

**Workshop on “Advances in Computer Aided Drug Design”
From August 2nd to August 4th 2010**

**Bioinformatics Infrastructure Facility (DBT-BIF)
and
Centre of Advanced Study in Crystallography and Biophysics
University of Madras, Guindy Campus, Chennai – 600025**

2nd August, 2010

9.00 AM– 10.00 AM	Registration
10.00 AM– 11.30 AM	Inauguration by The Vice Chancellor, University of Madras and Keynote Address: “Drug Design and Modelling” Dr. Mukesh Doble, Professor, IIT-Madras, Chennai
11.30 AM– 12.00 AM	High Tea
12.00 noon – 01.15 PM	“Introduction to Computer Aided Drug Design” Dr. Sami Mukhopadhyay, vLife Science Technology, Pune
1-15 P.M – 2.15 P.M	Lunch Break
2.15 PM – 3.15 PM	“Introduction to Macromolecular Crystallography” Prof. D. Velmurugan, CAS in Crystallography and Biophysics, University of Madras
3.15 PM – 4.00 PM	“DNA Crystallography” Prof. N. Gautham, CAS in Crystallography and Biophysics, University of Madras
4.00 PM – 4.15 PM	Tea Break
4.15 PM – 5.00 PM	“Structure of Hemoglobins” Prof. M.N.Ponnusamy, CAS in Crystallography and Biophysics, University of Madras
5.00 PM – 5.45 PM	“Herbal Drugs and their Structural Activity” Dr.K.Balasubramanian, Secretary&CEO, Ramoni Research Foundation, Chennai

3rd August, 2010

9.30 AM– 10.15 AM	“Structure, Conformation and Function of Carbohydrates” Prof. K. Veluraja, Department of Physics, MSU, Tirunelveli
10.15 AM – 11.00 AM	“Structural Basis for Diversity in SGNH Hydrolases” Dr. N. Manoj, Asst. Professor, Department of Biotechnology, IIT Madras, Chennai
11.00 AM– 11.15 AM	Tea Break
11.15 AM – 12.15 noon	“Virtual Library Generation and Screening” Dr. Sami Mukhopadhyay, vLife Science Technology, Pune
12.15 noon – 1.00 PM	“Introduction to Chemoinformatics and Pharmacophore Modelling” Dr. Sami Mukhopadhyay, vLife Science Technology, Pune
1.00 PM – 2.00 PM	Lunch Break
2.00 PM – 2.45 PM	“Evolution of Virulence Properties from Common Protein Folds in Pathogenic Bacteria” Dr.Rajan Sankaranarayanan, Structural Biology Laboratory, CCMB), Hyderabad
2.45 PM – 3.30 PM	“Structure and Function of Bacterial Surface Proteins” Dr. P. Karthe, CAS in Crystallography and Biophysics, University of Madras
3.30 PM – 4.15 PM	“Proteins from Filarial Parasites” Dr. K. Gunasekaran, CAS in Crystallography and Biophysics, University of Madras
4.15 PM – 4.30 PM	Tea Break
4.30 PM – 5.15 PM	“Molecular Dynamics Simulations” Prof. P. Gautam, Anna University, Chennai

2.00 PM – 5.15 PM

**Hands on Session for 20 participants at BIF
vLife Sciences Technologies, Pune.**

4th August, 2010

9.30 AM – 10.15 AM	<i>“Membrane Protein Crystallography”</i> Dr. S. Krishnaswamy, MKU, Madurai	
10.15 AM – 11.00 AM	<i>“Molecular Dynamics Simulation Studies on Glycan and Glycan-Protein Complexes”</i> Prof. K. Veluraja, Department of Physics, MSU, Tirunelveli	
11.00 AM – 11.15 AM	<i>Tea Break</i>	
11.15 AM – 12.00 noon	<i>“High Throughput Crystallography”</i> Dr. J. Jayakanthan, Department of Bioinformatics, Alagappa University, Karaikudi	
12.00 noon – 12.45 PM	<i>“Applications of Stem Cells in Modern Biology”</i> Dr. H. Devaraj, Department of Biotechnology, University of Madras, Chennai	
1.00 PM – 2.00 PM	<i>Lunch Break</i>	
2 PM – 2.40 PM	Batch I	<i>“Molecular Biology tools for Bioinformatics”</i> by Dr. K. Gunasekaran
	Batch II	<i>“Macromolecular Data Collection”</i> by Dr. P. Karthe
	Batch III	<i>“GNR Contributions”</i> by Prof. N. Gautham
2.40 PM – 3.20 PM	Batch I	<i>“Macromolecular Data Collection”</i> by Dr. P. Karthe
	Batch II	<i>“GNR Contributions”</i> by Prof. N. Gautham
	Batch III	<i>“Molecular Biology tools for Bioinformatics”</i> by Dr. K. Gunasekaran
3.20 PM – 4 PM	Batch I	<i>“GNR Contributions”</i> by Prof. N. Gautham
	Batch II	<i>“Molecular Biology tools for Bioinformatics”</i> by Dr. K. Gunasekaran
	Batch III	<i>“Macromolecular Data Collection”</i> by Dr. P. Karthe
4.00 P.M	<i>“Valedictory Function, Certificate Distribution and High Tea”</i>	

9.00 AM – 4.00 PM

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