

B. Tech. in BIOINFORMATICS ENGINEERING

Syllabus of Paper – 1

IMMUNOLOGY

Overview Of The Immune System: Introduction: overview of the immune system-Lymphatic system, Lymphoid organs, Cells of the immune system and their functions-Immune system. Innate and Acquired immunity: Cells and processes of Innate immunity—Cells and organs of the Acquired immunity- Anatomical and Physiological barriers; Innate immune response and their recognition structures; Pathogen elimination. Comparative immunity. Plant Immune system. Immunogens and Antigens: Requirements for immunogenicity; major classes of antigens; antigen recognition by B and T lymphocytes. Antibody Structure And Functions, B Cell Function: Immunoglobulins: Structure and function-- Monoclonal antibodies. B Cell generation and differentiation: BCR-Antibody diversity: Genetic basis—T-dependent activation of B cells – B – lymphocyte signal transduction. Cytokines. Complement. Antigen – Antibody Interactions: Antigen- antibody interaction: antibody affinity and activity- Isolation of lymphoid cells from blood and lymphoid organs--precipitation reaction, agglutination reaction -Radioimmunoassay, ELISA, Western Blot, Immunoprecipitation – Immunofluorescence, flow cytometry. Cell culture and Experimental animal models. Analysis of gene expression. T Cell Maturation, Activation & Differentiation : MHC, antigen processing and presentations: T-cell receptors-T-cell maturation, activation and differentiation-Cell mediated effector responses-Function of CD8+ T cells. Immune System In Health & Disease: Hypersensitive reactions--Immune responses to infectious diseases--Tumor Immunology- Vaccines-Autoimmunity.

MOLECULAR BIOLOGY AND GENETICS

Structure Of Nucleic Acid: Structure of DNA - Different forms of DNA and RNA - Identification of DNA as genetic material by Griffith –Avery, McLeod and McCarty - Frankel and Singer - Hershey and Chase - Messelson and Stahl experiment. DNA Replication And Mutation: Semi-Conservative replication - replication of DNA in Eukaryotes - molecular basis of Mutation - classification of mutation. Gene Expression And Regulation: Genetic code – transcription - prokaryotes and Eukaryotes - Post transcriptional modification - Translation in prokaryotes and Eukaryotes - Post translational modification - Gene Regulation - Lac operon model. Mendelian Genetics: Mendel's laws - monohybrid - dihybrid inheritance- multiple alleles -structure and organization of chromosome in prokaryote and Eukaryotes. Crossing Over And Linkage: Linkage - types of linkage -crossing over and their types- Recombination mapping by two point and three point test cross mapping in bacteria.

BIOPHYSICS

Elementary Biophysics: Definition of atom and its properties, size and charge of electron, nucleus, protons neutrons. Types of interaction between atoms: Bond distance, Bond angle, Torsion Angle, H-bonding, VdW interactions, Hydrophobic interactions, Electrostatics interactions. Classical Mechanics: Newton's laws of motion, Law of conservation of mass and energy. Thermodynamics: Laws, Enthalpy, Entropy, Free Energy, Gibbs & Helmholtz free energy, Internal energy, Boltzmann constant. Difference between classical and quantum mechanics. Lagrange's equation, Uncertainty

principle, Schrodinger equation: time dependent and time independent with its applications; Hamilton's equation with its applications. DNA Biophysics: Structure of A, B & Z forms of DNA with special emphasize to formation of phosphodiester bond, hydrogen bonding between the two strands of DNA, Helical parameters, DNA Backbone torsion angles, sugar backbone torsion angles, pseudorotation, sugar puckering. Comparison of various parameters of A, B & Z forms of DNA. Protein Biophysics: Amino acids, peptide bond, phi, psi & omega angles with distance, Zwitterion formation of amino acids, Levels of protein structure, Significance of Ramachandran Plot, Protein – DNA, drug, carbohydrate, small molecule interactions. Energetics of lipid bilayer. Molecular Mechanics & Dynamics protocol. Carbohydrate Biophysics: Structure of D-glucose & D-fructose; formation of glucosides & the cyclic structure of D- glucose; D-ribose & D-deoxyribose; Structure and conformation of disaccharides and polysaccharides- cellulose, amylose, amylopectin & glycogen, Chitin, carbohydrate conjugates. Techniques InBiophysics: X-ray crystallography, NMR, IR, Raman, AAS, UV, CD, Cosy, Noesy, spectroscopy, Mass spectrometry, Maldi TOF for protein prediction.

