

**BHARATHIAR UNIVERSITY-COIMBATORE-641046**  
**M. Phil./ Ph.D. Bioinformatics Degree Course**

**(For candidates admitted from October 2011 batch onwards)**

**PART I : PAPER I**  
**RESEARCH METHODOLOGY**

**UNIT I :**

Research Methodology: Introduction ;meaning of research; objectives of research; types of research; research approaches; significances of research; research methods vs methodology; research and scientific method ; importance of knowing how research is done; research process; criteria of good research; problem encountered by researchers in India; Defining the research problem; What is the research problem? Selecting the problem; Techniques involved in defining the problem; Research design; Need for research Design; Features of good Design, important concepts relating to design; different research designs; basic principles of experimental designs.

**UNIT II :**

Hypothesis testing: What is Hypothesis? Basic concepts concerning testing of hypothesis;procedure for hypothesis testing;Probability;Markov models and Hidden Markov Models;Probability distribution;Binomial;Poisson;Normal distribution and Multiple testing Methods ANOVA;Test of significance-t-test;F-test

**UNIT III :**

Interpretation and Report writing; Meaning of Interpretations; Techniques of interpretation;precautions of interpretations; significances of report writing; Different steps in report writing; layout of the research project;types of report; oral presentation;mechanics of writing a research project; precautions for writing research reports; conclusions

**UNIT IV :**

Elements of C Programming;Features of C;Variables;Constants;keywords;Data types;operators;statements;loops – simple programs using Loops,Arrays – integer arrays – character arrays – simple programs using arrays;Introductions to functions – simple programs using functions – Introduction to pointers,structures string Manipulations using pointers and arrays;Files;Defining and opening a file,Closing a file,input/output operations on files PERL:Basic syntax-I/O – Variables,strings & arrays-control structures – regular expressions – simple programs

**UNIT V:**

Algorithms in computer sciences inspired by biology genetic algorithms,Neural networks and path optimization

**Reference:**

- 1 Kothari. C.R. 2004 Research Methodology – Methods and Techniques,New Age International(P)Ltd
- 2 E Balagurusamy.Programming in ANSI C Tata Mc Graw Hill
- 3 Randa L.Schwartz,tom phoenix,learning perl,third edition

## **PART I : PAPER II – ADVANCES IN BIOINFORMATICS**

### **UNIT I**

High throughput genome sequencing and genome assembly, Gene finding algorithms, DNA Microarrays and large gene expression data sets, clustering algorithms

### **UNIT II**

Protein and Nucleic acid sequence alignments, Sequence databases, the use of algorithm BLAST, Multiple sequence alignments

### **UNIT III**

Protein Structure analysis; Protein structure databases; Protein Structure comparison; Fold Recognition; 3D – ID Profiles; Threading; Comparative Structure Modeling

### **UNIT IV**

Phylogeny (evolutionary trees) biological networks; pathway analysis

### **UNIT V**

Emerging new ideas on treating biological systems; Pharmacogenetics and its applications; SNPs and their applications

### **Reference:**

- 1 Andreas D Baxevanis and BF Francis Oueliene 2001 Bioinformatics A Practical Guide to the analysis of Genes and Proteins, A John Wiley & sons, INC, Pub
- 2 David W Mount, 2003 Bioinformatics – Sequence and Genome Analysis, CBS Publishers, Ian Korf, Mark Yandell & Joseph Bedell, 2003
- 3 Ian Korf, Mark Yandell & Joseph Bedell. 2003 BLAST (O' REILLY) SPD Pvt Ltd

## **PART I : PAPER- III “OMICS” COMPLEXES IN PHYTOMATICS**

### **UNIT-I Purification of Macromolecules**

Moving boundary and zonal sedimentations, Partition and Ion-exchange Chromatography; Electrophoresis Principles, Electrophoresis of Nucleic acids; SDS gel Electrophoresis; Capillary Electrophoresis and Purification.

### **UNIT-II Structural Proteomics**

Experimental Techniques for Protein Structure Elucidation, X-ray Crystallography, 2-D Electrophoresis, MALDI-TOF, Mass Spectrometry, Protein Microarrays & Bioseparation, Structure Visualization & Manipulation.

### **UNIT-III Biological Databases**

Secondary & Tertiary Structure Prediction Tools: FASTA, BLAST, PSI-BLAST, CLASTALW, Multialign, Dialign, Gene Bee, Motif Scan, TMPred, GOR, Chou-Fasman, Neural Network Prediction, Promoter Finder, NEB cutter, Genscan, ORF Finder and Intron- Exon Finder.

### **UNIT-IV Pointers in Sequence analysis**

Usage of Sequence alignment & Searching Tools for Gene Identification ,Genome Annotation, ORFs, ESTs, Codon Biases, Redundancy, Conserved Motifs, Patterns, Blocks & Domains.

