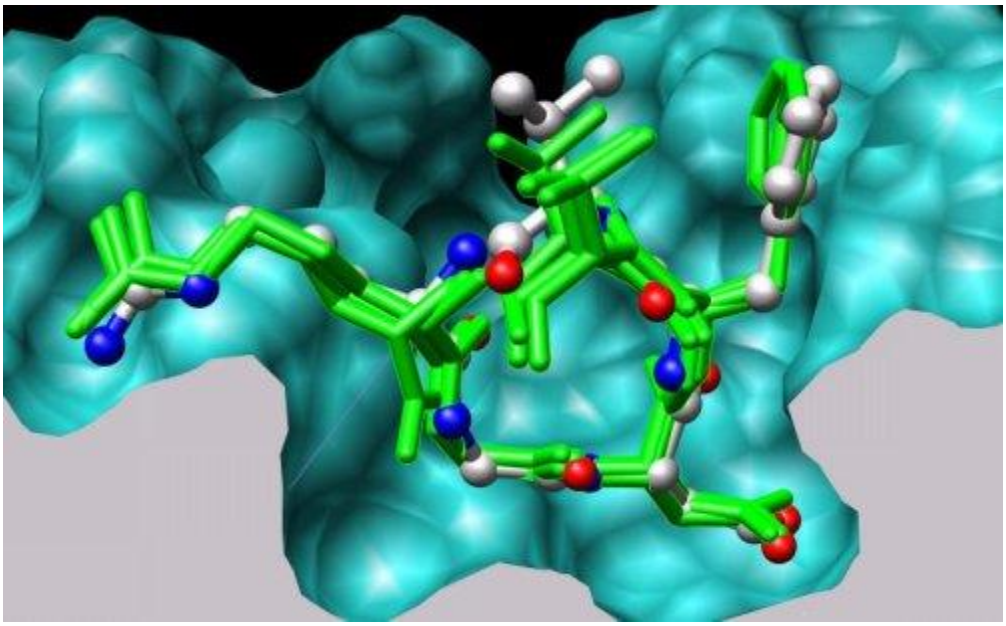
Syllabus of

MSc BIOINFORMATICS

with Specialization in Computer aided Drug Design

(Syllabus effective from 2020 Admission onwards)



UNIVERSITY OF KERALA

THIRUVANANTHAPURAM

2020

Course structure of MSc Bioinformatics with Specialization in Computer aided Drug Design Programme

MSc. Syllabus of the Programme					
Semester	**Course Code**	**Name of the course**	**Number of Credits**	**Max. Marks**	
				CA	ESA
I	BI-111	Introduction to Life Sciences & Bioinformatics	4	25	75
	BI-112	Applied Mathematics & Biostatistics	4	25	75
	BI-113	Python Programming	4	25	75
	BI-114	Biochemistry & Biophysics	4	25	75
	BI-115	Laboratory-I	4	25	75
II	BI-121	Introduction to Molecular Biology & Genetic Engineering	4	25	75
	BI-122	Computational Genomics	4	25	75
	BI-123	Micro-biology & Immunology	4	25	75
	BI-124	Pharmacology & Toxicology	4	25	75
	BI-125	Laboratory-II	4	25	75
III	BI-131	Drug Design-I	4	25	75
	BI-132	Computational Proteomics	4	25	75
	BI-133	Pharmacogenomics	4	25	75
	BI-134	NGS & Advanced topics in Bioinformatics	4	25	75
	BI-135	Laboratory-III	4	25	75
IV	BI-141	Drug Design-II	4	25	75
	BI-142	Professional Studies	4	25	75
	BI-143	Project & Viva Voce	12	-	100
		Grand Total		**1800**	

Programme Specific Outcomes (PSO) for MSc Bioinformatics with Specialization in Computer aided Drug Design

PSO 1: Life Science concepts (especially molecular biology) and skills relevant to Bioinformatics and Drug Design
PSO 2: Mathematical concepts and skills relevant to Bioinformatics and Drug Design
PSO 3: Concepts and skills in processing bio-sequence data
PSO 4: Basic wet lab skill and exposure to molecular biology experiments
PSO 5: Moderate skill in selected programming language
PSO 6: Thorough knowledge of basic concepts of Bioinformatics & Drug Design
PSO 7: Moderate skill in using basic computation tools of Bioinformatics & Drug Design
PSO 8: Basic Knowledge in the field of Machine Learning
PSO 9: Knowledge about scientific method and skill in research process
PSO 10: Knowledge and skill to process DNA/RNA sequence data
PSO 11: Knowledge and skill in computational drug design
PSO 12: Basic *in- silico* laboratory skills relevant to Bioinformatics & Drug Design
PSO 13: Enhanced skills and attitudes for becoming a better learner, thinker, professional and a human being
PSO 14: Awareness of emerging trends and concepts in Bioinformatics & Drug Design

Semester I

Course Title	Course Code
Introduction to Life Sciences & Bioinformatics	BI-111
Applied Mathematics & Biostatistics	BI-112
Python Programming	BI-113
Biochemistry & Biophysics	BI-114
Laboratory-I	BI-115

Semester I	Course Code: BI-111	Credits:4

INTRODUCTION TO LIFE SCIENCE & BIOINFORMATICS

Course Outcome

On completion of the course, students should be able to:

CO1: Articulate and exemplify basic knowledge of Life science and about macro biomolecules
CO2: Articulate basic knowledge about cells and subcellular processes
CO3: Articulate basic concepts of DNA, its functions and associated mechanisms
CO4: Articulate basics about amino acids and its classification, structure and function of proteins
CO5: Do basic bio sequence handling
CO6: Articulate basic knowledge about bio sequence databases

Semester I	Course Code: BI-111	Credits:4

INTRODUCTION TO LIFE SCIENCE & BIOINFORMATICS

COURSE CONTENT:

Module I: Characteristics of life, Levels of biological Organization- From atoms to molecules to life, general properties and biological functions of Macromolecules; carbohydrates, Lipids, Proteins and Nucleic acids, intermolecular interactions: covalent bonds, ionic bonds, Non covalent bonds: Hydrogen bonds, electrostatic interactions, Van der Waals interactions, systematics: Binomial nomenclature, Five Kingdom, Six kingdom and Three domain system of classification.

Module II: The cell as basic unit of life, cell theory, structure of Prokaryotic cell and Eukaryotic cell, structure and function of cell membrane, cell organelles- nucleus, endoplasmic reticulum, ribosomes, Golgi complex, mitochondria, peroxisomes, lysosomes, cell division- mitosis, meiosis, cell death: Brief overview about apoptosis and cell necrosis.

Module III: Primary and secondary structure of DNA, Chargaff's Rules, Different forms of DNA, RNA, structural organization of DNA: Major groove, Minor groove, Gene, chromatin threads, higher order structure of chromosomes.

Module IV: Amino acids, Functional classification of proteins, Representation of amino acids in bio sequence, Structural organization of proteins: Primary, Secondary, Tertiary and Quaternary structure of proteins; Protein folding.

Module V: Bioinformatics: History of Bioinformatics, Definition of Bioinformatics, Goals of Bioinformatics analysis, Biological data, File format, conversion of file format, Data retrieval system, Genome browsers.

Module VI: Databases: Bioinformatics databases, Types of databases -sequence databases, Primary nucleotide sequence databases-EMBL, Gene Bank, DDBJ; Secondary nucleotide databases-Ensembl, HapMap, RefSeq, Protein sequence databases-SwissProt/ TrEMBL, Protein structure databases-Protein Data Bank, SCOP and CATH.

References:

1. Devasena T. (2012), Cell Biology, Oxford University Press.
2. Karp G. (2014, 2016), Cell and Molecular Biology: Concepts and Experiments, John Wiley & Sons.
3. Hausman R.E., & Cooper G.M. (2019), The Cell: a molecular approach. ASM, Washington, DC.
4. Lewin B. (2011), Lewin's Genes X (Vol. 10, 11 &12), J. Krebs, S.T. Kilpatrick, & E. S. Goldstein (Eds.). Jones & Bartlett Learning.
5. Lodish H. (2008), Molecular cell biology, Macmillan.

