

## ANNEXURE-III

BHARATHIAR UNIVERSITY, COIMBATORE - 641 046

M.Phil. / Ph.D. : **BIOINFORMATICS**

### Part I-Syllabus

## 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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**M.Phil Degree Course**

**Part I - Syllabus**

**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.
- Searching for 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 similarity.
- 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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M.Phil Degree Course

Part I - Syllabus

**PAPER- III “OMICS” COMPLEXES IN PHYTOMATICS**

**UNIT-I Purification of Macromolecules**

Moving boundary and zonal sedimentations, Partion 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 (3<sup>rd</sup> edition), Springer International Edition.

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**M.Phil Degree Course**

**Part I - Syllabus**

**PAPER III – STRUCTURAL BIOLOGY AND BIOPHYSICS**

**UNIT-I**

PERL, C+, PYTHON, MySQL, SCOP, CATH, FSSP, BIND, DIP, FASTA, BLAST, PSI, KEGG, PDB.

**UNIT-II**

Ramachandran Plot, GOR, Chou-FASMAN method, secondary tertiary Structure Prediction, TMpred, ORFs, ESTs, MOTIF, Sequence alignment.

**UNIT-III**

Structure alignment, Structure validation, Refinement, Prediction, Protein-protein interaction, membrane protein, Microarrays, Docking, QSAR, Drug discovery.

**UNIT-IV**

X-ray crystallography, nuclear magnetic resonance, UV spectrophotometry, electron microscopy, cryo electron microscopy, atomic force microscopy, MALDI-TOF, Mass spectrophotometry.

**UNIT-V**

Fundamentals of protein, carbohydrates and nucleic acids, classification, biographies, management, Intellectual property rights.

**Books for References**

- 1) Principles of Proteomics by R.M.Twyman.
- 2) Bioinformatics principles and Applications by Zhumur Ghosh.
- 3) Introduction to Systems Biology by Sangdun Choi.

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**Part I – Syllabus**

### **PAPER III – COMPREHENSIVE ANALYSIS IN BIOCHEMATICS**

#### **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: Modeler, Rosetta, 3-D-PSSM, PHD, PSIPRED, JPRED. Motif databases: BLOCKS, PROSITE, PFAM, PRINTS, COG.

#### **UNIT-IV Metabolomics**

Analyzing databases for Metabolic Pathways (WIT, KEGG, PathDB, BIOCARTA, PathCase). Metabolic and Cellular simulation: Gepasi, XPP, Virtual cell. Reconstruction of metabolic pathways (Biocyc, ASGARD).

#### **UNIT-V Molecular Interaction and Docking**

Determination of active site and hot spots, Receptor-Ligand interactions, Pharmacophore identification (Catalyst, DISCO, GASP), Denovo drug designing (Group Build, Gen Star). Tools used for docking (DOCK, FLEX, GLIDE, SLIDE, GOLD, SURFLEX).

### **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 Lengauer (Ed). Bioinformatics - From Genomes to Drugs Volume I and II. Wiley-Vch, Germany.