

Chhatrapati Shahuji Maharaj University, Kanpur

Revised scheme & syllabus for M.Sc. Bioinformatics

Course Curriculum

Semester	Paper code	Subject/Paper	Total 100%
Semester I	MB1101. A/B	Mathematics & Statistics/ Cell & Molecular Biology	100
	MB1102.	Biochemistry & Structural Biology	100
	MB1103.	Introduction to Programming	100
	MB1104.	Computational Biology	100
	MB1105.	Basic Genetics	100
Semester II	MB1201.	Genomics & Transcriptomics	100
	MB1202.	Data Structure & Algorithm	100
	MB1203.	Object Oriented Programming using Java	100
	MB1204.	Immunology & Immunoinformatics	100
	MB1205.	Biochemical & Biophysical Methods	100
Semester III	MB1301.	Database Management & Data Security	100
	MB1302.	Programming using Perl & Python	100
	MB1303.	Pharmacogenomics & Metagenomics	100
	MB1304.	Data Mining & Data Analytics	100
	MB1305.	Technical Communication, Research and IPR	100
Semester IV	MB1401.	High throughput data generation and analysis	100
	MB1402.	Protein Engineering & Design	100
	MB1403. MB1403A/ MB1403B	Elective 1-Computer Aided Drug Design Elective 2-Systems Biology & Metabolomics	100
	MB1404.	Seminar Oriented Course	100
	MB1405.	Project Work	100
	✓ MB1406	MOOCs	Grade
Total marks			2000

Scheme is revised to include MOOCs Courses by following members (Experts) of Board of Studies (BOS), Bioinformatics, CSJM University, and Kanpur under the supervision of Prof. S.K. Agarwal, Biochemistry, Lucknow University on 11 October 2019

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Bio-Informatics
UJET, C.S.J.M. University, Kanpur

Chhatrapati Shahuji Maharaj University, Kanpur

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SEMESTER I

MBI 101A. Mathematics & Statistics

Unit 1. Matrices: Operations on Matrices, determinants, (Simple Calculations) Adjoint, Inverse of a matrix using determinant solution of Equations, Cramer's rule. 3d Geometry: Equation of line in space, Vectors: Definition, Addition, Dot product, Cross product.

Unit 2. Differentiation: Derivatives of important functions (Formulae), sum rule, product rule, Quotient rule, Chain rule.

Unit 3. Integration: Indefinite integrals as anti-derivatives. Integration of sum of two functions, Product rule.

Unit 4. Set Theory Russell's Paradox. The basic axioms, and some basic sets, classes, Ordered pairism, Basic cardinal arithmetic

Unit 5. Random variables, Poisson, normal and binomial distributions, Probability, Permutation and combination, mean, median, mode.

Unit 6. Regression and Correlation; t-test; Analysis of variance; Chi square Test

Programming in C for correlation and regression, standard deviation, testing of hypothesis etc. Using standard package like SPSS and R package

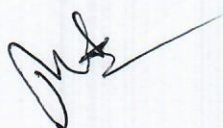
Text Books and References:

Mathematics

1. G.B.Thomas and R.L.Finney : Calculus and Analytical Geometry, 9th edition, Pearson Educaion.
2. B.S. Grewal, Higher Engineering Mathematics, Khanna Publishers, 2005 Modern Biology
3. Ewens, W.J. and Grant, 2001 Statistical Methods in Bioinformatics: An Introduction. Springer-Verlag.
4. Warren J.J., Ewens Warren, Ewens Gregory Grant, Statistical Methods in Bioinformatics: An Introduction, Springer-Verlag.
5. Ayers, F. , Matrices and Vectors, Schaum .

Statistics

1. Statistical Methods in Bioinformatics: An Introduction by W. Evans & G. Grant, Springer, 2001
2. First course in Probability by Sheldon Ross, Prentice-Hall (India), 2001
3. Larson, H.J., Introduction to Probability Theory and Statistical Inference, John Wiley & Sons.
4. Goon, A.M., Gupta, M.K. and Dasgupta B.: Fundamental of Statistics - Vol. 1, The World Press Pvt. Ltd.
5. Devore, J.L., 2002 Probability and Statistics, 5th edition, Thomson Asia.
6. Hoel, Port and Stone, Introduction to Statistics.
7. Miller & Freund: Probability and Statistics for Engineers, 7th Edition.
8. Chung, Kai Lai, Elementary Probability Theory with Statistical Processes (Student Edition) Springer International
9. Angela Dean & Daniel Voss (2006). Design and Analysis of Experiments, Springer Verlag
10. Campbell M.J, Machin D. & Walters S.J (2007). Medical Statistics – A Text Book for the Health Sciences, Wiley.
11. Das M.N. & Giri N.C. (2006). Design and Analysis of Experiments, New Age Publications



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12. Cochran, W.G. (2002). Sampling Techniques. Wiley Des Raj and Chandhok (1998). Sampling Theory, Narosa.
13. Murthy, M.N. (1967). Sampling Theory and Methods. Statistical Publishing Company, Calcutta.
14. Feller, W., An Introduction to Probability: Theory and its Applications, Wiley Eastern Limited.

MBI 101B. Cell and Molecular Biology

Unit 1. Structure of cell & Tissues; cell cycle, Cell-cell communication; Introduction to genome biology: Genome as the store house of information, DNA as the carrier of encoded messages; Organization and regulations of genes in prokaryotes and eukaryotes.

Unit 2. Intra-cellular transmission of genetic message and their cellular translation; Selective transmission of genetic messages- regulation of gene expression; logic of building body plans- developmental translation of encoded messages, cell signalling and signal transduction

Unit 3. Introduction to molecular and cellular biology from an engineering perspective. DNA sequencing methods, strategies for genome sequencing, Gene mapping methods: Linkage maps, tetrad analysis, mapping with molecular markers, mapping by using somatic cell hybrids, FISH, development of mapping population in plants.

Unit 4. DNA fingerprinting; Southern and northern blotting; In-situ hybridization Methods for analysis of gene expression at RNA and protein level, large scale expression, such as micro array based techniques. Isolation, separation and analysis of carbohydrate and lipid molecules RFLP, RAPD and AFLP techniques.

Unit 5. Generation of genomic and cDNA libraries in plasmid, phage, cosmid, BAC and YAC vectors. In vitro mutagenesis and deletion techniques, gene knock out in bacterial and eukaryotic organisms. Transposons and gene targeting; DNA labeling; DNA sequencing; Polymerase chain reactions; Gene isolation; Gene cloning; Expression of cloned gene; Applications of genetic engineering in drug design and therapeutics, agriculture and livestock improvement.

Text Books and References:

1. Lewin 2004, Genes VIII. Pearson.
2. Gerald Karp 2002, Cell and Molecular Biology. John Wiley.
3. Lodish et. al. 2004, Molecular Cell Biology. Freeman.
4. Molecular Biology of the Cell, by Alberts et al (4th edition or later), Garland Sciences, New York
5. Pollard & Earnshaw 2002, Cell Biology. Saunders.
6. Tobin & Morcel 1997, Asking about Cells. Saunders.
7. Watson et. al. 2004, Molecular Biology of the Gene. Pearson.
8. An Introduction to Genetic Engineering, Desmond S.T. Nicholl, third Edition.
- 9.

MBI 102. Biochemistry & Structural Biology

Unit 1. Structure of atoms, molecules and chemical bonds, Composition, structure and function of biomolecules (carbohydrates, lipids, proteins, nucleic acids and vitamins).

Unit 2. Principles of protein structure; anatomy of proteins – Hierarchical organization of protein structure -Internal coordinates of proteins; Internal, Cartesian and distance coordinate representations of protein structures. - Primary, Secondary, Super secondary, Tertiary and quaternary structure; Theory, Conformation of proteins (Ramachandran plot, secondary structure, domains, motif and folds). Stability



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of proteins stabilizing interactions and weak intermolecular interactions (Van der Waals, electrostatic, hydrogen bonding, hydrophobic interaction, etc.). Classification of Three Dimensional Structures in Brookhaven Protein Data Bank (HSSP, SCOP, FSSP, CATH)

Unit 3. Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics, colligative properties). Water as the universal biological solvent. Osmolarity.

Unit 4. Bioenergetics, glycolysis, oxidative phosphorylation, coupled reaction, group transfer, biological energy transducers, enzymes and enzyme kinetics, enzyme regulation, mechanism of enzyme catalysis, isozymes, Chemical and functional nature of enzymes.

