



DEPARTMENT OF BIOINFORMATICS
ALAGAPPA UNIVERSITY
(Reaccredited with 'A' Grade by NAAC)
KARAIKUDI-630 004, TAMIL NADU, INDIA



5th National Symposium cum Workshop on
"Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" (SBCADD'2013)

Program Schedule: 19th - 22nd February, 2013

19th February, 2013

09.00 am - 10.00 am	Registration	
10.00 am - 10.45 am	Inauguration	
10.45 am - 11.00 am	High Tea	
11.00 am - 11.45 am	Plenary Lecture-I	Anti-Cancer Drug Design using Marine Compounds - Dr. D. Velmurugan , University of Madras
11.45 am - 12.30 pm	Plenary Lecture-II	Elucidating Molecular Structure - Dr. K. Sivakumar , Anna University
12.30 pm - 01.15 pm	Plenary Lecture-III	Getting a handhold on designing proteins for human therapeutics - Dr. D. Sundar , Indian Institute of Technology, Delhi
01.15 pm - 02.00 pm	LUNCH & POSTER SESSION	
02.00 pm - 02.45 pm	Plenary Lecture-IV	Protein Structure and Folding - Dr. N. Gautham , University of Madras
02.45 pm - 03.30 pm	Plenary Lecture-V	Design of small molecules as anti-inflammatory agents - Dr. Mukesh Doble , Indian Institute of Technology, Chennai
03.30 pm - 04.15 pm	Plenary Lecture-VI	Rational Structure - Based Drug Discovery - Dr. Punit Kaur , All India Institute of Medical Sciences
04.15 pm - 04.30 pm	TEA	
04.30 pm - 05.15 pm	Plenary Lecture-VII	Molecular Dynamics Simulations of Lipases - Dr. P. Gautham , Anna University
05.15 pm - 06.00 pm	Plenary Lecture-VIII	Importance of protein binding cavity volume and ligand volume in docking and scoring studies - Dr. S. Selvaraj , Bharathidasan University

20th February, 2013 (Plenary Sessions)

10.00 am - 10.45 am	Plenary Lecture-IX	Cyclic peptides and peptidomimetic systems as molecular transporters and drug delivery systems - Dr. Arpita Yadav , C.S.J.M. University
10.45 am - 11.30 am	Plenary Lecture-X	Protein Structure Analysis - Dr. K. Sekar , Indian Institute of Science, Bangalore
11.30 am - 11.45 am	TEA	
11.45 am - 12.30 pm	Plenary Lecture-XI	Structure of collagen adhesin and its interaction with nanoparticle - Dr. P. Karthe , University of Madras
12.30 pm - 01.15 pm	Plenary Lecture-XII	Cation- π interactions in β -lactamases: The role in structural stability - Dr. A. Anand , VIT University, Vellore
01.15 pm - 02.00 pm	LUNCH & POSTER SESSION	
02.00 pm - 02.45 pm	Plenary Lecture-XIII	Applications of Molecular Dynamics Simulation and Molecular Docking to Collagen like Peptides and Identification of Inhibitors for Bromodomain - Dr. V. Subramanian , Central Leather Research Institute
02.45 pm - 03.30 pm	Plenary Lecture-XIV	Evolutionary analysis of the Neuropeptide S Receptor - Dr. N. Manoj , Indian Institute of Technology, Chennai
03.30 pm - 04.15 pm	Plenary Lecture-XV	The Genomic Organization of a Complex Biological System - Dr. Basant K. Tiwary , Pondicherry University
04.15 pm - 04.30 pm	TEA	
04.30 pm - 05.15 pm	Plenary Lecture-XVI	Success stories of computer aided drug design: IRAK4 and ACC - Mr. R. Raghu , Senior Director, Schrodinger
05.15 pm - 06.00 pm	Plenary Lecture-XVII	Structure of the C-terminal domain of transcription factor IIB from <i>Trypanosoma brucei</i> - Dr. B. Syed Ibrahim , Pondicherry University

21st February, 2013

Workshop on Recent Advances in Computational Biology and Computer Aided Drug Design

Mr. R. Raghu, Senior Director, Schrodinger

09:30 am - 10:30 am	Session-I	Importance of crystal structure refinement and ligand optimization in Molecular Modeling <i>Presentation and Hands-on</i>
10.30 am - 11.30 am	Session-II	Recent Developments in Docking Scoring Functions; Designing of Plasmeprin (malarial target) Inhibitors using Docking studies <i>Presentation and Hands-on</i>
11.30 am - 11.45 am	TEA	
11.45 am - 01.00 pm	Session-III	Advances in Homology Modeling of GPCR proteins, Homology modeling of Dopamine D3 structure <i>Presentation and Hands-on</i>
01.15 pm - 02.00 pm	LUNCH	
02.00 pm - 02.45 pm	Session-IV	Methods in Incorporation of Protein Flexibility in Ligand Docking Case Study on determining the Selectivity and Efficacy of Dopamine D3 Receptor Inhibitors Using Induced fit docking <i>Presentation and Hands-on</i>
02.45 pm - 03.45 pm	Session-V:	Recent methods in Antibody-specific homology modeling, case study with a Fab fragment of a monoclonal antibody (IgG) <i>Presentation and Hands-on</i>
03.45 pm - 04.00 pm	TEA	
04.00 pm - 04.45 pm	Session-VI	Recent advances in Protein-Protein Docking and Protein - protein aggregation prediction; Docking of FAB13B5 antibody to HIV-1 Capsid Protein <i>Presentation and Hands-on</i>
04.45 pm - 05.00 pm	REVISION	

22nd February, 2013

Workshop on Recent Advances in Computational Biology and Computer Aided Drug Design

Mr. R. Raghu, Senior Director, Schrodinger

09.00 am - 10.00 am	Session-VII	Recent Advances in in-silico Protein Engineering: Residue-scanning and associated property predictions, Cysteine scanning, Reactive hot spots prediction <i>Presentation and Hands-on</i>
10.00 am - 11.15 am	Session-VIII	Recent advances in Ligand based methods in Drug discovery; Case study on pharmacophore modelling and virtual screening of Anti-cancer compounds <i>Presentation and Hands-on</i>
11.15 am - 11.30 am	TEA	
11.30 am - 12.30 pm	Session-IX	QSAR modelling in Lead optimization Case study with case study with Mycobacterium tuberculosis inhibitors <i>Presentation and Hands-on</i>
12.30 pm - 01.15 pm	<i>Panel Discussion and Revision of the above topics</i>	
01.15 pm - 02.00 pm	LUNCH	
02.00 pm - 02.45 pm	VALEDICTORY FUNCTION	
02.45 pm - 03.15 pm	PRIZE DISTRIBUTION FOR POSTER PRESENTATION	

Sponsored by

Alagappa University, Tamilnadu

Department of Biotechnology (DBT), New Delhi

Department of Science & Technology (DST), New Delhi

