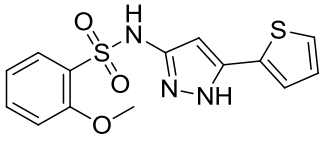
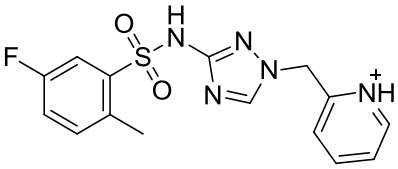
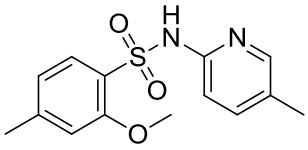
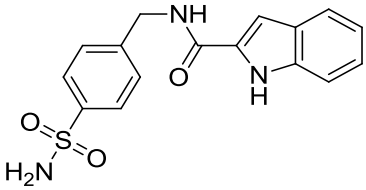
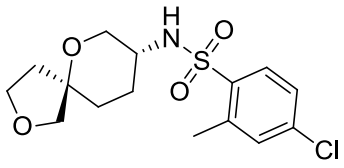
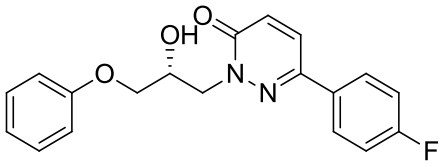
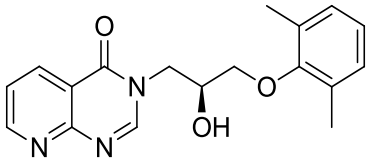
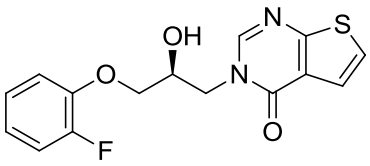
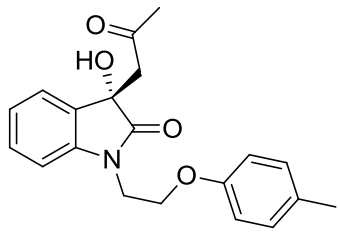
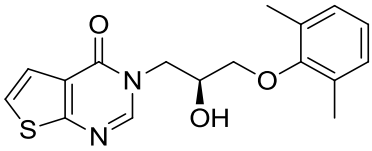
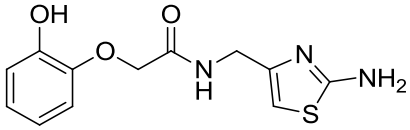
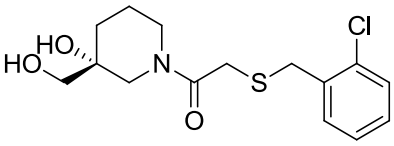
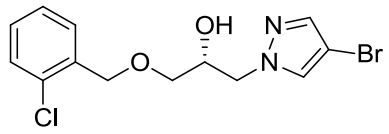
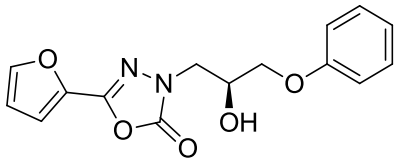
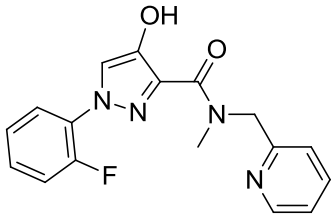
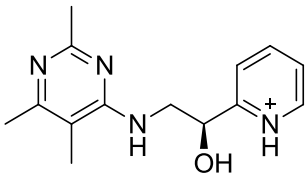
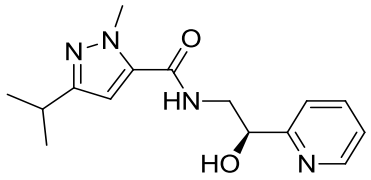
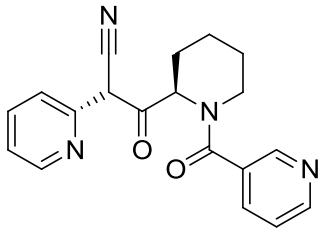
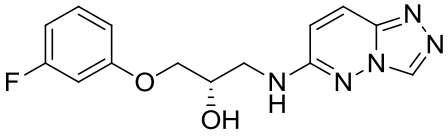
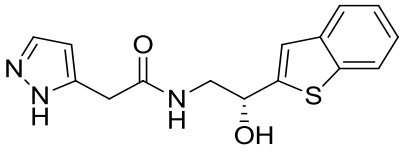
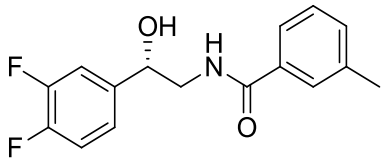
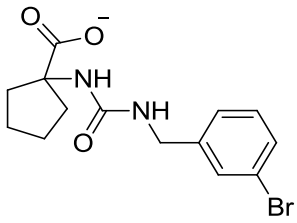
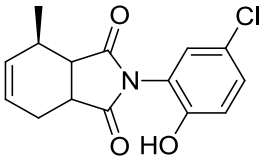
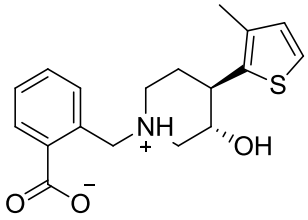
Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
1[a]		-69.11	3.14
2[a]		-60.48	2.52
3[a]		-56.03	2.80
4[a]		-53.66	2.33

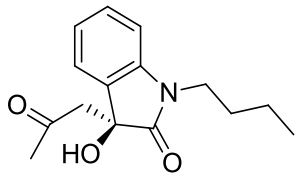
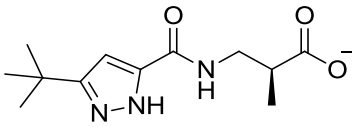
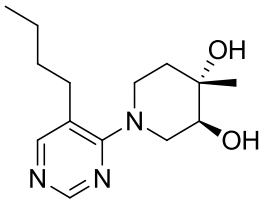
Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
5[a]		-46.75	2.12
6[a]		-39.96	1.60
7[a]		-38.81	1.62
8[a]		-37.87	1.72

Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
9[a]		-37.63	1.50
10[a]		-37.27	1.62
11[b]		-35.78	1.88
12[b]		-35.76	1.70

Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
13[a]		-35.29	1.86
14[a]		-34.53	1.57
15[a]		-32.38	1.35
16[b]		-32.32	1.70

Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
17[b]		-31.43	1.50
18[a]		-31.38	1.25
19[a]		-31.37	1.43
20[a]		-31.25	1.49

Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
21[a]		-31.24	1.49
22[a]		-31.22	1.56
23[b]		-31.08	1.55
24[b]		-26.77	1.16

Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol^{-1}× HAC^{-1}]
25[a]		-26.40	1.40
26[a]		-25.95	1.44
27[b]		-25.66	1.50

* Predicted ligand efficiency (see equation (1))

** Inhibition (see equation (2)) at 300 µM (100 µM in case of compound **24**)

† Assay interference due to autofluorescence

[a] Compounds have been purchased from Enamine

[b] Compounds have been purchased from Chembridge