

Name of the Programme: M.Sc. Marine Biotechnology

Course Code: MBT-521

Title of the Course: BIOINFORMATICS

Number of Credits: 2

Effective from AY: 2022-23

Pre-requisites for the Course:	GBT-509	
Course Objectives:	<p>The objectives of this course are</p> <p>1)to provide students with theory and practical experience of the use of common computational tools and databases especially marine databases</p> <p>2)To facilitate the investigation of molecular biology and evolution-related concepts.</p>	
Content:	<p style="text-align: center;"><u>MODULE I</u></p> <ul style="list-style-type: none"> • Introduction, Primary & Secondary database, Sequence file formats, Introduction to structures, Protein Data Bank (PDb), Molecular Modelling Database (MMDb), Structure file formats, Collection of sequences, sequence annotation, sequence description. • Evolutionary basis of sequence alignment, optimal alignment methods, Substitution scores & gap penalties, Statistical significance of alignments, • Database similarity searching, FASTA, BLAST, Low complexity regions, Repetitive elements, Multiple Sequence Alignment: Progressive alignment methods, Motifs and patterns, Clustal, Muscle; Scoring matrices, Distance matrices. • Alignment, tree building and tree evaluation, Comparison and application of Unweighted Pair Group Method with Arithmetic Mean (UPGMA), Neighbour Joining (NJ), Maximum Parsimony (MP), Maximum Likelihood (ML) methods, Bootstrapping, Jackknife; • Software for Phylogenetic analysis. DNA barcoding: Methods tools and databases for barcoding across all 	<p>No. of hours</p> <p style="text-align: center;">15</p>

	species, Applications and limitations of barcoding, Consortium for Barcode of Life (CBOL) recommendations, Barcode of Life Database (BOLD).	
	<p style="text-align: center;"><u>MODULE II</u></p> <ul style="list-style-type: none"> • 3-D structure visualization and simulation, Basic concepts in molecular modeling: different types of computer representations of molecules; External coordinates and Internal Coordinates, Molecular Mechanics, Force fields <i>etc.</i> Secondary structure elucidation using Peptide bond, phi, psi and chi torsion angles, Ramachandran map, anatomy of proteins – Hierarchical organization of protein structure –like CATH (class, architecture, topology, homology), SCOP (Structural Classification of Proteins), FSSP (families of structurally similar proteins). • Fundamentals of the methods for 3D structure prediction (sequence similarity/identity of target proteins of known structure, fundamental principles of protein folding <i>etc.</i>) Homology/comparative modeling, fold recognition, threading approaches, and ab initio structure prediction methods; CASP (Critical Assessment of protein Structure Prediction); Computational design of promoters, proteins & enzymes. • Chemical databases like NCI/PUBCHEM; Fundamentals of Receptor-ligand interactions; Structure-based drug design: Identification and Analysis of Binding sites and virtual screening; Ligand based drug design: Structure Activity Relationship– QSARs & Pharmacophore; <i>In silico</i> predictions of drug activity and ADMET. • Designing of oligo probes; Image processing and normalization; Microarray data variability (measurement and quantification); Analysis of differentially expressed genes; Experimental designs. 	15
Pedagogy:	Lectures, tutorials, assignments	
References/ Readings:	1. L. Arthur, Introduction to Bioinformatics. Oxford University Press, 2019.	

	<ol style="list-style-type: none"> 2. A. D. Baxevanis, G. D. Bader and D. S. Wishart, Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins Wiley Publisher, 2020. 3. N. Gautham, Bioinformatics databases and algorithms, 2007. 2. V.R. Srinivas, Bioinformatics: A modern approach, PHI Learning Pvt. Ltd., 2005. 3. S.C. Rastogi, N. Mendiratta and P. Rastogi, Bioinformatics: concepts skills and applications, 2004. 4. J. Xiong, Essential Bioinformatics, by Cambridge University Press, First edition, 2007. 5. S. Ignacimuthus, Basic Bioinformatics, Alpha Science International Ltd, 2013. 6. J. Pevsner, Bioinformatics and Functional Genomics, Wiley Blackwell Publication, 2015. 7. P. S. Neelakanta, A Textbook of Bioinformatics: Information-theoretic Perspectives of Bioengineering and Biological Complexes, World Scientific Publisher, 2020. 8. W. Even and G. Grant, Statistical methods in Bioinformatics: An introduction, 2005. 9. J. Xiong, Essential Bioinformatics, Cambridge University Press, 2006.
Course Outcomes:	<p>Students should be able to:</p> <ol style="list-style-type: none"> 1. develop an understanding of the basic theory of these computational tools. 2. gain working knowledge of these computational tools and methods. 3. appreciate their relevance for investigating specific contemporary biological questions. 4. Understand the process of drug designing