ADDITIONAL DIPLOMA IN COMPUTATIONAL BIOLOGY

ADDITIONAL DIPLOMA COURSE OFFERED

PG DIPLOMA IN COMPUTATIONAL BIOLOGY

Semester	Paper	Subject	Hrs Per week	University examination		Credits
				Duration in Hrs.	Max. Marks	
SEMESTER I	09MBTDA01	Basics of computational biology	4	3	100	4
SEMESTER II	09MBTDA02	Genomics and proteomics	4	3	100	4
SEMESTER III	09MBTDA03	Cheminformatics and Pharmacogenomics	4	3	100	4
SEMESTER IV	09MBTDAP	Computational biology lab	6	3	100	4

PAPER I : 09MBTDA01 INTRODUCTION TO BIOINFORMATICS

Unit I

Bioinformatics - Definition, History, Web servers, computer systems, languages, - machine, high level and assembly. Internet basics – internet connection, web browsing and URL.

Unit II

Introduction to biological databases - Sequence databases, structural databases, specialized databases, sequence retrieval system from net - SRS, Entrez

Unit III

Protein structure prediction – Gene and protein expression data, protein interaction data, similarity and database structure tools, FASTA, BLAST

Unit IV

Sequence analysis and phylogeny – Sequence and similarity – sequence alignment – local, global pairwise and multiple sequence, introduction to scoring matrix – PAM and Blossum, introduction to phylogenetic trees.

Unit V

Introduction to programming: C and Perl. Datatypes, operators, expressions, control flow, structures, in put and output, functions, pointers and references, string processing, file handling.Basic Level Program.

REFERENCES:

1. Introduction to bioinformatics by T.A Atwood
2. Introduction to computers by Alexis Leon and Mathews Leon
3. Trends in Bioinformatics by P.Shanmughavel
4. Programming C by Balaguruswamy
5. Beginning Perl to bioinformatics by James Tisdaal

PAPER II : 09MBTDAO2 GENOMICS AND PROTEOMICS

Unit I

Introduction to genomics: genome structure, physical mapping of genome, genome sequencing, functional genomics, genome wide mutation for annotation, plant transcriptomics and expression analysis by SAGE, MPSS, DDDPCR, and Microarray.

Unit II

Genome organization in pro and eukaryotes: whole genome sequencing technologies; assembly of sequence reads; annotation and other methods of genome; sequence analysis; minimal genome concept.

Unit III

Functional genomics of microbes, plants and animals: Transcriptome analysis methods, microarrays and serial analysis of gene expression. Data bases of expressed sequence tags. Data mining.

Unit IV

Principles of protein classification: Based on the structural features, phylogenetic relationship, CATH – Classification by class, architecture, Topology, 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

Proteomics of selected systems: Methods and applications of proteome analysis. Expression proteomics; 2D and multidimensional chromatography. MALDI method and applications in protoemics. Protein interaction analysis.

REFERENCES:

1. Genomics: The Science and Technology Behind the Human Genome Project (2000). Edited by C.Cantor and C.L.Smith, Wiley -Interscience, New York.
2. Genome Mapping – A Practical Approach (1997) by P.H. Dear, Oxford University Press, Oxford.
3. Reviews and Articles from Journals such as Nature, Science, PNAS (USA), Nucleic Acids Research, Trends Series & Current Opinion Series.
4. Proteine Research: New Frontiers in Functional Genomics (1997). Edited by M.R. Wilkins, K.L. Williams, R.D.Appel and D.F. Hochstrasser, Springer – Verlag, New York.
5. 2-D Proteome Analysis Protocols (1998). Edited by A.L. Link, Humana Press, Totowa, NJ.
6. Proteins and Proteomics. 2002. R.J. Simpson. Cold Spring Harbor Lab. Press. New York.

PAPER III: 09MBTDA03 CHEMINFORMATICS AND PHARMACOGENOMICS

Unit I

Chemical information sources: Chemical databases, chemical abstracts registry system, searching by structure, chemical reaction information, analytical chemistry information, chemical property information, patents.

Unit II

Spectroscopy and crystallography in chemoinformatics: overview of structure determination by NMR, NMR and combinatorial chemistry, the symmetry notations used in X-ray crystallography, molecular modeling of receptor sites.

Unit III

Chemical informatics applications: Computer aided drug design, combinatorial chemistry, SAR, chemoinformatics software statistical analysis tools. Bibliometrics, property prediction, phamacophore searching.

Unit IV

Pharmacogenetics: polymorphic genes encoding drug metabolism enzyme, transportors, receptors and other drug targets, man an animals. Effects of genetic polymorphism on the desposition and the metabolism of drugs, environmental and endogenous chemicals and other xenobioitcs. Regulation of drug metabolizing enzymes – examples.

Unit V

Pharmacogenomics in drug discovery: Drug discovery principle, target identification, screening methodologies and assays, mechanism based design, structure based design, invitro invivo testing, chemical analogues and development issues.

REFERENCES:

1. G H Grant and WG Richrds "Computational Chemistry" oxford science publication, Oxford 1995.
2. D M Hirst A computational approach to chemisty Blackwell scientific publication Morsby. 1990.
3. Wm. L Allen etal, Editors Pharmacogenomics: application to patient care. American College of clinical pharmacy 2004.

PRACTICAL: 09MBTDAP COMPUTATIONAL BIOLOGY LAB

1. **Introduction to sequence analysis software**

   Installation of EMBOSS; Use of EMBOSS and GCG; BioEdit; Public Domain Software; Internet access to software and databases

2. **Accessing Biological Databases:**

   Retreiving protein and nucleic acids sequences, structures, EST sequences, SNP data and biomedical information from databases; Using database browsers and genome browsers; Converting sequences between different formats; Using sequence editors; Sequence assembly

3. **Nucleic acid sequence analysis:**

   Detecting ORFs; Identification of translational and transcriptional signals; Gene predictions; Codon usage; RNA Fold analysis

4. **Sequence alignment and applications:**

Pairwise alignment – Dot matrix comparisons, Global and Local alignment; Database searching – different pairwise methods; Use of scoring matrices and gap penalties; Statistical vs Biological significance; Handling large datasets; genome comparisons.

5. **Multiple sequence alignment and applications:**

Use of Mutliple sequence editors; Progressive alignment and iterative alignment approaches; Use of Profile methods; Motif detection; Clustering and Phylogeny approaches; Protein family classification

6. **Protein sequence analysis:**

Composition analysis; Hydrophobicity and amphilicity analysis; Transmembrane predictions; Secondary structure prediction

7. **Integrating information:**

Report generation; Making presentations of results; Placing analysis in biological context; Limits of analysis

8. **3D structure retrieval and visualization using rasmol**
9. **Molecular modeling using swissmodel – analysis using swiss PDBviewer**
10. **Molecular docking – protein protein interaction- protein ligand interaction, analysis using online servers using whatif, lpc.**
11. **MALDI**