REGISTRATION DETAILS

REGISTRATION FEES

For PG, PhD, JRF, SRF & Research Scholars: **3500 INR**

For faculty & Industrial Delegates: **4000 INR**

ACCOUNT DETAILS

Account Name: AIIMS IMPREST HOD PHARMACOLOGY

Account Number: 6189000100050376

Bank Name: Punjab National Bank

IFSC Code: PUNB0618900

ACCOMMODATION

Accommodation will be provided in campus guest house for limited for first 15 peoples on

Rs 600/ day for separate room

Rs 300/day with sharing basis

Contact : 9414153849, 9870659280

REGISTRATION FORM

Last Date for Registration

30 August 2019

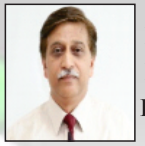
Filled Registration form should be sent to

aiimscadd@gmail.com

WORKSHOP ORGANIZING COMMITTEE

Patron
Prof Ravi Kant
Director, AIIMS, Rishikesh

Co-Patron
Prof Surekha Kishore
Dean, AIIMS, Rishikesh



Organizing Chairperson
Prof Shailendra Handu
Prof & Head, Department of Pharmacology
Dean (Paramedical)

Convener
Dr Puneet Dhamija
Additional Professor, Pharmacology

Organizing Secretary
Mr Rohitash Yadav
Research Scholar

Speakers Cum Resource Persons

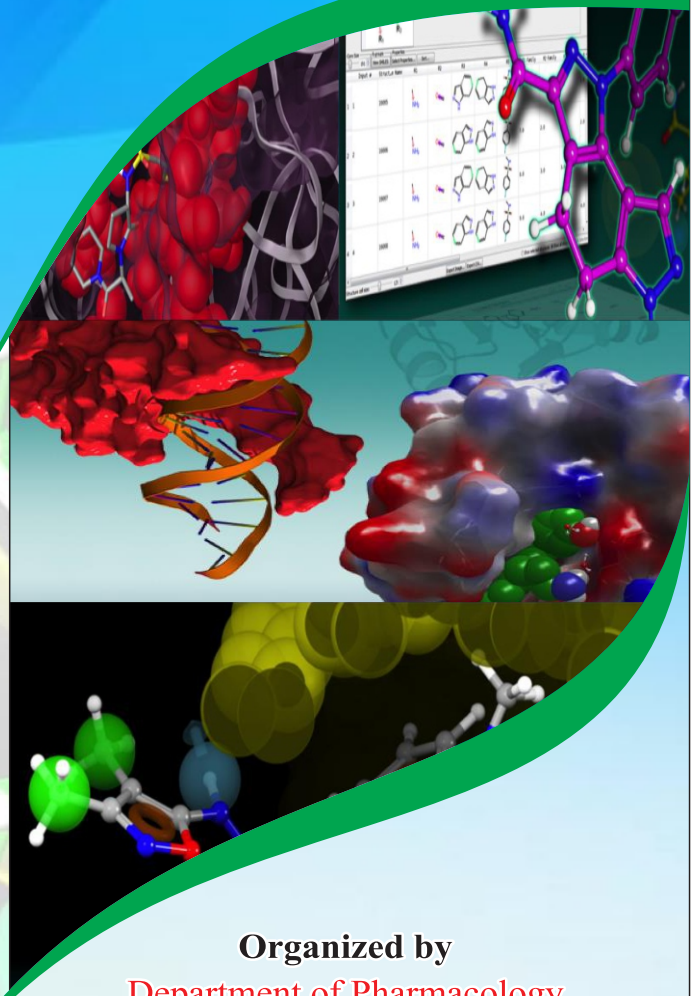
Dr Prajwal Nandekar, PhD, PDF
Scientist, Schrödinger Inc. Bangalore

Dr Vinod Devaraji, PhD
Scientist, Schrödinger Inc.
Bangalore

National Workshop on Advanced Computer Aided Drug Design and Computational Biology

using Schrodinger's Glide software

17th to 19th of September, 2019



Organized by

Department of Pharmacology
All India Institute of Medical Sciences,
Rishikesh (INDIA)

Co-Partner

Schrödinger Inc. Bangalore

Dear All,

Department of Pharmacology, All India Institute of Medical Sciences, Rishikesh is announcing National workshop on "Advanced Computer-Aided Drug Design and Computational Biology" from 17th to 19th September, 2019. In recent years, several computational techniques and bioinformatics softwares have revolutionized the field of drug discovery and development by reducing time and money required for either new drug development/repurposing of existing drugs.

Bioinformatics and Computational Biology have made significant advances that could accelerate translational research comprising of the development and discovery of drugs against combating diseases. The aim of this workshop is to create a friendly environment & train researchers with bioinformatics tools & techniques to keep pace with drug discovery process. We cordially invite you to participate in this 3days Hands-on Workshop cum Training Program.

About the Training Course cum workshop

The training course cum workshop has been designed to provide the theoretical background as well as a hands-on approach to Molecular Docking, Virtual screening, MD Simulation, homology modelling, ADMET and other Computational techniques for Computer Aided Drug Designing Using Most Reliable Software Like Schrodinger's Glide Software.

