DISCIPLINE SPECIFIC ELECTIVES (DSE-10):
Integrative Systems Biology and Bioinformatics

Credit distribution, Eligibility and Pre-requisites of the Course

Course Title & Code	Credits	Credit distribution of the Course			Eligibility criteria	Pre-requisite of the course	Department offering the course
		Lecture	Tutorial	Practical			
Integrative Systems Biology and Bioinformatics Zoo-DSE- 10	04	03	Nil	01	Passed Class XII with Biology/ Biotechnology	Basic knowledge of computer and biology	Zoology

Learning Objectives

The learning objectives of this course are as follows:

- to give an overview of the key principles of Systems Biology and Bioinformatics.
- to introduce students to a variety of *in silico* solution for biological problems and systems data by analysing biological databases, gene sequence alignments, gene annotation, structure predictions, and drug development, among other areas.
- to encourage undergraduate students to pursue higher education in this field as Bioinformatics has been identified as a critical area of study and development

Learning Outcomes

By studying this course, students will be able to:

- know more about the basic of systems biology and bioinformatics
- better understand about the availability of experimental data through biological databases, usage of small molecules, nucleic acids, protein sequences, in a variety of biological sciences domains
- gain more knowledge about the gene sequence annotation, protein structure prediction and gene enrichment prediction
- acquire skills to perform and understand pair-wise and multiple sequence alignment
- better understand a variety of computational tools and approaches, as well as their use in *in silico* drug discovery, structural bioinformatics, and functional genomics etc.

SYLLABUS OF DSE- 10

UNIT- 1: Introduction to Systems Biology and Bioinformatics **5 hrs**

Introduction to Systems Biology, Bioinformatics, Genomics, Proteomics, Transcriptomics, Metabolomics, Scope and their applications.

UNIT- 2: Systems Biology **10 hrs**

Computational models, modelling and their basic notions, networks (feed forwardgene circuit,transcription regulatory networks and protein-protein interaction networks)

UNIT- 3: Biological Databases **8 hrs**

Introduction to biological databases; Primary, Secondary and Composite databases; Nucleic acid databases (GenBank, DDBJ, EMBL and NDB); Protein databases (PIR, SWISS-PROT, TrEMBL, PDB); Metabolic pathway database (KEGG, Reactome, EcoCyc, and MetaCyc); Small molecule databases (PubChem, Drug Bank, ZINC, CSD)

UNIT- 4: Sequence Alignment and Phylogeny **10 hrs**

Scoring Matrices (PAM, BLOSUM), Methods of Alignment (Dot matrix, Dynamic Programming, BLAST and FASTA); HMM model, Local and global alignment, pair wise and multiple sequence alignments, Molecular Phylogeny.

UNIT- 5: Structural Biology and Drug Discovery **12 hrs**

Protein secondary structure prediction (Chou-Fasman & GOR methods), Protein tertiary structure prediction and its validation (Homology modelling, Threading and *Ab-initio* methods); Lipinski rule, Molecular docking (rigid and flexible docking), ADMET properties, Molecular Dynamics, Drug-DNA interactions.

Practical **(30 hrs)**

(Laboratory periods: 15 classes of 2 hours each)

1. Retrieval of DNA, RNA, protein sequences and structures from the biological databases and to create various datasets.
2. Perform pairwise and multiple sequence alignments from the generated datasets in Experiment 1, using online/offline tool.
3. Retrieval and analysis of any one disease network from KEGG pathway database.
4. Gene functional enrichment analysis using DAVID tool.
5. Protein structure prediction through homology modelling using Swiss Modeller.
6. Molecular docking (Protein-ligand) using AutodockVina/ SwissDock/ PatchDock/ZDock (anyone).
7. Project related to topics covered in theory/ project report based on visit to labs/institutions/industry etc.

Essential/recommended readings

1. Pevsner, J. (2015) Bioinformatics and Functional Genomics, 3rd edition, Wiley and Blackwell.
2. Xiong, J. (2012) Essential Bioinformatics, Cambridge University Press.
3. Claverie, JM and Notredame, C. (2006) Bioinformatics for Dummies 2nd edition, Wiley Publishing Inc.
4. Klipp, E., Liebermeister, W., Wierling, C. and Kowald, (2016) A. System Biology

Suggestive readings

1. Alon, U. (2019) An Introduction to Systems Biology 2nd edition, CRC, Taylor & Francis.
2. Jenny Gu, J. and Bourne, P.E.(2011) Structural Bioinformatics 2nd edition, Wiley Blackwell.
3. Harren Jhoti, H. & Leach, A. (2007) Structure-based Drug Discovery, Springer.
4. Kitano, H. (2001) Foundations of Systems Biology, MIT press Cambridge.

NOTE: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.