On-line Resources/MOOCs:

1. Introduction to Biology - The secret of life, Massachusetts Institute of Technology (Edx)
2. Preparation for Introductory Biology: DNA to organisms, University of California (Coursera)

Semester I	Course Code: BI-112	Credits:4

APPLIED MATHEMATICS & BIOSTATISTICS

Course Outcome

On completion of the course, students should be able to:

CO 1: Demonstrate the use of Number theory in DNA Sequences
CO 2: Demonstrate the use of linear algebra in database and computation
CO 3: Demonstrate the use of python for Computational thinking
CO 4: Apply functions in the microbial growth models/ curve fitting in epidemic models
CO 5: Demonstrate the use trigonometric function
CO6: Apply differentiation and integration for biological modelling
CO7: Formulate problems in the language of sets and perform set operations
CO8: Apply probability theory in prediction problems
CO9: Demonstrate the use of statistical approaches in Bioinformatics
CO10: Demonstrate the use of graph theory as modelling tool

Semester I	Course Code: BI-112	Credits:4

APPLIED MATHEMATICS & BIOSTATISTICS

COURSE CONTENT:

Module I: Number systems, Real numbers, Rational numbers and Complex numbers (Application in Numerical encoding of DNA Sequence), Solving equations- first-order equations, Quadratic equations, Simultaneous linear equations(Application in Evolutionary Tree), Linear Algebra: Scalars &Vectors, addition, subtraction, dot, cross & scalar triple products, Matrices, inverse of a matrix, Operations, solution of simultaneous equation by using matrix.

Module II: Functions, Inverse Functions, Exponentials and logs to represent Natural growth and decay, Bacteria/population growth model, Curve Fitting(Application in Epidemic Models), Basic trigonometric functions: Sine and Cosine, Sinusoidal oscillations, Amplitude, Frequency and phase of sinusoidal oscillation, Damped oscillations, Waves, Fourier theorem (basic Introduction only) Trigonometric functions in Python.

Module III: Introduction to Calculus: Limits, Derivatives & Integrals: Limits, continuity, derivative as rate of change. Graphical treatment of derivative, maxima and minima, Automatic Differentiation. Integrals: graphical treatment, Integrating simple expressions, Definite and indefinite integrals, The area under a curve. Introduction to Differential equations, Python implementation of automatic differentiation.

Module IV: Set theory, Permutation, combination & Probability: Set theory, sets, elements, set operation, finite & countable sets, counting, factorial, permutation, combination, binomial coefficients. Basic concepts; sample space & events, laws of probability, conditional probability: Baye's theorem, Random variables: probability distribution, Binomial, Poisson, normal and 't'.

Module V: Statistics: Scope of statistical methods, Categorical & Numerical data, frequency distribution, Data distribution-Uniform, Normal ; Measures of central tendency: mean, median, mode, geometric mean, harmonic mean, percentile; Measures of dispersion: range, mean deviation, variance, standard deviation, Z-value, confidence interval, p-value; Types of sampling methods.

Module VI: Applied Statistics: Covariance, Correlation; Linear regression; Statistical testing: Population, Sample, Central limit theorem, Null/alternative hypothesis, F-test, t-test, Chi- square test; ANOVA. Graph terminology: edges, vertices, loop, path, circuit, bridge, Eulers path; Graph representation: Adjacency matrix, incident matrix. Introduction to SAS, Case study on Clinical trial analysis using python packages.

References:

1. Olive J. (2000), Maths: A Self-study Guide, Cambridge University Press.
2. Fred S. [1998], Schaum's outline Theory and Problems of Pre-calculus, Tata McGraw Hill.
3. Dawn Griffiths. (2008), Head First Statistics, O'Reilly Media Inc.
4. P. Abbot & H. Neill. (2003), Teach Yourself Trigonometry, McGraw Hill.

Online Resources:

1. https://www.edx.org/course/ap-introduction-to-statistics
2. https://www.edx.org/course/pre-university-calculus-2

Semester I	Course Code: BI-113	Credits:4

PYTHON PROGRAMMING

Course Outcome

On completion of the course, students should be able to:

CO1: Acquire moderate Python programming skills
CO2: Write Python programs including control structures and collections
CO3: Practice modular programming constructs in Python
CO4: Use Numpy, Scipy, Pandas, Matplolib for developing biological models
CO5: Develop insight from dataset using python
CO6: Better Python programming ability by practicing higher level constructs

Semester I	Course Code: BI-113	Credits:4

PYTHON PROGRAMMING

COURSE CONTENT:

Module I: Review of basic programming environment**:** Computers, memory (RAM and Secondary memory), Typical configurations, binary representation, algorithms, programming, compilers, interpreters, Concept of program reuse – object orientation: classes, hierarchy, inheritance and encapsulation. History of Python.

Module II: Introduction to Python: Special features, Versions. Programming environments: Python shell, Command line, IDLE, other interactive environments including Jupitor Notebook. Programming elements: Reserved words, Variables, Naming conventions, Data types and type conversions. Real world problems to program logic: Developing program logic. Developing programs: Basic python syntax, Comments, Input and output function, Arithmetic operators, String data processing-string values and operators.

Module III: Language components- Control structures in Python**:** Relational, Logical & Membership operators, create expressions, Indenting in python, if statement, elif statement. Loops: while loop, for loop, break and continue. Collections: List, Tuples, Sets, Dictionaries, Copying Collections, Using Control Structures on Collections.

Module IV: Function & Modules: Functions**:** Built-in functions-using string handling methods, User defined functions: Calling & defining your own functions, Passing parameters, Passing collections to function, Passing varying number of parameters, Keyword & optional parameters, Function returning values, Anonymous functions-lambda & closure, Scope of variables.

Module V: Modules & Packages- Creating module, import statements. Python Packages- NumPy, Scipy, Matplotlib. Mathematical Computing with Python (NumPy): Creating a Numpy Array, Accessing the array Index, Basic Array Operations, Indexing/Slicing, datatypes, datatype object(dtype), Biopython.

Module VI: Data analysis and Visualization with Python, Creating DataFrame in Pandas, Indexing, DataFrames(iloc) , Indexing Using Labels in Pandas(loc), DataFrame Math with Pandas(statistical functions), Plotting with Matplotlib, Plotly, Seaborn, Analyze Biological/Bioinformatics data: Reading CSV/Excel files, Sorting, Filtering, Groupby, Case study using KAGGLE COVID dataset.

References:

1.Mark S. (2018), Programming in Python 3, Pearson Education.
2.Lutz M. (2013), Learning Python, O'Reilly Media.
3.Tim J. S., Wayne B. (2015), Python Programming for Biology Bioinformatics and Beyond, CUP.
4.Downey A. (2012), Think Python: How to Think Like a Computer Scientist, O'Reilly Media.
5.Punch W. F., Enbody R. (2016), The Practice of Computing Using Python, Pearson Education.

On-line Resources/MOOCs:

1. Python3 Programming, University of Michigan. (Coursera)
2. Python Programming Essentials, RICE University. (Coursera)

Semester I	Course Code: BI-114	Credits:4

BIOCHEMISTRY & BIOPHYSICS

Course Outcome

On completion of the course, students should be able to:

CO1: Acquire basic knowledge in stabilizing interactions and thermodynamics
CO2: Understand the structure and function of Biomolecules
CO3: Understand basic carbohydrate metabolism and photosynthesis
CO4: Articulate the role of vitamins and hormones in metabolic regulation
CO5: Use basic analytical methods for the separation of Biomolecules
CO6: Use basic analytical techniques for visualization of specimen, quantification etc.

Semester I	Course Code: BI-114	Credits:4

BIOCHEMISTRY & BIOPHYSICS

COURSE CONTENT:

Module I: Basics: Structure of atoms, molecules and chemical bonds, Stabilising forces in macromolecules– Ionic, covalent, H bonding, Vander Waals interaction, polar and nonpolar interactions Laws of thermodynamics, the concept of enthalpy, entropy and free energy, thermodynamic equilibrium, redox potential, high energy molecules- ATP, ADP, GTP, PEP, NADP, NAD, FAD, Phosphocreatine, acyl phosphate and thiol esters.

