

University of North Bengal
Department of Bioinformatics



CHOICE BASED CREDIT SYSTEM (CBCS) SYLLABUS FOR M.SC.
Duration: Two years (Four Semesters); Total marks 1600 [64 CREDITS]
Academic Year 2022-23
Semester I

Sem	Crs	Course	New Course-Code (ALPHA-NUMERIC)	Paper type	Course name	Course type	Full Marks (External)	Full marks (Practical)	Full marks (Internal)	Total FM	Credit
1	332	M.Sc. in Bioinformatics	BINFCCT0101N	T	Cell Biology, Genetics, and Molecular Biology	CORE	40		10	50	2
			BINFCCT0102N	T	Basic Bioinformatics		40		10	50	2
			BINFCCT0103N	T	Basic computer applications		40		10	50	2
			BINFCCP0104N	P	Cell Biology, Genetics, and Molecular Biology		50	50	50	2	
			BINFCCP0105N	P	Basic Bioinformatics				50	50	2
			BINFCCP0106N	P	Basic computer applications				50	50	2
			BINFDET0101A	T	Biochemistry and Biophysics	DSE* (Anyone has to be Chosen)	25		25	1	
			BINFDET0101B	T	Basic mathematics and statistics for Biology					25	25
			BINFDEP0101A	P	Biochemistry and Biophysics		25	25	1		
			BINFDEP0101B	P	Basic mathematics and statistics for Biology					50	2
			AEC-I (Choose any One from BASKET -1)	T	AEC I	AEC					
Total										400	16

Sem	Crs	Course	New Course-Code (ALPHA-NUMERIC)	Paper type	Course name	Course type	Full Marks (External)	Full marks (Practical)	Full marks (Internal)	Total FM	Credit
2	332	M.Sc. in Bioinformatics	BINFCT0201N	T	Genomics and Proteomics	CORE	40	50	10	50	2
			BINFCT0202N	T	Advanced statistical techniques for Bioinformatics		40		10	50	2
			BINFCT0203N	T	Computer programming for Bioinformatics		40		10	50	2
			BINFCCP0204N	P	Genomics and Proteomics		50		50	50	2
			BINFCCP0205N	P	Advanced statistical techniques for Bioinformatics					50	2
			BINFCCP0206N	P	Computer programming for Bioinformatics					50	2
			BINFDEP0201A	P	NCC/NSS/MOOC	DSE (Anyone has to be chosen)	50	50	50	2	
			BINFDEP0201B	P	Review Paper Writing/Industrial and Institutional visit and Report submission						
			SEC (Choose any One from BASKET - 2)	T	SEC I	SEC				50	2
Total										400	16

Semester II

Semester III

Sem	Crs	Course	New Course-Code (ALPHA-NUMERIC)	Paper type	Course name	Course type	Full Marks (External)	Full marks (Practical)	Full marks (Internal)	Total FM	Credit
3	332	M.Sc. in Bioinformatics	BINFCCT0301N	T	Structural Bioinformatics	CORE	40		10	50	2
			BINFCCP0302N	P	Structural Bioinformatics		40		10	50	2
			BINFDET0301A	T	Web-based Programming & Database management systems	DSE (Any Three to be chosen)	25+25+25			75	1+1+1
			BINFDET0301B	T	Phylogeny and Phylogenomic						
			BINFDET0301C	T	NGS and expression data analysis						
			BINFDET0301D	T	Advance computer programming for Bioinformatics						
			BINFDET0301E	T	Data Mining and Machine learning techniques for Bioinformatics						
			BINFDET0301F	T	Advanced omics technologies						
			BINFDEP0301A	P	Web-based Programming & Database management systems						
			BINFDEP0301B	P	Phylogeny and Phylogenomic	25+25+25			75	1+1+1	
			BINFDEP0301C	P	NGS and expression data analysis						
			BINFDEP0301D	P	Advance computer programming for Bioinformatics						
			BINFDEP0301E	P	Data Mining and Machine learning techniques for Bioinformatics						
			BINFDEP0301F	P	Advanced omics technologies						
			BINFGET0301A	T	Biological data analysis						GE* (Anyone to be chosen)
			BINFGET0301B	T	Cheminformatics						
			BINFGEP0301A	P	Biological data analysis	50			50	2	
			BINFGEP0301B	P	Cheminformatics						
				T	AEC II	AEC				50	2
Total										400	16

* Students pursuing M.Sc. (Bioinformatics) can choose chemoinformatics or any other GE paper offered by other departments. Students from other department can choose any one of them

Semester IV

Sem	Crs	Course	New Course-Code (ALPHA- NUMERIC)	Paper type	Course name	Course type	Full Marks (External)	Full marks (Practical)	Full marks (Internal)	Total FM	Credit
4	332	M.Sc. in Bioinformatics	BINFCCT0401N	T	Research Methodology & Scientific Writing	CORE	40		10	50	2
			BINFCCT0402N	T	Bioethics, Biosafety, and IPR		40		10	50	2
			BINFCCP0403N	P	Research Methodology & Scientific Writing					50	2
			BINFCCP0404N	P	Bioethics, Biosafety, and IPR					50	2
			BINFDEP0401A		Dissertation/Project work and viva	DSE (Anyone)				50	2
			BINFDEP0401B		Internship						
			BINFGET0401A	T	Comparative and Functional Genomics	GE (Anyone)	40		10	50	2
			BINFGET0401B	T	Computational Systems Biology						
			BINFGEP0401A	P	Comparative and Functional Genomics						
			BINFGEP0401B	P	Computational Systems Biology						
							T	SEC II	SEC		
Total									400	16	

Detailed Syllabus of M.Sc. in Bioinformatics:

Semester-I : Core Course	
Theory (Cr. 2)	Cell Biology, Genetics, and Molecular Biology
Course Objectives:	The main objective of the course is students to understand the structure and function of living systems at the molecular level and to understand genetics concepts from mendelian to modern era
Course Outcomes:	After completion of the course the learners will be able to: <ul style="list-style-type: none"> • Understand the concepts of cell and molecular biology and to utilize them in bioinformatics applications. • Understand the gene and its modular structure, mutation and its role in genome evolution, genetic and physical map • Understand the connection of Applied areas of cell and molecular biology and Bioinformatics for human diseases and health
Unit 1	Basics of cell biology: Structure and Functions of Cellular Organelles, Cell Cycle, Chromosome Structure, organization, and classification, chromosomal abnormalities, mutations and repair, idiogram, imprinting, Lampbrush chromosome, Polytene chromosome; DNA as the genetic material (experimental evidences); genome complexity; C-value paradox, Cot value, repetitive DNA, satellite DNA; gene structure in prokaryotes and eukaryotes; split genes, overlapping genes, pseudogenes
Unit 2	Mendel's Laws, the physical basis of inheritance; the concept of the gene, gene-gene interactions; multiple alleles; complementation; linkage, recombination, and chromosome mapping (genetic) with examples for linkage/genetic mapping extra-chromosomal inheritance; transposable elements. Chromosomal aberrations: Numerical variations: euploidy and aneuploidy; Structural variations: deletion, duplication, inversion and translocation, Chromatin structure; Epigenetic modifications.
Unit 3	Central Dogma in molecular Biology, DNA Replication; Transcription; Translation in prokaryotes and eukaryotes, Concept of genetic code (degeneracy of codons, codon bias), Regulation of gene expression in prokaryotes– the concept of the operon (lac and trp), transcriptional and post-transcriptional processing of mRNA in eukaryotes, Splicing, Editing; Translation machinery and its regulation in the eukaryotic system, post-translational modifications.
Unit 4	Gene Cloning: Restriction endonuclease, DNA modifying enzymes, cloning vectors; PCR; Different modified PCR; quantitative PCR; ddPCR; Molecular markers in genome analysis: RFLP, RAPD, and AFLP analysis, DNA fingerprinting; DNA, RNA, and protein probes (production, labeling by radioactive and nonradioactive method); Fluorescence in situ Hybridization (FISH); Microarray (Basic principles and technology of cDNA microarrays and their applications, case studies).
Suggested readings	<ol style="list-style-type: none"> 1. Concepts of Genetics- Klug W.S., Cummings M.R., Spencer C.A. and Palladino M.A. (Pearson Int. Edition). 2. Benjamin Lewin; Genes IX; Jones and Bartlett Publishers 3. James D Watson, Tania A Baker, Stephen P Bell; Molecular Biology of the Gene; Pearson Education Limited 2017 4. Gerald Karp; Cell and Molecular Biology; John Wiley 2013; 5thEdition; 5. H. Lodish, A. Berk, S. L. Zipursky, P. Matsudaira, D. Baltimore, and J. Darnell; Molecular Cell Biology; W. H. Freeman & Comp., 2007; 6th edition

Theory (Cr. 2)	Basic Bioinformatics
Course Objectives:	The course introduces Bioinformatics in general and online resources and tools related to sequences, structures, pathway, and genome databases in particular to the students
Course Outcomes:	After completing the course, the student will recognize various online bioinformatics resources, able to retrieve relevant information from biological databases and also learn to differentiate between file formats to store biological data. They will learn to compare sequence data
Unit 1	Genome projects, Human Genome Project, Nature of Biological data, Related disciplines of Bioinformatics (Branches of Bioinformatics), Applications of Bioinformatics, Major Bioinformatics Resources: NCBI, EBI, ExPASy, RCSB, JCVI, SANGER, etc. Biological file formats
Unit 2	Primary Sequence Databases - nucleic acid (GenBank, ENA, DDBJ) and protein (UniProt), Secondary databases (InterPro, PROSITE, PRINTS, Pfam, CATH and SCOP), Structure databases (PDB and MMDB), Visualization tools (RasMol, Pymol, SPDBV, and LIGPLOT), Database search tool: Entrez (GQuery), EBI Search (EB-eye)
Unit 3	Basic concepts and need for sequence alignment (Introduction to sequence alignment and sequence analysis), Basic terminologies: Identity, similarity, positives, score, E-Value, motifs, fingerprints, domains, family, superfamily, profile, matrix, fold, etc, Sequence comparison scoring systems: Dot matrix, PAM and BLOSUM, Pairwise sequence comparison: Dynamic Programming, use of scoring matrices and gap penalties in sequence alignments, Assessing the significance of sequence alignments, Database Searching for Similar Sequences: BLAST and FASTA
Unit 4	Multiple sequence alignment: Multiple sequence alignment as an extension of sequence pair alignment by dynamic programming, scoring multiple sequence alignments, Progressive methods of multiple sequence alignment, Iterative methods of multiple sequence alignment, Localized alignments in sequences, Phylogenetic analysis–Overview, Relation with multiple sequence alignment, Phylogenetic tree: topology & branch length, Overview of methods & tools available for Phylogenetic Analysis.

