

**Maulana Abul Kalam Azad University of Technology, West Bengal
(Formerly West Bengal University of Technology)
Syllabus for M.Tech. In Bioinformatics**

2-Year PG

MAKAUT Framework

w.e.f. AY 2021-22

MODEL CURRICULUM

For

M.Tech. in Bioinformatics

**Maulana Abul Kalam Azad University of Technology, West Bengal
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M.Tech Bioinformatics Course structure

For 1st Semester : Total 21 Credits

Code	Course Title	Contact Hrs./wk	Credits	Total
A	Theory	L-T-P		
MBIN 101	Cell and Molecular Biology	3-0-0	3	21
MBIN 102	Applied Biochemistry	3-0-0	3	
MBIN 103	Mathematics and Statistics	3-0-0	3	
MBIN 104	Bio tools and Bio database	3-0-0	3	
MBIN 105	Data Structure and Algorithm	3-0-0	3	
B	Practical			
MBIN 192	Applied Biochemistry Lab	0-0-4	2	
MBIN 194	Applied Bioinformatics Lab	0-0-4	2	
MBIN 195	Data Structure and Algorithm Lab	0-0-4	2	

For 2nd Semester : Total 21 Credits

Code	Course Title	Contact Hrs./wk	Credits	Total
A	Theory	L-T-P		
MBIN 201	Protein Engineering	3-0-0	3	21
MBIN 202	Genomics and Proteomics	3-0-0	3	
MBIN 203	Bio Molecular Dynamics	3-0-0	3	
MBIN 204	Python in Bioinformatics	3-0-0	3	
B	Practical			
MBIN 291	Protein Engineering Lab	0-0-6	3	
MBIN 292	Genomics and Proteomics Lab	0-0-6	3	
MBIN 294	Computational Programming Lab-I	0-0-6	3	

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For 3rd Semester : Total 21 Credits

Code	Course Title	Contact Hrs./wk	Credits	Total
A	Theory	L-T-P		
MBIN 301	Drug Design	3-0-0	3	21
MBIN 302	Systems Biology	3-0-0	3	
MBIN 303	Research Methodology and IPR	3-0-0	3	
	Elective (Any one):	3-0-0	3	
MBIN 304(A)	Omics Technology			
MBIN 304(B)	NGS Technology			
B	Practical			
MBIN 391	Drug Design Lab	0-0-6	3	
MBIN 395	Computational Programming Lab-II	0-0-6	3	
C	Sessional			
MBIN 381	Dissertation and Presentation		3	

For 4th Semester : Total 21 Credits

Code	Course Title	Credits	Total
C	Sessional		
MBIN 481	Major Project Work	15	21

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Syllabus:

MBIN 101: 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.

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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: Benjamin/Cummings.

MBIN 102: Applied Biochemistry (Credits-3)

Course Outcome: On completion of this course, the students are expected to:

1. Develop and understand the advance knowledge on computational biochemistry tools.
2. Obtain new insights on enzyme at the molecular level, their interactions, and design of biocatalyst.
3. Gain advance knowledge about the dynamics of enzyme, its reactions mechanism, and its computational design.
4. Producing the new hypothesis on designing and engineering of enzyme for industrial application.

Unit: 1 (8 Lectures)

Basic knowledge of Protein and Nucleic acid: General structure and properties of proteins; amino acid composition of proteins; structures of common amino acids, amino acid sequence in protein molecules, physicochemical properties of proteins, analysis of dihedral angle of residues and Ramachandran plot, denaturation of protein. Molecular structure of DNA, denaturation and renaturation of DNA, molecular structure of chromatin; molecular organization of messenger ribonucleic acid, transfer ribonucleic acid, ribosomal ribonucleic acid, Small Nuclear Nucleoproteins.

Unit: 2 (4 Lectures)

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Nature of Chemical Bonds in Biomolecules: Types of chemical bonds-covalent bonds, inter-atomic distances for fractional bond, characters of partial double bond, metallic bond-inter-atomic distance and bond number in metals, hydrogen bond-nature, physical properties of H-bonds, H-bonds in protein and nucleic acids, electrostatic and VDW interaction in biomolecules.

Unit: 3 (8 Lectures)

Enzyme Design and Its Computational Applications: Engineering protein solubility and aggregation, engineering enzyme activity and specificity, engineering protein stability, engineering multiple properties of enzyme. Structural organization, function, and identification method of the enzyme tunnels and channels, function and identification method of the enzyme gates and their molecular engineering. *In silico* construction of protein mutants and prediction of their activities.

Unit: 4 (8 Lectures)

Enzyme Kinetics and Metabolic Simulation: Characteristics and enzyme, kinetics - steady-state assumption; conformational change and allosteric regulation; Monod-Wyman-Changeux mechanism, Koshland-Nemethy-Filmer model; Environmental Effects- presence of inhibitors, pH and temperature, computational search of enzyme database; analysis of kinetic data. Primary metabolism, Secondary metabolism, xenometabolism; metabolic database and simulation - search for metabolic pathways and information.

Unit: 5 (8 Lectures)

Design of Biocatalyst using Computational tools: Biochemical reactivity, ligand binding, access pathways and ligand transport, hotspot identification and smart library design, mutagenesis, applications of computational design of biocatalysts: design of efficient biocatalysts, design of biocatalysts with novel activity, design of specific and enantio selective biocatalysts, design of biocatalysts with tailored flexibility.

Unit: 6 (4 Lectures)

Computational Protein Engineering: Computational tools for *de novo* design of active sites of enzyme, Computational tools for design of ligand exchange pathways, Computational tools for design of protein-protein interfaces, computational tools for analysis of mutation, Computational tools for design of protein stability. Protein design and evolution for biocatalysis.