Module II: Biomolecules: Biomolecules; Composition, structure and function (carbohydrates, lipids, proteins, nucleic acids), Carbohydrates (mono saccharides, disaccharides, polysaccharides, glycoproteins and peptidoglycans), Proteins (classification of amino acids with structure, Conformation of proteins and polypeptides, secondary, tertiary, quaternary , Domain and motif structure; Reverse turns), Nucleic acid : Nucleotides, Higher orders of DNA Structure: Chromatin Structure: Histones and Nucleosomes, Conformation of nucleic acids (helix (A, B, Z), t-RNA, m-RNA and r-RNA.

Module III: Carbohydrate metabolism: Glycolysis, Gluconeogenesis, TCA, HMP pathway, Mobile electron carriers. Proton transport during electron flow, Electron transport chain, oxidative phosphorylation, Biochemistry of photosynthesis (light reaction, dark reaction).

Module IV: Vitamins and hormones: Fat soluble and water soluble vitamins: structure and function, cofactors and coenzymes: structure and function Coenzymes and their functions - NAD, NADP+, FAD, FMN, lipoic acid, TPP, pyridoxal phosphate, biotin and cyanocobalamin. Hormones: Classification; site of formation, target organs; mechanism of action of peptide and steroid hormones: insulin, glucagon, epinephrine, norepinephrine, thyroid hormones, testosterone, estrogen, progesterone, pheromones.

Module V: Techniques: Principle, instrument design, working and applications of Dialysis, Ultrafiltration, Chromatography- Principle, instrument design, methods and applications of Paper, TLC, ion exchange, molecular sieve, affinity chromatography, GC, HPLC; Centrifugation and Ultra centrifugation; Principle, instrument design, methods and applications of AGE, PAGE, SDS PAGE, Capillary Electrophoresis, Isoelectric focusing, pH meter and Ion selective electrodes.

Module VI: Instrumentation: Light Microscopy: Introduction- Magnification, Resolution, and Numerical aperture. Principle, design, working, applications, advantages and disadvantages of Light, phase contrast, polarization, confocal and interference microscopes. Electron microscopy: SEM and TEM. Spectroscopy: Beer-Lamberts law-Principle; Design, working and applications of UV-Visible, IR, Raman, Fluorescence, NMR and ESR spectroscopes. Principle, instrument design, working and applications of Light scattering, Refractometry and Flowcytometry; X-ray diffraction and Electron diffraction-application in Biology; Autoradiography- GM counter and Liquid scintillation counter; Biosensors.

References:

1. Lehninger A.L., Benjamin. (2012), Bioenergetics -, 2nd Edn
2. David L. Nelson, Michael M.Cox. (2017), Lehninger, Principles of Biochemistry, Seventh Edition
3. RK Murray, DK Grammer, PA Mayes VW Rodwell. (2015), Harpers Biochemistry, MCGraw Hill USA

On-line Resources/MOOCs:

1. https://www.coursera.org/learn/energy-metabolism

Semester I	Course Code: BI-115	Credits:4

LABORATORY-I

Course Outcome

On completion of the course, students should be able to:

CO1: Hands on experience in basic laboratory protocols
CO2: Hands-on experience in cell division stages
CO3: Hands-on experience in basic qualitative and quantitative experiments of carbohydrates
CO4: Hands-on experience in biological databases
CO5: Hands on experience in writing programs in python

Semester I	Course Code: BI-115	Credits:4

LABORATORY-I

COURSE CONTENT:

Module I: Laboratory safety guidelines, equipment handling, and sterilization techniques, Preparation of buffer, acid, base and pH, Comparative study of prokaryotic and eukaryotic cells by staining and mounting.

Module II: Chromosome preparation: Mitosis onion root tip/ human lymphocytes, Meiosis-Crotalaria, Datura.

Module III: Identification of carbohydrates- glucose, fructose, sucrose, maltose, lactose, starch, Molisch's test, Fehling's, Benedict's, Estimation of Glucose – Anthrone method.

Module IV: Basic use of standard biological databases: NCBI, PDB, SWISS PROT, etc.

Module V: Writing programs using Python features : Sequence analysis – Reading DNA/Protein sequences, sequence length, GC%, handle string search; Programs using string handling function-substring search, count of nucleotides, check RNA/DNA, ORF finding, Transcription, Translation; File handling programs-ReadWrite Fasta; Program with regular expression, Define RE for a set of sequences, search for subsequences/patterns, locations; Programs for processing FASTA files; Analyze Biological/Bioinformatics data: Epidemic Modeling of COVID dataset.

References:

1. Norman S Cohn. (1969), Elements of cytology, HBJ College & School Division.
2. Harold Varley. (2005), Practical Biochemistry, CBS.
3. Rastogi, S.C., etal. (2019), Bioinformatics: Concepts, Skills and applications, CBS.
4. K.Mani & N. Vijayaraj. (2004), Bioiformatics: A Practical Approach, Aparna Publishers.
5. Mark S. (2018), Programming in Python 3, Pearson Education.
6. Lutz M. (2013), Learning Python, O'Reilly Media.

Case study:

Students must carry out an independent case study based on any of the topics in the courses covered during this semester.

Semester II

Course Title	Course Code
Introduction to Molecular Biology & Genetic Engineering	BI-121
Computational Genomics	BI-122
Micro-biology & Immunology	BI-123
Pharmacology & Toxicology	BI-124
Laboratory-II	BI-125

Semester II	Course Code: BI-121	Credits:4

INTRODUCTION TO MOLECULAR BIOLOGY & GENETIC ENGINEERING

Course Outcome

On completion of the course, students should be able to:

CO1: Demonstrate understanding of the concept and structure of genes
CO2: Demonstrate understanding the concept of DNA replication, mutation and repair
CO3: Demonstrate knowledge of Central Dogma of Molecular Biology and associated knowledge
CO4: Demonstrate understanding the concept of modification and regulation of gene expression
CO5: Demonstrate knowledge of recombinant DNA technology used for Genetic Engineering
CO6: Demonstrate application of selected latest molecular biology techniques

Semester II	Course Code: BI-121	Credits:4

INTRODUCTION TO MOLECULAR BIOLOGY & GENETIC ENGINEERING

COURSE CONTENT:

Module I. Gene structure: introns, exons, splicing; Control Elements- Promoters, Enhancers, Silencers, Insulators; Repeats- tandem, microsatellite, mini satellite, inverted repeats.

Module II. DNA Replication, Mutation & Repair**:** conservative, semi conservative and dispersive models of DNA replication, Prokaryotic and Eukaryotic DNA replication. Mutations- Gene mutations- silent, missense, nonsense and frameshift, Somatic and germline mutations, spontaneous and induced mutations. DNA repair- common types of DNA repair mechanisms- direct repair, base excision & nucleotide excision repair, mismatch repair.

Module III. Central Dogma of Molecular Biology: Transcription- Prokaryotic and Eukaryotic. Translation- Prokaryotic and Eukaryotic. Genetic code, Codon usage bias, Wobble hypothesis.

Module IV. Modification & Regulation of Gene Expression: Post transcriptional modification, post translational modification, gene expression regulation in prokaryotes - principles of gene regulation, negative and positive regulation, concept of operons, regulatory proteins, activators, repressors, regulation of lac operon, gene expression regulation in eukaryotes.

Module V. Genetic engineering: Genetic Engineering; recombinant DNA technology, Enzymes used in rDNA technology- Endonuclease, Exonuclease, restriction endonucleases, Ligase, Reverse transcriptase, DNA Polymerase; Foreign DNA, Cloning vectors- plasmids, phages, cosmids, BACs, YACs; cDNA, cDNA construction, cDNA library, Genomic library, Steps involved in rDNA technology.

Module VI. Technologies & Applications of Molecular Biology & Genetic Enginering: Technologies- overview of DNA sequencing, PCR, Gel Electrophoresis, Nucleic acid hybridization. Applications: DNA fingerprinting, RNA interference, gene editing, gene therapy.

References:

1. David R. H. (2010), Genetics and molecular biology. Special Indian edition, Tata McGraw Hill Education private limited.
2. Gerald K. (2015), Cell and molecular biology: concepts and experiments. John Wiley and Sons, Hoboken, NJ.
3. Hausman R. E., & Cooper G. M. (2018), The cell: a molecular approach. ASM, Washington, DC.
4. Jogdand S. N. (2016), Gene Biotechnology. Himalaya Publishing house.
5. Lewin B. (2017), Lewin's genes XII. J. Krebs, S. T. Kilpatrick, & E. S. Goldstein (Eds.). Jones & Bartlett Learning.

