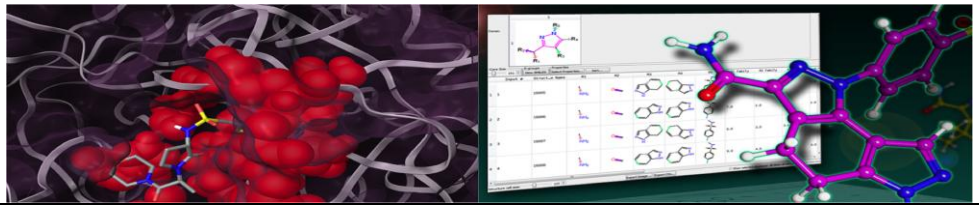
Self-financed Coursework

Advanced Workshop on Molecular Docking, Virtual Screening & Computational Biology

13th - 15th March 2019

Indian Institute of Information Technology- Allahabad
Jhalwa Campus, Devghat, Prayagraj, 211015, India



Level of Participants:
Academicians/Scientists/Research Scholars can participate.

Registration Fee: Rs. 3,000 (INR)-Professional & 2000(INR)-Student

Number of Participants: 30 (*On first-in, first-served basis*)

Deadline: *For the receipt of filled in Registration form is* ***05th March 2019***
(Mail it to: conference.iiita@gmail.com)

Phone: +91-9236666060 / +91-9582675181/ +91-8639243015

About the Training Course:
The training course for the workshop has been designed to provide the theoretical background as well as a hands-on approach to Molecular Docking and Virtual screening. The workshop will also cover the use of different software and will focus on Cheminformatics methods for lead identification and optimization.

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
- Water thermodinamics in lead optimisation
- Biologics Design and Protein engineering

"Advanced Workshop on Molecular Docking, Virtual Screening & Computational Biology"

	Time (9:30 AM to 5.00 PM)	Workshop Topics
Day 1: Lead Identification – Virtual screening and Fragment Based Drug Design		
1	9.30 am 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*
	10:15am to 10:30 am	**Tea Break**
2	10:30 am to 1.00 pm	**Structure Based Virtual Screening of potential inhibitors** a) Examination and selection of the crystal structure from public databases(PLDB) **b)** Refinement of the crystal structures **c)** Preparation of the drug like small molecule databases **d)** Refinement of binding pocket with ligand induced protein flexibility (Induced Fit Docking) **e)** Validation of docking protocol - Enrichment Calculations **f)** Consensus Molecular docking – Virtual Screening **g)** Identifying the potential and druggable hits based on binding affinity (MM-GBSA), interaction figure prints – SIFT and ADMET models *Presentation, Hands-on and Discussion*
	1:00 pm to 2:00 pm	**Lunch Break**
3	3.45 pm to 5.00 pm	**Fragment Based Drug Design** a) Identifying the potential fragments in the binding site using structure based pharmacophore b) Joining the fragments and generating the novel compounds c) Validation for ADMET Models *Presentation, Hands-on and Discussion*

Day 2. Lead Optimization		
4	9.30 am to 10.15 am	**Presentation on Molecular Modeling studies and success stories** *Presentation*
	10.15 am to 10.30 am	**Tea Break**
5	10.30 am to 1.00 pm	**Structure Based Lead Optimization** a) Binding site analysis and optimization of the Potential Virtual Screening Hits b) Selection of suitable fragments on Scaffold using Protein Ligand Database (PLDB) c) Modification of the lead compounds for potency and selectivity using hydration energetics for Lead optimization –using WaterMap Analysis *Presentation, Hands-on and Discussion*
	1:00 pm to 2:00 pm	**Lunch Break**
6	2.00 pm to 5.00 pm	**Ligand Based Lead Optimization** a) QSAR methods (2Dand 3D QSARs) in Lead optimization b) QSPR methods for druggable property optimization *Presentation, Hands-on and Discussion*

Day 3. Biopharmaceuticals (Biologics) Modeling		
7	9.30 am to 10.15 am	**Computational approaches in designing of biologics and bio-enhancers** *Presentation*
	10.15 am to 10.30 am	**Tea Break**
8	10:30am to 12.00 pm	**Homology modeling of unknown targets: case study with kinase receptor and antibody:** a) Starting with the selection of sequence, searching the proper homologus template, model building, refinement and Validation b) Advances in Homology Modeling/Antibody modeling and Loop prediction of GPCRs/Antibodies. *Presentation, Hands-on and Discussion*
9	12.00 pm to 1.00 pm	**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*
	1:00 pm to 2:00 pm	**Lunch Break**
10	2.00 pm to 3.30 pm	**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*
	3.30 pm to 3.45pm	**Tea Break**
11	3.45pm to 5.00pm	**Question & Answers**

Registration Form

Advanced Workshop on Molecular Docking, Virtual Screening & Computational Biology

Name(Dr./Prof./Mr./Mrs./Ms.) .....
Designation: .....

(Faculty /Industry /Student /Researcher /Scientist)
Department/Unit.....

Institution/Organization.....

Mailing Address.....

City..... State/Prov..... Postal Code.....
Mobile..... Email.....

Registration Fees (INR) (Tick the appropriate ✓)

Student, Scholar : Rs. 2000	**Industry, Researcher, Faculty, Scientist : 3000**

**To avail the student registration, please furnish the certificate proof signed by Head of the Institution.*

Method of Payment (#)

Demand Draft No/ Bank Transfer Reference: ..... UTR Number.....
Amount:..... (In words).....
Bank Name:.....
Date:.....

Name: Signature:
Date:

Bank Transfer details

Name of the Bank	:	State Bank of India
Bank Account Name	:	Indian Institute of Information Technology Jhalwa Allahabad
Bank Account Number	:	30996838478
Branch Code	:	10891
MICR Code	:	211002057
IFS Code	:	SBIN0010891
SWIFT Code	:	SBININBB00828

(#)The Demand Draft along with Signed registration form need to be submitted on Registration Desk

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Scanned copy of filled in signed form should be sent to conference.iiita@gmail.com on or before 05th March 2019