

**Workshop on
Protein Structure and Drug Discovery**
August 27 – September 5, 2017

School of Life Sciences, University of Hyderabad,
Prof. CR Rao Road, Hyderabad 500046, INDIA

<http://sls.uohyd.ac.in/gianpsdd>

Time	Title	Speaker
Sunday, August 27		
12:30-14:00	Registration	
14:00- 15:00	Inauguration	
15:00-16:00	Protein structure and fragment-based drug discovery in cancer & tuberculosis	Sir Tom Blundell
16:00- 16:30	Tea Break	
16:30- 17:30	Designing drugs to overcome resistance against HIV-1 reverse transcriptase and <i>Mycobacterium tuberculosis</i> RNA polymerase	Eddy Arnold
17:30- 18:30	Overview of protein crystallography and its application	Shekhar Mande
19:00- 21:00	Buffet Dinner	
Monday, August 28		
Session Chairman: H.A. Nagarajaram / M. Rami Reddy		
9:30-10:30	Principle of protein crystallization and structural determination	Shekhar Mande
10:30-11:00	Tea Brake	
11:30- 12:00	Understanding structural basis of electron transfer process in <i>M. tuberculosis</i>	Shekhar Mande
12:00- 13:00	Exploiting macromolecular structure data	Sameer Velankar
13:00- 14:00	Lunch	
14:00-15:00	Understanding random crystal screening with microseeding - how new strategies can improve productivity	Patrick Shaw Stewart
14:00- 17:30	Hands on: Protein Crystallization	Insaf A. Qureshi / Mohd. Akif
Tuesday, August 29		
Session Chairman: A.K. Kondapi / M. Rami Reddy		
9:30-10:30	Symmetry in protein crystallography	Anthony A.
10:30-11:00	Tea Brake	

11:00- 12:00	Development of specific inhibitors against a malarial enzyme	Anthony A.
12:00- 13:00	Data processing - introduction to imosflm & other softwares	S. Gourinath
13:00- 14:00	Lunch	
14:00- 17:30	Demonstration: Data processing and phase determination	Dileep Vasudevan / Mohd. Akif
Wednesday, August 30		
Session Chairman: S. Rajagopal / M. Rami Reddy		
9:30-10:30	Challenges in Cytoskeletal protein crystallography	S. Gourinath
10:30-11:00	Tea Brake	
11:00- 12:00	Mechanistic insights into the recognition of 5-methylcytosine oxidation derivatives on DNA and histone lysine methyl marks by the reader domains SUVH5 and UHRF1	Rajkumara Eerappa
12:00- 13:00	Crystallographic structure refinement and model building	Dileep Vasudevan
13:00- 14:00	Lunch	
14:00- 17:30	Demonstration: Model building and refinement	Insaf A. Qureshi / Dileep Vasudevan
Thursday, August 31		
Session Chairman: N. Siva Kumar / M. Rami Reddy		
9:30-10:30	A structural bioinformatics approach to understand gene expression in <i>Mycobacterium tuberculosis</i>	B. Gopal
10:30-11:00	Tea Brake	
11:00- 12:00	Insights into protein choreography by solution NMR	Mandar V. Deshmukh
12:00- 13:00	Introduction to cryo-electron microscopy (cryo-EM) in structural biology	Ramanathan Natesh
13:00- 14:00	Lunch	
14:00- 15:00	Visualizing the non-native protein at the chamber of secrets	Ramanathan Natesh
15:00- 17:30	Demonstration: Visualization, validation, analysis of structure	Insaf A. Qureshi / Mohd. Akif
Friday, September 1		
Session Chairman: R.S. Rathore / M. Rami Reddy		
9:30-10:15	Overview of computer aided drug discovery	M. Rami Reddy
10:15-11:00	Understanding biomolecular interactions using quantum mechanical calculations	U. D. Priyakumar

11:00-11:30	Tea Break	
11:30-12:15	Quantum mechanics in pharmaceutical formulation studies	Sudharsan Pandiyan
12:15-13:00	The overview of molecular mechanics	Lalitha Guruprasad
13:00-14:00	Lunch	
14:00-18:30	Hands on: Quantum Mechanics/ Molecular Mechanics	Schrodinger/ M. Rami Reddy
Saturday, September 2		
Session Chairman: A.K. Kondapi / M. Rami Reddy		
9:30-10:15	Protein-protein interaction network analysis and target selection toward drug design	H.A. Nagarajaram
10:15-11:00	Structural and functional insights from protein sequences for drug design	Lalitha Guruprasad
11:00-11:30	Tea Break	
11:30-12:15	Understanding biomolecular processes using molecular dynamics simulations	U.D. Priyakumar
12:15-13:00	Introduction to Solvent Models in Molecular Simulation	N. Prakash Prabhu
13:00-14:00	Lunch	
14:00-15:00	Hands on: Molecular property diagnostic suite	IICT/ Y. Soujanya (Dr. Sastry's group)
15:00- 18:30	Hands on: Homology modeling	Schrodinger/ R. S. Rathore/ M. Rami Reddy
Sunday, September 3		
Session Chairman: H.A. Nagarajaram / M. Rami Reddy		
9:30-10:15	Chemoinformatics in understanding the SAR's in substituted octahydropyrazino-pyridoindoles class of antihistamine H ₁	A.K. Saxena
10:15-11:00	QSAR methods: An overview	A.K. Kondapi
11:00-11:30	Tea Break	
11:30-12:15	Design, synthesis and biological evaluation of GSK-3 β inhibitors	P. Bharatham
12:15-13:00	Quantitating small molecule target engagement using traditional docking and machine learning techniques	Raghunadha Reddy Burri
12:00-13:00	Lunch	
14:00-18:30	Hands on: Docking & Virtual Screening and QSAR	Schrodinger/ R.S. Rathore/ M. Rami Reddy

Monday, September 4**Session Chairman: P. Bharatham / M. Rami Reddy**

9:30-10:15	Integrated Multidisciplinary Methods in Finding Novel C3aR Antagonists	V. Sreedhara
10:15-11:00	Structural analysis of the anti-cancer target human topoisomerase II	P. Bharatham
11:00-11:30	Tea Break	
11:30-12:15	Effect of water-restructuring mutations on ligand binding to human carbonic anhydrase: a theoretical study	Madhavi Sastry
12:15-13:00	CADD methods and their limitations and advantages of QM/MM based FEP method for drug discovery	M. Rami Reddy
13:00-14:00	Lunch	
14:00-18:30	Hands on: FEP	Schrodinger/ M. Rami Reddy

Tuesday, September 5**Session Chairman: V. Sreedhara / M. Rami Reddy**

9:20-10:00	Structural and functional diversity in lipoxygenases: implications in health and disease	P. Reddanna
10:00-10:40	Pharmaceutically acceptable fragment-based design of PTP-1B and P13K subtype/mTOR inhibitors	V. Sreedhara
10:40-11:20	Molecular docking studies: the success should overrule the doubts?	Awantika Shrivastava
11:20-11:40	Tea Break	
11:40-12:20	Structure-based approaches in design and discovery of novel compounds: few case studies	D. Raveendra
12:20-13:00	Use of novel computer aided drug design methods and structural biology in the discovery of clinical candidates for diabetes, cancer & a marketed drug for AIDS	M. Rami Reddy
13:00-14:00	Lunch	
14:00-15:00	Structural proteomics of plant seeds	Dinakar M Salunke
15:00-16:30	Valedictory Function	