Reference Books:

1. Computational Biochemistry and Biophysics by Oren M. Becker (Editor), Alexander D. MacKerell Jr. (Editor), Publisher: CRC Press, ISBN-13: 978-0824704551.
2. Computational Methods in Physics, Chemistry and Biology: An Introduction by Paul Harrison, Publisher: Wiley, John & Sons, Incorporated, ISBN: 0471495638.
3. Fundamentals of Enzymology by Nicholas C. Price, Publisher: Oxford/Panima Pub Corp, ISBN: 9780198064398.
4. Protein Design Methods And Applications by Guerois, Springer, ISBN:9781588295859.

MBIN 103: 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;

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- 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 (10 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 (6 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. 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.

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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, 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, 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, DNA databank of Japan, Introduction, Resources of DDBJ, Data submission to DDBJ, Protein information resource, Introduction, Resources of PIR, Data retrieval of PIR, Databases of PIR, Swiss-Prot: Introduction, Features of Swiss-prot Protein 3D structure and classification databases, Protein databank, Introduction, Harnessing data from PDB , Data deposition tools, PDB beta, RCSB PDB structural genomics information portal, Molecular modelling databases, Introduction, Retrieval of structural data from MMDB, Conserved domain database, E-MSD, Introduction, Resources of E-MSD, Data submission at E-MSD, Search system of E-MSD, 3D genomics, Introduction, Assessing 3D genomics, Gene 3D, Introduction, Retrieving data from gene 3D, 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 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.

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

MBIN 105: Data Structure and Algorithm (Credits- 3)

Course Objectives:

1. To teach efficient storage mechanisms of data for an easy access.
2. To design and implementation of various basic and advanced data structures.
3. To introduce various techniques for representation of the data in the real world.
4. To develop application using data structures.
5. To improve the logical ability.

Course Outcomes:

Upon completion of the course, the students are expected to:

CO1: Remember and **understand** the basics of data structure and prerequisite of the data structure and algorithm.

CO2: Understand and **apply** the knowledge of liner data structure, like array, linked list, stack and queue.

CO3: Explain and **apply** the knowledge of non-linear data structure, like graph and tree.

CO4: Analyze different types of the searching and sorting algorithms.

SYLLABUS

UNIT I (12 lectures): Introduction

Introduction: Concept about Data, Information, Data Structure and Information System, Why data structure? Linear and non-linear data structure, time analysis of algorithm, Asymptotic notation.

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Revision on related Concepts: Revision on Conditional and Repetitive statements, 1D & 2D-dimensional array representation in memory, multidimensional array, Algorithms on array, Strings, Scope of the variable, Storage class, Pointer concept, Function, Call by Value and Call by address, Array and Pointer, Array and Function, Structure, Structure and Pointer, Structure and function.

Recursion – Recursion, Tail recursion, recursive problem implementation, recursion tree, Tower of Hanoi problem.

UNIT II (10 lectures): Linear Data Structure

Linear list – Array vs. Linked list, singly linked list implementation, insertion, deletion and searching operations on linear list, circular linked list implementation, doubly linked list implementation, Applications of linked lists.

Stacks- Representation of expression, Conversion among different expression, Stack, representations of stacks, stack applications-infix to postfix conversion, postfix expression evaluation.

Queues- Operations, representations of queue, Circular Queue operations, Dequeues, applications of queues.

UNIT III (11 lectures): Non-linear Data Structure

Graph theory- Vertex, Edge and Graph concepts, connected graph, regular graph, undirected graph, directed graph, complete graph, null graph, isomorphic graph, multi-graph and weighted graph. Hamiltonian cycle. Degree of vertex, in-degree & out-degree. Representation of graphs (adjacency matrix & list representation), Breadth first search, Depth first search, Application of graph theory in Biological Science.

Trees- Definitions, tree representation, properties of trees, Binary tree, Binary tree representation, binary tree properties, binary tree traversals, binary tree implementation, Binary search tree, Heap concept, applications of trees in Biological Science.

UNIT IV (8 lectures): Sorting & Searching Methods

Searching- Linear search, Time analysis of linear search, Binary search, Time analysis of binary search, comparison of searching methods.

Sorting– Bubble sort, Time complexity of bubble sort, Selection sort, Time complexity of selection sort, Insertion sort, Time complexity of Insertion sort, Quick sort, Time complexity of quick sort, Merge sort, Time complexity of Merge sort, Comparison of sorting methods.

Text Books & Reference Books:

1. Fundamentals of Data Structures of C– by Ellis Horowitz, Sartaj Sahni, Susan Andersonfreed.
2. Data Structures in C– by Aaron M. Tenenbaum.

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3. Data Structures Using C– by Reema Thareja.
4. Data structures and Algorithm Analysis in C, 2nd edition, M.A. Weiss, Pearson.
5. Data structures and Program Design in C, 2nd edition, R. Kruse, C.L. Tondo and B. Leung, Pearson.

MBIN 192: Applied Biochemistry Lab (Credits- 2)

Visualization and analysis of protein databank. The basic concept of protein crystallographic data, Detail structural analysis of protein, DNA, RNA, tRNA, protein-DNA, and protein-RNA complexes. Measuring inter-atomic distances of protein-ligand structures.

Calculation of dihedral angles of important residues in protein and identification of their conformation. Analysis of Ramachandran plot and protein secondary structure.

Computation of H-bonds and VDW interactions in protein and protein-ligand complexes, active site analysis of enzyme, protein-water-ligand, and protein-water-metal interactions study.

Identification of enzyme tunnels, channels, gates, and ligands' transport by computational tools. *In silico* analysis of protein mutants.

Prediction of protein solubility from protein primary sequence. Transportation of substrate, a product, an inhibitor, a co-factor, or a co-solvent from the outside environment into the binding site and vice versa using computational tools.

Identification of 'hot spots' and design of smart libraries for engineering protein stability, catalytic activity, substrate specificity, and enantioselectivity.

