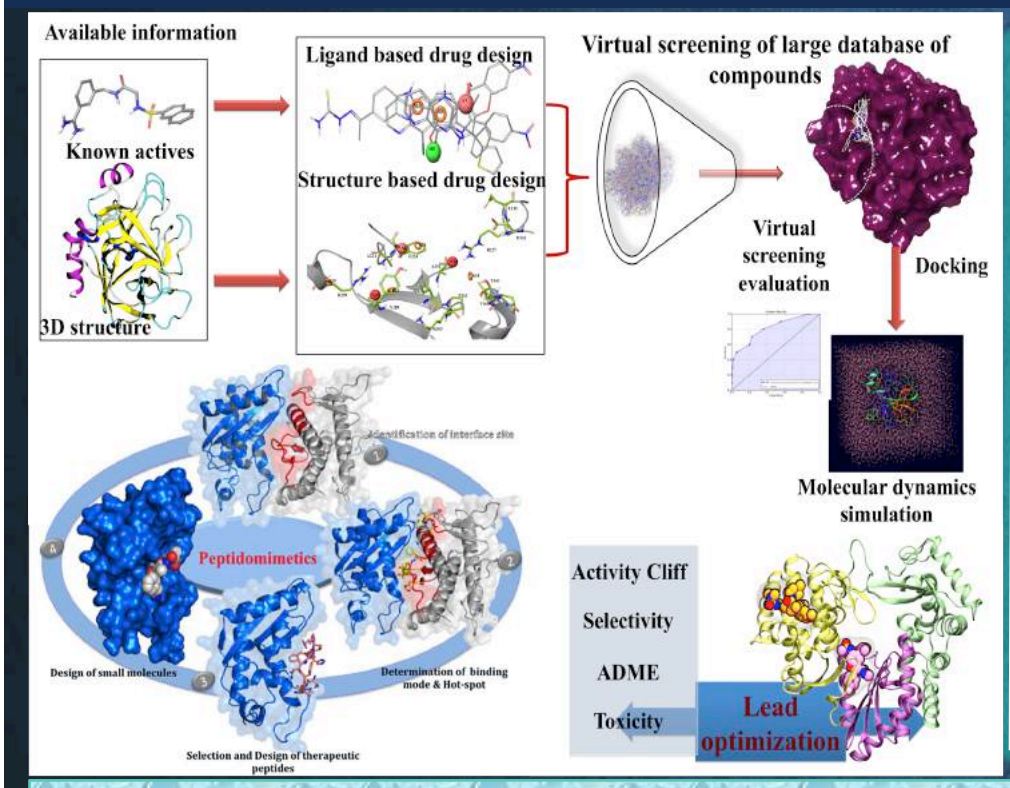
thsti ट्रांसलेशनल स्वास्थ्य विज्ञान एवं प्रौद्योगिकी संस्थान
TRANSLATIONAL HEALTH SCIENCE AND TECHNOLOGY INSTITUTE

SCHRÖDINGER

Practical Courses on

Computational methods in drug discovery



COURSE HIGHLIGHTS

- ❖Structure-based drug discovery
  - ➢Binding site identification
  - ➢Molecular docking
- ❖Biologics
  - ➢Molecular modelling
  - ➢Protein-Protein docking
  - ➢Pharmacophore modelling and Virtual screening
  - ➢Molecular dynamics simulation
- ❖Ligand-based drug discovery
  - ➢QSAR modelling
  - ➢Chemo-informatics
  - ➢Free energy perturbation
- ❖Case studies

01-03 May, 2018 | **THSTI, NCR Biotech Cluster, Faridabad**

Organizer
Jointly organized by THSTI and SCHRODINGER

Registration
Registration deadline :
22nd April, 2018

Student (B.tech, M.tech, M.Sc., M. Pharm and Ph.D.) : 2,000 INR
Postdoc : 3,000 INR
Faculty : 5,000 INR
Industry : 10,000 INR

Invited Speakers
Dr. Rambabu Gundala
Associate Professor
Computational and Medicinal Chemistry, GITAM University
Hyderabad, India

Dr. Sairam Kalapatapu
Deputy General Manager
Computational and Organic Synthesis, Sun Pharma Advance Research Company Ltd., Tandalja, Vadodara, India.

