Abstract

Cell cycle inhibition is important hallmark of anti cancer research. CDKs are divided into two types based on their Cell cycle controlling and transcriptional control. CDK 9, a transcriptional regulator serves as potential drug target. Only few drugs are under clinical trials phase 1/2/3 of CDK 9 inhibitory potential. 3BLR (pdb id) is used as docking target. Virtual screening is carried out based on the pharmacophore information generated from literature. Docking is carried out using Molegro virtual docker with all the compounds and top ranking compounds are shortlisted. The best compound (ZINC91643349) was identified and further analyzed by Invitro assays.

References

2. Suresh Gudala, Uzma Khan, Niteesh Kanungo, Srinivas Bandaru, Tajamul Hussain, MS Parihar, Anuraj Nayarisseri, Hema Prasad Mundluru. Identification and Pharmacological
Virtual Screening of CDK9 Inhibitors as Potential Anti Cancer Drugs


Virtual Screening of CDK9 Inhibitors as Potential Anti Cancer Drugs


Index Terms

Computer Science  
Applied Sciences

Keywords

CDK9, CDK9 inhibitors, Virtual Screening, Molecular Docking