103B : BIOINFORMATICS

BIOLOGICAL DATABASES: Genomes, DNA sequences. Sequence databases: GeneBank, European Molecular Biology Laboratory (EMBL) Nucleotide sequence databank, DNA Data Bank of Japan (DDBJ), Protein databases; primary databases and secondary databases, database formats. Structural databases; Protein Data bank (PDB), Nucleic Acid Data Bank (NDB), Molecular modeling Data Bank (MMDB).

SEQUENCE ALIGNMENTS: Introduction, Protein sequences, physicochemical properties based on sequence, sequence comparison. Pair-wise sequence alignment, gaps, gap-penalties, scoring matrices, Smith-Waterman and Needleman-Wunsch algorithms for sequence alignments, multiple sequence alignment, comparision, composition and properties, useful programs, ClustalW, BioEDIT, BLASTp, Phylogenetic analysis tools-Phylip, ClustalW, Online phylogenetic analysis.

GENE EXPRESSION AND DNA MICROARRAY: Introduction, Basic steps for gene expression, genome information and special features, coding sequences (CDS), untranslated regions (UTR's), cDNA library, expressed sequence tags (EST). Approach to gene identification; codon-bias detection, detecting functional sites in the DNA. Internet resources for gene identification, detection of functional sites. Types of microarrays; Tools for microarray analysis; soft-finder, xCluster, MADAM, SAGE, Applications of microarray technology.

STRUCTURAL BIOLOGY: Nucleic acid structures, RNA folding, RNA loops, conformational study, various ribose ring conformations, ribose-ring puckering, protein-protein interactions, protein-ligand interactions, DNA-binding proteins, RNA-binding proteins, Ramachandran plot, , 3-dimensional structures of membrane proteins, importance of 3^{10} helix and loops, biophysical aspects of proteins and nucleic acids.

PROTEIN STRUCTURE PREDICTION: Protein Structure Prediction; Homology modeling, prediction of protein structure from sequences, functional sites, Protein folding problem, protein folding classes, protein identification and characterization; structure determination by X-ray and NMR.

MOLECULAR MODELING: Introduction, force field, quantum chemistry, Schrödinger equation, potential energy functions, energy minimization, local and global

minima, saddle point, grid search, , various approximations; LCAO, HF, semi-empirical calculations; single point calculations, full-geometry optimization methods, ZDO, MNDO, CNDO, NDDO, AM1, PM3, RM1, conformational search, Z-matrix, docking, molecular modeling packages.

MOLECULAR MECHANICS: Definition, balls and springs, force fields, bond-stretching, bond-bending, dihedral motions, out of plane angle potential, non-bonded interaction, coulomb interactions, conformational search, united atoms and cut-offs, Derivative methods; First-order methods; Steepest descent, conjugate gradient, Second order methods; Newton-Raphson method.

MOLECULAR DYNAMICS: Introduction, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzman velocity, time steps, duration of the MD run.

FUNDAMENTALS OF UNIX SYSTEM: Introduction about UNIX, differentiation between UNIX and other Operating systems, various programs in the UNIX System, structure of the UNIX system, applications of the UNIX systems, basic UNIX commands, file access permissions, the file system hierarchy, terminating process, running jobs at background, controlling running programs, overview of system administration, managing deisk space, shutting down UNIX system.

BIOINFORMATICS APPLICATIONS: Agriculture, Molecular biology, Environment, Biotechnology, Neurobiology, Drug Designing, Biomedical genome medicines.

Reference books:

1. Bioinformatics Methods and Applications Genomics, Proteomics, and Drug Discovery (S. C. Rastogi, N. Mendiratta, and P. Rastogi).
2. Introduction to Bioinformatics, (Atwood, T. K. and Parry-Smith, D. J).
3. An introduction to Computational Biochemistry. (C. Stain Tsai, A John Wiley and Sons, Inc., publications).
4. Developing Bioinformatics Computer Skills. (Cynthia Gibas and Per Jambeck).
5. Molecular Modelling for Beginners (Alan Hinchliffe).
6. A user guide to the UNIX system (Rebecca Thomas and Jean Yates)
7. http://www.ncbi.nlm.nih.gov