On-line Resources/MOOCs:

1. Molecular Biology - Part 1: DNA Replication and Repair (Edx)
2. Molecular Biology - Part 2: Transcription and Transposition (Edx)
3. Molecular Biology – Part 3: RNA Processing and Translation (Edx)

Semester II	Course Code: BI-122	Credits:4

COMPUTATIONAL GENOMICS

Course Outcome

On completion of the course, students should be able to:

CO1: Articulate the basic structural features of DNA, with respect to sequence data
CO2: Articulate various types of sequence alignments and their relevance
CO3: Apply DNA scoring schemes, do visual comparison of sequence similarity & articulate the same
CO4: Apply pairwise & multiple sequence alignment algorithms using selected tools and articulate it
CO5: Articulate evolution and its molecular trace, basic types of phylogenetics & terminology thereof
CO6: Apply selected phylogenetic tree construction techniques and tools and articulate it
CO7: Articulate concept of transcriptomics, various techniques & use selected RNA databases & tools

Semester II	Course Code: BI-122	Credits:4

COMPUTATIONAL GENOMICS

COURSE CONTENT:

Module I: Functional elements of DNA & its Analysis: Reading frames +1, +2, +3 and -1, -2, -3, ORFs, Codon usage bias, Basic gene statistics – base counts, word (n-mer) frequencies, ORF finder, Gene finding, Transcription factor binding site identification.

Module II: Sequence alignment: Concepts and types – pairwise, multiple, global, local, Need of Scoring schemes/ matrices, Simple DNA scoring schemes, Penalizing gaps – End/ middle gaps, opening/ extension gaps, affine gap penalty, identical vs similar matches, Simple pairwise alignment, EMBOSS Needle, Dot plots for visual interpretation for sequence patterns.

Module III: Techniques/ Algorithm for sequence alignment: Dynamic programming (overview only)– Needleman-Wunsch algorithm, Smith-Waterman algorithm, Hand computing of toy alignments, Overview of BLAST algorithm, Interpreting the results, E-value, Bit score, Multiple sequence alignment – Need for MSA, Concept of MSA, Approaches to MSA (overview only) –MSA tools – ClustalW – options of word size, matrix, gap open, extension, output format – guide tree.

Module IV: Phylogeny: Basic concepts & terminologies: Molecular Evolution-Micro & Macro, Taxonomy Vs phylogeny, Traditional Vs Molecular phylogeny-Computational phylogeny, Terminology of phylogenetic tree: Root, Branch, Node, Leaf, Clade, Outgroup, Homology, Orthology, Paralogy, Xenology, Gene phylogeny vs Species phylogeny, Different types of trees- Rooted vs. Unrooted trees, Monophyletic vs. Paraphyletic, Dichotomy vs. Polytomy, Phylogram vs. Cladogram, Model Testing, Molecular clock hypothesis.

Module V: Phylogenetic Tree Construction methods: Clustering based -UPGMA and neighbor joining; Character based -Maximum Parsimony (MP) and Maximum Likelihood (ML) methods; Bayesian inference, Evaluation of phylogenetic trees-reliability and significance; Bootstrapping; Jackknifing, Tools: MEGA, RAxML, FigTree, ETE3.

Module VI: Transcriptomics: Introduction to Transcriptome and Transcriptomics, Types and functions of coding and non-coding RNAs- mRNAs, rRNA, tRNA, lncRNAs, miRNAs, piRNAs, siRNAs, ceRNAs; Overview to Transcriptomic techniques- EST, SAGE/CAGE, Microarray, RNAseq; RNA databases- RNAcentral, miRBase, NONCODE; RNA structure prediction tools- RNAFold, RNA123; Applications of Transcriptomics.

References:

1. Mount D. W. (2004), Sequence and genome analysis. Bioinformatics: Cold Spring Harbour Laboratory Press: Cold Spring Harbour, 2.
2. Pevsner J. (2009), Bioinformatics and Functional genomics. John Wiley & Sons
3. Salemi M., Lemey P., & Vandamme A. M. (Eds.). (2009), The phylogenetic handbook: a practical approach to phylogenetic analysis and hypothesis testing. Cambridge University Press
4. Zvelebil M. J., & Baum J. O. (2008), Understanding bioinformatics. Garland Science.

On-line Resources/MOOCs:

1. Bioinformatics: introduction and methods (Coursera)
2. Computational Molecular Evolution (Coursera)

Semester II	Course Code: BI-123	Credits:4

MICRO-BIOLOGY & IMMUNOLOGY

Course Outcome

On completion of the course, students should be able to:

CO1: Articulate on the principles of Microscopy
CO2: Demonstrate the staining techniques
CO3: Articulate the cell structure of bacteria, virus and fungi
CO4: Articulate on the control of microbes
CO5: Demonstrate the cultivation of bacteria
CO6: Articulate the concept of immunology

Semester II	Course Code: BI-123	Credits:4

MICRO-BIOLOGY & IMMUNOLOGY

COURSE CONTENT:

Module I: An overview of microbial world, Basic microbiology- contribution of scientists - discovery of antibiotics,– Microscopy- Principles and applications, dark field, bright field, phase contrast microscopy, fluorescent microscopy, electron microscopy- TEM and SEM; Basic principles and working of instruments, pH meter, spectrophotometer, Beer-Lambert's law, flame photometry, colorimeter.

Module II: Stains and staining- Principles of staining, simple staining, negative staining, differential staining, Gram and acid fast staining; Control of microbes- Sterilisation, physical agents, radiation, chemical agents, disinfection, pasteurization, Principles, functioning and types of Biosafety cabinets.

Module III: Significance of microorganisms, Principles of bacterial taxonomy, Molecular taxonomy, Species concept in Microbiology, Bergey's manual of systematic bacteriology; Cell structure and sub cellular organelles of bacteria, fungi & viruses, Gut microbiota.

Module IV: Cultivation of bacteria– Types of growth media, pure culture methods-streak plate, spread plate, pour plate, stab culture, slant culture, continuous cultures. Maintenance and transport of cultures. Culture Collection Centres, Growth of bacteria- Growth phases, kinetics of growth, direct and indirect measurement of growth, factors affecting growth -pH, temperature, oxygen. Nutritional types of bacteria-Autotrophs and Chemolithotrophs.

Module V: Fundamental concepts of the immune system; Components of innate and acquired immunity; Organs and cells of the immune system- primary and secondary lymphoid organs; Lymphatic system; Immune response; Antigens - immunogens, haptens, super antigens; Humoral & cell mediated immunity immunoglobulins- basic structure, classes & subclasses, function of immunoglobulins; antigenic determinants.

Module VI: Immunoinformatics: Basic concepts of immunology, active and passive immunity, antigen and antibodies, monoclonal antibodies. B & T lymphocytes, monocytes. Immunological memory, Vaccination, auto immunity, immunodeficiency, AIDS, Cancer immunity and immunotherapy. Computational immunology: MHC peptides- structure and interactions, QSAR-based predictions of epitopes, epitope modification, epitope mapping tools, Allergenicity prediction, Vaccine design-types of vaccines; Live, killed, attenuated, subunit vaccines; systems immunology.

References:

1. Dubey R. C. and Maheswari D. K. (2012), A text of Microbiology, S. Chand and Company Ltd., New Delhi.
2. Pelczar M. J. Chan E. C. S. and Kreig N. R. (2002), Microbiology, Tata Mc Graw-Hill INC. New York.
3. Madhavee Latha. (2012), A Text book Immunology, S.Chand & Company Ltd, New Delhi.
4. Kuby (2007), Immunology, W H Freeman and company. New York.

On-line Resources/MOOCs:

1. Small and Mighty: Introduction to Microbiology (FutureLearn)
2. Vaccines: from smallpox to technologies of the future (Coursera)

Semester II	Course Code: BI-124	Credits:4

PHARMACOLOGY & TOXICOLOGY

Course Outcome

On completion of the course, students should be able to:

CO1: Understand the basics of pharmacology and pharmacokinetics
CO2: Demonstrate knowledge of pharmacodynamics
CO3: Articulate basic concepts of drug mechanism and drug resistance
CO4: Articulate the strategies of chemical modification of natural products
CO5: Articulate the concepts of toxicology and toxicokinetics

Semester II	Course Code: BI-124	Credits:4

PHARMACOLOGY & TOXICOLOGY

COURSE CONTENT:

Module I: Introduction and scope of pharmacology: Definition, scope, sources of drugs and its classification, routes of administration of drugs, targeted drug delivery, newer drug delivery systems (DDSs). Overview of adverse drug reactions & drug interactions. Pharmacokinetics: drug absorption, distribution, biotransformations, and excretion; bioavailability, factors influencing drug absorption and bioavailability.

