

**M.TECH BIOINFORMATICS**  
**SEMESTER-I**

## **MBIN 101: Cell and Molecular Biology (Credits- 3)**

**Course Objectives:** The objectives of this course are to sensitize the students to the fact that as we go down the scale of magnitude from cells to organelles to molecules, the understanding of various biological processes becomes deeper and inclusive.

**Student Learning Outcomes:** Student should be equipped to understand three fundamental aspects in biological phenomena: a) what to seek; b) how to seek; c) why to seek?

### **Unit I: Dynamic organization of cell (6 lectures)**

Universal features of cells; cell chemistry and biosynthesis: chemical organization of cells; internal organization of the cell - cell membranes: structure of cell membranes and concepts related to compartmentalization in eukaryotic cells; intracellular organelles: endoplasmic reticulum and Golgi apparatus, lysosomes and peroxisomes, ribosomes, cellular cytoskeleton, mitochondria, chloroplasts and cell energetics; nuclear compartment: nucleus, nucleolus and chromosomes.

### **Unit II: Chromatin structure and dynamics (12 lectures)**

Chromatin organization - histone and DNA interactome: structure and assembly of eukaryotic and prokaryotic DNA polymerases, DNA-replication, repair and recombination; chromatin control: gene transcription and silencing by chromatin-Writers,-Readers and -Erasers; Transcriptional control: Structure and assembly of eukaryotic and prokaryotic RNA Polymerases, promoters and enhancers, transcription factors as activators and repressors, transcriptional initiation, elongation and termination; post-transcriptional control: splicing and addition of cap and tail, mRNA flow through nuclear envelope into cytoplasm, breakdown of selective and specific mRNAs through interference by small non-coding RNAs (miRNAs and siRNAs), protein translation machinery, ribosomes-composition and assembly; universal genetic codes, degeneracy of codons, Wobble hypothesis; Iso-accepting tRNA; mechanism of initiation, elongation and termination; co- and post-translational modifications, mitochondrial genetic code.

### **Unit III: Cellular signalling, transport and trafficking (3 lectures)**

Molecular mechanisms of membrane transport, nuclear transport, transport across mitochondria and chloroplasts; intracellular vesicular trafficking from endoplasmic reticulum through Golgi apparatus to lysosomes/cell exterior.

### **Unit IV: Cellular processes (8 lectures)**

Cell cycle and its regulation; cell division: mitosis, meiosis and cytokinesis; cell differentiation: stem cells, their differentiation into different cell types and organization into specialized tissues; cell-ECM and cell-cell interactions; cell receptors and trans-membrane signalling; cell motility and migration; cell death: different modes of cell death and their regulation.

### **Unit V: Manipulating and studying cells (3 lectures)**

Isolation of cells and basics of cell culture; observing cells under a microscope, different types of microscopy; analyzing and manipulating DNA, RNA and proteins.

### **Unit VI: Genome instability and cell transformation (8 lectures)**

Mutations, proto-oncogenes, oncogenes and tumour suppressor genes, physical, chemical and biological mutagens; types of mutations; intra-genic and inter-genic suppression; transpositions-transposable genetic elements in prokaryotes and eukaryotes, role of transposons in genome; viral and cellular oncogenes; tumor suppressor genes; structure, function and mechanism of action; activation and suppression of tumor suppressor genes; oncogenes as transcriptional activators.

**Recommended Textbooks and References:**

1. Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K., & Walter, P. (2002). Molecular Biology of the Cell. New York: Garland Science.
2. Lodish, H. F. (2000). Molecular Cell Biology. New York: W.H. Freeman.
3. Krebs, J. E., Lewin, B., Kilpatrick, S. T., & Goldstein, E. S. (2014). Lewin's Genes XI. Burlington, MA: Jones & Bartlett Learning.
4. Cooper, G. M., & Hausman, R. E. (2009). The Cell: a Molecular Approach. Washington: ASM; Sunderland.
5. Hardin, J., Bertoni, G., Kleinsmith, L. J., & Becker, W. M. (2012). Becker's World of the Cell. Boston: Benjamin Cummings.
6. Watson, J. D. (1987). Molecular Biology of the Gene (7th ed.). Menlo Park, CA: enjamin/Cummings.

**MBIN 102: Biochemistry (Credits- 3)**  
**Course Objectives**

**The objectives:** The objectives of this course are to build upon undergraduate level knowledge of biochemical principles with specific emphasis on different metabolic pathways. The course shall make the students aware of various disease pathologies within the context of each topic.

