Target Name	MMP-2
Target TTD ID	TTDC00104

Target Species	Human
Chemical Type	N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives
Mode of Action	Inhibitor
QSAR Model 1	MLR-MMP-2: $\log(10^6/\mathrm{IC}_{50}) = -0.042 \times \mathrm{ATS2v} - 110.925 \times \mathrm{MATS4m} - 55.421 \times \mathrm{MATS8m} - 8.431 \times \mathrm{MATS3v} + 2.379 \times \mathrm{GATS6e} + 5.227 \times \mathrm{GATS2p} + 162.799$ $N = 32; \quad R^2 = 0.808; \quad S = 0.420; \quad p < 10^{-5}$ $Q^2_{\mathrm{LOO}} = 0.721 \quad S_{\mathrm{CV\,LOO}} = 0.454 \quad Q^2_{\mathrm{L3O}} = 0.697 \quad S_{\mathrm{CV\,L3O}} = 0.479$
QSAR Model 2	MLR-MMP-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

Target Species	Human
Chemical Type	5-amino-2-mercapto-1,3,4-thiadiazoles
Mode of Action	Inhibitor
QSAR Model 1	*MMP-2* $\log(1/K_i) = [2.92822(\pm 0.860004)] + {}^3K_\alpha[0.255415(\pm 0.122169)] + \text{a\_nF}[0.110207(\pm 0.0556175)] + I[0.357692(\pm 0.191531)]$ $N = 27,\ r = 0.893,\ r^2 = 0.797,\ \text{SEE} = 0.152,\ F = 30.175(F_{3,23} = 4.765),$ $\text{chance} =< 0.001,\ q^2 = 0.682,\ S_{\text{PRESS}} = 0.189,\ S_{\text{DEP}} = 0.175.$
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); ${}^{1}K$: first kappa shape index; ${}^{2}K$: second kappa shape index; ${}^{3}K$: third kappa shape index; ${}^{1}K_{\alpha}$: first alpha modified shape index; ${}^{2}K_{\alpha}$: second alpha modified shape index; ${}^{3}K_{\alpha}$: 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	$\log(1/K_i) = 0.853(\pm0.309)S_S - 2.331(\pm0.598)S_N - 0.683(\pm0.325)I + 15.530(\pm3.227)$ $n = 24,\ r = 0.952,\ r_{cv}^2 = 0.87,\ R_A^2 = 0.89,\ s = 0.09,\ F_{3,20} = 64.35(4.94)$
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	Aryl sulfonyl ureido derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/K_i) = 0.853(\pm0.309)S_S - 2.331(\pm0.598)S_N - 0.683(\pm0.325)I + 15.530(\pm3.227)$ $n = 24,\ r = 0.952,\ r_{cv}^2 = 0.87,\ R_A^2 = 0.89,\ s = 0.09,\ F_{3,20} = 64.35(4.94)$
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