Target Name	Histone deacetylase 6
Target TTD ID	TTDR01167

Target Species	Human
Chemical Type	Substituted biaryl hydroxamates
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50}(HDAC6) = -1.429 \times I\text{-}NHCOCH_2SH + 0.711 \times I\text{-}Thiazole + 0.046 \times (ClogP)_2 + 7.799$ $R^2=0.86$, n=23, RMSE=0.384, $p<0.0001$
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. *Current Topics in Medicinal Chemistry*, 2009, 9, 241-256

Target Species	Human
Chemical Type	Substituted mercaptoacetamides
Mode of Action	Inhibitor

QSAR Model 1	$pIC_{50}(HDAC6) = -1.429 \times I\text{-}NHCOCH_2SH + 0.711 \times I\text{-}Thiazole + 0.046 \times (ClogP)_2 + 7.799$ $R^2=0.86$, n=23, RMSE=0.384, $p<0.0001$
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. *Current Topics in Medicinal Chemistry*, 2009, 9, 241-256