



MCC, Department of Botany

Paper 3b BIOINFORMATICS

M. Sc. va. (Candidates admitted from academic year 2008-2009)

Elective Theory

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UNIT I

Introduction to Bioinformatics: Internet, World Wide Web, web browsers, HTML, HTTP and URLs. EMB net, NCBI. Applications of Bioinformatics. Bioinformatics as multidisciplinary tool. Information Retrieval System.

UNIT II

Biological Databases: Structure, Sequence and literature databases. Protein sequence database - PIR, SWISS-PROT, MIPS. Protein structure database - PDB, SCOP. DNA sequence databases – Gen Bank, ENBL, MBL, DDBJ. Literature data base – Med Line, PubMed. Patterns, motifs and profile Databases: Metabolic Pathway Databases.

UNIT III

Sequence Alignment and Analysis: Local and Global alignment. Scoring matrices. Database Similarity Searches: BLAST, FASTA, PSI-BLAST algorithms; Pair wise sequence alignment - NEEDLEMAN and Wunsch, Smith Waterman algorithms; Multiple sequence alignments - CLUSTAL, PRAS; Patterns, motifs and Profiles in sequences.

UNIT IV

Protein Structure Prediction and Protein Folding: Protein architecture, classification of protein structures – Primary, Secondary, Tertiary and Quaternary structures. Protein stability and folding – Ramachandran Plot. Side chains. Protein stability and denaturation. Protein structure prediction – Critical assessment of structure prediction (CASP), fold recognition, conformational energy calculations and molecular dynamics.

UNIT V

Homology, Phylogeny and Evolutionary Trees: Sequence Analysis. Alignment and Phylogenetic Trees. Homology and similarity, Phylogeny and relationships, Approaches used in Phylogenetic analysis, Molecular approaches to Phylogeny, Phylogenetic Analysis databases, Hidden Markov Models for homology modeling.

UNIT VI

Pharmacogenomics: Important parameters in Drug Discovery and the role of computational methods. Process of drug discovery – Target identification, target validation, lead identification, lead optimization and preclinical pharmacology and toxicology. Computer Aided Drug Design (CADD). Molecular docking - Concept of receptor and target. Receptor binding and activation. Ligand-receptor interaction, non-covalent bonds. Ligand into the binding site. Concepts of pharmacophore.

Suggested Reading

- ANDREAS D. BAXEVANIS AND B. F. FRANCIS OUELLETTE. 2001. Bioinformatics. A Practical Guide to the Analysis of Genes and Proteins (Second Edition). John Wiley & Sons, Inc.
- ARTHUR M. LESK, 2003 Introduction to Bioinformatics Oxford University Press
- ATTWOOD T. K. AND PARRY-SMITH D. J. 2003. Introduction to Bioinformatics. Pearson Education (Singapore) Pvt. Ltd.
- BALASUBRAMANIAN, D., BRYCE, C. F. A., DHARMALINGAM, K., GREEN, J. AND KUNTHALA JAYARAMAN. 1996. Concepts in Biotechnology (Edts.) University Press (India) Ltd.
- BASU, O., S.K. THUKRAL. 2007. Bioinformatics-Databases, Tools and Algorithms. Oxford University Press, New Delhi.
- BRYAN BERGERON, M.D. 2006. Bioinformatics Computing. 2006. Prentice Hall of India Pvt Limited, New Delhi.
- GAUTHAM, N. 2006. Bioinformatics- Databases and Algorithms, Narosa Publishing House Hall of India Pvt. Ltd, New Delhi.
- IGNACIMUTHU, S.S.J. 2005. Basic Bioinformatics, Narosa Publishing House, India.
- JEAN-MICHEL CLAVERIE AND CEDRIC NOTREDAME. 2006. Bioinformatics- A Beginner's Guide. Wiley Publishing, Inc.
- LESK, A.M. 2006. Introduction to Bioinformatics. (2nd Edition). Oxford University Press, New Delhi.
- MALCOLM CAMPBELL, A. AND LAURIE J. HEYER. 2003. Discovering Genomics, Proteomics and Bioinformatics. Pearson Education (Singapore) Pvt. Ltd.
- MURTHY, C.S.V. 2003. Bioinformatics. (1st Edition). Himalaya Publishing House, New Delhi.
- RASTOGI, S.C., N. MENDIRATTA AND P. RASTOGI. 2005. Bioinformatics- Methods and Applications- Genomics, Proteomics & Drug Discovery, Prentice Hall of India Private Ltd.
- WALKER, J. M. AND RAPLEY. 2003. Molecular Biology and Biotechnology. (4th Edition). Panima Publishing Corporation. New Delhi.
- WESTHEAD, D.R., J. H. PARISH AND R.M. TWYMAN. 2003. Bioinformatics. Viva Books Pvt. Ltd., Chennai.
- ZOE LACROIX and TERENCE CRITCHLOW. 2003. Bioinformatics- Managing Scientific Data.. Morgan Kaufmann Publishers.