Target Name	MMP-8
Target TTD ID	TTDR01266

Target Species	Human
Chemical Type	5-amino-2-mercapto-1,3,4-thiadiazoles
Mode of Action	Inhibitor
QSAR Model 1	*MMP-8* $\log(1/K_i) = [2.96998(\pm 0.987275)] + I[0.413534(\pm 0.245314)] + \text{a\_nF}[0.272465(\pm 0.063659)] + {}^3K_x[0.242856(\pm 0.140256)]$ $N = 25,\ r = 0.916,\ r^2 = 0.840,\ \text{SEE} = 0.170,\ \ F = 36.846(F_{3,21} = 4.874),$ $\text{chance} =< 0.001, q^2 = 0.773,\ S_{\text{PRESS}} = 0.203,\ S_{\text{DEP}} = 0.186.$
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	$\log(1/K_i) = 0.977(\pm0.377)S_S - 3.579(\pm0.552)S_N + 19.495\ (\pm3.296)$ $n = 24,\ r = 0.957,\ r_{cv}^{2} = 0.90,\ R_A^{2} = 0.91,\ s = 0.21,\ F_{2,21} = 113.03(5.78)$
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	$\log(1/K_i) = 0.977(\pm 0.377)S_S - 3.579(\pm 0.552)S_N + 19.495\ (\pm 3.296)$ $n = 24,\ r = 0.957,\ r_{cv}^2 = 0.90,\ R_A^2 = 0.91,\ s = 0.21,\ F_{2,21} = 113.03(5.78)$
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