**Student Learning Outcomes:** On completion of this course, students should be able to:

- Gain fundamental knowledge in biochemistry;
- Understand the molecular basis of various pathological conditions from the perspective of biochemical reactions.

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**Unit I: Protein structure (7 lectures)**

Chemical basis of life: Miller-Urey experiment, abiotic formation of amino acid oligomers, composition of living matter; Water – properties of water, essential role of water for life on earth pH, buffer, maintenance of blood pH and pH of gastric juice, pH optima of different enzymes (pepsin, trypsin and alkaline phosphatase), ionization and hydrophobicity, emergent properties of biomolecules in water, biomolecular hierarchy, macromolecules, molecular assemblies; Structure-function relationships: amino acids – structure and functional group properties, peptides and covalent structure of proteins, elucidation of primary and higher order structures, Ramachandran

plot, evolution of protein structure, protein degradation and introduction to molecular pathways controlling protein degradation, structure-function relationships in model proteins like ribonuclease A, myoglobin, hemoglobin, chymotrypsin etc.; basic principles of protein purification; tools to characterize expressed proteins; Protein folding: Anfinsen's Dogma, Levinthal paradox, cooperativity in protein folding, free energy landscape of protein folding and pathways of protein folding, molten globule state, chaperons, diseases associated with protein folding, introduction to molecular dynamic simulation.

### **Unit II: Enzyme kinetics (6 lectures)**

Enzyme catalysis – general principles of catalysis; quantitation of enzyme activity and efficiency; enzyme characterization and Michaelis-Menten kinetics; relevance of enzymes in metabolic regulation, activation, inhibition and covalent modification; single substrate enzymes; concept of catalytic antibodies; catalytic strategies with specific examples of proteases, carbonic anhydrases, restriction enzymes and nucleoside monophosphate kinase; regulatory strategies with specific example of hemoglobin; isozymes; role of covalent modification in enzymatic activity; zymogens.

### **Unit III: Glycobiology (2 lectures)**

Sugars-mono, di, and polysaccharides with specific reference to glycogen, amylose and cellulose, glycosylation of other biomolecules-glycoproteins and glycolipids; lipids- structure and properties of important members of storage and membrane lipids; lipoproteins.

### **Unit IV: Structure and functions of DNA, RNA and Lipids (3 lectures)**

Self-assembly of lipids, micelle, biomembrane organization - sidedness and function; membrane bound proteins - **structure**, properties and function; transport phenomena; nucleosides, nucleotides, nucleic acids - structure, a historical perspective leading up to the proposition of DNA double helical structure; difference in RNA and DNA structure and their importance in evolution of DNA as the genetic material.

### **Unit V: Bio-energetics (8 lectures)**

Bioenergetics-basic principles; equilibria and concept of free energy; coupled interconnecting reactions in metabolism; oxidation of carbon fuels; recurring motifs in metabolism; Introduction to GPCR, Inositol/DAG//PKC and Ca<sup>++</sup> signaling pathways; glycolysis and gluconeogenesis; reciprocal regulations and non-carbohydrate sources of glucose; Citric acid cycle, entry to citric acid cycle, citric acid cycle as a source of biosynthetic precursors; Oxidative phosphorylation; importance of electron transfer in oxidative phosphorylation; F1-F0 ATP Synthase; shuttles across mitochondria; regulation of oxidative phosphorylation; Photosynthesis – chloroplasts and two photosystems; proton gradient across thylakoid membrane.

### **Unit VI: Role of vitamins & cofactors in metabolism (12 lectures)**

Calvin cycle and pentose phosphate pathway; glycogen metabolism, reciprocal control of glycogen synthesis and breakdown, roles of epinephrine and glucagon and insulin in glycogen metabolism; Fatty acid metabolism; protein turnover and amino acid catabolism; nucleotide biosynthesis; biosynthesis of membrane lipids and sterols with specific emphasis on cholesterol metabolism and mevalonate pathway; elucidation of metabolic pathways; logic and integration of central metabolism; entry/ exit of various biomolecules from central pathways; principles of metabolic

regulation; steps for regulation; TOR (target of rapamycin) & autophagy regulation in relation to C & N metabolism, starvation responses and insulin signalling.

**Recommended Textbooks and References:**

1. Stryer, L. (2015). Biochemistry. (8th ed.) New York: Freeman.
2. Lehninger, A. L. (2012). Principles of Biochemistry (6th ed.). New York, NY: Worth.
3. Voet, D., & Voet, J. G. (2016). Biochemistry (5th ed.). Hoboken, NJ: J. Wiley & Sons.
4. Dobson, C. M. (2003). Protein Folding and Misfolding. Nature, 426(6968), 884-890. doi:10.1038/nature02261.
5. Richards, F. M. (1991). The Protein Folding Problem. Scientific American, 264(1), 54-63. doi:10.1038/scientificamerican0191-54.

