Abstract

Zika virus is an arbovirus that spreads through mosquito bites, sexual transmission, pregnancy and blood transfusions. The infection can be severe leading to birth defects, Guillen- Barre syndrome or it may be mild showing no symptom at all. The present study, aims at using Computer aided drug design to speed up the process of drug discovery by rapid optimization of lead compounds through virtual screening and predicting bioactivity. Docking studies were conducted to screen compounds against NS5 protein of Zika virus. The pharmacokinetic properties of the lead compounds were analysed using online tools.


4. Issur, M. et al. The flavivirus NS5 protein is a true RNA guanylyl transferase that catalyze a two-step reaction to form the RNA cap structure. RNA 15, 2340–2350 (2009).


17. National Center for Biotechnology Information. PubChem Compound Database;

Index Terms

Computer Science	Biomedical

Keywords

Zika virus, NS5 protein, flavonoids,