Computational Biology

Credits – 3   L-T-P
                                                                                                                    2-0-2

Course objectives

1. Articulate importance & application of Computational Biology & Bioinformatics.
2. Understanding biological data of diverse types and their retrieval from various biological databases.
3. Develop computational workflows using bioinformatics techniques & tools used for analysis of biological data and interpret the results.
4. Familiarize with computational methods for biological sequence and structure analysis.
5. Perform biological sequence alignments and interpret the results.
6. Prediction of gene, RNA structure, and protein structure & function.
7. Familiarize with computational methods for performing evolutionary studies.

Course content

Module I: Computational Biology & Bioinformatics

History, importance & applications of computational biology & bioinformatics.

Module II: Biological Databases

Biological data, importance of biological databases & their biological design basis, file formats & types (primary, secondary, sequence, structure & other), information retrieval from various biological databases, databases of nucleic acids sequence & structure, protein sequence & structure, chemical structures, biological networks & metabolic pathways, biomedical image databases. Practical importance of biological databases in different segments of healthcare, pharmaceutical and biotech industries.

Module III: Sequence Alignment

Practical importance of aligning two or more than 2 genes/ genome sequences, Biological sequences alignment principles, its importance & applications, different alignment techniques (dot matrix, dynamic programming, heuristics), scoring matrices (BLOSUM & PAM), gaps, global versus local sequence alignment, pairwise sequence alignment & its methods, tools of similarity searches (BLAST, PSI-BLAST, & FASTA), multiple sequence alignment (practical issues, methods & tools: Clustal Omega, TCoffee, MUSCLE).

Module IV: Genome Annotation

Why need of genome annotation, Biological basis of gene prediction & its importance, pattern recognition, gene prediction using bioinformatics tools (Ab initio, homology based, statistical & HMM based gene prediction approaches), tools of gene prediction.

Module V: RNA and Protein Structure Prediction

Introduction & importance, secondary structure of RNA, methods of RNA secondary structure prediction & tools. Protein structural hierarchy, super secondary structures, structure determination, protein folding, sequence structure relation, methods of protein secondary structure prediction (ab initio modeling, threading, homology modeling), structure evaluation,

protein structure visualization tools, structure function relation, protein function prediction, motifs & domains. Introduction, importance & applications of patterns, motifs, and profiles, PROSITE, BLOCKS, PRINTS, Pfam. How to utilize RNA/Protein structures in drug designing and discovery with case studies of commercial importance

Module VI: Evolutionary studies
Importance & applications, methods of phylogenetic analysis (distance & character based), tree construction & topologies, tools for tree visualization.

Module VII: Biological Modelling & Biomedical Image Analysis
Computer models of population dynamics, biochemical kinetics, cell pathways, etc. Morphological image analysis, image classification and image-derived models for sue in clinical decision support systems

Recommended Books

1. Baxevanis, Andreas D., Gary D. Bader, and David S. Wishart, eds. *Bioinformatics*. John Wiley & Sons, 2020.
2. Zvelebil, Marketa J., and Jeremy O. Baum. *Understanding bioinformatics*. Garland Science, 2007.
3. Agostino, Michael. *Practical Bioinformatics*. Garland Science, 2012.
4. Tramontano, Anna. *Introduction to bioinformatics*. Chapman and Hall/CRC, 2007.
5. Pevsner, Jonathan. *Bioinformatics and functional genomics*. John Wiley & Sons, 2015
6. Rastogi, S. C., Parag Rastogi, and Namita Mendiratta. *Bioinformatics: Methods and Applications-Genomics, Proteomics and Drug Discovery*. PHI Learning Pvt. Ltd., 2022.