C(=C\c1ccco1)O2
predicted mean: [4.539]
predicted standard deviation: [0.711]
95% CI: [3.117] - [5.961]
aleatoric uncertainty: [0.674]
epistemic uncertainty: [0.244]
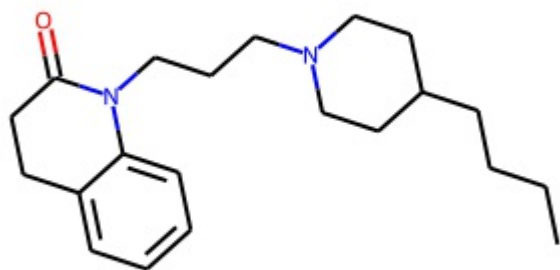p_risky at threshold of 5: [0.745]

interesting mol: CN(C)CCOc1ccc2ccccc2c1C=O
predicted mean: [4.941]
predicted standard deviation: [0.729]
95% CI: [3.483] - [6.4]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.346]
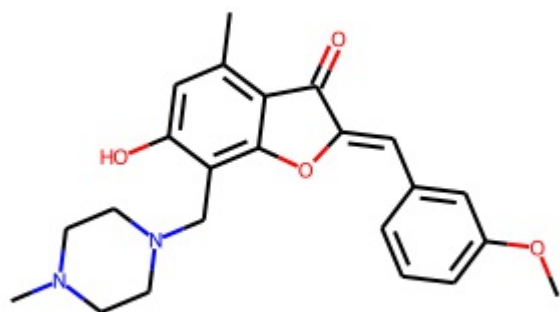p_risky at threshold of 5: [0.526]

interesting mol: Cc1cc(O)c(C[NH+](C)C)c2c1C(=O)/C(=C/c1ccccc1)O2
predicted mean: [4.778]
predicted standard deviation: [0.756]
95% CI: [3.266] - [6.291]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.332]
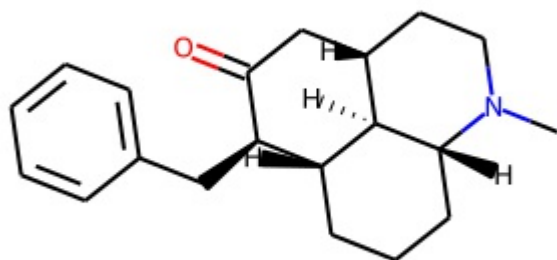p_risky at threshold of 5: [0.603]

interesting mol: COc1cccc(/C=C2\Oc3c(CN(C)C)c(O)cc(C)c3C2=O)c1
predicted mean: [4.644]
predicted standard deviation: [0.725]
95% CI: [3.194] - [6.093]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.345]
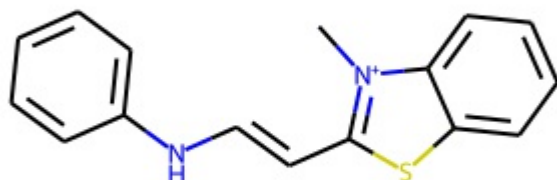p_risky at threshold of 5: [0.69]

interesting mol: CCCCC1CCN(CCCN2C(=O)CCc3ccccc32)CC1
predicted mean: [5.459]
predicted standard deviation: [0.761]
95% CI: [3.938] - [6.981]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.326]
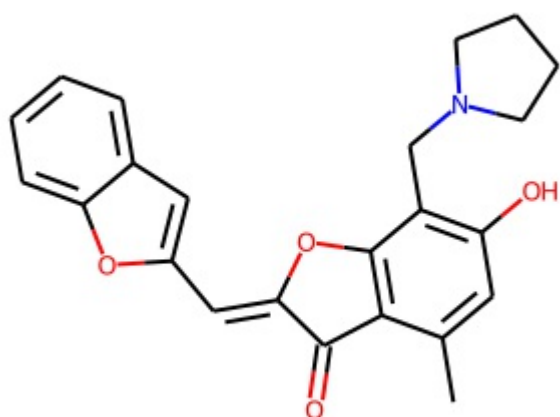p_risky at threshold of 5: [0.271]

