

20BT011**BIOINFORMATICS AND
MOLECULAR MODELING**

Hours Per Week :

L	T	P	C
3	-	-	3

Total Hours :

L	T	P	WA/RA	SSH/HSB	CS	SA	S	BS
45	-	45	-	-	-	-	-	-

Course Description and Objectives:

This course offers basic concepts in computational skills and computational methods to study, organise, analyse and interpret biological information at molecular, genetic and genomics levels. It also offers knowledge on an overall understanding about the critical relationship among biomolecular structure, function and force field models. The objective of this course is to introduce the analysis of biological data using software tools and is to train students in utilizing basic modelling techniques to explore biological phenomena at the molecular level

Course Outcomes:

The student will be able to:

- Demonstrate understanding of biological sciences by articulating the methods of science, explaining why current biological knowledge is both contestable and testable through further inquiry and explaining the role and relevance of biotechnology in society.
- Gain software skills to critically analyze and solve problems in biotechnology.
- Demonstrate cognitive skills in mastery of advanced theoretical knowledge in bioinformatics and apply this knowledge to solve complex problems.
- Understand the principles and practice molecular modelling and modern drug discovery

SKILLS:

- ✓ Design, conduct and interpret scientific research on bioinformatics.
- ✓ Conduct statistical analysis of biological data pertaining to genomics and proteomics.
- ✓ Apply a scientific approach to problems involving molecular phylogeny.
- ✓ Estimate energy minimization upon docking

ACTIVITIES:

- o Retrieval of FASTA format from databases.
- o Perform BLAST and FASTA software analysis for both nucleic acids and amino acid sequences.
- o Construct phylogenetic trees using software tools such as PHYLIP and PAUP.
- o Perform protein homology modelling.

Unit - I

Introduction: Scope of Bioinformatics, Elementary commands and protocols, ftp, telnet, http. Primer on information theory. DNAMapping and sequencing –Map alignment – Large scale sequencing methods - Shotgun – DNA sequencing – Sequence assembly.

Unit - II

Sequence Alignment and Dynamic Programming &Phlogeny: Heuristic Alignment algorithms. Global sequence alignments-Neddleman-Wunsch Algorithm, Smith-Waterman Algorithm-Local sequence alignments (Amino acid substitutionMatrices (PAM, BLOSUM). Ultrasonic trees – parsimony – Ultrametric problem – Perfect phylogeny – Phylogenetic alignment – connection betweenmultiple alignment and tree

Unit - III

Biological Database and their use: Introduction to Biological databases, Organization and management of databases. Searching and retrieval of information from the WorldWide Web. Structure databases - PDB (Protein Data Bank),MolecularModelingDatabases(MMDB). Primary DatabasesNCBI,EMBL,DDDB. Swissprot, PIR,KEGG. BioChemical databases- KEGG, EXGESCY, BRENDA, WIT.

Unit - IV

Introduction to Molecular Modelling: Introduction - Useful Concepts inMolecularModelling: Coordinate Systems. Potential Energy, Surfaces. Molecular Graphics. Surfaces.Computer Hardware and Software. TheMolecular Modelling Literature. Force Fields, Bond Stretching,Angle Bending, Introduction to Non-bonded Interactions. Electrostatic Interactions. Van der Waals Interactions.Hydrogen Bonding inMolecular Mechanics. Force FieldModels for the Simulation of LiquidWater.

Unit - V

EnergyMinimisation andRelatedMethods for Exploring the Energy Surface. Non-Derivativemethod, 1st and 2nd orderminimisationmethods.Computer SimulationMethods. Simple Thermodynamic Properties and Phase Space. Boundaries. Analyzing the Results of a Simulation.

TEXT BOOKS :

1. Mount. D. Cold, "Bioinformatics: Sequence andGenomeAnalysis",Spring Harbor Lab.: 2001
2. T KAttwood, D J parry-Smith, "Introduction to Bioinformatics", 1st Edition, 11th Reprint, Pearson Education, 2005.
3. A. R. Leach, "Molecular modelling principles and application", Longman Company, 2001.

REFERENCE BOOKS :

1. Harshawardhan P.Bal, "Bioinformatics – Principles andApplications " TataMac Graw Hill.
2. Arthur.M.Lesk , "Introduction to Bioinformatics", Oxford University Press.
3. J.M.Haile, "Molecular Dynamics Simulation ElementaryMethods",JohnWiley and Sons, 1997.
4. Satya Prakash Gupta, "QSAR andMolecular Modeling", Springer -Anamaya Publishers, 2008.