RECOMBINANT DNA TECHNOLOGY

Vector and Inserts: Vehicles for gene cloning – Biology of plasmids, Plasmid based vectors, Bacteriophage, Phage vectors, Cosmids, Phasmids, BAC and YAC vectors; Insert preparation – Restriction Digestion - Restriction enzymes, Polymerase chain reaction –Polymerase, Creation of restriction site by PCR. Cloning Technique: Ligation–Ligase, cohesive , Blunt end ligation; Other Modification enzymes – Nucleases, Phasphatase, Kinase; Transformation-Preparation of competent cell, chemical and electrical transformation; Transfection; Recombinant selection and screening - Blotting technique. Construction Of Gene Libraries: Construction of cDNA library- construction subtractive cDNA library – construction of genomic DNA library – BAC library – YAC library. Expression Of Recombinant Protein In E.Coli: Plasmid expression vectors-general features, promoters used in expression vectors -cloning of genes in correct reading frame in expression vector- purification of recombinant protein using Histidine tag, GST tag, chitin. Application Of Recombinant Dna Technology: Applications of rDNA technology in Diagnostics- HIV diagnosis; Therapeutic proteins-Vaccines, Human Insulin, Growth hormone; Agriculture - Golden rice, Insect resistant plant; Genetic diversity.

GENOMICS AND TRANSCRIPTOMICS

Genomes And Their Organization: Prokaryotic and eukaryotic genomes- structure- organization- Genomics: Genome Sequencing- Fragment Assembly- Genome Assembly- Human Genome Project- Aims- goals and achievements. General principles of Gene Therapy. Gene Expression Profiling: Aligning Whole Genome Alignment (WGA) - prediction of coding regions - gene structure - conserved motifs, comparative genomics, methods of gene discovery-Prediction of gene function - methods - annotation, Coding and non coding genes and RNA, Gene expression - regulatory mechanism, Expression profiling - Northern, RT-PCR, DD-RT-PCR, EST library - cDNA library, cDNA AFLP – SAGE-Mechanical methods of delivery- Example: Duchenne myotrophy- Liposomal methods of delivery- Cystic fibrosis. Gene Regulatory Network And Microarray: Gene regulatory network and the models- DNA micro array and the analysis of data using clustering methods. Functional And Comparative Genomics: Introduction to functional and comparative genomics- Methods to perform comparative genomics. Transcriptomics: Features of RNA secondary structure- Basics of RNAstructure prediction-Limitations of prediction- Development of RNA prediction

methods- Methods -Self- complementary regions in RNA- minimum free energy method- MFOLD- Sequence covariation method.

PROTEOMICS

An Overview of Proteomics: Proteomics- Need, scope and challenges of proteomics, how proteomics is applied in real-life scientific research, Protein structures, Making the extract, Clarification- Centrifugation, filtration and ultra-filtration, precipitation, dialyze, batch binding. Strategies for Protein Separation: Liquid 2D gel electrophoresis – principle and applications, multi dimensional chromatography – principle and applications. ChromatographyMass Spectrometry - principles, instrumentation and applications in proteomics. Strategies For Protein Identification Quantitation: Protein Identification with antibodies, protein sequence determination bychemical degradation, Edman's degradation, Short-gun proteomics for proteome profile, Quantitative proteomics with standard 2D gels, multiplexed proteomics, quantitative with mass spectrometry, Computational tools- advanced tools for data analysis. Structural Proteomics: Protein-Protein interactions- principles and methods to study proteins,Proteomic analysis of Post-translational Modification- Phosphorylation, ubiquitination, and glycosylation. Protein Chips: Protein Chips and Functional Proteomics- different types of protein chip-detecting and quantifying, Applications of Proteomics, Proteome database.

