conferenceseries.com

6th International Conference on

Bioinformatics & Systems Biology

August 22-23, 2016   Philadelphia, USA

Dhanvantari : An automated pipeline from genomes to hit molecules

Ruchika Bhat
Indian Institute of Technology Delhi, India

Dhanvantari: An automated pipeline starting from genome sequence leading to small molecules as potential drugs. It is a unique assembly of several independent programs developed by our team at Supercomputing Facility for Bioinformatics and Computational Biology, IIT Delhi. First module i.e ChemGenome, reveals the amino acid sequences, a given genome codes for. These predicted protein sequences are then fed to Bhageerath+which generates tertiary structures, ranked based on ProtSAV+Active Site finder (ASF) utilizes structure information to specify their respective active sites. A rapid screening (RASPD) against a molecular database, selects the best hits (small molecules) against all predicted active sites. Docking (ParDOCK) further refines hits and generates their best binding poses. Further, a short molecular dynamics simulation run on the selected pose brings valuable insights about the *in vivo* drug receptor interactions. Molecules found with stable binding affinity throughout are finally presented as potential drugs which could then be separately investigated *in vitro*. As of 2016, obtaining a drug molecule from just genomic information is a grand challenge. Dhanvantari is thus a vital contribution to the drug discovery community. This software suite aims at speeding up the drug discovery process to save time and resources without compromising on efficacy, apart from automating to make it user friendly. Case studies on HAV and HBV genomes lead to hit molecules through this protocol and their *in vitro* testing is underway at KSBS, IIT Delhi. This suite will be updated and revised regularly to keep up the standards of high level performance.

Biography

Ruchika Bhat is currently pursuing her second year of PhD from the Department of Chemistry at IIT Delhi. She has previously worked as Project Assistant in IIIM Jammu (CSIR Lab) for a tenure of 10 months before joining PhD. Her areas of experties lies in Computional Biology, Computer Aided Drug Designing, Bioinformatics, etc. She has done BE in Biotechnology from University of Mumbai in the year 2010. She has completed her MTech in Bioinformatics from Jamia Hamdard University, New Delhi.

ruchikabhat31@gmail.com

Notes:

J Comput Sci Syst Biol

ISSN: 0974-7230 JCSB, an open access journal

Systems Biology 2016
August 22-23, 2016

Volume 9, Issue 5 (Suppl)

Page 49