Sr. No	Lecture Title	Description	Category	Duration	
	Segment 5: Molecular Docking and Docking Complex Evaluation				
1	Molecular Docking of Protein Ligand using MOE	• Introduction to Molecular Operating Environment (MOE) and molecular docking. • Preparation of the receptor for docking. • Searching active site residues in receptor and ligand preparation. • Docking of receptor and ligand molecules and analysis of the docked complex.	Molecular Docking	9:23	
2	Protein-protein Docking using MOE	• Basic description of Molecular Operating Environment (MOE) software and protein-protein docking. • Procedure to dock a ligand protein against a receptor protein (protein-protein docking) using the MOE software. • Defines parameters to select the best docking conformation for a specific drug candidate.	Molecular Docking	11:38	
3	SwissDock	• Introduction to SwissDock server and its purpose. • Procedure to dock a ligand compound against a receptor molecule (Protein-Ligand Docking). • Defines parameters to be selected for docking process. • Creating ligand and receptor files in the required formats.	Molecular Docking	19:16	
4	Docking a Library of Compounds using MOE	• Introduction to Molecular Operating Environment (MOE) software and its uses. • Procedure of docking a library of compounds against a particular protein of interest using MOE software. • Defines parameters to analyse the best docking conformation to indicate the stable addict.	Molecular Docking	19:48	

5	ClusPro Protein-Protein Docking	• Introduction to ClusPro server and its purpose. • Utilization of various features of ClusPro to perform protein-protein doc king. • Describes advanced functionalities offered by ClusPro to select the best docked complex.	Molecular Docking	21:44	
6	patchDock	• Introduction to PatchDock server and its purpose. • Procedure to dock a receptor protein molecule against the ligand protein molecule (Protein-Protein docking) using the PatchDock server. • Analysis of results and the best complexes refined by FireDock server.	Molecular Docking	17:39	
7	MDockPEP protein peptide docking	• Introduction to MDockPEP server and its uses. • Procedure to dock a receptor protein molecule against the ligand peptide molecule (Protein-Peptide docking) using the MDockPeP server. • Description to prepare the receptor file for docking process and analysis of the results.	Molecular Docking		
8	ZDOCK	• Introduction to ZDOCK server and its purpose. • Procedure to dock a receptor protein molecule against the ligand protein molecule (Protein-Protein docking) using the ZDOCK server. • Procedure to dock a protein molecule against its multimers using the M-ZDOCK program and analysis of results.	Molecular Docking	19:35	
9	Structure Based Drug Desinging Using MOE	• Introduction to MOE software and structure based drug designing. • Procedure to design a drug based on knowledge of 3D structure of biological target. • Defines parameters and modifications to make the ligand molecule an effective drug candidate.	Molecular Docking	16:19	
10	Discovery Studio+	• Introduction to Discovery Studio+ software and structure based drug designing. • Procedure to design a drug based on knowledge of 3D structure of biological target. • Defines parameters and modifications to make the ligand molecule an effective drug candidate.	Molecular Docking	12:03	

11	AutoDock	• Introduction to AutoDock software and structure based drug designing. • Procedure to design a drug based on knowledge of 3D structure of biological target. • Defines parameters and modifications to make the ligand molecule an effective drug candidate.	Molecular Docking		
12	PDBsum Docking Complex Evaluation	• Introduction to PDBsum server and its uses. • Procedure to evaluate protein-protein and protein-ligand docking complex using PDBsum server. • Analysis and interpretation of evaluation results.	Docking Complex Evaluation	18:49	
13	PDBepisa Docking Complex Evaluation	• Introduction to PDBePISA server and its purpose. • Evaluation of protein-protein and protein-ligand docked complex through PDBePISA server. • Defines parameters for an optimal docking complex model.	Docking Complex Evaluation	23:27	
14	SwissADME	• Introduction to SwissADME server and its purpose. • Evaluation of pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules or ligands. • Defines parameters for an optimal docking complex model.	Docking Complex Evaluation		