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Abstract

Molecular Docking, PASS Prediction, Pharmacokinetic and Toxicity Studies of Focal Adhesion Kinase Inhibitors †

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Abstract: Drug discovery relies on computational medicinal chemistry for designing and identifying new drug-like chemicals, predicting properties and pharmacological activities of molecules, and optimizing lead structures. Focal Adhesion Kinase (FAK) is an emerging target for cancer chemotherapy with mounting evidence that FAK activation or elevated expression is associated with cancer progression, invasion, and drug resistance. This work envisages identification and in silico screening of potential FAK inhibitors which could further be evaluated. A total of 862 compounds were screened from the ZINC database and docked on the refined FAK enzyme using Autodock Vina. The best spotted hits were filtered for their drug-likeness using SwissADME. These potential hits were further evaluated for their in silico toxicity using ProTox II software. Promiscuous hits identified by the docking score and applying Lipinski's Rule of Five were ZINC43200601, ZINC95593660, and ZINC95595125. These hits showed high binding scores and passed the colander of in silico pharmacokinetic and toxicity proving these ligands propitious and worthy of further evaluation. For selecting the Activity Spectra for Substances, the PASS program was used to screen the anticancer potential of the compound. The hits displayed an antitumor profile.

Keywords: focal adhesion kinase; PASS; docking; toxicity

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