SRM
UNIVERSITY
(Under section 3 of UGC Act 1956)

M. TECH. (FULL TIME) - BIOINFORMATICS
CURRICULUM & SYLLABUS
2013 – 2014

FACULTY OF ENGINEERING AND TECHNOLOGY
SRM UNIVERSITY
SRM NAGAR, KATTANKULATHUR – 603 203

M. Tech. BIOINFORMATICS (FULL TIME)
CURRICULUM

SEMESTER- I

Code	Category	Course	L	T	P	C
BI2001	C	Advanced Biochemistry and Immunology	3	0	3	4
BI2002	C	Algorithms for Bioinformatics	3	2	0	4
BI2003	C	Bioinformatics – Techniques and Applications	3	0	3	4
MA2016	S	Numerical and Biostatistical Methods	3	0	0	3
E1	E	Elective I	3	0	0	3
Total			**15**	**2**	**6**	**18**
Total Contact Hours			**23**			**18**

SEMESTER- II

Code	Category	Course	L	T	P	C
BI2004	C	Applications of Matlab in Bioinformatics	3	0	3	4
BI2005	C	Functional Genomics and Proteomics	3	0	3	4
BI2006	C	Structural Bioinformatics	3	2	0	4
E2	E	Elective II	3	0	0	3
E3	E	Elective III	3	0	0	3
Total			**15**	**2**	**6**	**18**
Total Contact Hours -23						

SEMESTER- III

Code	Category	Course	L	T	P	C
E4	E	Elective IV	3	0	0	3
E5	E	Elective V	3	0	0	3
E6	E	Elective VI	1	0	6	3
E7	E	Interdisciplinary Elective	3	0	0	3
BI2047	C	Seminar	0	0	1	1
BI2048	C	Industrial Training	0	0	1	1
BI2049	P	Project Work - Phase I	0	0	12	6
Total			**10**	**0**	**20**	**20**
Total Contact Hours - 30						

SEMESTER- IV

Code	Category	Course	L	T	P	C
BI2050	P	Project Work - Phase II	0	0	32	16
Total			**0**	**0**	**32**	**16**
Total Contact Hours - 32						
TOTAL CREDITS TO BE EARNED FOR THE AWARD OF DEGREE:						**72**

CATEGORY OF COURSES:

C: Core courses **S: Supportive courses**
E: Elective courses **P: Project Work**

CONTACT HOUR/CREDIT:

L: Lecture Hours per week **T: Tutorial Hours per week**
P: Practical Hours per week **C: Credit**

LIST OF ELECTIVES

Program Electives (Theory)

Course Code	Name of the course	L	T	P	C
BI2101	Advanced Biology	3	0	0	3
BI2102	Object-Oriented Programming and Database Management	3	0	0	3
BI2103	Metabolic Engineering	3	0	0	3
BI2104	Microarray Bioinformatics	3	0	0	3
BI2105	Computational Chemistry	3	0	0	3
BI2106	Macromolecular Biophysics	3	0	0	3
BI2107	Unix & Java	3	0	0	3
BI2108	Molecular Mechanics and Simulation	3	0	0	3
BI2109	Systems Biology - Models and Approaches	3	0	0	3
BI2110	Python for Bioinformatics	3	0	0	3

Program Electives (Practical)

Course Code	Name of the course	L	T	P	C
BI2111	Computer Aided Drug Designing	0	1	6	3
BI2112	Molecular Dynamics	0	1	6	3
BI2113	Perl for Bioinformatics	0	1	6	3

SEMESTER I

Course Code	Course Title	L	T	P	C
BI2001	ADVANCED BIOCHEMISTRY AND IMMUNOLOGY	3	0	3	4
	Total Contact Hours - 90				

PURPOSE

The course helps the students to understand the underlying principles of biochemistry and immunology which form the basis of biosciences

INSTRUCTIONAL OBJECTIVES

1.	Understanding Proteins and Carbohydrates,
2.	Understanding Lipids, Nucleic acids and Enzymes
3.	Introducing the basics of immune system
4.	Understanding antigen-antibody reaction
5.	Understanding immune response.

UNIT I -PROTEINS AND CARBOHYDRATES (9 hours)

Proteins: amino acids– physical and chemical properties of amino acids, peptides,Ramachandran plot, Amino acid biosynthesis, Metabolism – Urea cycle. Sugars and polysaccharides: Monosaccharides, polysaccharides and glycoprotein, Metabolism of carbohydrates – Glycolysis-TCA cycle – gluconeogenesis- glycogen metabolism

UNIT II -LIPIDS, NUCLEIC ACIDS AND ENZYMES (9 hours)

Lipids: Lipid classification, properties of lipid aggregates, Biological membrane, Lipid linked proteins and lipoproteins, Biosynthesis – fatty acids, triglycerides, Cholesterol. Metabolism – oxidation of fatty acid, ATP synthesis. Nucleic acids: Structure of DNA, Forms of DNA - A, B, Z Structures, classification of RNA.

UNIT III -ENZYMES (9 hours)

Enzymes: Nomenclature, classification, substrate specificity, coenzymes, regulation of enzyme activity. Rate of enzyme reaction, kinetics, inhibition, effect of pH and temperature.

UNIT IV -IMMUNE SYSTEM (9 hours)

Innate vs. Acquired, humoral and cell mediated immunity, Immunity at Body Surfaces. Cells of the immune system, Organs of the immune system – primary and secondary lymphoid organ, Antibody structure and isotypes, Antigens.

UNIT V -IMMUNE RESPONSE **(9 hours)**

Major histocompatibility complex, HLA typing, Antigen processing and presentation Pathways.Lymphokines and Cytokines: The complement system, Cell-mediated effectors responses (CTL, NK, DH). Vaccines. Autoimmunity: Breakdown in Self-Tolerance. Transplantation: tissue and organ grafting.

LIST OF EXPERIMENTS **(45 hours)**

1. pH and Buffers
2. Protein isolation & estimation
3. 2D electrophoresis
4. Carbohydrate assays
5. Lipid assays
6. Nucleotide assays
7. DNA & RNA isolation & estimation
8. Blotting Techniques
9. Enzyme kinetics
10. Immunodiffusion
11. Agglutination
12. Immunoelectrophoresis
13. Western blotting.

REFERENCES

1. VoetD. and J.G. Voet, *"Biochemistry"*, Wiley Publications, Second Edition, 2005.
2. D.L Nelson and M.M Cox, *"Lehninger's Principles of Biochemistry"*, W.H FreemanPublications, 5th edition, 2008.
3. Thomas Devlin,*"Textbook of Biochemistry with Clinical Correlations"*, 7th edition,John Wiley &Sons,2010.
4. Roitt, *"Essential Immunology"*, 10th edition. Blackwell Science, 2005.
5. Richard A. Goldsby, Thomas J. Kindt and Barbara A. Osborne, Kuby*"Immunology"*,4th edition, W. H. Freeman & Company, 2000.
6. Janeway et al., *"Immunobiology"*, 4th edition, Current Biology Publications, 1999.
7. William E. Paul, *"Fundamental Immunology"*, 4th edition, Lippencott Raven, 1999.

