Segment No.	Lecture Title	Description	Category
1	Introduction to UniProt	• Introduction to UniProt, its purpose and uses. • Sub-databases hosted by UniProt database.	UniProt
1	UniProtKB & Protein Analysis	• Introduction to UniProtKB database. • Retrieval and analysis of protein seqeunces and genomic level information of proteins.	UniProt
1	UniProteome & Retreieval of an Entire Proteome	• Introduction to UniProteome • Retrieval of an entire proteome • Proteomics data and data annotation	UniProt
1	UniRef & Retrieve Protein Clusters	• Introduction to UniRef • Describes clusters sets from UniParc and UniProtKB • Sequence space at three resolution (UniRef100, UniRef90, UniRef50).	UniProt
1	UniParc & Find the Non-Redundant Entries	• Introduction to UniParc • Retrieval of non-redundant protein sequences. • Non-redundant protein sequence data and data annotation.	UniProt
1	Peptide Search: Searching for a Particular Peptide on UniProt	• Introduction to Peptide Search tool hosted by UniProt database. • Search methods of retrieving a particular amino acid sequence. • Retrieving regions of particular protein against the entire	UniProt
1	Introduction to Protein Data Bank (PDB)	• Introduction to Protein Data Bank (PDB). • Describes the repository of experimentally structured biomolecules.	PDB
1	Accurately Searching for a Protein Structure on PDB & Protein Analysis	• Describes different search methods to retrieve query protein molecule on PDB. • Defines parameters and filters to specify the searches. • Accurately seatching a protein structure on Protein Data	PDB

1	Browsing PDB According to Annotation	• Retrieval of a protein structure using Biological annotation on PDB. • Describes categories of annotation and their description.	PDB
1	Digging Out Categorized & Specific Protein Structures from PDB Archives	• Retrieval of detailed information for a particular protein structure through Protein Data Bank (PDB). • Accessing the PDB Archive using multiple sorts of parameters.	PDB
1	3D Structure Visualization on PDB	• Visualization and analysis of protein structure using visualization tool hosted by PDB. • Defines parameters to interactively visualize the protein.	PDB
1	Biological Annotation and Protein Features View & Analysis	• Visualization of features of the query protein through Protein Data Bank. • Procedure to look into the visualization and analysis of the protein features.	PDB
1	Protein Symmetry: Understanding the Protein Validation	• Description of protein symmetry page of Protein Data Bank (PDB). • Visualization and analysis of protein of interest.	PDB
1	NCBI BLAST Database Searching	• Describes NCBI BLAST searching to find regions of similarity between biological sequences. • Calculates statistical significance. • Compares nucleotide and protein seqeunces to seqeuence	NCBI
1	UniProt BLAST & Protein Database Searching	• Searching a query against the entire UniProt databse using UniProt BLAST • Detailed analysis of local similarity, functional and evolutionary relationship between different sequences	UniProt
1	Introduction to InterPro	• Protein family classification and analysis using InterPro database. • Proteome analysis of a particular protein. • Protein families domains analysis.	Protein Families Database
1	InterPro - Protein Family Classifcation and Analysis	• Introduction to UniProt BLAST searching tool. • Finds functional and evolutionary relationship between sequences. • Search query sequences against the entire UniProt database.	Protein Families Database

1	Protein & Protein Domain Analysis	• Protein and protein domain analysis through InterPro database. • Protein families domain analysis.	Protein Families Database
1	Pfam: Understanding Protein Families and their Members	• Detailed introduction of a database of curated protein families, Pfam. • Analyze a protein and retrieve significant information related to that protein.	Protein Families Database
1	PROSITE: Understanding and Analyzing Protein Motif and Domain Profiles	• Introduction to protein domain, families and functional sites database , PROSITE. • Analyze various informative sections provided by the documentation page.	Protein Families Database
1	Introduction to Molecular Modeling Database (MMDB)	• Introduction to Molecular Modeling Database (MMDB). • Retrieval and analysis of a particular dataset from MMDB. • Lists the tools provided by MMDB.	NCBI
1	STRING: Protein-Protein Network Database and Analyzing PPI Between Proteins	• Introduction to protein-protein iInteraction database, STRING. • Understading of protein interaction network through analyzing the query protein result and visualization.	PPI Database
2	NEEDLE: Pairwise Global Sequecne Alignment	• Introduction to EMBOSS Needle, a pairwise alignment tool. • Procedure to perform and analyse global alignment and track the optimum seqeunce.	Pairwise Sequence Alignment
2	WATER: Pairwise Local Sequence Alignment	• Introduction to EMBOSS Needle, a pairwise alignment tool. • Procedure to perform and analyse local alignment and how Needleman-Wunsch algorithm works.	Pairwise Sequence Alignment
2	UniProt Align & Alignment of 2 Proteins	• Description of UniProt Align tool hosted by UniProt Database. • Aligning multiple sequences using UniProt Align tool. • Annotation of alignment results.	Pairwise Sequence Alignment
2	Alignment Between Two PDB Sequences & Structures	• Alignment of biomolecular structures and sequeces through a PDB tool; sequence & structure alignment. • Defines parameters to align two query molecules and it's analysis.	Pairwise Sequence & Structure Alignment