MBIN 194: Applied Bioinformatics Lab (Credits- 2)

1. Conceptual background, Understanding the Unix command.
2. General purpose: Utilities, the file system, Handling ordinary files, Basic file attributes.
3. The vi editor, the shell, the process, Customize the environment, Simple filters, Essential shell programming.
4. Essential system administrator, The X window system.
5. All bio tool application.
6. Etc.

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MSBIN 195: Data Structure and Algorithm (credits- 2)

Course Outcome:

After completion of the course the students will be able to:

CO1: Apply appropriate logic and data structure to **solve** given problem.

CO2: Implement appropriate linear data structure respective problems.

CO3: Implement appropriate non-linear data structure related problems.

CO4: Apply appropriate logic and data structure to **solve** searching and sorting problems.

UNIT I: Introduction

1. Write a program to print first n Fibonacci numbers using function.
2. Write a program to distinguish between call-by-value and call-by-address.
3. Write a program to distinguish between automatic and static variables.
4. Write a program to distinguish between local and global variables.
5. Write a program to construct a Pascal triangle.
6. Write a program to print N.S.C. Bose (where the input string is Netaji Subhash Chandra Bose).
7. Create a structure STUDENT (id, name, roll, and marks of five subjects). Write a program to find out the name and roll of the student who got highest total mark among 50 students.
8. Write a program to find out the GCD and LCM using recursion.
9. Write a program to implement the Tower-of-Hanoi problem.

UNIT II: Linear Data Structure

1. Write a program to insert a specific element into a 1-D array as the following-
 - A. at the beginning
 - B. at the end
 - C. at any position
2. Write a program to delete a specific element from a 1-D array as the following-
 - A. at the beginning
 - B. at the end
 - C. at any position
3. Write a program to find out the mean, mode and standard deviation of a set of values using function.
4. Write a program to find out the sum of the two leading diagonal of a square matrix.
5. Write a program to multiply the two 2-D matrices.

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6. Implementation of Singly linked list related problems (creation, insertion, deletion, traversing etc.).
7. Implementation of Circular linked list related problems (creation, insertion, deletion, traversing etc.).
8. Implementation of Stack using Array and Linked List.
9. Implementation of Linear Queue using Array and Linked List.
10. Implementation of Circular Queue.

UNIT III: Non-linear Data Structure

1. Implementation of Binary Search Tree.
2. Implementation of Binary tree to display the nodes as per inorder, preorder, and postorder traversals.
3. Implementation of Breadth First Search Algorithm on a graph.
4. Implementation of Depth First Search Algorithm on a graph.

UNIT IV: Sorting and Searching methods

1. Implementation of Linear Search algorithm using array.
2. Implementation of Binary Search algorithm using array.
3. Implementation of Bubble Sort algorithm using array.
4. Implementation of Selection Sort algorithm using array.
5. Implementation of Insertion Sort algorithm using array.
6. Implementation of Quick Sort algorithm using array.
7. Implementation of Merge Sort algorithm using array.

MBIN 201: Protein Engineering (Credits- 3)

Student Learning Outcomes: On completion of this course, the students are expected to:

1. Understand basic knowledge of protein structure, function, and dynamics.
2. Create new methods of analysing and characterization of macromolecules to solve problems in protein chemistry.
3. Obtain accurate and comprehensive information about the structures and energies of proteins at an atomic level.

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4. A thorough overview of the computational tools, and some of the underlying theory, to study the dynamics of proteins by computational molecular dynamics simulations.

Unit 1: (8 Lectures)

Prediction of Protein Structure: Structural organization and function of Greek key, Jelly roll motif, and Rossmann fold, Protein structure prediction- template-based modelling; template-free modelling; homology modelling, Chou and Fasman and GOR method, Loop modelling, ab-initio modelling, fragment assembly, machine learning in protein structure prediction, contact predictions from residue covariation, model refinement. Methods for predicting irregular secondary structures –coil, different types of turns, omega loop, and beta hairpin.

Unit 2: (4 Lectures)

Protein Design by Computational study: *De novo* protein design, optimizing the protein sequence, validates computational predictions, applications of protein design-*de novo* interface design, scaffold design, ligand binding site design, design of protein switches.

Unit 3: (4 Lectures)

Classification of Protein 3D structure: Concept of 3D structure of protein; Algorithm-DALI, VAST, and CE. RMSD and Z-score for structural comparison, Database for structure based classification, CATH, SCOP, and FSSP.

Unit 4: (8 Lectures)

Computational Chemistry: Molecular mechanics, its advantage, disadvantage, and limitation. Force field-bond stretching, angle bending, cross-term, and non-bonded interaction, parameterization of force field. Different types of water model and its application. Wave-particle duality, Schrödinger wave equation, particle in a box model, simple harmonic oscillation, potential barrier, Expectation value, Aspect of computational chemistry, potential energy surface, single point energy calculation, geometry optimization, local minima, global minima, and saddle point, basic concept of energy landscape.

Unit 5: (8 Lectures)

Molecular Dynamic Simulation of Protein: Basic concept of MD-simulation, molecular interactions, configuration file of MD-simulation, equation of motion in MD simulation, finite difference method, integrating equation of motion, relationship between the solution of equation of motions and ensembles, solvation of protein, simulation with explicit solvent, constraints of MD-simulation, multiple time step dynamics, transport properties of MD simulation, MD simulation at constant temperature and pressure, multiple trajectory analysis.

Reference Books:

1. Structural Bioinformatics 2008 Edition by Forbes J. Burkowski, publisher Taylor & Francis Ltd, ISBN: 9781584886839.
2. Structural Bioinformatics Methods And Protocols 2021 Edition by Zoltan Gaspari, Publisher-Springer, ISBN: 9781071602720.
3. Structural Bioinformatics, 2nd Edition by Gu Jenne et.al, Publisher: Wiley India, ISBN: 9788126574711, 8126574712.