Suggested readings	<ol style="list-style-type: none"> 1. Web resources, Review papers 2. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003. 3. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001. 4. G. Gibson & S.V. Muse, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002. 5. A. Baxeavanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005. 6. A. M. Campbell & L. J. Heyer, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003. 7. S.R. Pennington & M.J. Dunn, Proteomics – from protein sequence to function, BIOS Scientific Publishers, 2002.
Theory (Cr. 2)	Basic Computer Application
Course Objectives:	The main objective of the course is for students to understand the basics of computer architecture, computer software and hardware. The concepts like principles of operating systems with special reference to Windows, Linux along with data communication and computer network, and computer graphics presentation will be introduced.
Course Outcomes:	After completion of the course the students will be able to do: <ul style="list-style-type: none"> ● webpage designing, ● 3D presentation using computer graphics ● Command line scripting in the operating system.
Unit 1	Computer Fundamentals - Number systems; Representation of integers, fixed and floating-point numbers, character representation: ASCII, EBCDIC. Functional units of computer, I/O devices, Computer memory, primary and secondary memories; Concepts of Hardware and Software.
Unit 2	Basics of Operating System; Popular Operating Systems (Windows, Linux, DOS); Basic commands of DOS operating system, File management in DOS, Linux Operating System Layers, The Linux Shell (different kinds of shell), Process: (parent and child processes), Files and Directories (File Structure and directory structure), Interaction with System, shell commands, Regular expressions of Linux (awk, grep, sed).
Unit 3	Basic of Computer networks; Types of Networking - LAN, MAN, WAN; Data communication; ISO-OSI references model, TCP/IP reference model. Concept of Internet; WWW and Web Browsers; Search Engines; Understanding URL, Internet protocol- FTP, SMTP. Web page designing – HTML.

Unit 4	Computer graphics basics; Graphics I/P Devices; Development of computer graphics: Basic graphics system and standards. Raster scan and random scan graphics, Frame buffer and bit operations, Concepts in raster graphics; Points, Lines and Curves; Scan conversion; Line-drawing algorithms; Circle and ellipse generation; Polygon filling; Conic-section generation. Three-dimensional concepts: 3-D representations and transformations; 3-D viewing; Algorithm for 3-D volumes, Spline curves and surfaces.
Suggested readings	<ol style="list-style-type: none"> 1. Buyens, Jim. 2002. Microsoft FrontPage -Inside Out. Microsoft Press. 2. Cox, V., Wermers L. and Reding E. E. 2006. HTML Illustrated Complete. Course Technology. 3. Niederst, J. 2001. Web Design in a Nutshell. O'Reilly Media, Inc. 4. Tanenbaum, A.S. 2003. Computer Networks. Prentice Hall of India, New Delhi. 5. Bach, M.J. 2008. Design of the UNIX Operating System. Pearson Education. 6. Deitel, H.M. 1990. An Introduction to Operating System. Addison Wesley. 7. Dhamdhare, D.M. 2007. Operating Systems: A Concept Based Approach. Tata McGraw Hill, New Delhi. 8. Hearn, D. and Baker, M.P. 2004. Computer Graphics. Prentice and Hall of India, New Delhi. 9. Marshal, G. 1983. Programming with Graphics. Granada Publishing, London
Practical (Cr. 2)	Cell Biology, Genetics, and Molecular Biology
	<ol style="list-style-type: none"> 1. Preparation of sample and identification of various stages of mitosis and meiosis 2. Linear differentiation of chromosomes through G-banding, C-banding and Q-banding 3. Microscopic studies of microbial morphology (shape, size, arrangement etc.) and Microbial staining techniques (Simple staining; Gram staining; Flagella staining; Cell wall staining; Negative staining) 4. Probability and chi-square test for genetic analyses for goodness of fit 5. Human genetics- study of simple human traits 6. Isolation of genomic and plasmid DNA and analysis by agarose gel electrophoresis 7. PCR primer designing; Plasmid vector designing 8. PCR and RAPD analysis.

<i>Suggested readings</i>	<ol style="list-style-type: none"> 1. Concepts of Genetics- Klug W.S., Cummings M.R., Spencer C.A. and Palladino M.A. (Pearson Int. Edition). 2. Benjamin Lewin; Genes IX; Jones and Bartlett Publishers 3. James D Watson, Tania A Baker, Stephen P Bell; Molecular Biology of the Gene; Pearson Education Limited 2017 4. Gerald Karp; Cell and Molecular Biology; John Wiley 2013; 5thEdition; 5. H. Lodish, A. Berk, S. L. Zipursky, P. Matsudaira, D. Baltimore and J. Darnell; Molecular Cell Biology; W. H. Freeman & Comp., 2007; 6th edition 6. Sambrook JF, Russell DW; Molecular Cloning: A Laboratory Manual (3rd Edition). Cold Spring Harbor Laboratory Press
Practical (Cr. 2)	Basic Bioinformatics
	<ol style="list-style-type: none"> 1. Retrieve information from Nucleotide databases (GenBank, ENA, DDBJ) 2. Retrieve information from Protein Primary sequence: UNIPROT 3. Retrieve information from RCSB 4. Explore Secondary databases (InterPro, PROSITE, PRINTS, Pfam, CATH and SCOP) 5. Download protein 3D structure from PDB 6. Molecular Visualization Tool: RasMol, SPDBV, PYMOL, LigPlot 7. Search tool: Entrez, EB-eye 8. Sequence Similarity search: BLAST (Online and Standalone) 9. Pairwise Sequence Alignment: Local and Global 10. Multiple Sequence Alignment: Clustal Omega <p>Phylogenetic analysis using MEGA</p>
<i>Suggested readings</i>	<ol style="list-style-type: none"> 1. Web resources, Research and Review articles. Help files, software tutorials. 2. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003. 3. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001. 4. G. Gibson & S.V. Muse, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002. 5. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005. 6. A. M. Campbell & L. J. Heyer, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003. 7. S.R. Pennington & M.J. Dunn, Proteomics – from protein sequence to function, BIOS Scientific Publishers, 2002
Practical (Cr. 2)	Basic Computer Application

	<ol style="list-style-type: none"> 1. Problems using system calls for process management, signaling, file management, directory management, protection; Critical section problem; Solution to the mutual exclusion by Peterson method; Producer consumer problem with fatal race conditions; Comparison of various CPU scheduling algorithms and Paging, segmentation and demand paging 2. Network and mail configuration, Web page designing using HTML; Designing a static website with features like tables, the hyperlink among pages, pictures, frames and layers 3. Shell: Basic commands of a shell, internal vs external commands (working on multiple shell commands and understanding of how it interacts with Linux) 4. Shell programming (working on core shell programming in sync with Linux) 5. Implementation of algorithms for drawing geometrical figures, rotation, and charts; Pixel handling on screen; Clipping – Line clipping – Polygon Clipping, Windowing; Use of primitive transformations and/or their combinations; Implementation of 3D Object Representation and Fractal programming and animation.
Suggested readings	<ol style="list-style-type: none"> 1. Buyens, Jim. 2002. Microsoft FrontPage -Inside Out. Microsoft Press. 2. Cox, V., Wermers L. and Reding E. E. 2006. HTML Illustrated Complete. Course Technology. 3. Niederst, J. 2001. Web Design in a Nutshell. O'Reilly Media, Inc. 4. Tanenbaum, A.S. 2003. Computer Networks. Prentice Hall of India, New Delhi. 5. Bach, M.J. 2008. Design of the UNIX Operating System. Pearson Education. 6. Deitel, H.M. 1990. An Introduction to Operating System. Addison Wesley. 7. Dhamdhare, D.M. 2007. Operating Systems: A Concept Based Approach. Tata McGraw Hill, New Delhi. 8. Hearn, D. and Baker, M.P. 2004. Computer Graphics. Prentice and Hall of India, New Delhi. 9. Marshal, G. 1983. Programming with Graphics. Granada Publishing,London
Department Skill Enhancement (DSE) (Any One to be chosen)	
Theory (Cr. 1)	Biochemistry and Biophysics
Course Objectives:	This is meant to introduce biochemistry and biophysics as a course in biosciences applying the theoretical language of chemistry and physics to aid functional understanding of molecular and cellular processes

Course Outcomes:	<p>After completion of the course the students will be able to:</p> <ul style="list-style-type: none"> ● Explain the structure of Biomolecules and their interactions ● Understand physical laws underlying biological systems ● Understand the structure, functions and classifications of proteins, nucleic acid, lipids and carbohydrate
Unit 1	<p>Biomolecules: Micro and Macromolecules, The chemical bonds involved in biomolecules, Three-dimensional structure are described by configuration and conformation, Basics of acids and bases, chemical equilibrium, pH, pKa, and buffer solutions, Physical Foundations of living organisms: energy, enthalpy and entropy, different types of systems, laws of thermodynamics, spontaneous reactions, Nucleotides and Nucleic Acids: Basics, Structure, Chemistry (Except sequencing technology) & Functions.</p>
Unit 2	<p>Secondary and Tertiary Structures of RNA, Amino Acids, Peptides, and Proteins, four levels of protein structure, Enzymes: Definition, Nomenclature & Classification, Active site, coenzyme and metal co-factor, Mechanism of enzyme action, Enzyme Inhibition, Carbohydrates -Classification, Structure and Functions, Lipids- Classification, Structure and Functions</p>
Suggested readings	<ol style="list-style-type: none"> 1. Davis L. Nelson, Michael M. Cox, Lehninger's Principles of Biochemistry, Seventh Edition, W. H. Freeman 2. Jeremy M. Berg, John L. Tymoczko, Lubert Stryer, Biochemistry, Seventh Edition, W. H. Freeman and Company, New York 3. Reginald H. Garrett, Charles M. Grisham, Biochemistry, Fifth Edition, Brooks/Cole Cengage Learning 4. Sathyanarayana, U. & Chakrapani, "Biochemistry", 2008, 3rd Ed., Books and Allied (P) Ltd. 5. Voet, D., Voet, J.G., Pratt, W.C., "Fundamentals of Biochemistry", 2011, 4th Ed., John Wiley Publications. 6. S.C. Rastogi, Biochemistry, Tata McGraw Hill publishing limited, 1996
Theory (Cr. 1)	Basic mathematics and statistics for Biology
Course Objectives:	<p>The course is designed to provide the students basic understanding of systems of linear equations, their associated matrices and their properties, characteristic polynomials, eigenvalues and eigenvectors, bilinear forms, and linear programming.</p>
Course Outcomes:	<p>The student will be able to-</p> <ul style="list-style-type: none"> ● analyze system of linear equations, ● solving linear recurrences, and, ● formulating linear programming problems and finding their feasible and optimal solutions.