2	Clustal Omega: Multiple Sequence Alignment	• Introduction to Clustal Omega, a multiple seqeunce alignment tool. • Procedure to align multiple sequence using Clustal Omega. • Interpretation of the output final alignment.	Multiple Sequence Alignment
2	Aln2Plot: Prediction of Hydrophobocity Between Two Proteins	• Introduction to Aln2Plot tool. • Generates graphical plots of hydrophobicity and side chain volumes for two or more query proteins using the Aln2Plot tool.	Protein Analysis
2	REPPER: Prediction of Gapless Repeats in Protein Sequences	• Introduction to REPPER to analyses regions with short gapless REPeats in protein sequences. • Analysis of output that is complemented by coiled coil prediction (COILS) and optionally by secondary structure	Protein Analysis
2	SignalP: Prediction of Signal Peptide in Proteins	• Introduction of SignalP tool. • Predicton of signal peptide from protein sequence.	Protein Analysis
2	TargetP: Prediction of Protein Localization	• Introduction to TargetP server. • Prediction and detailed analysis of Mitochondrial transfer peptide through TargetP.	Protein Analysis
2	ScanProsite: Prediciton of Important Functional Sites in Proteins Using Profiles	• Establishment of ScanProssite, an improved version of the web-based tool provided by PROSITE. • Scan proteins for matches against the PROSITE collection of motifs as well as against your own patterns.	Motif & Domain Analysis
2	HMMER: Prediction of Import Functional Sites in Proteins Using Hidden Markov Models	• Introduction of HMMER; hidden Markov model based database for protein profiling. • Retrieve the sequence homologs of the query protein using the HMM profile method and it's elaborated analysis.	Motif & Domain Analysis
2	SMART: Finding Domains in Proteins	• Introduction of SMART; Simple Modular Architecture Research Tool for the identification and analysis of protein domains. • Detection of protein domains from the multiple sequence alignments of proteins.	Protein Analysis
2	Ali2D	• Use of Ali2D tool for secondary structure prediction. • Detailed analysis of the secondary structure prediction results.	Secondary Structure Prediction

2	Quick2D	• Use of Quick2D tool for secondary structure prediction. • Detailed analysis and information retrieval of the secondary structure features like alpha-helices, extended beta-sheets, transmembrane helices and disorder regions of the query protein.	Secondary Structure Prediction
2	HHrepID: Prediction Secondary Structure of Proteins	• Introduction to HHrepID, a web-based tool for the prediction of secondary structures of the protein. • Find repetitive regions within a query protein sequence using the HHrepID tool.	Secondary Structure Prediction
2	DeepCoil: Prediction of the Coiled-coil Domain Regions	• Introduction to a web based tool, DeepCoil. • Prediction of the coiled coil domain regions within a query protein sequence.	Secondary Structure Prediction
2	MARCOIL: Analysis of Coiled-coil Domains of Proteins	• Introduction to Marcoil, an HMM for the recognition of proteins with a CCD. • Analysis and prediction of potential coiled-coil domains in protein sequences.	Secondary Structure Prediction
2	Jpred: Prediction Secondary Structure of the Proteins	• Use of Jpred server for secondary structure prediction. • A detailed analysis of secondary structure features' information of the query protein sequence.	Secondary Structure Prediction
3	PEPFOLD 3 Peptide Structure Modeling	• Introduction to PEPFOLD_3 server and its purpose. • Generating 3D models of a peptide using the query sequence. • Defines parameters and analysis of results.	Peptide Structure prediction
3	MODELLER	• Introduction to Modeller tool and its uses. • Procedure to predict a protein structure through Modeller. • Evaluation method of MODELLER to find out the most optimal and good protein structure predicted.	3D Structure Prediction
3	SwissModel	• Introduction to homology modeling and SwissModel, a homology modeling server. • Prediction of protein structure for a target sequence using SwissModel.	3D Structure Prediction
3	HHPRED	• Basic description of HHPred tool and its purpose. • Procedure to predict the protein structure from target sequence through HHPred tool. • Selecting a particular template structure for homology	3D Structure Prediction

