S-30th May, 2015 AC after Circulars from Circular No.1 & onwards++ - 43 -

DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY

CIRCULAR NO.SU/Sci./C.B.C. & G.S./P.G. Syll./39/2015

It is hereby inform to all concerned that, the revised Curriculum under <u>Choice Based Credit and Grading System</u> submitted by the various Ad-hoc Boards which are run at college level only and recommended by the Dean, Faculty of Science, the Hon'ble Vice-Chancellor has accepted the same on behalf of the Academic Council under Section-14[7] of the Maharashtra Universities Act, 1994 as under :-

[1] M.Sc. Forensic Science Ist Year, Semester-I & II Progressively

- [2] M.Sc. Electronics Ist & IInd Year, Semester-I to IV Progressively
 [3] M.Sc. Industrial Automation Ist & IInd Year, Semester-I to IV
- Progressively [Under Innovative Programme of U.G.C.]
- [4] M.Sc. Industrial Chemistry Ist & IInd Year, Semester-I to IV Progressively
- [5] M.Sc. Herbal Technology Ist & IInd Year, Semester-I to IV Progressively [Under Innovative Programme of U.G.C.]
- [6] M.Sc. Biophysics Ist & IInd Year, Semester-I to IV Progressively
 [7] M.Sc. Bioinformatics Ist & IInd Year, Semester-I to IV Progressively
- [8] M.Sc. Plant Breeding & Molecular Genetics
- Ist & IInd Year, Semester-I to IV Progressively

[9] M.Sc. Plant Biotechnology Ist & IInd Year, Semester-I to IV Progressively

[10] M.Sc. Geology Ist & IInd Year, Semester-I to IV Progressively.

This is effective from the Academic Year 2015-16 & onwards as appended herewith.

All concerned are requested to note the contents of the circular and bring the notice to the students, teachers and staff for their information and necessary action.

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Aurangabad-431 004. REF.NO.SU/S.S./C.B.C. & G.S. / P.G.Syll./2015/9893-10142_ Date:- 20-07-2015.

Director, Board of College and

* * **** University Development.

Copy forwarded with compliments to:-

- 1] The Principals, affiliated concerned colleges, Dr. Babasaheb Ambedkar Marathwada University Copy to :-
- 1] The Controller of Examinations,
- 2] The Director, [E-Suvidha Kendra], in-front of Registrar's Quarter, Dr. Babasaheb Ambedkar Marathwada University,

_=**=.

- 3] The Superintendent, [M.Sc. Unit],
- 4] The Programmer [Computer Unit-1] Examinations,
- 5] The Programmer [Computer Unit-2] Examinations,
- 6] The Record Keeper.

S*/-030815/-

Final MSc BioInformatics-CBCS-corrected



- 2 -



run at college level from the

Academic Year 2015-16 & onwards progressively

Dr Babasaheb Ambedkar Marathwada University, Aurangabad

1 st Year	1 st Semester						
Subject	Subject Name	Hrs/ Week		Exa	a Theory	Practic	Total
code		Т	Ρ	m Hrs.	Credits	al Credits	Credits
BI 401	Basic Biology, Mathematics and Statistics	4	0	3	4	0	4
BI 402	Biological Chemistry and Genetic information flow & Processing	4	0	3	4	0	4
BI 403	Basic concepts in computing and Introduction to Database systems	4	0	3	4	0	4
BI 404	Biological databases and Data Analysis	4	0	3	4	0	4
BI 451	Practicals based on BI401	0	4	3	0	2	2
BI 452	C programming	0	4	3	0	2	2
BI 453	Practicals based on BI403	0	4	3	0	2	2
BI 454	Practicals based on BI404	0	4	3	0	2	2
					16	8	24
1 st Year 2 nd Semester							
BI 405	Cell Biology and Immunology	4	0	0	4	0	4
BI 406	Structural Biology	4	0	3	4	0	4
BI 407	Chemo Informatics and Biodiversity Informatics	4	0	3	4	0	4
BI 408	Programming in object oriented languages, Computer Graphics, Networking and data security	4	0	3	4	0	4
BI 455	Practical based on BI 406	0	4	3	0	2	2
BI 456	Practicals based on BI407	0	4	3	0	2	2

