Target Name	Matrix Metalloproteinase 13 (MMP-13)
Target TTD ID	TTDC00150

Target Species	Human
Chemical Type	Anthranilic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = 8.699(\pm0.302) - 1.240(\pm0.247)\log P$ $n = 9, r = 0.976, r^2_{cv} = 0.92, s = 0.23, F_{1,7} = 140.93(12.25)$
QSAR Model 2	$\log(1/IC_{50}) = 7.902(\pm0.366) - 0.184(\pm0.138)\log P - 1.051(\pm0.552)I_1 + 1.079(\pm0.626)I_3 + 1.341(\pm0.527)I_4$ $n = 22, r = 0.919, r^2_{cv} = 0.75, s = 0.38, F_{4,17} = 23.06(4.67)$
QSAR Model 3	$\log(1/IC_{50}) = 0.410(\pm0.158)\mathrm{Pol} + 0.773(\pm0.325)I_1 + 5.960(\pm0.824)$ $n = 19, r = 0.914, r^2_{cv} = 0.79, s = 0.19, F_{2,14} = 40.71(6.51)$
QSAR Model 4	$\log(1/IC_{50}) = 8.220(\pm0.467) - 0.320(\pm0.192)\log P - 0.891(\pm0.422)I_{1,CC} - 0.531(\pm0.403)I_{1,N}$ $n = 17, r = 0.910, r^2_{cv} = 0.70, s = 0.29, F_{3,13} = 20.78(5.74)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** I1 stands for R1-substituents and has a value of unity for R1 = OCH2Ph and zero for others, I2 stands for R2-substituents and has a values of unity for R2 = CH2-3-pyridyl group and zero for others, I3 stands for R3-substiutents and is equal to 1 for R3 = an aromatic substituent and zero otherwise, I4, which stands for R4-substituents also has a value of unity for R4 = an aromatic moiety and zero for others.

Reference	A quantitative structure–activity relationship study on some series of anthranilic acid-based matrix metalloproteinase inhibitors. *Bioorganic & Medicinal Chemistry* 13 (2005) 5454–5462

Target Species	Human
Chemical Type	N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives
Mode of Action	Inhibitor
QSAR Model 4	MLR-MMP-13: $\log(10^6/\mathrm{IC}_{50}) = -86.944 \times \mathrm{MATS4m} - 33.782 \times \mathrm{MATS8m} - 5.375 \times \mathrm{MATS3v} + 8.188 \times \mathrm{MATS1p} + 1.103 \times \mathrm{GATS5e} + 122.338$ $N = 29; \quad R^2 = 0.787; \quad S = 0.397; \quad p < 10^{-5}$ $Q^2_{\mathrm{LOO}} = 0.703; \quad S_{\mathrm{CV\,LOO}} = 0.423; \quad Q^2_{\mathrm{L3O}} = 0.692; \quad S_{\mathrm{CV\,L3O}} = 0.434$
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

Target Species	TTDC00150
Chemical Type	N-hydroxy-α-phenylsulfonylacetamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(10^6/IC_{50}) = 0.017 \times ATS3m + 11.363 \times MATS6v - 1.118 \times MATS6e - 1.826 \times GATS1v + 11.911 \times GATS6v + 6.097 \times GATS1e + 1.297 \times GATS4e - 11.139$ $N_{training} = 68 \quad R^2 = 0.692 \quad S = 0.376 \quad p < 10^{-5} \quad R^2_{CV} = 0.598 \quad S_{CV} = 0.430 \quad N_{test} = 12$ $R^2_{EP} = 0.727 \quad S_{EP} = 0.429$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** MATS(p_k, l) and GATS(p_k, l), Moran's index and Geary's coefficient respectively at spatial lag l; p_k, value of property k; N_{test}, number of compounds included in the training and test sets respectively; R^2, square of correlation coefficients; S, standard deviation of regressions; p, significance of the variables in the models; R^2_{CV} and S_{CV}, correlation coefficients and standard deviations of the leave-one-out (LOO) cross-validation respectively; R^2_{EP} and S_{EP} the correlation coefficients and standard deviations of test set regressions respectively. $N_{training}$ and N_{test} are the number of compounds included in the training and test sets, respectively, R^2 is the square of correlation coefficients, S is the standard deviation of the regressions, p is the significance of the variables in the models, R^2_{CV} and S_{CV} are the correlation coefficients and standard deviations of the leave-one-out (LOO) cross-validation, respectively. $R2_{EP}$ and S_{EP} are the correlation coefficients and standard deviations of test set regressions, respectively. Broto–Moreau's autocorrelation coefficients (ATS), Moran's indices (MATS), and Geary's coefficients (GATS). Descriptors (MMP1): ATS3e, MATS3m, MATS3e, MATS5e, MATS6e, GATS1v, GATS7p; Descriptors (MMP9): ATS6m, MATS2m, MATS5v, MATS1e, GATS4v, GATS5e, GATS4p; Descriptors (MMP13): ATS3m, ATS6m, MATS1v, GATS7v, GATS3e, GATS4e, GATS6p.
Reference	QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-α-phenylsulfonylacetamide derivatives. *Bioorganic & Medicinal Chemistry* 15 (2007) 6298–6310