Unit 5. Structure of Nucleic Acids: DNA and RNA: types of base pairing – Watson-Crick and Hoogsteen; Conformation of nucleic acids (helix (A, B, Z), t-RNA, micro-RNA) structural and geometrical parameters of each and their comparison, stability of nucleic acids.

Unit 6. Metabolism of carbohydrates, lipids, amino acids nucleotides and vitamins. Biomolecules and their conformation;; Bioenergetics; Metabolism (Glycolysis, TCA and Oxidative phosphorylation); Membrane transport and pumps.

Text Books and Reference:

1. Cellular Biophysics I & II by Thomas F. Weiss 1995, Publisher : MIT Press
2. Introduction to Chemical Engineering Thermodynamics, J. M. Smith, H. C. Van Ness and M. M. Abbott, Mc Graw-Hill, 2005.
3. The Molecules of Life: Physical and Chemical Principles. John. Kurian, Boyana Konforti and D.Wemmer Garland Science, New York 2013
4. Introduction to Protein Structure. Carl Branden & John Tooze, Garland Science
5. Biochemistry by L. Stryer. Publishers : W.H. Freeman and Company(4th Edition)
6. Principles of Biochemistry by A.L. Lehninger, D.L. Nelson, M.M. Cox. Publisher : Worth Publishing.
7. Harper's Biochemistry by K. Robert, M.D. Murray, D.K. Granner, P.A. Mayes and V.I. Rodwell. Publisher: McGraw-Hill/Appleton and Lange.
8. Devlin's Textbook of Biochemistry with Clinical correlations. Publisher : John Wiley and Sons Inc.
9. Tools of Biochemistry by T.G. Cooper. Publisher : John Wiley and Sons
10. Biochemical calculations by I.H. Segal. Publisher : John Wiley and Sons

MBI 103. Introduction to Programming

Unit 1. Basic concepts of Computers, Basic UNIX Concepts and Vi – Editor, Learning OS Commands, Exposure to Windows environment, Practice of UNIX commands and Vi editor, Writing simple shell script.

Unit 2. Problem identification, analyzing requirements, research existing and alternative solutions, analyzing solutions quantitatively, synthesizing and evaluating data, prototyping, and testing.

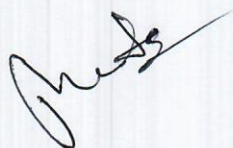
Unit 3. Introduction to C: Basic Programming concepts, Program structure in C, Variables and Constants, Data types, Basics of Algorithm, Pseudocode and Flowcharts.

Unit 4: C Programming: Practicing programs to get exposure to basic data types, algebraic expressions, sequential, conditional and loop constructs, control statements. Input, Output Formatting, Control structures, arrays, string, functions, structures, pointers and basic file handling.

Unit 5. Web technologies: HTML, XML, basic concepts of client-server computing. Editors and Word Processors, Spreadsheets and Database packages, data communication and computer networks.

Lab/Practical: Programming in C language

1. Program to carry out basic arithmetic operations (+, -, *, /, %), Integer division, Digit reversing



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2. Program to find whether a given number is prime or not
3. Program to find the biggest of 2/3 numbers
4. Program to print a series of odd/even numbers or Determining if a number is +ve / -ve /
5. Program to find factorial of an integer with or without using recursion
6. Program to check whether a string is palindrome or not
7. Arrange a series of numbers/strings in ascending/descending order
8. Sum of first n numbers, given n numbers
9. Program for matrix addition, Substataion, matrix multiplication
10. Program for string copying and String concatenation and File copying
11. Table generation for n, a^b, sine series, cosine series, ⁿC_r, Pascal Triangle, Factors of a number
12. Program using array and structures.

Text Books and References:

1. A Balanced Introduction to Computer science by David Reed, PE, 2000.
2. Introduction to Computing Systems: From Bits to Gates to C and Beyond. Yale N. Patt and Sanjay J. Patel. Prentice Hall India, 1999
3. Programming with C, K.R.Venugopal & Sudeep R. Prasad, Tata McGraw Hill
4. Programming in C, Herbert Schildt, THM, Fifth Edition, 2002
5. C How to program, Deitel & Deitel, Pearson Edition, Third Edition, 2001
6. Programming in C, Denis Ritchie, THM, Fourth Edition, 2000
7. Programming in C, Schaum Series, 3rd edition
8. The 'C' Programming, Denis Ritchi (PHI)
9. Programming in C, Venugopal (TMH)
10. Programming in C, Balaguruswami (TMH)


MBI 104. Computational Biology

Unit.1 Basic concepts: Sequence similarity, identity and homology, definitions of homologues, orthologues, paralogues, Introduction to Sequence analysis programs and structure prediction programs, Sequence assembly and finishing methods, Introduction to Genome and Genomic mapping, complexity of genome, Fragmentation of Genome. Primers design, mapping algorithms.

Unit 2. Pairwise sequence alignments: Basic concepts of sequence alignment: local and global alignments, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments, gap penalties, use of pairwise alignments for analysis of Nucleic acid and protein sequences and interpretation of results.

Unit 3. Scoring matrices: Basic concept of a scoring matrix, Matrices for nucleic acid and proteins sequences, BLAST and FASTA, PAM and BLOSUM matrices derivation, principles based on which these matrices are derived. Computation of various parameters using proteomics tools at the ExPASy server and EMBOSS

Unit 4. Multiple sequence alignments (MSA): The need for MSA, basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW and PileUp and their application for sequence analysis, concept of dendrogram, phylogram and cladogram, whole genome alignments: understanding significance. Use of HMM-based Algorithm for MSA (e.g. SAM method)



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Unit 5. Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, various types of pattern representations viz. consensus, regular expression (Prosite-type) and sequence profiles; profile-based database searches using PSI-BLAST, MEME, PHI-BLAST, SCanProsite and PRATT, Profile Analysis method of Gribskov, HMMer, PSI-BLAST

Unit 6. Basic concepts in systematics, taxonomy and phylogeny; molecular evolution; nature of data, Phylogenetic tree analysis algorithms such as maximum Parsimony, UPGMA, Transformed Distance, Character based method, Neighbor-Joining, Probabilistic models, Bayesian inference algorithm, Bootstrapping methods, use of tools such as PHYLIP, MEGA, PAUP Analysis of regulatory RNA's: Databases and tools.

Practical/Lab

1. Pair-wise global alignments of protein and DNA sequences using Needleman-Wunsch algorithm & interpretation of results to deduce homology between the sequences, use of scoring matrices
2. Pair-wise local alignments of protein and DNA sequences using Smith-Waterman algorithm and interpretation of results
3. Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences
2. Database (homology) searches using different versions of FASTA & interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences.
3. Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLUSTAL. Interpretation of results to identify conserved and variable regions and correlate them with physico-chemical & structural properties.
4. Profile-based database searches using PSI-BLAST, analysis and interpretation of profile-based searches. Conserved Motif search using MEME, PHI-BLAST

Text Books and References:

1. Developing Bioinformatics Computer Skills by C. Gibas and P. Jam beck, O' Reilly (2001)*
2. An Introduction to Bioinformatics Algorithms, Neil C Jones & Pavel A. Pevzner, Ane Books, 2005.
3. Bioinformatics: Sequence and Genome Analysis, David W Mount , 2nd Edition, cold Spring Harbor Press
4. Introduction to Computational Molecular Biology , Setubal and Meidanis, Thomson, 2003.
5. Introduction to Mathematical Method in Bioinformatics, Alexcender Isaev, Springer Universitext, 2004.
6. Biological Sequence Analysis Probablistic Models of Proteins and Nucleic Acid, R. Durbin, Eady, A. Krogh and Mitchison, Cambridge University Press, 1998.
7. Essential Bioinformatics-Jin Xiong, Cambridge University Press
8. Introduction to Bioinformatics – Attwood & Parry-Smith, Pearson Education
9. Bioinformatics- A beginner's guide by Jean-Michel Claverie, John Wiley & Sons.

MBI 105. Basic Genetics

Unit 1. Mendelian Inheritance, Extensions of Mendelian principles: Codominance, incomplete dominance, gene interactions, gene and environment interactions, pleiotropy, genomic imprinting, penetrance and



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expressivity, linkage and crossing over, sex linkage, Extra chromosomal inheritance: Inheritance of mitochondrial and chloroplast genes, maternal inheritance.