### **UNIT-V Metabolomics**

Understanding the Metabolic Pathways of Cyanobacteria, Microbes and Medicinal Plants. Metabolic analysis and Tools.

### **Books for References**

1. Andrew R Leach, Molecular Modeling-Principles and Applications, Prentice Hall Publications.
2. Andrews D.Baxevanis and BF. Francis Ouellette, Bioinformatics-A Practical guide to the Analysis of Genes and Proteins, A John Wiley & Sons Pub, 2001.
3. David W.Mount, Bioinformatics-Sequence and Genome Analysis, CBS Publishers 2003.
4. Ian Korf, Mark Xandell & Joseph Bedell, BLAST (O'REILLY), SPD Private Ltd, 2003.
5. Philip E Bourre, 2003, Structural Bioinformatics, A John Wiley & Sons Publication.
6. D.Bowtell and Sambrook, DNA Microarrays-A Molecular Cloning Manual, Cold Spring Harbor Laboratories Publication, Cold Spring Harbor, New York.
7. Robert K.Scopes, Protein Purification – Principles and Practice (3rd edition), Springer International Edition.

**Part I- PAPER-III**  
**BIOLOGICAL DATABASES, DATA MINING AND MICROARRAYS**

**UNIT-I**

Biological database - Sequence databases - Other specialized databases – Microarray databases - Database browsers and search engines.

**UNIT-II**

Data mining definition – Classification and clustering of data – Association rules – Data visualization.

**UNIT-III**

Introduction to Microarrays - Oligonucleotide and Spotted cDNA arrays - Design considerations for microarray experiments – Goals of a microarray experiment.

**UNIT-IV**

Basic research with DNA microarrays – Microarrays and Cancer - Myeloid leukemia (AML) vs. acute lymphoblastic leukemia (ALL) data analysis.

**UNIT-V**

Use of array analysis programs – SAM - TIGR programs – MEV.

**Books for References**

1. Analysis of DNA Microarray Data by Steen Knudsen.
2. Discovering Genomics, Proteomics, and Bioinformatics by A.M. Campbell and L.J. Heyer.

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**Part I – Syllabus**  
**PAPER III – COMPREHENSIVE ANALYSIS IN BIOCHEMICALS**

**UNIT-I Genome analysis**

Isolation of genomic and organelle DNA from Prokaryotes and Eukaryotes. Mapping and sequencing genes, Electrophoretic karyotyping, Construction and screening of genomic DNA libraries. Functional genomics: Sequence based, Microarray based approaches, in silico vector construction.

**UNIT-II Techniques for Isolation and Purification of Protein & Bio-active compounds**

Extraction (soxhlet and cold percolation), Isolation of Alkaloids and Flavonoids, Protein extraction from Micro organisms, Plants and Animals. Purification: Hanging drop, Native gel, Chromatographic methods (Column, Preparative TLC, HPLC, HPTLC, Ion exchange, Gel filtration, Affinity), Crystallization.

**UNIT-III Structure elucidation of Protein and Bioactive compounds**

Crystal studies, IR, NMR, MASS, CHN analysis, X-ray diffraction, 2-D Electrophoresis, Protein microarray. Tools used for protein structure prediction: BLAST, PDB, Swiss Model, Modeler, PSIPRED, JPRED; Structure validation: SAVS; Motif databases: BLOCKS, PROSITE, PFAM, COG.

**UNIT-IV Metabolomics and Evolutionary Biology**

Analyzing databases for Metabolic Pathways (WIT, KEGG, PathDB, PathCase); Reconstruction of metabolic pathways (Biocyc, ASGARD); Metabolic and Cellular simulation: Gepasi , Virtual cell; Tools for Phylogenetic analysis: CLUSTALW, PHYLIP, MEGA.

**UNIT-V Molecular Interaction and Docking**

Determination of active site and hot spots, Receptor-Ligand interactions, Pharmacophore identification (Catalyst, DISCO, GASP), De novo drug designing (Group Build, Gen Star). Tools used for docking (AUTODOCK, FLEX X, GLIDE).

**Books for references**

1. Sujata V. Bhat, Bhimsen A. Nagasampagi and Meenakshi Sivakumar. Chemistry of Natural Products, Narosa Publishing House.
2. Daniel M. Bollag, Michael D. Rozycki and Stuart J. Edelstein. Protein Methods. Wiley-Liss. A John Wiley & Sons, INC, Publications.
3. Mount, David W. Sequence and Genome Analysis. Cold Spring Harbor Laboratory Press Publications.
4. S.B.Primrose and R.M.Twyman. Principles of Gene Manipulation & Genomics. Black well Publishing.
5. Cynthia Gibas and Per Jambeck. Developing Bioinformatics Computer Skills. O'Reily and Associates.
6. Jin Xiong. Essential Bioinformatics. Cambridge University Press.
7. Thomas Lenganr (Ed). Bioinformatics - From Genomes to Drugs Volume I and II. Wiley-Veh, Germany.

