Workshop
New Vistas in Drug Discovery
School of Life Sciences, UoH
16th-17th March 2019
Program

Time	Title	Speaker
March 16th 2019, Venue: Seminar Hall, School of Life Sciences		
8.30 - 9.00 am	Registration	
9.30 - 10.00 am	Inauguration	
	Welcome by Prof. H. A. Nagarajaram, Coordinator, BIF Address by Prof. S. Dayananda, Dean, SLS Inaugural address by Prof. Appa Rao Podile, Vice Chancellor, UoH Vote of thanks by Dr. Manjari Kiran, Coordinator, Workshop	
Session I Time: 10:00 – 12:45 pm Chair Person: Dr.Sreedhara Voleti		
10.00 - 10:45 am	**Keynote Lecture:**Drug Repositioning: An Academic and Industrial Perspective	Dr. Sudhir Kulkarni
Tea Break (10:45 - 11:15 am)		
11:15 - 12:00 pm	In Quest of New Anti-microbial agents	Dr. Srinivas Nanduri
12.00 - 12.45 pm	Can Type-II Kinase Inhibitors be Designed?	Dr. Ramesh Sistla
Lunch (12:45 - 2:15 pm)		
Session II Time: 2:15 – 5:00 pm Chair Person: Prof. Anand K. Kondapi		
2:15 - 3:00 pm	Genomes to hit molecules in silico: Promises and Perspectives.	Prof. B. Jayaram
3:00 - 3:45 pm	How are new medicines discovered?	Dr. Uday Saxena
Tea Break (3:45 – 4:15 pm)		
4:15 – 5:00 pm	Fragment-based studies in PTP1B and PI3K-mTOR inhibitors in drug discovery	Dr. Sreedhara Voleti
Closing Remarks by Dr. Vivek, DoSCB		
March 17th 2019, Venue : Center for Modeling Simulation and Design (CMSD) Demo and practice session by M/s Schrödinger		

Dr. Sudhir Kulkarni, Vice President, Novalead Pharma

Title: Drug Repositioning: An Academic and Industrial Perspective

Abstract: Drug repurposing, repositioning and rescue are well accepted terms in Pharma industry which will be discussed along with examples. Advantages as well as challenges in drug repositioning will be discussed. Both computational and experimental methods used in drug repositioning will be presented. Academic and Industrial efforts along with success stories and failures will be presented.

Dr. Srinivas Nanduri, Associate Professor, NIPER, Hyderabad

Title:In Quest of New Anti-microbial agents

Abstract: *Staphylococcus aureus* and *Mycobacterium tuberculosis* are major causative agents responsible for serious nosocomial and community-acquired infections impacting healthcare systems globally. Over several decades, these pathogenshave developed resistance to multiple antibiotics significantly affecting morbidity and mortality. Thus, these recalcitrant pathogensare amongst the most formidable microbial pathogens for which international healthcare agencies have mandated active identification and development of new antibacterial agents for

chemotherapeutic intervention. In our efforts to find new anti-microbial agents, we have investigated several quinazolin-4(3*H*)-one, quinazoline and azole derivatives as potent anti-microbial agents. The results of our exploration will be presented.

Dr. Ramesh Sistla,Senior Lead Investigator, Biocon, Bangalore

Title: Can Type-II Kinase Inhibitors be designed?

Abstract: Kinases are an important therapeutic target class. Till 2019, the Foods and Drugs Administration (FDA) has approved the use of more than thirty kinase inhibitors, mainly in oncology and immunology. Several other kinase inhibitors are in the phase of development and preclinical discovery. The vast and ever growing repository of structural information makes kinases an attractive target class. Several kinases have been structurally characterized to exist in two distinct conformations viz. DFG (Asp-Phe-Gly)-in or DFG-out depending on the orientation of the activation loop. Kinase inhibitors which bind to a DFG-IN conformation are known as type I inhibitors and those that trap the kinase in a DFG-out conformation are known as type II inhibitors. The DFG-out structures of a few kinases have been experimentally solved in complex with the inhibitors. It has also been proposed that “suitable ligands” can induce DFG-out state in kinases that are not otherwise seen in such a conformation.

In this talk, I will share my experience of type I and type II inhibition of kinases and also exemplify a workflow for the modeling of DFG-out conformation of kinases for which an experimental DFG-out structure is not available. The workflow includes various aspects of the protein and inhibitor modeling and molecular dynamics simulations. The talk will present extensive validation of the workflow based on available public domain protein structures. Such models will aid in design of type II inhibitors.

Prof. B. Jayaram, Professor, IIT Delhi

Title: Genomes to hit molecules in silico: Promises and Perspectives

Dr. Uday Saxena, Chief Mentor, Reagene Innovations

Title: How are new medicines discovered?

Abstract: The discovery of new medicines is a long, expensive and risky process. On a average it takes about $500 million USD and about 12-15 years to bring an idea into the market as a new medicine. There are different ways to reduce the timelines, cost and the risk associated with discovery of medicines. My presentation will describe the process of drug discovery and development as well as strategies to accelerate brings medicines to the patient.

Dr. Sreedhara Voleti, CEO, INDRAS Pvt. Ltd, Hyderabad

Title: Fragment-based studies in PTP1B and PI3K-mTOR inhibitors in drug discovery

Abstract: The talk is based on smart utilization of fragments with novel cores towards generating pharmaceutically acceptable Kinase/Phosphatase inhibitors. In PTP1B, a simple fragment is grown organically towards finding leads which could be converted to qualified leads, while in search of inhibitors for PI3K/mTOR dual-targets in oncology, a novel core with suitable crystal fragments appropriately positioned are designed.