



GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Science (Industrial Biotechnology)

Level: PG Semester-3

Course / Subject Code: IB03001071

Course / Subject Name : Computational Biology

1. Learning Outcomes

Learning Outcome Component	Learning Outcome (Learner will be able to)
Theoretical and practical understanding of computational biology	<ul style="list-style-type: none">Develop required database extraction, integration, coding for computational tools and methods necessary for all Omics.Formation of hypothesis for investigating specific contemporary biological questions, provide help to experiment with or develop appropriate tools.
Value applications of Computational Biology in biological research as well as in biotech-industries	<ul style="list-style-type: none">Describe genomics, proteomics, pharmacogenomics and drug discovery.Explain human genome sequencing and assist in modeling biological systems.
Effective Communication	<ul style="list-style-type: none">Communicate concepts and ideas effectively.
Professional & Ethical Behaviour	<ul style="list-style-type: none">Transparency, honesty and ethical reasoning in handling databases for further research.

LO – PO Mapping: Correlation Levels:

1 = Slight (Low); 2 = Moderate (Medium); 3 = Substantial (High), “-“= no correlation

Sub Code:	PO1	PO2	PO3	PO4	PO5	PO6	PO7
LO1:Theoretical and practical understanding of computational biology	3	3	2	2	3	3	2
LO2:Value applications of computational biology in biological research as well as in biotech-industries	2	2	3	2	2	2	2
LO3: Effective communication	2	2	2	2	2	3	2
LO4: Professional & Ethical Behaviour	3	2	2	3	3	3	3

2. Course Duration: The course duration is of 45 sessions of 60 minutes each.

3. Course Contents:

Module No:	Module Content	No. of Sessions	70 Marks (External Evaluation)
1	<u>Introduction to computational biology basics and biological databases</u> Computers in biology and medicine; Overview of biological databases, nucleic acid & protein databases, primary,	6	10



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	secondary, functional, composite, structural classification database, Sequence formats & storage, Access databases, Extract and create sub databases, limitations of existing databases.		
2	<u>Pairwise and multiple sequence alignments</u> Local alignment, Global alignment, Scoring matrices - PAM, BLOSUM, Gaps and penalties, Dot plots. Dynamic programming approach: Needleman and Wunsch Algorithm, Smith and Waterman Algorithm, Hidden Markov Model: Viterbi Algorithm. Heuristic approach: BLAST, FASTA. Building Profiles, Profile based functional identification.	6	10
3	<u>Genome analysis</u> Polymorphisms in DNA sequence, Introduction to Next Generation Sequencing technologies, Whole Genome Assembly and challenges, Sequencing and analysis of large genomes, Gene prediction, Functional annotation, Comparative genomics, Probabilistic functional gene networks, Human genome project, Genomics and crop improvement; Study the available GWAS, ENCODE, HUGO projects, extract and build sub databases; Visualization tools including Artemis and Vista for genome comparison; Functional genomics case studies.	7	10
4	<u>Structure visualisation</u> Retrieving and drawing structures, Macromolecule viewing platforms, Structure validation and correction, Structure optimization, Analysis of ligand-protein interactions; Tools such as PyMol or VMD.	5	10
5	<u>Molecular modelling</u> Significance and need, force field methods, energy, buried and exposed residues; side chains and neighbours; fixed regions; hydrogen bonds; mapping properties onto surfaces; RMS fit of conformers and protein chains, assigning secondary structures; sequence alignment: methods, evaluation, scoring; protein curation: backbone construction and side chain addition; different types of protein chain modeling: ab initio, homology,	7	10



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	hybrid, loop; Template recognition and alignments; Modeling parameters and considerations; Model analysis and validation; Model optimization; Substructure manipulations, annealing, protein folding and model generation; loop generating methods; loop analysis; Analysis of active sites using different methods in studying protein–protein interactions		
6	<u>Structure-based drug development</u> Molecular docking: Types and principles, Semi-flexible docking: Flexible docking: Ligand and protein preparation, Macromolecule and ligand optimization, Ligand conformations, Clustering, Analysis of docking results and validation with known information. Extra precision docking platforms, Use of Small-molecule libraries, Natural compound libraries for virtual high throughput screening.	7	10
7	<u>Ligand-based drug development</u> Quantitative structure activity relationships. Introduction to chemical descriptors like 2D, 3D and Group-based; Radar plots and contribution plots and Activity predictions, Pharmacophore modeling, Pharmacophore-based screenings of compound library, analysis and experimental validation.	7	10

4. Pedagogy:

- ICT enabled Classroom teaching
- Practical / live assignment
- Interactive classroom discussions

5. Evaluation:

Students shall be evaluated on the following components:

A	Mid-Semester Examination	(Internal assessment-30 Marks)
B	End-Semester Examination	(External assessment-70 Marks)

6. Reference Books:

No	Author	Name of the Book	Publisher	Year of Publication / Edition



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1	Mount, D. W	Bioinformatics: Sequence and Genome Analysis	Cold Spring Harbor Laboratory Press	Latest Edition
2	Bourne, P. E., & Gu, J.	Structural Bioinformatics	Hoboken, NJ: Wiley-Liss	Latest Edition
3	Lesk, A. M.	Introduction to Protein Science: Architecture, Function, and Genomics	Oxford University Press	Latest Edition
4	Campbell, M & Heyer, L. J.	Discovering Genomics, Proteomics and Bioinformatics	Pearson Education	Latest Edition
5	Oprea. T.	Chemoinformatics in Drug Discovery, Volume 23	Wiley Online Library	Latest Edition
6	Gasteiger, J. and Engel, T.	Chemoinformatics: a Textbook	Wiley Online Library	Latest Edition

Note: Wherever the standard books are not available for the topic appropriate print and online resources, journals and books published by different authors may be prescribed.

7. List of Journals/Periodicals/Magazines/Newspapers / Web resources, etc

- <https://biology.mit.edu/faculty-and-research/areas-of-research/computational-biology/>

Course Outcomes:

On completion of this course, students should be able to:

- Develop an understanding of basic theory of these computational tools;
- Develop required database extraction, integration, coding for computational tools and methods necessary for all Omics;
- Formation of hypothesis for investigating specific contemporary biological questions, provide help to experiment with or develop appropriate tools;
- Critically analyze and interpret results of their study with respect to whole systems.