**MBIN 103: Basics of Mathematics and Statistics (Credits- 3)**

**Course Objectives:** The objective of this course is to give conceptual exposure of essential contents of mathematics and statistics to students.

**Student Learning Outcomes:** On completion of this course, students should be able to:

- Gain broad understanding in mathematics and statistics;
  - Recognize importance and value of mathematical and statistical thinking, training, and approach to problem solving, on a diverse variety of disciplines.
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**Unit I: Algebra (6 lectures)**

Linear equations, functions: slopes-intercepts, forms of two-variable linear equations; constructing linear models in biological systems; quadratic equations (solving, graphing, features of, interpreting quadratic models etc.), introduction to polynomials, graphs of binomials and polynomials; Symmetry of polynomial functions, basics of trigonometric functions, Pythagorean theory, graphing and constructing sinusoidal functions, imaginary numbers, complex numbers, adding-subtracting-multiplying complex numbers, basics of vectors, introduction to matrices.

**Unit II: Calculus (4 lectures)**

Differential calculus (limits, derivatives), integral calculus (integrals, sequences and series etc.)

**Unit III: Mathematical models in biology (3 lectures)**

Population dynamics; oscillations, circadian rhythms, developmental patterns, symmetry in biological systems, fractal geometries, size-limits & scaling in biology, modelling chemical reaction networks and metabolic networks.

**Unit IV: Statistics (5 lectures)**

Probability: counting, conditional probability, discrete and continuous random variables; Error propagation; Populations and samples, expectation, parametric tests of statistical significance, nonparametric hypothesis tests, linear regression, correlation & causality, analysis of variance, factorial experiment design.

#### **Unit IV: Numerical methods (15 lectures)**

Solution of non-linear equations: Bisection method, Regula-Falsi method, Newton Raphson.

Solution of linear equations: Gauss Jordan, Gauss-Seidal iterative method, LU Factorization method.

Interpolation: Lagrange's method, Newton's Forward and Backward, Symbolic operators

Numerical integration: Trapezoidal method, Simpson 1/3 method.

Solution of differential equation: Taylor's series, Euler's method, Runge-Kutta method.

#### **Recommended Textbooks and References:**

1. Stroud, K. A., & Booth, D. J. (2009). Foundation Mathematics. New York, NY: Palgrave Macmillan.
2. Aitken, M., Broadhursts, B., & Haldky, S. (2009) Mathematics for Biological Scientists. Garland Science.
3. Billingsley, P. (1986). Probability and Measure. New York: Wiley.
4. Rosner, B. (2000). Fundamentals of Biostatistics. Boston, MA: Duxbury Press.
5. Daniel, W. W. (1987). Biostatistics, a Foundation for Analysis in the Health Sciences. New York: Wiley.

#### **MBIN 104: Bio tools and Bio database (Credits- 3):--**

##### Unit I-Introduction to Bioinformatics

A word on Bioinformatics

- Introduction
- Branches of Bioinformatics
- Aims of Bioinformatics
- Scope/research areas of bioinformatics

##### Unit II-Biological tools and databases

###### **Sequence and molecular file form and ats**

- Introduction
- Sequence file formats
- Sequence conversion tools

- Molecular file formats
- Molecular file format conversion

#### Databases in bioinformatics & introduction: -

- Introduction
- Biological databases
- Classification schema of biological databases
- Biological database retrieval system

#### **Biological sequence databases**

##### *A. National Centre for biotechnology information (NCBI)*

- *Introduction*
- Tools and databases of NCBI
- Database retrieval tool
- Sequence submission to NCBI
- BLAST
- PSI-BLAST
- RPS-BLAST
- Specialized tools
- Nucleotide database
- Literature database
- Protein database
- Gene expression database
- GEO
- Structural database
- Chemical database
- Other databases

##### **B. EMBL Nucleotide Sequence Database**

- Introduction
- Sequence retrieval
- Sequence submission at EMBL
- Resources of EMBL
- Biological annotation and data curation
- Sequence analysis tools
- Features of database

##### **C. DNA databank of Japan**

- Introduction
- Resources of DDBJ
- Data submission to DDBJ

##### **D. Protein information resource**

- Introduction

- Resources of PIR
- Data retrieval of PIR
- Databases of PIR

#### **E. Swiss-Prot**

- Introduction
- Features of Swiss-prot

### **Protein 3D structure and classification databases**

#### **A. Protein databank**

- Introduction
- Harnessing data from PDB
- Data deposition tools
- PDB beta
- RCSB PDB structural genomics information portal