Course Code	Course Title	L	T	P	C
BI2002	ALGORITHMS FOR BIOINFORMATICS	3	2	0	4
	Total Contact Hours –75				

PURPOSE

The purpose of this subject is to study various Algorithm design techniques and applying it in bioinformatics

INSTRUCTIONAL OBJECTIVES

1.	Introduction to algorithms and dynamic programming
2.	Description of graph algorithms and their applications sequencing
3.	Description of pattern matching and clustering with reference to bioinformatics
4.	Description of evolutionary trees and phylogeny related algorithms
5.	Description Hidden Markov Models and randomized algorithms.

UNIT I - DYNAMIC PROGRAMMING ALGORITHMS (9 hours)

Introduction to Algorithms, Dynamic Programming, Sequence Alignment: Edit distance, LCS. PAM and BLOSUM Scoring Matrices. Global alignments: Needleman Wunsch Algorithm, Local Alignments: Smith Waterman Algorithm, Gap Penalties.

UNIT II- GRAPH ALGORITHMS (9 hours)

Graph Algorithms, SBH and Eulerian Paths, De-novo Peptide Sequencing: Longest Paths and Space Efficient Alignment Algorithms. Fast LCS using Table Lookup.

UNIT III- PATTERN MATCHING AND CLUSTERING (9 hours)

Exact Pattern Matching: KMP Algorithm, Keyword Trees, Aho-Corasick Algorithm. Clustering Basics: Hierarchical Clustering, Multiple Sequence Alignment: CLUSTAL, Center-based Clustering, Clustering via Cliques.

UNIT IV- EVOLUTIONARY TRESS AND PHYLOGENY (9 hours)

Evolutionary Trees and Ultrametrics, Additive distance trees, Perfect Phylogeny Problem, Small Parsimony Problem, Nearest Neighbor Interchange.

UNIT V- HIDDEN MARKOV MODELS, RANDOMIZED ALGORITHMS (9 hours)

Hidden Markov Models: Basics, Forward and Backward (Viterbi) Algorithms, Randomized algorithms and their applications.

TUTORIAL (30 hours)

REFERENCES

1. Neil C. Jones and Pavel A. Pevzner, *"An Introduction to Bioinformatics Algorithms"*, MIT Press, 2005.
2. Gusfields D, *"Algorithms on strings, trees and sequences: Computer Science and Computational Biology"*, Cambridge University Press, 1997.
3. Steffen Schulze-Kremer, *"Molecular Bioinformatics: Algorithms and Applications"*, Walter de Gruyter, 1996.
4. Gary Benson, Roderic Page (Eds.), *"Algorithms in Bioinformatics"*, Springer International Edition, 2004.
5. Richard Durbin, Sean R. Eddy, Anders Krogh, Graeme Mitchison. *"Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acid"*, Cambridge University Press, 1999.

Course Code	Course Title	L	T	P	C
BI2003	**BIOINFORMATICS – TECHNIQUES ANDAPPLICATIONS**	**3**	**0**	**3**	**4**
	Total Contact Hours –90				

PURPOSE	
To equip the students with the requisite background in areas of modern biology and computer science.	
INSTRUCTIONAL OBJECTIVES	
1.	To launch the students into core areas of Bioinformatics like sequence alignment,phylogenetic trees, genomics, proteomics
2.	To explore the students to applied areas of Bioinformatics like drug design, metabolicpathway engineering
3.	Practical exploration of tools in bioinformatics

UNIT I - BIOLOGICAL DATABASES (9 hours)

Biological data types, Major biological databases and its classification, sequence and structure file formats, data mining.

UNIT II - SEQUENCE ANALYSIS (9 hours)

Methods of sequence alignment. Pair wise alignment- Global, local, dot plot and its applications. Words method of alignment- FASTA and its variations, BLAST- Filtered and gapped BLAST, PSIBLAST, Multiple sequence alignment- methods and Tools for MSA, Application of multiple alignments, Viewing and editing of MSA

UNIT III - MOLECULAR PHYLOGENY (9 hours)

Concepts of trees- Distance matrix methods, Character based methods. Solving UPGMA, NJ and small parsimony problems. Methods of evaluating phylogenetic methods- boot strapping, jackknifing

UNIT IV - MACROMOLECULAR STRUCTURE ANALYSIS (9 hours)

Gene prediction, Conserved domain analysis, Protein visualization, Prediction of protein secondary structure, Tertiary structure prediction- Validation of the predicted structure using Ramachandran plot, steriochemical properties.

Unit V - COMPUTER AIDED DRUG DESIGNING (9 hours)

Protein Function Prediction,Metabolic Pathway analysis, Computer aided drug designing,Pharmacogenomics and Pharmacogenetics.

LIST OF EXPERIMENTS (45 hours)

1. Bioinformatics databases
2. Pairwise sequence alignment
3. Sequence similarity searching for sequences
4. Multiple sequence alignment and editing
5. Phylogenetic analysis using distance based methods & character based methods
6. Evaluation of trees
7. Gene prediction tools
8. Prediction Of secondary Structure of proteins
9. Sequence based prediction and Validation of 3d Protein structure
10. Docking studies

REFERENCES

1. Cynthia Gibas, Per Jambeck, *"Developing Bioinformatics Computer Skills"*, O'Reilly Media,Inc., 2001.

2. David Edwards, Jason Eric Stajich, David Hansen, *"Bioinformatics: Tools and Applications"*, Springer, 2009.
3. David W Mount, *"Bioinformatics: Sequence and genome analysis"*, Cold spring harbor laboratory press, 2nd edition, 2004.
4. Stan Tsai C., *"Biomacromolecules: Introduction to Structure, Function and Informatics"*, John Wiley & Sons, 2007.
5. Attwood T K, D J Parry-Smith, *"Introduction to Bioinformatics"*, Pearson Education, 2005.
6. ParagRastogi, *"Bioinformatics Methods And Applications: Genomics Proteomics And Drug Discovery"*, PHI Learning Pvt. Ltd., 3rdedition, 2008.

Course Code	Course Title	L	T	P	C
MA2016	**NUMERICAL AND BIOSTATISTICAL METHODS**	**3**	**0**	**0**	**3**
	Total Contact Hours – 45				

PURPOSE	
To provide an understanding of statistical methods and numerical methods.	
INSTRUCTIONAL OBJECTIVES	
1.	Know the techniques of numerical methods
2.	Learn the basics of Biostatistics
3.	Understand the concept of hypothesis

UNIT I - NUMERICAL CALCULATIONS (9 hours)

Numerical calculation: introduction and fundamental concepts, numerical methods for linear equation and matrices, Crammers rule, Gaussian elimination method , Crouts method, Similarity transformation, Eigen values and Eigen vectors of a matrix, Numerical solution of differential and integral equations.