Unit 2. Basic biological concepts in genetics, Mendel's law, Hardy Weinberg equilibrium, estimation of allele frequency (dominant/co-dominant cases), Approach to equilibrium for X-linked gene. The law of natural selection, mutation, genetic drift. Population genetics: Hardy Weinberg Law, Effect of mutation, migration, selection and genetic drift on population. Basic Human genetics: Pedigree analysis, linkage testing, karyotypes, genetic disorders.

Unit 3. Non-random mating, inbreeding, phenotypic assortative mating. I, T, O matrices, identity by descent. Family data-estimation of segregation ratio under ascertainment bias, pedigree data: Elston - Stewart algorithm for calculation of likelihoods. Linkage, estimation of re-combination fraction, inheritance of quantitative traits.

Unit 4. Simple Mendelian traits; Loss of function mutations; Gain of function mutations; Gene interactions; Dynamic mutations; Genetics of neoplasia; Genomic imprinting and human disease; X-inactivation and DNA methylation; Gene mapping and positional cloning; Multifactorial inheritance; Genetics of behavioural disorders. Gene duplication Pharmacogenetics and biochemical genetics; Animal models in human genetics: Methods used for diagnosis and detection of gene mutations; Gene Therapy.

Text books and References:

1. Atherly et. al. 1999, The Science of Genetics. Saunders.
2. Griffiths et. al. 2004, An Introduction to Genetic Analysis.
3. Hartl & Jones 1998, Genetics - Principles & Analysis. Jones & Bartlett.
4. Snustad et. al. 1998, Principles of Genetics. Wiley & Sons.
5. Strickberger 1985, Genetics. Macmillan.
6. Russell 2002, Genetics. Benjamin.
7. Anil Gore & Sharayu Paranjpe (2001). A Course in Mathematical And Statistical Ecology. Kluwer academic Publishers.
8. Gardner E.J. & Snustad D.P. Principles of Genetics, John Wiley & Sons Inc.
9. Lange, K (2002). Mathematical and Statistical Methods for Genetic Analysis, Springer.

SEMESTER II

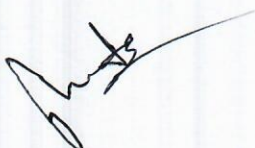
MBI 201. Genomics & Transcriptomics

Unit 1. Identification of alternatively spliced genes; Transcription binding sites, Identification of genes in prokaryotes and eukaryotes. Promoter identification.

Unit 2. Introduction; The impact of Genomics on biological research; Identification of a large set of genes involved in a biological process; High throughput expression analysis; Genome wide search for interacting partners; Sequence variations and disease susceptibility. Genome wide annotation methods, identification analysis of various genome.

Unit 3. Comparative genomics: Basic concepts and applications, MegaBlast algorithms, PipMaker, AVID, Vista, MUMmer, applications of suffix tree in comparative genomics, synteny and gene order comparisons, Comparative genomics databases: Clusters of Orthologous Groups (COGs), Ensembl

Unit 4. Functional genomics: Application of sequence based and structure-based approaches to assignment of gene functions – e.g. sequence comparison, structure analysis (especially active sites, binding sites) and



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comparison, pattern identification, etc. Use of various derived databases in function assignment, use of SNPs for identification of genetic traits, Gene/Protein function prediction using Machine learning tools; supervised/unsupervised learning, Neural network, SVM etc

Unit 5. Microarray data analysis, Principle of NGS technology, Next Generation Sequencing Methods, Workflows for various NGS experiments; Various file formats such as SAM, VCF, BED, ChIP-seq, Binary Alignment/Map (BAM) format.

Unit 6. Transcriptomics Types of RNAs and the respective roles in cells. Transcriptome and techniques used for transcriptomics; microarray and RNA-seq. Impact of transcriptomics on biology, volume of data produced and important repositories. Comparing transcriptomics with genomics and proteomics

Lab/Practical

1. Searching for particular gene from Biological Databases, Genome Databases, Viral Genomes, Archeal and Bacterial Genomes, Eukaryotic genomes with special reference to model organisms (Yeast, Drosophila, *C. elegans*, Rat, Mouse) Human, plants such as Arabidopsis thaliana, Rice, etc.
2. Retrieving protein and nucleic acid sequences, structures, ESTsequences, SNP data using database browsers and genome browsers.
3. Gene sequence analysis : Prediction of ORF's, transcription factor binding site and promoters
4. Prediction of gene features, codon usage and RNA fold analysis.
5. Phylogenetic analysis of gene orthologs and paralogs: Prediction of conserved motif.
6. Micro array data analysis using online tools.
7. Prediction of splice sites using-SIN-4, spidey, BLAT etc.

Text Books & References

1. Gupta, PK (2004) Biotechnology and Genomics, Rastogi Publications, Meerut, India (ISBN: 81-7133-676-0)
2. Stuart M. Brown "Next-Generation DNA Sequencing Informatics", Cold Spring Harbor Laboratory Press
3. Genomics: the science and technology behind human genome project, Cantor and Smith
4. Pevnezer, "Bioinformatics and Functional Genomics", John Wiley.
5. Genomics, Proteomics and Bioinformatics. A. Malcolm Campbell & Laurie J. Heyer, CSHL Press and Benjamin Cummings. Current Protocols in Bioinformatics, Edited by A.D. Baxevanis et al, Wiley Publishers.2005
7. Bioinformatics by David W. Mount, Cold Spring Harbor Laboratory Press. 2001
8. Fundamental concepts of Bioinformatics by D.E. Krane and M.L Raymer, Pearson Education. 2003

MBI 202. Data Structure & Algorithm

Unit 1. Basic Concepts and algorithmic mathematical notations, Introduction to algorithm analysis for Time and Space requirements,



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Unit 2. (a) Arrays and Linked lists (b) Stacks and Queues, Dynamic (c) Trees: Definition and basic concepts, Binary search trees and their usage, Trees: Definition and basic concepts linked tree representation, Binary tree traversal techniques, Binary search trees and their usage.

Unit 3. Searching Techniques, Basic concepts of Indexing, Sequential search, Indexed sequential search, Binary search, Hashing, B+ Tree indexed files.

Unit 4. Graphs: Definition and Representations of graphs, Depth-first search, Breadth-first search, Introduction to Greedy algorithms. Sorting algorithms, Bubble sort, Insertion sort, selection sort, merge sort and quick sort; Divide and Conquer method

Lab/ Practical: Write Program in C for following:

1. Searching, traversing, insertion, deletion operations on Arrays
2. Traversing, searching, insertion and deletion on Stack.
3. Traversing, searching, insertion and deletion on Queue, Circular Queue
4. Linked list implementation using Dynamic memory Allocation, deletions and insertions
5. Programming to implement algorithms on Tree Structures, Binary Tree, Tree Traversals, Binary Search Tree, Insertion and Deletion in BST.
6. Programming to implement Searching algorithms (sequential search and binary search)
7. Programming to implement Sorting Algorithms
8. Programming to create Graph structure and its searching algorithms BFS, DFS.

Text Books and References:

1. AV Aho, J Hopcroft, JD Ullman, Data Structures and Algorithms, Addison Wesley, 1983.
2. TH Cormen, CF Leiserson, RL Rivest, C Stein, Introduction to Algorithms, 3rd Ed., MIT Press, 2009.3. AV Aho, J
3. Hopcroft, JD Ullman, The Design and Analysis of Algorithms, AddisonWesley, 1974.
4. MT Goodrich, R Tamassia, DM Mount, Data Structures and Algorithms in Java, 5th Ed., Wiley, 2010. (Equivalent book in C also exists.)
5. Y. Langsam, M.J. Augenstein and A.M. Tenenbaum, Data Structure Using C and C++. Second Edition, Pearson education 2nd edition 2002.
6. John R. Husband – Schaum outline Data structure with C++, McGraw Hill
7. Design and Analysis of algorithms, David M Mount, University of Maryland 2003.

MBI 203. Object Oriented Programming using Java

Unit 1. Object Oriented Concepts, Introduction to Object Oriented Programming using Java programming language, Abstraction, encapsulation, Inheritance.