#### **B. Molecular modelling databases**

- Introduction
- Retrieval of structural data from MMDB
- Conserved domain database

#### **C. E-MSD**

- Introduction
- Resources of E-MSD
- Data submission at E-MSD
- Search system of E-MSD

#### **D. 3D genomics**

- Introduction
- Assessing 3D genomics

#### **E. Gene 3D**

- Introduction
- Retrieving data from gene 3D

#### **F. Protein structural classification**

##### **Databases**

- Introduction
- CATH-Class, Architecture, Topology, Homologous
- SCOP (Structural Classification of Proteins)

### **Unit III: Bio-algorithms and tools**



## Sequence alignments

- Introduction
- Concept of alignment
- Scoring Matrices
- PAM
- BLOSUM
- Alignment of pairs of sequences
- Alignment algorithms
- Heuristic methods
- Multiple sequence Alignment (MSA)

## Gene prediction methods: principles and challenges

- Introduction
- Biological overview
- What is gene prediction?
- Computational methods of gene prediction
- Combination of two methods
- Why is gene prediction difficult?

## Molecular Phylogeny

- Introduction
- Phenotypic phylogeny and molecular phylogeny
- Molecular clocks
- Methods of phylogeny
- Statistical Evaluation of the obtained phylogenetic trees or validation methods
- Software for phylogenetic analysis
- Reliability of molecular phylogenetic prediction

## Molecular Viewers

- Introduction
- A few molecular viewers
- RasMol
- Deep view- The Swiss-PDB viewer
- (SPDBV)
- Cn3D

## **Unit IV: Protein Modelling**

### Protein structure and modelling

#### **A. Protein and secondary structure prediction**

- Introduction
- Levels of protein structure
- Conformational parameters Secondary structure of a protein
- Secondary structure types

- Secondary structure prediction
- Software for secondary structure prediction
- Limitations of secondary structure prediction

#### **B. Protein modelling**

- Introduction
- Methods of protein modelling
- Homology or comparative modelling
- Model refinement
- Evaluation of the model
- Hands on in comparative modelling using Swiss-model
- Threading or fold recognition
- *Ab initio*/De novo method

#### **Recommended Textbooks and References:**

1. Mount, D. W. (2001). Bioinformatics: Sequence and Genome Analysis. Cold Spring Harbor, NY: Cold Spring Harbor Laboratory Press.
2. Bourne, P. E., & Gu, J. (2009). Structural Bioinformatics. Hoboken, NJ: Wiley-Liss.
3. Lesk, A. M. (2004). Introduction to Protein Science: Architecture, Function, and Genomics. Oxford: Oxford University Press.
4. Campbell, M & Heyer, L. J. (2006), Discovering Genomics, Proteomics and Bioinformatics, Pearson Education.
5. Oprea, T. (2005). Chemoinformatics in Drug Discovery, Volume 23. Wiley Online Library.
6. Gasteiger, J. & Engel, T. (2003), Chemoinformatics: a Textbook, Wiley Online Library

#### **MBIN 105: Computational Techniques (Credits- 3)**

**Course Objectives:** The objective of this course is to give conceptual exposure of essential contents of programming languages in procedural and object oriented way to students.

**Student Learning Outcomes:** On completion of this course, students should be able to:

- Gain broad understanding about procedural oriented concept and syntactical concept of C language to problem solving on a diverse variety of disciplines.
- Recognize importance of object oriented thinking and syntactical concept of C++ language to problem solving on a diverse variety of disciplines.

#### **PROCEDURAL ORIENTED PROGRAMMING C**

**Introduction (2 lectures):** Programming Language concepts & Introduction to C. C character set, Constants, variables and keywords, Type of variables & constants. Rules of constructing variable identifier.

**Operators (2 lectures):** Types of C Instructions (Type declaration, Arithmetic & Control Instructions), Data Types, Operators, Hierarchy of operators, Associativity of operators, Type conversion (explicit and implicit),

**Control Instructions (1 lecture):** if-else, switch case, conditional operator.

**Loop (2 lectures):** for, while, do-while, break & continue statement.

**Array (3 lectures):** one-dimensional & multi-dimensional (2D) array.

**Function and pointer (6 lectures):** Prototype, definition and calling of function, Recursive functions, Call-by-value & Call-by-address, passing array to function, Pointer concept, pointer to pointer, pointer operations, pointer and array.