	<ol style="list-style-type: none"> 1. Systems of linear equations, Matrices and elementary row operations, Row reduced Echelon matrices 2. Matrix multiplication, Invertible matrices, Transpose of a matrix 3. Systems of homogeneous equations, Equivalence of row rank and column rank of a matrix, Determinant and volume of the fundamental parallelepiped 4. Permutation matrices, Cramers rule 5. Vector spaces and subspaces, Bases and dimensions, Coordinates and change of bases, Direct sums, 6. The Rank-Nullity theorem, Matrix of a linear transformation, Linear operators and isomorphism of vector spaces, Determinant of a linear operator 7. Others
Suggested readings	<ol style="list-style-type: none"> 1. Abertson, M.O. and Hutchinson, J.P. 1988. Discrete Mathematics with Algorithms. John Wiley. 2. Deo, N. 1984. Graph Theory with Application to Engineering and Computer Science. Prentice Hall of India, New Delhi. 3. Knuth, D.E. 1968. Art of Computer Programming, Vol. I. Fundamental Algorithms. Addison Wesley. 4. Tremblay, J.P. and Manohar, R.P. 1975. Discrete Mathematical Structures with Applications to Computer Science. McGraw Hill 5. Gupta, S.C. and Kapoor, V.K. 2007. Fundamentals of Mathematical Statistics. Sultan Chand and Sons. 6. Campbell, R.A. 1974. Statistics for Biologists. Cambridge University Press. 7. W. Warren John Ewens, Gregory Robert Grant 2001. Statistical Methods in Bioinformatics: An Introduction. Springer
Practical (Cr. 1)	Biochemistry and Biophysics
	<ol style="list-style-type: none"> 1. Standard buffer solution preparation and pH determination 2. Estimation of protein concentration using Lowry and Bradford methods 3. Estimation of carbohydrates by DNSA method 4. Assay activity of Amylase 5. Assay activity of Acid phosphatase 6. Effect of substrate concentration on enzyme activity 7. Estimation of amino acids by Ninhydrin method 8. Separation of plant pigments by thin-layer chromatography 9. Separation of proteins by SDS-PAGE, followed by silver staining
Suggested readings	<ol style="list-style-type: none"> 1. Abertson, M.O. and Hutchinson, J.P. 1988. Discrete Mathematics with Damodaran Geetha K, Practical Biochemistry, Jaypee Brothers Medical Publishers 2. Rashmi A. Joshi, A Text Book of Practical Biochemistry, B.Jain Large Print
Practical (Cr. 1)	Basic mathematics and statistics for Biology

	<ol style="list-style-type: none"> 1. Data analysis using descriptive statistics measures in Microsoft excel 2. Histogram, Box- plots, Stem & leaf plot 3. Correlation studies of data 4. Regression analysis and calculation of regression coefficients 5. Error analysis and error bars 6. Fitting of distributions: Binomial, Poisson and Normal distributions and deviates 7. Testing of hypothesis using t-test, F-test, chi-square test <p>Nonparametric tests – Wilcoxon Mann Whitney tests, Kruskal Wallis test</p>
<i>Suggested readings</i>	<ol style="list-style-type: none"> 1. Abertson, M.O. and Hutchinson, J.P. 1988. Discrete Mathematics with Algorithms. John Wiley. 2. Deo, N. 1984. Graph Theory with Application to Engineering and Computer Science. Prentice Hall of India, New Delhi. 3. Knuth, D.E. 1968. Art of Computer Programming, Vol. I. Fundamental Algorithms. Addison Wesley. 4. Tremblay, J.P. and Manohar, R.P. 1975. Discrete Mathematical Structures with Applications to Computer Science. McGraw Hill 5. Gupta, S.C. and Kapoor, V.K. 2007. Fundamentals of Mathematical Statistics. Sultan Chand and Sons. 6. Campbell, R.A. 1974. Statistics for Biologists. Cambridge University Press. 7. W. Warren John Ewens, Gregory Robert Grant 2001. Statistical Methods in Bioinformatics: An Introduction. Springer
<i>Theory (Cr. 2)</i>	AEC I
	The course will be offered jointly along with students of other departments

Semester-II Core Course	
Theory (Cr. 2)	Genomics and Proteomics
Course Objectives:	The goal is to determine how all the genes in a genome act and how their products interact to produce a functional organism. The different methods of sequencing, microarrays, protein fingerprints and the role of bioinformatics tools applied to analyse and interpret the protein-protein interactions in different cell types will be detailed
Course Outcomes:	After completion of the course the learners will be able to: <ul style="list-style-type: none"> ● explain the genomic and proteomic strategies and apply bioinformatics tools for the same ● Understand how the proteins act and how their products interact ● Learn different computational resources available for genomics and Proteomics ● understand the nature of transcriptome data, normalize it and perform differential expression analysis ● able to compare 2D gel images for difference of protein expression
Unit 1	Genome sequencing: Whole genome shotgun sequencing; Principle of Sanger's dideoxy method versus NGS, comparative study of standard NGS methods; Introduction to various databases, genome browsers & associated tools: ENSEMBL, GeneCards, UCSC Genome Browser, Galaxy and their application; Overview of various genome scale projects: Human genome project, HapMap project, 1000 genome projects, Expressed sequence Tag (EST) project; Concept of Epigenomics, microRNA, long non-coding RNA; Concept of three dimensional genome; SNPs and genome-wide association studies (GWAS)
Unit 2	Overview of metagenomics principles, microbial and ecological aspects underlying metagenomic experiments; Transcriptome and techniques used for transcriptomics; microarray and RNA-seq; Application of transcriptomics; Methylation of DNA and genetics; histone modifications, HATs and HDACs in the context of gene expression regulation; ChIP-chip and ChIPseq techniques.
Unit 3	The origin and scope of proteomics, Post-translational modification, Proteomics: Technologies and Their Applications, General principles of protein separation in proteomics, Methods to study protein-protein interactions, Library-based methods for the global analysis of binary interactions, Two-hybrid/protein complementation assays; Modified two-hybrid systems for membrane, cytosolic, and extracellular proteins, Phosphoproteomics, Glycoproteomics, Application of Proteomics to Disease Diagnostics, Applications of proteomics in drug development, Artificial intelligence for proteomics and biomarker discovery
Unit 4	Proteomics resources at the EBI & ExPASy, A Golden Age for Working with Public Proteomics Data, Bioinformatic analysis of proteomics data, Functional annotation and biological interpretation of proteomics data, Web Resources for Mass Spectrometry-based Proteomics, Protein post-translational modifications: In silico prediction tools and molecular modeling, Glycobioinformatics: Current strategies and tools for data mining in MS-based glycoproteomics
Suggested readings	<ol style="list-style-type: none"> 1. T. A. Brown; Genomes; Bios Scientific Publishers Limited, 2002. 2. B. R. Korf and M. B. Irons; Human Genetics and Genomics; Wiley, 2013, 4th edition. 3. A. M. Lesk; Introduction to Genomics; Oxford University Press, 2012, 2nd edition 4. Genomics: Application in Human Biology -S.B. Primrose and R. M. Twyman. (Blackwell Pub.) 5. Twyman, R. M. (2014). Principles of proteomics. Second Edition, Garland Science, Taylor & Francis Group, LLC

Theory (Cr. 2)	Advanced statistical techniques for Bioinformatics
<i>Unit 1</i>	Statistical Inference: Properties of estimation theory, Methods of estimation; Maximum likelihood estimation, Ordinary least square, Confidence Intervals, Classical Hypothesis Testing, P-Values, Testing for the Parameters in a Multinomial Distribution, Association tests, Likelihood Ratios.
<i>Unit 2</i>	Simultaneous hypothesis testing, Adjusted p-value, Differential Expression – Multiple Genes: The False Discovery Rate (FDR), Bootstrap Methods: Estimation and Confidence Intervals, Bayesian inference: Monte Carlo Markov Chain, The Hastings–Metropolis Algorithm, Gibbs Sampling.
<i>Unit 3</i>	Concept of sampling, sampling vs complete enumeration, planning of sample survey. Sampling from a finite population, simple random sampling, inverse sampling, stratified sampling, cluster sampling, systematic sampling, multistage sampling, double sampling. Ratio and regression method of estimation. Non-sampling errors.
<i>Unit 4</i>	General Gauss Markoff set up, Gauss-Markoff's theorem, Aitken's transformation. Theory of linear estimation, test of hypothesis in linear models. Analysis of variance, partitioning of degrees of freedom. Restricted least squares. Special cases of one- and two-way classifications (including disproportionate cell frequencies and interaction, cross and nested classifications).
<i>Suggested readings</i>	<ol style="list-style-type: none"> 1. Bapat, R.B. 1993. Linear Algebra and Linear Models. Springer-Verlag. 2. Graybill, F. A. 1976. Theory and Application of the Linear Model. Duxbury, North Scituate. 3. Casela, G. and Berger, R.L. 2001. Statistical Inference. Duxbury Thompson Learning. 4. Cochran, W.G. 1977. Sampling Techniques. John Wiley. 5. Des Raj 1976. Sampling Theory. Tata-McGraw-Hill
Theory (Cr. 2)	Computer programming for Bioinformatics
Course Objectives:	The course introduces the- (1) basic concepts of algorithm writing and flowchart (2) Programming script writing using C, JAVA, PERL (3) Usage of programming script for bioinformatics data analysis.
Course Outcomes:	The student who completes the course will have the ability- <ul style="list-style-type: none"> ● to develop algorithm for solving complex biological problem ● to write problem specific script for biological data analysis ● to write programming script for algorithm development
<i>Unit 1</i>	Techniques of problem solving, Algorithm development, Flowcharting, Stepwise refinement. Concepts of programming language, types of programming language, imperative language, procedural programming language and object-oriented programming language. Compiler, Interpreter, Loader and Linker.
<i>Unit 2</i>	Procedural programming language; C programming language, data types, keywords, operators and expressions; I/O library function, control statements, function, function prototype, type of functions; local and global variables.
<i>Unit 3</i>	Structured programming; Object oriented programming, Java; Classes, objects, Abstract data types, Data types, Operators (Arithmetic, Logical and Comparison) and expressions. Branching and iteration, Arrays, Object/Message paradigm. Data encapsulation- modules and interfaces; Polymorphism - Static and dynamic binding, Inheritance: class and object inheritance.

Unit 4	Perl: Introduction, Scalar, Arrays and List Data, Control Structures, Hashes, String Handling, Regular Expressions; Subroutines, File handling, Directory Access and Formatting, CGI Programming: CGI Module, Passing Parameters via CGI and Perl, Object oriented, Creating Objects.
Suggested readings	<ol style="list-style-type: none"> 1. Petersen, R. 2007. Linux: The Complete Reference, Sixth Edition. McGraw-Hill Education. 2. Sethi, R., 1996, Programming Languages, Addison-Wesl. 3. Gottfried, B.S., 1998 Schaum's Outline of Theory and Problems of Programming with C, McGraw-Hill. 4. James Tisdall. 2001. Beginning Perl for Bioinformatics. O-Reilly. 5. Randal L. Schwartz, Tom Phoenix, brian d foy. 2008. Learning Perl. O-Reilly.
Practical (Cr. 2)	Genomics and Proteomics
	<ol style="list-style-type: none"> 1. Explore genomic resources like Ensemble, CoGe etc. 2. Assembling and editing of Genomic data; Genome alignment and analysis tools- BWA (BurrowsWheeler Aligner), SAMtools, GATK (The Genome Analysis Toolkit), IGV (Integrative Genomics Viewer) 3. Assembling short reads from a organism using SPAdes 4. Variant calling and SNP detection 5. Map reads from CHiPseq experiment to the respective reference genome and identify peaks using MACS 6. Explore Proteomics resources at ExPASy, EBI 7. Explore and query the protein-Protein, protein-small molecule and biomedical interaction databases 8. Explore post-translational modifications databases 9. Analysis of 2D Gel Electrophoresis image Analysis of mass spectrometry data.
Suggested readings	<ol style="list-style-type: none"> 1. Twyman, R. M. (2014). Principles of proteomics. Second Edition, Garland Science, Taylor & Francis Group, LLC 2. Web resources and tutorials of respective databases and tools
Practical (Cr. 2)	Advanced statistical techniques for Bioinformatics
	<ol style="list-style-type: none"> 1. Exercises on estimation of parameters using methods of maximum likelihood, minimum χ^2 and moments. Obtaining confidence interval estimates, MP and UMP tests, large sample tests, non-parametric tests, Sequential probability ratio test, Decision functions. 2. Selection of a random sample, use of random number tables, estimation using simple random sampling. Exercises on inverse sampling, stratified sampling, cluster sampling and systematic sampling. Estimation using ratio and regression estimators, Estimation using multistage design and double sampling. Exercises on various non-parametric tests. 3. ANOVA, ANCOVA, MANOVA for biological data 4. Simultaneous hypothesis testing, Adjusted p-value, Differential Expression – Multiple Genes: The False Discovery Rate (FDR).
Practical (Cr. 2)	Computer programming for Bioinformatics

	<ol style="list-style-type: none"> 1. Writing C script, variable declaration, functions, arithmetic and logical operations 2. Working with arrays single and multi-dimensional; control/condition statements; iterations and looping 3. Programming in Java, declaring objects, methods and constructor, packages and arrays, multithreading, file handling, exception handling. 4. Designing PERL program for analysis of nucleotide and protein sequences; Uses of Scalar and Array Variables to manipulate DNA/RNA/Protein sequence data 5. Reading a sequence data from a file and writing the results to a file; Concatenation DNA fragments, Transcribing DNA into RNA; Calculating the Reverse complement of a DNA strand; Uses of subroutine to read FASTA files 6. Uses of Regular Expressions 7. Uses of Bio-PERL modules for sequence manipulation, accessing local database.
Department Skill Enhancement (DSE) (Any One to be chosen)	
NCC/NSS/MO OC (Cr. 2)	Students can opt for courses offered by the SWAYAM portal. They will have to produce the course completion certificate. Students can join the NCC or NSS for acquiring the required credit.
Review Paper Writing/Industrial and Institutional visit & Report submission (Cr. 2)	Students can earn credit by writing a review article on a relevant topic on bioinformatics or by visiting an advanced center of learning/ R&D institute A report on the visit is required to be submitted.
SEC I (Cr. 2)	
	The course will be offered jointly along with students of other departments.