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4. Understanding Molecular Simulation: From Algorithms to Applications (Computational Science Series, Vol 1) by Daan Frenkel. ISBN: 978-0122673511

MBIN 202: Genomics and Proteomics (Credits- 3)

Course Objectives:

Theory with practical: This course will introduce advancement in the proteomics field. Large scale genomics and proteomics data analysis will be done with a good command in bioinformatics.

Prerequisites: Basic knowledge in molecular biology, biochemistry, bioinformatics.

Student Learning Outcome:

By the end of this course students will be able to:

1. Browse, search, submit and retrieve genomics and proteomics data from widely used public repositories
2. Use tools to perform functional annotation of lists of genes and proteins
3. Proficiently use and understand bioinformatics tools to analyse genomics and proteomics data, involving identification and quantification approaches
4. Examine Genome and Proteome data and their functional analysis.

Course Content / Syllabus:

Genomics:

Unit:1 (5 lectures)

Genomics: Structural and Functional Genomics, Sequence based approach, EST and dbEST, SAGE analysis Microarray based approach, Software: Arrayplot, SNOMAD, Mutational genomics, Comparative genomics, Organization of Genome, Strategies of Genome Sequencing, Model Plant Genome Project, Functional Analysis of Genes.

Unit:2(5 lectures)

Human Genome Project: GENOME. FLOW CHART OF HUMAN GENOME. NUCLEAR GENOME. MITOCHONDRIAL GENOME. REPETITIVE DNA

Unit:3(5 lectures)

Single Nucleotide Polymorphism, Concept, Classification, Search Method, Assay Method, Clinical application, SNP mapping, SNP and cancer

Unit:4(5 lectures)

The Human Genome Project, International HapMap Project, www.hapmap.org, The 1000 Genomes Project –www.1000.genomes.org, Encyclopedia of DNA Elements (ENCODE) Project, The Cancer Genome Atlas (TCGA), Human Microbiome Project (HMP) –

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www.hmpdacc.org, The eMERGE (Electronic Medical Records and Genomics) Network
Common Features of Projects, High throughput, Use of technology, in particular –
Automation (Robotics, AI) – Databases – Visualization, simulation/computational models –
Groupware: Coordination and communication, Public domain tools, Open sharing of data.

Proteomics:

Unit I: (4 lectures)

Proteomics Data and Databases; UniProtKB, IntAct, Reactome, PRIDE, peptides Atlas, Software and open source tools; Reusing shared data, Application, challenges and opportunities of proteomics, Human Proteome Project; The human protein atlas

Unit II: (7 lectures)

Protein identification and quantification; PeptideShaker; Postprocessing of proteomics data; Post-translational modifications identification; Biomarker candidate identification; Utilities of Galaxy server

Unit III: (7 lectures)

Protein-Protein interaction data analysis; PPI databases (primary, secondary and predictive databases); Network analysis of PPI data (Cytoscape); proteins to pathways (Reactome); Proteogenomics: Database creation, Database search, Novel peptide analysis

Unit IV: (2 lectures)

Differential expression; ProStaR; Statistical methods for expression analysis of proteomics data; FDR; PCA; Enrichment analyses

Reference Books:

1. Principles of Genome Analysis and Genomics. Primrose SB & Twyman RM. 2007. Blackwell. ISBN-10: 1405101202
2. Introduction to Genomics. A.M Lesk, Oxford University press, 2007. ISBN-10: 0199557489
3. A Primer of Genome Science. Greg Gibson and Spencer V. Muse. 2nd ed. 2004. SINAUER Associates Inc. ISBN-10: 0878932364
4. Introduction to Proteomics: Tools for the New Biology. Daniel C. Liebler, Humana Press Inc., 2002. ISBN-10: 0896039919
5. Other research papers, review articles and web resources

MBIN 203: Bio-Molecular Dynamics (Credits- 3)

Student Learning Outcomes: On completion of this course, the students are expected to:

1. Gain basic knowledge about the advance technique in computational chemistry to solve complex biochemical problems.
2. Generate dynamic models by computational method and justify with experimental data.

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3. Obtain insights into biological systems using multi-scale engineering methods to analyze data in non-intuitive ways.
4. Know how computer simulations of biomolecules can be used to investigate biological problems at the molecular and atomic level.
5. Propose the best future and dynamic model development.

Unit 1: (8 Lectures)

Replica Exchange Molecular Dynamics Simulation: Replica Exchange Molecular Dynamics Simulation, Modified Replica Exchange MD Simulation, Hamiltonian Replica Exchange Molecular Dynamics, Multiplexed-replica exchange molecular dynamics, application of replica exchange MD Simulation.

Unit 2: (8 Lectures)

Application of advance MD Simulation techniques: Meta Dynamics, Constant-pH Molecular Dynamics Simulations, Temperature-accelerated MD Simulation and ab-initio MD Simulation. Basic idea of Inhomogeneous Solvation Theory (IST), Application of IST in WaterMap, structure-based ligand discovery and Grid Inhomogeneous Solvation Theory (GIST), GIST algorithm and its application in Molecular Dynamics Simulation, convergence of entropy and energy, end state analysis.

Unit3: (8 Lectures)

Justification of MD Simulation Results: Umbrella Sampling method, Steered Molecular Dynamics (SMD) Simulations, adaptive steered molecular dynamics (ASMD) and Nudged Elastic Band (NEB) simulations. Validation and verification of MD Simulation results and their correlation with experimental data.

Unit 4: (8 Lectures)

Modelling of Complex Biological System in Multi scale Level: Coarse-Grained Protein Models and their Applications: Brief History, Sampling Schemes, Examples of Protein Coarse-Grained Models, Applications of Coarse-Grained Models in Multiscale Modeling Pipelines, Multiscale Modeling Simulation: Example and Strategies, Reconstruction of Atomic Representation from Coarse-Grained Models.

