

6th Workshop on Bioinformatics and Molecular Modeling in Drug Design

January 21-23, 2016

Venue: Seminar Hall, ACBR, University of Delhi

Programme

DAY 1

21 January, 2016, Thursday

08:45– 09:15 a.m.

Registration

09:15 – 9:30 a.m.

Welcome and Administrative Announcements

9:30 –10:15 a.m.

Madhu Chopra, ACBR

Basics of Bioinformatics and Molecular Modeling

10:15 – 11:00 a.m.

Madhu Chopra, ACBR,

Computational approaches Drug Design and Discovery -I

11:00 – 11:30 a.m.

Tea

11:30 – 12:30 p.m.

Prof. Vani Brahmachari, ACBR

Title Awaited

12:30 – 01:30 p.m.

Madhu Chopra

Computational approaches Drug Design and Discovery -II

01:30 – 02 :00 p.m.

Lunch

02:00 – 03:00 p.m.

Hands on training session by Madhu Chopra

- Building Molecules, Visualization and Analysis
- Energy Minimization and Dynamics

03:00 – 03:15 p.m.

Tea

03:15 – 05:00 p.m.

- Use of the Binding Site tool panel to define a binding site using receptor cavities or known ligands for use in the Receptor-Ligand Interactions protocols

DAY 2

22 January 2016, Friday

09:00 – 10:00 a.m.

Dr. Gitanjali Yadav, NIPGR, New Delhi

Perturbation Analysis of Complex Networks: An Example from the Plant Kingdom

10:00 – 11:00 a.m.

Dr. Vineet Sharma, IISER Bhopal,

A novel approach for the prediction of human gut microbial mediated biotransformation of xenobiotic/drug

11:00 – 11:30 a.m.

TEA

11:30 am – 12:30 p.m.

Dr. Anshu Bhardwaj, OSDD, New Delhi

dPABBs: A Novel in silico Approach for Predicting and Designing Anti-biofilm Peptides

12:30 – 1:30 p.m.

Dr. Dinesh Gupta, ICGB, New Delhi

Big data analysis for cancer diagnostics and prognostics

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| 1:30 p.m. – 2.30 pm | LUNCH |
| 02:30 – 03:30 p.m. | <i>Hands-on-Training session By Dr. Madhu Chopra</i> <ul style="list-style-type: none"> • Docking and scoring |
| 03.30 – 03.45 pm | Tea |
| 3.45 – 5.00 pm | <i>Hands-on-Training session By Dr. Madhu Chopra contd.</i> <ul style="list-style-type: none"> • Conformational Analysis • Pharmacophore Modeling |

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| <u>DAY 3</u> | <u>23 January 2016, Saturday</u> |
| 09:30 – 10:30 a.m. | Prof. P. V. Bharatam, NIPER, Mohali, Punjab <i>Pharmacoinformatics, synthesis and biology in the design of anti-malarial agents.</i> |
| 10:30 – 11:00 a.m. | TEA |
| 11:00 – 12:00 noon | Prof. B. Jayaram, IIT New Delhi <i>Genomes to Hit Molecules In Silico: A country path today, a highway tomorrow</i> - An update |
| 12:00 – 01:00 p.m. | Prof. Indira Ghosh, JNU New Delhi <i>Title Awaited</i> |
| 01:00 – 02:00 p.m. | LUNCH |
| 02:00 – 3:00 p.m. | Prof. Punit Kaur , AIIMS New Delhi <i>The journey from Crystals to Drugs</i> |
| 03:00 – 03:15 p.m. | TEA |
| 03.30 – 4.30 pm | Hands –on- training session continued.... |
| 04:30 – 5.00 pm | <i>Distribution of Certificates and Vote of Thanks</i> |