Coordinator/Tutor
Dr. Shailendra Asthana
Dr. Ravi Kumar Muttineni
Mr. Vinod Devaraji

Organizing Members
Dr. Charu Suri
Mitul Srivastava
Mrityunjay Singh
Lovika Mittal
Anita Kumari

Contact
cmdd2018@gmail.com
Phone
+91-9911914205
+91-9999411243

Computational Methods in Drug Discovery
1st- 3rd May, 2018
Last Date for Registration: 22nd April, 2018

Overview

Drug discovery and development is an interdisciplinary, expensive and time-consuming process. Understanding the interactions between proteins and ligands is crucial for the pharmaceutical industries. The experimental structures of these protein/ligand complexes are usually obtained, under highly expert control, by time-consuming techniques such as X-ray crystallography or NMR. These techniques are therefore not suitable for routinely screening the possible interaction between one receptor and thousands of ligands. Scientific advancements during the past two decades have changed the way pharmaceutical research generate novel bioactive molecules. Advances in computational techniques and in parallel hardware support have enabled *in silico* methods are becoming inevitable tools for the discovery of small molecule drugs in various stages of drug discovery including new target selection, identification of hits optimizing affinity, reducing off-target effects and improving pharmacokinetic properties.

This workshop provides the theoretical and hands-on experience on the application of various computational methods and techniques including basic and advanced methods in structure and ligand based drug design including. The workshop will focus on (a) the fundamentals of the algorithms of the docking program (with particular emphasis on their strengths and limitations); (b) normal and advance docking methods to achieve precise outcomes (c) how the results from different docking algorithms compare (d) reverse docking to find unknown targets of natural products and existing old drugs and (e) the future perspectives and challenges for docking techniques and the role of molecular dynamics simulation in all atom wise and via biased methods.

COURSE DETAILS:

Time	Workshop Topics
1st Day: SBDD	
8:00 to 9:00 AM	**Breakfast and Registration**
9:00 to 9:15 AM	**Welcome Note**
9:15 to 9:45 AM	**Talk by Invited Speaker**
9:45 to 10:45 AM	**Computational methods and advances in the discovery of small drug design-Success stories:** Advanced methods to improve virtual screening enrichment. Success stories: Clinical candidates designed using modeling methods. *Presentation*
10:45 to 11:00 AM	**Tea Break**
11:00 to 12:00 PM	**Selection and refinement of crystal structure of target for SBDD; Preparation of ligands for SBDD:** Selection of PDB structures (target structures) and explanation about the pitfalls in structures and how to refine the structures for SBDD. *Hands-on*
12:00 to 12:45 PM	**Binding site analysis and its importance in Structure based lead identification and optimization:** *Hands-on*
12:45 to 1:30 PM	**Lunch Break**
1:30 to 3:00 PM	**Recent Developments in Docking Scoring Functions:** Docking studies of P2Y12 inhibitors Structure Based Virtual screening of novel P2Y12 inhibitors *Presentation and Hands-on*
3:00 to 3:45 PM	**Method in achieving the Protein flexibility upon ligand binding** (INDUCEDFIT): Case study with MK5 receptor *Presentation and Hands-on*
3:45 to 4:00 PM	**Tea Break**
4.00 to 5.15 PM	**Homology modeling of unknown targets: case study with kinase receptor:** Homology modeling of MK5 (mitogen-activated protein kinase [MAPK]-activated protein kinase 5): Starting with the selection of sequence, searching the proper homologues template, model building and refinement. Further validation of final model. Advances in Homology Modeling of GPCRs. *Presentation and Hands-on*
5:45 PM	**Institute Bus Departure**
2nd Day: Biologics	
8:30 to 9:00 AM	**Breakfast**
9:00 to 9:30 AM	**Talk by invited speaker**
9:30 to 10:30 AM	**Protein-Protein Docking** Protein-protein docking and building complex of Trypsin-trypsin inhibitors Understanding protein-protein interface using Schrodinger PPI tool

