

M. TECH. BIOINFORMATICS

Semester I

S.No.	Paper Code	Subject Title	Credit	L.T.P.
1.	BCBT-715	BioMolecules	2	2-0-0
2.	COMP-704	Object Oriented Programming	3	2-0-1
3.	PHY-701	Molecular Biophysics	2	2-0-0
4.	CBBI-701	Fundamental of Bioinformatics & Information Technology	3	2-0-1
5.	MBGE-701	Molecular Cell Biology	3	2-0-1

Deficiency Course

S.No.	Paper Code	Subject Title	Credit	L.T.P.
1.	MAS-312	Elementary Mathematics	4	3-1-0

Semester II

S.No.	Paper Code	Subject Title	Credit	L.T.P.
1.	MAS-814	Applied Biostatistics	3	2-0-1
2.	CBBI-702	Biological Databases and Data Analysis	3	2-0-1
3.	CBBI-703	Phylogenetic Analysis	3	2-0-1
4.	CBBI-704	Genomics and Proteomics	3	2-0-1
5.	CBBI-705	Sequence Analysis and Data Mining	3	2-0-1
6.	CBBI-706	IPR Issues in Bioinformatics	2	2-0-0
7.	CBBI-708	Biomolecular Modeling	3	2-0-1
8.	CBBI-780	Seminar-I	1	0-0-1

Deficiency Course

1.	MAS-411	Engineering Mathematics-I	4	3-1-0
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1.	CBBI-800	Summer Training	1	0-0-1
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Semester III

S.No.	Paper Code	Subject Title	Credit	L.T.P.
1.	CBBI-707	Artificial Neural Networks	2	2-0-0
2.	CBBI-802	Chemo Informatics	3	2-0-1
3.	CBBI-803	Computer Aided Drug Designing	3	2-0-1
4.	CBBI-804	Biodiversity & Informatics	3	2-0-1
5.	CBBI-805	Bio-Image Processing	2	2-0-0
6.	CBBI-806	Pattern Recognition	2	2-0-0
7.	ME -749	Design Theory & Methodology	3	3-0-0
8.	CBBI-880	Seminar-II	1	0-0-1

Deficiency Courses

1.	MAS-490	Engineering Mathematics-II	4	3-1-0
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Semester IV

S.No.	Paper Code	Subject Title	Credit	Credit
1.	CBBI-899	Research Project (Dissertation)	15	0-0-15

SYLLABUS

BCBT-850 BioMolecules 2 2-0-0

Unit 1

Carbohydrates: Classification and function, metabolism of carbohydrates; Glycolysis, TCA, glyconeogenesis.

Unit 2

Lipids: classification and function, plasma membrane, isoprenoids, eicosanoids and their biological importance, metabolism of lipids, beta oxidation and fat synthesis.

Unit 3

Proteins: amino acids and their structures, functions, protein folding, protein biosynthesis and breakdown.

Unit 4

Nucleic acid: Nucleoside, structure of RNA and DNA, structural forms of DNA, denaturation and renaturation and hybridization of DNA, different forms of RNA, protein nucleic acid interaction.

Unit 5

Enzyme: classification and nomenclature, factors affecting enzyme activity, coenzyme, cofactors, enzyme kinetics, different types of inhibition, covalent and non covalent regulation of enzymes, allosteric enzymes, feed back control of enzymes, multi enzyme complexes.

COMP-704 Object Oriented Programming 3 2-0-2

Unit 1

Programming concepts: Reduction of a given problem to a computer program; flow chart concepts, Conversion of the flow chart to code, Key concepts in programming: variables and constants; different kind or types of variables; storage needs.

Unit 2

Arrays; concept of address and value; keywords and reserved words; syntax, Programming tools: sequential execution; branching; conditional branching; different kinds of loops.

Unit 3

Machine dependent conditions: address; segment. Pointers, function calls, memory allocation, entry, exit codes, large programs (overlays).

Unit 4

Introduction to C: general features of a C program, Arrays and pointers in C: detailed discussion, Input and output: files: basic concepts of stream I/O, Strings and string operations, string handling.

Unit 5

Classes and structures, Overloading operations, Objects, composition, inheritance and other properties, Template and iterators, Libraries, Compilers, options and optimizations, Loading, linking and debugging, Good programming practices.

