

SBCADD-2016
16th - 19th, February, 2016
PROGRAMME SCHEDULE

DAY I - 16th February, 2016

VENUE: L. CT. L. Palaniappa Chettiar Memorial Auditorium

09.00-10.30 am	Registration
10.30-12.00 pm	Inaugural Session
HIGH TEA	
PLENARY SESSION	
Chairperson: Dr. R. Sowdhamini Co-Chairperson: Dr. Sanjeev Kumar Singh	
12.15-01.00 pm	<i>Structure based drug design and exploitation of proteins of innate immune system as protein antibiotics</i> Dr. T. P. Singh All India Institute of Medical Sciences, New Delhi
LUNCH	
Chairperson: Dr. Vikash Kumar Dubey Co-Chairperson: Dr. J. Jeyakanthan	
02.00-02.40 pm	<i>Bridging the islands of protein families in sequence space using artificial sequences</i> Dr. N. Srinivasan Indian Institute of Science, Bangalore
02.40-03.20 pm	<i>Analysis and Prediction of Domain Swapping in Proteins</i> Dr. R. Sowdhamini National Centre for Biological Sciences, Bangalore
03.20-04.00 pm	<i>Insilico studies supporting the antidiabetic and anticancer activities of some medicinally important plant compounds of North East India</i> Dr. D. Velmurugan University of Madras, Chennai
HIGH TEA	
Chairperson: Dr. D. Velmurugan Co-Chairperson: Dr. M. Karthikeyan	
04.10-04.50 pm	<i>Designing novel antituberculosis and antimalarial agents against prioritized drug targets of Mycobacterium tuberculosis and Plasmodium falciparum</i> Dr. Naidu Subbarao Jawaharlal Nehru University, New Delhi
04.50-05.30 pm	<i>Recent development on Leishmania research: Promising drug candidates in pipeline</i> Dr. Vikash Kumar Dubey Indian Institute of Technology Guwahati, Guwahati

DAY II - 17th February, 2016

VENUE: Physics seminar Hall, Science Block

Chairperson: Dr. P. Karthe		Co-Chairperson: Dr. P. Boomi	
09.30-10.10 am	<i>Role of the drug and hormone disposition in pharmacogenetics of anti-epileptic drugs</i>	Dr. Ritushree Kukreti Institute of Genomics & Integrative Biology, New Delhi	
10.10-10.50 am	<i>Structure And Simulation of A Zundel Ion Stabilized By - Hydroxyquinoline-5,7 Disulfonic Acid</i>	Dr. P. Gautam Anna University, Chennai	
10.50-11.30 am	<i>Accelerating "Candidate Gene" Discovery through Genomics and Bioinformatics</i>	Dr. M. Raveendran Tamil Nadu Agricultural University, Coimbatore	
HIGH TEA			
Chairperson: Dr. Sanjeev Kumar Singh		Co-Chairperson: Dr. J. Joseph Sahayarayan	
11.45-12.25 pm	<i>Structural and functional studies on surface proteins of Gram-positive bacteria</i>	Dr. P. Karthe University of Madras, Chennai	
12.25-01.05 pm	<i>New insights into mammalian Target of Rapamycin (mTOR) signaling pathway: Identification and Exploration of new drug like molecules for mTOR domain activation and stabilization.</i>	Dr. A. Dinakara Rao Pondicherry University, Puducherry	
LUNCH & POSTER SESSION			
02.00-02.40 pm	<i>Exploring the role of non-classical hydrogen bonds and its impact on stability and specificity of β-lactamases and Penicillin binding proteins</i>	Dr. A. Anand VIT University, Vellore	

WORKSHOP SESSION

VENUE: Department of Bioinformatics, Science Block

02.40 pm–07.00 pm	<i>Thermodynamic analysis of water and its applications in Drug discovery</i> Presentation
	<i>Recent advances in Computer aided Drug discovery</i> Presentation
	<i>Selection and Refinement of protein and ligands for docking studies</i> Presentation and Hands-on
	HIGH TEA
	<i>Advances in docking methods in addressing the receptor flexibility, polarization and covalent binding</i> <i>Docking and virtual screening on human P2Y12 receptor as antithrombotic drug target</i> Presentation and Hands-on
	<i>Binding site analysis and designing of potential antithrombotic agents against P2Y12 receptor</i> Hands-on
	<i>Practice session on docking studies</i> Hands-on
07.00 pm–10.00 pm	Practice session



DAY III - 18th February, 2016

09.00 am–07.00 pm	Post Docking analysis: Selection of hits from virtual screening results a) Fingerprint calculations, Data clustering b) Analysis of virtual screening results and selection of hits based clustering, pose filter, SIFT c) MM-GBSA and other accurate method of binding free energy calculations Presentation and Hands-on
	HIGH TEA
	Protein –protein docking and analysis of protein-protein interaction interface: Case study of PORCINE PANCREATIC TRYPSIN/ SOYBEAN TRYPSIN INHIBITOR interactions Hands-on
	Watermap: Using Hydration Energetics in a Lead Optimization Case Study of HSP-90 Demo
	LUNCH & POSTER SESSION
	Residue scanning and cys-scanning: Case study of Barnease-Barster Complex and Analysis of results, biologics design Presentation and Hands-on
	HIGH TEA
07.00 pm–10.00 pm	Practice session

DAY IV - 19th February, 2016

09.00 am–04.30 pm	Advances in Ligand-based drug design a) Pharmacophore modeling using Phase b) Phase database design/management & screening Presentation and Hands-on
	HIGH TEA
	Methods and advances in cheminformatics Case study on property calculations and clustering, diversity, classification, and data reduction of Anti-tubercular compounds Presentation and Hands-on
	LUNCH & POSTER SESSION
04.30 pm–05.30 pm	Methods in ADMET modeling. a. Case study on QSPR studies of solubility prediction b. Membrane permeability prediction Presentation and Hands-on
	VALEDICTORY FUNCTION
05.30 pm–10.00 pm	Practice session

