

Target Name	Glycogen Synthase Kinase-3 $\beta$
Target TTD ID	TTDC00162

Target Species	Human
Chemical Type	Indirubin derivatives
Mode of Action	Inhibitor
Activity Type	No information
QSAR Model 1	$pIC_{50} = - (14.01 \pm 7.773) - (171.6 \pm 13.74)Zefirov's\ PC - (48.89 \pm 0.34)QC1$ $- (75.03 \pm 1.0435)QC2 - (19.85 \pm 0.2934)SaaN + (62.54 \times 10 \pm 13.35 \times 10)QC3$ $n = 36, R^2 = 0.94, R^2_{pred} = 0.6, F = 81.73, s = 0.27$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p>Here, n stands for the total number of compounds in the training set, F signifies the ratio of variance explained by the model and the variance not explained by the model. Larger the value of F means better models, while the values below 1 means that the model is completely useless. Descriptors refer to the minimum partial charge for a N atom (Zefirov=s PC), minimum total bond order (&gt;0.1) of a N atom (QC1), atomic orbital electronic population (QC2), SaaN (E-state index) and Minimum valency of a H atom (QC3).</p>
Reference	QSAR Models for Prediction of Glycogen Synthase Kinase-3 $\beta$ Inhibitory Activity of Indirubin Derivatives. <i>QSAR Comb. Sci.</i> 27, 2008, No. 6, 718 – 728