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 2023-24 onwards

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
			BINFCCT0101N	Т	Cell Biology, Genetics, and Molecular Biology		40		10	50	2
			BINFCCT0102N	Т	Basic Bioinformatics		40		10	50	2
			BINFCCT0103N	Т	Basic computer applications	-	40	-	10	50	2
1			BINFCCP0104N	Р	Cell Biology, Genetics, and Molecular Biology	CORE		50		50	2
1			BINFCCP0105N	Р	Basic Bioinformatics	-		50	-	50	2
		M.Sc. in	BINFCCP0106N	Р	Basic computer applications	-		50	-	50	2
	332	Bioinformatics	BINFDET0101A	Т	Biochemistry and Biophysics		25			25	
			BINFDET0101B	Т	Basic mathematics and statistics for Biology	DSE* (Anyone	23			25	1
			BINFDEP0101A	Р	Biochemistry and Biophysics	has to be Chosen)		25		25	
			BINFDEP0101B	Р	Basic mathematics and statistics for Biology	Chosen)		25		25	1
			AEC-I	Т	AEC I					50	
			(Choose any One from BASKET -1)			AEC					2
				•		•	•		Total	400	16

Semester II

Sem	Crs	Course	New Course-Code	Pape	Course name	Course	Full Marks	Full marks	Full marks	Total	Credit
			(ALPHA-	r		type	(External)	(Practical)	(Internal)	FM	
			NUMERIC)	type							
			BINFCCT0201N	Т	Genomics and Proteomics		40		10	50	2
			BINFCCT0202N	Т	Advanced statistical techniques for Bioinformatics		40		10	50	2
			BINFCCT0203N	Т	Computer programming for Bioinformatics	GODE	40		10	50	2
			BINFCCP0204N	Р	Genomics and Proteomics	CORE		50		50	2
			BINFCCP0205N	Р	Advanced statistical techniques for Bioinformatics			50		50	2
	332	M.Sc. in Bioinformatics	BINFCCP0206N	Р	Computer programming for Bioinformatics			50		50	2
2			BINFDEP0201A	Р	NCC/NSS/MOOC	DSE					
			BINFDEP0201B	Р	Review Paper Writing/Industrial and Institutional visit and Report submission	(Anyon e has to be chosen)		50		50	2
			SEC (Choose any One from BASKET -2)	Т	SEC I	SEC				50	2
	• • •			•	•	•	•	•	Total	400	16

Semester III

Sem	Crs	Cour se	New Course-Code (ALPHA- NUMERIC)	Paper type	Course name	Course type	Full Marks (External)	Full marks (Practical)	Full marks (Internal)	Total FM	Credit
			BINFCCT0301N	Т	Structural Bioinformatics		40		10	50	2
			BINFCCP0302N	Р	Structural Bioinformatics	CORE	40		10	50	2
			BINFDET0301A	Т	Web-based Programming & Database management systems					75	
			BINFDET0301B	Т	Phylogeny and Phylogenomic	_	25 25 25				
			BINFDET0301C	Т	NGS and expression data analysis	_	25+25+25				1.1.1
			BINFDET0301D	Т	Advance computer programming for Bioinformatics						1+1+1
			BINFDET0301E	Т	Data Mining and Machine learning techniques for Bioinformatics						
		MG	BINFDET0301F	Т	Advanced omics technologies	DSE (Any					
		M.S c. in	BINFDEP0301A	Р	Web-based Programming & Database management systems	Three to be chosen)			-	75	
	332	Bioi nfor	BINFDEP0301B	Р	Phylogeny and Phylogenomic	_					
		mati cs	BINFDEP0301C	Р	NGS and expression data analysis			25+25+25			1+1+1
			BINFDEP0301D	Р	Advance computer programming for Bioinformatics						1+1+1
3			BINFDEP0301E	Р	Data Mining and Machine learning techniques for Bioinformatics	_					
U			BINFDEP0301F	Р	Advanced omics technologies						
			BINFGET0301A	Т	Biological data analysis					50	_
			BINFGET0301B	Т	Cheminformatics	GE*	40		10		2
			BINFGEP0301A	Р	Biological data analysis	(Anyone to be chosen)		50		50	
			BINFGEP0301B	Р	Cheminformatics	1 1					2
				Т	AEC II	AEC				50	2
	1	1	1	1	1			1	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	Paper type	Course name	Course type	Full Marks	Full marks	Full marks	Total	Credit
			(ALPHA-NUMERIC)				(External)	(Practical)	(Internal)	FM	
			BINFCCT0401N	Т	Research Methodology & Scientific Writing		40		10	50	2
			BINFCCT0402N	Т	Bioethics, Biosafety, and IPR		40		10	50	2
			BINFCCP0403N	Р	Research Methodology & Scientific Writing	CORE				50	2
			BINFCCP0404N	Р	Bioethics, Biosafety, and IPR					50	2
			BINFDEP0401A		Dissertation/Project work and viva					50	
	332	M.Sc. in Bioinformatics	BINFDEP0401B		Internship	DSE (Anyone)				50	2
4			BINFGET0401A	Т	Comparative and Functional Genomics		10		10	-	
			BINFGET0401B	Т	Computational Systems Biology		40		10	50	2
			BINFGEP0401A	Р	Comparative and Functional Genomics	GE (Anyone)		50		50	-
			BINFGEP0401B	Р	Computational Systems Biology	•		50		50	2
				Т	SEC II	SEC				50	2
			1	1		1		I	То	tal 4	00 16

