Abstract

Cyclin Dependent Kinases go about as potential remedial focuses in cancer disease and several efforts are under way to find out more specific, potent and selective CDK inhibitors. In this paper, reported a computational molecular docking approach to screen approved drugs from DrugBank database. Docking and scoring of all compounds was done using Molegro Virtual Docker software, evaluated the binding affinities towards CDK-2, 4, 5 and 9 enzymes 2W9F, 2UZO, 1UNH and 3BLR resulted in variable dock scores. The resultant top 14 hits from a dataset of 1584 approved drugs were found to be more specific towards CDK inhibition. Further, re-scoring of 14 best docked poses followed by a consensus scoring approach retrieved top hits. In this study, tested three different scoring functions such as MolDock score of Molegro software, GOLD score and AutoDock. From the analysis, it was observed that Olmesartan and Telmisartan were reported to have high binding affinities with all CDKs tested.


Identification of Novel CDK Inhibitors by Molecular Docking and Consensus Scoring Approach


Index Terms

Computer Science

Information Sciences

Keywords

Cyclin-dependent kinases, Molecular docking, Consensus scoring, Binding affinity, DrugBank database, Olmesartan, Telmisartan, Protein Data Bank.