Semester III : Core Course	
Theory (Cr. 2)	Structural Bioinformatics
Course Objectives:	This course introduces the concept of how the biomolecules act, their structural properties and how their products interact. The students will learn about different computational resources available for structural bioinformatics
Course Outcomes:	A student who completes this course is expected to: <ul style="list-style-type: none"> ● Know the structure of the different biological molecule ● Predict the structures and grasp the idea of experimental structure and determination using x-ray crystallography ● To explain the structural Bioinformatics strategies and apply bioinformatics tools for the same
Unit 1	Proteins: Primary, secondary, tertiary, quaternary and supra-molecular structures; Ramachandran plots; motifs and folds; Methods for determining the structure of biomolecules (X-ray crystallography, NMR spectroscopy, and electron microscopy). Defining bioinformatics and structural bioinformatics, Search and sampling in structural bioinformatics, Molecular visualization
Unit 2	The PDB format, MMCIF formats, and other data formats, Other structure-based databases, Structural quality assurance, The impact of local accuracy in protein and RNA structures: validation as an active tool, Structure comparison and alignment, Secondary structure assignment, Identifying structural domains in proteins, Inferring protein function from structure, Structural annotation of genomes, Electrostatic interactions, Prediction of protein–nucleic acid interactions, Prediction of protein–protein interactions from evolutionary information,
Unit 3	CASP and other community-wide assessments to advance the field of structure prediction, Prediction of protein structure in 1D: secondary structure, membrane regions, and solvent accessibility, Homology modeling, Fold recognition methods, de novo protein structure prediction: methods and application, RNA structural bioinformatics
Unit 4	Structural bioinformatics in drug discovery, B-Cell epitope prediction, Methods to classify and predict the structure of membrane proteins, Protein motion: Simulation, The significance and impacts of protein disorder and conformational variants, Protein designability and engineering, Structural genomics of protein superfamilies
Suggested readings	<ol style="list-style-type: none"> 1. Web resources, Review papers 2. F. J Burkowski; Structural Bioinformatics An Algorithmic Approach; CRC Press, 2009 3. P. E. Bourne and J. Gu; Structural bioinformatics; 2nd edition. John Wiley and Sons. 2009. 4. A. Leach; Molecular modelling – principles and applications; Pearson Education Ltd, 2001 5. M.J.E Sternberg ; Protein Structure Prediction: A Practical Approach. Publisher: USA; Oxford University Press, 1997

Practical (Cr. 2)	Structural Bioinformatics
	<ol style="list-style-type: none"> 1. Explore Protein Secondary and 3D structure databases 2. Evaluation and visualization of 3D structure of biomolecules using open source resource 3. Protein 3D Structure Predictions - Homology modelling, Threading and <i>Ab initio</i> methods 4. Refine the Predicted structure 5. Evaluation and Validation of protein models 6. Protein 3D Structure Comparison 7. Protein and Ligand Visualization Software
Suggested Readings:	Web resources, Research and Review articles. Help files, software tutorials
Department Skill Enhancement (DSE) (Any Three to be chosen)	
Theory (Cr. 1)	Web-based Programming and Database management systems
Course Objectives:	This course is intended to provide students with an in-depth understanding of the web page designing using CSS, HTML, PHP etc. and database development and management using SQL, ORACLE. The concept of establishment the connectivity of web page with database will also be introduced.
Course Outcomes:	<p>After completion of the course the learners will be able to</p> <ol style="list-style-type: none"> (1) Understand the procedure of creation of biological database and its management (2) Develop webpage as graphical interface of algorithm (3) Handle database integration with the webtool for storing data.
Unit 1	Introduction to CSS, CSS Properties, CSS Styling: Background, Text Format, Controlling Fonts, Working with Lists and Tables, CSS ID and Class, Writing JavaScript into HTML, Basic Programming using JavaScript, JavaScript Client Validations, Evaluation of PHP, Basic Syntax, Defining variable and constant, Introduction to WAMP/XAMPP Server – Configuration and Web Application Deployment, PHP Server Variables.
Unit 2	Overview of DBMS; Data associations - Entities, Attributes and Associations, Entity Relationship model. Relational Database Design - Anomalies in a Database, Normalization Theory, and Normal forms; Query processing and optimization; Security, backup and recovery. Distributed Databases- concepts, architecture, design; Structured Query Language (SQL) - Data Definition Language (DDL), Data Manipulation Language (DML). Transaction management: ACID properties.

Suggested Readings:	<ol style="list-style-type: none"> 1. Robert W. Sebesta, Programming the World Wide Web, Addison Wesley 2. Ivan Bayross, HTML 5 and CSS 3 Made Simple, BPB 3. Bayross, Web Enabled Commercial Application Development Using HTML, JavaScript, DHTML and PHP, BPB 4. Dick Oliver, Michael Morrison, Sams Teach Yourself HTML and CSS in 24 Hours, Pearson Education 5. Date, C. J. 2000. Introduction to Database System. Addison Wesley. 6. Desai, B. C. 2000. Introduction to Database Systems. Galgotia Publications, New Delhi. 7. Elmasri and Navathe. 2006. Fundamentals of Database Systems. Addison Wesley. 8. Garcia-Molina, H., Ullman, J. D. and Widom J. 2002. Database Systems: The Complete Book. Prentice Hall.
Theory (Cr. 1)	Phylogeny and Phylogenomics
Course Objectives:	The main goal of this course is to help students in learning the basic concepts and computational methods involved in the molecular evolutionary analysis of genes and proteins
Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● understand the theoretical aspects of classical, molecular evolution and applications. ● Measuring the rate of evolution and concept of molecular clock hypothesis. ● Various algorithms and their comparison for deducing phylogenetic tree among species
Unit 1	Concepts of neutral evolution, molecular divergence and molecular clocks; Molecular tools in phylogeny, classification and identification; Protein and nucleotide sequence analysis; Gene duplication and divergence. Concepts and rate of change in gene frequency through natural selection, migration and random genetic drift; Adaptive radiation; Speciation; Convergent evolution; Co-evolution
Unit 2	Phylogenetic representations, Definition and description, various types of trees; Phylogenetic Algorithms: UPGMA ,neighbor joining, Maximum Parsimony (MP) and Maximum Likelihood (ML) methods; Bayesian inference; Boot strapping; Jackknifing; Phylogenetic software & applications: Multiple sequence alignment & Tree building software - ClustalW, Mega, Phylip, Phylodraw, Phylml, RaxML

Suggested Readings	<ol style="list-style-type: none"> 1. Page, R. D., & Holmes, E. C. (1998). Molecular evolution: a phylogenetic approach. John Wiley & Sons 2. L. Bromham ; Reading the Story in DNA: A Beginner's Guide to Molecular Evolution; Oxford University Press, 2008 3. G. Bernardi; Structural and Evolutionary Genomics: Natural Selection in Genome Evolution (New Comprehensive Biochemistry); Elsevier Science, 2005. 4. M. Salemi and Anne-Mieke Vandamme; The phylogenetic handbook: a practical approach to DNA and protein phylogeny; Cambridge University Press, 2003.
Theory (Cr. 1)	NGS and expression data analysis
Course Objectives:	The major goal of this course provides the student with a strong foundation for principles, methods and concepts of sequencing, Impact of transcriptomics on biology and familiarize them with tools and method to analyze the NGS, Microarray, RNA-Seq data
Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● Comprehend the ideas of NGS data processing and workflow ● Understand metagenomics and its data workflow ● Understand the Differential expression analysis of gene
Unit 1	Comparison of Next generation sequencing techniques, NGS File formats, & applications; <i>De novo</i> Genome sequence assembly, Reference sequence assembly, Challenges of Genome assembly, Use of paired – end reads in the assembly, Data Preprocessing methods and sequencing read correction methods, Evaluation of assembly methods; Overview of metagenomics principles, 16SrRNA data analysis, clustering/phylogenetic tree based of alignment, clustering based on composition, Concepts behind self organizing maps, principal component and other clustering tools
Unit 2	DNA microarray- understanding of microarray data, normalizing microarray data, detecting differential gene expression, correlation of gene expression data to biological process and computational analysis tools (especially clustering approaches); RNA-Seq Data Analysis: Data Quality Control and Reads Mapping, RNA-Seq Data Normalization, Identification of Differentially Expressed Genes, Differential Splicing Analysis, Visualization of RNA-Seq Data, Functional Analysis of Identified Genes; RNA-Seq as a Discovery Tool

Suggested Readings	<ol style="list-style-type: none"> 1. Ali Masoudi-Nejad, Zahra Narimani, Nazanin Hosseinkhan; “Next Generation Sequencing and Sequence Assembly”, Methodologies and Algorithms, Springer; 2013. 2. Stuart M. Brown, “Next-Generation DNA Sequencing Informatics”, Cold Spring Harbor Laboratory Press, 2013. 3. Y. M. Kwon and S. C. Ricke; HighThroughput Next Generation Sequencing: Methods and Applications; Humana Press; 2011. 4. Wang, Xinkun. Next-Generation Sequencing Data Analysis, CRC Press; 2016.
Theory (Cr. 1)	Advance computer programming for Bioinformatics
Course Objectives:	This lab course introduces the basic concept of of python and R programming and develop programming capability to write scripts to solve bioinformatics problems
Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● Understand Python programming syntax ● Able to write python scripts for various bioinformatics applications. ● Implement statistical application for solving biological problems using R packages.
Unit 1	Introduction to Python Programming, Features of Python, Python interpreter interactive and non-interactive mode. Functions: Introduction, Defining and Calling a Void Function, designing a Program to Use Functions, Local Variables, Passing Arguments to Functions, Global Variables and Global Constants, Value-Returning Functions Generating Random Numbers, Writing Our Own Value-Returning Functions, the math Module, Storing Functions in Modules.Application of Bio-python in Bioinformatics.
Unit 2	R: open-source language and environment for statistical computing and graphics Bioconductor - open-source software for the analysis of biomedical and genomic data, mainly R packages. Analysis of microarray data, Next Generation Sequencing (NGS) data, DNA/protein sequence data.
Suggested Readings	<ol style="list-style-type: none"> 1. Kinser J. 2008 Python for Bioinformatics, Series in Biomedical Informatics, Jones & Bartlett. 2. Martin C. Brown 2001 Python: The Complete Reference, Complete Reference Series, McGraw-Hill. 3. Hadley W, and Garrett G. 2017 R for Data Science, OREILLY 4. Norman M. 2011 The Art of R Programming - A Tour of Statistical Software Design, No Starch Press.
Theory (Cr. 1)	Data Mining and Machine learning techniques for Bioinformatics
Course Objectives:	The course gives an idea of the different algorithms to be used to train and test systems along with mining relevant data from a system. This course will also introduce the basics of data analysis with machine learning techniques.