Detailed Syllabus of M.Sc. in Bioinformatics

Semester-I

Core Course	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: 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	 Concepts of Genetics- Klug W.S., Cummings M.R., Spencer C.A. and Palladino M.A. (Pearson Int. Edition). Benjamin Lewin; Genes IX; Jones and Bartlett Publishers James D Watson, Tania A Baker, Stephen P Bell; Molecular Biology of the Gene; Pearson Education Limited 2017 Gerald Karp; Cell and Molecular Biology; John Wiley 2013; 5thEdition; 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	 Web resources, Review papers Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi, 2003. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001. G. Gibson &S.V.Muse, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005. A. M.Campbell& L. J. Heyer, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003. 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: 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	 Buyens, Jim. 2002. Microsoft FrontPage -Inside Out. Microsoft Press. Cox, V., Wermers L. and Reding E. E. 2006. HTML Illustrated Complete. Course Technology. Niederst, J. 2001. Web Design in a Nutshell. O'Reilly Media, Inc. Tanenbaum, A.S. 2003. Computer Networks. Prentice Hall of India, New Delhi. Bach, M.J. 2008. Design of the UNIX Operating System. Pearson Education. Deitel, H.M. 1990. An Introduction to Operating System. Addison Wesley. Dhamdhere, D.M. 2007. Operating Systems: A Concept Based Approach. Tata McGraw Hill, New Delhi. Hearn, D. and Baker, M.P. 2004. Computer Graphics. Prentice and Hall of India, New Delhi. Marshal, G. 1983. Programming with Graphics. Granada Publishing, London

Practical (Cr. 2)	Cell Biology, Genetics, and Molecular Biology
Suggested	 Preparation of sample and identification of various stages of mitosis and meiosis Linear differentiation of chromosomes through G-banding, C-banding and Q-banding Microscopic studies of microbial morphology (shape, size, arrangement etc.) and Microbial staining techniques (Simple staining; Gram staining; Flagella staining; Cell wall staining; Negative staining Probability and chi-square test for genetic analyses for goodness of fit Human genetics- study of simple human traits Isolation of genomic and plasmid DNA and analysis by agarose gel electrophoresis PCR primer designing; Plasmid vector designing PCR and RAPD analysis.
Suggested readings	 Concepts of Genetics- Klug W.S., Cummings M.R., Spencer C.A. and Palladino M.A. (Pearson Int. Edition). Benjamin Lewin; Genes IX; Jones and Bartlett Publishers James D Watson, Tania A Baker, Stephen P Bell; Molecular Biology of the Gene; Pearson Education Limited 2017 Gerald Karp; Cell and Molecular Biology; John Wiley 2013; 5thEdition; H. Lodish, A. Berk, S. L. Zipursky, P. Matsudaira, D. Baltimore and J. Darnell; Molecular Cell Biology; W. H. Freeman & Comp., 2007; 6th edition Sambrook JF, Russell DW; Molecular Cloning: A Laboratory Manual (3rd Edition). Cold Spring Harbor Laboratory Press
Practical (Cr. 2)	Basic Bioinformatics
	 Retrieve information from Nucleotide databases (GenBank, ENA, DDBJ) Retrieve information from Protein Primary sequence: UNIPROT Retrieve information from RCSB Explore Secondary databases (InterPro, PROSITE, PRINTS, Pfam, CATH and SCOP) Download protein 3D structure from PDB Molecular Visualization Tool: RasMol, SPDBV, PYMOL, LigPlot Search tool: Entrez, EB-eye Sequence Similarity search: BLAST (Online and Standalone) Pairwise Sequence Alignment: Local and Global Multiple Sequence Alignment: Clustal Omega Phylogenetic analysis using MEGA

Suggested	1. Web resources, Research and Review articles. Help files, software tutorials.
readings	 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.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.
	 A. M.Campbell& L. J. Heyer, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003.
	 S.R. Pennington & M.J. Dunn, Proteomics – from protein sequence to function, BIOS Scientific Publishers, 2002
Practical (Cr. 2)	Basic Computer Application
	1. Problems using system calls for process management, signalling, 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	1. Buyens, Jim. 2002. Microsoft FrontPage -Inside Out. Microsoft Press.
readings	2. Cox, V., Wermers L. and Reding E. E. 2006. HTML Illustrated Complete. Course
	Technology.
	 Niederst, J. 2001. Web Design in a Nutshell. O'Reilly Media, Inc.
	 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. Dhamdhere, 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	This is meant to introduce biochemistry and biophysics as a course in biosciences
Objectives:	applying the theoretical language of chemistry and physics to aid functional
0	understanding of molecular and cellular processes
Course	After completion of the course the students will be able to:
Outcomes:	• 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	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.
Unit 2	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
	and Functions
Suggested	1. Davis L. Nelson, Michael M. Cox, Lehninger's Principles of Biochemistry, Seventh
readings	Edition, W. H. Freeman
U U	2. Jeremy M. Berg, John L. Tymoczko, LubertStryer, 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	The course is designed to provide the students basic understanding of systems of linear
Objectives:	equations, their associated matrices and their properties, characteristic polynomials,
	eigenvalues and eigenvectors, bilinear forms, and linear programming.
Course	The student will be able to-
Outcomes:	• analyze system of linear equations,
	• solving linear recurrences, and,
	• formulating linear programming problems and finding their feasible and optimal
	solutions. 1. Matrices and elementary row operations, Matrix multiplication, Invertible matrices,
	1. Matrices and elementary row operations, Matrix multiplication, Invertible matrices, Transpose of a matrix, Cramers rule, Determinant, Combination and Permutation,
	3-D coordinate geometry, set theory.
	 Descriptive statistics, Probability theory, probability distribution function, testing of
	hypothesis, Parametric and non- parametric methods, Correlation and regression
	method, statistical inference, methods of statistical estimations.