UNIT II - BIOSTATISTICS (9 hours)

Biostatistics: Introduction to Biostatistics, Distributions – Binomial, Poisson and Normal, Handling Univariate, Bivariate and Multivariate data-Introduction to Probabilities, Interval Estimation.

UNIT III- TESTING OF HYPOTHESIS (9 hours)

Hypothesis testing: Testing hypothesis, Examining relationships using Correlation & Regression.

UNIT IV - ANALYSIS OF VARIANCE (9 hours)

Analysis of Variance, Multiple Correlation, PCA, Factor analysis, Discriminant functional analysis.

UNIT V - DESIGN EXPERIMENTS (9 hours)

Concepts & Methods of Design Experiments, Randomization & Blocking, Analysis OF variance technique, Factorial & Fractional designs, Taguchi's concepts & Methods and second- order designs.

REFERENCES

1. George W. Collins, II, "*Fundamental Numerical Methods and data analysis"*, George W. Collins, II Press, 2003.
2. Hildebrand. F.B,"*Introduction to Numerical Analysis"*, McGraw- Hill book Co, 1956.
3. Householder A.S., "*Principles of Numerical Analysis"*, McGraw Hill Book Co; 1953.
4. Hamming, R.W, "*Numerical methods for scientists and engineers"*, McGraw Hill Book Co; 1962.
5. Daniel W.W., "*Biostatistics a Foundation for Analysis in the Health Sciences"*, John Wiley & sons, 2000.
6. Warren J. Ewens, Gregory R. Grant, "*Statistical methods in Bioinformatics*: *An Introduction"*, 2nd edition,Springer 2004.

SEMESTER II

Course Code	Course Title	L	T	P	C
BI2004	**APPLICATIONS OF MATLAB IN BIOINFORMATICS**	**3**	**0**	**3**	**4**
	Total Contact Hours –90				

PURPOSE

This course enables the students to understand various applications of MATLAB in Bioinformatics, Biological image analysis and Systems Biology.

INSTRUCTIONAL OBJECTIVES

1.	Basic functionalities of Matlab
2.	Application of Matlab for solving various problems in biological sciences- sequence analysis, gene expression analysis, biomedical image analysis, metabolic pathway analysis
3.	Additional plug-in's to Matlab

UNIT I -INTRODUCTION TO MATLAB (9 hours)

Matlab key features, basic functionalities-tool box, data types,variables, operators, vectors, matrix operations, trigonometric functions, 2D,3D-graphics , Limits. Control structures, function handling, class file handling, mat file creation, symbolic mathematics. Numerical Methods- solving linear equations, solving differential equations-ODE suite, integration, interpolation, regression. Statistical analysis- probability, hypothesis testing, ANOVA and cluster analysis.

UNIT II - BIOINFORMATICS TOOL BOX (9 hours)

Sequence Analysis**,** NGS,Graph Theory, Gene Ontology, Importing Data and Deploying.

UNIT III - BIOLOGICAL DATA ANALYSIS (9 hours)

Microarray Data Analysis, Mass Spectrometry Data Analysis, statistical classification of biological data

UNIT IV- IMAGE PROCESSING (9 hours)

Key Features,Importing and Exporting Images, image file formats and format conversion, Pre- and Post-Processing Images, Spatial Transformations and Image Registration. Microarray image analysis

UNIT V- SYSTEMS BIOLOGY **(9 hours)**

Basics of enzyme kinetics, Kinetic Laws.Modeling Biological System, Simulation, sensitivity analysis, parameter estimation using simbiology.Pharmacokinetic modeling- simulation, population study.Model of the Yeast Heterotrimeric G Protein Cycle and glycolysis.

LIST OF EXPERIMENTS **(45 hours)**

1. MATLAB basic commands.
2. Sequence analysis tools including functions for pairwise, MSA and phylogenetic tree construction
3. Microarray data import from GEO and affymetrix and expression analysis and normalization
4. Microarray image analysis
5. Gene expression data analysis from gene ontology.
6. Mass spectrometry data import and base line correction and normalization
7. Model creation and simulation using simbiology
8. Node knock out of model generated in simbiology using graph theory
9. Pharmakokinetic model building and population fitting

REFERENCES

1. Alterovitz G., M. F. Ramoni, *"Systems Bioinformatics: An Engineering Case-Based Approach"*,Artech House, 2007.
2. Michael R. King, Nipa A. Mody, *"Numerical and Statistical Methods for Bioengineering: Applications in MATLAB", Cambridge University Press, 2011.*
3. Gibas C., Per Jambeck,*"Developing bioinformatics computer skills"*,O'Reilly Media, Inc., 2001.
4. Semmlow, *"Biosignal and Biomedical Image Processing"*, Marcel Dekker, Inc., 2004.
5. Hoppensteadt, Peskin, *"Modeling and Simulation in Medicine and Life Sciences"*, Springer, 2010.

Course Code	Course Title	L	T	P	C
BI2005	**FUNCTIONAL GENOMICS AND PROTEOMICS**	**3**	**0**	**3**	**4**
	Total Contact Hours - 90				
PURPOSE					
This course enables the students to understand various applications of genomics and proteomics in Bioinformatics.					

INSTRUCTIONAL OBJECTIVES	
1.	This course provides a foundation in the following four areas; whole genome analysis; genome sequencing; annotation of genome and proteome analysis

UNIT I - GENOMICS **(9 hours)**

Prokaryotes and Eukaryotes, The structure, function and evolution of the human genome.Foundations of genomics. Strategies for large-scale sequencing projects, Genome library construction: YAC, BAC and PAC libraries of genome.

UNIT II- SEQUENCING AND MAPPING **(9 hours)**

Genome sequencing, Hierarchical and shot gun sequencing methods, variation in sequencing methods, Pyroseqencing, Automation in genome sequencing, New generation sequencing methods, Mapping of genome: linkage mapping, High resolution physical mapping, Marker associated and clone assisted genome mapping

UNIT III- SEQUENCE AND GENE EXPRESSION ANALYSIS **(9 hours)**

Sequence analysis, Databanks, data mining, Annotation of genome, Bioinformatics for the analysis of sequence data, approaches for determining gene expression patterns and functions, Functional genomics, Human disease genes Expression, Gene knockouts, gene expression profiling, microarrays, cDNA and Oligo array.

UNIT IV - PROTEOMICS TOOLS **(9 hours)**

Tools for proteomics: 2D Electrophoresis, Liquid chromatography in proteomics,Protein identification – Mass spectrometry, peptide mass fingerprinting, protein sequencing, Structural proteomics- X-ray crystallography, NMR.

UNIT V - PROTEIN INTERACTIONS AND MICROARRAYS **(9 hours)**

Protein-Protein interactions, Library based methods, systematic complex analysis by Mass spectrometry, Protein interaction maps .Functional proteomics – protein chips, detection and quantification.