Course Outcomes:	<p>After completion of the course the learners will be able to-</p> <ul style="list-style-type: none"> ● Learn the different classification and clustering algorithms ● Biological data analysis using supervised and unsupervised techniques for better understanding of biological events ● Integration of biological data using machine learning and data mining techniques.
Unit 1	Overview of machine learning techniques; supervised and unsupervised techniques. Empirical Risk Minimization, Structural Risk Minimization; Measuring the accuracy of learned hypotheses. Comparing learning algorithms: cross-validation, learning curves, and statistical hypothesis testing.
Unit 2	Introduction to Data mining, Data mining Functionalities, Classification of Data mining Systems, Data Mining Task Primitives, Integration of Data mining systems, Major issues of Data mining. Data mining: Basic concepts of Knowledge discovery and Data Mining, Application of data mining in bioinformatics. Data Pre-processing, Data Cleaning, Data Integration and Transformation, Data Reduction, Data discretization and concept hierarchy generation.
Suggested readings	<ul style="list-style-type: none"> ● Witten, H. I., Frank, E. and Hall, M. A. 2011. Data Mining: Practical Machine Learning Tools and Techniques. ● Hastie, T., Tibshirani, R., Friedman, J. H. 2009. The Elements of Statistical Learning: Data Mining Interface and Prediction. ● Clarke, S. B., Fokoue, E. and Zhang, H. H. 2009 Principles and Theory for Data Mining and Machine Learning.
Theory (Cr. 1)	Advanced omics technologies
Course Objectives:	This course will familiarize the students with advanced tools and techniques used in omics studies. They will learn about different computational resources available for high throughput data coming from different omics platform
Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● Explain the Peptidomics, Allergens, Metabolomics, Interactomics, etc ● Understand the principles of integrative analysis methods for biological system analysis and interactions ● Implement database search and suits for –omics ● Analyze data coming from different omics experiments
Unit 1	Current peptidomics: Applications, purification, identification, quantification, and functional analysis; Plant Peptides: Bioactivity, Opportunities and Challenges; Antimicrobial Peptides; Introduction to Bacteriocin & its type / Classes, Genetics and Regulation of Bacteriocin Synthesis, Mode of Action, Applications of Bacteriocins; In Silico Search for Biologically Active Peptides; Pheromone Peptides, Prebiotic Peptides; Allergen Peptides, Recombinant Allergens and Hypoallergens for Allergen-Specific Immunotherapy; In silico Identification of Potential Peptides or Allergen Shot Candidates Against <i>Aspergillus fumigatus</i> ; Secretomics-Overview; Methodologies to decipher the cell secretome; Lipidomics-Overview; Techniques, Applications, and Outcomes Related to Biomedical Sciences; Prospects from a technological perspective

<i>Unit 2</i>	Metabolomics-Overview, Metabolomics techniques and technologies, Analytical platform and Analysis of metabolomic data; Overview of Extremophiles; Extremozymes: A Potential Source for Industrial Applications; Stability and solubility of proteins from extremophiles, Survival Mechanisms of Extremophiles, Protein Adaptations in Archaeal Extremophiles; Interactome & Interactomics – Overview; Interactomics: Connecting the dots; Interactomics: toward protein function and regulation; Proteome-Scale Human Interactomics; Pathway analysis- Overview; Integrating Networks and Proteomics: Moving Forward; Pathway and network analysis in proteomics; Introduction to Network Analysis in Systems Biology; List of visualization tools for network biology
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Suggested readings

1. Web resources, Review papers
2. Handbook of Biologically Active Peptides (Second Edition); Edited by:AbbaKastin; 2013 Elsevier Inc; ISBN: 978-0-12-385095-9
3. Dallas, D. C., Guerrero, A., Parker, E. A., Robinson, R. C., Gan, J., German, J. B., ... Lebrilla, C. B. (2015). Current peptidomics: Applications, purification, identification, quantification, and functional analysis. *Proteomics*, 15(0), 1026–1038. <http://doi.org/10.1002/pmic.201400310>
4. Sarethy IP. Plant Peptides: Bioactivity, Opportunities and Challenges. *Protein Pept Lett*. 2017;24(2):102-108. doi: 10.2174/0929866523666161220113632. Review. PubMed PMID: 28000568.
5. Bahar, A. A., & Ren, D. (2013). Antimicrobial Peptides. *Pharmaceuticals*, 6(12), 1543–1575. <http://doi.org/10.3390/ph6121543>
6. Martínez, B., Rodríguez, A., & Suárez, E. (2016). Antimicrobial Peptides Produced by Bacteria: The Bacteriocins. In *New Weapons to Control Bacterial Growth* (pp. 15-38). Springer International Publishing
7. Babu, P., Chandel, A. K., & Singh, O. V. (2015). Survival Mechanisms of Extremophiles. In *Extremophiles and Their Applications in Medical Processes* (pp. 9-23). Springer International Publishing.
8. Burgess, K., Rankin, N., & Weidt, S. (2014). Chapter 10 - Metabolomics - Padmanabhan, Sandosh; *Handbook of Pharmacogenomics and Stratified Medicine* (pp. 181-205). San Diego: Academic Press.
9. Dammeyer T., Schobert M. (2010) Interactomics. In: Timmis K.N. (eds) *Handbook of Hydrocarbon and Lipid Microbiology*. Springer, Berlin, Heidelberg
10. Dumorné K, Córdova DC, Astorga-Eló M, Renganathan P. Extremozymes: A Potential Source for Industrial Applications. *J MicrobiolBiotechnol*. 2017 Apr 28;27(4):649-659. doi: 10.4014/jmb.1611.11006. Review. PubMed PMID: 28104900.
11. Feng S, Zhou L, Huang C, Xie K, Nice EC. Interactomics: toward protein function and regulation. *Expert Rev Proteomics*. 2015 Feb;12(1):37-60. doi: 10.1586/14789450.2015.1000870. Epub 2015 Jan 12. Review. PubMed PMID: 25578092.
12. Finkelstein, J. M. (2015). Interactomics: Connecting the dots. *Nature Chemical Biology*, 11, 449. doi:10.1038/nchembio.1855
13. Goh WW, Wong L. Integrating Networks and Proteomics: Moving Forward. *Trends Biotechnol*. 2016 Dec;34(12):951-959. doi: 10.1016/j.tibtech.2016.05.015. Epub 2016 Jun 13. Review. PubMed PMID: 27312055.
14. Greaves RB, Warwicker J. Stability and solubility of proteins from extremophiles. *BiochemBiophys Res Commun*. 2009 Mar 13;380(3):581-5. doi: 10.1016/j.bbrc.2009.01.145. Epub 2009 Jan 29. PubMed PMID: 19285004.

	<p>15. List of visualization tools for network biology: http://bioinformaticsonline.com/pages/view/35386/list-of-visualization-tools-for-network-biology</p> <p>16. Luck K, Sheynkman GM, Zhang I, Vidal M. Proteome-Scale Human Interactomics. <i>Trends Biochem Sci.</i> 2017 May;42(5):342-354. doi: 10.1016/j.tibs.2017.02.006. Epub 2017 Mar 8. Review. PubMed PMID: 28284537; PubMed Central PMCID: PMC5409865.</p> <p>17. Ma'ayan, A. (2011). Introduction to Network Analysis in Systems Biology. <i>Science Signaling</i>, 4(190), tr5. http://doi.org/10.1126/scisignal.2001965</p> <p>18. Marth, K., Focke-Tejkl, M., Lupinek, C., Valenta, R., &Niederberger, V. (2014). Allergen Peptides, Recombinant Allergens and Hypoallergens for Allergen-Specific Immunotherapy. <i>Current Treatment Options in Allergy</i>, 1(1), 91–106. http://doi.org/10.1007/s40521-013-0006-5</p> <p>19. Mukherjee, P., & Mani, S. (2013). Methodologies to decipher the cell secretome. <i>Biochimica et Biophysica Acta</i>, 1834(11), 2226–2232. http://doi.org/10.1016/j.bbapap.2013.01.022</p> <p>20. Neifar, M., Maktouf, S., Ghorbel, R. E., Jaouani, A. and Cherif, A. (2015) Extremophiles as source of novel bioactive compounds with industrial potential, in <i>Biotechnology of Bioactive Compounds: Sources and applications</i> (eds V. K. Gupta and M. G. Tuohy), John Wiley & Sons, Ltd, Chichester, UK. doi: 10.1002/9781118733103.ch10</p> <p>21. What is metabolomics: https://www.ebi.ac.uk/training/online/course/introduction-metabolomics/what-metabolomics</p> <p>22. Wu X, Hasan MA, Chen JY. Pathway and network analysis in proteomics. <i>J Theor Biol.</i> 2014 Dec 7;362:44-52. doi: 10.1016/j.jtbi.2014.05.031. Epub 2014 Jun 6. Review. PubMed PMID: 24911777; PubMed Central PMCID: PMC4253643.</p> <p>23. Yang K, Han X. Lipidomics: Techniques, Applications, and Outcomes Related to Biomedical Sciences. <i>Trends Biochem Sci.</i> 2016 Nov;41(11):954-969. doi: 10.1016/j.tibs.2016.08.010. Epub 2016 Sep 20. Review. PubMed PMID: 27663237;PubMed Central PMCID: PMC5085849.</p>
Practical (Cr. 1)	Web based programming and database management

	<ol style="list-style-type: none"> 1. Web page designing using CSS, JSP, PHP 2. E-R diagram construction; SQL - Command Syntax, SQL constraints, Data types, DDL Statements, DML Statements, SQL-expressions, Creating database using SQL, CREAT, DROP or DELETE table SQL operators, SELECT, INSERT, WHERE, AND, OR. SQL UPDATE query, DELETE query, Integrity constraints; Triggers, creating stored procedures/ functions; 3. Normalization of database and Case study on a database design and implementation using SQL and Oracle. Relational DBMS using SQL. SQL Transactional control commands, COMMIT, ROLLBACK, SAVEPOINT, SET TRANSACTION
Practical (Cr. 1)	Phylogeny and Phylogenomics
	<ol style="list-style-type: none"> 1. Reconstruction of phylogenetic trees using molecular data – UPGMA, Neighbour-joining, Maximum parsimony and Maximum likelihood method 2. Using bootstrapping tool to generate multiple datasets from the original input data & generation of consensus tree 3. Plotting, visualizing & formatting phylogenetic trees: TreeView and FigTree 4. Molecular divergence or clock analysis 5. Reconstruction of phylogenetic trees using whole genome data of viruses 6. Identification of horizontal gene transfer events from phylogenetic trees
<i>Suggested readings</i>	<ol style="list-style-type: none"> 5. Page, R. D., & Holmes, E. C. (1998). Molecular evolution: a phylogenetic approach. John Wiley & Sons 6. L. Bromham ; Reading the Story in DNA: A Beginner's Guide to Molecular Evolution; Oxford University Press, 2008 7. G. Bernardi; Structural and Evolutionary Genomics: Natural Selection in Genome Evolution (New Comprehensive Biochemistry); Elsevier Science, 2005. 8. M. Salemi and Anne-Meike Vandamme; The phylogenetic handbook: a practical approach to DNA and protein phylogeny; Cambridge University Press, 2003.