**C Pre-processor (2 lectures):** Concept, File inclusion & Macro expansion, Symbolic constants. Type modifiers (long, short & signed), Storage class (auto, extern, static & register).

**String (3 lectures):** Pointer and String, Standard library functions (strlen(), strcpy(), strcmp(), strcat()).

**Structure (2 lectures):** Structure and Union, Self-referential structure.

**File handling (3 lectures):** File opening modes, Reading from file, writing into file.

## **OBJECT ORIENTED PROGRAMMING C++**

**Introduction (2 lectures):** What is object oriented programming? Why do we need object oriented? Programming characteristics of object oriented languages C and C++.

**C++ Programming basics (1 lecture):** Output using cout. directives, Input with cin, Type bool, Type conversions.

**Functions (3 lectures):** Returning values from functions, Reference arguments, Overloaded function, Inline function, Default arguments, Returning by reference.

**Object and Classes (5 lectures):** Making sense of core object concepts (Encapsulation, Abstraction, Polymorphism, Classes, Messages Association, Interfaces), Implementation of class in C++, C++ Objects as physical object, C++ object as data types constructor, Object as function arguments, The default copy constructor, returning object from function, Structures and classes, Classes objects and memory static class data, Const and classes, Arrays and string arrays fundamentals, Arrays as class Member.

**Data (1 lecture):** Arrays of object, string, the standard C++ String class.

**Operator overloading (2 lectures):** Overloading unary operations, Overloading binary operators, data conversion, pitfalls of operators overloading and conversion keywords, Explicit and Mutable.

**Inheritance (5 lectures):** Concept of inheritance, Derived class and based class, Derived class constructors, member function, inheritance in the English distance class, class hierarchies, inheritance and graphics shapes, public and private inheritance, Classes within classes, inheritance and program development.

**Virtual Function (2 lectures):** Virtual Function, friend function, Static function, Assignment and copy initialization, this pointer, dynamic type information.

**Streams and Files (3 lectures):** Streams classes, Stream Errors, Disk File I/O with streams, file pointers, error handling in file I/O with member function, overloading the extraction and insertion operators, memory as a stream object, command line arguments, and printer output.

**Templates and Exceptions (2 lectures):** Function templates, Class templates Exceptions

Reference Books:

- Programming with C – by Byron Gottfried
- Let Us C -by Yashavant P. Kanetkar
- C++: The Complete Reference, 4th Edition - The Complete Reference -by Schildt Herbert)
- Mastering C++ Programming –by Jeganathan Swaminathan
- The C++ Programming Language – by Bjarne Stroustrup

### **MBIN 192: Biochemistry Lab & Analytical Techniques Lab (Credits- 3)**

**Course Objectives:** The objective of this laboratory course is to introduce students to experiments in biochemistry. The course is designed to teach utility of experimental methods in biochemistry in a problem oriented manner.

**Student Learning Outcomes:** Students should be able to:

- Elaborate concepts of biochemistry with simple experiments;
- Understand principle and working of basic laboratory instruments.

1. Estimation of sugars – Reducing and non-reducing sugars.

2. Titration of Amino Acids and separation of aliphatic, aromatic and polar amino acids by thin layer chromatography.

3. Purification and characterization of an enzyme from a recombinant source (such as Alkaline Phosphatase or Lactate Dehydrogenase or any enzyme of institution's choice).

a. Preparation of cell-free lysates

b. Ammonium Sulphate precipitation

c. Ion-exchange Chromatography

d. Gel Filtration

e. Affinity Chromatography

f. Generating a Purification Table (protein concentration, amount of total protein)

g. Computing specific activity of the enzyme preparation at each stage of purification

h. Assessing purity of samples from each step of purification by SDS-PAGE Gel Electrophoresis

i. Enzyme Kinetic Parameters:  $K_m$ ,  $V_{max}$  and  $K_{cat}$ .

j. Dialysis of the purified protein solution against 60% glycerol as a demonstration of storage method

4. Identification of an unknown sample as DNA, RNA or protein using available laboratory tools.

5. Biophysical methods (Circular Dichroism Spectroscopy, Fluorescence Spectroscopy).

6. Determination of mass of small molecules and fragmentation patterns by Mass Spectrometry.

#### **MBIN 194: Bio tools and Bio database Lab (Credits- 3):-**

1 Downloading macromolecular sequences from the NCBI database in different file formats.

2 Using BLAST search creation of a data-set on the basis of the E-value.

3. Different secondary structure of RNA molecules. Experiment on clover-leaf structure of tRNA molecule. Experiment on stemloop structure of miRNA molecule for prediction of ideal miRNA candidate.