PHY-701

Molecular Biophysics

2

2-0-0

Unit 1

Physical Techniques: Diffraction/Sedimentation: Determination of molecular weight of macromolecules using Diffraction & Sedimentation.

Unit 2

X-Ray Diffraction: X-Ray Diffraction, Principles of X-Ray, the unit cell & space group, Bragg's law, Structure determination, the Patterson method.

Unit 3

Spectroscopy: UV, IR & Raman spectroscopy, basic principles, instrumentation & application, NMR/ESR: classical description of magnetic resonance, spin lattice relaxation process, Spin labeling in biological molecules.

Unit 4

Nucleic Acid: Introduction to Nucleic Acid. Definition of terms for nucleic acid, Watson-Crick hypothesis of DNA structure and its biological implication.

CBBI-701

Fundamental of Bioinformatics & Information Technology

3

2-0-1

Unit 1

Introduction to Bioinformatics, philosophical, directional and application oriented background of Bioinformatics. Biological databanks: NCBI data model, GenBank sequence database, structural database, biodiversity information, virology information database, Chemoinformatics databases, practicals on data retrieval involving internet based Bioinformatics tools.

Unit 2

Introduction to database: Data abstraction, data models, E-R Models, E-R Diagrams and their reduction to tables, basic concepts, Network data models, Hierarchical data models, Multimedia data models, Basic concept of Indexing: B, B+ tree indexed files, Static and Dynamic Hashing, Text database, Introduction to distributed Database Processing.

Unit 3

Information network - Internet, Web Browser and address (NCBI, EBI etc). Use of INTERNET & WWW; Ethernet and TCP/IP family of protocols

Unit 4

Computer Networking - LAN, WAN, MODEM; Network structure; Network architecture; Hierarchical networks, Optical Vs. Electronic Networking; Security of the network, Fire-walls; Network Goals; Applications Network.

Practicals:

1. Understanding Linux Operating System and Commands.
2. Introduction to NCBI.
3. Using Entrez to search Literature Databases.
4. Retrieving DNA sequence from GenBank and analyzing various formats of the data stored.
5. Retrieving Protein sequence from GenPept (NCBI) and Expasy.
6. Analyzing Protein Sequences.
7. Analyzing DNA sequence.
8. Setting up NFS server for file sharing.
9. Using SSH for secure login.
10. Using FTP and SFTP to transfer data across the network.

MBGE-610

Molecular Cell Biology

3

2-0-2

Unit 1

Diversity of cell size and shape. General structure and constituents of prokaryotic and eukaryotic cells, Cell wall, cell membrane, cell surface related functions.

Unit 2

Endoplasmic reticulum, Golgi apparatus, nuclear membrane, tonoplast, vacuoles, their molecular structure and function.

Unit 2

Structure and function of major cell organelles-nucleus, chloroplast, mitochondria and ribosome in relation to cell growth and division Regulation of cell cycle and cell division.

Unit 4

Introduction and concepts in Molecular Biology, Macromolecules-major classes and understanding of macromolecules, Proteins- structural organization, conformation and biological function.

Unit 5

Enzymes- classification, active site, kinetics and regulation Nucleic acids- classification, structure, stereochemistry and secondary structure

Unit 6

Organization of prokaryotes, eukaryotes and organelle genomes Gene structure in prokaryotes and in eukaryotes

Unit 7

Examination of cells- plant, animal and microbial cells, Examination of tissues- epidermis, parenchyma, chlorenchyma, collenchyma, sclerenchyma Preparation of microscopic slides and mounting of transverse and longitudinal sections of stem, root and leaf samples, Preparation of microscopic slides to study different stages of mitosis and meiosis

MAS-313

Elementary Mathematics

4

3-1-0

Algebra: Theory of Quadratic equations, Partial fractions, Binomial theorem (for positive index), Exponential and Logarithmic series, Elementary concepts of Permutation and Combination.

Trigonometry: Elementary concepts of Complex numbers, De-Moivre's theorem and its application.

Co-ordinate Geometry: Equation of standard curves and their identification.

Differential Calculus: Function, Limit, Continuity and Differentiability, Differentiation of standard functions, Method of Differentiation, Tangent and Normal, Maxima and Minima.

Integral Calculus: Indefinite integration of standard functions, Integration by substitution, by parts, by partial fraction.

