Meetings International WITH US
International Conference on
Bioinformatics & System Biology
Bioinformatics 2019
March 20-21, 2019 | Singapore City, Singapore

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

JAINUL FATHIMA A[1], MURUGABOOPATHI G[2], SELVAM P[3]

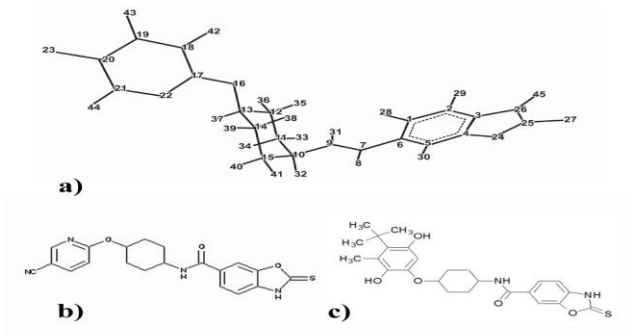
Affiliations:
[1,2] Department of Computer Science and Engineering, Kalasalingam Academy of Research and Education, TN , INDIA
[3] President, Anti-viral Research Society, Kalasalingam Academy of Research and Education, TN, INDIA

Keywords: Dengue NS2B/NS3 protease; De nova simulation ; ADMET; HighThroughputScreening (HTS).

1. Abstract

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 biding 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 valve towards enhancing the discovery of NS2B/NS3 protease target specific drug molecules with the least cost and time.

Image



Reference:

1. A. Jainul Fathima*, G. Murugaboopathi and P. Selvam, "Pharmacophore Mapping of Ligand Based Virtual Screening, Molecular Docking and Molecular Dynamic Simulation Studies for Finding Potent NS2B/NS3 Protease Inhibitors as Potential Anti-dengue Drug Compounds", Current Bioinformatics (2018) 13: 606. https://doi.org/10.2174/1574893613666180118105659
2. Murugaboopathi Gurusamy* and Jainul Fathima, "Lead Optimization Studies Towards Finding NS2B/NS3 Protease Target-specific Inhibitors as Potential Anti-dengue Drug-like Compounds", Current Drug Discovery Technologies (2018) 15: 1. https://doi.org/10.2174/1570163815666180709155131

2. Biography:

A.JainulFathima received her B.Tech. degree in Information Technology from Anna University- Chennai and M.Tech degree in Computer Science and Engineering from Anna University – Tirunelveli . She has 3 years of teaching experience. She is currently pursuing Ph.D. degree in Kalasalingam Academy of Research and Education , Krishnankoil. 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).

3. Presenting author details



Full Name: A. JAINUL FATHIMA
Contact number: +91 - 8072337226
Email-id(s): jainulfathima.a@klu.ac.in
Category: Poster presentation
Passport Number: k8992748