Suggested	1. Abertson, M.O. and Hutchinson, J.P. 1988. Discrete Mathematics with Algorithms.
readings	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.
	 Campbell, R.A. 1974. Statistics for Biologists. Cambridge University Press. W. Warren John Ewens, Gregory Robert Grant 2001. Statistical Methods in
	Bioinformatics: An Introduction. Springer
Practical (Cr. 1)	Biochemistry and Biophysics
	1. Standard buffer solution preparation and pH determination
	 Standard outlet solution preparation and predetermination Estimation of protein concentration using Lowry and Bradford methods
	 2. Estimation of protein concentration using Lowry and Bradiord 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	1. Abertson, M.O. and Hutchinson, J.P. 1988. Discrete Mathematics with Damodaran
readings	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
	1. Matrices and elementary row operations, Matrix multiplication, Invertible matrices,
	Transpose of a matrix, Cramers rule, Determinant, Combination and Permutation, 3-
	D coordinate geometry, set theory.
	2. Data analysis using descriptive statistics measures in Microsoft excel, Correlation
	studies of data, Regression analysis and calculation of regression coefficients, Fitting
	of probability distribution functions. Testing of hypothesis, parametric and non-
	parametric methods.
Theory (Cr. 2)	AEC I
	The course will be offered jointly along with students of other departments

Semester-II

Core Course	Companies and Protocomies
Theory (Cr. 2)	Genomics and Proteomics
Course	The goal is to determine how all the genes in a genome act and how their products interact
Objectives:	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	After completion of the course the learners will be able to:
Outcomes:	• 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
Onu 4	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
Care a serie 1	MS-based glycoproteomics
Suggested	1. T. A. Brown; Genomes; Bios Scientific Publishers Limited, 2002.
readings	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

Cr. 2) Advanced statistical techniques for Bioinformatics	
Analysis of One DNA Sequence, weighted matrices: independence, Markov dep	pendence
maximal dependence decomposition, analysis of patterns, occurrence of overlap	
approximation to the distribution, overlap not counted, motifs.	, councea,
Two Sequences: Frequency Comparisons. Simple Tests for Significant Simila	rity in an
Alignment, Alignment Algorithms for Two Sequences, Gapped Global Compar	
Dynamic Programming Algorithms, fitting linear gap model, local alignment w	
gap model, Analysis of Multiple DNA or Protein Sequences.	vitil illicai
Concept of sampling, sampling vs complete enumeration, planning of sampl	o survou
Sampling from a finite population, simple random sampling, Classical estimation	-
plug-in concept, Bootstrap Methods: Estimation and Confidence Intervals.	on meory,
	lized and
BLAST, BLAST random walk, parameter calculation, choice of score, norma	
bit score, Karlin–Altschul Sum Statistic, Comparison of Two Unaligned So	
MinimumSignificance Lengths, Gapped BLAST and PSI BLAST. Modelin	
Families and gene finding using HMM, Sources of Bias and Variation in gene en	xpression
data, Evolutionary models and phylogenetic tree estimation.	
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.	1
3. Casela, G. and Berger, R.L. 2001. Statistical Inference. Duxbury T	nompson
Learning.	
4. Cochran, W.G. 1977. Sampling Techniques. John Wiley.	
1. Des Raj 1976. Sampling Theory. Tata-McGraw-Hill	
Cr. 2) Computer programming for Bioinformatics	
Course 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 The student who completes the course will have the ability-	
• to develop algorithm for solving complex biological problem	
• to write problem specific script for biological data analysis	
to write programming script for algorithm development	F D
R-programming, R Data Types: Vectors, Lists, Matrices, Arrays, Factors, Data I	
- Variables: Variable assignment, Data types of Variables, Finding Variable, and	
Variables. R Operators: Arithmetic Operators, Relational Operators, Logical	·
Assignment Operators, Miscellaneous Operators. R Decision Making: if stater	
else statement, if – else if statement, switch statement. R Loops: while loop, f	for loop -
Loop control statement: break statement, next statement.	11.
R-Function : function definition, Built in functions, user-defined function,	
function, calling a function without an argument, calling a function with argume	
: R-Strings – Manipulating Text in Data; R Vectors – Sequence vector, rep	
vector access, vector names, vector math, vector recycling, vector element sortin	
- Creating a List, List Tags and Values, Add/Delete Element to or from a List	
List, Merging Lists, Converting List to Vector; R -Matrices – Accessing Elem	
Matrix, Matrix Computations: Addition, subtraction, Multiplication and Div	
Arrays; R Factors –creating factors; Data, Expand Data Frame; Loading and	nandling
Data in R.	
	o •
Perl programming; Perl Components: variables, operations, statements, f	
modules. Perl syntax and parsing rules; Variables and data: Naming rule	es, scalar
modules. Perl syntax and parsing rules; Variables and data: Naming rule variables, literals, arrays, hashes, lists, special variables. Loops: while, until, for	es, scalar r, foreach
modules. Perl syntax and parsing rules; Variables and data: Naming rule variables, literals, arrays, hashes, lists, special variables. Loops: while, until, for loops, loop control. Functions & packages: arguments, return values, context,	es, scalar r, foreach attribute,
modules. Perl syntax and parsing rules; Variables and data: Naming rule variables, literals, arrays, hashes, lists, special variables. Loops: while, until, for loops, loop control. Functions & packages: arguments, return values, context, prototypes; Working with file: Basic File Management, Reading and Writing File	es, scalar r, foreach attribute, e handles.
modules. Perl syntax and parsing rules; Variables and data: Naming rule variables, literals, arrays, hashes, lists, special variables. Loops: while, until, for loops, loop control. Functions & packages: arguments, return values, context,	es, scalar r, foreach attribute, e handles.