LIST OF EXPERIMENTS **(45 hours)**

1. Genome comparison
2. Genome rearrangements
3. Phylogenetic Reconstruction
4. Methods for detecting trans-membrane helices
5. Identification of proteins using database searches
6. Predicting Gene-Gene (Protein-Protein) interactions

REFERENCES

1. Twyman, RM and Primrose, SB, "*Principle of Genome Analysis"*, Blackwell Publisher, 2003.
2. Brown TA ,"*Genomes 2"*, Wiley-Liss,2006.
3. Veenstra TW and Tates III, JR, "*Proteomics for biological discovery"*, Wiley, 2006.
4. Durbin R, Eddy SR, Krogh A and Mitchison G, "*Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids"*, Cambridge University Press, 2000.

Course Code	Course Title	L	T	P	C
BI2006	**STRUCTURAL BIOINFORMATICS**	**3**	**2**	**0**	**4**
	Total Contact Hours - 75				

PURPOSE	
The structural bioinformatics course, aimed for life-scientists and chemists alike, will present thelatest tools available in the field and their usage for derivation of Biological insight	
INSTRUCTIONAL OBJECTIVES	
1.	To provide various data format for structural databases
2.	Students can learn importance of structure-function relationship of biomolecules
3.	To learn how various interactions played major for biomolecules
4.	To provide knowledge about predicting the structure of biomolecules
5.	To provide the essence of structural validation

UNIT I – DATA REPRESENTATION AND DATABASES (9 hours)

PDB, mmCIF and other formats, structure based databases for proteins and nucleic acids. Comparative features-the CATH domain structure Database, Protein structure evolution and the SCOP Database.

UNIT II – DATA INTEGRITY AND COMPARATIVE FEATURES **(9 hours)**

Structural Quality Assurance, Structure Comparison and Alignment.Structure and Functional Assignment-Identifying Structural Domains in Proteins**,** Inferring Protein Function from Structure.

UNIT III – BIOMOLECULES INTERACTIONS (9 hours)

Electrostatic interactions, Prediction of Protein- protein interactions, Prediction of Protein- nucleic acid interactions, Docking Methods: Introduction, Docking and scoring, Application in the drug design

UNIT IV – STRUCTURAL MODELING (9 hours)

Scoring functions: forcefields, surface area based functions, knowledge based potentials, searching procedures: grid based, stochastic methods, building complete protein structures using homologymodeling, fold recognition, Ab initio methods, Analysis of Folds.

UNIT V– STRUCTURAL VALIDATIONAND APPLICATION **(9 hours)**

Validation: CASP and CAFASP experiments and their findings, Structural bioinformatics in drug design: Modern drug discovery, Drug target, Lead identification, Lead Optimization.

TUTORIAL (30 hours)

REFERENCES

1. Philip E. Bourne, HelgeWeissig, *"Structural Bioinformatics"*, John Wiley & Sons, Inc, 2003.
2. Becker OM., MackKerell AD Jr., Roux B., Watanabe M (Eds.), "*Computational Biochemistry and Biophysics"*, Dekker, 2001.
3. Hinchliffe A., "*Molecular Modelling for Beginners"*, Wiley, 2003.
4. Orengo CA, Jones DT, Thornton, JM (Eds.), "*Bioinformatics - Genes, Proteins and Computers"*, Bios Scientific Publishers Ltd., 2003.

SEMESTER III

Course Code	Course Title	L	T	P	C
BI2047	**SEMINAR**	**0**	**0**	**1**	**1**

PURPOSE

This course gives an opportunity to the students to present what they have learnt to an audience. This will train the students in giving scientific presentations.

INSTRUCTIONAL OBJECTIVES

1.	Teach the students to learn prepare for scientific presentations and present it to an audience and face the discussions.

Topics Included

1. Synthetic Biology
2. Thermodynamics and Statistical kinetics
3. Pharmacogenomics
4. Immunoinformatics
5. IPR and Bioethics
6. Linux
7. Advances in Bioinformatics
8. Applications of Systems Biology

Course Code	Course Title	L	T	P	C
BI2048	**INDUSTRIAL TRAINING**	**0**	**0**	**1**	**1**
	3 week practical training in industry				

PURPOSE

This course gives an opportunity to the students to get exposure to Bioinformatics Industry/Research Institutions. This will help the students to get hands-on training in carrying out scientific activities at Bioinformatics Industries.

INSTRUCTIONAL OBJECTIVES

1.	To help the students to get exposure to Bioinformatics Industry.
2.	Enable the students to get hands-on training at Bioinformatics Industries.

The student has to undergo Industrial Training for a period of two to four weeks during summer vacation between II and III semesters and submit a report which will be evaluated.

Course Code	Course Title	L	T	P	C
BI2049	**PROJECT WORK PHASE I (III semester)**	**0**	**0**	**12**	**6**
BI2050	**PROJECT WORK PHASE II (IV semester)**	**0**	**0**	**32**	**16**

PURPOSE

To undertake research in an area related to the program of study

INSTRUCTIONAL OBJECTIVE

The student shall be capable of identifying a problem related to the program of study and carry out wholesome research on it leading to findings which will facilitate development of a new/improved product, process for the benefit of the society.

M.Tech projects should be socially relevant and research oriented ones. Each student is expected to do an individual project. The project work is carried out in two phases – Phase I in III semester and Phase II in IV semester. Phase II of the project work shall be in continuation of Phase I only. At the completion of a project the student will submit a project report, which will be evaluated (end semester assessment) by duly appointed examiner(s). This evaluation will be based on the project report and a viva voce examination on the project. The method of assessment for both Phase I and Phase II is shown in the following table:

Assessment	Tool	Weightage
In- semester	I review	10%
	II review	15%
	III review	35%
End semester	Final viva voce examination	40%

Student will be allowed to appear in the final viva voce examination only if he / she has submitted his / her project work in the form of paper for presentation / publication in a conference / journal and produced the proof of acknowledgement of receipt of paper from the organizers / publishers.

PROGRAM ELECTIVES

Course Code	Course Title	L	T	P	C
BI2101	**ADVANCED BIOLOGY**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE	
This course enables the students to understand biology in detail.	
INSTRUCTIONAL OBJECTIVES	
1.	It enables to survey the biological world which includes topics of Genetics, Cell biology and molecular biology

UNIT I - MOLECULES AND MACROMOLECULES OF THE CELL **(9 hours)**

Elements, molecules and macromolecules of the cell, Formation of macromolecules, Types of bonds, Structure of carbohydrates, lipids, DNA, RNA and proteins

UNIT II - CELL STRUCTURE AND FUNCTIONS **(9 hours)**

Unity and diversity in life forms, Structure of virus and bacteria, Features of prokaryotic and eukaryotic cells, Levels of biological organization – cell, tissue and organs.

