Therapeutic Targets Database





Target Name	Histone deacetylase 10
Target TTD ID	TTDR01338

Target Species	Human
Chemical Type	Substituted biaryl hydroxamates
Mode of Action	Inhibitor
QSAR Model 1	pIC ₅₀ (HDAC10)= -2.029 ×I-NHCOCH ₂ SH + 1.007 ×I-Thiazole + 7.192 R^2 =0.92, n=22, RMSE=0.328, p <0.0001
Molecular Descriptor 1	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon Five QSAR equations were developed from the 23 compounds (biphenyl or phenylthiazoles bearing hydroxamates or mercaptoacetamides) against HDACs 1, 2, 8, 10 and 6 incorporating the binary indicators I-NHCOCH2SH and I-Thiazole and calculated LogP (ClogP). If the compound is mercaptoacetamide, then I-NHCOCH2SH = 1.0; otherwise it is 0. If the compound is phenylthiazole, then I-Thiazole = 1.0; otherwise it is 0.
Reference	Computational Studies on the Histone Deacetylases and the Design of Selective Histone Deacetylase Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2009, 9, 241-256

Target Species	Human
Chemical Type	Mercaptoacetamides
Mode of Action	Inhibitor

QSAR	$pIC_{50}(HDAC10) = -2.029 \times I-NHCOCH_2SH + 1.007 \times I-Thiazole + 7.192$
Model 1	R ² =0.92, n=22, RMSE=0.328, p<0.0001
	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon
Molecular Descriptor	Five QSAR equations were developed from the 23 compounds (biphenyl or phenylthiazoles bearing hydroxamates or mercaptoacetamides) against HDACs 1, 2, 8, 10 and 6 incorporating
1	the binary indicators I-NHCOCH2SH and I-Thiazole and calculated LogP (ClogP). If the compound is mercaptoacetamide, then I-NHCOCH2SH = 1.0; otherwise it is 0. If the compound is phenylthiazole, then I-Thiazole = 1.0; otherwise it is 0.
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