Practical (Cr. 1)	NGS and expression data analysis
	<ol style="list-style-type: none"> 1. Exploring the Gene expression databases like GEO, SRA etc 2. Microarray data analysis- understanding of microarray data, normalizing microarray data, detecting differential gene expression, microarray Data Cluster Analysis 3. Mapping RNAseq dataset onto the reference genome; extract read counts per gene using a gtf file; compute RPKM; find out genes differentially expressed between two samples using DESeq (R package). 4. Classify the phylum using a dataset of 16SrRNA sequencing of a microbiome using QIIME
Suggested readings	<ol style="list-style-type: none"> 1. Stuart M. Brown, “Next-Generation DNA Sequencing Informatics”, Cold Spring Harbor Laboratory Press, 2013. 2. Y. M. Kwon and S. C. Ricke; HighThroughput Next Generation Sequencing: Methods and Applications; Humana Press; 2011. 3. Wang, Xinkun. Next-Generation Sequencing Data Analysis, CRCPress; 2016
Practical (Cr. 1)	Advance computer programming for Bioinformatics
	<ol style="list-style-type: none"> 1. R programming for analysing gene expression data, RNA seq data. 2. Bio-conductor and R package for analysis of biological data 3. Declaring function in R, creating package in R. 4. Basic syntax; variables; operators (basic python programming) 5. Decision making; loops (selection and iterations in python programming) 6. Numbers, lists, strings, tuples and dictionary (advanced data structures in python programming). 7. Functions in python; modules in python (function and module orientation in python programming)
Practical (Cr. 1)	Data Mining and Machine learning techniques for Bioinformatics
	<ol style="list-style-type: none"> 1. Generalized linear model prediction based on real data, error minimization of the model and cross validation using ROC curve. 2. Regularized regression model, Ridge regression, LASSO for prediction 3. Decision tree, random forest-based prediction 4. Classification techniques: ANN, SVM, KNN. 5. Case based reasoning and its applications on biological data. 6. Clustering techniques; Clustering of high dimensional data; clustering of gene expression data. 7. Dimensional reduction techniques; Principal component analysis, feature selection technique. 8. Re-sampling techniques; bootstrap for estimation and model validation. <p>Text mining and Web mining. Soft Computing and Fuzzy logic system and application in bioinformatics</p>
Practical (Cr. 1)	Advanced omics technologies

	<ol style="list-style-type: none"> 1. Explore the Antimicrobial peptide database 2. Explore the Bacteriocin database 3. Explore the cyclotide database 4. Explore the allergen database 5. Explore the Secretome database 6. Explore the metabolic pathway databases 7. Explore Biomolecule interaction databases 8. Explore visualization tools for network biology
Suggested Readings	Web resources, Research and Review articles. Help files, software tutorials.
Generic Elective (GE) (Any One to be chosen)	
Theory (Cr. 2)	Biological data analysis
Course Objectives:	The main objective of this course is to introduce general concepts of computational methods of biological data analysis to the allied department students of the university
Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● Understand the essential features of the interdisciplinary field of science for better understanding biological data. ● Look at a biological problem from a computational point of view ● Find out the methods for analyzing the structure, function and expression of DNA, RNA and proteins ● Interact with algorithms, tools and data in current scenario
Unit 1	Overview of molecular biology, the cell as basic unit of life-Prokaryotic cell and Eukaryotic cell - Central Dogma: DNA-RNA-Protein, Introduction to DNA and Protein sequencing, Human Genome Project, Introduction to Data types and source; Protein Sequence and Structural Databases; Nucleic acid databases; Genome databases; Specialized Databases;; Information retrieval from Biological databases
Unit 2	Algorithms in Computing; Analyzing algorithms-Asymptotic notation, Standard notations, Big 'O' notations; Algorithm design techniques- Exhaustive Search, Branch-and-Bound Algorithms, Greedy Algorithms, Dynamic Programming, Divide-and-Conquer Algorithms, Machine Learning, Randomized Algorithms; Time and space complexity of algorithms, common Sort and Search algorithms
Unit3	Concepts in sequence analysis- sequence similarity, identity and homology; Scoring matrices- PAM and BLOSUM matrices, Global alignments: Needleman Wunsch Algorithm, Local Alignments: Smith Waterman Algorithm, Gap Penalties,Pairwise sequence alignments: BLAST, Multiple sequence alignments (MSA); Phylogeny: Basic concepts of phylogeny; molecular evolution; Brief introduction to Phylogenetics and phylogenetic tree construction

Unit4	Structure classification of proteins (SCOP, CATH), Secondary structure prediction of various protein categories; Patterns, motifs and Profiles in sequences, Databases of patterns, motifs and profiles e.g.Prosite, Blocks, Prints-S, Pfam; Protein structure prediction by comparative modeling approaches (homology modeling and fold recognition); ab initio structure prediction methods.
Suggested Readings:	<ol style="list-style-type: none"> 1. Neil C. Jones and Pavel A. Pevzner, “An Introduction to Bioinformatics Algorithms”, MIT Press, 2005 2. Wing-kin Sung, “Algorithms in Bioinformatics: A Practical Introduction”, CRC Press, 2011. 3. David W Mount, “Bioinformatics sequence and Genome analysis”, Second Edition, Cold Spring Harbor Laboratory Press, 2013 4. P. G. Higgs and T. K Attwood, “Bioinformatics and Molecular Evolution”, Blackwell Publishing, 2005 5. D. W. Mount, “Bioinformatics Sequence and Genome Analysis”, Cold Spring Laboratory Press, 2001.

Theory (Cr. 2)	Cheminformatics
Course Objectives:	This course will familiarize the students with tools and techniques used in Cheminformatics, especially Computer-aided drug discovery. The course is designed to provide basic understanding of computational drug design and applicability of tools for novel drug discovery
Course Outcomes:	Students would be able to- <ul style="list-style-type: none"> ● Get insights on the modern drug discovery and development process ● Identify the drug targets and understand the mode of action ● Knows the basics of drugs, the rules that govern drug behavior and its classification ● Learn different computational resources available for Structural Bioinformatics
Unit 1	Introduction to Cheminformatics: Development of the Field, The Basis of Cheminformatics and the Diversity of Applications, Databases, Fundamental Questions of a Chemist, Drug Discovery, Additional Fields of Application; Applications of Cheminformatics in Drug Discovery; Representation of Chemical Structures; Overview of small molecule databases (Database needs to be covered from the latest database issue of Nucleic Acids Research journals); Overview of Drugs and drug design databases(Database needs to be covered from the latest database issue of Nucleic Acids Research journals); Resources for Chemical, Biological, and Structural Data on Natural Products; Free Marine Natural Products Databases for Biotechnology and Bioengineering.
Unit 2	Computational/in silico methods in drug target and lead prediction; Computational approaches in target identification and drug discovery; Using reverse docking for target identification and its applications for drug discovery; Tools for in silico target fishing; A review of ligand-based virtual screening web tools and screening algorithms in large molecular databases in the age of big data; In Silico Target Druggability Assessment: From Structural to Systemic Approaches; Modern Computational Strategies for Designing Drugs to Curb Human Diseases: A Prospect; A Structure-Based Drug Discovery Paradigm; Virtual Screening Techniques in Drug Discovery: Review and Recent Applications; Recent Advances in Scaffold Hopping; Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity
Unit3	Computational Methodologies in the Exploration of Marine Natural Product Leads; Polypharmacology by Design: A Medicinal Chemist's Perspective on Multitargeting Compounds Repurposing; Web-Based Tools for Polypharmacology Prediction; Molecular Docking: Shifting Paradigms in Drug Discovery; Molecular docking: current advances and challenges; An Overview of Scoring Functions Used for Protein-Ligand Interactions in Molecular Docking; Virtual Screening Techniques in Drug Discovery: Review and Recent Applications; Benchmarking of different molecular docking methods for protein-peptide docking; Concepts and Core Principles of Fragment-Based Drug Design; Computational Fragment-Based Drug Design: Current Trends, Strategies, and Applications

<i>Unit4</i>	Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview; Molecular Dynamics Simulation for All; Molecular mechanics; Quantitative Structure-Activity Relationship (QSAR): Modeling Approaches to Biological Applications; QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery; The Pharmacophore Concept and Its Applications in Computer-Aided Drug Design; In Silico Approaches for Predictive Toxicology; In silico ADME-Tox modeling: progress and prospects; In silico toxicology protocols; Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases; Advancing Drug Discovery via Artificial Intelligence
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Suggested Readings:

1. Cereto-Massagué, A., et al (2015). Tools for in silico target fishing. *Methods*, 71, 98-103. doi:<https://doi.org/10.1016/j.ymeth.2014.09.006>
2. Chan HCS, et al. Advancing Drug Discovery via Artificial Intelligence. *Trends Pharmacol Sci*. 2019 Oct;40(10):801. doi: 10.1016/j.tips.2019.07.013. Epub 2019 Aug 23. PubMed PMID: 31451243.
3. Rifaioglu AS, et al. Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases. *Brief Bioinform*. 2019 Sep 27;20(5):1878-1912. doi: 10.1093/bib/bby061. PubMed PMID: 30084866
4. Neves, B. J., et al. (2018). QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. 9(1275). doi:10.3389/fphar.2018.01275
5. Vanommeslaeghe K, et al. Molecular mechanics. *Curr Pharm Des*. 2014;20(20):3281-92. Review. PubMed PMID: 23947650; PubMed Central PMCID: PMC4026342.
6. Salmaso V, Moro S. Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview. *Front Pharmacol*. 2018 Aug 22;9:923. doi: 10.3389/fphar.2018.00923. eCollection 2018. Review. PubMed PMID: 30186166
7. De Vivo, et al (2016). Role of Molecular Dynamics and Related Methods in Drug Discovery. *Journal of Medicinal Chemistry*, 59(9), 4035-4061. doi:10.1021/acs.jmedchem.5b01684
8. Zheng, L., et al (2019). Molecular Dynamics and Simulation. In S. Ranganathan, M. Gribskov, K. Nakai, & C. Schönbach (Eds.), *Encyclopedia of Bioinformatics and Computational Biology* (pp. 550-566). Oxford: Academic Press.
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10. Merk D, et al. De Novo Design of Bioactive Small Molecules by Artificial Intelligence. *Mol Inform*. 2018 Jan;37(1-2). doi: 10.1002/minf.201700153. Epub 2018 Jan 10. PubMed PMID: 29319225
11. Myatt GJ, et al. In silico toxicology protocols. *Regul Toxicol Pharmacol*. 2018 Jul;96:1-17. doi: 10.1016/j.yrtph.2018.04.014. Epub 2018 Apr 17. PubMed PMID: 29678766
12. Alqahtani S. In silico ADME-Tox modeling: progress and prospects. *Expert Opin Drug Metab Toxicol*. 2017 Nov;13(11):1147-1158. doi: 10.1080/17425255.2017.1389897. Epub 2017 Oct 13. Review. PubMed PMID: 28988506.
13. Engel, T., & Gasteiger, J. (2018). *Chemoinformatics: Basic Concepts and Methods*: Wiley.
14. Thomas Engel Johann Gasteiger, *Applied Chemoinformatics: Achievements and Future Opportunities*, First published: 20 April 2018, Print ISBN: 9783527342013 | Online ISBN: 9783527806539 | DOI: 10.1002/9783527806539
15. Warr, W. A. (2011). Representation of chemical structures. 1(4), 557-579. doi:10.1002/wcms.36
16. Kinghorn AD, Falk H, Gibbons S, et al.: eds. *Progress in the Chemistry of Organic Natural Products 110: Cheminformatics in Natural Product Research*. Cham: Springer International Publishing. 2019

