National Workshop on

Drug Discovery Technology | A Molecular Modeling, Simulations & Dynamics Approach

30th November - 2nd December 2017

Organised by
Department of Pharmacology,
Jawaharlal Institute of Postgraduate Medical Education and Research (JIPMER)

Venue: Department of Pharmacology,
3rd floor, Old Institute block, JIPMER,
Puducherry– 605006

Chief Patron

Dr. DG.Shewade
Professor (Senior scale) of Pharmacology,
Head, Pharmacy JIPMER

Organizing Chairman

Dr. R. Raveendran
Professor (Senior scale) and Head
Department of Pharmacology JIPMER

Organizing Secretary

Dr.R.Kesavan
Assistant Professor
Department of Pharmacology
JIPMER
Pondicherry -605006
jipmerdrugdiscovery@gmail.com

About the workshop

The Department of Pharmacology, JIPMER, Pondicherry in collaboration with BioDiscovery Group, India will conduct 3 day training cum workshop on Drug Discovery Technology entitled Drug Discovery Technology | A Molecular Modeling, Simulations & Dynamics Approach. During these 3 days workshop, hands-on training course will focus on the use of efficient technologies used in Structure based drug design and Molecular Simulations & Dynamics and how the structural data can be used in molecular modeling to design lead molecules based on the structural features of the active site that can lead to design of new molecules which can be drugs and have good target potency.

Practical approach in Molecular Modeling Dynamics & Simulations | Insights of Computational Biophysics will highlight this powerful computational technique and provide hands on practical experience on this technique. After lecture and discussions, participants will learn how to model a biological molecule such as a particular protein, solvate the protein, run minimization, equilibration and protein simulation and analyze the simulations. We invite you to participate in the National workshop on "Drug Discovery Technology | A Molecular Modeling, Simulations & Dynamics Approach". We look forward to meeting you at JIPMER, Puducherry

COURSE CONTENT

- Introduction of Drug Discovery Technology
- Science involved in disease target identification
- Virtual screening
- In-silico generation of ligands
- Conversion of .mol files to .pdb files
- Protein optimization & Energy Minimization
- Molecular Docking
- Creation of Grid Parameter & Dock Parameter files
- Running autogrid & autodock Algorithm
- Selection of inhibitors on the basis of binding energies(delta G) and Lipinski's Rule of 5
- Creating docking complex
- Structure Analysis- Protein & ligand complex
- Prediction of Molecular Properties
- Prediction of Bioactivity
- Drug Likeness
- Bioavailability, ADME & Toxicity
- Introduction to DNA, RNA & Protein
- Different Structures of Proteins
- Introduction to Different DATABASES
- Homology Modelling
- Making a protein structure file.
- Solvating the protein in a water box- parameter generation for the protein or the small molecule
- Adding ions to the solvated protein.
- NAMD configuration file.
- Minimization & equilibration.
- Simulations parameters and running the simulations.
- Analysis of the simulations

Who Should Attend:

The target audience comprises Student & Faculty: Bachelor, Masters, PhD, students as well as Faculty and Professors from Pharmacology, Microbiology, Biochemistry, Biotechnology, Immunology, Pharmacy, Pharmaceutical Chemistry, Biomedical Technology, Genetics, Bioinformatics, Plant Science and Life Sciences.

Professionals: Biotechnology, Bioinformatics and Pharmaceutical scientists from industry, academia and regulatory agencies. Hands-on exercises will be performed individually using software tools (no prior experience required).

Registration fee:

Students*	₹ 4000 /-
Faculty	₹ 6000 /-
Industry delegates	₹ 10000 /-

*Students must attach a bonafide certificate from the Head of the department of their parent institute Scanned copies of filled registration forms must be sent to jipmerdrugdiscovery@gmail.com The last date for sending filled applications- 25th October 2017. The late registrations after 25th October have to pay extra ₹ 1500 to the above fees structure

The interested candidates may register for this workshop through demand draft in the name of "Pharmacology Research Forum" payable at Pondicherry (or) through online bank transfer:

Account Name : Pharmacology Research Forum
Account Number : 98340100002069
Bank :- Bank of Baroda
Branch : JIPMER Extension Counter Pondicherry
IFSC Code : BARB0JIPMER; MICR Code : 605012003

Important points

- Only limited seats are available. The selection of the participants is purely based on " First Come, First Serve (FCFS)" basis.
- On confirmation of your participation, the candidate must bring their own laptop and a mouse to do the hands on training. Candidates who cannot bring a laptop and a mouse need not apply. Attendance for 3 days is prerequisite for getting certificate.
- In the case of cancellation by the participants on or before 30 days of the scheduled date of the workshop, 50% of the fee will be returned. Only 25% of the fee will be returned within 30 days of the scheduled date of the workshop.

Accommodation

1. Participants will have to make their own arrangements for accommodation. A list of hotels in Pondicherry along with the tentative tariff will be provided on request.
2. Subject to the availability of the rooms in JIPMER Guest house, we will try our best to accommodate the participants in the Guest House and they will be charged as per the private tariff of JIPMER. Please send your request at the earliest to the organizing secretary for the assistance: jipmerdrugdiscovery@gmail.com

Registration form

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Name: .....

Qualification:.....

Designation: (Student/ Faculty/ Industry delegate)

Department .....

Institute (Name & address):

.....

.....

.....

Mobile.....

E-mail.....

Demand draft /Bank Transfer Details:

Please send the filled Registration form to

Dr.R.Kesavan
Organizing Secretary
Department of Pharmacology
3rd floor Institute block JIPMER
Pondicherry -605006
jipmerdrugdiscovery@gmail.com
kes7ramasamy@gmail.com
9360532592, 9443958957