Unit 5: (8 Lectures)

Electron transfer mechanism and Energy Landscape study of Bio-molecules: Electron transfer in peptides and proteins: Electron transfer by superexchange, Electron hopping, Amino acid side chains as intermediates in electron hopping, Electron tunnelling. Free energy and potential energy landscape study of biomolecules and its application, Protein Dynamics in the Living Cytoplasm.

Reference Books:

1. Multiscale Approaches to Protein Modeling by Andrzej Kolinski, ISBN: 9781441968883, 1441968881, Publisher: Springer-Verlag New York Inc.
2. Multiscale Modelling and Simulation by Sabine Attinger, Publisher: Springer-Verlag Berlin and Heidelberg GmbH & Co. KG., ISBN: 9783540211808, 9783540211808.

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3. Innovations in Biomolecular Modeling and Simulations (Volume 1) Editor: Tamar Schlick. Print ISBN: 978-1-84973-461-5.
4. Theory and Practice in Replica-Exchange Molecular Dynamics Simulation Paperback – Import, 1 May 2012 by Cooke Isard, Benjamin Perry Publisher: Proquest, Umi Dissertation Publishing (1 May 2012), ISBN-13: 978-1248997017.

MBIN 204: Python in Bioinformatics (Credits- 3)

Course Objective: The objective of this course is to give conceptual exposure of essential contents of modern Python programming languages to students. Students should be able to gain broad understanding about control structures, looping, strings, functions, file, lists, dictionaries and tuples concept and syntactical concept of python to problem solving on a diverse variety of disciplines.

Course Outcomes:

CO1: Describe the basic concepts of python installation, operators and control structures programming syntax, and debugging.

CO2: Understand and apply several types of String operation, List, and Function used in programming.

CO3: Describe and apply the concepts of File, Dictionaries, Tuples, and different useful Packages.

CO4: Application of python in bioinformatics.

Syllabus:

UNIT 1: 6L

Introduction- Why Python, Introduction to Python, Python history and version, Python installation and debugging.

Basics- Tokens, character set, variables and keywords, constants, numbers, datatypes, rules of constructing variable identifier, statements, operators and operands, Different types of operators, Hierarchy of operators, Associativity of operators, Type conversion (explicit and implicit), Expression, Boolean expression, Logical expression.

Instruction- Types of instructions, Control Instructions, Repetitive instruction (for, while), Definite and indefinite loop, range function, break and continue statement.

UNIT 2: 15L

String operations- Asking the user for input, Comments, various string operators, String slices, String length, Strings are immutable, in operator, String comparison, String methods, Parsing strings, Format operator.

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Function calls- Built-in functions, Type conversion functions, Math functions, adding new functions, Function Definitions and uses, Flow of execution, Parameters and arguments, Fruitful functions and void functions.

Lists- list is a sequence, Lists are mutable, traversing a list, List operations, List slices, List methods, deleting elements, Lists and functions, Lists and strings, Objects and values, List arguments.

UNIT 3:15L

Files- Persistence, opening files, Text files and lines, reading files, searching through a file, User choose the file name, using try-except-open, Writing files, Different types of file operation.

Dictionaries- Dictionary as a set of counters, Dictionaries and files, Looping and dictionaries.

Tuples- Tuples are immutable, comparing tuples, Tuple assignment, Dictionaries and tuples, Multiple assignment with dictionaries, Using tuples as keys in dictionaries.

Modules and packages – numpy, pandas, matplotlib, biopython packages, etc.

UNIT 4: 9L

Application-

Genome sequence analysis- Parsing DNA/RNA sequence data, Sequences reading and writing, Transcription of sequence, Translation of sequence, Find the CODON table, Identify proteins, Protein-Protein Interaction analysis, Visualization of DNA/RNA/Protein sequences, Sequence alignment and similarity comparison, Phylogenetic analysis of the complete viral genome.

Microarray data analysis- Data preparation with pandas (import label, recode label to numeric, visualization of training and testing data, transform all string values to numbers, transposing of data), Data cleaning, Data cross-fold, Principal Component Analysis, Model building, clustering, classification.

Reference Books:

1. Introduction to Python Programming language- Chaitanya Singh
2. Python programming language- by G van Rossum
3. Python Programming: An Introduction to Computer Science, by John Zelle.

MBIN 291: Protein Engineering Lab (Credits- 3)

Visualization and analysis of Greek key, Jelly Roll motif, and Rossmann fold in protein. Homology and template-free modeling of protein structure. Modeling the loop region of the protein, analysis of different types of turns. Computational tools of scaffold design, ligand binding site design, and design of protein switches.

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Analysis of force field of protein, nucleic acids, and ligands, computational visualizations of different water molecules.

Energy minimization of protein, protein-water complexes, and identification of local minima, global minima, and saddle point.

Molecular dynamics simulation of protein, protein-water, protein-nucleic acid, and protein-ligand complexes. Parameterization technique of new ligand. Water dynamics study.

Free energy calculation of ligand using LIE and MM/PBSA method.

MBIN 292: Genomics and Proteomics Lab (Credits- 3)

Genomics Lab:

1. Data format (FASTQ, BED, GTF, GFF3, SAM, BAM and VCF);
2. Quality control, FastQC, Trimmomatic
3. Genome assembly,
4. Read mapping TopHat, Bowtie, Picard, Cufflinks, CuffMerge
5. Read Count, HTSeq-count, RSEM
6. Differential expression analysis, edgeR, DESeq
7. Biological interpretation: DAVID, Reactome, Gene Ontology
8. Biological Network analysis using Cytoscape
9. Utilities of Galaxy Server and GEO2R

Proteomics Lab:

1. Protein identification and quantification; MaxQuant; SearchGUI and PeptideShaker;
2. Post-translational modifications identification
3. Utilities of Galaxy Server: ProteoRE
4. Protein-Protein interaction network analysis using Cytoscape
5. Etc.