4. Experiment on codon usage and its significance for biosystem. Synonymous and non- synonymous codon usage analysis for prediction of evolution of mRNA gene. Relative Synonymous Codon Usage(RSCU),Codon Adaptation Index(CAI) & Codon Impact Parameter(CIP) analysis for evolution study.

5. Using EMBOSS for local and global alignment of nucleotide & proteins.

6. Determination of domains present in proteins and comparison of domain architecture (DA) across different proteins.

7. Identification of repeats in proteins using Pfam.

8. Pair wise alignment analysis & Multiple sequence alignment analysis : Preliminary experiment for formation of the backbone of different types of phylogeny

9. Construction of phylogenetic tree using PHYLIP, MegaX. Bootstrap analysis.

#### **MBIN 195: Computational Techniques Lab (Credits- 6)**

**Course Objectives:** The objective of this laboratory course is to introduce students to solve several problems in different discipline using C and C++ programming languages.

**Student Learning Outcomes:** Students should be able to:

- Familiar in Linux operating system and commands.
- Understand the concepts of Perl programming syntax and solve various problems.
- Understand the concepts of C programming syntax and solve various problems.
- Understand the concepts of C++ programming syntax and solve various problems.

## **Part I (Credits- 3):**

### **Unit I: The Linux Operating System**

1. Brief history of Linux.
2. Overview of Linux OS – Kernel, Shell, Applications, File system organization, Desktops like GNOME, KDE.
3. Linux Command Line Utilities – General purpose utilities, File system navigation, File attributes and handling, Environment variables, Shell, Wild cards and Regular Expression, Filters.
4. Bash Shell scripting
5. Working with vi/vim editor.
6. System Administration with Reference to Linux File System – Partitions, File system organization, ext2 file system, Inodes, Super block, Boot block, Data block, Mounting other file systems, symbolic link etc.
7. User management and remote login.

### **Unit II: Perl Programming**

1. Introduction – History, availability, support and use with special reference to bioinformatics.
2. Scalar data – Concept, numbers, strings, operators, variables and functions.
3. Array and List Data – Concept, literal representation, variables, operators and functions.
4. Hashes – Concept, Literal representation, variables, hash functions and slices, Hash of Hashes and Hash of arrays.
5. Basic I/O
6. Regular Expressions – Concept, Uses of Regex and Pattern matching, Operator and substitutions, split and join functions.
7. Subroutines – System and user functions, local operator, Parameter list, parameter passing by value and by reference.
8. Various control structures.
9. File Handles and File Tests – Concept, Opening and closing of File Handles, Using path and file names, Using file handle, die, -x File tests.
10. Process Management – Using system, exec, and back quotes.
11. Data Transformations – Finding substring, Extracting and Replacing a Substring.
12. Formatting Data – Sorting and Transliteration.
13. Objecting Oriented Perl – Introducing to modules, Creating Objects.

14. Bioperl – Introduction, Installation procedures and uses of Bioperl.

**Part II (Credits- 3):**

**Procedure oriented Programming using C**

- C basics - Variables, Constant, Data types, Keywords
- Logical or decision making block
  - If
  - If – else
  - Nested if – else
  - If – else ladder
  - Switch case
- Repetition of same process: Loops
  - While loops
  - Do – While loops
  - For loops
- Array
  - Type of array, Declaration of array, creation of array
  - One dimensional array
  - Two dimensional array
  - Matrix creation and manipulation and calculation using array
- Functions
  - Types, need, features
  - Library function
  - User defined function
  - Returnable and non-returnable function
- Structures
  - Creation, Declaration
  - Difference between Array and Structure
  - Array of Structure
- Pointers
  - Importance and uses
  - Difference between pointer and array
  - Structure using pointer
  - Memory handling

## **Object oriented Programming using C++**

Write programs on the following –

- demonstrate call by reference
- demonstrate the Constructor Overloading, assume desired parameters.
- create the class shape, and overload the function to return the perimeters of the different shapes.
- demonstrating the public, protected and private parameters.
- demonstrating the Static Data member.
- demonstrate constructor with default argument.
- demonstrate destructor in inheritance.
- demonstrate unary and binary operator over complex number class.
- demonstrate multiple and multilevel inheritance.
- demonstrate public, private and protected inheritance.
- demonstrate constructor and destructor call in the derived class.
- demonstrate virtual function.
- demonstrate friend function.
- implement a class for complex numbers with add and multiply as member functions.
- Overload ++ operator to increment a complex number.