Unit 2. Java Programming: Data types, control structured, arrays, strings, and vector, classes, Polymorphism, package, exception handling, Multithreading,

Unit 3. Java applets, AWT controls layout manager, string handling Java applet basics, Simple events and inter activity, creating user interfaces with AWT, Modifiers, Serialization, Streams and I/O, Data structure and Java image filters.

Unit 4. Networking, event handling, JDBC, Java Servlets: Introduction, Servlet Basics, The Servlet Lifecycle, Retrieving Information, Sending HTML Information, Database Connectivity, Java Server Pages: Introducing Java Server Pages.



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Lab/Practical

1. Simple Programming to create class, initialise an object and use constructor and method.
2. Programming to derive the class from base class using single level inheritance.
3. Programming to derive the class from base class using multi-level inheritance.
4. Programming to implement multiple inheritances using interface.
5. Programming to implement conditional statement.
6. Programming to implement different types of Loops.
7. Programming to implement different types of operators.
8. Programming to use various types of Java data structures (array, string, vectors, hashes)
9. Use of try and catch for exception handling.
10. Initialising and running a thread, implementation of other lifecycle state of thread.
11. Creation applet using awt classes and viewing it in applet viewer
12. File handling (read, write and open) to manage input/output data.

Text Books and References:

1. Patrick Naughton and Herbert Schildt, "Java-2 The Complete Reference" 199, TMH.
2. Hopcroft, JD Ullman, The Design and Analysis of Algorithms, Addison Wesley, 1974.4.
3. MT Goodrich, R Tamassia, DM Mount, Data Structures and Algorithms in Java, 5th Ed., Wiley, 2010. (Equivalent book in C also exists.)
4. Ivor Horton, "Beginning Java-2" SPD Publication
5. Jason Hunter, "Java Servlet Programming" O'Reilly
6. Hans Bergsten, "Java Server Pages", 3rd Ed. O'reilly

MBI 204. Immunology & Immunoinformatics

Unit 1. Immunology: Overview of immune system, Immunoassays, Antibody generation. Immune systems: Innate and adaptive immunity in vertebrates, Antigen processing and presentation, Infectious diseases, Autoimmune diseases

Unit 2. Antibodies: Immunoglobulin classes and subclasses, CDR and LDR regions and sequence numbering, Immunogenetics & immunogenomics, Membrane receptors for antigen, The B-cell surface receptor for antigen (BCR), T-cell surface receptor for antigen (TCR), The major histocompatibility complex (MHC), MHC polymorphism Recognition of Antigen by B cells

Unit 3. Immunoinformatics overview, Reverse vaccinology, Rational Vaccine design o Evolution and escape due to variations, Immunoinformatics databases & tools, Molecular interactions, Specificity, characterization; Sequential and conformational epitopes, MHC- peptide HLA: nomenclature, HLA-peptide interactions & matrices

Unit 4. Epitope prediction algorithms: B-cell epitope predictions using sequence-based approaches o B-cell epitope predictions using structure-based approaches, T-cell epitope prediction methods, Epitope Predictions;

Unit 5. Predicting Peptide-MHC Binding using Profiles, Machine Learning Techniques for MHC Binders, Methods for Predicting T-Cell Epitopes, MHC-Class I and II Binding Affinity. MHC-Molecular Affinity and QSAR Models, Nonlinear Predictive Modelling of MHC Class II-Peptide Binding using Bayesian, Neural Networks; Vaccine design, Codon optimization, application of genetic



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engineering in vaccine design. Vaccine design: Pipeline & workflows o Prediction of immunogenicity, Case studies: Hepatitis B

Lab/ Practicals

Prediction of Antigenic properties and Epitopes

1. Prediction of structural features of antibodies using computational tools
2. Retrieval of sequence & structure of Immunoglobulin in databases.
3. Study of Antibody sequence and structure: visualisation of structure & mapping CDRs on structure
4. Study of variable and constant domains
5. Characterization of binding sites on the basis of molecular interaction
6. Sequence analysis to study conserved regions and variable regions.
7. Prediction of conformational epitopes
8. Prediction of cytotoxic and helper T cell epitopes
9. Prediction of immunogenicity for vaccine design: Combination of MHC and Proteasome predictions

Vaccine Design

1. Screening of Antigenic protein using vaccine databases.
2. Study of model organisms.
3. Data base searching using MHCDB
4. Epitope prediction using NetMHC.
5. Mapping and identification of Epitopes
6. Codon optimisation of reverse translated sequence.
7. Study of open reading frame.

Text Book References:

1. Flower Darren R. Bioinformatics for Vaccinology Publisher: UK, John Wiley & Sons Inc. 2008.
2. Flower Darren R. Immunoinformatics: Predicting Immunogenicity In Silico Publisher: New Jersey, Humana Press. 2007.
3. Kindt, Thomas J., Osborne Barbara A. Goldsby Richard A. Kuby Immunology 6th Edition. Publisher: New York, W. H. Freeman. 2007. ISBN: 9780716785903.
4. Lund Ole , Nielsen Morten , Lundegaard Claus, Kesmir Can, Brunak SÃ,ren. Immunological Bioinformatics. Publisher: London, MIT Press 2005 ISBN: 0262122804.
5. Foundation Novartis. Immunoinformatics: Bioinformatic Strategies for Better Understanding of Immune Function. Publisher: Chichester, John Wiley & Sons Inc. 2003. ISBN: 0470853565.
6. Roitt Ivan, Delves Peter. Roitt's Essential Immunology 10th Edition. Publisher: Canada, Blackwell. 2001, ISBN: 0632059028.

MBI 205. Biochemical & Biophysical Method

Unit 1: Biophysical Thermodynamics, the thermodynamics of biopolymer structure formation. First and Second Laws, Phase Rule and Phase Equilibria, Thermodynamics of Adsorption and Binding. Isolation and purification of RNA, DNA (genomic and plasmid) and proteins, Analysis of RNA, DNA and

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proteins by gel electrophoresis, Isoelectric focusing gels, 2D-PAGE, Chromatography, HPLC Protein sequencing methods, detection of post translation modification of proteins.

Unit 2: Proteomics: Protein sequencing analysis, protein and peptide sample preparation, Gel Electrophoresis, analytical proteomics, combined method, recombinant protein purification, protein-protein and protein-DNA interactions, newly emerging methods for the investigation of the proteome, allowing to analyze the expression of genes. Methods for studying molecular interactions of protein – Protein, Protein – DNA, Protein – carbohydrate, DNA – small molecules and Protein-drug. Emulsion PCR approach with small magnetic beads and single molecule real time (SMRT) sequencing;

Unit 3: Biophysical Method: Molecular analysis using UV/visible, fluorescence, circular dichroism, NMR and ESR spectroscopy Molecular structure determination using X-ray diffraction and NMR, FTIR Molecular analysis using light scattering, different types of mass spectrometry and surface plasma resonance methods. Mass spectrometry, analysis of post-translational modifications, Luminescence, fluorescence, phosphorescence.

Text Books and References:

1. Jan Drenth Principles of Protein X-ray Crystallography (Springer Advanced Texts in Chemistry), Springer-Verlag Telos.
2. Lipson, H. and Steeple, H., Interpretation of X-Ray Powder Diffraction Patterns. St. Martin's Press.
3. Bovey, F.A., Mirau, P.A. and Gutowsky, H.S., Nuclear Magnetic Resonance Spectroscopy (2nd Edition). Academic Press.
4. Hallet, F.R., Stinson, R.H., Speight, P.A. and Graham, W.G., 2004 Physics for the Biological Science. Toronto: Nelson Can.
5. Yadav, L.D.S., Organic Spectroscopy (1st Edition). Springer.
6. Hollas, J.M., High Resolution Spectroscopy (2nd Edition). John Wiley & Sons.
7. Mass spectrometry: Principles and applications; E.D. Hoffmann & V. Stroobant; Wiley, 3rd edition, 2007.
8. Biological Thermodynamics, D. T. Haynie, Cambridge University Press, 2008.

SEMESTER III

MBI 301. Database Management and Data Security

Unit 1. Databases, ER-model, Relational model (relational algebra, tuple calculus), Database design (integrity constraints, normal forms), Query languages (SQL), Transactions and concurrency control, Introduction to Biological databases.

Unit 2. Relational database design: Normalisation - 1NF, 2NF and 3NF. File structures (sequential files, indexing, Indexing and Hashing. Security of databases. Design example on a popular RDBMS package.

