

QSAR STUDIES ON THIAZOLES HAVING ANTIPLATELET ACTIVITY

G. A. Kashid^{1*} J. Sarvanan² N. P. Jain¹

¹ Department of Pharmaceutical Chemistry, S N D College of Pharmacy, Babhulgaon, Yeola, Nashik, Maharashtra, India-423401,

² Department of Pharmaceutical Chemistry, P E S College of Pharmacy, Bangalore, Karnataka.

Received 03 April 2015; Revise 12 May 2015; Accepted 15 April 2015

Abstract

Recently thiazole derivatives were identified antiplatelet activity. Using with multiple regression method, partial least square method, principal component regression and kNN-MFA 3D-QSAR models were generated. One of these models was selected on the basis of q^2 and pred_r^2 values. The selected model has shown good internal and external prediction for training set of 16 molecules and test set of 4 molecules with validation q^2 and cross validation (pred_r^2). QSAR analysis of thiazole derivatives has been applied to develop of relationships between physicochemical properties of chemical substances and their antiplatelet activities, to obtain a reliable statistical model for prediction. The best model shown by 3D QSAR study was obtained from Partial least square regression forward method having r^2 value = 0.9665 and for 2D QSAR study was obtained from Multiple regression forward method r^2 value=0.9151 with good predictive ability. The results obtained from QSAR studies could be used in designing better anticancer agents among the congeners in future.

Keywords: Thiazoles, Antiplatelet Activity, 3D & 2D QSAR.