J.J COLLEGE OF ARTS AND SCIENCE (AUTONOMOUS)

PUDUKKOTTAI - 622422

P.G. DIPLOMA IN BIOINFORMATICS

ELIGIBILITY: Any Bachelor Degree in science from a recognized University

(For students admitted from 2019 - 2020 onwards)

SEMESTER I				
S. NO.	**TITLE OF THE PAPER**	**I.A**	**U.E**	**TOTAL**
01	Basics of bioinformatics (PDR1BI1)	25	75	100
02	Statistics for bioinformatics (PDR1BI2)	25	75	100
03	Basic structural biology (PDR1BI3)	25	75	100
04	Object oriented programming and web publishing (PDR1BI4)	25	75	100
05	Practical-I: C++ Programming and web publishing lab (PD1BI5P)	10	40	50
	Total			**450**
	SEMESTER II			
06	Data base management systems (PDR1BI6)	25	75	100
07	Bio-physics (PDR1BI7)	25	75	100
08	Genome and proteomics (PDR1BI8)	25	75	100
09	Computational biology (PDR1BI9)	25	75	100
10	Elective (anyone of the following) (PDR1BI10) a) Commercial applications of bio-informatics b) Molecular modelling and drug design c) Data communication networks	25	75	100
11	Practical-II bioinformatics lab (PDR1BI11P)	10	40	50
	Total			**550**

PROGRAMME OUTCOMES

- PG Diploma Grandaunts are Professionally Competent with characteristic Knowledge-bank, Mind-set and Pragmatic Wisdom in their chosen fields.
- Spiritedness with excellent qualities of productive contribution to society and nation in the arena Science and Technology.
- PG Grandaunts are mentored such that they exert Leadership Latitude in their chosen fields with commitment to novelty and distinction.
- PG Grandaunts are directed in understanding of ethical principles and responsibilities, moral and social values in day-to-day life thereby attaining Cultural and Civilized personality.
- PG Grandaunts of are able to Collate information from different kinds of sources and gain a coherent understanding of the subject.

Programme Specific Outcome

At the end of the programme, students will be able to:

- Explain the fundamental principles of Bioinformatics and statistical applications in bio informatics.
- Outline the process of generation, manipulation and representation of molecules for drug modeling.
- Describe the basic structure of biological molecules, process of acquiring the structures and the interaction between the molecules.
- Develop and apply basic computer programming to build biological algorithms and models to study their relationships.
- Deduce the interrelationship between genomics and Proteomics, techniques involved in analyzing proteomics and its applications

BASICS OF BIOINFORMATICS

Course Code: PDR1BI1 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To understand concepts of molecularbiology that are basic to bioinformatics.
- To provide the basic knowledge of computer programming required for bioinformatics.
- To introduce the basics, models and applications of different biological sequence.
- Describe the database designing concepts and the languages
- Describe the widely used relational database model and biological sequence databases

Total Instructional Hours: 60

UNIT I Hours: 12

Bioinformatics- an overview, definition and history- information networks- internet in bioinformatics, EMNnet- commercial databases and software's, intranet and internet packages, bioinformatics glossary.

UNIT II Hours: 12

Languages- basics of programming, Perl- basics, string handling, subroutines.HTML- basics, tags, text handling, image handling, links, frames and tables.XML- basics, data binding and record sets.

UNIT III Hours: 12

Proteins information resources- biological databases, primary sequence databases, composite protein sequence databases- secondary databases- prosite, prints, blocks profiles and identity.

UNIT IV Hours: 12

Genome information resources- DNA sequence databases- EMBL, DDBJ, Genbank GSDB (Genome Sequence Database), UniGene.

UNIT V Hours: 12

Evolution of bioinformatics- Scope- potentials of bioinformatics human genome project- bioinformatics in India- future of bioinformatics.

REFERENCE BOOKS

1. T.K. Attwood and D.J. Parry-smith, introduction to bioinformatics, Pearson Education Ltd., New Delhi 2004.
2. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi 2001.
3. D. Higgins and W. Taylor, Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi 2006.
4. A. Baxevanis and B.F Ouellette, Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, wiley- Interscience, Hoboken, NJ 2008.

