

Kumar V. Topological models for the prediction of tyrosine kinase inhibitory activity of 4-anilinoquinazolines. *Bull. Pharm. Res.* 2011;1(2):53-9.

Abstract: The relationship of *Wiener's index* - a distance-based topological descriptor, *Zagreb group parameter* - M_1 , an adjacency-based topological descriptor and *eccentric connectivity index* - an adjacency-cum-distance based topological descriptor with the tyrosine kinase inhibitory activity of 4-anilinoquinazolines has been investigated. A training set comprising of 30 analogues of substituted 4-anilinoquinazolines was selected for the present investigations. The values of the *Wiener's index*, *Zagreb group parameter*, *eccentric connectivity index* and each of 30 analogues comprising the data set, were computed. Resultant data was analyzed and suitable models developed after identification of active ranges. Subsequently, a biological activity was assigned to each analogue involved in the data set using these models, which was then compared with the reported tyrosine kinase inhibitory activity. Accuracy of prediction was found to vary from a minimum of ~82% for model based on *Zagreb group parameter* to a maximum of ~87% for model based on *Wiener's index* and *eccentric connectivity index*.

Key words: Wiener's index, Eccentric connectivity index, Zagreb group parameter, 4-Anilinoquinazolines, Tyrosine kinase inhibitory activity.

References: [29](#)

Total Pages: 07

Cited by: [00](#)

*Author to whom correspondence should be addressed:

Dr. Vipin Kumar (vipbhardwaj@rediffmail.com)

Department of Pharmaceutics, Institute of Pharmaceutical Sciences,
Kurukshetra University, Kurukshetra, Haryana, India