Unit 3. Introductory data security concepts, Discretionary and mandatory access controls, secure database design and architectures, information flow controls, inference controls. Role based access control and Encryption.

Unit 4. Application of database management in biological areas, Agrininformatics, Medical Informatics, Patient database system, Telehealth and Telemedicine.



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Lab/Database Practical

1. Learning SQL commands and development of database.
2. Defining data structure for building a database.
3. Managing database objects within a database.
4. Normalization of tables in databases.
5. Manipulation of the data.

Text Books and References:

1. Ralph Kimball, "The Data Warehouse Lifecycle Tool Kit", John Wiley.
2. H GarciaMolina, JD Ullman and Widom, Database Systems: The Complete Book, 2nd Ed., PrenticeHall, 2008.
3. A Silberschatz, H Korth and S Sudarshan, Database System Concepts, 6th Ed., McGrawHill, 2010.
4. R Elmasri, S Navathe, Fundamentals of Database Systems, 6th edition, AddisonWesley, 2010.4.
R Ramakrishnan, J Gehrke, Database Management Systems, 3rd Ed., McGrawHill, 2002.

MBI 302. Programming using Perl & Python

Unit 1. Introduction: An Introduction to Perl, The Perl Interpreter, How the Perl Interpreter Works, Variables and Data Types: Perl Variables, Scalar Values, Variable Definition, Special Variables. Arrays and Hashes: Arrays, Array Manipulation, Hashes Control Structures, Comparisons, Conditional statements, Loops, Operators, Subroutines: Creating a Subroutine, Arguments, Passing Arguments with References, String Manipulation: Array-Based Character Manipulation, Regular Expressions, Patterns

Unit 2. Input and Output: Program Parameters, File I/O (File handles, Working with Files, Built-in File, Handles, File Safety, The Input Operator, Binary I/O). Object oriented Perl: Introduction to modules and Packages, Objects creation Bioperl : Introduction, Installation procedures, Architecture, Uses of bioperl, Class, Method, Method overriding, Inheritance, Perl Database access.

Unit 3. Introduction to Python, Python features, Python Environment, Basic syntax, variables, function and method, operators, conditional statements, Looping, control statements, List, Tuple, string manipulation, Dictionaries, python standard Library. Modules, Input-Output, Exception handling

Unit 4. OOPs Concept: Class and object, Attributes, Inheritance, Overloading, Overriding, Data hiding, Regular expression, CGI, Database, Networking multithreading, GUI

Practical/Lab

1. Data storage and manipulation using array and hashes
2. Programming to implement conditional statement.
3. Programming to implement different types of Loops.
4. Programming to implement different types (eight) of operators.
5. Use of subroutines and references in programming.
6. Searching of patterns in sequences.
7. Programs to read and analyze DNA and Protein sequences in different file formats.
8. File handling to manage input/output.
9. Programming to predict genome annotation.
10. Programs to read and analyze PDB structure files
11. Scripts to automate other standalone Bioinformatics software.
12. Simple Programming to create class, method and initialise an object using Python programming..



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13. Python Programming to inherit the class from base class.
14. Python Programming to perform operations on data structures.

Text Books and references:

1. Beginning Perl for Bioinformatics, James Tisdall, 2001, O'Reilly & Associates, (2001) Learning Perl, 3rd Edition.
2. Mastering Perl for Bioinformatics"James Tisdall, 2003, O'Reilly & Associates, (2001) Learning Perl, 3rd Edition.
3. Perl programming for Bioinformatics Bal, H.P.. Publisher: Tata McGraw-Hill New Delhi.
4. Bioinformatics, Biocomputing and Perl: an Introduction to bioinformatics computing skills and practice, Moorhouse Michael, Barry Paul.. Publisher: John Wiley and Sons, 2004
5. Curtis Jamison D. Perl programming for biologists. Publisher: John Wiley & sons, inc., 2003
6. Genomic Perl; *R.A. Dwyer*; Cambridge University Press, 2003.
7. Perl tutorial ,Tutorial point,.www.tutorialpoint.com
8. Python for Data Analysis: Data Wrangling with Pandas, NumPy, and IPython by Wes McKinney
9. Python Essential Reference (4th Edition) by David Beazley

MBI-303. Pharmacogenomics & Metagenomics

Unit 1. Sequence variations and disease susceptibility; Pharmacogenomics; Functional Genomics in model organisms; High-throughput phenotypic analysis; Recent developments in Genomics. Comparative Genomics, Genetic profile and its analysis using Microarrays and other techniques. Gene therapy, SiRNA Technology,

Unit 2. Pharmacogenomics databases, Introduction to Pharmacogenomics, Pharmacogenomics vs Pharmacogenetics. drug metabolism, drug interactions, pharmacological actions of drugs, Pharmacokinetics and Pharmacodynamics, SNP array, SNP's and drug response: Genetic variations, types of polymorphisms, Personalized medicine; Inter-individual variability, Personalized sequencing, precision therapies.

Unit 3. Metagenomics and Population genomics Overview of metagenomics principles, microbial and ecological aspects underlying metagenomic experiments, applications and limitations of metagenomics, differences between metagenomics and single-cell genomics. Definition and principle of population genomics, difference between metagenomics and population genomics, applications of population genomics.

Unit 4. Metagenomics, study of environmental effects on gene expression and biodiversity. Metagenomics: Concept, Approaches for metagenome analysis & ecological inference, QIIME pipeline for microbial community, SeqEnv: annotating sequences with environmental information; Introduction to shotgun metagenomics, Read based metagenomic profiling & analysis; Taxonomic classification and clustering of contigs.

Lab/practical

Pharmacogenomics

1. Study of genetic profile of various types of population.
2. Study of antibiotic sensitivity in these population
3. Prediction of drug's effect on population based on clinical data analysis.
4. Study of SNP variation.

Metagenomics

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1. Metagenomic analysis using Megan
2. Searching in MGRast,IMG, WebMG,EBI

Text Books & References

1. Emily D. Aulicino, "Genetic Genealogy: The Basics and Beyond" 4. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
2. Joseph S. Bertino, "Pharmacogenomics An Introduction and Clinical Perspective", McGraw Hill
3. Lorenz, P and Eck, J (2005) Metagenomics and Industrial Applications, Nat. Rev. Microbiol., Vol 3, pp. 510-516.
4. Handelsman, J (2004) Metagenomics: Application of Genomics to Uncultured Microorganisms, Microbiol. Mol. Biol. Rev., Vol 68-4, pp. 669-685.
5. Riesenfeld, CS, Schloss, PD, Handelsman, J (2004) Metagenomics: Genomic analysis of Microbial Communities, Annu. Rev. Genet.,

MBI-304. Data Mining & Data Analytics

Unit 1. Data Warehousing: Need for data warehousing, Basic elements of data warehousing, Data Warehouse and Online analytical processing (OLAP) technology Data Mart, DMQL. Data Integration methods.

Unit 2. Data Mining: Basics, Architecture for Data Mining, Data Preprocessing, Data Integration and Transformation. Data mining techniques, KDP (Knowledge Discovery Process). Data Mining & Machine Learning methods: Clustering, Feature selection, Classification, Correlation analysis, Supervised and Unsupervised learning with regression etc. Application and Challenges of Data Mining in Bioinformatics.

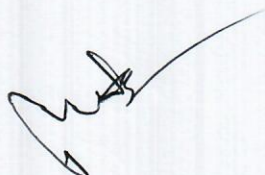
Unit 3. Big data analytics: Overview of big data analytics in context of bioinformatics, Types of big data in bioinformatics, Big data analytics applications, Theory and methods for big data analytics, Technologies and tools for big data analytics.

Unit 4. Analytics life cycle, Need, Structured and multi-structured data analysis, Big-data analytics major components, Analytical models and approaches, Application areas, Design and analysis of Analytics model-Analytics design steps, Understanding different data processing models, Statistical models, Predictive models, Descriptive models.

Unit 5. Introduction to Data analysis using R- Basics of R Language, Statistical models in R, Statistical techniques applied using R, Graphical analysis techniques, Practical examples/case studies. Tools for big data analytics in bioinformatics, GWAS, pathway analysis.

