Target Name	MMP-3
Target TTD ID	TTDC00105

Target Species	Human
Chemical Type	N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(10^6/\mathrm{IC}_{50}) = -0.042 \times \mathrm{ATS2v} - 110.925 \times \mathrm{MATS4m} - 55.421 \times \mathrm{MATS8m} - 8.431 \times \mathrm{MATS3v} + 2.379 \times \mathrm{GATS6e} + 5.227 \times \mathrm{GATS2p} + 162.799$ $N = 32; \quad R^2 = 0.808; \quad S = 0.420; \quad p < 10^{-5}$ $Q^2_{\mathrm{LOO}} = 0.721 \quad S_{\mathrm{CV\,LOO}} = 0.454 \quad Q^2_{\mathrm{L3O}} = 0.697 \quad S_{\mathrm{CV\,L3O}} = 0.479$
QSAR Model 2	$\log(10^6/\mathrm{IC}_{50}) = -0.049 \times O[\mathrm{ATS2v}] - 110.925 \times O[\mathrm{MATS4m}] - 32.131 \times O[\mathrm{MATS8m}] - 2.739 \times O[\mathrm{MATS3v}] + 4.427 \times O[\mathrm{GATS6e}] + 4.716 \times O[\mathrm{GATS2p}] + 37.443$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** N is the number of compounds included in the models; R^2 are the square of correlation coefficients; S is the standard deviation of the regressions; p is the significance of the variables in the models; Q^2_{LOO} and $S_{CV\ LOO}$ are the correlation coefficients and standard deviations of the LOO cross-validation, respectively, and Q^2_{L3O} and $S_{CV\ L3O}$ are the correlation coefficients and standard deviations of the L3O cross-validation, respectively; ${}^1\chi^v$ or log P: hydrophobicity-related descriptors; Descriptors of MMP1 include ATS2v, MATS5m, MATS7m, GATS1v, GATS1e, GATS4p; Descriptors of MMP2 include MATS5m, MATS5v, MATS5p, GATS4v, GATS7v, GATS7p; Descriptors of MMP3 include ATS2v, MATS1m, MATS6m, MATS6e, GATS1v, GATS5v; Descriptors of MMP9 include MATS6m, MATS2v, MATS1p, GATS3v, GATS7v, GATS8v; Descriptors of MMP13 include ATS2v, MATS4m, MATS7v, MATS1p, MATS5p, GATS7p; Contribution C_i^{39} of descriptor i is given by:

	$C_i = \frac{100 \times \Delta m_i}{\sum \Delta m_i}$.
Reference	Linear and nonlinear QSAR study of N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives as matrix metalloproteinase inhibitors. *Bioorganic & Medicinal Chemistry* 14 (2006) 4137–4150