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**PAPER- III COMPUTATIONAL BIOLOGY**

**UNIT I: DATA MINING AND SEQUENCE ANALYSIS**

- Biological background for sequence analysis.
- Searching for database for similar to a new sequence.
- Identification of protein primary sequence from DNA sequence.
- Searchingfor database for similar to a new sequence.
- Calculation of sequence alignment for evolutionary interferences and to aid in structural and functional analysis.

**UNIT II: SIMILARITY SEARCHES & CONSTRUCTION OF PHYLOGENETIC GUIDE TREE**

- Distance and similaity.
- The evolutionary basis for sequence alignment.
- Substitution scores and gap penalties.
- Optimal alignment method.
- Database similarity searching.
- FASTA and BLAST.
- Conclusion and internet software availability.

**UNIT III: PRACTICAL ASPECT OF MULTIPLE SEQUENCE ALIGNMENT**

- Introduction.
- MULT ALIN.
- BLOCKS.
- MOST.
- Probe.
- MacBoxshade.

**UNIT IV: PHYLOGENETIC ANALYSIS**

- Introduction.
- Phylogenetic tree building methods.
- Multiple tree alignment procedures.
- Searching for trees.
- Evaluating trees and data.
- Phylogenetic software's.
- Internet resources.

## **UNIT V: PREDICTIVE METHODS USING PROTEIN AND NUCLEIC ACID SEQUENCES**

- Introduction.
- Detecting functional sites in DNA.
- Internet tools for identification of protein coding genes.
- Internet resources for repeat analysis.
- Predictive methods using protein sequences.
- AACompIdent and AACompsin.
- Secondary structures and folding classes.
- nnPredict, predict protein, ssPRED, SOPMA.
- Tertiary structures.

### **Books for References**

1. Computer methods for macromolecular sequence analysis. Doolittle R.F (Ed.). Academic Press, San Diego (1996).
2. Introduction to Bioinformatics. Teresa K. Attwood and David J. Parry-Smith.
3. Bioinformatics-concepts, skills, applications. S.C. Rastogi, Namita Mendiratta, Parag Rastogi.
4. Bioinformatics – A practical approach 2004. K. Mani and N. Vijayaraj. Aparna publications.
5. Hand book of computational Molecular Biology. Edited by Srinivas Aluru. Chapman and Hall 2006.
6. Computational Methods in Molecular Biology Edited by S. Salzberg, D. Searls, and S. Kasif. Elsevier Science, 1998.
7. Sequence and Genome Analysis. By David W. Mount Published 2004 CSHL Press Science.
8. Trends in Bioinformatics. By Dr. P. Shanmughavel. 2006 Pointer publishers, Jaipur, India.
9. Principles of Bioinformatics. By Dr. P. Shanmughavel. 2005 Pointer publishers, Jaipur, India.

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Part I - Syllabus

**PAPER III – STRUCTURAL BIOLOGY AND BIOPHYSICS**

**UNIT-I:**

**Basics:** Fundamentals of proteins, carbohydrates and Nucleic Acids, Classification of proteins, Helix, Sheet, Strand, Loop and Coil, Active site, Class and Domains, Fold, motif, Profile, Protein stability, protein folding.

**UNIT-II:**

**Structural classification of proteins:** Understanding various structure of protein, globular and fibrous protein, membrane protein.

**Functional classification of proteins:** Cell surface receptors, GPCR, kinases, channel proteins, Ubiquitin.

**UNIT-III:**

**Structure Prediction:** Protein sequencing; Secondary structure prediction tools and methods, tertiary structure prediction tools and methods; Structure alignment, validation, refinement, prediction; protein- protein interactions.

**UNIT-IV:**

**Scope and methods of Biophysics:** Basics of X-rays, crystals and symmetry; X-ray crystallography, nuclear magnetic resonance, UV spectrophotometry, electron microscopy, cryo electron microscopy, atomic force microscopy, MALDI-TOF, Mass spectrophotometry, synchrotron radiation and its uses, Protein and DNA microarray.

**UNIT-V:**

**Databases:** Protein Sequence databases; Structure Databases (CATH, SCOP, FSSP, MMDB, PDB, MPDB, TMPDB, SARF); Docking, QSAR, Drug Discovery, Intellectual Property rights.



**Books for References:**

- 1) **Outline of Crystallography for Biologists**- David Blow
- 2) **Principles of Proteomics** - R.M.Twyman
- 3) **Structural Biology of Membrane Proteins** – Reinhard Grisshammer and Susan K Buchanan
- 4) **Proteins Structures and Molecular Properties** - Thomas. E. Creighton
- 5) **Biophysical Chemistry Part II Techniques for the study of biological structure and function** - Cantor and Schimmel
- 6) **Foundations of Structural Biology** - Leonard Banaszak
- 7) **Structural Bioinformatics** - Philip E. Bourne
- 8) **Textbook of Biochemistry** - Thomas M Devlin