BI 457	Practicals based on BI408	0	4	3	0	2	2	
BI 458	Computer graphics and structure visualization	0	4	3	0	2	2	
					16	8	24	
2 nd Year		3 rd Semester						
BI 501	Taxonomy & Phylogeny	4	0	3	4	0	4	
BI 502	Object Oriented and Relation Databases	4	0	3	4	0 4		
BI 503	Genomics, Proteomics and Genome to Drug and Vaccine	4	0	3	4	0	4	
BI 504	Parasite Bioinformatics	4	0	3	4	0	4	
BI 551	Practicals based on BI501	0	4	3	0	2	2	
BI 552	Practicals based on BI502	0	4	3	0	2	2	
BI 553	Practicals based on BI503	0	4	3	0	2	2	
BI 554	Programming in Perl	0	4	3	0	2	2	
					20	8	24	
2 nd Year 4 th Semester								
BI 505	Advanced Techniques for Sequence and Structure Analysis and Data mining	4	4	3	4	0	4	
BI 506	Metabolomes and Metabolic Pathway Engineering	4	6	3	4	0	4	
BI 507	Emerging Areas in Bioinformatics	4	6	3	4	0	4	
BI 555	Practicals based on BI505	0	4	3	0	2	2	
BI 556	Practicals based on BI506	0	4	3	0	2	8	

BI 557	Practicals based on BI507	0	4	3	0	2	2
BI 558	Project	0	8	3	0	4	2
						10	26

Seminar should be based on any one of the following

- 1. Seminars on Applications of Bioinformatics in Agriculture
- 2. Seminars on Applications of Bioinformatics in Human Health
- 3. Seminars on Applications of Bioinformatics in Environment
- 4. Seminars on Applications of Bioinformatics in Biotechnology
- 5. Seminars on Applications of Bioinformatics in Molecular Biology
- 6. Seminars on Applications of Bioinformatics in Neurobiology
- 7. Seminars on Applications of Bioinformatics in Drug Designing
- 8. Seminars on Applications of Bioinformatics in Veterinary Sciences

Project should be based on the following topics

- 1. Parasite bioinformatics
- 2. Biodiversity informatics
- 3. Microbial informatics
- 4. Immunology bioinformatics
- 5. Plant bioinformatics
- 6. Molecular modeling
- 7. Any recent advance topic

Semester I

BI 401 Basic Biology, Basic Mathematics and Statistics Objectives:

The course aims at exposing the students of the non-biology stream to the diversity of microbial, plant and animal life. At the conclusion of the course the student would have become familiar with outlines of the classification of the organisms, their structural organization and functional complexities.

To upgrade the skills of the students (biology) in mathematics that is essential for learning Bioinformatics.

To upgrade the skills of the students (biology) in statistics that is essential for learning Bioinformatics

Syllabus:

Origin of life: Prebiological chemical evolution, proteinoids, proto cells.

Systematics: Species concept; kingdom to species; the five kingdoms; classical, phenetic and cladistic approaches

Bacteria: Structure of bacterial cell; bacterial types; transformation, transfection, transduction and conjugation; nutrition; phylogeny

Viruses: Biology of viruses; bacteriophages, plant and animal viruses; replication of viral genome; HIV

Protists: Endosymbiont theory of eukaryotic origin; protozoan, algae, slime and water molds

Fungal World: Feeding, reproduction, diversity and relationships

Plant Diversity: Broad classification and inter-relationships of non-vascular and vascular plants; tissue organization; reproductive patterns; transport mechanisms, growth, photosynthesis, hormones.

