I Year & I Sem.; M.Tech. Biotechnology & Bioprocess Engg.

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(BT537) BIOINFORMATICS AND MOLECULAR MODELLING

Objectives of the Course :

To equip students with computational skills and to help them use computational methods to study, organise, analyse and interpret biological information at molecular, genetic and genomics levels.

UNIT I : Introduction:

Scope of Bioinformatics, Elementary commands and protocols, ftp, telnet, http. Primer on information theory. DNA Mapping and sequencing –Map alignment – Large scale sequencing methods - Shotgun – DNA sequencing – Sequence assembly.

UNIT II: Sequence Alignement and Dynamic Programming & Phlogeny

Heuristic Alignment algorithms. Global sequence alignments-Neddleman-Wunsch Algorithm, Smith-Waterman Algorithm-Local sequence alignments (Amino acid substitution Matrices (PAM, BLOSUM). Ultrasonic trees – parsimony – Ultrametric problem – Perfect phylogeny – Phylogenetic alignment – connection between multiple alignment and tree.

UNIT III: Biological Database and their use:

Introduction to Biological databases, Organization and management of databases. Searching and retrieval of information from the World Wide Web. Structure databases - PDB (Protein Data Bank), Molecular Modeling Databases (MMDB). Primary Databases NCBI,EMBL, DDB. Swissprot, PIR,KEGG. BioChemical databases- KEGG, EXGESCY,BRENDA, WIT.

UNIT IV: Introduction to Molecular Modelling :

Introduction - Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy, Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature. Force Fields, Bond Stretching, Angle Bending, Introduction to Non-bonded Interactions. Electrostatic Interactions. Van der Waals Interactions. Hydrogen Bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

UNIT V: Energy Minimisation and Computer Simulation:

Energy Minimisation and Related Methods for Exploring the Energy Surface. Non-Derivative method, 1st and 2nd order minimisation methods. Computer Simulation Methods. Simple Thermodynamic Properties and Phase Space. Boundaries. Analyzing the Results of a Simulation.

TEXT BOOKS :

1. D. Baxivanis and Foulette,"Bioinformatics: A Practical guide to the Analysis of Genes and Proteins", Wiely Indian Edition, 2001.
2. Mount. D. Cold, "Bioinformatics: Sequence and Genome Analysis", Spring Harbor Lab.: 2001
3. T K Attwood, D J parry-Smith, "Introduction to Bioinformatics", 1st Edition,11th Reprint, Pearson Education, 2005.
4. C S V Murthy, "Bioinformatics",1st ed., Himalaya Publishing House, 2003.

REFERENCE BOOKS :

1. Harshawardhan P.Bal, "Bioinformatics – Principles and Applications " Tata Mac Graw Hill.
2. Arthur.M.Lesk , "Introduction to Bioinformatics", Oxford University Press.
3. A.R.Leach, "Molecular Modelling Principles and Application", Longman,1996.
4. J.M.Haile, "Molecular Dynamics Simulation Elementary Methods", John Wiley and Sons, 1997.
5. Satya Prakash Gupta, "QSAR and Molecular Modeling", Springer - Anamaya Publishers, 2008.

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