Unit 4	Introduction to BioPerl for biologists, Reading and writing detailed data associated with sequences, Create, manage, and query BLAST databases with NCBI blast+, Parsing reports from sequence comparison programs like BLAST, retrieve genomic sequences, Create and analyze alignments using BioPerl, Use SearchIO to create robust alignments, Using BioPerl to analyze phylogenetic trees, Query NCBI Entrez via the Eutilities, Submitting sequence data to Web forms and retrieving results, Population genetics, molecular evolution, and BioPerl.
Suggested readings	 Lang, J.D. Teetor, P. 2019. R Cookbook, Second edition. O'Reilly Media, Inc. Cotton, R. 2013. Learning R. O'Reilly Media, Inc. Grolemund, Garrett. 2014. Hands-On Programming with R. O'Reilly Media, Inc. Kabacoff, R.I. 2011. R in Action, Third Edition. Manning. Schmuller, J. 2017. Statistical Analysis with R For Dummies John Wiley & Sons, Inc. Brown, M.C. 2001. Perl The Complete Reference. The McGraw-Hill Companies. Chromatic. 2015. Modern Perl, Fourth Edition. The Pragmatic Programmers, LLC. Schwartz, R. L., Phoenix, T., & foy, b. d. (2005). Learning Perl, Fourth Edition. O'Reilly Media, Inc.
Practical (Cr. 2)	 James Tisdall. 2001. Beginning Perl for Bioinformatics. O-Reilly. Genomics and Proteomics
Suggested readings	 Explore genomic resources like Ensemble, CoGe etc. Assembling and editing of Genomic data; Genome alignment and analysis tools- BWA (BurrowsWheeler Aligner), SAMtools, GATK (The Genome Analysis Toolkit), IGV (Integrative Genomics Viewer) Assembling short reads from a organism using SPAdes Variant calling and SNP detection Map reads from CHiPseq experiment to the respective reference genome and identify peaks using MACS Explore Proteomics resources at ExPASy, EBI Explore and query the protein-Protein, protein-small molecule and biomedical interaction databases Explore post-translational modifications databases Analysis of 2D Gel Electrophoresis image Analysis of mass spectrometry data. Twyman, R. M. (2014). Principles of proteomics. Second Edition, Garland Science, Taylor & Francis Group, LLC Web resources and tutorials of respective databases and tools
Practical (Cr. 2)	Advanced statistical techniques for Bioinformatics
	1. Analysis of One DNA Sequence, weight matrix calculation,
	2. Analysis of Multiple DNA or Protein Sequences, linear gap model
	3. sample generation, SRS with/without replacement,
	4. Boot strap method for estimation
	5. Exercises on BLAST using R
	6. Phylogenetic tree estimation and evolutionary models.

Practical (Cr. 2)	Computer programming for Bioinformatics
	 Writing R script, variable declaration, functions, arithmetic and logical operations Working with arrays single and multi-dimensional; control/condition statements; iterations and looping Designing PERL program for analysis of nucleotide and protein sequences; Uses of Scalar and Array Variables to manipulate DNA/RNA/Protein sequence data 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, Uses of Regular Expressions. Uses of Bio-PERL modules for sequence manipulation, accessing local database.
NCC/NSS/MOO C	kill Enhancement (DSE) (Any One to be chosen) 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
(Cr. 2)	required credit.
Review Paper Writing/Industri al 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	This course introduces the concept of how the biomolecules act, their structural
Objectives:	properties and how their products interact. The students will learn about different
	computational resources available for structural bioinformatics
Course	A student who completes this course is expected to:
Outcomes:	 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, quarternary 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	 Web resources, Review papers F. J Burkowski; Structural Bioinformatics An Algorithmic Approach; CRC Press, 2009 P. E. Bourne and J. Gu; Structural bioinformatics; 2nd edition. John Wiley and Sons. 2009. A. Leach; Molecular modelling – principles and applications; Pearson Education Ltd, 2001 M.J.E Sternberg ; Protein Structure Prediction: A Practical Approach. Publisher: USA; Oxford University Press, 1997

