Target Name	PDGFR
Target TTD ID	TTDS00261

Target Species	Human
Chemical Type	Pyrido[2,3-d]pyrimidine derivatives
Mode of Action	Inhibitor
QSAR Model 1	2DA-PDGFR-TK: $\log(10^6/IC_{50}) = -24.042 \times MATS1m - 3.213 \times MATS8v - 9.196 \times MATS6e + 25.481$ $N = 18, \quad R_2 = 0.716, \quad S = 0.634, \quad p < 10^{-5} \quad Q^2 = 0.598, \quad S_{CV} = 0.672$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Three 2D autocorrelation MLR models are reported in this work. In total, nine descriptors from the whole 2D autocorrelation pool were employed. N is the number of compounds included in the training set, R^2 is the square of correlation coefficients, S is the standard deviation of the regression, p is the significance of the variables in the model, and Q^2 and S_{CV} are the correlation coefficients and standard deviations of the leave-one-out (LOO) cross validation. Three spatial autocorrelation vectors were employed for modeling the inhibitory activities: Broto-Moreau's autocorrelation coefficients (ATS), Moran's indices (MATS), and Geary's coefficients (GATS). $$ATS(p_k, l) = \sum_i \delta_{ij} p_{ki} p_{kj}$$ $$MATS(p_k, l) = \frac{N}{2L} \frac{\sum_{ij} \delta_{ij} (p_{ki} - \bar{p}_k)(p_{kj} - \bar{p}_k)}{\sum_i (p_{ki} - \bar{p}_k)}$$

	$$\mathrm{GATS}(p_k, l) = \frac{(N-1)}{4L} \frac{\sum_{ij} \delta_{ij}(p_{ki} - \bar{p}_k)(p_{kj} - \bar{p}_k)}{\sum_i (p_{ki} - \bar{p}_k)}$$ where ATS(pk, l), MATS(pk, l), and GATS(pk, l) are Broto-Moreau's autocorrelation coefficient, Moran's index, and Geary's coefficient at spatial lag l, respectively; pki and pkj are the values of property k of atoms, i and j, respectively; _pk is the average value of property k, L is the number of nonzero values in the sum, N is the number of atoms in the molecule, and d (l,dij) is a Dirac-delta function defined as $$\delta(l, d_{ij}) = \left\{ \begin{array}{lll} 1 & \text{if} & d_{ij} = l \\ 0 & \text{if} & d_{ij} \neq l \end{array} \right\}$$ where dij is the topological distance or spatial lag between atoms i and j. Spatial autocorrelation measures the level of interdependence between properties, and the nature and strength of that interdependence. In a molecule, Moran's and Geary's spatial autocorrelation analysis tests whether the value of an atomic property at one atom in the molecular structure is independent of the values of the property at neighboring atoms. If dependence exists, the property is said to exhibit spatial autocorrelation. The autocorrelation vectors represent the degree of similarity between molecules.
Reference	2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinases' inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. *Bioorganic & Medicinal Chemistry* 16 (2008) 810–821

Target Species	Human
Chemical Type	1-phenylbenzimidazoles
Mode of Action	Inhibitors
QSAR Model 1	$\mathrm{Log}(1/\mathrm{IC}_{50}) = 7.0050 - 1.3877 \cdot {}^{3}\chi_c^f - 11.3749/{}^{1}\chi^f + \exp(0.4970 \cdot B_5 - 1.98 \cdot B_{2,2',4,7})$ $n = 55 \quad s = 0.363 \quad F = 43.03 \quad r^2 = 0.78$
Molecular	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**

Descriptor	${}^{m}\chi_k$: *m*th-order connectivity index; ${}^{m}\chi_k^v$: the valence connectivity index; ${}^{3}\chi_c^f$: third-order variable cluster connectivity index; ${}^{1}\chi^f$: first-order variable connectivity index; B_5 is a position index, which is assigned the value of 1 when a substituting group is present at 5-position, and a value of 0 is assigned otherwise. $B_{2,2',4,7}$: another position index, which is assigned to 1 if a substituting group presents at the 2-, 2'-, 4-, or 7-position, and a value of 0 otherwise.
Reference	A QSAR study on inhibitory activities of 1-phenylbenzimidazoles against the platelet-derived growth factor receptor. *Bioorganic & Medicinal Chemistry* 12 (2004) 4009–4015