**SEMESTER-II**

## **Course: MBIN 201:- Biomolecular structure and function**

### **1. Structural Biology & Statistical Thermodynamics**

Laws of thermodynamics, concepts of entropy and free energy, isothermal and adiabatic processes, the Carnot cycle, specific heats at constant pressure and volume, concepts of statistical thermodynamics, calculation of partition functions, rotation about single bonds and intramolecular energy, conformational entropy of hydrogen bonded molecules, cooperative phenomena in proteins and DNA, zipper model for helix-coil transitions in proteins, solution behavior of macromolecules.

### **2. Structural Biology & XRay Crystallography**

Translational vectors, unit cell, symmetry operations on crystals: rotation, reflection and inversion, point and space symmetry groups, x-ray diffraction and Bragg's law, Miller indices, reciprocal lattice, structure factors and Fourier transforms, Diffraction pattern for DNA, protein crystallography, calculation of bond lengths, bond angles and dihedral angles from protein data base (PDB) files.

### **3. Structural Biology & Molecular Spectroscopy**

UV-visible spectroscopy for molecular electronic spectra: signal to noise ratio, inherent line broadening, transition probability and population difference, Fourier transformation Circular dichroism (CD) and optical rotatory dispersion (ORD), the Cotton effect and their applications in structural biology Nuclear Magnetic Resonance (NMR), chemical shifts, coupling constant, applications of 2D NMR in structural biology. IR & Raman spectroscopy for molecular vibrations and rotations and its applications in determination of macromolecular structure Fluorescence spectroscopy and its applications in structural biology

## **Course: MBIN 203; Computational Methods in Biology**

### **Nucleic Acid Structure:**

- Watson-Crick
- Base Pairs.
- Double Helix.
- Triple Helix.
- Quadruplet Helix.
- DNA-Ligand Interaction.
- Structural features of A-DNA, B-DNA, Z-DNA.
- Sequence directed structure [Crick's Rule].
- Base-pair parameters .

### **Macromolecular Interaction:**

- Vanderwaals force .
- Coulombic Forces .
- Receptor-Ligand interaction .
- Monte Carlo simulation.
- Genetic Algorithm .
- Molecular mechanics force field .
- Energy minimization (Steepest Descent, Conjugate gradient, NR)

### **Drug Design:-**

1. Basic concept

## 2. Drug Development: Lead modification

1. Identification of the the active part: The Pharmacophore
2. Functional group modification
3. StructureActivity Relationships
4. Structure modification to increase potency
  - Homologation
  - Chain branching
  - Ring-Chain transformation
  - Bioisosterism
5. Quantitative Structure-Activity Relationships
  - Physicochemical parameters
  - Electronic effects: The Hammett Equation
  - Lipophilicity effects: The basis for the Hansch equation
  - Steric effect
  - Correlation between physicochemical parameters and biological activity: Hansch equation.

### **Advanced Statistics**

1. Stochastic process, Markov properties, Markov chains, Markov matrices. Hidden Markov model. Forward algorithm, Viterbi algorithm, Baum-Welch algorithm.
2. Maximum Likelihood Test; Likelihood ratio test. MLE estimation for univariate Gaussian distribution, Poisson distribution and Binomial distribution.
3. Cluster Analysis: Hierarchical clustering. Computing metric, computing linkage. Single linkage, complete linkage and average linkage clustering.
4. Cluster Analysis: kmeans clustering. Convergence of the algorithm. Weakness of kmeans clustering.
5. Principal Component Analysis: Change of basis; Variance of noisy data, Reduction of dimension; Diagonalization of covariance matrix.
6. Singular Value Decomposition: Full singular value decomposition; Reduced singular value decomposition.

### **Course: MBIN 204; Proteomics and Genomics**

Modern concepts of metabolomics, genomics, proteomics, functional genomics, systems biology. Wholistic concepts of Omics. Overview of technologies, driving work in these areas.

Problems related to genomes in Biology: Cvalue paradox, genome assembly, genome evolution, comparative genomics synteny, gene detection, conservation, gene volatility, linkage, SNP, alternate splicing. General application using Neural Networks.

Regulatory signals on genome: promoters, attenuators, terminators, riboswitches.

Functional signatures in genomes: repeats, epigenetics

Transcriptomics: basic concepts and technology, data normalization, clustering (Hierarchical, kmeans, SOM), detection of over expression and under expression (PCA). Modeling using Boolean Networks. EST, Unigene.