• Workshop Topics include

- Methods and Advances in computer aided drug design.
- Approaches in Target selection and refinement for docking studies.
- Identidication and evaluation of Binding Pocket / Active site.
- Docking approches in virtual screening and Lead idenitfication.
- Modeling the unknown proteins for docking and virtual screening.
- Pharmacophore modeling and virtual screening of novel compounds.
- Refinement of novel leads using ADME prediction.
- Similiraty and disslimiaraity based methods in lead identification.
- 3D-QSAR Modeling and Lead optimization
- Biologics Design and Protein engineering.

Who can Attend

Academicians, Scientists, Research Scholars, students and industrial delegates can participate.

Note: *Participants need to bring their own laptop.*

Number of Participants

Total 40 seats (On first come, first-served basis)

S/N	Delegates From	No. of Delegate
1.	Indian institutes/Universities (Academic & research Institution)	20
2.	Delegates From AIIMS, Rishikesh	10
3.	Industrial Delegates	10

National Workshop on Advanced Computer Aided Drug Design and Computational Biology

using Schrodinger's Glide software

17th to 19th of September, 2019

Venue: AIIMS Rishikesh.

Workshop Details:

	Time (9:30 AM to 5.00 PM)	Workshop Topics
Day 1: Structure-based drug design and virtual screening		
1	9.30 to 10.15 am	**Computational methods and advances in the discovery of small drug designing:** Advanced methods to improve virtual screening enrichments. Examples of success stories: Clinical candidates designed using modeling methods. *Presentation, Hands-on and Discussion*
	10:15 to 10:30 am	**Tea Break**
2	10:30 am to 1.00 pm	**Maestro GUI –** Introduction and familiarity with interface **Structure Based Virtual Screening of potential inhibitors** a) Examination and selection of the crystal structure from public databases (PDB) b) Refinement and preparation of the crystal structures c) Preparation of the drug like small molecule databases d) Molecular docking – Virtual Screening *Hands-on and Discussion*
	1:00 to 2:00 pm	**Lunch Break**
3	2:00 to 4:15 pm	e) Validation of docking protocol and interactions analysis f) Identifying potential hits based on interaction finger prints (SIFT) g) Binding site properties analysis using SiteMap. h) De-novo molecular design: Library enumeration, Reaction pathway enumeration, Bioisosteric modifications *Hands-on and Discussion*
	3:30 to 3:45 pm	**Tea Break**
4	4:15 to 4.40 pm	Method in achieving the Protein flexibility upon ligand binding (Induced Fit Docking) *Presentation, Hands-on and Discussion*
	4:40 to 5:00 pm	**Practice and Q/A session**

Day 2. Lead Optimization and MD simulation		
5	9:30 to 10.15 am	**Homology modeling of unknown targets: case study with kinase receptor** a) Starting with the selection of sequence, b) Searching the proper homologous template, c) Model building, d) Model refinement and Validation *Presentation, Hands-on and Discussion*
	10.15 to 10.30 am	**Tea Break**
6	10.30 am to 1.00 pm	**Structure Based Lead Optimization** a) Identifying the potential and druggable hits based on binding affinity (MM-GBSA) b) Optimization of the Potential Virtual Screening Hits for binding affinity and potency using Lead optimization tool c) Calculation of physiochemical properties and ADMET profiling *Hands-on and Discussion*
	1:00 to 2:00 pm	**Lunch Break**
7	2.00 to 3:30 pm	**Ligand Based Lead Optimization** a) Pharmacophore modeling using Phase b) Database screening for identifying potential HITS. c) Energetically optimized structure-based pharmacophore modelling d) QSAR methods (3D QSAR) in Lead optimization. *Hands-on and Discussion*
	3.30 to 3.45 pm	**Tea Break**
8	3.45 to 4.45 pm	**Molecular dynamics simulations** a) Introduction to Molecular dynamics simulations b) Setting-up of protein-ligand complex for MD simulation using Desmond c) MD simulation advanced analysis using Simulation interaction diagram *Hands-on and Discussion*
	4.45 to 5.00 pm	**Practice and Q/A session**

Day 3. Biologics Modeling		
	9.30 to 10.00 am	**Computational approaches in designing of biologics and bio-enhancers** *Presentation*
9	10.00 to 10.30 am	**Identifying the hotspots at protein-protein interfaces using protein-protein docking** a) Protein-protein docking and building b) Understanding protein-protein interface and identifying the hotspots *Presentation, Hands-on and Discussion*
	10.30 to 10.45 am	**Tea Break**
10	10:45 am to 12:00 noon	**Computational protein engineering for enhancing the binding affinity and properties** a) Residue scanning and affinity maturation to identify suitable amino-acids for higher affinity b) Cysteine scanning for increasing the stability of the biologics c) Prediction of the post-translation sites in biologics d) Protein-aggregation predictions *Presentation, Hands-on and Discussion*
	12:00 noon to 12:30 pm	**Question & Answers** **Distribution of certificates**