PBT6I102 BIOINFORMATICS

Module-I:

Searching Biological Data From databases: Finding the information stored and its retrieval methods at NCBI, EMBL and DDBJ, Protein Data Bank, CSD, Uniprot, PIR, SwissProt, TrEMBL, SNP, Metabolic pathways databases KEGG, MetaCyc, Domain classification databases: SCOP, CATH, Pfam Retrieving microbial and viral genome information.

Module-II:

Sequence alignment and analysis: Local and global alignment, Gap penalty and substitution matrix, Pairwise and Multiple sequence alignment, Fast Alignment method, dynamic programming, Sequence profile and HMM, Basic algorithms for prediction of ORF, promoters, splice sites

Module-III:

Molecular modelling and drug design: Homology modelling, Molecular mechanics and force fields, molecular dynamics simulation, Drug design Process, drug like Property of a molecule, target identification, Docking methods, Basic idea about Molecular descriptors and QSAR analysis.

Text Books:

1. Mount DW, Bioinformatics: Sequence and Genome Analysis, Spring Harbor Press
2. Arthur Lesk, Introduction to Bioinformatics, Oxford University Press.
3. Baxevanis AS and Ouellette BF, Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, Wiley International Science.
4. Bryan Bergeron, Bioinformatics computing, Prentice Hall Inc
5. Bernhard houbold ,Thomas Wiehe,Introduction to computational biology : an evolutionary approach Blkhauser verlag press

Reference:

1. Tao Jiang, Ying Xu, Michael Q. Zhang, Current Topics in Computational Molecular Biology, MIT press.
2. Thomas lengauer,Bioinformatics from genome to drug .WILLEY-VCH press.

BIOINFORMATICS LAB

1. Retrieving Human genome data, OMIM, SNP databases to understand genetic and metabolic disorders. (At least 2 each)
2. Mining genomic data to identify genomic features: codon usage, repeats, Homologous sequences etc.
3. Making Phylogenetic tree of given sequences by using ClustalW and PHYLIP.
4. Gene and promoter prediction for Prokaryotes and eukaryotes (comparative analysis by using different tools: at least 3)
5. Learning about molecule visualisation software like Rasmol, Pymol etc.
6. Primary Structural databases: pdb, ndb, csd and Derived databases of structures: DSSP, FSSP, CATH & SCOP.
7. Prediction of secondary structures of proteins: at least 3 methods
8. Prediction of Tertiary structure of proteins and Validation of model protein structure: Energy minimization, Procheck, verify 3D, Prosa II, ERRAT etc.
9. Molecule drawing. Conversion of 2D structure to 3D structure.
10. Molecular docking and analysis of receptor with ligand
11. Molecular Dynamics simulation