Practical/Lab

1. Implementation of data mining algorithms using R package
2. Big data & Machine learning tools: Spark & SparkML , H2O , Azure ML
3. Use of Hadoop and Hadoop related tools, MapReduce, Pig and HIVE for big data analytics
4. Microarrays and Gene Expression (differentially expressed) data analysis by R
5. Cluster Analysis of microarray information
6. Analysis of NGS data R and bioconductor
7. Analysis of Transcriptome data by R and Bioconductors packages
8. Constraint based modeling in R using metabolic reconstruction databases Constraint based modeling in R using metabolic reconstruction databases (BiGGR)
9. An R interface for computational modeling of tumor progression (Cancer InSilico)
10. Protein-Protein Interaction Statistical Package (ppiStats)
11. MATLAB use for statistical analysis for big data



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Text Books and References:

1. J. Han, M. Kamber, "Data Mining: Concepts and Techniques", Harcourt India / Morgan Kaufman P.Ponnian, "Data Warehousing Fundamentals", John Wiley.
2. M.H.Dunham, "Data Mining Introductory & Advanced Topics", Pearson Education.
3. Ralph Kimball, "The Data Warehouse Lifecycle Tool Kit", John Wiley.
4. M.Berry , G.Linoff, "Master in Data Mining", John Wiley.
5. E.G. Mallach , "The Decision Support & Data Warehouse Systems", TMH
6. Sam Anahory, Dennis Murry, "Data Warehousing in the real world", Pearson Education 2003.
7. David Hand, Heikki Manila, Padhraic Symth, "Principles of Data Mining", PHI 2004.
8. Alex Bezon, Stephen J.Smith, "Data Warehousing, Data Mining & OLAP", McGraw-Hill Edition.
9. Klir G.J. and Folger T.A, Fuzzy sets, Uncertainty and Information, PHI
10. Kosco B., Neural networks and fuzzy systems: A dynamic approach to machine Intelligence, Prentice Hall USA, 1992.
11. Michael Minelli, Michelle Chambers, and Ambiga Dhiraj, "Big Data, Big Analytics: Emerging Business Intelligence and Analytic Trends for Today's Businesses", Wiley, 2013.
12. Big-Data Black Book, DT Editorial Services, Wily India.
13. Biological Data Mining, George Tzanis, Christos Berberidis and Ioannis Vlahavas, Aristotle University of Thessaloniki, Greece.
14. Introduction to Datamining and Knowledge Discovery by Two Crows Corporation.
15. Big Data Analytics in Bioinformatics and Healthcare, Baoying Wang and Ruowang Li, Idea Group,U.S.; 1 edition
16. P. Ponnian, "Data Warehousing Fundamentals", John Wiley.
17. M.H.Dunham, "Data Mining Introductory & Advanced Topics", Pearson Education.

MBI 305. Technical Communication, Research & IPR

Unit 1. Critical reasoning and verbal deduction. Numerical Ability: Numerical computation, numerical estimation, numerical reasoning and data interpretation.

Unit 2. Basics of Technical Communication: Technical Communication: features; Distinction between General and Technical communication; Constituents of Technical Written Communication: Technical Terms; Paragraph-Text Readings, Mechanics of writing, Forms of Technical Communication: Letters. Reports: Types; Significance; Structure, Style & Writing of Reports and Proposal; Significance.

Unit 3. Presentation Strategies: Defining Purpose; Audience & Locale; Organizing Contents; Preparing, Outline, Seminar, workshop and Conference.

Unit 4. Research, Methods of Scientific research, Format of Project Report, Thesis, Research Article, Review Article, Searching in bibliographic databases

Unit 5. Ethics and Technology: Intellectual property rights, patenting, Entrepreneurship development, Risk Assessment and Management Information Security. IPR issues in Biotechnology and Bioinformatics, impacts of IT on language & culture localization issues – Unicode – IT and regional languages, Integrated Practice Management Systems, Various IPR laws Copyright and Patents.

Students will have to submit a draft of project report for internal assessment (shall be evaluated by course instructor) and final copy of project report for external evaluation (shall be evaluated by external examiner) based on two months (20 May to 20 July) summer training work from R& D Institution. Each student must present summer training work in series of presentations for internal assessment (20%



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presentation+ 10% written exam of above course) and one final viva/ presentation for external evaluation (30% project report+30% presentation of work +10% query/viva)

Text Books and References:

1. Improve Your Writing ed. V.N. Arora and Laxmi Chandra, Oxford Univ. Press, New Delhi.
2. Technical Communication – Principles and Practices by Meenakshi Raman & Sangeeta Sharma, Oxford Univ. Press 2007, New Delhi.
3. Effective Technical Communication by Barun K. Mitra, Oxford Univ. Press, 2006, New Delhi
4. Developing Communication Skills by Krishna Mohan, Meera Banerji- Macmillan India Ltd. Delhi.
5. Manual of Practical Communication by L.U.B. Pandey & R.P. Singh; A.I.T.B.S. Publications India Ltd.; Krishan Nagar, Delhi.
6. The Language of Literature and Science by A.Huxley
7. Core referel. AnithaRao and BhanejiRao, "Intellectual Property rights: A primer", Eastern Book Company.
8. Rowena Murray, "How to Write a Thesis", Tata McGraw Hill Education Pvt. Ltd.
9. C.R.Kothari, "Research Methodology, New Age Publishers
10. Jeffrey A. Lee, "The scientific endeavor: a primer on scientific principles and practice", Benjamin Cummings.
11. Robert A. Day, "How to Write and Publish a Scientific Paper", Cambridge University Press.
12. Dr. Marlene Caroseli, "Quick Wits: 50 Activities for Developing Critical Thinking Skills", Ane Books.
13. Gregory Bassham, William Irwin, Henry Nardone and James Wallace, "Critical Thinking: A Student's Introduction", Tata McGraw Hill education Pvt. Ltd.
14. Rhonda Abrams and Julie Vallone, "Winning Presentation in a Day", PHI Pvt Ltd. 6. Weisberg, R., "Creativity - Beyond the Myth of Genius", W.H. Freeman and Company, New York, 1993.

IV SEMESTER

MBI 401. High throughput Data analysis

Unit 1: DNA microarray: understanding of microarray data, normalizing microarray data, detecting differential gene expression, correlation of gene expression data to biological process and computational analysis. Expression matrix, intensity ratio, various methods of Normalisation, Clustering algorithms, Distance method, and applications. Bioconductors for short read analysis. Gene Expression Omnibus (GEO), ArrayExpress, SAGE databases,

Unit 2: Highthroughput sequencing based association studies, Genome analysis Sequence assembly concepts and challenges in assembling short reads; Algorithms for assembling short reads using graph theory, Gene prediction and annotation; gene ontology (GO); Identification genetic variations from genome sequence: SNPs, SNVs, translocation, copy number variation. Concepts behind genome-wide association studies. Highthroughput analysis of metabolomics data generated by GC-MS and LC-MS, Transcriptome analysis and database tools. Measuring gene, lncRNA, siRNA from RNA-seq data, Introduction to Chip-Seq data and analysis, Differential expression for RNA-Seq. Method for single cell RNA-seq data analysis.

Unit 3. Computational epigenomics Concepts and algorithms to measure transcriptional regulation; methylation and alternative splicing; small RNA analysis, validation of whole-genome datasets. Allele specific expression and eQTL.



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Unit 4. Genome sequencing technology, Sanger's dideoxy method versus NGS; shotgun sequencing methods and library preparations, comparative study of standard NGS methods. Next Generation sequencing & assembly: Elements of big data analysis, NGS Platforms based on pyrosequencing, sequencing by synthesis. Handling and analysis of HT & PCR data and data driven normalisation strategy

Lab/Practical

1. Analysis of Chip-Seq data and short read using online tools
2. Prediction of quantitative trait loci.
3. Prediction of transcription factor binding site and co regulated genes using microarray data.
4. Prediction of genome features using online tools.
5. Analysis of NGS data from plants
6. Statistical Analysis of High throughput data using MATLAB

Textbooks and References

1. Experimental design and data analysis for biologists; G.P. Quinn and M.J. Keough; Cambridge University Press, 2002.
2. Guide to analysis of DNA microarray data; S. Knudsen; Wiley, 2nd edition, 2004.
3. Microarray Data Analysis and Visualization by Arun Jogota, Bioinformatics, the Bay Press, 2001.
4. Advanced analysis of gene expression microarray data; A. Zhang; World Scientific Publishing, 2006. 5. Bioinformatics for High Throughput Sequencing; N Rodriguez-Ezpeleta; Springer; 2012.
5. Causton, HC, Quackenbush, J and Brazma, A (2004) Microarray gene expression Data Analysis: A Beginner's Guide, Blackwell Publishing Co., Oxford, UK (ISBN: 1-4051-2735-X)
6. High-Throughput Next Generation Sequencing: Methods and Applications; Y. M. Kwon and S. C. Rieke, Humana Press; 2011.
7. NCBI Science Premier on MicroArrays.
8. Albala, JS and Humphery-Smith, I (2003) Protein arrays, Biochips and Proteomics: The Next Phase of Genomic Discovery, Marcel Dekker Inc., USA (ISBN: 0-8247-4312-1)

MBI 402. Protein engineering and Design

Unit 2. Fundamentals of the methods for 3D structure prediction (sequence similarity/identity of target proteins of known structure, Homology Modelling, Structural Alignment Methods, Structure superposition, Structure – structure alignment tool, DALI, CE, VAST, TM-align, Visualization and comparison of 3D structures of proteins, nucleic acids, rRNA. functional implications of protein domains, fold recognition, threading approaches, and ab-initio structure prediction methods.