Vector Analysis: Scalar and Vectors, sum and Difference of Vectors, Dot and Cross product. (Double, triple).

CBBI-702 **Biological Databases and Data Analysis** **3** **2-0-1**

Unit 1

Biological databanks: Types, Nucleic Acid and Protein Sequence Databases and Structural Databases, primary, secondary & tertiary databases sequence and composite databases, Genome & Organism-specific database ex. OMIM, TAIR, NCBI, TIGR, GOLD etc, specialized sequence databases ex. r-RNA & tRNAseq, introns, promoters & other regulatory elements, ESTs etc., Literature databases.

Unit 2

Building biological databases, Submitting sequences to databases, Database tools for displaying and annotating sequence data, Retrieval of biological data for ex. with Entrez, DBGET/Link DB & SRS.

Unit 3

Sequence analysis, Database similarity searches: FASTA & BLAST, Amino-acid substitution matrices, and Statistical significance of database-searches.

Unit 4

Data-warehousing, Data-capture, Data-analysis.

Practicals:

1. Introduction to NCBI and its contents.
2. Using Entrez to search Literature Databases.
3. Exploring KEGG (Kyoto Encyclopedia of Genes and Genomes).
4. Introduction to the structure database PDB.
5. Sequence alignment using BLAST (Basic Local Alignment Search Tool).
6. Sequence alignment using FASTA.
7. Multiple sequence alignment using ClustalW.
8. Sequence analysis using EMBOSS.

CBBI-703 **Phylogenetic Analysis** **3** **2-0-1**

Unit 1

Molecular-Phylogenetics, Phylogenetic-trees, Terminology of tree-reconstruction, rooted and unrooted trees, gene vs species trees, character and distance data.

Unit 2

Phylogenetic analysis algorithms/methods: (a) Distance based methods: UPGMA, Transformed distance method, Neighbor's relation method, Neighbor-Joining Method, Multiple sequence alignment. (b) Character based methods: Parsimony, Weighted & unweighted parsimony, Branch & Bound method and Heuristic searches.

Unit 3

Probabilistic models and associated algorithms; Probabilistic models of evolution, Maximum likelihood algorithm

Unit 4

Approaches for tree reconstruction; Character optimization; delayed and accelerated transformation. Reliability of trees: Bootstrapping, parametric tests jackknife, decay and randomization tests.

Unit 5

Comparisons of Trees, Consensus (Strict, semi strict, Adam's majority rule, Nelson), Data partitioning and combination. Tree to tree distances and similarity.

Unit 6

Applications of Phylogenetic analyses Comparison of Phylogenetic Trees obtained using DNA sequences vs. Protein. Sequences vs. Full genomes. Need for addition of other properties towards total Phylogenetic analysis, Comparative methods for detection of species / organism relationships Gene duplication, Horizontal transfer, Domain evolution, Study of co-evolution: Plant-insect interactions. Host-parasite interactions, viral evolution.

Practicals:

CBBI-704

Genomics and Proteomics 3

2-0-1

Unit-1

Overview- Structure and organization of Prokaryotic and eukaryotic genome, gene structure and gene density of prokaryotes and eukaryotes, variations in the general structure and organization in genomes expression profiles.

Unit-2

Brief outlook of various genome projects and their outcome, Nucleotide and protein sequencing, Genome sequencing; various techniques: shot gun, clone contig approach, chromosome walking, primer walking, chromosome jumping, contig assembly, genome marking and mapping techniques, genomic DNA-library, cDNA-library.

Unit-3

Mapping and Sequence Assembly, Genetic markers- RFLP, STR, SSLP, VNTR. Physical markers, ESTs, STS, FISH, Radiation hybrid, Sequence marker, SNP'S, Expression analysis, Obtaining & Evaluating gene expression profiles with microarray.

Unit-4

Human genome project - transcript on structural and functional genomics, comparative and population genomics, Pharmacogenomics and Phylogenetics, Functional Proteomics, genotype-phenotype relationship, polygenic nature of proteins

Unit-5

Proteomics experimental techniques: 2-D electrophoresis, Mass spectrometry & Protein Microarray, DrugDesign, Empirical Methods and prediction techniques, X-ray and NMR-structures, Post-translational modification prediction: protein sorting, proteolytic cleavage, glycosylation and phosphorylation.

