CENTER FOR BIOINFORMATICS
PONDICHERRY UNIVERSITY

SEMINAR NOTICE

From Virtual Screening to Real Molecules: Exploiting Protein Structures in Search for Inhibitors of Therapeutically Relevant Drug Targets.

by

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Date and Time: 27-03-2017 (Monday) 10.30 AM
Venue: Seminar Hall, Center for Bioinformatics

ABSTRACT OF THE TALK

Protein structure-based approach for the identification of inhibitors targeted to therapeutically relevant drug targets play an increasingly important role in modern drug discovery process. For the purpose of finding novel inhibitors of selected proteins involved in cancer and infectious disease like tuberculosis, an integrated pharmacophore and structure-based virtual screening of small molecule compound libraries, subsequently followed by Structure Interaction Fingerprints generation to prioritize the virtual screening leads for biological evaluation have been effectively employed. The structural models of the ligands in the protein binding site together with optimizing the bio-molecular interactions facilitate further medicinal chemistry efforts in search and rational design of more potent inhibitors as anti-infective and anti-cancer agents.

Dr. R. Krishna
Seminar coordinator
22/3/17

22/03/2017.
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ALL ARE WELCOME