Module II: Pharmacodynamics: site and mechanism of drug action, drug receptors and receptor regulation, concepts of agonists, antagonists, partial agonist and inverse agonist drugs.

Module III: Pharmacology of drugs and drug resistance: Pharmacological screening of herbal drugs: Introduction and evaluation of herbal drugs for antidiabetic, hepatoprotective, cardiovascular, antifertility, antioxidant, anticancer, antimalarial, anti-inflammatory, analgesic and antipyretic properties. Chemotherapy; general principles and side effects. Drugs for metabolic disorders; Mechanism of drug resistance.

Module IV: Drugs obtained by chemical modification of natural products: general features of natural products, structural features and stereochemistry. Different modification strategies; molecular size and complexity based individualized manipulation, unnecessary chiral centres removal. Successful modifications of phytochemicals from Indian medicinal plants.

Module V: Toxicology: Toxins; types, mechanism of action. General concepts of toxicity, Factors affecting toxicity; Acute, Subacute, Subchronic and Chronic toxicity; EC50, ED50, LC50, LD50, TD50; Classification of toxicants; Metals; Pesticides; Xenobiotics; Teratogens; Food additives and contaminants; Toxins of animal and plant origin; Radiation types, detection and effects. Detoxification enzymes.

Module VI: Toxicokinetics: Absorption; Digestion; Metabolism; Excretion; Mutagenicity; Carcinogenicity; Teratogenicity; Biotransformation; Bioactivation; Mechanism of Toxicity. Methods in toxicity testing; Cytotoxicity and genotoxicity.

References:

1. Klaassen, Curtis D., ed. Casarett and Doull's. (2013), Toxicology: the basic science of poisons. McGraw-Hill.
2. Katzung B.G. (2018), Basic & Clinical Pharmacology. McGraw-Hill.
3. Hartmut Derendorf and Stephan Schmidt. (2019), Rowland and Tozer's Clinical Pharmacokinetics and Pharmacodynamics: Concepts and Applications 5th Edition. LWW.
4. David E Golan, Armen H Tashjian Jr, Ehrin J Armstrong, April W Armstrong. (2011), Principles of pharmacology: the pathophysiologic basis of drug therapy. Lippincott Williams and Wilkins.
5. Shashank Kumar and Chukwuebuka Egbuna. (2019), Phytochemistry: An In-silico and In-vitro Update: Advances in Phytochemical Research. Springer.

On-line Resources/MOOCs:

1. Chemicals and Health (Coursera)
2. Toxicology 21: Scientific Applications (Coursera)

Semester II	Course Code: BI-125	Credits:4

LABORATORY-II

Course Outcome

On completion of the course, students should be able to:

CO1: Hands-on experience in basic Molecular Biology experiments
CO2: Hands-on experience in Computational Genomics software
CO3: Hands-on experience in basic Microbiology experiments
CO4: Hands-on experience in basic Immunology experiments

Semester II	Course Code: BI-125	Credits:4

LABORATORY-II
COURSE CONTENT:

Module I: Molecular Biology: Extraction and Quantification of DNA, Agarose Gel Electrophoresis, Southern Blotting, Polymerase Chain Reaction (Demonstration only, not for examination).

Module II: Genomics: ORF Finder, Gene finder, Pairwise sequence alignment, BLAST, EMBOSS, Dot plot analysis, Multiple sequence alignment, Phylogenetic analysis – MEGA.

Module III: Microbiology: Microscopic examination of bacteria by simple and differential staining, Differential staining of WBC, Blood typing. Cleaning and sterilization of glassware, Preparation of media – nutrient broth, nutrient agar, Cultivation of microorganisms on agar plate (point inoculation), broth cultivation.

Module IV: Microbiology: Isolation of microorganisms by spread plate, pour plate and streak plate methods, Isolation of air-borne microorganisms (bacteria and fungi) by Petri plate exposure method, Antibiotic sensitivity test, Microbial growth curve.

Module V: Immunology: Ouchterlony diffusion on gels for antibody titration, Antibiotic sensitivity test, Diffusion experiments for testing common epitopes on antigens, ELISA, B cell epitope prediction using DiscoTop and ElliPro.

References:

1. Chaitanya, K. V. (2013). Cell and Molecular Biology: A Lab Manual. PHI Learning Pvt. Ltd.
2. Carson S., Miller H. B., Srougi M. C., & Witherow D. S. (2019). Molecular biology techniques: a classroom laboratory manual. Academic Press.
3. Russell, D. W., & Sambrook, J. (2001). Molecular cloning: a laboratory manual. Cold Spring Harbor, NY: Cold Spring Harbor Laboratory.
4. Agostino M. (2012). Practical bioinformatics. Garland Science.
5. Krane D. E., & Raymer M. L. (2003).Fundamental concepts of bioinformatics. 2003.Pearson Education India.
6. Myers, Mika, Klein (2013). Microbiology and Immunology Laboratory Manual. Pearson Learning Solutions.

Case study:

Students must carry out an independent case study based on any of the topics in the courses covered during this semester.

Semester III

Course Title	Course Code
Drug Design-I	BI-131
Computational Proteomics	BI-132
Pharmacogenomics	BI-133
NGS & Advanced topics in Bioinformatics	BI-134
Laboratory-III	BI-135

Semester III	Course Code: BI-131	Credits:4

DRUG DESIGN-I

Course Outcome

On completion of the course, students should be able to:

CO1: Have molecular view of drug
CO2: Have molecular view of diseases, drug-target molecules
CO3: Have Knowledge about peptides
CO4: Working knowledge of ligand databases
CO5: Working knowledge of drug properties
CO6: Have knowledge about CADD

Semester III	Course Code: BI-131	Credits:4

DRUG DESIGN-I

COURSE CONTENT:

Module I: Drugs and vaccines: Drug Molecules: Molecular and chemical properties of drugs, Lipinski's rule of five, Ligands, small molecules, Leads, Phytochemicals (example: Curcumin), peptide drugs (Oxytocin), Mechanism of drug action: Agonist, antagonist, Functional groups of drugs, Vaccines, Drug Vs Vaccines.

Module II: Drug Targets : Molecular Concept of Disease, Types of diseases: Infectious disease, Deficiency disease, hereditary diseases: genetic nor non genetic, Physiological diseases, Disease Pathway (example of inflammation pathway), Drug-Targets; Types of Drug targets: Proteins/Enzymes, Receptor Proteins, Nucleic Acids & other drug targets, Overview of SARS-CoV-2 drug candidates (Remdesivir, Ritonavir), Active sites pharmacophores and allosteric sites, Drug Targets Intermolecular binding force of drugs with targets: electrostatic or ionic bonds, Hydrogen bonds, Vander Waals forces, Dipole- dipole and ion dipole interaction, Repulsive interaction and Pi-Pi interaction.

Module III: Petides and peptide analogs as drugs: Natural peptides: Food peptides, Marine peptides; Peptide drug discovery, Peptide designing, Peptidomimetics, Peptidomimetic-Based Therapy.

Module IV: Ligand Databases: Pub Chem, Drug Bank, Chem spider, Representation of Drugs: Smile notation, IUPAC name, Chemical formula, molecular descriptors, 2D representation, Formats: SDF, MOL, MOL2. Softwares: Building chemical structures with Chem sketch. Chemical descriptors, predicting biological activities of drug molecules using SAR, QSAR.

Module V: Physico chemical properties of drug molecules in relation to biological activity – Solubility, lipophilicity, partition-coefficient, Ionization, hydrogen bonding, Chelation, redox potential and surface activity. Bioisosterism and steric features of drugs, drug distribution and protein binding: Introduction to Pro and soft drug approaches.