Unit 3. Protein design: Principles of Protein Folding, Dynamics and Structural Evolution. Elementary ideas of bonding and structure, stereochemistry; Random, site directed mutagenesis; Strategies to alter catalytic efficiency; structure prediction and modelling proteins, Molecular graphics in protein engineering; and Dynamics.

Unit 4. Biomolecular Simulation: Computer simulation as a powerful research tool, atomic force field models, MD algorithm, numerical integration of equations of motion, ergodic hypothesis, long range interactions, microcanonical ensemble, NVT, NPT ensembles, limitations of MD simulation, simulation quality analysis, event analysis, time and size limitations, QM/MM techniques, steered MD simulation, free energy methods, examples of simulations on conformational changes in protein and inhibitor binding to proteins. Calculation of conformational energy for bio-macromolecules, Simulation of

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molecular mechanics and dynamics and free energy changes, Molecular Simulation, Molecular dynamics.

Lab/Practicals

A. Prediction of gene/protein for the selection of target and template protein (model)

1. Collection of Protein sequences related to specific biological activity from NCBI/SWISSPROT & UniProtKB to select Model protein and target protein
2. Pair-wise global alignments of protein and gene/ protein sequences using BLAST/FASTA & interpretation of results to deduce homology between the sequences, use of scoring matrices
3. Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences for the selection of plant protein, to modify protein using protein engineering approaches.
4. Database (homology) searches using different versions of FASTA & interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences.
5. Pattern searching using ScanProsite and PRATT

B. Protein Designing

1. Searching for a particular protein and its folds in Structural and Related Databases:PDB, NDB, CCSD, Prosite, PRODOM, Pfam, PRINTS, CATH, SCOP, DSSP, FSSP, DALI
2. Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLUSTAL W. Interpretation of MSA to identify conserved and variable regions which can be analysed for physico-chemical & structural properties in order to identify the residues which can be modified in plant proteins.
3. Visualization of structures: Search for modification sites (active site) to alter catalytic efficiency of protein

C. Modelling

1. Modeling protein structure using modeling tool Geno3D.
2. 3-D structure visualization and simulation: Visualization of structures using Pymol Rasmol or SPDBV or CHIME or VMD
3. Structure analysis and validation: Pdbsum, Whatcheck, Procheck, Verify3D , Critical Assessment of Structure Prediction (CASP) Structures of oligomeric proteins and study of interaction interfaces, DALI, CE, VAST TM-align, Visualization and comparison of 3D structures of proteins
4. Visualization and comparison of 3D structures of proteins, nucleic acids, rRNA

D. Simulation

1. Simulation of protein structure to analyse conformation of modelled protein using Desmond.

Text Books and References:

1. Molecular Modelling: Principle and Applications, Andrew R. Leach, Longman Singapore Publisher, 1999.
2. The Molecules of Life: Physical and Chemical Principles. John. Kurian, Boyana Konforti and D.Wemmer Garland Science, New York 2013
3. Introduction to Protein Structure. Carl Branden & John Tooze, Garland Science



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4. Biochemistry by L. Stryer. Publishers : W.H. Freeman and Company(4th Edition)
5. Structural bioinformatics; P. E. Bourne and J. Gu. 2 nd Edition. John Wiley and Sons. 2009.
6. Bioinformatics vol:2: Structure, function & applications; J. M. Keith Humana Press. 2008.
7. An Introduction to Bioinformatics Algorithms, Neil C Jones & Pavel A. Pevzner, Ane Books, 2005.
8. Introduction to Computational Molecular Biology, Setubal and Meidanis, Thomson, 2003.
9. Biological Sequence Analysis Probablistc Models of Proteins and Nucleic Acid, R. Durbin, Eady, A. Krogh and Mitchison, Cambridge University Press, 1998.
10. Introduction to Mathematical Method in Bioinformatics, Alexcender Isaev, Springer Universitext,
11. Bioinformatics: From Genome to Drugs (Vol. I and II), Thomas Lengau, Wiley- VCH, 2000.
12. Structural bioinformatics: An algorithmic approach; F. J.Burkowski. CRC Press. 2008.
13. Computational molecular biology: an introduction; P. Clote and R. Backofen, Wiley & Sons, 2000.

Elective 1

MBI 403. Computer Aided Drug Design

Unit 1. Introduction to drug discovery, drug discovery pipeline, Role of Bioinformatics in drug design, Aspect for new drug like safety, effectiveness, stability, solubility, synthetic feasibility and novelty and patent issue. Introduction to Retrometabolic drug design.

Unit 2. Enzyme Kinetics, line weaver plot for competitive and non-competitive inhibition, IC₅₀, ED₅₀, Therapeutic index, LD₅₀, Lipinski Rule and Jorgensen Rule-of-Three. Pharmacokinetics: *In silico* prediction ADMET properties for Drug Molecules, Pharmacodynamics, Pharmacogenetics. Reactions of drugs and approaches for toxicity predictions.

Unit 3. Target identification and validation and lead optimization, Different systems for representing chemical structure of small molecules like SMILES etc Generation of 3D coordinates of small molecules, Structure-based drug design: Identification and Analysis of Binding sites and scoring function, Ligand based drug design, Pharmacophore modeling and mapping. Docking Concepts, Scoring functions, Software tools for Docking.

Unit 4. Structure Activity Relationship: Introduction to QSAR, QSPR, Various Descriptors used in QSARs: Electronics; Topology; Quantum Chemical based Descriptors. Regression Analysis, The Significance and Validity of QSAR Regression Equations, Partial Least Squares (PLS) Analysis, Multi Linear Regression Analysis. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations. Efficient search for drug candidates in chemical databases-library design and virtual screening, combinatorial library, automated synthesis. Pre-clinical and Clinical Testing.

Unit 5. Traditinal medicine system, Natural compounds, tribal medicines, ethno biology and traditional medicinal plants, their scope, folk herbal medicines, Ethnobotany, Databases and IT resources on traditional medicines.

Practical/Lab

Modelling



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1. Drawing chemical structures by using the ChemSketch/ChemDraw software.
2. Protein-ligand docking by using the HEX program.
3. Protein-protein and Protein-Drug docking by using the open source docking software.
4. Virtual screening of ligands by using the open source software program.
5. QSAR modelling.
6. Molecular Dynamic Simulation using Desmond.
7. Database searching for traditional and ethno medicines.
8. Prediction of chemical compounds which is found in natural medicines.

Text Books and References:

1. Bioinformatics: From Genome to Drugs (Vol. I and II), Thomas Lengauer, Wiley- VCH, 2000.
2. The Molecules of Life: Physical and Chemical Principles. John. Kurian, Boyana Konforti and D.Wemmer Garland Science, New York 2013
3. Novartis Foundation, J. Craig Venter. From Genome to Therapy: Integrating New Technologies with Drug Development - No. 229. Publisher: Wiley; 1 edition, 2000.
4. Wyler David J. Modern Parasite Biology: Cellular, Immunological, and Molecular Aspects. Publisher: New York, W H Freeman & Co. 1990.
5. Burger's Medicinal Chemistry and Drug Discovery (Vol I to Vol IV) by Donald J Abraham, Wiley Inter-science
6. Computer-Aided Drug Design: Methods and Applications by Thomas J. Perun, Catherine Lamb Propst, Taylor & Francis
7. Rational Drug Design: Novel Methodology and Practical Applications (ACS Symposium Series) by Abby L. Parrill (Editor), M. Rami Reddy (Editor) American Chemical Society; Second Enlarged ed. edition (1 April 1999)

Elective 2.