Practicals:

1. Retrieval of genomic & proteomic data through different biological databases.
2. Prediction of ORF in DNA sequence.
3. Prediction of Amino Acid sequence from predicted ORF.
4. Calculation of physio-chemical properties of protein sequence.
5. Prediction of post translational modifications for a given protein.
6. Prediction of restriction sites in a given sequence of nucleotide by using different restriction enzymes

CBBI-705 **Sequence Analysis and Data Mining** **3** **2-0-1**

Unit 1

Analysis of protein and nucleic acid sequences e.g. Genome analysis, Microarray-data analysis etc.

Unit 2

Pairwise sequence alignment: Basics and techniques, Local alignment and Global alignment, NEEDLEMAN and Wunsch algorithm, Smith and Waterman algorithm, The Dot Plot, Dynamic Programming Algorithm.

Unit 3

Multiple Sequence Alignment: The goal of MSA, Definition, Consensus Sequence, Computational Complexity, Methods for MSA: Heuristic approaches, Combined approaches (Dynamic programming and Heuristic), Dynamic programming approaches or Progressive approaches.

Unit 4

Datamining: Architecture for Data-discovery process and Datamining, Datamining methods, Differences between Datamining and machine learning, Data-visualization, Datamining models, Decision Tree, Datamining applications in Bioinformatics.

Practicals:

1. Sequence alignment using BLAST (Basic Local Alignment Search Tool).
2. Sequence alignment using FASTA.
3. Multiple sequence alignment using ClustalW.
4. Comparative genomics and BLAST.
5. Cluster analysis on gene expression data using GENESIS.
6. Comparative Genome Analysis of two sequences using MUMmer.
7. Gene Finding using GLIMMER.
8. Sequence analysis using HMMER.
9. Sequence analysis using EMBOSS.

CBBI-706 **IPR Issues in Bioinformatics** **2** **2-0-1**

Unit 1

General Introduction, Patent Claims, The Legal Decision-Making Process, Ownership of Tangible and Intellectual Property.

Unit 2

Patentable Subject Matter, Novelty and the Public Domain, Non-obviousness.

Unit 3

Disclosure Requirements, Collaborative Research, Competitive Research, Plant Biotechnology, Foreign Patents.

Unit 4

Substantive Aspects of Patent Litigation, Procedural Aspects of Patent Litigation, Recent Developments in Patent System and Patentability of Biotechnological invention, IPR issues in the Indian Context.

Unit-5

Legal aspects of Genomics and Proteomics, bioethics, IPR and patents in Bioinformatics.

CBBI-707

Artificial Neural Networks

2

2-0-1

Unit 1

Probabilistic Framework & NP-Complete Problem, Bayesian Modeling, The Cox Jaynes Axioms, Numerical Probabilistic Algorithms, Las Vegas Algorithms.

Unit 2

Polynomials, Polynomial-time verification, NP-Completeness and Reducibility, NP-Completeness Proof, NP-Complete problems, Machine Learning Algorithms.

Unit 3

Gradient Descent, Expectation Maximization, Generalized Expectation Maximization Algorithms, Neural Networks, Back propagation, Markov Chains Monte Carlo algorithm, Simulated Annealing, Fuzzy Logic & Evolutionary/Genetic algorithm

CBBI-708

Bimolecular Modeling

3

2-0-1

Unit 1

Concepts of Molecular Modeling, Simulation of molecular mechanics and dynamics, Empirical representation of molecular energies, Simulations of Free Energy changes, Force fields, Use of Force Fields. A Energy minimization of small molecules, Local and global energy minima. Molecular Mechanics methods, Techniques in Molecular Dynamics, Monte Carlo Simulation for conformational analysis and semi-empirical methods, Application of molecular graphics.

Unit 2

Methods for Prediction of Secondary and Tertiary structures of Proteins - Knowledge-based structure prediction, Principles of Protein Folding, Fold recognition, Methods for comparison of 3D structures of proteins; Methods to predict three dimensional structures of nucleic acids.

Unit 3

Analysis of structures and correctness of structures, Submission of data to PDB: atomic coordinates and electron density maps; Anatomy of Proteins - Ramachandran plot. Evaluation of stereo-chemical properties of protein structures.

