## CENTRE FOR ADVANCED TRAINING AND RESEARCH, LUCKNOW INDIA

## WINTER TRAINING BIOINFORMATICS COURSE MODULE

S.NO.	Name of the topic	Main Category
	UNIT-I Introduction of Bioinfor	matics
1.	Basic Molecular Biology (Central Dogma)	Introduction
2.	Introduction and Applications of Bioinformatics	Introduction
3.	Origin, History, and Scope of Bioinformatics	Introduction
	UNIT-II Data, Database and Database Mining	Tools in Bioinformatics
4.	Importance of Data and Databases in Bioinformatics	Databases
5.	Different types of Databases	Databases
6.	Nucleotide Databases	Databases
7.	Protein Databases	Databases
8.	Structural Databases and Enzyme Databases	Databases
	Bibliographic Databases	Databases
9.	BLAST, FASTA, HMMER, MSPROBS, MULTALIN	Data Mining tools
10.	GENSCAN, GENOMESCAN AND GENEMARK	Data Mining tools

UNIT-III Sequence Retrieval from Sequence Database		
11.	Sequence Retrieval from NCBI	Bioinformatics Databases
12.	Sequence Analysis	Bioinformatics Databases
13.	PubMed Central & ENTREZ	Bioinformatics Databases
14.	GenBank: Nucleotide Database on NCBI	Bioinformatics Databases
15.	FASTA vs. GenBank	Bioinformatics Databases
16.	Gene Database: A Comprehensive Gene Database	Bioinformatics Databases
17.	NCBI Genomes & NCBI Assembly: Retrieval of Genomes	Bioinformatics Databases
18.	Introduction to ENSEMBL	Bioinformatics Databases
19.	Retrieval of a Gene-Protein-Chromosomal Region	Bioinformatics Databases
20.	RefSeq Database: Retrieval of Single Reference Sequences	Bioinformatics Databases
21.	BLAST Database Searching	Bioinformatics Databases
22.	GenBank (Sequence Annotation Format) FASTA (Sequence Format)	Bioinformatics File Formats
23.	Gene File Format/Gene Transfer Format	Bioinformatics File Formats
24.	SDF and Mol File Format	Bioinformatics File Formats
25.	PDB File Format	Bioinformatics File Formats
26.	Introduction to MolecularModeling Database (MMDB)	Protein Databases & Analysis
27.	Introduction to UniProt	Protein Databases & Analysis
28.	UniProtKB & Protein Analysis	Protein Databases & Analysis
29.	Introduction to Protein Data Bank (PDB)	Protein Databases & Analysis

30.	Accurately Searching for a Protein Structure on PDB & Protein	Protein Databases & Analysis
	Analysis	
31.	Introduction to InterPro	Protein Databases & Analysis
32.	InterPro - Protein Family	Protein Databases & Analysis
UNIT-IV Sequence Analysis-Comparative Tools		
33.	Introduction of Sequence Alignment	Sequence Alignment & Analysis
34.	Local and Global Sequence Alignment	Sequence Alignment & Analysis
35.	EMBOSS NEEDLE: Global Alignment of Sequences	Sequence Alignment & Analysis
36.	Clustal Omega: Most Reliable Multiple SequenceAlignment Tool	Sequence Alignment & Analysis
37.	Clustal Omega Alignment Format	Bioinformatics File Formats
38.	MEGA - Multiple Sequence Alignment	Sequence Alignment & Analysis
39.	MEGA (Alignment Format)	Bioinformatics File Formats
40.	Mega (Phylogenetic Analysis)	Phylogenetic Analysis
UNIT-V PREDICTION and Analysis TOOLS		
41.	Gene prediction tools	Gene Analysis
42.	ORF finding tool	Gene Analysis
43.	Prediction of potential cleavage sites by ExPasy web tool	Gene Analysis
44.	Secondary structure prediction tool	Structure Analysis

45.	PubChem and Drug bank Introduction and analysis	Chemoinformatic Databases and
		Analysis
46.	Introduction of Pharmacokinetics and	Chemoinformatic Databases and
	Lipinski's Rule of Five (Draggability)	Analysis
47.	Properties prediction of Ligands/Drugs/Metabolites/Synthetic	Pharmacokinetics analysis/ Drug
	Compounds	Designing
48.	Toxicity and Drugs ADME properties prediction toolSwissADME,	Pharmacokinetics analysis/ Drug
	PreADMET, ProToX-II	Designing
49.	EDMET Lab 4.0 (Big Data Analysis)	Pharmacokinetics analysis/ Drug
		Designing
UNIT-VI Computer-Aided Drug Designing Approach (Molecular Docking of Protein and		

## Ligand)

50.	Introduction of Computer-Aided Drug Design	Drug Designing
51.	Preparation of Enzyme Target by DS tool	Drug Designing
52.	Active Site Prediction	Drug Designing
53.	Interconversion of various file Conversion using software	Drug Designing
54.	Molecular Docking Analysis	Drug Designing
55.	Installation of Software for CADD	Drug Designing
56.	Analysis of Drug Vs Target (Binding Affinity) by AutoDcok4.2	Drug Designing
57.	Binding Energy and Inhibition constant	Drug Designing

58.	Analysis of Interactive Amino Acids	Drug Designing	
59.	Analysis of H-Bond Interactions	Drug Designing	
60.	Pose Selection	Drug Designing	
61.	Results interpretation	Drug Designing	
UNIT-VII Homology Modelling			
62.	Introduction & applications of Homology Modelling	Modelling of Protein	
63.	Role of Homology Modelling in virtual Drug Design	Modelling of Protein	
64.	Installation of software MODELLER and PyMOL	Modelling of Protein	
65.	Technique for Homology Modelling employing MODELLER software	Modelling of Protein	
66.	Preparation of Script files and Input files	Modelling of Protein	
67.	Template Recognition & Initial Alignment, Backbone Generation	Modelling of Protein	
68.	Loop Modelling, Side Chain Modelling	Modelling of Protein	
69.	Model Validation and Result Analysis	Modelling of Protein	
UNIT-VIII Molecular Dynamics Simulations (MDS)			
70.	Introduction to Molecular Dynamics (MD) Simulations	MDS	
71.	Running MD Simulations	MDS	
72.	Analyzing MD Simulation Results	MDS	