3	M4T	• Introduction to M4T, a protein structure prediction tool. • Procedure to predict the protein structure from a Target protein sequence, using the M4T server.	3D Structure Prediction
3	IntFOLD	• Introduction to IntFOLD and its purpose. • Procedure to predict the protein structure from target protein sequence, using the IntFOLD server. • Interpretation of results.	3D Structure Prediction
3	ROBETTA	• Introduction to Robetta, a protein structure prediction tool. • Procedure to predict and analyse protein structure. • Prediction of protein structure for a query sequence using ab-initio	3D Structure Prediction
3	Homology Modeling Using MOE	• Introduction to homology modeling and Molecular Operating Enviroment (MOE) tool. • Generating a homology 3D model of a target protein using MOE.	3D Structure Prediction
4	Chimera	• Introduction to UCSC Chimera and its uses. • Visualization and analysis of a protein 3D model using Chimera. • Comparing and analysis of more than one protein structure for research	3D Structure Visualization
4	PyMol	• Introduction to PyMol. • Defines parameters to visualize and analyze the protein 3D model. • Commands used in PyMol to visualize and manipulate protein 3D model.	3D Structure Visualization
4	WhatCheck	• Introduction to WhatCheck, a protein model evaluation tool. • Utilization of WhatCeck tool for protein model evaluation. • Analysis and implication of results for protein structure evaluation.	3D Structure Evaluation
4	ProCheck	• Introduction to ProCheck, a protein model evaluation tool. • Utilization of ProCheck to check quality of protein model based on certain parameters. • Interpretation of results to select the best model.	3D Structure Evaluation
4	ERRAT	• Introduction to ERRAT, a protein model evaluation tool. • Procedure to evaluate experimentally determined protein model. • Analysis and interpretation of results to evaluate the best model.	3D Structure Evaluation

4	Verify3D	• Introduction to Verify3D, a protein model evaluation tool. • Procedure to evaluate a protein model using the web server of Verify3D. • Interpretation and analysis of the results provided by Verify3D	3D Structure Evaluation
4	RAMPAGE	• Introduction to RAMPAGE, a protein model evaluation tool. • Procedure to evaluate protein model based on Ramachandran plotting by RAMPAGE. • Interpretation of Ramachandran plotting to select the best	3D Structure Evaluation
4	PROSA	• Introduction to ProSA server. • Procedure to evaluate protein model predicted using different methods. • Analysis of three different structures of the protein predicted from three	3D Structure Evaluation
4	SAVES	• Introduction to SAVES tool and its purpose. • Procedure to evaluate a predicted protein model using Saves server. • Analysis of Ramachandran plot generated by the SAVES server for the	3D Structure Evaluation
5	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	Molecular Docking
5	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-	Molecular Docking
5	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.	Molecular Docking
5	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	Molecular Docking
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	Molecular Docking

5	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.	Molecular Docking
5	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.	Molecular Docking
5	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	Molecular Docking
5	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.	Molecular Docking
5	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	Molecular Docking
5	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	Molecular Docking
5	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
5	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
5	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

6	Getting Started With Molecular Dyanmics Simulation - Pre-processing of Protein Structure and Removal of Unncessary Structural Features	• Introduction to GROMACS and its installation. • Pre-processing of the protein structure and removal of unnecessary structural features.	Protein Simulation
6	pdb2gmx - Construction of Topology File for Simulation	• Introduction to pdb2gmx tool of GROMACS. • Construction of topology file for simulation.	Protein Simulation
6	Defining a Solvant Box for Simulation	• Introduction to GROMACS for defining solvant box. • Definig a solvant box to prepare the protein for simulation.	Protein Simulation
6	Solvation - Adding Water Molecules in Solvant Box	• Introduction to GROMACS for defining solvant box. • Adding water molecules in solvant box to prepare the protein for simulation.	Protein Simulation
6	Generating Input Run File Replacement of Water Molecues With Ions	• Generating input run file. • Replacing the water molecules with ions for protein simulation.	Protein Simulation
6	genion - Replacement of Water Molecules With Ions	• Introduction to genioin tool of GROMACS. • Replacing the water molecules with ions for protein simulation.	Protein Simulation
6	Energy Minimization - Relaxing and Fixing the Structure for Simulation	• Introduction to gmx energy tool of GROMACS. • Relaxing and fixing the structure for protein simulation.	Protein Simulation
6	GRACE - Visualization and Analysis of Minimized Structure	• Introduction to gmgrace tool of GROMACS. • Visualization and analysis of minimized structure of the protein.	Protein Simulation
6	Equibiliration of Protein Structure NVT ENSEMBLE Phase 1	• Introduction to nvt tool of GROMACS. • Phase 1 of NVT ENSEMBLE to equilibrate the protein structure.	Protein Simulation

6	Equibiliration of Protein Structure NPT ENSEMBLE Phase 2	• Introduction to nvt tool of GROMACS. • Phase 2 of NVT ENSEMBLE to equilibrate the protein structure.	Protein Simulation
6	mdrun - Executing Simulation Analysis	• Introduction to mdrun tool of GROMACS. • Execution of MD simulation on the protein structure.	Protein Simulation