Unit 4

Internal and external co-ordinate system; Generation of co-ordinates of biopolymers in Cartesian and cylindrical polar co-ordinate system; Methods of single crystal X-ray diffraction of

macromolecules: molecular replacement method and direct method - Fiber diffraction. Structural data banks - Protein Data Bank, Cambridge small molecular crystal structure data bank.

Practicals:

1. Introduction to the structure database PDB.
2. Visualization of the protein structure using VMD.
3. Secondary structure prediction using GOR algorithm.
4. Tertiary structure prediction using SWISS-MODEL, ModWeb and Geno3D.
5. Homology modeling of a protein by using the MODELLER software.
6. Protein Structure validation using SAVS server.
7. Protein active site prediction using CastP and Pocket Finder.
8. Automated docking using PATCH DOCK webservice.
9. Structural alignment using DaliLite and SSAP.

MAS-411

Engineering Mathematics-I

4

3-1-0

Matrices: Theory of Matrices, Types, Addition, Subtraction, Multiplication, Transpose, Ad joint and Inverse of Matrices, Rank of Matrix, Solution of simultaneous equations, Eigen values, Cayley-Hamilton theorem.

Differential Calculus: Partial Differentiation, Euler theorem, Total differential coefficient, Partial higher order derivatives, Application of partial differentiation, Maxima-Minima of function of two variables, Jacobians.

Integral Calculus: Definite integrals and their properties, Application of determining area length, area, surface and volume. Simpson's rule for approximate integration, Mean values, Root mean square values.

Differential Equations: Ordinary differential equations their order, degree and formation, Solution of the equation of the first order, first degree, Homogenous differential equations, Linear differential equations, Exact differential equations, Linear differential equations of second order with constant coefficient, Homogenous linear equations, Applications.

CBBI-802

Chemoinformatics

3

2-0-1

Unit 1

Role of computers in chemical research, Introduction to Chemoinformatics, Representation and manipulation of 2D and 3D molecular structures, Chemical Databases - Design, Storage & Retrieval methods.

Unit 2

Reaction databases, Representation of chemical reactions, Search techniques (Full, Sub and Super structure), Similarity searches, Modeling of small molecules.

Unit 3

Combinatorial chemistry and Library design -Introduction, Diversed and focused Libraries, Combinatorial library design strategies, Product-based library design, Multiobjective library design.

Unit 4

Analysis of high-throughput screening data- Introduction, Data visualization, Data mining methods, Prediction of ADMET properties, Chemoinformatics tools for drug discovery.

Practicals:

1. To draw and analyze the chemical structures by using the ChemSketch / ChemDraw software.
2. To convert the chemical structure data from one file format to other file formats by using the CHIMERA / BABEL software.
3. To study about the different types of chemical structure databases.
4. To visualize the chemical structure in different views by using the visualization softwares.
5. To calculate the descriptors of few ligands by using the DRAGON software.
6. To perform the virtual screening of ligands by using the AUTODOCK program.

CBBI-803

Computer Aided Drug Designing

3

2-0-1

Unit-1

What are drugs? Various routes of Drug Administration, Pharmacokinetics - Absorption, Distribution, Metabolism, Elimination and Toxicity, Pharmacodynamics - Receptor Types, Theories of Receptor, Molecular mechanism of drug action through Enzymes, Ion channels and Carrier Proteins.

Unit-2

Drug discovery and development, Devising a Research Strategy, Challenges in Drug Discovery.

Rational

drug design, Structure based drug design- de novo drug design and Virtual screening of drugs.

Unit-3

Ligand based drug design- Quantitative Structure Activity Relationship, Molecular descriptors, 2D and 3D

QSAR analysis, Methods to derive 3D Pharmacophores, Pharmacophore mapping and its applications.

Unit-4

Docking- protein-ligand, protein-protein and protein-DNA docking, Algorithms, Scoring functions used in docking.

Practicals:

1. To perform the homology modeling of a protein by using the MODELLER software.
2. To evaluate the 3D structure of a protein by using the different tools on the SAVS server.
3. To find the active site/cavity in a receptor by using the SURFACE RACER program.
4. To draw the chemical structures by using the ChemSketch/ChemDraw software.
5. To perform the de novo Drug Designing by using the LIGBUILDER software.
6. To perform the protein-ligand docking by using the HEX program.
7. To perform the protein-protein docking by using the AUTOCOOCK software.