Module VI: Computer Aided Drug Design: Traditional Drug Discovery: Blind search/Serendipitous discovery -limitations in high throughput screening; In-silico Drug discovery Pipeline: Disease Pathways in KEGG, Target identification & validation, Active site identification, pharmacophore, removal of water molecules, Lead/Ligand identification, Binding energy prediction by docking (Auto dock), Energy Minimisation, concept of Molecular Dynamics; In-Vitro & In-Vivo clinical trials Overview of in-vitro & in vivo clinical trials, and approval IP issues related to drugs IdMOC for drug testing.

References:

1. Kessel A., Ben-Tal N, (2018), Introduction to Proteins: Structure, Function, and Motion. CRC Press.
2. Lesk A. (2013), Introduction to bioinformatics. Oxford University Press.
3. K. Anand Solomon. (2019), Molecular Modelling and Drug Design. MJP Publishers.

On-line Courses/MOOCs:

1. Drug Discovery: Coursera: https://www.coursera.org/learn/drug-discovery

Semester III	Course Code: BI-132	Credits:4

COMPUTATIONAL PROTEOMICS

Course Outcome

On completion of the course, students should be able to:

CO1: Working knowledge of primary, secondary, tertiary & quaternary protein structures
CO2: Articulate enzymes, their classification and Kinetics
CO3: Have working knowledge of concepts in Mass spectrometry data
CO4: Familiarity with standard protein databases and visualization tools
CO5: Have working knowledge of concepts & techniques related to AA sequence alignment
CO6: Assess and interpret protein structure prediction models

Semester III	Course Code: BI-132	Credits:4

COMPUTATIONAL PROTEOMICS

COURSE CONTENT:

Module I: Protein Basics: Proteins as work-horse molecules, protein diversity, types of proteins and examples; Proteins as amino acid chains - basic structure of amino acids, classification of amino acids; Peptides, Polypeptides, Primary & secondary, tertiary and quaternary structures, active site, allosteric site of protein, Protein folding, Protein stability, Protein denaturation; Case study of Hemoglobin and NSP3 (SARS-CoV-2).

Module II: Enzymes: Classification - IUB system, Characteristics of enzymes, enzyme substrate complex. Concept of active centre, binding sites and ES complex formation. Effect of temperature, pH and substrate concentration on reaction rate. Activation energy. Transition state theory. Enzyme activity, international units. Enzyme Kinetics: Michaelis - Menten Equation, steady state enzyme kinetics. Vmax and Km. Enzyme inhibition - types of inhibitors - competitive, noncompetitive and uncompetitive, mode of action, experimental determination.

Module III: Quantitative Proteomics: Protein MS applications – identifying unknown proteins by peptide mass fingerprinting; de novo sequencing of peptides from fragment ion spectra obtained by tandem MS; Protein arrays: basic principles. Bioinformatics tools for proteomics (SEQUEST, MASCOT etc.).

Module IV: Databases: Sequence: UniprotKB, Structure: PDB, Structural Classification- SCOP and CATH; Visualization tools: RasMol, Swiss PDB viewer, Overview of ExPASy Proteomic Tools. Active site prediction using Casp2 Server, protein interaction database: BioGRID, IntAct, protein interaction network: STRING, EIIP. Functional annotation and Protein families (ProtoNet-tracing Protein families, ProtoNet based tools.

Module V: Basic Computational Proteomics: AA Sequence Alignment: Review of basic sequence alignment concepts, Aligning amino acid sequences, scoring matrices (PAM & BLOSUM), scoring schemes, Bit scores & e-values, Dot Plots, Algorithm for Global alignment (Needleman & Wunch) and Local alignment (Smith-Waterman): Hand computing alignment, Online tools: EMBOSS Needle & BLAST; Molecular Phylogeny using AA sequences, Case Study of Covid-19.

Module VI: Protein Structure Prediction: Secondary structural elements – Structural elements: backbone, domains, side chains, native state/conformation, Backbone flexibility- Φ and ψ, α and β propensities, Ramachandran plot, Prediction methods : Chou-Fasman Method & GOR Method; Tertiary Structure Prediction: Need for structure prediction, role of hydro-phobicity and chaperones in protein folding, Levinthal's paradox, Denovo Vs Ab-initio approaches to folding prediction, CASP for assessing structure models; Homology Modeling: Swiss Modeller for homology Modelling; Case study of Papain-like protease (NSP3) of Coronavirus.

References:

1. Kessel A., Ben-Tal N, (2018), Introduction to Proteins: Structure, Function, and Motion. CRC Press.
2. Charifson P. S. (1997), Practical application of computer-aided drug design. Marcel Dekker, Inc.
3. Leach, Andrew R. (2010), Molecular modelling: principles and applications. 2001. Harlow: Prentice Hall 24.744 2.

On-line Courses/MOOCs:

1. https://www.classcentral.com/course/swayam-introduction-to-proteomics-7910

Semester III	Course Code: BI-133	Credits:4

PHARMACOGENOMICS

Course Outcome

On completion of the course, students should be able to:

CO1: Familiarity with basic human genetics
CO2: Familiarity with pharmacogenomics
CO3: Have working knowledge pathway analysis and functional annotation
CO4: Familiarity with genetic markers
CO5: Familiarity with personalized medicine
CO6: Familiarity with allied areas

Semester III	Course Code: BI-133	Credits:4

PHARMACOGENOMICS
COURSE CONTENT:

Module I: Heredity: Human genome organization, gene orders on human chromosomes, Structure of eukaryotic genes, Mendelian inheritance and atypical inheritance patterns: Mitochondrial inheritance, Genetic variation in individuals and populations, Mutation and polymorphism. Hardy - Weinberg law, allele and genotype frequency calculation. Pedigree construction and analysis.

Module II:Introduction to Pharmacogenomics**:** Definition and scope; History, pharmacogenomics vs pharmacogenetics, The genetics of therapeutic targets and gene-based targets, drug metabolism, drug interaction, pharmacological action of drugs, pharmacokinetics and pharmacodynamics, Adverse effects of drugs, Genome projects, SNP's, alleles, Human genetic variation.

Module III: Structural and functional genomics: Genomics approaches in target identification, and validation- comparative genomics approaches, functional annotation, Gene expression data analysis, pathway analysis, Target variability, functional and structural analysis of genetic variation.

Module IV: SNP's and drug response: Genetic variation, types of polymorphism, genetic markers, Single nucleotide polymorphisms, SNP's at structural and functional level, SNP'S and metabolism, SNP and emergence of drug resistance, multidrug resistance-tuberculosis, Development of drug derivatives with improved activity.

Module V:P4 Medicine: Concept of P4; Personalized medicine, Inter- individual variability, factors affecting drug response, personal genomics, non-genetic markers, design of drugs less prone to variations, common genetic variants affecting drug response, dose-response relationship, personalized sequencing, precision therapies.

Module VI: Allied areas: Chemogenomics, Toxicogenomics, Clinomics. Mitochondrial haplogroups and disease correlation, Ethical issues in pharmacogenomics, Pharmacogenomics of the following diseases: Bipolar disease, Schizophrenia, Neurodegenerative Diseases, cancer, alchoholism.

References:

1. Joseph S. Bertino. (2009), Pharmacogenomics An Introduction and Clinical Perspective, McGraw Hill
2. Yan and Qing. (2008), Pharmacogenomics in Drug Discovery and Development
3. P.N. Bannet and M.J.Brown. (2018), Clinical Pharmacology. Elsevier, 12th Edition

On-line Courses/MOOCs:

1. https://www.coursera.org/courses?query=pharmacology
2. https://www.classcentral.com/university/penn

Semester III	Course Code: BI-134	Credits:4

NGS & ADVANCED TOPICS IN BIOINFORMATICS

Course Outcome

On completion of the course, students should be able to:

CO1: Demonstrate the understanding of NGS
CO2: Demonstrate Understanding of RNASeq Pipeline
CO3: Articulate NGS tools and techniques
CO4: Demonstrate understanding of clinical applications of NGS
CO6: Articulate systems and synthetic biology

Semester III	Course Code: BI-134	Credits:4

NGS & ADVANCED TOPICS IN BIOINFORMATICS

COURSE CONTENT:

Module I: Introduction to NGS technology (includes different types of NGS – WGS, ChiPseq, RNAseq etc.), advantages, limitations and applications. NGS Platforms, NGS Data sources: NCBI SRA, EBI-ENA, DDBJ-SRA; Format conversion, SRA toolkit.

