COURSE TITLE	**INTRODUCTION TO STRUCTURAL & SYSTEMS BIOLOGY**
COURSE CODE	**01CB1403**
COURSE CREDITS	**4**

Objective:

1 To provide comprehensive knowledge of structural and systems biology, emphasizing macromolecular structures, interactions, and functions.

2 To develop skills in computational modeling, structure prediction, and network analysis for biological research and drug design.

Course Outcomes: After completion of this course, student will be able to:

1 Apply structural biology concepts to study macromolecular interactions.

2 Analyze protein folding to determine structural stability and misfolding risks.

3 Evaluate computational predictions of protein/RNA structures for accuracy.

4 Apply mathematical models to understand system robustness and control.

5 Analyze network models to interpret gene, metabolic, and host–pathogen systems.

Pre-requisite of course:NA

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
3	0	2	50	30	20	25	25

Contents : Unit	Topics	Contact Hours
1	**Introduction to Structural Biology** Overview of structural biology and its importance in molecular biology and drug design, X-ray crystallographic and NMR-structures of proteins and nucleic acids, General macromolecular structures, bonding forces, Types of macromolecular interactions including protein-protein and protein-nucleic acid interactions, Chemical basis for interactions with enzyme inhibitors and other ligands, Nucleosome and Chromatin structure, Cytoskeleton structure and protein-protein network	10

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Contents : Unit	Topics	Contact Hours
2	**Protein Sequence & Structure** Physicochemical Properties of Proteins, Protein Structural Motifs and Domains, Secondary structures : alpha helix, beta sheet (parallel & antiparallel), loops and turns, Tertiary and Quaternary structures of proteins and cooperativity, Super-secondary Structures and Folds, Structural characteristics of fibrous, globular, and membrane proteins, Characterization of Folding Pathways and Mutagenesis Studies, Protein Folding & Flexibility and Thermodynamics of folding, Protein misfolding and aggregation	8
3	**Overview of Structural Bioinformatics** Protein structure databases, Protein structure visualization methods, Protein structure prediction by homology modelling and ab initio modelling, Ramachandran Plots, Structural Alignment, Protein Structure Validation and Quality Assessment, Classification of RNA tertiary structures, RNA tertiary structure prediction	8
4	**Introduction to Systems Biology** What is system biology, Introduction to Mathematical Modelling in Systems Biology, System level understanding of biological systems, Whole cell simulation, Principle and levels of simulation, Virtual erythrocytes, Pathological analysis, Fermentation analysis , Flux balance analysis, Minimal gene complement, system state, steady states, variables, parameters & constants, Properties of models-robustness, redundancy, control, modular design, model assignment, Model development, model behavior, process classification, purpose & adequateness of models, Advantages of computational modeling, Aspects of biological systems & corresponding models	8
5	**Introduction to Network Biology** Introduction to Static Networks, Network Biology and Applications, Constraint-based approaches to Modelling Metabolic Networks, Modelling Gene Regulation, Host-pathogen Interactions, Genetic circuits-toggle switches, genetic circuits, lambda phage lysogeny-lysis model	8
Total Hours		**42**

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	**Experiment 1** To Identify different levels of protein structure and visualize them using PyMol and Chimera	2
2	**Experiment 2** To predict the secondary structure of proteins from their amino acid sequences	2
3	**Experiment 3** To predict the solvent accessibility of amino acid residues in a protein	2

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Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
4	**Experiment 4** To predict the subcellular localization and intrinsic disorder regions of proteins from their amino acid sequences	2
5	**Experiment 5** To identify protein motifs and domains from amino acid sequences	2
6	**Experiment 6** To predict 3D structure of protein using SWISS MODEL	2
7	**Experiment 7** To predict the 3D structure of proteins using threading (template-based) methods and ab initio modeling techniques.	2
8	**Experiment 8** To evaluate the stereochemical quality of protein structures using Ramachandran plots.	2
9	**Experiment 9** To analyze protein structural features using the PDBsum database	2
10	**Experiment 10** To predict binding sites in proteins using computational tools and sequence-based methods	2
11	**Experiment 11** To predict binding sites in proteins using computational tools and structure-based methods	2
12	**Experiment 12** To model host-pathogen interactions using STRING Database	2
13	**Experiment 13** To construct and analyze genome-scale metabolic models (GEMs) of organisms	2
14	**Experiment 14** To build and simulate models of biological systems	2
Total Hours		**28**

Textbook :

1 Structural Bioinformatics, Jenny Gu, Philip E. Bourne, John Wiley & Sons, 2009
2 A First Course in Systems Biology, Eberhard O. Voit, Garland Science, 2018
3 Systems Biology: A Textbook, Edda Klipp et al.,, Wiley-Blackwell, 2016
4 Introduction to Protein Structure, Carl Branden & John Tooze, Garland Science, 1934
5 Molecular Biology of the Cell, Bruce Alberts et al, Garland Science, 2002
6 An Introduction to Systems Biology: Design Principles of Biological Circuits, Uri Alon, CRC Press, 2007

References:

1 Proteins: structures and molecular properties, Proteins: structures and molecular properties, Creighton, Thomas, W.H. Freeman, 1993

References:

2 An Introduction to Systems Biology: Design Principles of Biological Circuits, An Introduction to Systems Biology: Design Principles of Biological Circuits, Uri Alon, Chapman and Hall/CRC, 2006

3 An Introduction to Computational Systems Biology Systems-Level Modelling of Cellular Networks, An Introduction to Computational Systems Biology Systems-Level Modelling of Cellular Networks, Karthik Raman, Chapman & Hall/CRC Press, 2021

4 Evolutionary Dynamics: Exploring the Equations of Life, Evolutionary Dynamics: Exploring the Equations of Life, Martin A. Nowak, Belknap Press, 2006

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery					
Remember / Knowledge	**Understand**	**Apply**	**Analyze**	**Evaluate**	**Higher order Thinking / Creative**
0.00	0.00	35.00	35.00	30.00	0.00

Instructional Method:

1 The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.

2 The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.

3 Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory.

Supplementary Resources:

1 https://www.coursera.org/courses?query=bioinformatics

2 https://www.coursera.org/learn/network-biology

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