Target Name	Matrix Metalloproteinase 1 (MMP-1)
Target TTD ID	TTDC00147

Target Species	Human
Chemical Type	Anthranilic acid derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = 7.286(\pm0.331) - 2.473(\pm1.279)\log P + 1.098(\pm0.683)(\log P)^2$ $n = 7, r = 0.960, r^2_{cv} = 0.80, s = 0.18, F_{1,4} = 23.53(21.20), [\log P_o = 1.13]$
QSAR Model 2	$\log(1/IC_{50}) = 1.020(\pm0.396)I_2 + 0.596(\pm0.487)I_3 - 0.192(\pm0.118)\log P + 5.979(\pm0.432)$ $n = 16, r = 0.919, r^2_{cv} = 0.67, s = 0.28, F_{3,12} = 21.86(5.95)$
QSAR Model 3	$\log(1/IC_{50}) = 0.234(\pm0.147)I_{4,Br} + 0.317(\pm0.186)I_3 + 0.629(\pm0.173)I_2 + 0.534(\pm0.251)I_1$ $- 0.062(\pm0.060)\log P + 6.801(\pm0.150)$ $n = 19, r = 0.935, r^2_{cv} = 0.74, s = 0.13, F_{5,13} = 18.15(4.86)$
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-1: $\log(10^6/IC_{50}) = -166.804 \times MATS4m - 51.519 \times MATS8m - 13.020 \times MATS3v + 4.817 \times GATS1e - 6.913 \times GATS2e + 219.442$ $N = 26; \quad R^2 = 0.834; \quad S = 0.383; \quad p < 10^{-5}$ $Q^2_{LOO} = 0.745; \quad S_{CV\,LOO} = 0.421; Q^2_{L3O} = 0.708; \quad S_{CV\,L3O} = 0.455$
QSAR Model 2	MLR-MMP-1: $\log(10^6/IC_{50}) = -79.680 \times O[MATS4m] - 61.543 \times O[MATS8m] - 5.561 \times O[MATS3v] + 4.817 \times O[GATS1e] - 4.981 \times O[GATS2e] + 65.454$
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	Human

Species	
Chemical Type	5-amino-2-mercapto-1,3,4-thiadiazoles
Mode of Action	Inhibitor
QSAR Model 1	*MMP-1* $\log(1/K_i) = [4.39725(\pm 1.03418)] + {}^1\chi_c^V[-0.207152(\pm 0.0851363)] + {}^3K_\alpha[0.201545(\pm 0.0927689)]$ $+ \text{a\_nF}[0.0832763(\pm 0.0471238)]$ $N = 27,\ r = 0.913,\ r^2 = 0.834,\ \text{SEE} = 0.122,\ F = 38.645(F_{3,23} = 4.765),$ $\text{chance} =< 0.001,\ q^2 = 0.734,\ S_{\text{PRESS}} = 0.154,\ S_{\text{DEP}} = 0.142.$
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	$\log(1/K_i) = 1.522(\pm 0.398)S_S - 3.690(\pm 0.779)S_N - 1.624\ (\pm 0.420)I + 22.598(\pm 4.183)$ $n = 24,\ r = 0.934,\ r_{cv}^2 = 0.81,\ R_A^2 = 0.85,\ s = 0.11,\ F_{3,20} = 45.83(4.94)$
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	Human

Species	
Chemical Type	Aryl sulfonyl ureido derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/K_i) = 1.522(\pm0.398)S_S - 3.690(\pm0.779)S_N - 1.624\ (\pm0.420)I + 22.598(\pm4.183)$ $n = 24,\ r = 0.934,\ r_{cv}^2 = 0.81,\ R_A^2 = 0.85,\ s = 0.11,\ F_{3,20} = 45.83(4.94)$
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	$\log(10^6/IC_{50}) = -17.557 \times MATS4m - 5.396 \times MATS3v + 17.908 \times MATS6v - 4.396 \times MATS5e - 4.375 \times MATS6e + 10.359 \times GATS6v - 5.118 \times GATS7v + 15.274$

	$N_{\text{training}} = 63$ $R^2 = 0.736$ $S = 0.312$ $p < 10^{-5}$ $R^2_{\text{CV}} = 0.559$ $S_{\text{CV}} = 0.403$ $N_{\text{test}} = 10$ $R^2_{\text{EP}} = 0.664$ $S_{\text{EP}} = 0.282$
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. $R2_{\text{EP}}$ 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