MBIN 294: Computational Programming Lab-I (Credits 3)

1. Implement different types of operators, control instructions: if-else, switch case, conditional operator. loops (for, while), break & continue statement based problems.
2. Implement different string operations and string methods.
3. Implement different user defined function calls and its application using python language.
4. Implement different list operations, lists and functions, lists and strings etc.
5. Implement different Dictionaries and Tuples based problems.
6. Implement different problems based on files and its application.
7. Usefulness of Packages in bioinformatics domain.
8. Application of packages for sequence analysis in bioinformatics domain.

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9. Application of packages for microarray data analysis in bioinformatics domain.
10. Etc.

MBIN 301: Drug Design (Credits- 3)

Student Learning Outcomes: On completion of this course, the students are expected to:

1. Explain the different methods of drug discovery.
2. Obtain knowledge about the physicochemical Properties and the techniques involved in computational QSAR.
3. Gain advance concept on Bioinformatics and Cheminformatics methods.
4. Explanation about various structure based drug design methods (Molecular docking, Denovo drug design).
5. Learn the concept of pharmacophore and modelling techniques.

Unit 1: (8 Lectures)

Computational Molecular Docking: Drug-likeness and Lipinski's 'rule of five'. -Docking: Introduction, basic steps of docking, Types of Docking-Rigid and flexible docking Search algorithm: Random searching, systematic searching, simulation based searching, Scoring/evaluation functions- Force-Field Based scoring, Empirical Scoring Function, Knowledge-Based scoring function, Virtual screening: Ligand based virtual screening (LBSV)- Pharmacophore based screening, Descriptor based screening Structure based virtual screening (SBVS).

Unit 2: (8 Lectures)

Concept of Pharmacophores Modelling: Modeling and mapping of pharmacophore- constrained systemic search approach, Clique detection, genetic algorithm based approach, pharmacophore generation: Ligand based pharmacophore generation, receptor based pharmacophore generation. Pharmacophore fingerprints. Pharmacophore applications: Pharmacophore searching, Pharmacophore based de-novo design of ligands, pharmacophore based Lead optimization. Salt-bridge-complete and incomplete salt bridge in protein and its role in drug discovery.

Unit 3: (8 Lectures)

QSAR Study: molecular descriptors: Based on 2D structure Physicochemical properties, Molar refractivity, topological indices, 2D fingerprints. Based on 3D structure 3D fragment screens, Pharmacophore keys, other 3D descriptors. Data verification and manipulation. QSAR: Deriving a QSAR equation, Designing of QSAR experiment, QSAR models: Free Wilson analysis, Hansch constant, Hammett Substituent Constant 3D QSAR: common 3D molecular field, 3D-QSAR model- Comparative Molecular Field Analysis (CoMFA), Comparative Molecular Similarity Index Analysis (CoMSIA).

Unit 4: (8 Lectures)

Computational ADMET: Prediction of ADMET properties, Toxicity prediction, Introduction to combinatorial chemistry and Chemoinformatics, Combinatorial libraries: Diverse and focused libraries, Library enumeration, combinatorial library design strategies, Approaches to product based library design, multi-objective library design.

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Unit 5: (8 Lectures)

Basic concept of drug discovery: Drug discovery methods and basic steps of drug designing process, drug target identification, fundamentals of pharmacokinetics, absorption- bio-availability, distribution-volume of distribution, drug barriers, Metabolism, Elimination-drug elimination kinetics, Drugs affinity and efficacy, Response of Drug on receptor: Agonist, antagonist. Quantification of drug safety: Effectiveness, Toxicity, Lethality, Therapeutic Index Impact of pharmacogenomics.

Reference Books:

1. An introduction to chemoinformatics- Andrew R. Leach and Valerie J. Gillet (springer)
2. Molecular Modeling-Principles and Applications-Andrew R. Leach.
3. Bioinformatics-from Genomes to drugs- Thomas Lengauer.
4. Fundamentals of Medicinal Chemistry by Gareth Thomas.

MBIN 302: Systems Biology (Credits- 3)

Course Objectives:

Theory: This course will introduce complex biological systems and students will think biological world as seen by mathematicians, physicists, engineers and computer scientists.

Prerequisites: Basic knowledge in molecular biology, bioinformatics, mathematics.

Student Learning Outcome:

By the end of this course students will be able to:

1. Understand systems based approaches in biological sciences
2. Proficiently select Systems Biology web-resources and tools that will help them in reconstructing and re-defining complex biological processes.
3. Choose an appropriate modeling technique to be used to a complex biological system

Course Content / Syllabus:

Unit I: Introduction to Systems Biology (6 lectures)

Basic concepts of Systems Biology, Top-down and bottom-up approaches for Systems Biology, Databases for Systems Biology, Multi-omics data integration, Robustness in biological systems, Potential limitations of systems biology.

Unit II: Fundamentals of biological networks (10 lectures)

Basics of network and its properties (node, edge, density, degree, shortest path, diameter, characteristic path length, degree distribution, directed and undirected network, hub), Network motifs, Feed Forward Loops, Auto-regulation, Network topologies (random, small-world, scale-free/power-law), Network perturbation, Cluster detection

Unit III: Reconstruction of biological networks (8 lectures)

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Gene regulatory networks (GRN), Noise in GRN, Protein networks, Signalling networks, Metabolic network from genome information and its structural and functional analysis, Metabolic Flux Analysis, Biochemical reaction networks and stoichiometry

Unit IV: Dynamic nature of biological networks (3 lectures)

Mathematical models in biology, Dynamical modeling, Parameter Estimation, Simulation. Deterministic versus Stochastic approaches.

Unit V: Multiscale representation of cells and emerging phenotypes (5 lectures)

Spatio-temporal Systems Biology, The IUPS Physiome project, Cytomics - From cell states to predictive medicine, Synthetic Biology, Recent developments and trends of Systems Biology.

