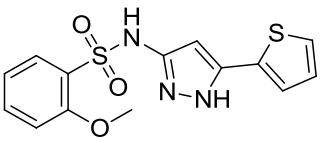
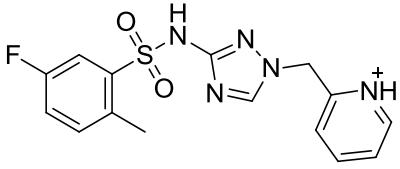
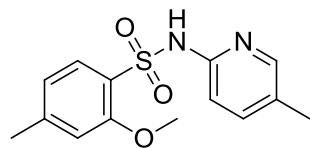
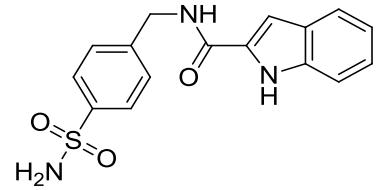
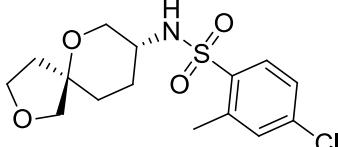
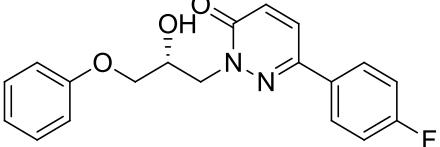
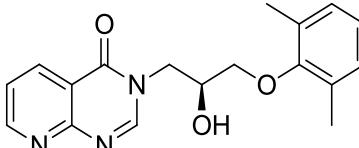
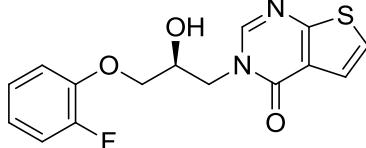
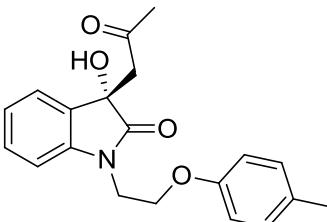
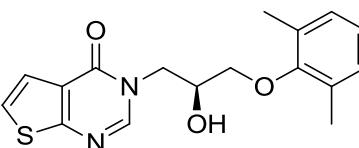
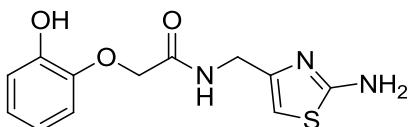
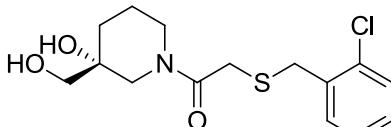
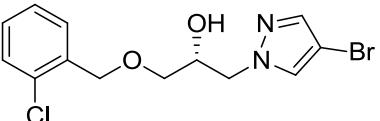
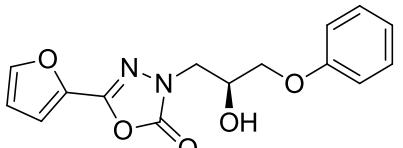
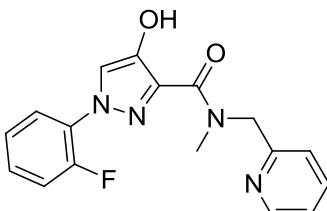
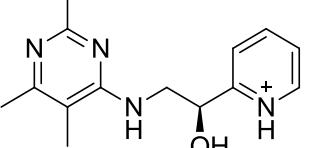
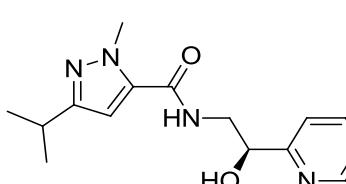
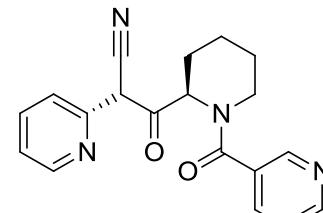
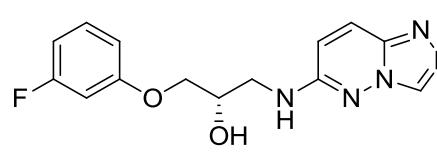
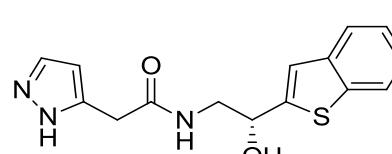


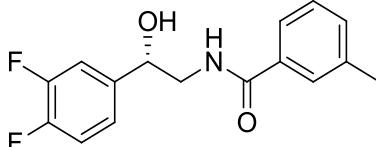
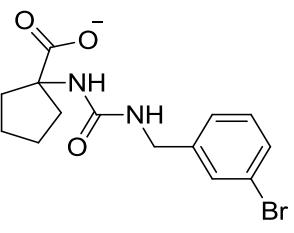
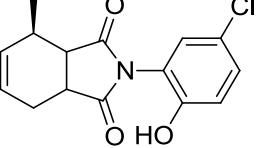
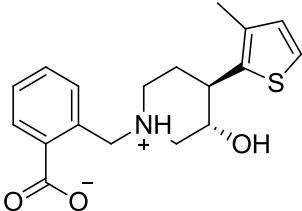
Compound	Molecular structure	Score [kJ/mol]	Predicted LE* [kJ×mol ⁻¹ × HAC ⁻¹]
1 ^a		-69.11	3.14
2 ^a		-60.48	2.52
3 ^a		-56.03	2.80
4 ^a		-53.66	2.33

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	 <p>Chemical structure of compound 21a: (S)-2-(2,4-difluorophenyl)-2-(4-methylphenyl)propan-1-ol.</p>	-31.24	1.49
22^a	 <p>Chemical structure of compound 22a: 1-[2-(4-bromophenyl)ethyl]cyclopentanecarboxylic acid.</p>	-31.22	1.56
23^b	 <p>Chemical structure of compound 23b: 2-(4-chlorophenyl)-3-hydroxy-2,3-dihydro-1H-inden-1-one.</p>	-31.08	1.55
24^b	 <p>Chemical structure of compound 24b: 2-(4-carboxyphenyl)-N-[2-(2-methylthiophenyl)cyclohexyl]ethylammonium cation.</p>	-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