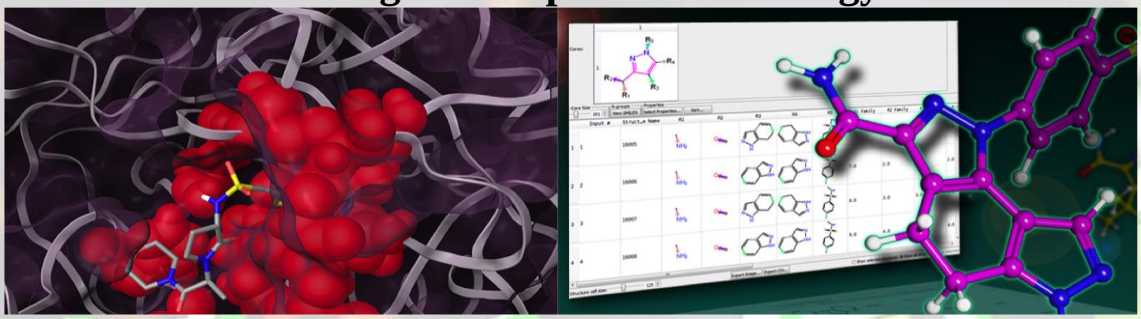
"Advanced Workshop on Molecular Docking, Virtual Screening & Computational Biology"



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 softwares and will focus on Chem-informatics 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

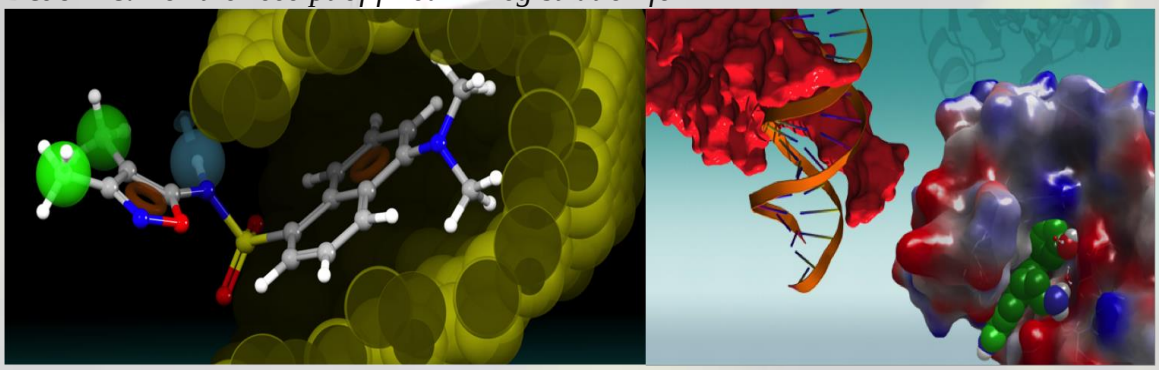
Level of Participants:

Academicians/Scientists/Research Scholars can participate.

Registration Fee: Rs. 1500

Number of Participants: 40

Deadline: *For the receipt of filled in Registration form*



Three Day Workshop on

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

Date: 15-17 November, 2017
Venue: Central University of Punjab, Bathinda

Workshop Details:

	Time (9:00 AM to 5.00 PM)	Workshop Topics
Day 1: Lead Identification – Virtual screening and Fragment Based Drug Design		
1	9:00 am to 9:30 am	**Inauguration and welcome address**
2	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**
	10:15 to 10:30	**Tea Break**
3	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**
4	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		
5	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**
6	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**
7	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		
8	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**
9	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**
10	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**
11	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 e) *Presentation, Hands-on and Discussion* **Question & Answers**
	3.30 pm to 3.45pm	**Closing ceremony**