

Target Name	VEGF receptor I
Target TTD ID	TTDS00007

Target Species	Human
Chemical Type	N- (Aryl)-4-(Azolyethyl) Thiazole-5-Carboxamides
Mode of Action	Agonist
Activity Type	VEGFR inhibitory activity
QSAR Model 1	$BA = [9.20894 (\pm 0.694867)] + I_1 [-1.21417 (\pm 0.190454)]$ $+ Xv (P)(5) [-1.49191 (\pm 0.317222)]$ <p> <math>n=16</math>, <math>r=0.968464</math>, <math>r^2=0.937922</math>, <math>std=0.125256</math>, <math>F=98.2067</math>, <math>(F_{(2,13)} = 6.36)</math>,  <math>Q^2= 0.897918</math>, <math>S_{PRESS}= 0.160621</math>, <math>S_{DEP}= 0.144782</math> </p>
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p><math>I_1</math>, indicator variable given for the presence of isoxazole nucleus in the structure; <math>Xv (P)(5)</math>, fifth order path type valence connectivity indices; <math>n</math>, number of data points; <math>r</math>, correlation coefficient; <math>r^2</math>, squared correlation coefficient; <math>std</math>, standard deviation; <math>F</math>, Fischer ratio between the variances of calculated and observed activities; <math>Q^2</math>, cross validated squared correlation coefficient; <math>S_{PRESS}</math> and <math>S_{DEP}</math>, 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"; <math>n</math> is number of data points, <math>r</math> is correlation coefficient, <math>r^2</math> is squared correlation coefficient, <math>std</math> is standard deviation, <math>F</math> represents Fischer ratio between the variances of calculated and observed activities.</p>

<b>Reference</b>	QSAR study on N- (Aryl)-4-(Azolyethyl) Thiazole-5-Carboxamides: Novel Potent Inhibitors of VEGF Receptors I and II. <i>Medicinal Chemistry</i> , 2009, 5, 455-461
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