COURSE OUTCOME

- Students learned problem solving, execution of programs, thinking the problems in procedure manner and apply the concepts
- Understand the features of DNA sequence analysis
- Analyze the pair wise sequence alignment methods
- Use and explain the application of bioinformatics.
- Follow the details on Watson and Crick model.
- Decipher the importance of bioinformatics.

STATISTICS FOR BIOINFORMATICS

Course Code: PDR1BI2 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To achieve skills in mathematics that are essential for application in bioinformatics.
- Mathematical and statistical frameworks are being increasingly employed to understand and investigate biological processes.
- Apply knowledge in modern industry, teaching, or secure acceptance in high-quality graduate programs of Bioinformatics.
- For better integration of the concepts at the intercepts of mathematical methods and biological codes, sequences, structures, networks, and systems biology.
- Understand and apply statistical techniques that are essential to process and interpret biological data.

Total Instructional Hours: 60

UNIT I

Hours: 12

Measures of central tendency- Arithmetic mean- median- mode- quartiles- range- quartile deviation- Mean deviation- Standard deviation.

UNIT II

Hours: 12

Probability- Addition theorem- multiplication theorem- Bayes’s theorem and related problems.

UNIT III

Hours: 12

Theoretical distribution- binomial, poison and normal- fitting of the distribution and its properties- Z-score, P-value and E-value.

UNIT IV

Hours: 12

Theory of attributes- introduction- dichotomy- consistency of data- independence of attributes- association of attributes- rules coefficient of association.

UNIT V

Hours: 12

Sampling distributors- Large and small sample tests- student’s t◦ test, X2 test, F-test and normal test and their applications.

TEXT BOOK

1) S.C. Gupta and V.K. Kapoor, Fundamentals of Mathematical Statistics, 11th edition, Sultan Chand and sons, New Delhi, 2002.

REFERENCE BOOKS

1. S.P. Gupta, Statistical Methods, Sultan Chand and sons, 1996.
2. L. Forthofer, Introduction to Biostatistics, Academic press, 1995.
3. Robert R. Sokal and F.J. Rohlf, Introduction to Biostatistics ,W.H. Freeman and company, New York, 1997.

COURSE OUTCOME

- Formulate as well as analyze mathematical and statistical problems, precisely define the key terms, and draw clear and reasonable conclusions.
- Use mathematical and statistical techniques to solve well-defined problems and present their mathematical work.
- understand and construct correct mathematical and statistical proofs and use the library and electronic data-bases to employ information on mathematical problems.
- Explain the importance of mathematics and its techniques to solve real life problems and provide an alternative paradigm for the limitations of such techniques and validate the results accordingly.
- Biostatistics is essential to ensure that the knowledge has been incorporated in places such as public health sector and biomedicine to henceforth bring viable solutions that could ease the complexity of biological problems.

BASIC STRUCTURAL BIOLOGY

Course Code: PDR1BI3 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To make the students understand the basic concept of cell.
- To know the central dogma of life plays a pivotal role in cell biology.
- To analyze the different structural form of DNA and protein.
- To understand the cell cycle and molecules of life in various aspects
- Proteomics based research such as crystal and solution structure determination of bimolecular.

Total Instructional Hours: 60

UNIT I **Hours: 12**

Cell structure and ultracell structure of pro and eukaryotic cells- cell wall- cell membrane- bio membranes- organelles- Diffusion- active and passive transport- osmoregulation.

UNIT II **Hours: 12**

Carbohydrates- classification types- structure- function, lipids- classification types- structure- function.

UNIT III **Hours: 12**

Classification of amino acids, classification and three dimensional structures of proteins. Overview of proteins structure- primary, secondary, tertiary and quaternary structures- α helix, β pleated sheet, Ramachandran plot and bonds stabilizing protein structure.

UNIT IV **Hours: 12**

Principles of structural organization and conformational analysis.Prediction of protein structure- Fold recognition (threading), comparative modelling (homology), the Chou and FasmanSheme, basic principles of X-ray diffraction studies. NMR, mass spectroscopy in identifying protein conformation.

UNIT V **Hours: 12**

Introduction and physiochemical properties of nucleic acids- DNA and RNA. Watson and Crik model of DNA and the different forms of DNA, RNA structure- principles and prediction. Gene structure.

