S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR
Chemical and Biological Sciences

22nd November, 2022 **3.00 PM** **ONLINE / FERMION**

SPEAKER

Prof. Arnab Mukherjee
Professor, Chemistry Department,
Indian Institute of Science Education and Research, Pune

TITLE OF THE TALK

Approaching de-novo drug-design using a combination of physics-based and machine learning algorithms

ABSTRACT

Most biological processes in our body are regulated by proteins in our cells. As a result, they are also part of many biological pathways that are perturbed during an illness. Drugs are small molecules that interfere with these biological processes in an attempt to correct them by interacting with these proteins. Hence, finding small-molecule drugs that have strong interactions with a target active site on a protein is very important. A computational approach to these problems started with screening. Screening has been a standard protocol where a large number of preexisting molecules are compared with the target active site to shortlist a few for further testing. De-novo drug-design is more recent and focuses on constructing completely new molecules with desired properties. We have recently developed one such algorithm capable of constructing molecules one atom at a time in such a way that the molecule's structure is optimized to interact with the protein active site, using a force field-based scoring function to compute the interaction energy with the protein. This method of generation allows our algorithm to circumvent the docking step as the molecule is being generated in its bound state. However, a drawback shared by most atomistic de-novo generation protocols is that the molecules predicted are synthetically challenging. For the case of drugs, we also need these molecules to be ADMET property. We are therefore trying to develop a reinforcement learning method that will produce not only strong binders to a protein receptor, but also have the desired properties (such as ADMET and synthesizability).

HOST FACULTY

Dr. Suman Chakrabarty
ASSOCIATE PROFESSOR, CHEMICAL and BIOLOGICAL SCIENCES
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