Module II: Pre-processing – Quality, Trimming, Alignment analysis - Aligners- Principles and tools-BWA, Bowtie, Denovo assemblers - SOAP denovo, Velvet, Exome Variant calling. Introduction to BAM, SAM, Variant calling tools – GATK, SAMTools.

Module III: Concepts and Pipelines-Preprocessing, Alignment, Differential expression analysis, GO term enrichment analysis. WGS Pipelines for reference assembly and variant calling.

Module IV: Systems Biology: System Concept- Properties of Biological systems, Self-organization, emergence, chaos in dynamical systems, linear stability, bifurcation analysis, limit cycles, attractors, stochastic and deterministic processes, continuous and discrete systems, modularity and abstraction, feedback, control analysis, well steirres system, Mathematics modeling; Biological Networks- Signaling pathway, GRN, PPIN, Flux Balance Analysis.

Module V: Synthetic Biology: Systems biology v/s synthetic biology; Parts, device and systems; Biobricks, circuitry and chassis; bacterial camera, toggle switch, logic gates, oscillators; softwares for synthetic biology, case study of Tinkercell.

References:

1. Stuart M. Brown. (2015), Next-Generation DNA Sequencing Informatics, Cold Spring Harbor Laboratory Press,U.S. 2nd ed. Edition.
2. Lloyd Wai Yee Low, Martti Tapani Tammi. (2017), Bioinformatics: A Practical Handbook Of Next Generation Sequencing And Its Applications, World Scientific Publishing Co Pte Ltd.
3. Borbala Mifsud, Kathi Zarnack, Anaïs F Bardet. (2018). Practical Guide to ChIP-seq Data Analysis, CRC Press.
4. Christophe Lambert, Darrol Baker, George P. Patrinos. (2018). Human Genome Informatics: Translating Genes into Health (Translational and Applied Genomics), Academic Press.

On-line Courses/MOOCs:

1. Bodi, K.. 2011. "Tools for Next Generation Sequencing Data Analysis." Journal of Biomolecular Techniques : JBT 22: S18.
2. Comprehensive compilation of tools and forums for NGS Data analysis: https://bioinformaticssoftwareandtools.co.in/ngs.php

Semester III	Course Code: BI-135	Credits:4

LABORATORY-III

Course Outcome

On completion of the course, students should be able to:

CO1: Hands-on experience in quantification of DNA and protein
CO2: Hands-on experience in separation methods
CO3: Hands-on experience in databases and tools
CO4: Hands-on experience in protein sequence analysis
CO5: Hands-on experience in protein structure prediction tools
CO6: Hands-on experience in molecular docking and molecular dynamic simulation

Semester III	Course Code: BI-135	Credits:4

LABORATORY-III

COURSE CONTENT:

Module I: Extraction: Extraction of RNA and protein from plant/ animal tissue, Estimation of DNA by Diphenylamine method, Estimation of protein by Lowry's method.

Module II: Separation methods: Extraction and quantification of secondary metabolites from plant tissue, separation techniques: Paper, Thin layer and column chromatography, Electrophoresis, native page, SDS page.

Module III: Databases and tools: Uniprot, Sequence manipulation suite, Expasy, PDB, Chemical databases: Pubchem, Chem spider, Drug bank, Chemical format conversion: Open Babel. Drawing tools: Chemsketch, Chemdraw. ADME prediction: Swiss ADME.

Module IV: Protein sequence analysis: Perform pairwise sequence alignment of protein sequences using BLAST and EMBOSS. Draw Dot plot for visual representation of optimal alignment between two sequences Perform multiple sequence alignment of protein sequence using ClustalW.

Module V: Protein structure prediction: File format conversion: open Babel, Swiss modeling, and ITASSER. Procheck: Ramachandran plot for structure stability, Active site prediction: CASTp server. Docking software: Docking software: Autodock, Argus lab, Protein small molecule docking, protein protein docking (cluspro), molecular dynamic simulation (GROMACS).

Module VI: Accessing NGS data from SRA/ENA/DDBBJ; Quality Control analysis- FASTQC; Mapping of NGS data- Bowtie/BWA; Variant calling- GATK; Data analysis using Galaxy.

References:

1. Experiments in Microbiology, Plant pathology & Biotechnology-K.R. Aneja-New Age International Publishers-4th Edn.
2. Practical Biochemistry, Harold Varley
3. Bioinformatics: Concepts, Skills and applications-Rastogi, S.C., etal-CBS Publishers, NewDelhi
4. Bioiformatics: A Practical Approach- K.Mani& N. Vijayaraj-Aparna Publishers NewDelhi
5. Biological Sequence Analysis-Durbin et al, Cambridge University press
6. Computer aided Drug Design: Methods and Application. Thomas J Perun, Marcel Dekker
7. Practical Applications of Computer Aided Drug Design, Paul S. -Marcel Dekker
8. Lloyd Wai Yee Low, Martti Tapani Tammi. (2017), Bioinformatics: A Practical Handbook Of Next Generation Sequencing And Its Applications, World Scientific Publishing Co Pte Ltd. ISBN: 9789813144743

Case study:

Students must carry out an independent case study based on any of the topics in the courses covered during this semester.

Semester IV

Course Title	Course Code
Drug Design-II	BI-141
Professional Studies	BI-142
Project & Viva Voce	BI-143

Semester IV	Course Code: BI-141	Credits:4

DRUG DESIGN-II

Course Outcome

On completion of the course, students should be able to:

CO1: Articulate structure based drug design
CO2: Perform molecular dynamic simulation using Gromacs
CO3: Articulate structure based drug design
CO4: Demonstrate understanding the concept of QSAR
CO5: Articulate the steps in de novo drug design
CO6: Articulate the concept of IP issues in drug design process

Semester IV	Course Code: BI-141	Credits:4

DRUG DESIGN-II

COURSE CONTENT:

Module I: Molecular Modeling: History of molecular modeling, mechanical, graphical & computational models, molecular surface, molecular properties, interactions. Protein modeling and engineering, Structure validation using Ramachandran plot and its significance.

Module II: Molecular Docking: Definition, lock & key hypothesis, Mechanics of docking: search algorithm; Genetic algorithm, Monte carlo algorithm, Scoring functions: Shape and chemical complementary scores, Empirical scoring, Force field scoring, knowledge based scoring, consensus scoring, Rigid and flexible docking, Application of docking in drug discovery, Docking tools Argus lab, Gold, Autodock.

Module III: Structure Based Drug Design: Elucidation of target structure, active site characterization- cavity detection, critical residues; Combinatorial chemistry, ligand libraries-Chembank, KEGG, Ligand info, CSD, Drug bank; Structure based virtual screening; De Novo design-fragment assembly and sequential grow; Ligand based design: ligand based screening, pharmacophore; QSAR studies, Lead optimization, ADME properties and prediction.

Module IV: Energy calculations: force fields, AMBER and CHARMM; Various constraints, Force fields for protein simulations, types of force fields in NAMD and Gromacs and its importance.

Module V: Molecular dynamics: Setting and running a molecular dynamic simulation. Molecular dynamics using simple models, Implicit and explicit Solvation models, Temperature and pressure control in molecular dynamics simulations, Trajectory analysis, CHARMM, Monte Carlo Simulation.

Module VI: Allied topics: Nature and scope of traditional medicines including Ayurveda, Known compounds in Ayurvedic medicines and their activity, Medicinal plants of India, Food as medicine; IP issues in Drug Design-process & product patents, drug licensing; Central Drugs Standard Control Organization; Ethical issues in drug use abuse and trials.

References:

1. Leach, Andrew R. (2010), Molecular modelling: principles and applications, Harlow: Prentice Hall 24.744 2.
2. Flower, Darren R., ed. (2007), mmunoinformatics: Predicting immunogenicity in silico, Springer Science & Business Media.
3. Leach, Andrew R., and Valerie J. Gillet. (2007), An introduction to chemoinformatics, Springer Science & Business Media.
4. Alon, Uri. (2006), An introduction to Systems Biology: design principles of biological circuits, CRC press.
5. Zhou, Xiaobo, and Stephen TC Wong. (2008), Computational Systems Bioinformatics â Methods and Biomedical Applications, World Scientific Publishing Co Inc.