UNIT III - SUPRAMOLECULAR ASSEMBLIES OF THE CELL **(9 hours)**

Self assembly of macromolecules – ribosome, chromosomes, membrane, collagen, actin and cellulose

UNIT IV - ENERGY AND CELLULAR WORK **(9 hours)**

Energy input and output in cell, The role of ATP, Electron transfer reactions, Electron transfer molecules, Electron transport chains, Light-driven electron flow, Catabolism and Metabolism, Metabolic pathways

UNIT V - CELL CYCLE **(9 hours)**

Different phases of cell cycle, mitosis and meiosis, Regulation of cell cycle, Apoptosis

REFERENCES

1. Roberts MBV and King TJ,"*Biology: A functional approach"*, Nelson ThornesLimited, USA, 1987.
2. Edwards, G.I, *Biology: "The easy way*; Barrons Educational Series, USA, 2000.
3. Murray, R.K., Mayes, P.A. and Graner, D.K, "*Harpers Biochemistry"*, Appleton and Lange Publishers, USA, 1996.
4. De Robertis, EDP, De Robertis EMF,"*Cell and Molecular Biology"*, 8th edition. Lippincott Williams & Wilkins, 2010.

Course Code	Course Title	L	T	P	C
BI2102	**OBJECT-ORIENTED PROGRAMMING AND DATABASE MANAGEMENT**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE	
Designing database for different applications is an important area of program development and C++ as tools for solving problems.	
INSTRUCTIONAL OBJECTIVES	
1.	Using C++ introduce the concept of object oriented programming
2.	Describe the concepts of Classes, objects and overloading using C++
3.	Introduce the Database management architecture and languages
4.	Description of Database models using ER model as an example
5.	Description of Structured query language

Unit I - OBJECT ORIENTED PROGRAMMING (OOP) (10 hours)
OOP concepts (Using C++): data hiding, encapsulation, inheritance, overloading, polymorphism.

Unit II - CLASSES AND OBJECTS, OVERLOADING (10 hours)
Classes and objects (Using C++); constructor and destructor, Inheritance: single, multiple, multilevel- overloading: Function overloading, Operator overloading.

Unit III - DBMS ARCHITECTURE, LANGUAGES (8 hours)
DBMS Architecture & Data Abstraction, DBMS Languages, DBMS System Structure.

Unit IV - ENTITY RELATIONSHIP MODEL (8 hours)

ER Model: Objects, Attributes and its Types, Entity and Entity Set, Relationship & Relationship Set. Design Issues in choosing attributes or entity set or relationship set: Constraints, Super Key, Candidate Keys, Primary Key, ER Diagram Notations.

Unit V - STRUCTURED QUERY LANGUAGE (9 hours)

SQL: Overview, the Form of Basic SQL Query, UNION, INTERSECT, and EXCEPT- Nested Queries- Aggregate Functions- Null Values.

REFERENCES

1. Herbert Schildt, *"The Complete Reference C++"*, Tata McGraw Hill, 2001.
2. Robert Lafore, *"Object Oriented Programming in Microsoft C++"*,Galgotia Publications, 2002.
3. Abraham Silberschatz, Henry F. Korth, S. Sudarshan, *"Database System Concepts"*, McGraw-Hill, 4th edition, 2002.
4. Elmashri&Navathe, *"Fundamentals of Database System"*, Addison-Wesley Publishing, 3rd edition, 2000.

Course Code	Course Title	L	T	P	C
BI2103	**METABOLIC ENGINEERING**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE

This course provides the fundamental knowledge on upcoming field of Metabolomics and themetabolic engineering in post genomic era.

INSTRUCTIONAL OBJECTIVES

1.	Metabolome and its study
2.	Applications of Metabolomics
3.	Comprehensive models cellular reactions
4.	Metabolic flux analysis and its applications

UNIT I -METABOLOMICS (5 hours)

Overview- Background and definitions of Metabolomics- importance of Metabolomics.

UNIT II -TECHNOLOGIES IN METABOLOMICS (10 hours)

Technologies-Mass spectrometry: principles, definitions, nomenclature, Metabolite isolation andanalysis by Mass Spectrometry, metabolite library, HPLC- capillaryelectrophoresis coupled with Mass spectrometry

UNIT III -APPLICATIONS (9hours)

Applications of Metabolomics to biology:examples and case studies,Metabolome informatics, data integration and mining.

UNIT IV- METABOLIC ENGINEERING (8 hours)

Metabolic engineering: introduction, mass balance, black box, metabolic flux analysis,stochiometry, Principles of metabolic engineering

UNIT V- FLUX BALANCE ANALYSIS (13 hours)

Flux balance analysis, flux balance methods, group based flux balance, metabolic control analysis: overview, control coefficients, methods of measuring control. Flux analysis of networks- top down approach, bottom up approach.

REFERENCES

1. Tomita M., T. Nishioka, "*Metabolomics:The Frontier of Systems Biology"*, Springer, 2003.
2. Gregory N. Stephanopoulos, "*Metabolic Engineering: Principles and Methodologies"*,Academic press, First Edition, 1998.
3. Wolfram Weckwerth, *"Metabolomics: Methods and Protocols"*, Humana Press, 2007.
4. Sang Yup Lee, E. Terry Papoutsakis, "*Metabolic engineering"*, CRC Press, 1999.
5. William J. Griffiths, "*Metabolomics, metabonomics and metabolite profiling"*, RoyalSociety of Chemistry, 2008.

Course Code	Course Title	L	T	P	C
BI2104	**MICROARRAY BIOINFORMATICS**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				
PURPOSE					
This course gives the technical knowledge on Microarray techniques and data analysis					
INSTRUCTIONAL OBJECTIVES					
1.	DNA Microarray and its statistical analysis				
2.	Analysis of RNA data				
3.	Statistical computing and Statistical Genetics				

UNIT I -DNA MICROARRAY (7 hours)

The Technical Foundations, Why are MicroArray Important?,What is a DNA MicroArray?, Designing a MicroArray Experiment-The Basic steps, Types of MicroArray.

UNIT II -MICROARRAY DATABASES (8 hours)

NCBI and MicroArray Data Management, GEO (Gene Expression Omnibus), MAML, The benefits of GEO and MAML, The Promise of MicroArray Technology in Treating Disease

UNIT III – MICROARRAY DATA NORMALIZATION (10 hours)

MicroArray DataPreprocessing, Data-Data normalization, Measuring Dissimilarity of Expression Pattern-Distance Motifs and Dissimilarity measures, Visualizing MicroArray Data-Principal Component Analysis,MicroArray Data.

UNIT IV– MICROARRAY DATA ANALYSIS (10 hours)

KMeans Clustering, Hierarchical Clustering, Self Organization Maps (SOM), Identifying Genes: Expressed usually in a sample- Expressed significantly in population-Expressed differently in two populations, Classifying Samples from two populations using Multilayer Perceptron, Support Vector Machines and their applications, Using genetic algorithm and Perceptron for feature selection and supervised classification.

UNIT V– MICROARRAY APPLICATIONS (10 hours)

Gene Ontology and pathway analysis, Promoter analysis and gene regulatory network, Coexpression analysis, CGH & Genotyping chips, Chromosome aberration and polymorphism via genome-wide scanning, Future direction of microarray approach, Pharmacogenomics, Toxicogenomics, Data mining.