REFERENCE BOOKS

1. Principles of Physical Biochemistry- Van Holde, Prentice Hall.
2. Basic one and two dimensional NMR spectroscopy, Horst FriebolinWitey- VCH 1990.
3. Lechninger Principles of Biochemistry- David I.Nelson, Michael M.Cox, 3rd edition Macmillan worth Publishers.
4. Principles of Protein structure, G.E. Shuttz and R.H. Schirmer, springer- verlag, New York.

COURSE OUTCOME

- Describe the Physical and chemical properties of amino acids and model 2D and 3D structure of a target from the sequence.
- Interpret the model refinement and validation of Protein structure.
- Evaluate the atomic scattering factor and structure factor of macromolecules.
- Understand the basic concepts on macromolecular structures and their interactions with special emphasis on computational biology.
- Grasp the structural basis for biological phenomena.

OBJECT ORIENTED PROGRAMMING AND WEB PUBLISHING

Course Code: PDR1BI4 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To make the students understand the basic aspects of programming.
- Develop an in-depth understanding of functional, logic, and object-oriented programming paradigms.
- Explain and be able to use fundamental programming constructs such as sequencing, decisions and iteration.
- To understand the concept of object oriented programming and to have through knowledge of c++ features
- To learn the fundamental programming concepts and methodologies which are essential to building good HTML programs.

Total Instructional Hours: 60

UNIT I **Hours: 12**

Introduction to the basic concepts of C++ language- Tokens, keywords, identifiers, data types, Variables, Manipulators- Expression and control structures.Functions: Main function- function prototyping- call by reference- function overloading- friend and inline functions.

UNIT II **Hours: 12**

Classes and objects- constructions and destructors- operator overloading- type conversions.

UNIT III **Hours: 12**

Inheritance- single inheritance- multiple inheritance- hierarchical, hybrid inheritance- polymorphism-pointers- console I/O operations.

UNIT IV **Hours: 12**

Files- classes for file operations- opening, closing and processing files- end of file detection- file pointers-error handling during file operations- command line arguments- exception handling.

UNIT V **Hours: 12**

Internet- WWW- browser- designing website- basic of creating a web page with HTML- linking- text formatting- adding images and background to HTML pages- tables- image maps.

TEXT BOOKS

1. For Units 1 to 4 “Object Oriented programming with C++”- E Balagurusamy- TMH.
2. For unit 5: “Web publishing”- Monica D’souza and judeD’souza- TMH 2001.
3.

REFERENCE BOOKS

1. Object Oriented Programming in C++- Robert Lafors, Galgoita.
2. Let us C++- Yeshwant Kanetkar- BPB.
3. Instant HTML Programmer’s Reference- Steve Wright- WROX Press Ltd.,

COURSE OUTCOME

- Good understanding about the concept of C & C++.
- Make use of data types, variables, constants, assignment statements, and arithmetic and Boolean expressions in writing programs;
- Understand object-oriented programming using C++
- Explain the concept of function overloading. Create the arrays of objects in C++.
- Understand the inline function in HTML

PRACTICAL- I - C++ PROGRAMMING AND WEB PUBLISHING LAB

Course Code: PDR1BI5P **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

C++

1) Factorial of a given number
2) Sorting and merging two arrays of numbers
3) Sorting names in alphabetical order
4) Reversing a given string
5) Checking for palindrome
6) String manipulation- string copy, string length, string concentration, string comparison and string reverse
7) Mean, median, mode and standard deviation calculations
8) Storing and retrieving amino acid sequences using structure data types
9) Swapping two values using pointers
10) File processing- creation and simple processing
11) Computing amino acid composition of a given protein sequence

WEB PUBLISHING

1) Create a web page for your university/ college using HTML. The opening page should provide hyperlink to other pages (add animation and sound effects appropriately).
2) Creating a web page to get protein sequence data and compute and display amino acid composition
3) Creating a web page to nucleic acid sequence data and compute and display base composition

COURSE OUTCOME

- **Describe the C programming concepts like Structures, Pointers and Command line arguments and data structures**
- **Identify the application of some basic programs in C and Web based application**
- **Acquire the knowledge Practice the use of conditional and looping statements.**
- **Illustrate the structure; implement arrays, functions and pointers.**
- **Improve the new skills to handle strings and files.**

DATABASE MANAGEMENT SYSTEMS

Course Code: PDR1BI6 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To gain knowledge on relational data and its management.
- To set the data into formats suitable for feeding in traditional RDBMS.
- To design Logical Database Schema and Mapping it to implementation level schema through Database Language Features.
- To study about relational databases, database design, structured query language and concurrency control, trends in database technology.
- Make the latest modification to the database available immediately.