17. Chen Y., de Bruyn Kops C., Kirchmair J. (2019) Resources for Chemical, Biological, and Structural Data on Natural Products. In: Kinghorn A., Falk H., Gibbons S., Kobayashi J., Asakawa Y., Liu JK. (eds) Progress in the Chemistry of Organic Natural Products 110. Progress in the Chemistry of Organic Natural Products, vol 110. Springer, Cham
18. Overview of small molecule databases: <http://www.oxfordjournals.org/nar/database/subcat/4/11>
19. Overview of Drugs and drug design databases: <http://www.oxfordjournals.org/nar/database/subcat/11/35>
20. Database issue of Nucleic Acids Research journals: <http://www.oxfordjournals.org/nar/database/c/>
21. Barbosa, A.J.M. and Roque, A.C.A. (2019), Free Marine Natural Products Databases for Biotechnology and Bioengineering. *Biotechnol. J.*, 14: 1800607. doi:10.1002/biot.201800607
22. Agamah FE, et al. Computational/in silico methods in drug target and lead prediction. *Brief Bioinform.* 2019 Nov 10. pii: bbz103. doi: 10.1093/bib/bbz103. PubMed PMID: 31711157.
23. Katsila T, et al. Computational approaches in target identification and drug discovery. *Comput Struct Biotechnol J.* 2016 May 7;14:177-84. doi: 10.1016/j.csbj.2016.04.004. eCollection 2016. Review. PubMed PMID: 27293534
24. Batool M, Ahmad B, Choi S. A Structure-Based Drug Discovery Paradigm. *Int J Mol Sci.* 2019 Jun 6;20(11). pii: E2783. doi: 10.3390/ijms20112783. Review. PubMed PMID: 31174387
25. Dar KB, et al. Modern Computational Strategies for Designing Drugs to Curb Human Diseases: A Prospect. *Curr Top Med Chem.* 2018;18(31):2702-2719. doi: 10.2174/1568026619666190119150741. Review. PubMed PMID: 30659543.
26. da Silva Rocha SFL, et al. Virtual Screening Techniques in Drug Discovery: Review and Recent Applications. *Curr Top Med Chem.* 2019;19(19):1751-1767. doi: 10.2174/1568026619666190816101948. Review. PubMed PMID: 31418662.
27. Trosset JY, Cavé C. In Silico Drug-Target Profiling. *Methods Mol Biol.* 2019;1953:89-103. doi: 10.1007/978-1-4939-9145-7_6. Review. PubMed PMID: 30912017.
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29. Pereira F, Aires-de-Sousa J. Computational Methodologies in the Exploration of Marine Natural Product Leads. *Mar Drugs.* 2018 Jul 13;16(7). pii: E236. doi: 10.3390/md16070236. Review. PubMed PMID: 30011882; PubMed Central PMCID: PMC6070892.
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31. Pinzi L, Rastelli G. Molecular Docking: Shifting Paradigms in Drug Discovery. *Int J Mol Sci.* 2019 Sep 4;20(18). pii: E4331. doi: 10.3390/ijms20184331. Review. PubMed PMID: 31487867

32. Proschak E, Stark H, Merk D. Polypharmacology by Design: A Medicinal Chemist's Perspective on Multitargeting Compounds. *J Med Chem*. 2019 Jan 24;62(2):420-444. doi: 10.1021/acs.jmedchem.8b00760. Epub 2018 Aug 3. PubMed PMID: 30035545.
33. Awale M, Reymond JL. Web-Based Tools for Polypharmacology Prediction. *Methods Mol Biol*. 2019;1888:255-272. doi: 10.1007/978-1-4939-8891-4_15. PubMed PMID: 30519952.
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35. Bian Y, Xie XS. Computational Fragment-Based Drug Design: Current Trends, Strategies, and Applications. *AAPS J*. 2018 Apr 9;20(3):59. doi: 10.1208/s12248-018-0216-7. Review. PubMed PMID: 29633051
36. Hu Y, Stumpfe D, Bajorath J. Recent Advances in Scaffold Hopping. *J Med Chem*. 2017 Feb 23;60(4):1238-1246. doi: 10.1021/acs.jmedchem.6b01437. Epub 2016 Dec 21. PubMed PMID: 28001064.
37. Grisoni, F., Merk, D., Consonni, V. et al. Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. *Commun Chem* 1, 44 (2018). <https://doi.org/10.1038/s42004-018-0043-x>
38. Torres PHM, et al. Key Topics in Molecular Docking for Drug Design. *Int J Mol Sci*. 2019 Sep 15;20(18). pii: E4574. doi: 10.3390/ijms20184574. Review. PubMed PMID: 31540192
39. Li J, Fu A, Zhang L. An Overview of Scoring Functions Used for Protein-Ligand Interactions in Molecular Docking. *Interdiscip Sci*. 2019 Jun;11(2):320-328. doi: 10.1007/s12539-019-00327-w. Epub 2019 Mar 15. Review. PubMed PMID: 30877639
40. Fan, J., Fu, A., & Zhang, L. J. Q. B. (2019). Progress in molecular docking. 7(2), 83-89. doi:10.1007/s40484-019-0172-y
41. Prieto-Martínez, et al (2019). Molecular docking: current advances and challenges. *TIP Revista Especializada en Ciencias Químico-Biológicas*, 21(S1), 65-87.
42. da Silva Rocha SFL, et al. Virtual Screening Techniques in Drug Discovery: Review and Recent Applications. *Curr Top Med Chem*. 2019;19(19):1751-1767. doi: 10.2174/1568026619666190816101948. Review. PubMed PMID: 31418662.
43. Agrawal P, et al. Benchmarking of different molecular docking methods for protein-peptide docking. *BMC Bioinformatics*. 2019 Feb 4;19(Suppl 13):426. doi: 10.1186/s12859-018-2449-y. PubMed PMID: 30717654.
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45. Peter, S. C., et al. (2019). Quantitative Structure-Activity Relationship (QSAR): Modeling Approaches to Biological Applications. In S. Ranganathan, M. Gribskov, K. Nakai, & C. Schönbach (Eds.), *Encyclopedia of Bioinformatics and Computational Biology* (pp. 661-676). Oxford: Academic Press.
46. Seidel T, et al. The Pharmacophore Concept and Its Applications in Computer-Aided Drug Design. *Prog Chem Org Nat Prod*. 2019;110:99-141. doi: 10.1007/978-3-030-14632-0_4. Review. PubMed PMID: 31621012.

	47. Parthasarathi, R., & Dhawan, A. (2018). Chapter 5 - In Silico Approaches for Predictive Toxicology. In A. Dhawan & S. Kwon (Eds.), In Vitro Toxicology (pp. 91-109): Academic Press.
Practical (Cr. 2)	Biological data analysis
<i>Unit 1</i>	Overview of molecular biology, the cell as basic unit of life-Prokaryotic cell and Eukaryotic cell - Central Dogma: DNA-RNA-Protein, Introduction to DNA and Protein sequencing, Human Genome Project, Introduction to Data types and source; Protein Sequence and Structural Databases; Nucleic acid databases; Genome databases; Specialized Databases;; Information retrieval from Biological databases
<i>Unit 2</i>	Algorithms in Computing; Analyzing algorithms-Asymptotic notation, Standard notations, Big 'O' notations; Algorithm design techniques- Exhaustive Search, Branch-and-Bound Algorithms, Greedy Algorithms, Dynamic Programming, Divide-and-Conquer Algorithms, Machine Learning, Randomized Algorithms; Time and space complexity of algorithms, common Sort and Search algorithms
<i>Unit3</i>	Concepts in sequence analysis- sequence similarity, identity and homology; Scoring matrices- PAM and BLOSUM matrices, Global alignments: Needleman Wunsch Algorithm, Local Alignments: Smith Waterman Algorithm, Gap Penalties,Pairwise sequence alignments: BLAST, Multiple sequence alignments (MSA); Phylogeny: Basic concepts of phylogeny; molecular evolution; Brief introduction to Phylogenetics and phylogenetic tree construction
<i>Unit4</i>	Structure classification of proteins (SCOP, CATH), Secondary structure prediction of various protein categories; Patterns, motifs and Profiles in sequences, Databases of patterns, motifs and profiles e.g.Prosite, Blocks, Prints-S, Pfam; Protein structure prediction by comparative modeling approaches (homology modeling and fold recognition); ab initio structure prediction methods.
Suggested Readings:	<ol style="list-style-type: none"> 1. Neil C. Jones and Pavel A. Pevzner, "An Introduction to Bioinformatics Algorithms", MIT Press, 2005 2. Wing-kin Sung, "Algorithms in Bioinformatics: A Practical Introduction", CRC Press, 2011. 3. David W Mount, "Bioinformatics sequence and Genome analysis", Second Edition, Cold Spring Harbor Laboratory Press, 2013 4. P. G. Higgs and T. K Attwood, "Bioinformatics and Molecular Evolution", Blackwell Publishing, 2005 5. D. W. Mount, "Bioinformatics Sequence and Genome Analysis", Cold Spring Laboratory Press, 2001.
Practical (Cr. 2)	Cheminformatics

	<ol style="list-style-type: none"> 1. Explore the Chemical molecule databases, Drug database 2. Utilization of Chemical Drawing tools 3. Drug Target identification through Subtractive Genomics approach 4. Predict Vaccine candidates through the Reverse Vaccinology approach 5. Reverse Docking 6. Target fishing 7. Protein and Ligand preparation for Docking (Online) 8. Pocket Prediction (Active site Prediction) 9. Protein-Ligand, Protein-Protein Docking 10. ADME/T and Drug likeliness Prediction 11. Pharmacophore generation and analysis, mapping 12. Tools for QSAR studies
<i>Suggested Readings:</i>	<ol style="list-style-type: none"> 1. Web resources, Research and Review articles. Help files, software tutorials.
<i>AEC II (Cr. 2)</i>	The course will be offered jointly along with students of other departments.

Semester-IV: Core Course	
Theory (Cr. 2)	Research Methodology & Scientific Writing
Course Objectives:	The major objective of this course is to provide an overview of how to identify research problems and conduct research.
Course Outcomes:	After completion of the course the learners will be able to: <ul style="list-style-type: none"> ● Understand the basics of how to design, conduct research, analyze and communicate the results to research community ● Organize and conduct research (advanced project) in a more appropriate manner ● Explain and apply techniques for scientific writing and research methodology to prepare the writing of a scientific report
Unit 1	Introduction to Research- Definition, Objectives and Characteristics of research, Types of Research- Basic, Applied and Action research, Exploratory and Descriptive, Ex-post facto research; Review of literature, meaning of concept, construct, laws, theory and hypothesis.
Unit 2	Identification of Research Problem Sources of research problem, Criteria for the selection of research problem. Research design, Rationale, Statement of problem, Setting objectives. Definition of concepts, operational definition, variables independent and dependent, control and intervening variables, limitations and delimitation. Hypothesis - Meaning and importance, types of hypotheses; Representation of Data - Diagrammatic and graphical representation - significance of diagrams and graphs
Unit3	Introduction - Types of scientific writings - Thesis or dissertation writing – Research paper writing; Types of publications - Open access and subscription based resources; Scientific paper writing - Choosing a journal- Instructions to authors - Structure and Style- Authorships –figures tables with legends - References and citations - Acknowledgements- Conflict of interest; Peer review mechanism and publication process; Scientometric Analyses of a paper/journal; Ethics in publishing and Plagiarism issues. Use of software for Reference Management – (Mendeley/endnote) and detection of Plagiarism (turnitin).
Unit4	Knowledge Management Skills: Advanced internet search skills – specialized academic search; Google scholar and scopus; Bibliometrics and webometrics – Concept of impact factor, i-10 index, H-index; Current awareness: RSS feeds, TOC alerts, DB alerts
Suggested Readings:	<ol style="list-style-type: none"> 1. R. A. Day; Scientific English: A Guide for Scientists and other Professionals. Greenwood Press; 3rd Revised edition, 2011. 2. Y.N. Bui; How to Write a Master's Thesis Paperback; 2nd edition, 2013. 3. Kothari, Chakravanti Rajagopalachari. Research methodology: Methods and techniques. New Age International, 2004. 4. Kumar, Ranjit. Research methodology: A step-by-step guide for beginners. Sage Publications Limited, 2019. 5. Leedy, P.D. and Ormrod, J.E., 2004 Practical Research: Planning and Design, Prentice Hall.