Practical (Cr. 2) Structural Bioinformatics	
1. Explore Protein Secondary and 3D structure databases	
2. Evaluation and visualization of 3D structure of biomolecules using	g open source
resource	
3. Protein 3D Structure Predictions - Homology modelling, Thread	ding and Ab
<i>initio</i> methods	C
4. Refine the Predicted structure	
5. Evaluation and Validation of protein models	
6. Protein 3D Structure Comparison	
7. Protein and Ligand Visualization Software	
SuggestedWeb resources, Research and Review articles. Help files, software tutorials	8
Readings:	
Department Skill Enhancement (DSE) (Any Three to be chosen)	
Theory (Cr. 1) Web begad Dragonoming and Database management systems	
Theory (Cr. 1) Web-based Programming and Database management systems	6.1 1
Course This course is intended to provide students with an in-depth understandin	•
Objectives: page designing using CSS, HTML, PhP etc. and database development and	-
using SQL, ORACLE. The concept of establishment the connectivity of w	beb page with
database will also be introduced.	
Course After completion of the course the learners will be able to	
Outcomes: (1) Understand the procedure of creation of biological database and its ma	anagement
(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, T	
Controlling Fonts, Working with Lists and Tables, CSS ID and Class, Writir into HTML, Basic Programming using JavaScript, JavaScript Client	•
Evaluation of PHP, Basic Syntax, Defining variable and constant, Int	
WAMP/XAMPP Server – Configuration and Web Application Deployment	
Variables.	
<i>Unit 2</i> Overview of DBMS; Data associations - Entities, Attributes and Associa	-
Relationship model. Relational Database Design - Anomalies in	
Normalization Theory, and Normal forms; Query processing and optimizati backup and recovery. Distributed Databases- concepts, architecture, design	
Query Language (SQL) - Data Definition Language (DDL), Data N	
Language (DML). Transaction management: ACID properties.	I
Suggested 1. Robert W. Sebesta, Programming the World Wide Web, Addison V	Wesley
Readings: 2. Ivan Bayross, HTML 5 and CSS 3 Made Simple, BPB	
3. Bayross, Web Enabled Commercial Application Development U	sing HTML,
JavaScript, DHTML and PHP, BPB 4. Dick Oliver, Michael Morrison, Sams Teach Yourself HTML and	d CSS in 24
Hours, Pearson Education	u CSS III 24
5. Date, C. J. 2000. Introduction to Database System. Addison Wesle	y.
6. Desai, B. C. 2000. Introduction to Database Systems. Galgotia	-
New Delhi.	
	ms. Addison
7. Elmasri and Navathe. 2006. Fundamentals of Database System	
7. Elmasri and Navathe. 2006. Fundamentals of Database System Wesley.	
7. Elmasri and Navathe. 2006. Fundamentals of Database System	

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	After completion of the course the learners will be able to:
Outcomes:	 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, Phyml, RaxML
Suggested Readings	 Page, R. D., & Holmes, E. C. (1998). Molecular evolution: a phylogenetic approach. John Wiley & Sons L. Bromham ; Reading the Story in DNA: A Beginner's Guide to Molecular Evolution; Oxford University Press, 2008 G. Bernardi; Structural and Evolutionary Genomics: Natural Selection in Genome Evolution (New Comprehensive Biochemistry); Elsevier Science, 2005. M. Salemi and Anne-MiekeVandamme; The phylogenetic handbook: a practical approach to DNA and protein phylogeny; Cambridge University Press, 2003.
Theory (Cr. 1)	NGS and expression data analysis
Course	The major goal of this course provides the student with a strong foundation for
Objectives:	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:	 After completion of the course the learners will be able to: Comprehend the ideas of NGS data processing and workflow Understand metagenomics and its data workflow Understand the Differential expression analysis of gene

T T 1 . 1	
Unit 1 Unit 2	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 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	1. Ali Masoudi-Nejad, Zahra Narimani, Nazanin Hosseinkhan; "Next Generation
Readings	Sequencing and Sequence Assembly", Methodologies and Algorithms, Springer;
0	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	This lab course introduces the basic concept of of python and R programming and
Objectives:	develop programming capability to write scripts to solve bioinformatics problems
Course	After completion of the course the learners will be able to:
	After completion of the course the learners will be able to.
Outcomes:	 Understand Python programming syntax
Outcomes:	*
Outcomes: Unit 1	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages.
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. Introduction to Python Programming, Features of Python, Python interpreter interactive
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. Introduction to Python Programming, Features of Python, Python interpreter interactive and non-interactive mode. Functions: Introduction, Defining and Calling a Void
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. 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
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. 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
	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. 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. R: open-source language and environment for statistical computing and graphics
Unit 1	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. 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. R: open-source language and environment for statistical computing and graphics Bioconductor - open-source software for the analysis of biomedical and genomic data,
Unit 1	 Understand Python programming syntax Able to write python scripts for various bioinformatics applications. Implement statistical application for solving biological problems using R packages. 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. R: open-source language and environment for statistical computing and graphics

