

Course: MBIN 101; Biomolecular structure and function –I

1. Elements of Quantum Theory

Wave-particle duality and the uncertainty principle, Schrödinger equation, probabilistic interpretation of the wave function, energy levels in rectangular potential well with applications, linear oscillator and rigid rotator models for diatomic molecules, energy levels of hydrogen-like atoms and the nature of atomic orbitals.

2. Chemical Bonding in Molecules

Formation of chemical bonds, molecular orbital (MO) theory and linear combination of atomic orbitals (LCAO), electronic energy levels and the nature of molecular orbitals in a hydrogen molecule, hybridized orbitals of carbon with applications to organic and biologically important molecules.

3. Structure Reactivity and Mechanism

Chemical bond breaking: homolytic or heterolytic cleavage, factors influencing electron availability: inductive and resonance effects and their time variable properties, dipole moments; stereo-electronic requirement for a reaction, structure and physico-chemical properties of amino acids, peptides and proteins, implication of stereo-electronic requirements in peptide and protein structural hierarchy.

4. Energetics, Kinetics and Spontaneous Process

Covalent and non covalent interactions for stabilization, chemical kinetics and thermodynamic principles, criteria for aromaticity, reaction kinetics and energy profile diagram, pseudo order reaction, isotope labeling, kinetically and thermodynamically controlled reaction, implications in peptide and protein structural stabilization and folding pathways.

Course: MBIN 102, Molecular Cell Biology and Genetics

Genetics

Unit I: Basic Genetics: Mendelian genetics, Meiosis, Linkage & Recombination, Hardy Weinberg Principle.

Unit II: Molecular Genetics: DNA Replication, transcription, translation, Mutations, Gene technology, cloning vectors, Restriction enzymes, PCR and its applications, Northern, Southern & Western blotting, Automated DNA sequencing

Unit III: Human Genetics: X-linked and autosomal diseases, Chromatin structure of eukaryotes, Chromosomal and genetic syndromes, Genetic markers, Human Genome mapping, Gene therapy, Cancer Genetics

Biochemistry

Lipids: Storage lipids (fatty acids, triglycerides), membrane lipids, glycerophospholipids, sphingolipids, sterols, Biosynthesis of fatty acids, triglycerides and membrane phospholipids

Water: Summary of its properties, hydrogen bonds, ionization of water, weak bases and weak acids, pH scale, buffering, Henderson-Hasselbach equation, Buffer systems in biology

Catabolism of Hexoses : Glycolysis, Fates of pyruvate under aerobic and anaerobic conditions, Degradation of sugars, Regulation of carbohydrate catabolism, TCA cycle, Gluconeogenesis, Biosynthesis of glycogen, glucose

Enzymes: Reaction rates, specificity, transition state, Enzyme kinetics (Michaelis-Menten equation, inhibition mechanisms)

Bioenergetics and Metabolism : Oxidative phosphorylation (ATP synthesis driven by electron transfer and electron flow in mitochondria) ; ATP synthesis and respiratory electron flow; Regulation of ATP synthesis, thermogenin and brown fat, hibernation

Carbohydrates of Physiological Significance

1. **Carbohydrates:** Monosaccharides, Oligosaccharides, Aldoses & Ketoses, Conversion of aldose to ketose and vice versa, D and L – sugars, Mutarotation, Conversion of pentose to hexose and vice versa,

Glucose with Fisher projection formula and Haworth pyranose structure,
Reaction of glucose, Test of Glucose

2. Polysaccharides: Starch, Cellulose, Chitin and chitosan, Application, Glycosaminoglycans, Hexoses of physiologic significance, Disaccharides of physiologic significance

3. Glycoproteins: Classification, Type of glycoprotein, Function of glycoprotein

4. Carbohydrate-mediated interaction: Fundamentals of protein-carbohydrate interaction, Glycobiology of diseases

Course: MBIN 103; Computational Methods in Biology- I

File formats – GenBank, FASTA, MSF, NBRF-PIR, GCG.

Definition of terms -Orthology, paralogy, xenology and analogy. Similarity and Identity.

Substitution matrices – PAM, BLOSUM, principles based on which these matrices are derived, Scoring Schemes, gap penalty, concept of distance and similarity matrix

Database searches – BLAST algorithm, Significance of the result, statistical parameters, filtering – DUST & SEG

Alignments – pairwise alignment, Dynamic Programming, Needleman Wunsch & Smith-Waterman algorithms

Multiple sequence alignment, Progressive method, Iterative method, sum of pairs method, ClustalW

Secondary Structure Prediction Methods – Chou-Fasman, GOR, Neural Networks

Algorithms for generation of sequence profiles: Profile Analysis, PSSM, PSI-BLAST

Protein and Nucleic acid properties - EMBOSS

Concept of domains, motif, repeat -Pfam, Prosite. CATH, SCOP

Phylogenetic Tree Construction – Distance-based method, character based methods. concept of dendograms and its interpretation. UPGMA, Fitch-Margoliash, Neighbour-Joining, Maximum Parsimony, Maximum Likelihood. Bootstrapping, Jack-knifing.