	Presentation and Hands-on
10:30 to 11:30 AM	**Residue-scanning and associated property predictions** protein aggregation predictions & analysis of results *Hands-on* **Protein Aggregation Analysis** Residue-scanning and associated property predictions, Cysteine scanning, Reactive hot spots prediction and Affinity Maturation in peptide designing and vaccine modeling *Hands-on*
11:30 to 11:45 AM	**Tea Break**
11:45 to 1:30 PM	**Pharmacophore modeling and virtual screening of Anti-cancer compounds:** Case study with AT1 receptor inhibitors: Identification of common pharmacophore, scoring and validation of pharmacophore, virtual screening of database with diverse compounds. *Presentation and Hands-on*
1:30 to 2:30 PM	**Lunch Break**
2:30 to 3:45 PM	**Molecular Dynamics** Analysis of Dynamics results of Arora Kinase, analysis of protein-ligand interactions using SID tool for Arora Kinase *Presentation and Hands-on*
3:45 to 4:00 PM	**Tea Break**
4:00 to 5:15 PM	Accelerated MD approaches *Presentation and Hands-on*
5:45 PM	**Institute Bus Departure**
3rd Day: LBDD	
9:00 to 9:30 AM	**Breakfast**
9:30 to 10:30 AM	**Calculation of physiochemical properties and ADME modeling:** *Presentation and Hands-on*
10:30 to 10:45 AM	**Tea Break**
10:45 to 12:00 PM	**Methods in QSAR modeling** Machine learning methods in ADMET modeling *Presentation and Hands-on*
12:00 to 12:45 PM	**Chemo-informatics methods in Similarity and dissimilarity based virtual screening** *Presentation and Hands-on*
01:00 to 2:00 PM	**Lunch Break**
02:00 to 03:30 PM	**Advances in Free Energy Perturbation (FEP) for prediction of accurate binding affinity** Hands-on session involves the setting the options in FEP/REST for the calculation of relative free energies of congeneric series of Kinase inhibitors and analyzing the generated results and calculating the correlation with biological activity *Demo/Hands-on*
3:30 to 3:45 PM	**Tea Break**
03:45 to 4:30 PM	**Panel Discussion**
4:30 to 5:00 PM	**Concluding Ceremony**
5:45 PM	**Institute Bus Departure**

You should attend if…	You are BTech/MSc/MTech/M.Pharm./PhD, Faculties and scientists from central government funded reputed academic institutions, technical institutions and research institutions. **Number of participants for the course will be limited to twenty five.**
Fees	The participation fees for taking the course is as follows: **Industry/ Pvt. Research Organizations**: Rs. 10,000/- **Academic Institutions**: Rs. 5000/- for faculty Rs. 3000/- for post-docs Rs. 2000/- for B.Tech/M.Tech/M.Sc/M.Pharma/Ph.D. students. The above fee includes all instructional materials, computer tutorials. Breakfast, Lunch, Tea and Snacks will be provided during lecture sessions. **For Registration: Application form is attached below** Registration deadline: **22th April, 2018** Payment deadline: **25th April, 2018** **Interested candidates should fill the application form below and send it to** cmdd2018@gmail.com. **The shortlisted candidates will be notified through mail along with the payment details. Registration and accommodation fee has to be paid after selection.**

Accommodation Fees:

Accommodation can be availed on campus at nominal cost of Rs. 650 per night, on sharing basis. Accommodation has to be booked separately. Payment has to be made along with the registration fee. Accommodation fee is exclusive of Food. We have limited accommodation. It would be provided on first come first serve basis. Preference for accommodation will be given to participants coming from outside Delhi.

Patron:

Prof. Gagandeep Kang

Executive Director, THSTI

Organizer

Dr. Shailendra Asthana, DDRC, THSTI

Organizing Members:

Dr. Charu Suri

Mitul Srivastava

Mrityunjay Singh

Lovika Mittal

Anita Kumari

For any further queries/details:
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Email id: cmdd2018@gmail.com

Application Form

Workshop on "Computational methods in drug discovery"
at THSTI, NCR Biotech Cluster, Faridabad.
1st - 3rd May, 2018

Name		
Gender		
Designation		
Institution		
Address		
Email id		
Contact No.		
Education Details (Please mention subject, Institution and Year)	PhD	
	Masters	
	Bachelors	
Area of Research		
Accommodation Required (Yes/No) and Dates.		
Amount paid for accommodation		

Venue

Translational Health Science and Technology Institute, NCR Biotech Science Cluster, 3rd Milestone, Faridabad – Gurgaon Expressway, Faridabad, Haryana 121001.

Phone: 0129 287 6300

Accommodation

The participants who are willing to make stay will be accommodated in THSTI Guest House at above mentioned address.

Transport

THSTI is 35 km from Indira Gandhi International Airport-New Delhi, 36 km from New Delhi Railway Station, 7.8 Km from Old Faridabad Railway Station. The venue can be reached by taxi from either the airport or railway station.

Also, it can be reached through the nearest metro station: Sector 28 on Violet line.

Use Ctrl+Click to open the map