Suggested	1. Kinser J. 2008 Python for Bioinformatics, Series in Biomedical Informatics, Jones
Readings	& Bartlett.
85	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	The course gives an idea of the different algorithms to be used to train and test systems
Objectives:	along with mining relevant data from a system. This course will also introduce the basics
	of data analysis with machine learning techniques.
Course	After completion of the course the learners will be able to-
Outcomes:	• 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	• Witten, H. I., Frank, E. and Hall, M. A. 2011. Data Mining: Practical Machine
readings	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	This course will familiarize the students with advanced tools and techniques used in
Objectives:	omics studies. They will learn about different computational resources available for high
~	throughput data coming from different omics platform
Course	After completion of the course the learners will be able to:
Outcomes:	 Explain the Peptidomics, Allergens, Metabolomics, Interactomics, etc Understand the principles of integrating analysis methods for high size of an explanation of the second second
	• Understand the principles of integrative analysis methods for biological system
	 analysis and interactions Implement database search and suits for –omics
	 Implement database search and suits for –omics Analyze data coming from different omics experiments
	Anaryze data coming nom different onnes 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 Aspergillus fumigatus; Secretomics-Overview; Methodologies to decipher the cell secretome; Lipidomics-Overview; Techniques, Applications, and Outcomes Related to Biomedical Sciences; Prospects from a technological perspective
Unit 2	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

Suggested	1. Web resources, Review papers
readings	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. <u>http://doi.org/10.3390/ph6121543</u>
	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.TrendsBiotechnol.2016Dec;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. 15. List of visualization tools for network biology:
	15. List of visualization tools for network biology: http://bioinformaticsonline.com/pages/view/35386/list-of-visualization-tools-
	for-network-biology
	16. Luck K, Sheynkman GM, Zhang I, Vidal M. Proteome-Scale Human
	Interactomics. Trends Biochem Sci. 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.
	17. Ma'ayan, A. (2011). Introduction to Network Analysis in Systems Biology.
	Science Signaling, 4(190), tr5. http://doi.org/10.1126/scisignal.2001965
	18. Marth, K., Focke-Tejkl, M., Lupinek, C., Valenta, R., & Niederberger, V. (2014).
	Allergen Peptides, Recombinant Allergens and Hypoallergens for Allergen-
	Specific Immunotherapy. Current Treatment Options in Allergy, 1(1), 91–106.
	http://doi.org/10.1007/s40521-013-0006-5
	19. Mukherjee, P., & Mani, S. (2013). Methodologies to decipher the cell secretome.

	D' 1' ' D' 1 ' A (1024(11) 020(0220
	 Biochimica et Biophysica Acta, 1834(11), 2226–2232. http://doi.org/10.1016/j.bbapap.2013.01.022 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 Biotechnology of Bioactive Compounds: Sources and applications (eds V. K. Cunta and M. C. Tuchy). John Wiley & Sana Ltd. Chickaster, UK, daire
	Gupta and M. G. Tuohy), John Wiley & Sons, Ltd, Chichester, UK. doi: 10.1002/9781118733103.ch10
	21. What is metabolomics:
	https://www.ebi.ac.uk/training/online/course/introduction-metabolomics/what- metabolomics
	 22. Wu X, Hasan MA, Chen JY. Pathway and network analysis in proteomics. J Theor Biol. 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.
	23. Yang K, Han X. Lipidomics: Techniques, Applications, and Outcomes Related
	to Biomedical Sciences. Trends Biochem Sci. 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.
Practical (Cr. 1)	Web based programming and database management
	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;
	 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
	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
Suggested	5. Page, R. D., & Holmes, E. C. (1998). Molecular evolution: a phylogenetic approach.
readings	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
	Evolution (New Comprehensive Biochemistry); Elsevier Science, 2005.
	8. M. SalemiandAnne-MeikeVandamme; The phylogenetic handbook: a practical
	approach to DNA and protein phylogeny; Cambridge University Press, 2003.

Practical (Cr. 1)	NGS and expression data analysis
	 Exploring the Gene expression databases like GEO, SRA etc Microarray data analysis- understanding of microarray data, normalizing microarray data, detecting differential gene expression, microarray Data Cluster Analysis 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). Classify the phylum using a dataset of 16SrRNA sequencing of a microbiome using QIIME
Suggested readings	 Stuart M. Brown, "Next-Generation DNA Sequencing Informatics", Cold Spring Harbor Laboratory Press, 2013. 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
	 R programming for analysing gene expression data, RNA seq data. Bio-conductor and R package for analysis of biological data Declaring function in R, creating package in R. Basic syntax; variables; operators (basic python programming) Decision making; loops (selection and iterations in python programming) Numbers, lists, strings, tuples and dictionary (advanced data structures in python programming). Functions in python; modules in python (function and module orientation in python programming)
Practical (Cr. 1)	programming) Data Mining and Machine learning techniques for Bioinformatics
	 Generalized linear model prediction based on real data, error minimization of the model and cross validation using ROC curve. Regularized regression model, Ridge regression, LASSO for prediction Decision tree, random forest-based prediction Classification techniques: ANN, SVM, KNN. Case based reasoning and its applications on biological data.
	 Clustering techniques; Clustering of high dimensional data; clustering of gene expression data. Dimensional reduction techniques; Principal component analysis, feature selection technique. Re-sampling techniques; bootstrap for estimation and model validation. Text mining and Web mining. Soft Computing and Fuzzy logic system and application in bioinformatics
Practical (Cr. 1)	 Clustering techniques; Clustering of high dimensional data; clustering of gene expression data. Dimensional reduction techniques; Principal component analysis, feature selection technique. Re-sampling techniques; bootstrap for estimation and model validation. Text mining and Web mining. Soft Computing and Fuzzy logic system and application
Practical (Cr. 1)	 Clustering techniques; Clustering of high dimensional data; clustering of gene expression data. Dimensional reduction techniques; Principal component analysis, feature selection technique. Re-sampling techniques; bootstrap for estimation and model validation. Text mining and Web mining. Soft Computing and Fuzzy logic system and application in bioinformatics