Total Instructional Hours: 60

UNIT I **Hours: 12**

Data base: Introduction- basic technology and data bases- objective of a data base organization- entities and attributes.

UNIT II **Hours: 12**

Data models: Introduction- schemes and sub schemes- data base management systems- tree structures- plex structures- relational databases- normal forms.

UNIT III **Hours: 12**

Data base languages: Introduction- data description languages- the CODASYL Data description language- query languages- data dictionaries.

UNIT IV **Hours: 12**

Physical organization: Introduction- criteria affecting physical organization- differences between physical and logical organization- addressing techniques- index sequential organization- hashing.

UNIT V **Hours: 12**

Pointers- chains and ring structures: Introduction- physical representation of tree structures- physical representation of plex structures- virtual and storage hierarchies.

TEXT BOOK

1) James Martin, Computer Database Organization, Prentice Hall of India.

REFERENCE BOOKS

1) James Martin, Computer Database Organization, Prentice Hall of India.
2) C.J. Date, An Introduction to database system, 3rd edition, Narosa Publishing House.

COURSE OUTCOME

- Analyzed Relational Data Base design methodology.
- Acquire knowledge in fundamentals of Relational Data Base Management System.
- Able to handle with different Data Base languages.
- Be able to effectively develop applications with full functionality and a graphical user interface using the language Visual Basic.
- Decide which probabilistic method is the best one for sequence alignment.
- Apply the bioinformatics principles discussed in the design of genome comparison and pattern recognition problems. Critically review bioinformatics research studies and new technologies.

BIOPHYSICS

Course Code: PDR1BI7 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To make the students to learn the laws of thermodynamics principles and techniques involved in qualitative and quantitative methods.
- To make the students understand the basic aspects and applications of crystallography.
- To know the computational software‟s to visualize and compare the protein structure and sequences.
- To analyze the conformational properties of protein using Ramachandran plot.
- To learn molecular interactions and electronic structure of atoms

Total Instructional Hours: 60

UNIT I **Hours: 12**

Levels of structure in biological macromolecules, central questions in biophysics, basic strategies in biophysics.

UNIT II **Hours: 12**

Forces that determine protein and nucleic acid structure, basic problems, polypeptide chain geometrics, potential energy calculations, observed values for rotaion angles, hydrogen bonding, hydrophobic interactions and water structure ionic interactions, disulphide bonds.

UNIT III **Hours: 12**

Prediction of protein structures nucleic acids, general characteristics of nucleic acid structure, geometrics, glycosidic bond rotational isomers and ribose puckering backbone rotational isomers and ribose puckering forces stabilizing ordered forms, base pairing, base stacking tertiary structure of nucleic acids.

UNIT IV **Hours: 12**

Biochemical kinetics studies, unimolecular reactions, simple biomolecular multiple intermediates, steady stake kinetics, catalytic efficiency, relaxation spectrometry, ribonuclease as an example.

UNIT V **Hours: 12**

Size and shape of macromolecules- method of direct visualization- macromolecules as hydrodynamic particles- macromolecular diffusion- ultracentrifugation- viscometry X-ray crystallography determination of molecular structure X-ray fibre diffraction electron minoscopy neutron scattering- light scattering.

REFERENCES

1. C.R. Cantor and P.R. Schimmel, Biophysical chemistry part – I,II and III, W.H. Freeman and Co., in San Fransisco, 1980.
2. C. Branden and J. Tooze, Introduction to Protein Structure, Garland Publishing Inc., New York, 1991.
3. R. Glaser, Biophysics, Springer, 2000.

COURSE OUTCOME

- Describe the Physical and chemical properties of amino acids and model 2D and 3D structure of a target from the sequence.
- Interpret the model refinement and validation of Protein structure.
- Evaluate the atomic scattering factor and structure factor of macromolecules.
- Visualize and compare the protein structures using bioinformatics tools.
- Understand the physico chemical techniques to study biomolecules.

