Target Name	Matrix Metalloproteinase 9 (MMP-9)
Target TTD ID	TTDC00076

Target Species	Human
Chemical Type	Anthranilic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = 8.525(\pm 0.193) - 0.576(\pm 0.147)\log P$ $n = 10, r = 0.954, r^2_{cv} = 0.86, s = 0.15, F_{1,8} = 81.56(11.26)$
QSAR Model 2	$\log(1/IC_{50}) = 8.336(\pm 0.492) - 0.265(\pm 0.183)\log P - 1.241(\pm 0.725)I_1 + 1.183(\pm 0.691)I_4$ $n = 19, r = 0.882, r^2_{cv} = 0.64, s = 0.50, F_{3,15} = 17.47(5.42)$
QSAR Model 3	$\log(1/IC_{50}) = 0.503(\pm 0.477)\mathrm{Pol} - 1.806(\pm 0.567)I_{1,CC} - 0.807(\pm 0.559)I_{1,N} + 5.916(\pm 2.137)$ $n = 16, r = 0.920, r^2_{cv} = 0.64, s = 0.37, F_{3,12} = 21.92(5.95)$
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 1	MLR-MMP-9: $\log(10^6/\mathrm{IC}_{50}) = 109.844 \times \mathrm{MATS2m} - 51.167 \times \mathrm{MATS4m} + 8.380 \times \mathrm{MATS2v} + 13.240 \times \mathrm{MATS6e} + 7.864 \times \mathrm{GATS6e} + 13.015 \times \mathrm{GATS2p} - 72.742$ $N = 32; \quad R^2 = 0.767; \quad S = 0.478; \quad p < 10^{-5}$ $Q^2_{LOO} = 0.644; \quad S_{\mathrm{CV\,LOO}} = 0.544; \quad Q^2_{L3O} = 0.605; \quad S_{\mathrm{CV\,L3O}} = 0.597$
QSAR Model 2	MLR-MMP-9: $\log(10^6/\mathrm{IC}_{50}) = 91.121 \times O[\mathrm{MATS2m}] - 96.892 \times O[\mathrm{MATS4m}] + 10.538 \times O[\mathrm{MATS2v}] + 13.240 \times O[\mathrm{MATS6e}] + 6.716 \times O[\mathrm{GATS6e}] + 6.278 \times O[\mathrm{GATS2p}] - 0.631$
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	Human
Chemical Type	5-amino-2-mercapto-1,3,4-thiadiazoles
Mode of Action	Inhibitor
QSAR Model 1	*MMP-9* $\log(1/K_i) = [2.59183(\pm 1.56751)] + I[0.789148(\pm 0.349099)] + \text{a\_nF}[0.237027(\pm 0.101373)]$ $N = 27,\ r = 0.885,\ r^2 = 0.784,\ \text{SEE} = 0.276,\ F = 27.834(F_{3,23} = 4.765),$ $\text{chance} =< 0.001,\ q^2 = 0.676,\ S_{\text{PRESS}} = 0.338,\ S_{\text{DEP}} = 0.312$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** **Functional families of the descriptors**-Descriptor: definition **Physical properties**-apol: sum of the atomic polarizabilities; bpol: sum of the absolute value of the difference between; atomic polarizabilities of all bonded atoms in the molecule; mr: molecular refractivity; Weight: molecular weight; TPSA: topological polar surface area; log P(O/W): log of the octanol/water partition coefficient. **Atom counts and bond counts**-a_aro: number of aromatic atoms; a_nN: number of nitrogen atoms; a_nO: number of oxygen atoms; a_nF: number of fluorine atoms; a_nS: number of sulfur atoms; a_nCl: number of chlorine atoms; a_nBr: number of bromine atoms; b_1rotN: number of rotatable single bonds; b_ar: number of aromatic bonds; b_ singlet: number of single bonds; b_double: number of double bonds; b_triple: number of triple bonds. **Kier and Hall connectivity indices and Kier shape indices**-$^0\chi$: atomic connectivity index (order 0); $^0\chi_c$: carbon connectivity index (order 0); $^1\chi$: atomic connectivity index (order 1); $^1\chi_c$: carbon connectivity index (order 1); $^0\chi^V$: atomic valence connectivity index (order 0); $^0\chi_c^V$: carbon valence connectivity index (order 0); $^1\chi^V$: atomic valence connectivity index (order 1); $^1\chi_c^V$: carbon valence connectivity index (order 1); ^1K: first kappa shape index; ^2K: second kappa shape index; ^3K: third kappa shape index; $^1K_\alpha$: first alpha modified shape index; $^2K_\alpha$: second alpha modified shape index; $^3K_\alpha$: third alpha modified shape index; KierFlex: Kier molecular flexibility index. **Adjacency and distance matrix descriptors**-balabanJ: Balaban's connectivity topological index; petitjeanSC: Petitjean graph shape coefficient; weinerPath: Wiener path number; weinerPol: Wiener