REFERENCES

1. ArunJogota, *"Microarray Data Analysis and Visualization"*, the Bay Press, 2001.
2. Ernst Wit and John McClure, *"Statistics for Microarrays Design, Analysis and Inference"*,John Wiley & Sons, 2004.
3. Steen Knudsen, *"Guide to analysis of DNA Microarray data"*, John Wiley & Sons, 2004.
4. DovStekel, *"Microarray Bioinformatics"*, Cambridge University Press, 2003.

5. Draghic S., Chapman, *"Data Analysis tools for DNA Microarray"*, Hall/ CRC Press, 2002.
6. Uwe R. Müller, Dan V. Nicolau,*"Microarray Technology and Its Applications"*, Springer, 2005.
7. Emanuele de Rinaldis, Armin Lahm, *"DNA Microarrays: Current Applications"*, Horizon Scientific Press, 2007.

Course Code	Course Title	L	T	P	C
BI2105	COMPUTATIONAL CHEMISTRY	3	0	0	3
	Total Contact Hours - 45				

PURPOSE	
This course provides knowledge on upcoming field of chemoinformatics.	
INSTRUCTIONAL OBJECTIVES	
1.	Providing the knowledge of 2D and 3D molecular structures
2.	To teach importance of structural descriptors
3.	Provide knowledge of data analysis
4.	To teach QSAR model generation and virtual screening
5.	Provide Applications of computational models

UNIT I -REPRESENTATION OF MOLECULAR STRUCTURES (9 hours)

Representation and Manipulation of 2D Molecular Structures, Representation and Manipulation of3D Molecular Structures, Representations of Chemical Reaction, Databases and data sources in chemistry.

UNIT II-MOLECULAR STRUCTURE DESCRIPTORS (9 hours)

Calculation of structure descriptors: structure keys and 1D fingerprints, topological descriptors, 3D Descriptors, Chirality descriptors, Further descriptors, Descriptors that are not structure based, properties of structure descriptors.

UNIT III - METHODS OF DATA ANALYSIS (9 hours)

Introduction, machine learning techniques, decision trees, Chemometrices, Neural Networks, Data mining.

UNIT IV- COMPUTATIONAL MODELS (9 hours)

Deriving a QSAR Equation: Simple and Multiple Linear Regression, Designing a QSAR "Experiment", Analysis of High-Throughput Screening Data, Virtual Screening.

UNIT V- APPLICATION OF IN SILICO MODELS (9 hours)

Predictions of properties of compounds, structure- spectra correlations, chemical reactions and synthesis design, Drug designing: molecular docking- De-novo ligand designing- and structure-based methods.

REFERENCES

1. Andrew R Leach, Valerie J Gillet, "*An Introduction to Chemoinformatics"*, Kluwer AcademicPublishers, 2003.
2. Johann Gasteiger, Thomas Engel, "*Chemoinformatics: A Textbook"*, Wiley-VCH, 2003.
3. Hugo Kubinyi,"*3D QSAR in drug design: theory, methods and applications"*, Springer,1993.
4. Smith and Williams,"*Introduction to the principles of drug design and action"*, CRC Press, 2006.
5. Barry A. Bunin, Brian Siesel, "*Chemoinformatics: theory, practice, & products"*, Springer, 2007.

Course Code	Course Title	L	T	P	C
BI2106	**MACROMOLECULAR BIOPHYSICS**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE

To understand the structural properties of various biomolecules and the energetics involved invarious biological process.

INSTRUCTIONAL OBJECTIVES

1.	Understand the various structural properties of biomolecules
2.	The various physical techniques to view the molecule
3.	Understanding signal transmission in neurons
4.	Understanding the energetics involved in various biochemical processes

UNIT I - STRUCTURAL PROPERTIES OF PROTEINS AND NUCLEIC ACIDS (10 hours)

Structural Properties of Proteins And Nucleic Acids: Dissociation Characteristics of Amino acids,Ramachandran plot, Water and its properties, Collagen, Keratin, Elastin, Resilin, Ribose-phosphatebackbone, B and Z family of DNA.

UNIT II - PHYSICS OF BIOMOLECULES (9 hours)

Physics Of Biomolecules: Molecular Forces, Strong Force,Inter-molecular weak forces, Van der Waals Force, Lenard-Jones Potential, Hydrogen Bond,Hydrophobic-Hydrophilic Force, Principle of Molecular recognition.

UNIT III - TECHNIQUES IN STRUCTURE DETERMINATION (10 hours)

Physical Techniques inStructure Determination: Optical Rotary Dispersion, Circular Dichroism, Absorption Spectroscopy,Absorption by oriented molecules, X-ray absorption Spectroscopy, Flow Cytometry, UltravioletSpectroscopy, Infrared Spectroscopy.

UNIT IV- NEUROBIOPHYSICS (9 hours)

Neurobiophysics: Concepts of membrane transport,Membrane-pore diffusion, Active transport, Action potential, Signal transmission, Signal reception,Photoreceptors.

UNIT V- BIOENERGETICS (7 hours)

Bioenergetics: Bioenergetics and ATP Molecules, Energetics of cellularrespiration, Chemiosmotic Theory, Photosynthesis, Emersion Effect, Mechanism and energetics ofmuscle contraction.

REFERENCES

1. Narayanan P., *"Essentials of Biophysics"*, New Age International Ltd., 2nd edition, 2007.
2. Srivastava P.K., *"Elementary Biophysics an Introduction"*, Narosa Publishing House, 2005.
3. Charles R. Cantor, Paul ReinhardSchimmel, *"Biophysical Chemistry: The conformation ofbiological macromolecule PART I"*, W. H. Freeman, 1980.

Course Code	Course Title	L	T	P	C
BI2107	**UNIX & JAVA**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				
PURPOSE					
An introduction to the UNIX operating system primarily focused on command line usage. It also covers the fundamentals of Java.					
INSTRUCTIONAL OBJECTIVES					
1.	Introduce the basics of Unix				
2.	Describe Shell programming in Unix				

3.	Software development using Unix
4.	Introduce Java programming concepts
5.	Object oriented programming using Java

UNIT I - BASICS OF UNIX (9 hours)

File system, KDE, Gnome, Bourne shells, manipulating files and directories, managing user groups. File security and permissions, file name and substitutions, shell input and output.

UNIT II - SHELL PROGRAMMING IN UNIX (9 hours)

Text Editors. Shell programming, variables, flow control. Regular expressions merge and divide, login environment, creating screen input and output.

UNIT III - SOFTWARE DEVELOPMENT IN UNIX (9 hours)

Software development, source code management, revision control system, version control systems, GNU utility, GDB debugger

UNIT IV - BASICS OF JAVA (9 hours)

JAVA: data types with variables and constants, Program control statements including if else, while, for and the switch as well as debugging techniques and recursion.