Generic Elective	(GE) (Any One to be chosen)
Theory (Cr. 2)	Biological data analysis
Course	The main objective of this course is to introduce general concepts of computational
Objectives:	methods of biological data analysis to the allied department students of the university
Course	After completion of the course the learners will be able to:
Outcomes:	 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;
Unit 2	Specialized Databases;; Information retrieval from Biological databases 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	1. Neil C. Jones and Pavel A. Pevzner, "An Introduction to Bioinformatics
Readings:	Algorithms", MIT Press, 2005
	 Wing-kin Sung, "Algorithms in Bioinformatics: A Practical Introduction", CRC Press, 2011.
	 David W Mount, "Bioinformatics sequence and Genome analysis", Second Edition, Cold Spring Harbor Laboratory Press, 2013
	 P. G. Higgs and T. K Attwood, "Bioinformatics and Molecular Evolution", Blackwell Publishing, 2005
	 D. W. Mount, "Bioinformatics Sequence and Genome Analysis", Cold Spring Laboratory Press, 2001.

Theory (Cr. 2)	Cheminformatics
Course	This course will familiarize the students with tools and techniques used in
Objectives:	Cheminformatics, especially Computer-aided drug discovery. The course is designed to provide basic understanding of computational drug design and applicability of tools for neural drug discovery.
0	for novel drug discovery
Course	Students would be able to-
Outcomes:	 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 Chemoinformatics and the Diversity of Applications, Databases, Fundamental Questions of a Chemist, Drug Discovery, Additional Fields of Application; Applications of Chemoinformatics 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
Unit4	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

Suggested	1. Cereto-Massagué, A., et al (2015). Tools for in silico target fishing. Methods, 71,
Readings:	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
	4. Reves, 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.
	9. Ramesh, V. and Gillet, V.J. (2020). Applications of Chemoinformatics in Drug
	Discovery. In Biomolecular and Bioanalytical Techniques, V. Ramesh (Ed.).
	doi:10.1002/9781119483977.ch2
	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. RegulToxicolPharmacol. 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 MetabToxicol. 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: 10.2174/1568026610666100110150741. Paviaw. PubMed PMID: 20650542
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.
 Trosset JY, Cavé C. In Silico Target Druggability Assessment: From Structural to Systemic Approaches. Methods Mol Biol. 2019;1953:63-88. doi: 10.1007/978-1-
4939-9145-7_5. PubMed PMID: 30912016.
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.
30. Banegas-Luna AJ, et al. A review of ligand-based virtual screening web tools and screening algorithms in large molecular databases in the age of big data. Future
Med Chem. 2018 Nov;10(22):2641-2658. doi: 10.4155/fmc-2018-0076. Epub 2018
Nov 30. Review. PubMed PMID: 30499744.
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.
34. Kirsch P, Hartman AM, Hirsch AKH, Empting M. Concepts and Core Principles of Fragment-Based Drug Design. Molecules. 2019 Nov 26;24(23). pii: E4309. doi:
10.3390/molecules24234309. Review. PubMed PMID: 31779114

	
	 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 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 RevistaEspecializadaenCienciasQuímico-Biológicas, 21(S1), 65-87.
	 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.
	 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.
	44. Lee A, Lee K, Kim D. Using reverse docking for target identification and its applications for drug discovery. Expert Opin Drug Discov. 2016 Jul;11(7):707-15. doi: 10.1080/17460441.2016.1190706. Epub 2016 Jun 1. Review. PubMed PMID: 27186904.
	 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.
	 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
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 Unit3	 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 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
Unit4	 concepts of phylogeny; molecular evolution; Brief introduction to Phylogenetics and phylogenetic tree construction 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:	 Neil C. Jones and Pavel A. Pevzner, "An Introduction to Bioinformatics Algorithms", MIT Press, 2005 Wing-kin Sung, "Algorithms in Bioinformatics: A Practical Introduction", CRC Press, 2011. David W Mount, "Bioinformatics sequence and Genome analysis", Second Edition, Cold Spring Harbor Laboratory Press, 2013 P. G. Higgs and T. K Attwood, "Bioinformatics and Molecular Evolution", Blackwell Publishing, 2005 D. W. Mount, "Bioinformatics Sequence and Genome Analysis", Cold Spring Laboratory Press, 2001.
Practical (Cr. 2)	Cheminformatics
	 Explore the Chemical molecule databases, Drug database Utilization of Chemical Drawing tools Drug Target identification through Subtractive Genomics approach Predict Vaccine candidates through the Reverse Vaccinology approach Reverse Docking Target fishing Protein and Ligand preparation for Docking (Online) Pocket Prediction (Active site Prediction) Protein-Ligand, Protein-Protein Docking ADME/T and Drug likeliness Prediction Pharmacophore generation and analysis, mapping Tools for QSAR studies
Suggested Readings:	1. Web resources, Research and Review articles. Help files, software tutorials.
AEC II (Cr. 2)	The course will be offered jointly along with students of other departments.

