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In Silico Study of FAK Inhibitors Containing Pyrimidine Fragment as Anticancer Agents

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Research Article

In Silico Study of FAK Inhibitors Containing Pyrimidine Fragment as Anticancer Agents

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Abstract

A series of diaminopyrimidine derivatives were collected from various literatures and subjected to *in silico* 3D-QSAR (Quantitative Structure Activity Relationship) study. Particularly, a field-based 3D-QSAR by using steric, H-bond donor and acceptor, electrostatic and hydrophobic fields was performed. Field-based 3D-QSAR models were generated with a data set of 62 diaminopyrimidine derivatives using its inhibitory activity against focal adhesion kinase (FAK) receptor. The data set were comprised of the training set (45 compounds; 72%) and test set (17 compounds; 28%), which were randomly assigned. The relationship of molecular field versus inhibitory activity was established using the partial least square (PLS) method. Assessment of the model for stability and predictability was done by the leave-one-out method. The QSAR model (PLS factor 6) with good predictivity showed R^2 value 0.98, value 0.6321, Q^2 value 0.6151, RMSE value 0.6, SD value 0.1527 based on different fields.

Key words: Anticancer agents, Diaminopyrimidines, FAK inhibitors, Field-based 3D QSAR

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