interesting mol: COc1cccc(/C=C2\Oc3c(CN4CCN(C)CC4)c(O)cc(C)c3C2=O)c1
predicted mean: [5.006]
predicted standard deviation: [0.793]
95% CI: [3.42] - [6.592]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.413]
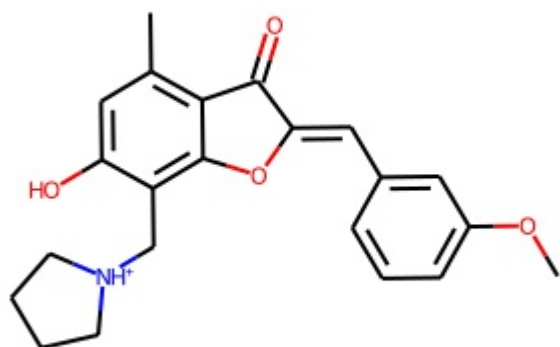p_risky at threshold of 5: [0.501]

interesting mol: CN1CC[C@H]2CC(=O)[C@H](Cc3ccccc3)[C@H]3CCC[C@@H]1[C@H]23
predicted mean: [5.468]
predicted standard deviation: [0.763]
95% CI: [3.941] - [6.994]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.29]
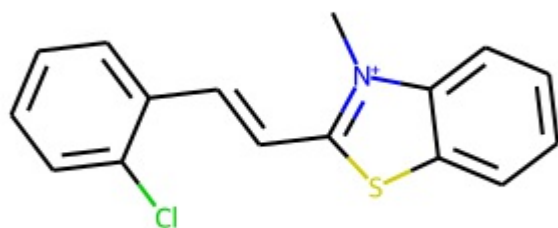p_risky at threshold of 5: [0.341]

interesting mol: C[n+]1c(/C=C/Nc2ccccc2)sc2ccccc21
predicted mean: [4.832]
predicted standard deviation: [0.744]
95% CI: [3.343] - [6.32]
aleatoric uncertainty: [0.675]
epistemic uncertainty: [0.244]
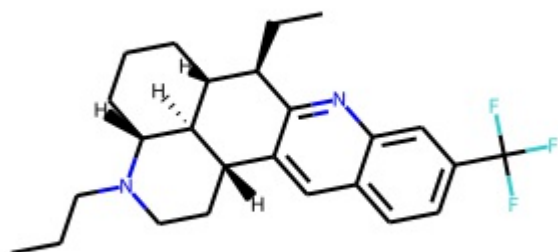p_risky at threshold of 5: [0.659]

interesting mol: Cc1cc(O)c(CN2CCCC2)c2c1C(=O)/C(=C/c1cc3ccccc3o1)O2
predicted mean: [4.452]
predicted standard deviation: [0.734]
95% CI: [2.984] - [5.919]
aleatoric uncertainty: [0.675]
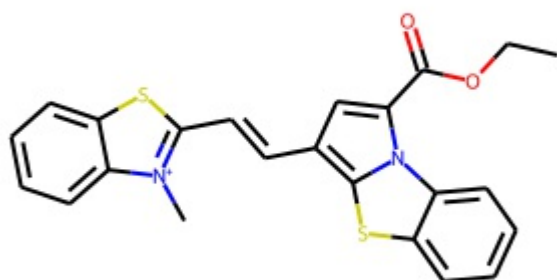epistemic uncertainty: [0.24]
p_risky at threshold of 5: [0.802]

interesting mol: COc1cccc(/C=C2\Oc3c(C[NH+]4CCCC4)c(O)cc(C)c3C2=O)c1
predicted mean: [5.357]
predicted standard deviation: [0.873]
95% CI: [3.611] - [7.102]
aleatoric uncertainty: [0.678]
epistemic uncertainty: [0.401]
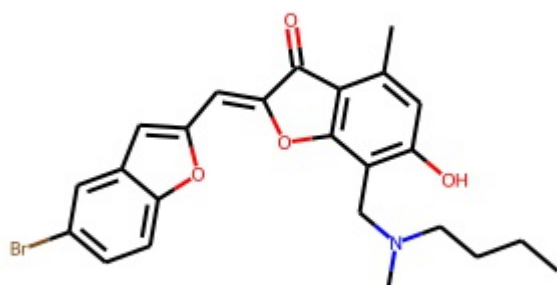p_risky at threshold of 5: [0.326]