Animal Life: Major animal phyla, characteristics and interrelationships; tissues, organs and organ/systems; principles of nutrition, digestion, thermoregulation, osmoregulation

and excretion, muscle contraction, neural reflexes, circulation, respiration and endocrines.

Calculus: Limits, Complete Differentials, Partial differentials of functions with one variable and multiple variables

Integration: Definite and non-definite integral; Series, Logarithms Mathematical Techniques Ordinary differential equations (first order), Partial differential equationsexample from biology. Special functions -Bessel, Legendre

2D Coordinate geometry: Equation of a line, circle, ellipse, parabola, hyperbola

3D Geometry: Equation of sphere, cone Trigonometric functions: Sin, Cos, Tan, Co~ Series expansion of these. Functions and other related functions Vector -Addition, subtraction, dot, cross, scalar triple product, divergence, curl of a vector, equation of normal

Matrix algebra: Addition, subtraction, multiplication, transpose inverse, and conjugate of matrix etc.

Logic: Boolean logic Addition, subtraction, multiplication and division using binary, octal and hexadecimal systems. Fundamentals of Set theory. Fourier transform, Laplace Transform & other standard transforms.

Statistics:

Introduction to principles of statistical sampling from a population

Random sampling, Frequency distributions and associated statistical measures,

Probability Distributions, Correlation and regression analysis, Multivariate analysis, Hypothesis testing, Markov Models, Cluster Analysis,Nearest neighbor search,Search using stem numbers, Search using text signatures,,Phylogenetic Analysis Tools: Maximum Likelihood, Parsimony methods

References

Bio molecule Structure and function; Paul F. Agis Fundamentals of Mycology; L. H. Burnett Microbial Genetics; David Frifilder Microbiology; Presscot Microbiology; Tortora, Funk and Case Mathematics for life Scientist; E.Batschelet, Springer

BI 402: Biological Chemistry, Genetic Information Flow and Processing

Objectives:

The objective of the course is to make the students understand the chemistry of different classes of bimolecular, their interactions in an aqueous environment, the structure-function relationships of macromolecules, the principles of enzyme catalysis and regulation, organization of metabolic systems and the pathways for the complete oxidation of glucose.

Syllabus:

Water as the universal biological solvent; concept of osmolarity.

Carbohydrates: monosaccharides, oligosaecharides, polysaccharides, proteoglycans and glycoproteins.

Lipids: fatty acids, acylglycerols; phospholipids, sphingolipids, cholesterol and membranes lsoprenoids, icosanoids and their biological importance.

Proteins: amino acids and peptides; primary, secondary, tertiary and quaternary structures;

structure, function and evolutionary relationships; protein -protein interactions protein folding; allosteric proteins.

Nucleic acids: bases, nucleotides, RNA and DNA; different structural forms of DNA; denaturation, renaturation and hybridization of DNA; different types of RNA; Proteinnucleic acid interaction.

Enzymes: details of enzyme nomenclature and classification; units of enzyme activity; coenzymes and metal cofactors; temperature and pH effects; Michaelis-Menten kinetics; Inhibitors and activators; active site and catalytic mechanisms; covalent and non-covalent regulations; isoenzymes; osmolytes and intracellular modulation of enzymes

Organization of metabolic systems: enzyme chains, multi enzyme complexes and multifunctional enzymes; anaplerotic sequences and amphibolic pathways; pacemaker enzymes and feedback control of metabolic pathways; shuttle pathways; energy charge.

Oxidation of glucose in cells: high-energy bon~ glycolysis, citric acid cycle and oxidative phosphorylation.

The objective of the course is to make the student, understand the current concepts in gene organization, transcription, translation and regulation of gene regulation as well as the biotechnological implications of recent developments in cloning genome sequencing.