GENOMICS AND PROTEOMICS

Course Code: PDR1BI8 **Max Marks: 100**
Hours/Week: 5 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVES

- To understand the genome architecture and to extract information like gene function, gene regulation, protein evolution and targets for drug designing.
- To provide students with the skills from acquisition of genomic data to its analysis.
- To make the students understand the structure of entire cellular proteins.
- To know the phylogenetic relationship via tree construction.
- To study prokaryotic and eukaryotic genomes, general methods of genome sequencing techniques, genome analysis and annotations, genome mapping techniques and applications of genomics.

Total Instructional Hours: 60

UNIT I Hours: 12

The genetic material- identification of genetic material, genetic code, concept of gene- operon concept- lac and trp operons, promoters and repressors.

UNIT II Hours: 12

Genomics- definitions- pharmacogenomics- taxicogenomics- prokaryotic and eukaryotic genome- genome relationships- human genomics.

UNIT III Hours: 12

Genomics methodologies: whole genome analysis- physical methods of sequencing- automated sequencing- genome expression and analysis- serial analysis- oligo NT array technology- code micro assay and micro chips.

UNIT IV Hours: 12

Proteomics: Definitions- transcriptomics; proteomics, metabolomics, techniques of proteomics- 2D PAGE, multidimensional protein identification (Mud PIT)isotopically coded affinity tag (ICAT), mass spectrophotometer- (MALDI- TOF) MS.

UNIT V Hours: 12

Application of functional genomics in basic biology, target/ marker identification, target valediction/ toxicology, microbial drug resistance, tumour immunology, vaccine discovery, drug design. A brief account of genetic engineering and protein engineering.

REFERENCES

1. Baxevanis AD and B.F.F. Ouellette, Wiley Bioinformatics- A practical guide to the analysis of genes and proteins- Interscience, New York, 2001.
2. Doolittle RF (1990), Molecular evolution, Computer Analysis of Protein and Nucleic acid Sequences, Methods in Enzymology, Academic Press, New York.
3. Faber K (1992) Biotransformation in organic chemistry, Springer Verlag.

4. Gerbardt P. Murray RG, Wood WA, Kreig NR (1994) Methods for general and molecular Bacteriology- American Society for Microbiology Washington D.C.

COURSE OUTCOME

1. Explain genomic technologies and the ways in which genomic data are stored.
2. Have hands-on experience on various bioinformatics tools available for analyzing genes and genomes.
3. Gain the knowledge on the computational methods for gene expression analysis.
4. Explain the details about constraint-based metabolic modelling and metabolic simulation.
5. Describe the methods, algorithms and tools involved in computational proteomics analysis.

COMPUTATIONAL BIOLOGY

Course Code: PDR1BI9	**Max Marks: 100**
Hours/Week: 5	**Internal Marks: 25**
	External Marks: 75

COURSE OBJECTIVES

- To understand various computational techniques employed to analyze biological data with the use of sequence information.
- Understand Genomic data acquisition and analysis, comparative and predictive analysis of DNA and protein sequence,
- To learn the phylogenetic inference etc.
- To provide an elementary knowledge of bioinformatics and biological information on the web.
- To understand the scope of bioinformatics, types of data bases and their use pairwise and sequence alignment, predictive methods

Total Instructional Hours: 60

UNIT I Hours: 12

Structure of DNA and protein- sequence analysis- pairewise sequence comparison- sequence queries against biological databases- BLAST and FASTA- multifunctional tools analysis.

UNIT II Hours: 12

Multiple sequence alignments, phylogenetic alignment- profiles and motifs distance and similarly-evolutionary basis of sequences alignments- scores and gaps.

UNIT III Hours: 12

Protein structure visualization- tools structure- classification. Alignment and analysis, solvent accessibility and interactions- physic chemical properties, structure optimization. Protein resource databases.

UNIT IV Hours: 12

Protein structure and function from sequence- determination of structure- feature detection- secondary structure prediction- predicting 3D structure, protein modeling.

UNIT V Hours: 12

Genomics and proteomics- Sequencing genomes- sequence assembly- genome on the web- annotating and analyzing genome sequences- proteomics- biochemical pathway databases- submitting sequence to the databases.

