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Computational screening of potent anti-dengue inhibitors against dengue NS2B/NS3 protease

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Globally, the Dengue Virus (DENV) infection has become a major threatening health issue. The World Health Organization (WHO) has reported 390 million people are getting affected with DENV every year. Though there are some anti-viral available in the market to reduce the severity of the disease, Still there is a need of drug to completely block the virus replication and cures the disease. Therefore, it is of utmost urgency to adopt innovative techniques to advance the drug discovery process. In our study, we focused on the identification of inhibitors against DENV NS2B/NS3 protease complex. NS2B/NS3 protease acts as a therapeutic target in computational anti-viral drug discovery. Based on the drug repurposing studies, several anti-viral were listed out from the previous studies. Out of which, Bromocriptine was selected as a reference ligand, pharmacophore-based virtual screening is

performed. The NS2B/NS3 protease was docked with drug compounds of ZINC library. Each compound from the library is virtually screened using Argus lab based on its 3D pharmacophore feature of the existing ligand. Followed by this semi-flexible docking studies were performed to predict the best binding pose along with its binding energy and IC50 value. The potential lead compound is filtered based on the binding energy. Further, the lead compound is optimized using scaffold hopping mechanism. Molecular dynamic simulation studies were performed to reveal the plausible mode of its action against the NS2B/NS3 protease of DENV. It is concluded that knowledge gained through this study would be of the high value towards enhancing the discovery of NS2B/NS3 protease target specific drug molecules with the least cost and time.

Biography

A JainulFathima received her BTech degree in Information Technology from Anna University, Chennai and MTech degree in Computer Science and Engineering from Anna University, Tirunelveli. She has 3 years of teaching experience. She is currently pursuing PhD degree in Kalasalingam Academy of Research and Education, Krishnankoil, India. Her Research area includes Big data analytics, Computational Drug discovery, and Bioinformatics. She is a Life Member of the Indian Society for Technical Education (ISTE).

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