On-line Resources/MOOCs:

1. Modeling and Simulation (Coursera)
2. Drugs, drug use, drug policy and health (Coursera)

Semester IV	Course Code: BI-142	Credits:4

PROFESSIONAL STUDIES

Course Outcome

On completion of the course, students should be able to:

CO1: Enhance creative and critical thinking skills
CO2: Articulate and exemplify the scientific method
CO3: Draft & Review a simple research paper
CO4: Articulate the practices of publications
CO5: Enhance knowledge processing skills
CO6: Demonstrate general awareness of IPR
CO7: Demonstrate technical communication skills

Semester IV	Course Code: BI-142	Credits:4

PROFESSIONAL STUDIES
COURSE CONTENT:

Module I: Creativity & Thinking Skills: Various views on creativity; stimulating creativity; obstructions to creativity; creativity & innovation, creativity & craft; critical thinking; problem solving strategies, logical thinking– common logical fallacies.

Module II: Research and Research Reporting: Various outlooks on research; Types of research: pure versus applied, incremental versus innovative, qualitative versus quantitative; The scientific method, the research process –creative question – hypothesis –– Critical discussions.

Module III: Format of a science research paper – the IMRAD format – objectives of each section – reference citing styles; Proof reading & editing; Publication process -Peer review – single/double blind and open; plagiarism, Open Access Publications.

Module IV: Knowledge Management Skills: Advanced internet search skills – specialized academic search; Google scholar; Bibliometrics – impact factors –h-index, – pitfalls in interpreting impact; Current awareness: RSS feeds, TOC alerts, DB alerts.

Module V: IPR awareness: Copylefts, copyrights and patents; IPR of software and life forms; Brief overview of IPR laws in India - Protection of traditional knowledge; Patent amendment of 2005 and its impact; Economic benefits of IPR protection.

Module VI: Making effective multi-media presentations, Time Management, Task Management. Communication Skills.

References:

1. Anitha Rao and Bhaneji Rao. (2010), Intellectual Property rights: A primer, Eastern Book Company.
2. Rowena Murray. (2010), How to Write a Thesis, Tata McGraw Hill Education Pvt. Ltd.
3. Robert A. Day and Barbara Gastel. (2017), How to Write and Publish a Scientific Paper, Cambridge University Press.
4.Gregory Bassham, William Irwin, Henry Nardone and james Wallace.(2005), Critical Thinking: A Student's Introduction, Tata McGraw Hill education Pvt. Ltd.
5. Rhonda Abrams and Julie Vallone. (2006), Winning Presentation in a Day, PHI Pvt Ltd.
6. Weisberg, R. (1993), Creativity - Beyond the Myth of Genius, W.H. Freeman and Company.

Semester IV	Course Code: BI-143	Credits: 12

PROJECT & VIVA-VOCE

Course Outcome

On completion of the course, students should be able to:

CO1: Experience in solving a real-life problem using knowledge and skills acquired in the courses.
CO2: Experience in Professional Project Management and Scientific Reporting
CO3: Experience in Popular Science Communication in mother tongue

Specific Outcome of Project

MO1	A dissertation embodying a project work (30-50 pages) as per prescribed format
MO2	Experience of professional work environment in either R & D/ Industry (optional)
MO3	Evidence of compliance with project management system (lab notebooks, progress reports, plagiarism report, peer-review reports)
MO4	Evidence of attempt to publish/patent the solution developed in the project (optional)
MO5	(a) Critical analysis of project work and (b) thorough knowledge related to the area of the project (as articulated in a viva voce)
MO6	Oral presentation of the project work (using multi-media support) in a professional manner, (a) in 20 minutes and (b) in 3 minutes
MO7	Summary of the project work in research paper format (3-4 pages)
MO8	Summary of the project in popular science style, in mother tongue

Students are required to carry out an industrial visit in any of the institution before the project work. The student shall do an individual project work spanning 90 working days (including reviews, evaluation etc.), preferably in an external R & D or industry organization, the result of which shall be embodied in a dissertation of (30-50 pages) in prescribed format. The project work shall relate to state-of-the-art in Computer aided drug design or allied areas and shall preferably involve an attempt to innovate. *In silico* work is intended, but students may add *in vitro*/*in vivo* components, if they wish. The student shall demonstrate technical/scientific writing skills and critical mind in compiling the dissertation and articulating the same. The student shall demonstrate professional presentation skills in presenting the work in a viva-voce. They shall also demonstrate overall knowledge related to the area of the project during the viva-voce. They shall summarize the work in a research paper format and produce the same along with dissertation. A summary in popular science format in mother tongue shall also be submitted.

Projects should be selected at least 6 months prior to commencement. Students are expected to spend a minimum of clear 8 hours per day, ideally 10-12 hours on the project work. This is sure to reflect on the quality and quantity of work. Students are encouraged to do their project in an external organization, to expose themselves to professional R&D work culture. Students shall submit 3 Project Progress Reporting Reports along with Work Reports (around 5 pages). Students shall maintain Lab

Notebooks, with brief notes for each day. Thesis writing should be done in a distributed manner and not in haste after finishing work. Project Report shall conform to Green Charter of the University of Kerala.

EVALUATION COMPONENTS & SUB COMPONENTS (Weightage out of 100 in brackets) **(2-6 TO BE awarded BY BOTH EXAMINERS AND AVERAGE AWARDED)**
1. PROJECT MANAGEMENT (10)(To be given by internal Supervisor)
Lab Notebook is regular & detailed (2.5)
Detailed & Precise Progress Reports (2.5)
Regular Peer Review/Supervisor review & Action (5)
2. PROJECT REPORTING (10)
Scientific Reporting Standards, Formatting (5)
Citing Practice, Avoidance of Plagiarism (5)
3. TECHNICAL WORK (35)
Quantum of work (10)
Meetings Objectives (10)
Demonstration of Results (15)
4. SCHOLARSHIP (15)
Demonstration of Critical Analysis (5)
Contextualizing the work (5)
Knowledge as demonstrated in Viva (5)
5. COMMUNICATION SKILLS (10)
Presentation Skills in Viva (5)
Use of language in Dissertation (5)
6. Publishing (15)
Summary of Project in Research paper format (5)
Publication/Attempt for Publication in journals/conferences approved by the Department council (10)
7.Weightage for project done in external organization (5)

1. Entry qualifications and infrastructure requirements

The board recommended the following common entry qualification for admission to MSc Bioinformatics (Specialisation in Drug Design): *Candidates for admission to MSc Bioinformatics (Specialisation in Drug Design) (i) should have studied Biology along with Mathematics/Computer Science at the +2 or equivalent level and (ii) hold a Bachelor's degree under faculty of Science/Applied Science & Technology/Engineering & Technology/Medicine/Ayurveda/Homeopathy or a degree recognized as equivalent thereto.*

2. Infrastructure for the programme:

Colleges which run MSc Bioinformatics (Specialisation in Drug Design) must have the following library & laboratory facilities: *1. Augmented library with at least 100 books related to the syllabus, of which 50 at least must be in Bioinformatics/Drug Design/Data Science. 2. Basic Wet-lab (if the college already has life science UG/PG programmes, their labs will suffice) 3. Net-connected computing facility with minimum of 4-hours/individual student/week.*

It was also recommended that one batch should be limited to 15 students.

3. Qualifications of Teachers to teach the programme

After detailed deliberations, in view of the existence of the PhD, MPhil and MSc in Computational Biology & Bioinformatics in the University of Kerala for nearly 15 years, it was resolved to recommend that the MSc Bioinformatics (Specialisation in Drug Design) should be taught by *persons holding MSc in Computational Biology/Bioinformatics, and in their absence, by persons holding MPhil in Computer Aided Drug Design/Bioinformatics) or PhD in Computational Biology and/or Bioinformatics*

4. Equivalence of the programme or eligibility of the degree holders

The Board recommended that the MSc Bioinformatics (Specialisation in Drug Design) *shall be equivalent to both MSc (Bioinformatics) and MSc (Computational Biology). F*urther, it is recommended that candidates holding MSc Bioinformatics (Specialisation in Drug Design) shall be *eligible for admission to MPhil in Computer Aided Drug Design/Bioinformatics) and PhD in Computational Biology and/or Bioinformatics.*