Target Name	Histone deacetylase 8
Target TTD ID	TTDR01337

Target Species	Human
Chemical Type	Substituted biaryl hydroxamates
Mode of Action	Inhibitor
QSAR Model 1	pIC_{50}(HDAC8) = -0.461 × I-NHCOCH$_2$SH + 5.668 R^2=0.52, n=23, RMSE=0.176, p<0.0001
Molecular Descriptor	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. *Current Topics in Medicinal Chemistry*, 2009, 9, 241-256

Target Species	Human
Chemical Type	Mercaptoacetamides
Mode of Action	Inhibitor

QSAR Model 1	$pIC_{50}(HDAC8) = -0.461 \times I\text{-}NHCOCH_2SH + 5.668$ $R^2=0.52$, n=23, RMSE=0.176, $p<0.0001$
Molecular Descriptor	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. *Current Topics in Medicinal Chemistry*, 2009, 9, 241-256