Unit VI: Tools for Systems Biology (8 lectures)

SBML, Cytoscape, Reactome, Ontologies in systems biology, E-cell, V-cell, ChEBI, Metaboanalyst, COBRA toolbox, CellDesigner, ReconMap, 3Omics

Recommended Textbooks and References:

1. Systems Biology PROPERTIES OF RECONSTRUCTED NETWORKS. By Bernhard Ø. Palsson. Published by Cambridge University Press, ISBN: 9780521859035
2. Uri Alon, An Introduction to Systems Biology: Design Principles of Biological Circuits, 2/e, CRC Press, (2006)
3. Systems Biology: Applications and Perspectives. By Peter Bringmann. Published by Springer, 2007, ISBN 3540313389
4. Systems Biology: Principles, Methods and Concepts. By Andrzej K, Konopka. Published by CRC Press, 2007, ISBN 0824725204
5. Systems Biology: Definitions and Perspectives. By Lilia Alberghina, Hans V. Westerhoff. Published by Birkhauser, 2005, ISBN 354022968X
6. R.Heinrich and S. Schuster, The Regulation of Cellular Systems, Chapman & Hall, 1996.ISBN 978-1-4613-1161-4
7. E.O. Voit, Computational Analysis of Biochemical Systems. Cambridge University Press, 2000.
8. Other research papers, review articles and web resources

MBIN 303: Research Methodology and IPR (Credit 3)

Course Outcomes: At the end of this course, students will be able to-

1. Understand research problem formulation.
2. Analyze research related information
3. Follow research ethics
4. Understand that today's world is controlled by Computer, Information Technology, but tomorrow world will be ruled by ideas, concept, and creativity.

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5. Understanding that when IPR would take such important place in growth of individuals & nation, it is needless to emphasise the need of information about Intellectual Property Right to be promoted among students in general & engineering in particular.
6. Understand that IPR protection provides an incentive to inventors for further research work and investment in R & D, which leads to creation of new and better products, and in turn brings about, economic growth and social benefits.

Course Outline:

Unit 1: Meaning of research problem, Sources of research problem, Criteria Characteristics of a good research problem, Errors in selecting a research problem, Scope and objectives of research problem. Approaches of investigation of solutions for research problem, data collection, analysis, interpretation, Necessary instrumentations

Unit 2: Effective literature studies approaches, analysis Plagiarism, Research ethics,

Unit 3: Effective technical writing, how to write report, Paper Developing a Research Proposal, Format of research proposal, a presentation and assessment by a review committee

Unit 4: Nature of Intellectual Property: Patents, Designs, Trade and Copyright. Process of Patenting and Development: technological research, innovation, patenting, development. International Scenario: International cooperation on Intellectual Property. Procedure for grants of patents, Patenting under PCT.

Unit 5: Patent Rights: Scope of Patent Rights. Licensing and transfer of technology. Patent information and databases. Geographical Indications.

Unit 6: New Developments in IPR: Administration of Patent System. New developments in IPR; IPR of Biological Systems, Computer Software etc. Traditional knowledge Case Studies, IPR and IITs.

Learning Resources:

1. Stuart Melville and Wayne Goddard, "Research methodology: an introduction for science & engineering students"
2. Wayne Goddard and Stuart Melville, "Research Methodology: An Introduction"
3. Ranjit Kumar, 2 nd Edition, "Research Methodology: A Step by Step Guide for beginners"
4. Halbert, "Resisting Intellectual Property", Taylor & Francis Ltd, 2007.
5. Mayall, "Industrial Design", McGraw Hill, 1992.
6. Niebel, "Product Design", McGraw Hill, 1974.
7. Asimov, "Introduction to Design", Prentice Hall, 1962.
8. Introduction to Research, NPTEL online certification course.

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MBIN 304(A) (Elective): Omics Technology (Credit 3)

Course Objectives:

Theory: This course will introduce different genomics, transcriptomics, proteomics and other 'omics' technology by acquiring methodological skills in experimental and/or computational techniques addressed through experimental design methods, overview of analytical platforms, bioinformatics tools, and databases used to decode sequence, structure and functional data.

Prerequisites: Basic knowledge in molecular biology, biochemistry, recombinant DNA technology, bioinformatics.

Student Learning Outcome:

By the end of this course students will be able to:

1. Browse and retrieve functional omics data
2. Find information on the abundance and localisation of RNA (and proteins) in different species and biological conditions
3. Recognize and validate the plans towards annotation, analysis pipelines and network modeling for scientific use.
4. Extend the concepts of sequencing, transcriptomics and other 'omics' methods applied and deduce logical interpretations from the data analysis.
5. Apply their bioinformatics knowledge and skills to critically assess the data characteristics, experimental design for efficient progress in high throughput biology.

Course Content / Syllabus:

Unit I: Genome, Genomics and Metagenomics (10 lectures)

Organization of genome structure, Variations in genome, Genome Molecular markers, First, second and third generation sequencing techniques; De novo and reference based Whole genome sequencing using Next Gen sequencing; Data format (FASTA, BED, GTF, GFF3, and VCF); Quality control, Genome assembly, Read mapping, BWA, SAM, BAM, Taxonomic investigation, Variant calling, Genome annotation; Variants of interest; Personal genomics; Genome-Wide Association Studies (GWAS); Metagenomics; Analysis of Metagenomic Data; QIIME, PICRUSt; Epigenomics; Genomics resources: TCGA, Ensembl, Genome Browser, The ENCODE project;

Unit II: Transcriptomics (10 lectures)