	polarity number; zagreb: Zagreb index. *N* is the number of data points, *r* is correlation coefficient, r^2 is squared correlation coefficient which when multiplied by 100 gives explained variance in biological activity, SEE is standard error of estimate, *F* represents Fischer ratio between the variances of calculated and observed activities.
Reference	QSAR analysis of some 5-amino-2-mercapto-1,3,4-thiadiazole based inhibitors of matrix metalloproteinases and bacterial collagenase. *Bioorganic & Medicinal Chemistry Letters* 16 (2006) 3847–3854

Target Species	Human
Chemical Type	Aryl sulfonyl amido derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/K_i) = 0.990(\pm 0.259)S_S - 3.132(\pm 0.380)S_N + 18.383\,(\pm 2.267)$ $n = 24,\ r = 0.971,\ r_{cv}^2 = 0.93,\ R_A^2 = 0.94,\ s = 0.15,\ F_{2,21} = 170.65(5.78)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; S_S and S_N, the E-state indices of sulfur and nitrogen atoms; R_A^2, the square of adjustable correlation coefficient [$R_A^2 = r^2(1 - 1/F)$]; r, correlation coefficient; r_{cv}^2, the squre of cross-validated correlation coefficient obtained from leave-one-out jackknife procedure; s is the standard deviation; F, F-ratio; $^1\chi^v$ is Kier's first-order valence molecular connectivity index and electrotopological state (E-state) indices of atoms (S); The intrinsic state of atom I_i;
Reference	A Quantitative Structure-Activity Relationship Study on Some Aryl Sulfonyl Amido and Ureido Derivatives Acting as Matrix Metalloproteinase and *Clostridium histolyticum* Collagenase Inhibitors. *Letters in Drug Design & Discovery*, 2007, 4, 496-501

Target Species	Human

Chemical Type	Aryl sulfonyl ureido derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/K_i) = 0.990(\pm 0.259)S_S - 3.132(\pm 0.380)S_N + 18.383\,(\pm 2.267)$ $n = 24,\ r = 0.971,\ r_{cv}^2 = 0.93,\ R_A^2 = 0.94,\ s = 0.15,\ F_{2,21} = 170.65(5.78)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *n* is the number of compounds; S_S and S_N, the E-state indices of sulfur and nitrogen atoms; R_A^2, the square of adjustable correlation coefficient [$R_A^2 = r^2(1 - 1/F)$]; r, correlation coefficient; r_{cv}^2, the squre of cross-validated correlation coefficient obtained from leave-one-out jackknife procedure; s is the standard deviation; F, F-ratio; $^1\chi^v$ is Kier's first-order valence molecular connectivity index and electrotopological state (E-state) indices of atoms (S); The intrinsic state of atom I_i;
Reference	A Quantitative Structure-Activity Relationship Study on Some Aryl Sulfonyl Amido and Ureido Derivatives Acting as Matrix Metalloproteinase and *Clostridium histolyticum* Collagenase Inhibitors. *Letters in Drug Design & Discovery*, 2007, 4, 496-501

Target Species	Human
Chemical Type	N-hydroxy-α-phenylsulfonylacetamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(10^6/IC_{50}) = -0.005 \times ATS6m + 0.018 \times ATS3e + 8.881 \times MATS2e - 7.718 \times MATS4e - 4.655 \times GATS1v + 14.788 \times GATS1e + 2.379 \times GATS6p - 4.571$ $N_{training} = 66 \quad R^2 = 0.731 \quad S = 0.416 \quad p < 10^{-5} \quad R^2_{CV} = 0.605 \quad S_{CV} = 0.504 \quad N_{test} = 12$ $R^2_{EP} = 0.713 \quad S_{EP} = 0.415$
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