

**BHARATHIDASAN UNIVERSITY, TIRUCHIRAPPALLI – 620 024**

## **CERTIFICATE PROGRAMME IN BIOINFORMATICS**

**(UGC sponsored Career Oriented Programme)**

**(For the candidates to be admitted from the academic year  
2005 – 2006 onwards)**

### **PAPER – I**

## **BIOPHYSICS AND STRUCTURAL BIOLOGY**

### **UNIT – I**

Bioinformatics – an overview, Definition & History – Internet resources - Cell structure and function – cell organelles - Key Biomolecules – lipids, polysaccharides, proteins, nucleic acids – overview of protein and nucleic acid structure

### **UNIT – II**

Proteins – Amino acids – Peptide bond – Ramachandran map – Protein denaturation and renaturation – Levels of protein structure -  $\alpha$ -helix,  $\beta$ -sheet and  $\beta$ -turns – Super secondary structures – Domains - quaternary structure –DNA and RNA structure - helical structures of DNA - Watson and Crick model - A, B and Z forms of DNA - RNA secondary structure – different forms of RNA

### **UNIT – III**

Methods for structure determination – Spectroscopic techniques - Infrared (IR), Ultraviolet (UV)–Visible spectroscopy - Fluorescence spectroscopy - Nuclear Magnetic Resonance (NMR) techniques – application to bio-macromolecules – X-ray crystallographic method of structure determination – Phase problem – Electron density map and interpretation – structure refinement.

### **UNIT – IV**

Methods of structure prediction - secondary structure prediction methods – Chou-Fasman, GOR – tertiary structure prediction - Homology (comparative) modeling – Fold recognition (threading) – ab initio method – Monte Carlo – Rosetta – CASP

## UNIT - V

Genetic Engineering – DNA sequencing – Introduction to human genome project - Genomics & Proteomics - Protein engineering – Structure-based drug discovery – binding sites detection – docking.

### Reference Books

1. T.K. Attwood and D.J. Parry-Smith, *Introduction to Bioinformatics*, Pearson Education Ltd., New Delhi (2004).
2. D.R. Westhead, J.H. Paris and R.M. Twyman, *Instant Notes: Bioinformatics* – Viva Books Private Ltd, New Delhi (2003).
3. J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, 5<sup>th</sup> edition, W. H. Freeman & Co. New York (2002).
4. C. Branden and J. Tooze, *An Introduction to Protein Structure*, Garland Publishing, House, New York (1998)
5. C.R.Cantor & P.R.Schimmel, *Biophysical Chemistry Part - II Techniques for the Study of Biological Structure and Function*, W.H. Freeman & Co., in San Fransisco, 1980
6. D. S. T. Nicholl, *An Introduction to Genetic Engineering*, Cambridge University Press, New Delhi (2002).

## **PAPER – II**

### **COMPUTATIONAL METHODS IN BIOINFORMATICS**

#### **UNIT - I**

DNA & Protein Sequence analysis – Pairwise sequence comparison – Sequence databases and searches – Swiss-Prot, NBRF-PIR, GenBank, DDJB - BLAST and FASTA search.

#### **UNIT II**

Algorithms for pairwise sequence alignment – Scoring matrices - PAM and BLOSUM - Local and Global alignment concepts - dynamic programming methodology - Needleman and Wunsch algorithm - Smith-Waterman algorithm - Statistics of alignment score - Multiple sequence alignments - Phylogenetic trees – Profiles and motifs – distance and similarity – Evolutionary basis of sequence alignment.

#### **UNIT III**

Protein structure data base (PDB) - Protein structure visualization tools – RasMol, Swiss PDB Viewer - Structure – Classification, alignment and analysis – SCOP, CATH, FSSP databases - Solvent accessibility and Interactions – Physico-chemical properties – Homology modeling using SPDBViewer or Insight II.

#### **UNIT IV**

Predicting Protein structure and function from sequence – Feature detection – Domains & Motifs – BLOCKS, PRINTS, PFAM – Secondary structure prediction – algorithms for predicting protein folds - Predicting 3D structure – comparative (homology) modeling.

#### **UNIT V**

Genomics and Proteomics – Sequencing genomes - Sequence assembly – Genome databases on the web (GDB) – Annotating and analyzing genome sequences – Proteomics.

## Reference Books

1. Arthur M. Lesk, *Introduction to Bioinformatics*, Oxford University Press, New Delhi (2003).
2. D. Higgins and W. Taylor (Eds), *Bioinformatics- Sequence, structure and databanks*, Oxford University Press, New Delhi (2000).
3. R.Durbin, S.R.Eddy, A.Krogh and G.Mitchison, *Biological Sequence Analysis*, Cambridge Univ. Press, Cambridge, UK (1998). (Chaps 1 & 2)
4. A. Baxevanis and B.F. Ouellette. *Bioinformatics: A practical Guide to the Analysis of Genes and Proteins*, Wiley-Interscience, Hoboken, NJ (1998).
5. Arthur M. Lesk, *Introduction to Protein Science*, Oxford University Press, New Delhi (2004).

## **PAPER – III**

### **BIOINFORMATICS AND COMPUTATIONAL BIOLOGY LAB**

1. Study of Internet resources in Bioinformatics. E.g. NCBI, CGEB, EMBL.
2. Searches on MEDLINE, PubMed and CDROM bibliographic databases.  
Concept of boolean operators in searching.
3. Introduction to sequence data bases  
  
Protein sequence databank, NBRF-PIR, SWISSPROT, EMBL.  
Nucleic acid sequence databank – Gene bank, EMBL
4. Pair wise alignment- Needleman-Wunsch and Smith-Waterman algorithms
5. Multiple alignment- CLUSTALW & PRINTS
6. BLAST, FASTA programs for sequence database search
7. Genome data bank – study the features of human genome.
8. Evaluation of protein structure by Swiss PDB viewer and by other molecular visualization tools.
9. Calculation of phi – psi angles - Ramachandran plot.
10. Homology modeling of a given protein sequence.

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**SCHEME OF EXAMINATIONS**

<b>Semester</b>	<b>Title of Paper</b>		<b>Marks</b>
<b>I</b>	Paper I - Biophysics and Structural Biology		100
	Paper II - Computational Methods in Bioinformatics		100
	Paper III - Bioinformatics and Computational Biology Lab		100
<b>Total</b>			<b>300</b>