Quantitative transcriptomics: qRT-PCR; Delta-Delta Ct method; Advanced transcriptomics: gene expression microarrays, Normalization and experimental design models for microarray data; Next-generation sequencing in transcriptomics: RNA-seq experiments; Quality control of raw reads: FASTQC and Trimmomatic; Read alignment: TopHat, Bowtie, HISAT2; Quantification of expression (HTSeq-count) and differential expression analysis (edgeR, limma-voom and DESeq2); Isoform Discovery and Alternate Expression; Analysis of transcription factor binding sites; miRNomics; Functional genomics resources: ArrayExpress, Expression Atlas, Single Cell Expression Atlas

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Unit III: Proteomics (8 lectures)

Protein identification and quantification; PeptideShaker; Postprocessing of proteomics data; Post-translational modifications identification; Biomarker candidate identification; Shotgun proteomics; Proteogenomics: Database creation, Database search, Novel peptide analysis; Proteomics resources: UniProtKB, IntAct, PRIDE, peptides Atlas, GPMDB and neXtProt; Software and open source tools

Unit IV: Interactomics and metabolomics (3 lectures)

Interactomics; Chromatin immunoprecipitation (ChIP), Chip-Seq data analysis; Protein-Protein interaction and network; Metabolomics

Unit V: Multiscale representation of cells and emerging phenotypes (2 lectures)

The IUPS Physiome project, Cytomics - From cell states to predictive medicine, Recent developments and trends of omics technologies.

Unit VI: EDA and Network Analysis of -omics Data (3 lectures)

Exploratory data analysis: tools and techniques; Basics of network and its properties (node, edge, density, degree, shortest path, diameter, degree distribution, directed and undirected network, hub etc.), Network motifs, Cluster detection

Unit VII: Bioinformatics Tools for Omics Technology (4 lectures)

Cytoscape, Reactome, Gene Ontologies, ChEBI, Metaboanalyst, CellDesigner, 3Omics

Recommended Textbooks and References:

1. High Throughput Screening: Methods and Protocols (Methods in Molecular Biology) 29 Nov 2011 - William P. Janzen (Editor), Paul Bernasconi (Editor) ISBN-13: 978-1617794919.
2. RNA Bioinformatics (Methods in Molecular Biology) Hardcover – 22 Jan 2015 - Ernesto Picardi (Editor) ISBN-13: 978-1493922901.
3. Discovering Genomics, Proteomics and Bioinformatics, 2nd Edition. Campbell AM & Heyer LJ, Benjamin Cummings 2007; CSH Press, NY. ISBN-10: 8131715590
4. Principles of Proteomics. R.M Twyman (2004). (BIOS Scientific publishers). ISBN-10: 1859962734
5. Principles of Gene Manipulation and Genomics- Primrose S & Twyman R, 7th Edition, Blackwell, 2006. ISBN-10: 1405135441
6. Principles of Genome Analysis and Genomics. Primrose SB & Twyman RM. 2007. Blackwell. ISBN-10: 1405101202
7. Introduction to Genomics. A.M Lesk, Oxford University press, 2007. ISBN-10: 0199557489
8. A Primer of Genome Science. Greg Gibson and Spencer V. Muse. 2nd ed. 2004. SINAUER Associates Inc. ISBN-10: 0878932364

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9. Introduction to Proteomics: Tools for the New Biology. Daniel C. Liebler, Humana Press Inc., 2002. ISBN-10: 0896039919
10. Other research papers, review articles and web resources

MBIN 304(B) (Elective): NGS Technology (Credit 3)

Course outcome:

After completing the course the student is expected to be able to:

- Identify the different NGS technologies available in the market
- Learn about chemistry behind NGS applications
- Evaluate the main parameters influencing the design of a sequencing project
- Detect good quality data
- Apply the different pipelines in the analysis of NGS data
- Interpret and analyse the results obtained from the different NGS applications

Unit I (5L)

History of sequencing, Generations of sequencing, Principle and theories behind NGS technologies, Accessing public sequencing repositories, Galaxy server

Unit II (8L)

NGS data formats and tools, Unix command line, FASTQ, Read alignment+QC, FASTQC, Picard, Bowtie, Samtools, BEDTools, SNP/indel, Structural variation, Integrated Genomics Viewer (IGV)

Unit III (12L)

Next generation sequencing: Methods and applications, 454 sequencing, Illumina sequencing, Ion Torrent: Proton / PGM sequencing, ONT nanopore sequencing, Whole genome sequencing

Unit IV (10L)

RNA-seq experimental design, Comparison of different RNA sequencing platforms, Tophat, Cufflinks, Differential gene expression, Downstream analysis: pathway analysis, clustering and Gene ontology

Unit V (5L)

ChiP-seq analysis, MACS, functional annotation and detect potential binding sites (motif)

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MBIN 391: Drug Design Lab (Credits- 3)

Preparation of receptor and ligand, molecular docking study-protein with ligand, protein with protein, protein with DNA, protein with RNA.

Comparative analysis of ligand conformation using different molecular docking programs.

Analysis of scoring function and validation of docking results with crystal data.

Binding energy calculation of ligand and correlation coefficient analysis between calculated and experimental data.

Identifications of salt bridge in protein using computational program and calculation their geometry.

Pharmacophore modelling, measuring the volume of ligand binding cavity in protein and Virtual screening from different chemical libraries and selection of specific ligand.

Computational tools for analysis of QSAR properties of ligands. Calculations of molecular descriptor using different computational tools.

Modification of ligand and structure based, water based, and salt-bridge based ligand design.

In silico analysis of ADMET and toxicity test of new identified ligands.

MBIN 395: Computational Programming Lab-II (Credits- 3)

1. Construct and execute basic programs in R using elementary programming techniques, e.g. import/export of data from file or Internet, assign and manipulate data structures, create user-defined functions, loops, condition statements and debugging.

2. Use R for statistical calculations.

3. Implement and describe Monte Carlo techniques as well as perform simulation studies with analysis and evaluation of result

4. Graphically visualize data and results of statistical calculations

5. Use external R-packages in statistics and data mining

6. Application of R packages in bioinformatics domain.

7. Etc.