Syllabus of Paper - 2

COMPUTATIONAL BIOLOGY

History, Scope And Importance: Important contributions - aims and tasks of Bioinformatics- applications of Bioinformatics - challenges and opportunities - internet basics- HTML - introduction to NCBI data model- Various file formats for biological sequences. Databases - Tools And Their Uses: Importance of databases - Biological databases-primary sequence databases-Composite sequence databases- Secondary databases- nucleic acid sequence databases- Protein sequence data bases - structure databases- bibliographic databases - specialized genomic resources- analysis packages. Sequence Alignment Methods: Sequence analysis of biological data-Significance of sequence alignment-pairwise sequence alignment methods- Use of scoring matrices and gap penalties in sequence alignments- multiple sequence alignment methods - Tools and application of multiple sequence alignment. Predictive Methods Using DNA And Protein Sequences: Gene predictions strategies - protein prediction strategies - molecular visualizationtools-phylogenetic analysis: Concept of trees- phylogenetic trees and multiplealignments. Drug Discovery Process: Discovering a drug - target identification and validation - identifying the lead compound - optimization of lead compound - chemical libraries.

BIOINFORMATICS ALGORITHMS

Introduction: Algorithms and Complexity- Biological algorithms versus computer algorithms - The 'Change problem' - Recursive Algorithms - Iterative versus Recursive Algorithms - Big-O Notations - Algorithm design techniques and the different types of algorithms. Greedy Algorithms: Molecular Biology Primer - Exhaustive Search: Mapping Algorithms - Motif Finding problem - Search Trees - Finding a Median String. Greedy Algorithms: Genome Rearrangements - Sorting by Reversals - Approximation Algorithms - A Greedy Approach to Motif Finding. Dynamic Programming Algorithms: DNA Sequence comparison - Manhattan Tourist Problem- Edit Distance and Alignments - Longest Commons Subsequences - Global Sequence Alignment - Scoring Alignment - Local Sequence Alignment - Alignment with Gap Penalties - Multiple Alignment. Graph Algorithms: Graphs - Graphs and Genetics - DNA Sequencing - Shortest Superstring ProblemDNA arrays as an alternative sequencing techniques - Sequencing by Hybridization - Path Problems - Fragment assembly in DNA Sequencing - Protein Sequencing and Identification - The Peptide Sequencing Problem - Spectrum Graphs. Clustering And Trees: Gene expression analysis - Hierarchical clustering-k-means clustering - Clustering and corrupted Cliques - Evolutionary Trees - Distance-based tree reconstruction - Reconstruction trees from additive matrices - Evolutionary trees and hierarchical clustering - Character-based tree reconstruction - Small and large Parsimony Problem - Hidden Markov Models.

MOLECULAR PHYLOGENY AND EVOLUTION

Phylogenetic Trees: Types- topological differences- tree building methods- Distance methods - UPGMA- LS methods- minimum evaluation methods- NJ methods- phylogenetic reconstruction. Methods: Maximum parsimony methods- Strategies of searching for MP trees- consensus trees- branch length estimation - weighted parsimony- MP methods for protein data- Maximum likelihood methods. Statistical Approach: Optimization principle and topological errors- interior branch tests- bootstrap tests- Tests of topological differences- advantages and disadvantages- molecular clocks and

linearized trees. Ancestral Sequences: Inferences of ancestral sequences- parsimony and Bayesian approaches-synonymous and non-synonymous substitutions- convergent and parallel evolution. Evolution: Molecular basis of evolution- synonymous and non-synonymous mutations-genetic polymorphism and evolution- Population trees from genetic markers.

