

Target Name	VEGF receptor II
Target TTD ID	TTDS00008

Target Species	Human
Chemical Type	N- (Aryl)-4-(Azolylethyl) Thiazole-5-Carboxamides
Mode of Action	Agonist
QSAR Model 1	$BA = [5.35111 (\pm 0.639971)] + I_2 [1.21889 (\pm 0.28205)] + X (\text{Ch})(6) [-4.40829 (\pm 1.95195)] + X_v (\text{PC})(5) [0.399077 (\pm 0.307898)]$ <p> $n=23$, $r=0.905808$, $r^2=0.820487$, $\text{std}=0.229413$, $F=28.9474$ ($F_{(3,19)} = 4.94$) $Q^2=0.753$, $S_{\text{PRESS}}=0.268718$, $S_{\text{DEP}}=0.244236$ </p>
QSAR Model 2	$BA = [7.16667 (\pm 0.251731)] + I_1 [-1.18213 (\pm 0.242998)] + DL [-0.102785 (\pm 0.0607741)]$ <p> $n=13$, $r=0.963524$, $r^2=0.928378$, $\text{std}=0.178149$, $F=64.8112$ ($F_{(2,10)} = 7.56$), $Q^2= 0.876577$, $S_{\text{PRESS}}= 0.233862$, $S_{\text{DEP}}= 0.20511$ </p>
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>I_1, indicator variable given for the presence of isoxazole nucleus in the structure; $X_v (\text{P})(5)$, fifth order path type valence connectivity indices; n, number of data points; r, correlation coefficient; r^2, squared correlation coefficient; std, standard deviation; F, Fischer ratio between the variances of calculated and observed activities; Q^2, cross validated squared correlation coefficient; S_{PRESS} and S_{DEP}, standard deviation based on predicted residual sum of squares and standard deviation of error of prediction respectively; Topological and physicochemical descriptors were calculated using QSAR software Modeslab electronic descriptors were calculated on the Chem3D software using the "Compute Properties Module"; n is number of data points, r is correlation coefficient, r^2 is squared correlation coefficient, std is standard deviation, F represents Fischer ratio between the variances of calculated and observed activities.</p>
Reference	QSAR study on N- (Aryl)-4-(Azolylethyl) Thiazole-5-Carboxamides: Novel Potent Inhibitors of

