

Target Name	Histone deacetylase 2
Target TTD ID	TTDR01156

Target Species	Human
Chemical Type	Substituted biaryl hydroxamates
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50}(HDAC2) = -2.127 \times I-NHCOCH_2SH + 0.606 \times I-Thiazole + 6.813$ $R^2=0.92, n=22, RMSE=0.318, p<0.0001$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p>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-NHCOCH<sub>2</sub>SH and I-Thiazole and calculated LogP (ClogP). If the compound is mercaptoacetamide, then I-NHCOCH<sub>2</sub>SH = 1.0; otherwise it is 0. If the compound is phenylthiazole, then I-Thiazole = 1.0; otherwise it is 0.</p>
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	Substituted mercaptoacetamides
Mode of Action	Inhibitor

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