Semester-IV

Core Course	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: 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:	 R. A. Day; Scientific English: A Guide for Scientists and other Professionals. Greenwood Press; 3rd Revised edition, 2011. Y.N. Bui; How to Write a Master's Thesis Paperback; 2nd edition, 2013. Kothari, Chakravanti Rajagopalachari. Research methodology: Methods and techniques. New Age International, 2004. Kumar, Ranjit. Research methodology: A step-by-step guide for beginners. Sage Publications Limited, 2019. Leedy, P.D. and Ormrod, J.E., 2004 Practical Research: Planning and Design, Prentice Hall. 	

Theory (Cr. 2)	Bioethics, Biosafety, and IPR
Unit 1	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.
Unit 2 Unit3	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
Unus	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.
Unit4	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:	 Web resources, Review papers J. Pila; The Subject Matter of Intellectual Property; Oxford University Press, 2017. N. S. Sreenivasulu; Intellectual Property Law Dynamic Interfaces; Aggarwal Law House, 2017. K. C. Kankanala; Fundamentals of Intellectual Property (FUN IP); Published by Dr. Kalyan C. Kankanala, 2013. K. C. Kankanala; Indian Patent Law and Practice (Oxford India Paperbacks); Oxford India Paperbacks, 2012. 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
	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
	 Utilization of reference management tools like Mendeley and Endnote in scientific writing

Suggested Readings:	 R. A. Day; Scientific English: A Guide for Scientists and other Professionals. Greenwood Press; 3rd Revised edition, 2011. Y.N. Bui; How to Write a Master's Thesis Paperback; 2nd edition, 2013. Kothari, Chakravanti Rajagopalachari. Research methodology: Methods and techniques. New Age International, 2004. Kumar, Ranjit. Research methodology: A step-by-step guide for beginners. Sage Publications Limited, 2019. Leedy, P.D. and Ormrod, J.E., 2004 Practical Research: Planning and Design, Prentice
	Hall.
Practical (Cr. 2)	Bioethics, Biosafety, and IPR
	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:	1. Web resources, Research and Review articles. Help files, software tutorials.
Department Skill	Enhancement (DSE) (Any One to be chosen)
Dissertation/	Each student will be required to undertake dissertation/review work assigned to him
Project work and Viva (<i>Cr. 2</i>)	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
	(GE) (Any one to be chosen)
Theory (Cr. 2)	Comparative and Functional Genomics
Course	This course will provide an overview of the concept of comparative and functional
Objectives:	Genomics and contemporary approaches used to understand the genome functionalities.

After completion of the course the learners will be able to:
 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
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
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
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
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
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
Computational System Biology
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:	 Junker, B. H. 2008. Analysis of Biological Networks. Koch, I. Reisig, W. Schreiber F. 2010. Modeling in Systems Biology: The Petri Net Approach. Ramadan, E.Y. 2008. Biological Networks: Modeling and Structural Analysis. Lautenbacher, R. 2007. Modeling and Simulation of Biological Networks. System Biology: Computational Systems Biology (Hardcover) by Andres Kriete (Editor), Roland Eils (Editor).
Practical	Comparative and Functional Genomics
<u>(Cr. 2)</u>	 Exploring comparative genome databases like- Ensembl, CoGe,EDGARetc Genome browsers and Visualization tools like- Vista, IGV, ACT etc Dot plot, Gene order and Synteny analysis Utilization of tools for pan genome and core genome analysis Prokaryotic and eukaryotic gene prediction tools Searching of adjacent and patterned repeats of nucleotide sequences using Tandem Repeat Finder or Repeat Masker OrthoMCL for ortholog prediction Gene interaction network visualization
Suggested Readings:	 Richard, J.R. (2003). Analysis of Genes and Genomes. Wiley Publication Deonier, R. C., Tavaré, S., & Waterman, M. (2005). Computational genome analysis: an introduction. Springer Pevsner, J. (2009). Bioinformatics and functional genomics. John Wiley & Sons Altman, R. B., Flockhart, D., & Goldstein, D. B. (Eds.). (2012). Principles of pharmacogenetics and pharmacogenomics. Cambridge University Press Lam, Y. W. F., & Scott, S. R. (Eds.). (2013). Pharmacogenomics: Challenges and Opportunities in Therapeutic Implementation. Academic Press

Practical (Cr. 2)	Computational System Biology
	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.
	GO enrichment and DAVID analysis
SEC II	The course will be offered jointly along with students of other departments.
(Cr. 2)	