

Discovery of small molecules inhibitors against Chikungunya virus reflection

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Abstract

Chikungunya virus (CHIKV) has emerged as a major viral threat, affecting over a million people worldwide per year. It is a vector-borne disease transmitted to the human by Aedes mosquitoes and primarily affects people by causing viral fever, severe joint pain, and other symptoms, like a rash, joint swelling, muscle pain, and in rare cases can be fatal. CHIKV is a deadly virus, with its mutation rate found to be significantly higher as compared to other viruses. To date, there has been no reported FDA approved drug against this virus. Thus, keeping in mind the urgent need to scrutinize potential therapies against CHIKV, the present study identified various plant bioactive compounds that are available at low prices and do not have associated adverse effects. For identification of active potentials molecules the pharmacoinformatics- based perspective was applied against CHIKV structural (E1) and non-structural (nsP2) proteins using molecular docking and scoring. The selected molecules were further studied for pharmacokinetics (PK) and pharmacodynamics (PD) associated parameters such as initial absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles based on in silico study. The results reveal potential lead molecules having high binding energy that can help in the development of commercial drugs with favorable ADMET characteristics.

Biography:

Naushad received a B.Sc. degree in Biotechnology from Meerut University in 2008 and enrolls to Jamia Hamdard for M.Sc. Toxicology in 2009. Further, he received M. Phil degree in Nanobiotechnology from the Jamia Millia Islamia, India. To select ongoing Indo-US project titles "Human Immunity to Chikungunya Virus" as a Junior Research Fellow. Therefore, join the Molecular Virology and Vaccinology Laboratory, Department of Biotechnology, Jamia Hamdard for a Ph.D. degree in 2016. During a short time of spam participate to deliver oral talk in national and international conferences and published approx. 12 research articles including Scientific Reports and JCI Insight. He selected for DST PURSE Fellow, Junior Research Fellow, Silver Jubilee Fellow, HNF (Hamdard National Fellow), Senior Research Fellow, NET, etc.

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