Semester: 7	
Course: Minor 4	
Paper Title: Computational Biology	
Paper code:	**Credits: 4 (3+1)**
Hours/week: 4	
Category: Core/MDC/SEC/VAC: Core	
Theory / Practical / Composite: Composite	
No of Modules: Theory - 3	

Course Overview:

This course provides an introduction to the principles and applications of Computational Biology with a focus on the analysis of biological data using computational tools and databases. Students will learn to navigate primary and secondary biological databases, perform sequence alignment, analyze phylogenetic relationships, and predict macromolecular structures. The course also covers genome analysis and introduction to computer aided drug discovery (CADD), enabling students to understand how complex biological information can be integrated and interpreted and their practical applications in healthcare. Practical modules emphasize hands-on training in the use of bioinformatics software, structural modeling, genome annotation, and data mining. By the end of the course, students will be equipped with both the theoretical foundation and computational skills required to solve biological problems and engage in modern research in the life sciences.

Course outcome:

1. Remember details of major biological databases, data formats, and their applications in computational biology.
2. Understand, explain and explore, sequence alignment methods, substitution matrices, and phylogenetic tree construction techniques. Perform protein structural predictions using computational tools such as homology modeling, and Alphafold.
3. Analyze macromolecular interactions, docking simulations, and molecular dynamics data using appropriate bioinformatics software.
4. Evaluate and compare genomes and understand structural and functional annotation of biological data.

Syllabus

Unit/Module	CONTENT	Hours / Number of Classes	Co Mapping	Cognitive Level
Theory [45 Marks] MODULE A 15 Marks	a) Importance of Biological macromolecules; b) Data types and Databases of organisms and biological macromolecules such as DNA and proteins;	10 hours	**CO 1 to CO6**	**K1 to K6**

	c) Sequence Analysis: Pairwise and Multiple Sequence alignments; Importance of substitution matrices in Bioinformatics. d) Phylogenetic analysis.			
Module B: 15 marks	a) Protein Structure Comparison and Classification; b) Protein Structure Prediction: Secondary Structure Prediction; Tertiary structure prediction: Homology modelling; Application of AI in modelling of protein structure (Alphafold). c) Protein-ligand/peptide docking; Molecular dynamics simulation.	10 hours	**CO 1 to CO6**	**K1 to K6**
Module C: 15 marks	a) Introduction to Genome, Transcriptome, and Metagenome analysis b) Quality Control of Data and Functional Annotation c) Basics of Computer-Aided Drug Discovery.	10 hours	**CO 1 to CO6**	**K1 to K6**
Practical [40 marks]	(1) Hands-on training on database analysis, similarity searches, sequence alignment, modelling and docking, genome analysis **(2)** Project work	30 hours	**CO 1 to CO6**	

Text books:	Text Books 1. Bioinformatics: Sequence and Genome Analysis, Second Edition David W Mount; CSHL Press 2. Bioinformatics and Molecular Evolution Paul G. Higgs, Teresa K. Attwood Wiley-Blackwell 3. Introduction to Protein Structure, Carl Ivar Branden and John Tooze; Garland Science 4. Computational Genome Analysis; An Introduction; Richard C. Deonier, Michael S. Waterman, Simon Tavaré; https://doi.org/10.1007/0-387-28807-4 5. Essential Bioinformatics – Jin Xiong	
Evaluation	**Theory** CIA- 10; Assignment – 02; Attendance – 03; Semester Exam- 45	**Practical** CA (38 marks) **;** Attendance (2 marks)
Question paper structure: Module A (15 Marks): Any 3 out of 4 questions (5 marks each with subparts not less than 1 Mark) Module B (15 Marks): Any 3 out of 4 questions (5 marks each with subparts not less than 1 Mark) Module C (15 Marks): Any 3 out of 4 questions (5 marks each with subparts not less than 1 Mark)		

COURSE OUTCOMES (COs) AND COGNITIVE LEVEL MAPPING

COs	CO Description	Cognitive levels
CO1	Remember the techniques of data and information retrieval from different biological databases and tools.	K1 to K6
CO2	Understand algorithms for searching the biological databases.	K1 to K6
CO3	Apply different sequence alignment methods and phylogenetic tree construction algorithms.	K 1 to K6

CO4	Analyze protein secondary and tertiary structure. Perform homology modeling, docking and molecular dynamic simulations	K1 to K6
CO5	Evaluate and annotate methods for genome, transcriptome and metagenome analyses and perform functional annotation.	K1 to K6
CO6	Explore, and create suitable pipelines in Computer Aided Drug Design for proposing new drug candidates	K1 to K6