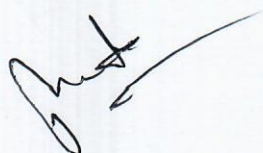
MBI 403. Systems Biology & Metabolomics

Unit 1. Basic properties of network, Adjacency matrix, bipartite network. Random vs. Scale free network: power laws, hubs, ultra-small property, degree exponent and the Barabasi-Albert model. Degree correlations, Network topology.

Unit 2. Introduction to systems biology. Properties of Biological network, Concept of signal transduction network, Gene regulatory network and metabolic networks. Intercellular network: Neuronal networks, Network motifs, Network medicine, Disease Networks.

Unit 3. Systematic Determination of Biological Network Topology: Nonintegral Connectivity Method (NICM), Storing, Searching, and Disseminating Experimental Proteomics Data, Representing and Analyzing Biochemical Networks using BioMaze. Genome scale metabolic reconstruction, Self-organizing maps and Connectivity maps.

Unit 4. Metabolomics: pathways determinations and analysis. Technologies in metabolomics. Metabolic network Simulation: Mass/Flux balance analysis, Extreme Pathways, Elementary mode analysis, Minimal metabolic behaviors (MMBs), Dynamic simulation and parameter estimation, Synthetic Accessibility. Metabolic pathways resources: KEGG, Biocarta, MetaCyc BioCyc, Biogrid, String, Ingenuity Pathways Knowledge Base, EMP, AraCyc, MAPman , Biomodels, Human metabolome database.



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Unit 5. Synthetic Biology: Introduction to synthetic biology Computational tools in synthetic Biology, Applications in synthetic biology.

Lab/Practical

1. File Formats for Pathways: Gene Ontology, PSIMI, CellML, BioPAX , CSML/CSO, SBML Models and MathSBML.
2. Enzyme Nomenclature and Classification, Compounds and Reactions databases: LIGAND - Biochemical Compounds and Reactions, ENZYME - Enzymes, BRENDA - Comprehensive Enzyme Information System
3. Numerical simulation of regulatory pathways and pharmacokinetics data.
4. Browse& search metabolic pathway databases: KEGG, EcoCyc and MetaCyc, EMP, Malaria Parasite Metabolic Pathways, Boehringer Mannheim - Biochemical Pathways.
5. Prokaryotes Vs Eukaryotes – single cell Vs multi cell species biology from a modeling. Rational Metabolic engineering design.
6. Interaction networks: Databases and visualization exercise
7. Structural and topological properties of biochemical networks SBML Models and MathSBML, CellDesigner: A Graphical Biological Network Editor and Workbench Interfacing Simulator, Systems Biology Workbench (SBW), Setting up Genome scale models
8. Computations of phenotypes and interpretation using genome scale models.
9. Cell Illustrator, Cellular Simulation: Towards a Virtual Biological Laboratory
10. Visualization of Integrated models of biomolecular interaction networks by cytoscape

Text Books & References:

1. Bjo Rn H. Junker , Falk Schreiber. Analysis of Biological Networks. 2008. John Wiley & Sons, Inc., Hoboken, New Jersey
2. Choi Sangdun. Introduction to Systems Biology. Humana Press Inc. Totowa, New Jersey.2007. ISBN: 978-1-58829-706-8
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MBI 404. Seminar Oriented Course

Students will have to present seminar in a series of presentation and submit the report and review article on one of the following topic

S.N.	Topic of seminar	Number of Presentations
Seminar I	Molecular Modelling & Protein Engineering	10
Seminar II	Microarray & NGS data Analysis	10
Seminar III	Database development & Software Engineering	10
Seminar IV	Data mining using R/MATLAB	10
Seminar V	Immunoinformatics & Vaccine design	10
Seminar VI	Pharmacogenomic & Metagenomics	10
Seminar VII	Systems Biology & Metabolomics,	10
Seminar VIII	Computer Aided Drug Design	10
Seminar IX	Agriinformatics & Geoinformatics	10
Seminar X	Medical Informatics	10

- (1) **Internal Assessment (30%):** Regular presentation of seminar report under the supervision of Course instructor(30 marks)
- (2) **External Evaluation (70%):** Review of Seminar Reports and review article by External examiner, which must be awarded on the basis of
 - (a) Scientific Reporting Standards (10)
 - (b) Lack of Plagiarism, Citing Literature (10)
 - (c) Explanation of problems and challenges in the specified area(10)
 - (d) Explanation of Method (20)
 - (e) Presentation Skills (10 marks)
 - (f) Viva (10 marks)

MBI 405. Project Work (practical based course)

The Postgraduate project provides students with an opportunity to undertake research in bioinformatics. A wide variety of projects are offered each year in such diverse areas as microarray analysis, structure prediction, mining biomedical texts and genome analysis. Every student is expected to carry out computational work such as designing a database, or writing programs to analyse biological data or analysis of data to provide useful prediction for future research. Sometimes students suggest projects of their own that we are able support. Some of the following areas Systems Biology & Metabolomics, Molecular Modelling & Protein Engineering, Immunoinformatics, Pharmacogenomic, Metagenomics Analysis of Microarray Data, Database development, Data mining and tool development using computational algorithm and other Data mining algorithm.

Student will have to submit a draft of project report for internal assessment (shall be evaluated by the project supervisor) and final copy of project report for external evaluation (shall be evaluated by external examiner) based on six (6) month project work/dissertation (January to June) in final semester. Each student must present project work in series of presentations with the progress report for internal assessment (10% presentation+ 20% first draft of project report) and one final presentation/viva for



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computational work such as designing a database, or writing programs to analyse biological data or analysis of data to provide useful prediction for future research. Sometimes students suggest projects of their own that we are able support. Some of the following areas Systems Biology & Metabolomics, Molecular Modelling & Protein Engineering, Immunoinformatics , Pharmacogenomic, Metagenomics Analysis of Microarray Data, Database development, Data mining and tool development using computational algorithm and other Data mining algorithm.

Students will have to present seminar in a series of presentation and submit the report and review article on one of the following topic

S.N.	Topic of seminar	Number of Presentations
Seminar I	Molecular Modelling & Protein Engineering	10
Seminar II	Microarray & NGS data Analysis	10
Seminar III	Database development & Software Engineering	10
Seminar IV	Data mining using R/MATLAB	10
Seminar V	Immunoinformatics & Vaccine design	10
Seminar VI	Pharmacogenomic & Metagenomics	10
Seminar VII	Systems Biology & Metabolomics,	10
Seminar VIII	Computer Aided Drug Design	10
Seminar IX	Agriinformatics & Geoinformatics	10
Seminar X	Medical Informatics	10

Student will have to submit a draft of project report for internal assessment (shall be evaluated by the project supervisor) and final copy of project report for external evaluation (shall be evaluated by external examiner) based on six (6) month project work/dissertation (January to June) in final semester. Each student must present project work in series of presentations with the progress report for internal assessment (10% presentation+ 20% first draft of project report) and one final presentation/viva for external evaluation (40% second draft copy of project report+20% presentation of work +10% query/viva).

- (1) **Internal Assessment (30%):** Regular Review of monthly progress report and project report by supervisor (20 marks) and presentation (10 marks)
- (2) **External Evaluation (70%):** Review of Project Report (40) by External examiner, which must be awarded on the basis of
 - (a) Scientific Reporting Standards (10)
 - (b) Lack of Plagiarism, Citing Literature (10)
 - (c) Work done (10)
 - (d) Results & Discussion (10)
 - (e) Presentation Skills (20 marks)
 - (f) Viva (10 marks)



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external evaluation (40% second draft copy of project report+20% presentation of work +10% query/viva).

- (3) **Internal Assessment (30%):** Regular Review of monthly progress report and project report by supervisor (20 marks) and presentation (10 marks)
- (4) **External Evaluation (70%):** Review of Project Report by External examiner, which must be awarded on the basis of
 - (g) Scientific Reporting Standards (10)
 - (h) Lack of Plagiarism, Citing Literature (10)
 - (i) Work done (10)
 - (j) Results & Discussion (10)
 - (k) Presentation Skills (20 marks)
 - (l) Viva (10 marks)

