Target Name	c-Src
Target TTD ID	TTDS00247

Target Species	Human
Chemical Type	Pyrido[2,3-d]pyrimidine derivatives
Mode of Action	Inhibitor
QSAR Model 1	2DA-c-Src-TK: $\log(10^6/IC_{50}) = 0.160 \times ATS1v + 2.262 \times MATS3v - 7.634 \times GATS1v + 5.328$ $N = 18, \quad R^2 = 0.860, \quad S = 0.654, \quad p < 10^{-5} \quad Q^2 = 0.772, \quad S_{CV} = 0.739$
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 $$\delta(l, d_{ij}) = \begin{Bmatrix} 1 & \text{if} & d_{ij} = l \\ 0 & \text{if} & d_{ij} \neq l \end{Bmatrix}$$ 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	4-Anilino-3-quinolinecarbonitriles
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/\mathrm{IC}_{50}) = -102.947(\pm 23.388) + 1.784(\pm 0.974)\mathrm{DECC} + 0.010(\pm 0.003)\mathrm{T(O...Cl)} + 6.842(\pm 3.183)\mathrm{IDE} + 22.240(\pm 5.283)\mathrm{BEHe4} + 0.012(\pm 0.003)\mathrm{TIC2} - 0.047(\pm 0.011)\mathrm{AEige} + 0.001(\pm 0.0003)\mathrm{Whetv} + 6.428(\pm 2.982)\mathrm{BELv4}$

	$n=64,\ R^2=0.825,\ \mathrm{RMS}=0.350,\ S=0.378$ (training set) $n=16,\ R^2=0.745,\ \mathrm{RMS}=0.398,\ S=0.601$ (test set)
QSAR Model 2	$\log(1/\mathrm{IC}_{50})=24.079(\pm 18.619)+13.174(\pm 4.579)\mathrm{BEHe4}-0.002(\pm 0.0006)\mathrm{QZZm}$ $+10.676(\pm 2.653)\mathrm{BELv4}+1.874(\pm 0.456)\mathrm{DP04}+2.670(\pm 0.970)\mathrm{ICR}$ $+0.743(\pm 0.139)\mathrm{G2}-51.320(\pm 7.073)\mathrm{BELm1}-1.392(\pm 0.196)\mathrm{S2K}$ $n=64,\ R^2=0.835,\ \mathrm{RMS}=0.340,\ S=0.367$ (training set) $n=16,\ R^2=0.788,\ \mathrm{RMS}=0.363,\ S=0.548$ (test set)
QSAR Model 3	$\log(1/\mathrm{IC}_{50})=23.971(\pm 19.270)+13.487(\pm 4.728)\mathrm{BEHe4}-0.001(\pm 0.0005)\mathrm{QYYm}$ $+10.407(\pm 2.751)\mathrm{BELv4}+1.468(\pm 0.427)\mathrm{DP04}+3.481(\pm 1.046)\mathrm{ICR}$ $+0.794(\pm 0.163)\mathrm{G2}-51.128(\pm 7.293)\mathrm{BELm1}-1.578(\pm 0.235)\mathrm{S2K}$ $n=64,\ R^2=0.829,\ \mathrm{RMS}=0.347,\ S=0.374$ (training set) $n=16,\ R^2=0.756,\ \mathrm{RMS}=0.389,\ S=0.588$ (test set)
QSAR Model 4	$\log(1/\mathrm{IC}_{50})=19.745(\pm 4.680)-119.266(\pm 22.561)\mathrm{VEA2}+0.230(\pm 0.035)\ \mathrm{L1s}$ $+0.204(\pm 0.072)\mathrm{G2}+0.017(\pm 0.003)\mathrm{TIC5}-0.108(\pm 0.032)\mathrm{Tm}$ $+3.124(\pm 0.586)\mathrm{DECC}-0.086(\pm 0.022)\mathrm{L1e}-0.038(\pm 0.004)\mathrm{AEige}$ $n=64,\ R^2=0.854,\ \mathrm{RMS}=0.320,\ S=0.345$ (training set) $n=16,\ R^2=0.840,\ \mathrm{RMS}=0.315,\ S=0.476$ (test set)
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Topological descriptors: DECC T(O...Cl): Eccentric sum of topological distances between O...Cl; ICR: Radial centric information index; S2K: 2-Path Kier k-modified shape index; Whetp: Wiener-type index from polarizability weighted distance matrix. Burden eigenvalue descriptors: BELm1: Lowest eigenvalue no. 1 of Burden matrix/weighted by atomic masses; BELv4: Lowest eigenvalue no. 4 of Burden matrix/weighted by atomic van der Waals volumes; BEHe4: Highest eigenvalue no. 4 of Burden matrix/weighted by atomic Sanderson electronegativities. Geometrical descriptor: QZZm G2: Qzz COMMA2 value/weighted by atomic masses Gravitational index G2 (bond-restricted).

	Information indices descriptor: IDE TIC2 TIC5: Mean information content on the distance equality total information content index (neighborhood symmetry of 2-order) total information content index (neighborhood symmetry of 5-order). WHIM descriptors: Tm: T total size index/weighted by atomic masses; L1e L1s: First component size directional WHIM index/weighted by atomic Sanderson electronegativities first component size directional WHIM index/weighted by atomic electrotopological states. Eigenvalue-based indices descriptors: AEige: Absolute eigenvalue sum from electronegativity weighted distance matrix; VEA2 Average eigenvector coefficient sum from adjacency matrix. Randic molecular profiles descriptor: DP04: Molecular profile no. 04. *n* is the number of samples. R^2, RMS, and S represent explained variance, RMS error, and standard error for regressions, respectively
Reference	Enhanced Replacement Method-based Quantitative Structure – Activity Relationship Modeling and Support Vector Machine Classification of 4-Anilino-3-quinolinecarbonitriles as Src Kinase Inhibitors. *QSAR Comb. Sci.* 28, 2009, No. 3, 312 – 324