REFERENCES

- Bioinformatics: A practical guide to the analysis of genes and proteins- 2001- AD Baxevanis and BFF Ouelltte- Wiley interscience- New York.
- Bioinformatics: Methods and Protocols- 2000- Stephen Misener and Stephen A. Krawetz, Human Press, New Jersey.
- Bioinformatics: Sequence, structure and databanks- 2000- Des Higgins and Willie Taylor – Oxford University Press.

COURSE OUTCOME

- The goal of this course is to introduce the main principles of bioinformatics.
- The coverage will include concepts like sequence alignments, phylogenetic trees, and structure prediction
- Students will create computer programs using the learned algorithms that facilitate bioinformatics.
- Students will interpret relationships among living things and analyze and solve biological problems, from the molecular to ecosystem level using basic biological concepts, grounded in foundational theories.
- Students will be able to conduct basic bioinformatics research and examine the source and underlying principle of large datasets and conclude which molecular processes of living organisms are informed by such data.

COMMERCIAL APPLICATIONS OF BIOINFORMATICS

Course Code: PDR1BI10	**Max Marks: 100**
Hours/Week: 3	**Internal Marks: 25**
	External Marks: 75

COURSE OBJECTIVES

- To launch the students into core areas of Bioinformatics like sequence alignment,phylogenetic trees, genomics, proteomics
- To explore the students to applied areas of Bioinformatics like drug design, metabolic pathway engineering
- Practical exploration of tools in bioinformatics
- To know the bioinformatics patents and its process.
- To provide the knowledge on IPR.

Total Instructional Hours: 60

UNIT I **Hours: 12**

Commercial bioinformatics, definition of bioinformatics company, genetic technology, high throughput sequencing and assembly.

UNIT II **Hours: 12**

Micro arrays and genome wide expression analysis, transcriptome, proteome, genome in medicine, disease monitoring, profiles for therapeutic molecular targeting.

UNIT III **Hours: 12**

Diagnosis drug discovery and genomic, pharmacogenomics and its applications, SNP’s and their applications.

UNIT IV **Hours: 12**

Proteomics in medicine and therapeutic target identification comparative proteomics and its applications.

UNIT V **Hours: 12**

Patenting and data generation from literature for commercial benefits.IPR and bioinformatics, bioinformatics patents.

REFERENCES

1. Drug Discovery Today, Trends journals.
2. Functional genomics, http://www.functionalgenomics.org.uk/

COURSE OUTCOME

- The development of computational infrastructure (eg. algorithms, programs, databases) and their use to analyze a wide variety of biological data.
- Evaluate and interpret current literature in areas of bioinformatic practice.
- Demonstrate the ability to obtain quantitative results from mathematical and statistical models through analytical and computational methods.
- Describe and apply a variety of methods in bioinformatics, including computer programming.
- Evaluate current research procedures across a range of topics in bioinformatics.

MOLECULAR MODELING AND DRUG DESIGN

Course Code: PDR1BI10 **Max Marks: 100**
Hours/Week: 3 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVE

- Understand the genome architecture and extracting information like gene function, gene regulation, protein evolution and targets for drug designing
- To let students to understand the use of informatics in drug design and development, finding new targets to treat disease; mechanism of drug designing
- To understand the concept of molecular modeling, mechanics and interactions
- To provide clear concepts on bond angle, bond stretching, bond distance and role on different types of bonds in interactions
- To study about protein structure prediction and conformational changes throughout the simulation
- To provide brief idea of receptor and receptor-ligand complex, inhibition and inactivation of enzyme, receptor theories

Total Instructional Hours: 36

UNIT I **Hours: 07**

Recent advances in drug design methodologies, biomolecular structure, structure activity relationship, pharmacokinetics, structure-based drug design.

UNIT II **Hours: 07**

Pharmacophoric pattern, ADME, properties, quantitative structure activity relationship, use of genetic algorithms and principle component analysis in the OSAR equations.

UNIT III **Hours: 07**

Molecular modeling, quantum mechanical and molecular orbital methods, introduction to semi-empritical, molecular mechanics and abintio techniques, simulation techniques, potential energy surfaces, docking and modeling substrate- receptor interactions.

UNIT IV **Hours: 07**

Software tools for modeling bio-molecules. Molecular electrostatic potentials, charge analyses.Protein conformations, folding and mutation through modeling.

UNIT V **Hours: 08**

Use of tools for proteomics for understanding diseases at molecular level strategies for target identification and lead design.