interesting mol: C[n+]1c(/C=C/c2ccccc2Cl)sc2ccccc21
predicted mean: [4.786]
predicted standard deviation: [0.68]
95% CI: [3.427] - [6.146]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.239]
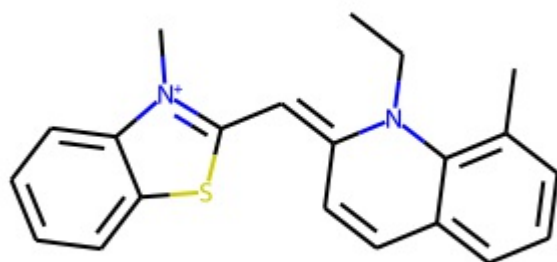p_risky at threshold of 5: [0.601]

interesting mol: CCCN1CC[C@H]2c3cc4ccc(C(F)(F)F)cc4nc3[C@H](CC)
[C@H]3CCC[C@@H]1[C@@H]32
predicted mean: [4.765]
predicted standard deviation: [0.732]
95% CI: [3.302] - [6.228]
aleatoric uncertainty: [0.675]
epistemic uncertainty: [0.286]
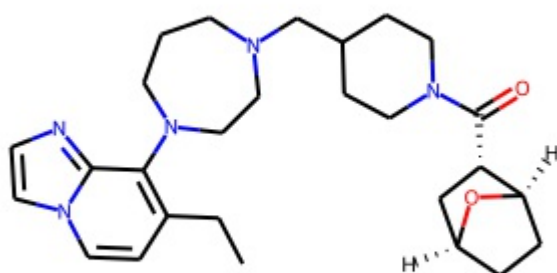p_risky at threshold of 5: [0.583]

interesting mol: CCOC(=O)c1cc(/C=C/c2sc3ccccc3[n+]2C)c2sc3ccccc3n12
predicted mean: [4.892]
predicted standard deviation: [0.742]
95% CI: [3.409] - [6.375]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.298]
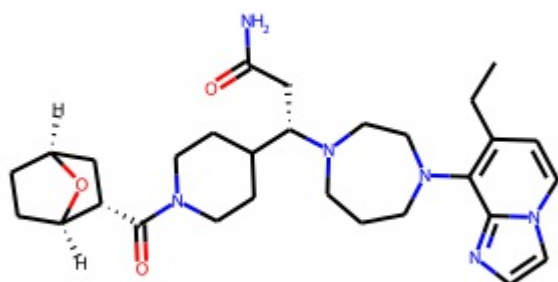p_risky at threshold of 5: [0.534]

interesting mol: CCCCN(C)Cc1c(O)cc(C)c2c1O/C(=C\c1cc3cc(Br)ccc3o1)C2=O
predicted mean: [4.126]
predicted standard deviation: [0.711]
95% CI: [2.704] - [5.548]
aleatoric uncertainty: [0.675]
epistemic uncertainty: [0.242]
p_risky at threshold of 5: [0.879]

interesting mol: CCN1C(=Cc2sc3ccccc3[n+]2C)C=Cc2cccc(C)c21
predicted mean: [5.185]
predicted standard deviation: [0.723]
95% CI: [3.738] - [6.631]
aleatoric uncertainty: [0.677]
epistemic uncertainty: [0.338]
p_risky at threshold of 5: [0.377]

interesting mol: CCc1ccn2ccnc2c1N1CCCN(CC2CCN(C(=O)
[C@H]3C[C@@H]4CC[C@H]3O4)CC2)CC1
predicted mean: [5.192]
predicted standard deviation: [0.713]
95% CI: [3.766] - [6.618]
aleatoric uncertainty: [0.676]
epistemic uncertainty: [0.322]
p_risky at threshold of 5: [0.393]

interesting mol: CCc1ccn2ccnc2c1N1CCCN([C@@H](CC(N)=O)C2CCN(C(=O)
[C@H]3C[C@@H]4CC[C@H]3O4)CC2)CC1
predicted mean: [5.795]
predicted standard deviation: [0.782]
95% CI: [4.231] - [7.359]
aleatoric uncertainty: [0.678]
epistemic uncertainty: [0.351]
p_risky at threshold of 5: [0.155]

In [27]: