BHARATHIAR UNIVERSITY
COIMBATORE-641 046

PG DIPLOPMA IN BIOINFORMATICS

SEMESTER PATTERN

(For the Candidates admitted during the academic year 2008-09 onwards)

Semester	Subject Code	Title of the Paper	Marks
I	**08PGDBI01**	Paper-I : Fundamentals of Biological Systems	100
	08PGDBI02	Paper-II : Molecular interactions	100
	08PGDBI03	Paper-III : Programming for Bioinformatics	100
	08PGDBIP01	Practical –I: Computer Programming	100
II	**08PGDBI04**	Paper-IV : Computational methods for Sequence analysis.	100
	08PGDBI05	Paper-V : Genomics & Proteomics	100
	08PGDBI06	Paper-VI : Molecular Modeling & Computer Aided Drug Design	100
	08PGDBIP02	Practical-II : Biological Databanks, Sequence Analysis, Modeling and Drug Design	100

* Includes 25% continuous internal assessment marks.
Practical examinations to be conducted at the end of the academic year.

08PGDBI01 **SEM.I**

FUNDEMENTALS OF BIOLOGICAL SYSTEMS

Objective: To understand the basics of organization, biology and functions of cell, the basic unit of life.

Unit I :

Biology of cells: Cells as a unit of life, structure of prokayotic and eukaryotic cells. An overview of organells (Mitochondria, chloroplasts, ER, Golgi, ribosomes, lysosomes and peroxysomes, nucleus and nucleolus). Differences and similarities in plant and animal cells. Cellular membrane: structure, transport, channels, carriers, receptors, endocytosis, membrane potentials.

Unit II:

DNA replication; Transcription and Translation.

Cell-cell interactions and signal transductions: Intercellular junctions, signaling by hormones and neurotransmitters; receptors, G-proteins, protein kinases and second messangers.Protein traffic in cells.

Unit III:

Cell Cycle and regulation – Mitosis, Meiosis.

Mutation – Types of mutations, types of mutagenic agents and their molecular mechanism; DNA repair; Chromosomal types and structure; Mechanism by which genome undergoes changes, recombination, mutation, inversion, duplication, and transposition.

UNIT-IV

Molecules of Life: Introduction to carbohydrates-Monosacharides and their derivatives, Disacharides, Polysacharides.

Proteins –Structure of aminoacids, Different levels of organization-Primary, secondary tertiary and Quarternary structures.

Nucleic acids – Purines, pyrimidines, Nucleosides and Nucleotides, Different structural form of DNA, denaturation and renaturation of DNA

Lipids-Structure and function of Fatty acids, Triacylglycerols, sphingolipids, steroids and glycerophospholipids.

Water, small molecules-Alkaloids, glycosides, phenols, oligopeptides, Flavonoids, and terpenoids

UNIT-V

Enzymes: Units of Activity,coenzymes and metal cofactors, temperature and pH effects, Michaelis – Menten kinetics, inhibitors and activators, active site and mechanism of enzyme action, Isoenzymes, allosteric enzymes.

Metabolism of glucose: glycolysis, TCA cycle, glycogenesis, glycogenolysis and

gluconeogenesis, pentophosphate shunt, ETC. Digestion of protein and protein metabolism, nitrogen balance: transamination, oxidative deamination and urea cycle. Lipid metabolism: beta oxidation. Interconnection of pathways, metabolic regulations.

REFERENCES:

1. Lehninger, A. L. 1984. **Principles of Biochemistry.** CBS publishers and distributors, New Delhi, India
2. Horton, Moran, Ochs, Rawn, Scrimgeour **Principles of Biochemistry** Prentice Hall Publishers.
3. David. E. Sadava **Cell Biology: Organelle Structure and Feunction** Jones & Bartlett publishers.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.

08PGDBI02 **SEM.I**

MOLECULAR INTERACTIONS

Objective: to understand the basic concepts of interaction, how biological molecules interact with each other and the experimental techniques to study these molecules.

UNIT-I

Fundamentals of atomic and molecular orbitals:

Theory of atomic and molecular orbitals; Linear combination of atomic orbitals; Quantitative treatment of valency bond theory and molecular orbital theory; Resonance structures; σ-bonds and π-bonds.

UNIT-II

Fundamentals of chemical bonding and non-bonding interactions:

Electrovalent bond, stability of electrovalent bond. Co- valent bond – partial ionic character of co-valent bonds. Shape of orbitals and hybridization. Co-ordination bond, Vander Waals forces; Metallic bond. Molecular geometry- VSEPR Theory.

UNIT-III

Folding pathways: Principles of protein folding, hydrophobic interactions, electrostatic interactions, non-bonded interactions. Beta turns, gamma turns, types of helices, disulphide bridge.

UNIT –IV

Molecular interactions: **protein-protein, protein-DNA, DNA-Drug, Protein-Lipid, Protein-Ligand, Protein-Carbohydrate interaction, Metalloproteins, Pi … Pi interactions, C-H…Pi interactions.**

UNIT-V

Spectroscopy: **Principles, Theory, Instrumentation and Application of UV, IR, NMR and Circular dichroism (CD) to macro molecules.**

REFERENCES:

1. Albert cotton, F. 1971. **Chemical Application of Group Theory**. John Wiley and Sons, Inc. New York. 386 pp.
2. Spice, J. E. 1964. **Chemical Bonding and Structure**. Pergamon Press Ltd., Headington Hill Hall, Oxford. 395 pp.
3. Winter, m. j. 1996. **Chemical Bonding**. Oxford University Press, Inc., New York. 91 pp.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.

08PGDBI03 **SEM.I**

PROGRAMMING FOR BIOINFORMATICS

Objective: To develop programming skills in C,C++ & PERL.

UNIT-I:

Programming in C

Introduction, Data types, Operators, Expressions, Control Flow, Structures, Input and Output, Functions, Pointers and References, String Processing, File Handling

UNIT-II

Programming in C++

Basic concepts of OOPS-Introduction to C++,C vs C++-data types, variables, constants, operators and statements in c++- Functions in c++- function prototype-definition-inline functions-overloaded functions.

UNIT- III

Programming in PERL

Introduction, Basic Operators and Control Structures, Scalars, Lists, Hashes, File Manipulation, Pattern Matching and Regular Expressions, Subroutines, Text and String Processing

UNIT-IV

Python Programming

Overview, Data structures, Control Flow, Modules, Basic I/O, Exception Handling, Regular Expressions, File Manipulation, Classes, Standard library

UNIT-V

BioPERL Programming

General Bioperl classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local Database)

REFERENCES:

1. B.W.Kernighan and D.M. Ritchie **The C Programming Language**, II Edition. Prientice Hall of India.
2. Larry Wall, Tom Christiansen & John Orwant **Programming Perl** –3 ed 2000- O' Reilly
3. Mark Lutz, **Programming Python,** II Edition., O' Reilly
4. E. Balagurusamy , **Programming in C++ -** Tata Mc. Graw Hill Edition
5. Byron Gottfried.1998. **Programming with C** (Schaum's Outline Series) - Tata McGrawHill Publishing Company .
6. Robert Laffore , **Object oriented programming with c++** -Waite series.
7. Larry. Wall, **Programming Perl** - Tom Christiansen, Orielly Publications

08PGDBIP01 **SEM.I**

PRACTICAL – I –COMPUTER PROGRAMMING

MS-Office and HTML.

1. Working with MS-Office Packages –One Exercise each in Word, Excel, Power Point and Access.
2. Working with HTML Tags and HTML Forms. Creating HTML Pages (At least five different pages to be created using all tags learnt).
3. Basic commands in MS-DOS and command line execution in LI NUX.

Programming in C, VB & PERL

1. Program to check odd or even numbers
2. Program to find the greatest of the three numbers and sum of average
3. Program to check leap year
4. Program to Matrix Multiplication
5. Program to Convert DNA to RNA and Vice versa
6. Program to read a protein sequence data from a file

REFERENCES:

1. K. Mani and N. Vijayaraj , **Bioinformatics a Practical Approach**, Aparna Publications, Coimbatore.
2. Byron Gottfried.1998. **Programming with C** (Schaum's Outline Series) - Tata McGrawHill Publishing Company .
3. Content Developments Group " Visual Basic 6 Programming " TMH Publishers 2002.

08PGDBI04 **SEM.II**

COMPUTATIONAL METHODS FOR SEQUENCE ANALYSIS

Objectives: To understand various computational techniques employed to analyze biological data with the use of sequence information.

UNIT-I

Introduction to bioinformatics, Classification of biological databases, Biological data formats, Application of bioinformatics in various fields. Introduction to single letter code of aminoacids, symbols used in nucleotides, data retrieval- Entrez and SRS.

UNIT-II

Introduction to Sequence alignment. Substitution matrices, Scoring matrices – PAM and BLOSUM. Local and Global alignment concepts, Dot plot. Dynamic programming methodology: Needleman and Wunsch algorithm. Smith–Waterman algorithm. Statistics of alignment score. Multiple sequence alignment. Progressive alignment. Database search for similar sequences using FASTA and BLAST Programs.

UNIT-III

Evolutionary analysis: distances, Cladistic and Phenetic methods. Clustering Methods. Rooted and unrooted tree representation. Bootstrapping strategies, Use of Clustal and PHYLIP.

UNIT-IV

Gene finding methods. Gene prediction: Analysis and prediction of regulatory regions. Fragment assembly. Genome sequence assembly, Restriction Mapping, Repeat Sequence finder.

UNIT-V

Concepts of secondary structure prediction of RNA and Protein. Probabilistic models: Markov chain, Hidden Markov Models-other applications.

REFERENCES

1. S.C. Rastogi, Namita Mendiratta, Parag Rastogi. **Bioinformatics – Concepts, Skills, Applications".**
2. Andréa's D. Baxevanis, B.F. Francis Ouellette. **Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins.**
3. Richard Durbin et al.**Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids.**
4. Doolittle R.F **Computer Methods for Macromolecular Sequence Analysis**.. (Ed.) (Methods in Enzymology, VOl. 266).
5. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
6. Bishop M.J. Rawlings C.J. (Eds.) **DNA and Protein Sequence Analysis. A Practical approach.**
7. Teresa. K. Atwood and David J. Parry-Smith **Introduction to Bioinformatics.**

08PGDBI05 **SEM.II**

GENOMICS & PROTEOMICS

Objectives: To understand the genome architecture and to extract information like gene function, gene regulation, protein evolution and targets for drug designing. Taxonomy, structure - function relationship and functional aspects of the entire set of cell proteins.

UNIT I

Annotation of the Genome

- Various approaches in gene prediction

ORF prediction, Gene prediction in prokaryotes, Gene prediction in eukaryotes, Pattern discrimination, Evaluation of gene prediction method, Prediction of promoter sequences.

- **Genome analysis**

Chromosome rearrangement, Compositional analysis, Clustering of genes, Composite genes.

UNIT II

Functional Genomics

Gene expression analysis by cDNA micro arrays, SAGE, Strategies for generating ESTs and full length inserts; EST clustering and assembly; EST databases (DBEST, UNIGENE); Expression and regulation of entire set of genes, Sporulation Vs Vegetative condition in yeast and *Bacillus.*

UNIT III

Comparative Genomics

- **Purpose and Methods of comparison**

Methods of comparison, Comparison at Nucleotide level, Breakpoints level, Gene cluster level.

- **Applications of comparative Genomics**

Predicting function, Predicting regulatory elements, Analysis of conserved strings.

UNIT-IV

- **Principles of Protein classification:**

Based on Structural features, Phylogenetic relationship, CATH - Classification by Class, Architecture, Topology, Homology, SCOP - Structural Classification Of Protein, FSSP - Fold classification based on structure - structure alignment, MMDB - Molecular Modeling Database, SARF - Spatial arrangement of backbone fragments

UNIT - V

Proteome analysis

- 2D Electrophoresis

Immobilized pH gradient, Sample preparation, First dimension criteria, second dimension criteria, Stabilization, Detecting protein on gel, Electro blot, Image analysis,
Digital imaging, Spot detection and quantification, Gel matching

REFERENCES

1. David W. Mount, 2001. **Bioinformatics Sequence and Genome Analysis**. Cold Spring Harbor laboratory Press.
2. S.R. Pennigton and M.J. Dunn. 2002. **Proteomics**. Viva Books Private Limited. New Delhi. (for Units III and IV and V.)
3. Carl Branden and John Tooze 1999. **Introduction to Protein Structure**. Garland Publishing. New York. (for Units I and II)
4. Laszlo Patthy, 1999. **Protein Evolution** Blackwell Science
5. Shanmughavel, P. 2005. **Principles of Bioinformatics**, Pointer Publishers, Jaipur, India.
6. Inna Dubchak et al. 2000, Active conservation of noncoding sequences revealed by three way species comparisons. *Genome Research*. **10**, 1304-1306

08PGDBI06 **SEM.II**

MOLECULAR MODELING & COMPUTER AIDED DRUG DESIGN

Objectives: To understand the concepts of molecular modeling and computational approaches for drug design.

UNIT-I

Introduction to the concepts of molecular modeling. Molecular structure and internal energy. Application of molecular graphics. Energy minimization of small molecules: Empirical representation of molecular energies. Use of force fields and the molecular mechanics method. Discussion of local and global energy minima.

UNIT-II

The techniques of molecular dynamics and Monte Carlo. Simulation for conformational analysis. *Ab initio,* dft and semi empirical methods.

UNIT-III

Macromolecular modeling. Design of ligands for known macromolecular target sites. Principles of Docking studies, Drug – receptor interactions. Classical SAR. / QSAR studies and their implications to the 3-D modeler. 2-D and 3-D database searching. Pharmacophore identification and novel drug design.

UNIT-IV

Docking-Rigid and Flexible.Finding new drug targets to treat disease, new targets for anti-cancer drugs, Drugs that rescue mutant p53's.

UNIT-V

Structure-based drug design for all classes of targets. Enzyme Inhibition strategies.

REFERENCES

1. Andrew R. Leach, **Molecular Modeling: Principles and Applications.**
2. Hans-x, **Basic principles and applications**
3. Yvonne C. Martin**, Designing bioactive molecules three-dimensional techniques and applications.**
4. Leo, Albert, Hockma, D.H.– Hansch, Corwin, **Exploring QSAR.**
5. Shanmughavel, P. 2005 ,**Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
6. Shanmughavel, P. 2006. **Trends in Bioinformatics,** Pointer Publishers, Jaipur, India.

08PGDBIP02 **SEM.II**

PRACTICAL II- BIOLOGICAL DATABANKS, SEQUENCE ANALYSIS, MODELING AND DRUG DESIGN

- Biological Databanks Sequence Databases, Structure Databases, Specialized Databases
- Data retrieval tools and methods
- Molecular visualization
- Gene structure and function prediction (using GenScan, GeneMark)
- Sequence similarity searching (NCBI BLAST)
- Protein sequence analysis (ExPASy proteomics tools)
- Multiple sequence alignment (Clustal)
- Molecular phylogeny (PHYLIP)
- Small molecule building, using ISIS DRAW and CHEM SKETCH
- Homology Modeling using SPDBV
- Model structure refinement using SPDBV
- Model validation using What Check and Pro Check
- Docking using DOCK or AUTODOCK or AMBER

REFERENCE:

K. Mani and N. Vijayaraj , **Bioinformatics a Practical Approach**, Aparna Publications, Coimbatore.