3D structure visualization

Comparative Genomics - Basic concepts and applications: Full Genome alignments: basic concepts, the need for genome alignments, MUMs, suffix tree, Ukkonen's algorithm, synteny and gene order comparisons

Course: MBIN 104, Mathematics and Statistics

Module 1: Recapitulation of Determinants & Matrices, Adjoint and Determinant of a matrix, Inverse of a matrix, Elementary Transformations in a matrix, Row Echelon form of a matrix, Inversion by Gauss-Jordan Method, Eigen Values and Eigen Vectors, Rank of a matrix, Solution of a system of simultaneous linear equations, Cayley Hamilton Theorem, Complete set of linearly independent vectors, Diagonalization of a matrix, Power series of a matrix, like exponential, trigonometric or hyperbolic functions (Only expanded expressions, without teaching Sylvester's theorem)

Module 2: Recapitulation of functions and their graphical representation. Review of basic functions. Functions of several variables. Recapitulation of the concepts of limits, continuity and derivatives. Recapitulation of differential calculus: derivative of function of a function, derivative of implicit functions, derivative in a parametric form, higher order differentiation. Recapitulation of integral calculus: indefinite integrals, definite integrals, tangent and normal, maxima and minima. Recapitulation of Vector algebra.

Module 3: Setting up of a ordinary differential equation, Initial value and Boundary value problems, First order differential equations: separation of variables, homogeneous equations, exact differential equations; Higher order differential equations: homogeneous equations with constant coefficients, non-homogeneous equations with constant coefficients, Method of undetermined coefficients, Method of variation of parameters; Solution of a system of simultaneous linear differential equations, Introduction of basic concepts of Partial Differential Equations. Examples of application of differential equations in bioinformatics.

Module 4: Numerical methods: : Solution of algebraic and transcendental equations: Newton-Raphson, Gauss-Jordan, Jacobi's iteration; Finite Differences and Interpolation: Newton's forward & Backward, Gauss's forward & Backward; Numerical integration: Trapezoidal, Simpson; Solution of differential equation: Taylor's series, Euler's method, Runge-Kutta, Milne; Finding Maxima nad Minima, Optimization problem: Single variable optimization, Gradient descent methods (Students should practice writing C/C++ codes for all these numerical problems)

Module 5: Population, sample, parameter, statistic, random sample, stratified sample, treatment group, control group, double-blind study, confounding factors, crosssectional and longitudinal study, population (sample) variance and standard deviation, Concept of probability: Joint probability, Conditional probability. Linear Regression and Correlation : Correlation coefficient, explained and unexplained deviations, coefficient of determination. Probability Distribution, Probability curve, Tossing of a coin, Binomial Distribution. Hypothesis testing : Null hypothesis, Alternate hypothesis, test statistic, critical

region, level of significance, Type I error, Type II error. Gaussian and Poisson distribution, Standard Normal distribution, level of confidence, confidence interval, p-value. Central Limit Theorem.

Module 6: t-distribution, checking for normality, F-distribution, One-way ANOVA, two-way ANOVA. CHI-square test for goodness of fit, Tests of independence, Contingency Table, Tests of Homogeneity.

Module 7: Objective and subjective views of statistics, Bayes' formula, frequentist vs. Bayesian interpretation of probability, simple problems using Bayesian analysis, Nontrivial results using Bayesian Analysis. Stochastic process, random walk, Markov Processes, Markov chain, Markov matrix, Hidden Markov model.

Course: MBIN 105, Computational Techniques

1. Basic Concepts in Computing

1. **Overview and functions of a computer** – Input and Output devices, Storage devices (Hard disk, Diskette, Magnetic tape, CD-ROM, DVD etc.), Main circuit board (Chips, ports, Expansion slots, etc.), Memory (Register, Buffers, RAM, ROM, PROM, EPROM concepts.).
2. **History of Computers** – Generation of Computers (I, II, III, IV, V), Classification of computers (Mainframe, minicomputers, microcomputers, Workstations, Servers).
3. **Introduction to Operating Systems** – Concept of operating systems, Types of Operating systems (Real time, Batch, Multiuser, Multitasking, etc.).
4. **Internet and its Resources** – World Wide Web(www), Associated tools, services and terminologies.

2. 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.

3. 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 backquotes.
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.

4. Introduction to Database Systems

1. Concepts of various types of databases
2. Data Abstraction
3. Data Models
4. Instances and Schemes
5. ER Model
6. Basic Concept - Hierarchical Data Model

5. SQL and MySQL

1. Select Statements
2. Data Definition Statements
3. Data Manipulation Statements
4. Data Control Statements
5. Variables and Procedures.

Course: MBIN 201; Biomolecular structure and function –II

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 intra-molecular 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.

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2. Structural Biology & X-Ray 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- II

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 [Caldine's Rule].
- ❖ Base-pair parameters .

Macromolecular Interaction:

- ❖ Van-der-waals force.
- ❖ Columbic 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. Structure-Activity 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: k-means clustering. Convergence of the algorithm. Weakness of k-means 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: C-value 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, k-means, 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 de novo 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
 - Object-Oriented 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 built-in 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.