UNIT V - CLASSES AND OBJECTS, ADVANCED METHODS (9 hours)

Classes and objects (Object Oriented Programming OOP), Interfaces, Event handling, AWT, Applets, multithreading, Java Library.

REFERENCES

1. Katherine Wrightson, Joseph Merlino, *"Mastering UNIX"*, Sybex Publishers, 2000.
2. Jerry Peek, Grace Todino& John Strang, *"Learning the Unix operating systems"*, Reilly Publications, 1997.
3. Bruce Eckel, *"Thinking in Java"*, Prentice Hall, 1999.
4. Herbert Schildt&FatrickNanghton, *"The complete reference Java 2.0"*, Tata McGraw-Hill, 2002.

Course Code	Course Title	L	T	P	C
BI2108	**MOLECULAR MECHANICS AND SIMULATION**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE	
This course tries to understand the various mechanical properties of biomolecules	
INSTRUCTIONAL OBJECTIVES	
1.	Basic concepts in Molecular Mechanics
2.	Empirical Force Field Models
3.	Computer Simulation Techniques
4.	Conformational analysis

UNIT I - CONCEPTS IN MOLECULAR MECHANICS (10 hours)

Concepts In Molecular Mechanics: Introduction, Coordinate systems, Units of Length and Energy, Potential Energy surfaces, other surfaces, Molecular Graphics.

UNIT II - COMPUTATIONAL QUANTUM MECHANICS (9 hours)

Computational Quantum Mechanics: One-electron atoms, Polyelectron atoms and molecules, Molecular orbitals, Hartree- Fock Equations, Molecular Properties using *ab initio* methods, Semi-empirical methods, Huckel Theory.

UNIT III - EMPIRICAL FORCE FIELD METHODS (10 hours)

Empirical Force Field Methods: Bond Stretching, Angle Bending, Torsional Terms, Nonbonded and ectrostatic interactions, Van der Waals Interaction, Hydrogen bonding parameterization, United atom force field representation, Force field parameterization.

UNIT IV- COMPUTER SIMULATION METHODS (9 hours)

Computer Simulation Methods: Simple Thermodynamic properties, Phase space, Practical aspects of Computer simulation, Boundaries, Truncating the potential, Minimum Image convention, Longrange forces. Conformational Analysis: Systematic methods for exploring conformational space, Random search methods, Evolutionary algorithms, Simulated Annealing, Restrained molecular methods, Molecular fitting, Clustering algorithm, Reducing dimensionality of data set, Pooling.

UNIT V- MONTE CARLO SIMULATIONS (7 hours)

Monte Carlo Simulations: Calculating properties by integration, metropolis methods- metropolisMonte Carlo methods- simulations of molecules-models- biased methods- different ensemblescalculatingchemical potentials-Gibbs ensemble methods.

REFERENCES

1. Andrew R. Leach, *"Molecular Modeling: Principles and applications"*, Prentice Hall, 2nd edition, 1996.
2. Alan Hinchliffe, *"Modelling Molecular Structures"*, John Wiley, 2000.
3. Ramachandran K. I., G. Deepa, K.Namboori,*"Computational Chemistry and Molecular Modeling: Principles and Applications"*, Springer, 2008.
4. Charles R. Cantor, Paul ReinhardSchimmel, *"Biophysical Chemistry: The Behavior of Biological Macromolecules PART III"*, W. H. Freeman, 1980.

Course Code	Course Title	L	T	P	C
BI2109	**SYSTEMS BIOLOGY- MODELS AND APPROACHES**	**3**	**0**	**0**	**3**
	Total Contact Hours - 45				

PURPOSE	
The course aims at introducing various concepts of systems biology, required for modeling and simulation of biological systems	
INSTRUCTIONAL OBJECTIVES	
1.	Learning the Principles of Systems Biology
2.	Learning the Standard models and approaches
3.	To understand signal transduction and other biological processes
4.	To understand modeling of gene expression.
5.	To understand modeling of evolution and self organization.

UNITI - PRINCIPLES OF SYSTEMS BIOLOGY (9 hours)

Systems Biology and modeling, Properties of models, Variables, parameters and constants. Model development, Data integration, Techniques involved in systems biology: Elementary experimental techniques, advanced experimental techniques.

UNIT II - STANDARD MODELS AND APPROACHES (9 hours)

Standard models and approaches in systems biology. Metabolism: Law of mass action. Michaelis-Menton Kinetics, Enzyme inhibition, Elementary flux models and extreme pathways, Flux balance analysis,Metabolic control analysis.

UNIT III - SIGNAL TRANSDUCTION, BIOLOGICAL PROCESSES (9 hours)

Signal transduction, Quantitative measures of properties of signaling pathway. Selected Biological process: Glycolytic oscillation, coupling of oscillator, cell cycle, Minimal cascade model, models of budding yeast cell cycle, ageing, Evolution of ageing process, Accumulation of defective mitochondria, Dilution of membrane damage, choice of parameters and simulation.

UNIT IV - GENE EXPRESSION MODELING (9 hours)

Modeling of Gene expression, Bayesian networks, Boolean Networks, The Model according to Griffith, The model according to Nicolis and Prigogine. Evolution and self organization: Quasispecies and Hypercycles.

UNIT V EVOLUTION AND SELF ORGANIZATION (9 hours)

The Genetic Algorithm, Spin-glass Model of Evolution, Boolean Network Models Data integration: Basic Concepts of database integration and data management, Biclustering and data integration. Applications of Systems Biology

REFERENCES

1. EddaKlipp, Ralf Herwig, *"Systems Biology in Practice-Concepts, Implementation and Application"*, Wiley VCH, I Edition, 2005.
2. Bernhard Ø. Palsson, *"Systems Biology: Properties of reconstructed network"*, Cambridge University Press, 2006.

Course Code	Course Title	L	T	P	C
BI2110	PYTHON FOR BIOINFORMATICS	3	0	0	3
	Total Contact Hours - 45				
PURPOSE					
To apply Python for bioinformatics applications.					
INSTRUCTIONAL OBJECTIVES					
1.	Introduce Python with reference to bioinformatics				

2.	Describe Object oriented programming in Python and different modules
3.	Biological sequence analysis using Python
4.	Describe advanced analysis techniques using Python
5.	Describe expression analysis using Python

UNIT I –PYTHON FUNDAMENTALS (7 hours)

Running programs, types and operations, Functions, modules, classes, Exceptions,

UNIT II -OBJECT ORIENTED PROGRAMMING, MODULES (11 hours)

Object Oriented Programming, Threads, process, synchronization, databases and persistence, NumPy, SciPy, image manipulation, Akando and Dancer modules.

UNIT III - BIOLOGICAL SEQUENCE ANALYSIS (9 hours)

Biopython: Parsing DNA data files, Sequence Alignment, Dynamic programming, Hidden Markov Model, Genetic algorithms, Multiple Sequence Alignment, gapped alignment.