REFERENCE BOOKS

1. Andrew Leach, Molecular Modelling principles and applications (2nd edition), Addison Wesley Longman, Essex, England, 1996.
2. Alan HInchliffe, Molecular Modelling for Beginners, John Wiley, 2003.

3. N. Cohen, Guide book on Molecular Modeling in Drug Design, Academic press, San Diego, 1996.

COURSE OUTCOME

- The students would know the steps for designing new drugs, target identification and validation
- They would be able to apply concepts of molecular modeling, quantum and molecular mechanics, bond and bond angles in molecular interactions, energy concepts and its importance in drug action
- The students would be able to perform protein structure prediction, loop searching, generating methods and analysis
- The students would be able to understand the concepts of molecular dynamics with constant temperature, pressure, time-dependent properties and solvent effects
- They would be able to perform drug designing basis on structure, ligand and De novo, screening types

DATA COMMUNICATION NETWORKS

Course Code: PDR1BI10 **Max Marks: 100**
Hours/Week: 3 **Internal Marks: 25**
External Marks: 75

COURSE OBJECTIVE

- Gain the knowledge of building different types of networks.
- Identify and differentiate the functionalities of each layer in the protocol stack.
- Choose the different standards of Ethernet and suggest one for the organization based on their applications.
- Able to develop different routing protocols for real world scenarios.
- Enhance the ideas gained to higher order communication systems.

Total Instructional Hours: 36

UNIT I **Hours: 07**

Data communication: Introduction- data communication system- data communication software- data communication concepts, digital and analog communication, parallel and serial communication, synchronous and asynchronous communication, simplex, half- duplex, full- duplex communication.

UNIT II **Hours: 07**

Communication hardware: communication adapter- acoustic couples and modems- communication processing- communication channels: wired transmission- optical, fibre, microwave, laser, radio and satellite transmission- applications of data communication.

UNIT III **Hours: 07**

Topologies and transmission media: Bus topology- ring topology- star broad band coaxial cable topology- star- ring topology- twisted pair wire- base band coaxial cable- fibre optic cables.

UNIT IV **Hours: 07**

Networks: Introduction- use of computer networks- network hardware: local area network- metropolitan area network- wide area network- wireless network- internet works.

UNIT V **Hours: 08**

Network software: Introduction to protocol- LAN protocols, protocol hierarchies- open system interconnection reference model- design issues for the layer- service primitives.

TEXT BOOKS

1. For Unit- I, II and III: Computer Networks, Andrews S. Tannenbaum, Prentice Hall of India, New Delhi, July 1998- 3rd edition.
2. For Unit – IV and V: Local Area Networks by S.K. BasandraJaiswal, Galgotia Publishing.

COURSE OUTCOME

- Understand the basic concepts of data communications and Networking
- Compare different switching techniques and Transmission media
- Classify different types of networks and Recognize the different internetworking devices and their functions Describe how TCP and UDP function and Explain the role of protocols in networking
- List the functions performed by layers in the OSI model

PRACTICAL - II
PRACTICAL - II BIOINFORMATICS LAB

Course Code: PDR1BI11P
Hours/Week: 5

Max Marks: 100
Internal Marks: 25
External Marks: 75

1. Biological Databanks Sequence Databases, Structure Databases, Specialized
2. Databases
3. Data retrieval tools and methods
4. Molecular visualization
5. Gene structure and function prediction (using GenScan, GeneMark)
6. Sequence similarity searching (NCBI BLAST)
7. Protein sequence analysis (ExPASy proteomics tools)
8. Multiple sequence alignment (Clustal)
9. Molecular phylogeny (PHYLIP)
10. Small molecule building, using ISIS DRAW and CHEM SKETCH
11. Homology Modeling using SPDBV
12. Model structure refinement using SPDBV
13. Model validation using What Check and Pro Check
14. Docking using DOCK or AUTODOCK or AMBER

REFERENCE

Bioinformatics- A Practical Approach, K. Mani and N. Vijayaraj, Aparna Publications, Coimbatore.

COURSE OUTCOME

- Describe about sequencing alignment and similar search tool Provide hands on training on various tools and techniques employed in biological sequence analysis
- Explain about protein structural analysis using Bioinformatics tools
- Expose to several DNA and protein databases.
- Practice methods and tools used for phylogenetic analysis.