PERL PROGRAMMING & BIOPERL

Introduction To Linux: Linux OS-Working Environment- editors-Navigation commands, File handling - creating and manipulating sequence files-text processing, System administration commands, Archival commands, process management networking and advanced commands. Introduction To PERL: Data types, variables, operators, formatting of input/output, Array operations, Hashes, @ARGV, control structures and file handling, Debugging. PERL Subroutines And Regular Expressions : Built-in functions, subroutines, scoping of variables, Regular expressions-metacharacters and special operators, translation and substitution operators, pattern matching. PERL Modules: OOP concepts in Perl, Packages, libraries and modules- basic modules - getopts::long, LWP, CWD, file::basename. BIOPERL: Bioperl installation and applications, Bioperl modules- Databases, sequence retrieval & alignment, phylogenetic tree construction, restriction enzyme analysis, mutation studies.

IMMUNOINFORMATICS

Sequence Analysis: Alignments- DNA alignments- Molecular evolution and phylogeny- viral evolution and escape- prediction of functions. Methods: Methods applied in Immunological Bioinformatics- starting from sequence weighing methods to cluster analysis- Gibbs Sampling- HMM- Neural network-microarray and its applications. MHC- I Prediction: Prediction of Cytotoxic T Cell (MHC Class I) Epitopes- Antigen Processing in the MHC Class I Pathway. MHC-II Prediction: Prediction of Helper T Cell (MHC Class II) Epitopes- Processing of MHC Class II Epitopes. B Cell Epitope Prediction And Web Sources: Recognition of Antigen by B Cells- vaccine design- Web-Based Tools for Vaccine Design.

CHEMOINFORMATICS & DRUG DESIGNING

Molecular Modeling In Drug Design: Molecular modeling in drug discovery- Molecular docking- De-novo ligand designing- and structure-based methods. Drug Discovery And Development: Drug discovery: targets and receptors- target identification and validation- drug interactions- small molecule drugs- Pharmacodynamics- Pharmacokinetics-toxicology- animal tests- formulations and delivery systems. Representation Of Structures And Molecular Descriptors : Representation and Manipulation of 2D Molecular Structures- Representation and Manipulation of 3D Molecular Structures. - Descriptors Calculated from the 2D Structure- Descriptors Based on 3D Representations. Similarity And Qsar Methods: Similarity Methods- Similarity Based on 2D Fingerprints- Similarity Coefficients- 2D Descriptor Methods- 3D Similarity- Selecting Diverse Sets Of Compounds-Introduction- deriving a QSAR Equation- Simple and Multiple Linear Regression-Designing a QSAR "Experiment"- Principal Components Regression- Partial Least Squares- Molecular Field Analysis. High Throughput And Virtual Screening: Analysis of High-Throughput Screening Data- Data Visualization- Data Mining Methods- Virtual Screening- Drug-Likeness and Compound Filters- Structure-Based Virtual Screening- chemical libraries.

MOLECULAR DYNAMICS

Basics: Introduction of molecular dynamics – Statistical mechanics- Entropy and temperature, Classical Statistical Mechanics, ergodicity- Monte Carlo Simulations-Sampling Method, Algorithm, applications- Molecular dynamics simulations: the Idea. Algorithms: Introduction- Periodic boundary conditions, Constraint algorithm- Shake, Lincs, Simulated Annealing, Stochastic Dynamics, Brownian Dynamics- Energy minimization- Steepest Descent- Conjugate Gradient. Force Field And Interaction Functions: Non-bonded interactions- Lennard-Jones interaction- Coulomb interaction- Bonded interactions- Bond stretching, Morse potential bond stretching- Cubic bond stretching- Torsional angles- Force field- GROMOS87, OPLS, AMBER, CHARMM. Molecular Dynamics: Molecular dynamics simulations- the Idea, Initialization, force calculation, integrating equations of motions- Higher order schemes- Liouville formulation of time reversible algorithm- Computer experiment: Diffusion, Order-n Algorithm to measure correlations- Applications. Monte Carlo And Molecular Dynamics In Various Ensembles: Monte Carlo Simulations- General approach, Canonical ensemble, Microcanonical Monte Carlo, Isobaric-isothermal ensemble, applications- Molecular dynamics: The Andersen Thermostat, Nose-Hoover Thermostat, MD at constant pressure.