Theory (Cr. 2)	Bioethics, Biosafety, and IPR
<i>Unit 1</i>	Good laboratory practice, Good manufacturing practice and National and International regulations - Regulations for recombinant DNA research and manufacturing process - Bio-safety and Bioethics - Regulations for clinical trials, Documentation and Compliance, in India and selected countries - Rules for import and export of biological materials.
<i>Unit 2</i>	The importance and needs of bioethics; Bioethical business practices; Laws and bioethics; Environmental protection; Creating awareness and safeguarding health of consumers; Fair trade practices; Combating plagiarism; Various ethical issues related to genetic studies, human genome project-stem cell applications and ethical issues in stem cell research- cloning- instrumentality
<i>Unit3</i>	Concept of property, rights/protection, duties, and their correlation; History and evaluation of intellectual property rights (IPR); Distinction among various forms of IPR, WTO - Definition — Functions- International treaties for IPR Protection.
<i>Unit4</i>	Introduction to patents; Key concepts; International Law of Patents; Indian Patent Act and practice; Patentability; Types of patents; Procedure of obtaining patents- Rights of patents- Infringement of patent rights. Other forms of IPR protection: Copyright - Trademark - Designs - Importance in Indian Scenario & laws in India for IPR protection.
Suggested Readings:	<ol style="list-style-type: none"> 1. Web resources, Review papers 2. J. Pila; The Subject Matter of Intellectual Property; Oxford University Press, 2017. 3. N. S. Sreenivasulu; Intellectual Property Law Dynamic Interfaces; Aggarwal Law House, 2017. 4. K. C. Kankanala; Fundamentals of Intellectual Property (FUN IP); Published by Dr. Kalyan C. Kankanala, 2013. 5. K. C. Kankanala; Indian Patent Law and Practice (Oxford India Paperbacks); Oxford India Paperbacks, 2012. 6. All (updated) statutes: Trade Marks Act 1999; Indian Copyright Act 1957; Design Act of 2000; Patents Act 1970
Practical (Cr. 2)	Research Methodology & Scientific Writing
	<ol style="list-style-type: none"> 1. Students are expected to write the research design on Exploratory and Descriptive Research 2. Report presentation methods, ex: Power Point Presentation, etc 3. Utilization of statistical data analysis softwares, MS-EXCEL, SPSS 4. Data representation using charts, graphs etc 5. Plagiarism checking using turnitin, viper etc 6. Utilization of reference management tools like Mendeley and Endnote in scientific writing

Suggested Readings:	<ol style="list-style-type: none"> 1. R. A. Day; Scientific English: A Guide for Scientists and other Professionals. Greenwood Press; 3rd Revised edition, 2011. 2. Y.N. Bui; How to Write a Master's Thesis Paperback; 2nd edition, 2013. 3. Kothari, Chakravanti Rajagopalachari. Research methodology: Methods and techniques. New Age International, 2004. 4. Kumar, Ranjit. Research methodology: A step-by-step guide for beginners. Sage Publications Limited, 2019. 5. Leedy, P.D. and Ormrod, J.E., 2004 Practical Research: Planning and Design, Prentice Hall.
Practical (Cr. 2)	Bioethics, Biosafety, and IPR
	<ol style="list-style-type: none"> 1. Explore U.S. Patent Database 2. Explore Indian Patent Advanced Search System 3. Explore EUIPO's Database Search 4. Explore WIPO-PATENTSCOPE 5. Patent search from China National Intellectual Property Administration 6. Explore various organizations and Databases 7. Explore different ethical committees information resources and Databases
Suggested Readings:	<ol style="list-style-type: none"> 1. Web resources, Research and Review articles. Help files, software tutorials.
Department Skill Enhancement (DSE) (Any One to be chosen)	
Dissertation Thesis (Cr. 2)	Each student will be required to undertake dissertation/review work assigned to him related to R&D in any area of Bioinformatics under the supervision of a faculty member. In principle, the research work is to be carried out by the student himself/herself taking advice from his/her supervisor when problem arises. The work will be allotted at the beginning of the fourth semester specifying the different aspects to be carried out by the student. At the end of the semester the student will submit a report on his work in typed and bound form. Evaluation shall include oral presentation and a viva-voce. Defense of the viva on the project should be done in presence of an external examiner along with the faculties
Internship (Cr. 2)	In-plant training in an industry which utilizes bioinformatics for R&D or an advanced centre of learning is to be undertaken by each student. A report on the training is required to be submitted
Generic Elective (GE) (Any one to be chosen)	
Theory (Cr. 2)	Comparative and Functional Genomics
Course Objectives:	This course will provide an overview of the concept of comparative and functional Genomics and contemporary approaches used to understand the genome functionalities.

Course Outcomes:	<p>After completion of the course the learners will be able to:</p> <ul style="list-style-type: none"> ● To familiarize students with the tools and databases available for genomic analysis, with an appreciation of the quantitative concepts that form the basis of those tools ● understand and perform genome-level comparative studies of molecular sequences isolated from multiple individuals within and across species ● Understand the basics of pharmacogenomics and its application in personalized medicine
Unit 1	Databases for genomics resources; Comparative genomics – Basic concepts and applications, whole genome alignments: understanding the significance; Artemis, BLAST2, MegaBlast algorithms, PipMaker, AVID, Vista, MUMmer, applications of suffix tree in comparative genomics, synteny and gene order comparisons; Representational display analysis of genome comparisons; Comparative genomics databases: COG, VOG
Unit 2	Whole genome annotation, resources for annotation; Analyzing Genomes with Reversals of Oriented Conserved Segments, Applications to Complex Genomes; Gene prediction methods and tools, Regulatory motifs in DNA sequences, Profiles, The motif finding problem, Search Trees, Finding Motifs and Median strings; Transposable elements and their organization within chromosomes, Virulence factors / Pathogenicity islands
Unit3	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 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 viz. Neural network, SVM etc
Unit4	Historical aspects of Pharmacogenetics- Pharmacogenomics- Biomarkers- and the promise of personalized medicine, Pharmacogenetics at population level, Pharmacogenomics vs. Structural Pharmacogenomics, Identification of Pharmacogenomics Biomarker Classifiers in Cancer, Toxicogenomics Application to Oncology Drug Development, Strategies to Identify Pharmacogenomic Biomarkers: Candidate Gene, Pathway-Based, and Genome-Wide Approaches
Suggested Readings:	<ol style="list-style-type: none"> 1. Richard, J.R. (2003). Analysis of Genes and Genomes. Wiley Publication 2. Deonier, R. C., Tavaré, S., & Waterman, M. (2005). Computational genome analysis: an introduction. Springer 3. Pevsner, J. (2009). Bioinformatics and functional genomics. John Wiley & Sons 4. Altman, R. B., Flockhart, D., & Goldstein, D. B. (Eds.). (2012). Principles of pharmacogenetics and pharmacogenomics. Cambridge University Press. 5. Lam, Y. W. F., & Scott, S. R. (Eds.). (2013). Pharmacogenomics: Challenges and Opportunities in Therapeutic Implementation. Academic Press
Theory (Cr. 2)	Computational System Biology

Unit 1	Introduction to biological networks, Graph theoretic modelling and analysis of biological networks; Discrete Dynamic modelling (Boolean networks, Petri nets); Continuous dynamic modelling (ODEs, stochastic simulation, etc.)
Unit 2	Mathematics of networks: Networks and their representation, adjacency matrix, weighted networks, bipartite networks; Measures and metrics: Clustering coefficient, centrality measures (degree, eigenvector); Random graphs, metabolic networks and flux balance analysis.
Unit3	Generation of regulatory networks using WGCNA; Generation of protein interaction networks via the String database; Comparisons and interpretations of protein networks; Pathways and regulatory networks in the context gene/protein functions; Transcriptional regulation significance of non-coding RNAs; Visualization of gene-gene interactions via Cytoscape.
Unit4	Probabilistic modelling (Probabilistic Boolean networks, Bayesian networks, Mutual Information); Network inference from experimental data, Genome-scale modelling and network integration; Evolution of molecular networks, Network-guided GWAS studies, FBA and epistasis detection, protein function prediction.
Suggested Readings:	<ol style="list-style-type: none"> 1. Junker, B. H. 2008. Analysis of Biological Networks. 2. Koch, I. Reisis, W. Schreiber F. 2010. Modeling in Systems Biology: The Petri Net Approach. 3. Ramadan, E.Y. 2008. Biological Networks: Modeling and Structural Analysis. 4. Lautenbacher, R. 2007. Modeling and Simulation of Biological Networks. 5. System Biology: Computational Systems Biology (Hardcover) by Andres Kriete (Editor), Roland Eils (Editor).
Practical (Cr. 2)	Comparative and Functional Genomics
	<ol style="list-style-type: none"> 1. Exploring comparative genome databases like- Ensembl, CoGe, EDGAR etc 2. Genome browsers and Visualization tools like- Vista, IGV, ACT etc 3. Dot plot, Gene order and Synteny analysis 4. Utilization of tools for pan genome and core genome analysis 5. Prokaryotic and eukaryotic gene prediction tools 6. Searching of adjacent and patterned repeats of nucleotide sequences using Tandem Repeat Finder or Repeat Masker 7. OrthoMCL for ortholog prediction <p>Gene interaction network visualization</p>

Suggested Readings:	<ol style="list-style-type: none"> 1. Richard, J.R. (2003). Analysis of Genes and Genomes. Wiley Publication 2. Deonier, R. C., Tavaré, S., & Waterman, M. (2005). Computational genome analysis: an introduction. Springer 3. Pevsner, J. (2009). Bioinformatics and functional genomics. John Wiley & Sons 4. Altman, R. B., Flockhart, D., & Goldstein, D. B. (Eds.). (2012). Principles of pharmacogenetics and pharmacogenomics. Cambridge University Press 5. Lam, Y. W. F., & Scott, S. R. (Eds.). (2013). Pharmacogenomics: Challenges and Opportunities in Therapeutic Implementation. Academic Press
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Practical (Cr. 2)	Computational System Biology
	<ol style="list-style-type: none"> 1. Visualization and topological analysis of biological networks (graph) using Cytoscape/other tools. 2. Implementation of modeling methods for metabolic network 3. Flux Balance Analysis using computational tools 4. Designing customized synthetic genes using computational genes 5. Working with CellDesigner or other biological network editing tools. <p>GO enrichment and DAVID analysis</p>
SEC II (Cr. 2)	The course will be offered jointly along with students of other departments.