Proteomics: limitations and advantages over transcriptomics, outline of a typical proteome experiment, example applications of proteomics technologies, mass spectrometry different instrumental configuration, its advantages in terms of accuracy and sensitivity, spectra deconvolution, tandem mass spectrometry peptide.

sequencing using denovo and database search (different ion nomenclatures, scoring), outline of quantitative proteomics experiment

Structural proteomics: fundamentals of protein/peptide structure, energetics (including Poisson Boltzmann Equation). Molecular mechanical energy functions and force fields, Monte Carlo, Simulated Annealing, Genetic Algorithm, Introduction to molecular dynamics simulation.

**Course: MBIN 205; Intellectual Property Rights Law**

**Module 1: General Overview of Intellectual Property** Introduction *in rem*: Nature and Objectives of Intellectual property A General Overview, Justifications for Protection and Historical Perspectives, Basic Principles and Acquisition of IPRs

**Module 2:** Industrial Property: Patents, Designs

**Module 3:** Industrial Property: Trademarks, Geographical Indications, Trade Secrets and Role of Unfair Competition with practical examples

**Module 4:** Protection of Copyrights and Related Rights (National & International Regimes)

**Module 5:** Semiconductors Integrated Circuits Layout Designs and Layout Designs Topography

**Module 6:** Contemporary Intellectual Property Issues

**Module 7:** Ownership and Enforcement of Intellectual Property Rights

**Module 8:** Nanotechnology & IPRs : A Corporate Overview in the Indian Perspective through Primary Source Materials

**Cases and Statutes:**

**Course: MBIN 292; Computer language**

**Procedure oriented Programming using C**

- **C basics**
  - Variables, Constant, Data types, Keywords
- **Logical or decision making block**
  - If
  - If – else
  - Nested if – else
  - If – else ladder
  - Switch case
- **Repetition of same process: Loops**
  - While loops
  - Do – While loops
  - For loops
- **Array**
  - Type of array, Declaration of array, creation of array
  - One dimensional array
  - Two dimensional array
  - Matrix creation and manipulation and calculation using array
- **Functions**
  - Types, need, features
  - Library function
  - User defined function

- Returnable and non returnable function
- **Structures**
  - Creation, Declaration
  - Difference between Array and Structure
  - Array of Structure
- **Pointers**
  - Importance and uses
  - Difference between pointer and array
  - Structure using pointer
  - Memory handling

## **Object oriented Programming using JAVA**

- **Java Basics**
  - An Introduction to Java Programming
  - ObjectOriented
  - Programming and Java
  - Arrays, Conditionals, and Loops
- **Creating Classes and Applications in Java**
  - Working with Objects
- **More About Methods**
  - Main Method
  - User defined
  - Abstract Method
- **Packages**
  - What is packages
  - Types of Packages
- **Inheritance**
  - What is Inheritance
  - Types of Inheritance
  - Extends keyword
- **Interfaces**
  - Why Interface
  - What is Interface
  - Implements keyword
- **Exception Handling**
  - Error and Exception
  - Types of Exceptions
  - Try, Catch, Finally block
- **Multithreading**
  - What is Threading
  - Need and Purpose of Threading
  - Creating Threads
  - Thread Life Cycle
  - Managing Threads from one state to another
- **Applet**
  - Applet Life Cycle
  - Graphics, Fonts, and Color
  - Simple Animation and Threads
  - Images and Threads

## **PHP**

1. Basic HTML Introduction, HTML Tags, HTML documents / Web Pages, Elements, Element Syntax, Attributes, Headings, Paragraphs, Lines, Comments, Line break, Text Formatting – bold, italics, font, color, size etc., Background, HTML links, hyperlinks, Images, Tables, Lists, Forms – various objects / elements and their attributes in forms like text, text area, radio, check box, button submit, option etc.
2. Brief Overview of Web servers, Web Browsers and Apache HTTP server.
3. Introduction to PHP What is PHP?, requirements, Why PHP? Basic PHP syntax, tag, Comments in PHP, variables, different operators (arithmetic, assignment, comparison, logical and concatenation).
4. PHP Conditional Statements if, if ... else, if ... elseif ... else, Nested if ... else, Switch Statement.
5. PHP array Numeric, Associative, Multidimensional array. Creation, Assign values, retrieve values and Dynamic creation.
6. PHP Loops :while, do ... while, for, foreach
7. PHP form handling.
8. PHP functions Declaring functions, Adding parameters, Returning values.
9. Working with PHP \$\_GET, \$\_POST, \$\_SELF.
10. Using various builtin functions array\_pop(), array\_push(), array\_reverse(), array\_shift(), array\_unshift(), sort, print, printf, split, join, strlen, substr.
11. PHP MySQL Connect, Create, Insert, Select etc.