UNIT IV - ADVANCED ANALYSIS TECHNIQUES (9 hours)

Trees, text mining, clustering, Self Organizing Map, Principal Component Analysis, Fourier transforms, Numerical Sequence Alignment.

UNIT V - EXPRESSION ANALYSIS (9 hours)

Gene expression array analysis, Spot finding and Measurement, Spreadsheet Arrays and Data Displays, Applications with Expression Arrays.

REFERENCES

1. Jason Kinser, "*Python for Bioinformatics"*, Jones & Bartlett Publishers, 2008.
2. Mark Lutz, "*Learning Python"*, 3rd edition, O'Reilly, 2007.
3. Alex Martelli, David Ascher, "*Python cookbook"*, O'Reilly, 2002.
4. http://www.biopython.org

ELECTIVE PRACTICAL COURSES

Course Code	Course Title	L	T	P	C
BI2111	**COMPUTER AIDED DRUG DESIGNING**	**0**	**1**	**6**	**3**
	Total Contact Hours - 105				

PURPOSE	
To design a novel drug through *in silico*approach.	
INSTRUCTIONAL OBJECTIVES	
1.	*In silico* docking/scoring
2.	ADME and Toxicity prediction
3.	Pharmacophore modeling

Computer aided drug design, methods of computer aided drug design, ligand design methods, docking algorithms and programs, drug design approaches, absorption, distribution, metabolism, and excretion (ADME) property prediction, computer based tools for drug design. Pharmacophoric approach, Pharmacophore based ligand design, Pharmacophore concept, Pharmacophore elements and representation, active conformation, molecular superimposition, examples of 3D Pharmacophore models and their uses.

TUTORIAL **(15 hours)**

LIST OF EXPERIMENTS **(90 hours)**

1. Homology modeling of a protein
2. Evaluate the 3D structure of a protein
3. Active site/cavity in a receptor
4. Building small molecules
5. ADME Predictions
6. Protein-ligand docking
7. Protein-protein docking
8. Combinatorial library generation
9. Pharmacophore modeling
10. Virtual screening: Structure based designing and ligand based designing

REFERENCES

1. Leach A. R., "*Molecular Modeling- Principles and applications"*, Prentice Hall, 2nd edition, 1996.

2. Paul S Charifson, *"Practical application of CADD"*, Informa Health Care, 1997.
3. PerunT.J. and C.L. Propst, *"Computer Aided Drug Design"*, Informa Health Care, 1992.
4. Rastogi et al, *"Bioinformatics – Genomics, proteomics, and drug discovery"*, PHI Publishing, 2008.
5. Lab Manual.

Course Code	Course Title	L	T	P	C
BI2112	**MOLECULAR DYNAMICS**	**0**	**1**	**6**	**3**
	Total Contact Hours - 105				

PURPOSE

This course gives an insight into the kinetics and dynamics of the biomolecules

INSTRUCTIONAL OBJECTIVES

1.	Introduction to the dynamics of biomolecules
2.	Understanding the structural properties
3.	Energy Minimization in the folding process

Introduction to molecular dynamics (MD), Statistical mechanics for MD, Energy minimization, Equations of motion-finite difference methods Constant energy MD simulations, Constant temperature and pressure MD simulations,Brownian dynamics MD simulations, Molecular dynamics packages- CHARMM, AMBER, GROMACS, Energy calculations for complex interaction potentials, Energy minimization for complex interaction potential. Molecular dynamics simulation of macromolecules, Free energy calculations, Molecular dynamics trajectories for activated processes.

TUTORIAL **(15 hours)**

LIST OF EXPERIMENTS **(90 hours)**

1. Simulation of A, B and Z forms of DNA
2. Constant energy and constant temperature simulations of macromolecules.
3. Molecular dynamics simulation of a peptide fragment with known structures using AMBER
4. Energy minimization
5. Non-polarizable and polarizable rigid models and Flexible models in water and smallorganic molecules
6. Structural and dielectric properties of a polar medium

7. Calculation of structure, energy and free energy through simulations.
8. Concept of hydrophobic and hydrophilic interactions

REFERENCES

1. Andrew R. Leach, *"Molecular Modelling- Principles and applications"*, Prentice Hall, 1996.
2. Carl Branden and John Tooze, *"Introduction to protein structures"*, Garland publishing Inc.,1999.
3. Heerman D.W., *"Computer Simulation Methods"*, Springer- Verlag, 1990.
4. McCammonJ.A. and Stephen C. Harvey, *"Dynamics of proteins and nucleic acids"*, Cambridge U. Press, 1987.
5. Lab Manual.

Course Code	Course Title	L	T	P	C
BI2113	**PERL FOR BIOINFORMATICS**	**0**	**1**	**6**	**3**
	Total Contact Hours - 105				
PURPOSE					
To understand the applications of Perl in Bioinformatics.					
INSTRUCTIONAL OBJECTIVES					
1.	Introduce Perl language of computing				
2.	To apply Perl to biological sequenceanalysis				
3.	Practical exposure to tool developing				

Perl in Bioinformatics: Basic concepts, Scalar data, Arrays and list data, Control structures, Hashes, Regular expressions: Concepts about regular expressions, simple uses of regular expressions, patterns, matching operator, substitutions, the split and join functions, Subroutines: System and user functions, the local operator, variable-length parameter lists, lexical variables. Filehandles and file tests: Opening and closing a filehandle, using pathnames and filenames, die, using Filehandles. Other data transformation: Finding a substring, extracting and replacing a substring. Formatting data: Sorting, Transliteration CGI programming: The CGI.pm Module, CGI program in context, simple CGI programs, passing parameters via CGI, Perl and the Web. Bioperl: Introduction, Installation procedures, Architecture, Uses of Bioperl.

TUTORIAL **(15 hours)**

LIST OF EXPERIMENTS **(90 hours)**

1. chop, chomp based simple Perl program
2. Program based on control structures- dowhile, foreach and with control flow statements-redo, next, goto etc.
3. Subroutines
4. Retrievingsequence file and searching for a pattern
5. Comparing files. Combining and extracting data from different files using modules
6. MSA using Perl and conserved domain identification and hast table creation
7. Blast usingBioperl
8. CGI- Perl Programs for developing MSA.

REFERENCES

1. Harshawardhan P Bal, *"Perl Programming for Bioinformatics"*, Tata McGraw Hill, 2003.
2. James Tisdall, *"Mastering Perl for Bioinformatics"*, O'Reilly, 2010.
3. James Lee, *"Beginning Perl"*, Apress, 2004.
4. Curtis Jamison D., *"Perl Programming for Bioinformatics & Biologists"*, John Wiley & Sons, INC., 2004.
5. Michael Moorhouse, Paul Barry, *"Bioinformatics Biocomputing and Perl"*, Wiley, 2004.
6. Rex A. Dwyer, *"Genomic Perl: From Bioinformatics Basics to Working Code"*, Cambridge University Press, 2003.
7. http://www.bioperl.org.
8. Lab manual.

AMENDMENTS

S.No.	Details of Amendment	Effective from	Approval with date