

**Workshop**  
**On**  
**“Recent advances in Computational biology and Structural Based Drug Designing”**

Presenters:

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	<b>Time (9:30 AM to 5.00PM)</b>	<b>Seminar Topics</b>
<b>Day 1: Computational Biology</b>		
1	9:30 to 10:15	Recent advances in Computational Biology techniques
	<b>10:15 to 10:30</b>	<b>Tea Break</b>
2	10:30 to 11:30	<i>In Silico</i> Protein engineering: Residue-scanning and associated property predictions, case study of barnase-barstar protein - Presentation and Demo
3	11.30-12.30	<i>In Silico</i> Protein engineering: Cysteine scanning, Reactive hot spots prediction; case study with Poplar Apoplastocyanin (Plant protein) - Presentation and Demo
4	12:30 to 1:30	Recent methods in Antibody-specific homology modeling, case study with A FAB FRAGMENT OF A MONOCLONAL ANTIBODY (IgG) - Presentation cum demo
	<b>1:30 to 2:30</b>	<b>Lunch Break</b>
5	2:30 to 3:00	How to analyse and rectify the quality of the protein structures, case study of IgG and many proteins – Presentation and demo
6	3:00 to 4:00	Presentation on Recent advances in Protein-Protein Docking; Demo on docking of FAB13B5 antibody to HIV-1 Capsid Protein Case study-2: Protein – DNA Docking
7	4:00 to 4:30	Tea Break
9	4:30 to 5.00	Presentation and demo on Protein –protein aggregation prediction

<b>Day 2: STRUCTURE BASED DRUG DESIGN (SBDD)</b>		
1	9:30 to 10:15	Recent advances in Structure Based Drug Design
	<b>10:15 to 10:30</b>	<b>Tea Break</b>
2	10:30 to 11:00	Importance of Protein preparation in Molecular modeling and Prioritizing ligand protonation states in docking
3	11:00 to 11.30	How binding site analysis can help in Structure guided drug design (Case study with Matrix Metalloproteinase Inhibitors). <i>In silico</i> Prediction of ADME properties of compounds
4	11:30 to 1.00	Presentation and Demo on Glide docking, case study of factor Xa receptor inhibitors
	<b>1:00 to 2:00</b>	<b>Lunch Break</b>
5	2:00 to 3:15	Recent success in Modeling GPCRs - Demo on GPCR Modeling, Case study with Dopamine D3 structure prediction
6	3:15 to 3:45	Importance of prediction of Ligand Induced protein Conformational change in SBDD. Case study on Dopamine D3 inhibitor design
	<b>3:45 to 4:00</b>	<b>Tea Break</b>
7	4.00 to 5.00	Revision/ discussion/ Q & A Session