Genetic Information Flow and Processing:

Prokaryotic gene expression, operons -positive & negative regulation, sigma factors Initiation, elongation and termination of transcription -template & enzyme properties Eukaryotic RNA polymerize I, II & III transcribed genes, promoter & regulatory sequences, transcription factors, Techniques -foot printing, Reporter genes Organization of globin, immunoglobulin, HLA, rRNA and 5 sRNA genes Processing of RNA and Proteins -Transport and Stability Stress & hormones regulated gene expression Organization of human genome . RFLP, Fingerprinting, RAPDs, Micro arrays, ESTs.

References Biochemistry; Deb Outline of Biochemistry; Cohn and Stumpf General Biochemistry; Lehninger, Nicolson and Cox Gene VII; Benjamin Lewin Recombinant DNA technology; Watson Molecular Biology; Watson General Biochemistry; Lehninger, Nicolson and Cox

BI 403 Basic concepts in computing and Introduction to Database systems

Objective:

To introduce the students to fundamentals of computers, computing and software. Basic understanding of the concepts of data, data models and relationships Basic understanding of Data representation, indexing and hashing Basic concepts of various types of databases Understand, appreciate and implement relational database design Acquiring the skills of using Oracle dbms, SQL skills and basic skill in using VB as a front

end

Syllabus:

Overview and functions of a computer System

Input and output devices Storage devices: Hard Disk, Diskette, Magnetic Tape, RAID, ZIP devices, Digital Tape, CD- ROM, DVD (capacity and access time) Main Circuit Board of a PC: Chips, Ports, Expansion Slots

Memory: Register, buffer, RAM, ROM, PROM, EPROM, EEPROM (comparison)

Types of Processing: Batch, Real-Time, Online, Offline.

History of -Computers: Evolution, Generation of computers (I, II, III, IV, V), Classification of computers (mainframes, mini computers, Microcomputers, special purpose) - comparison with memory, power, cost, size -then and now

Types of modem computers: The workstation, The Minicomputer, Mainframe Computers, Parallel Processing Computer, The Super Computer

An overview of Computer viruses: What is a virus? Virus symptoms, How do they get transmitted? What are the dangers, General Precautions

Introduction to operating systems: Operating System concept, Windows 98/XP, Windows server NT/2000, UNIX/LINUX

The Internet and its Resources, World Wide Web (WWW): Associated tools, services, resources and various technologies. Searches on Medline, bibliographic databases, etc.

Computer Networking

OSI Reference Model

Network Topologies and Protocols

Networking gadgets (Router, Switch, etc)

Data Communication (ISDN, VPN, DSL, cable modem, cellular modem, etc)

Communication Links (Wire pairs, Coaxial cables, Fiber optics, Microwave, Satellite, etc) .Local Area Network (LAN), Wide Area Network (WAN), Metropolitan Area Network (MAN) .Network Security (Firewall, Packet filtering, etc)

Data Abstraction

Data Models; Instances & Schemes;E-R Model;Entity and entity sets;Relations and relationship sets; E-R diagrams; Reducing E-R Diagrams to tables;Network Data Model: Basic concepts;Hierarchical Data Model: Basic Concepts;Multimedia Databases -Basic Concepts and Applications;Indexing and Hashing;Basic concepts-ISAM,B+ Tree indexed

Introduction to Distributed Database Processing

ORACLE, SQL, Visual Basic Front End

Relational database design

Oracle Architecture

Oracle objects -Tables, Views, Indexes, Sequences; Synonyms, Snapshots, Clusters Database -Table space, Data files, Blocks, Extents, Segments; Oracle Background Processes: PMON, SMON, LGWR, CKPT; Oracle Instance Startup, Shutdown/Init.ora. Control files; Oracle Memory Management -SGA; Rollback Segments; Redo logs/Archival; Transaction Control & Locking / Dead Lock; Security, Grants, Roles, Privileges

Oracle Utilities & SQL *DBA -Oracle Server Manager; Export-Import/SQL Monitor Backup & Recovery (Archiving); Physical Storage & Logical Storage

Oracle * Reports -Reports Features; Full Integration with Fonns and Graphics; Data Model and layout editors

Layout Objects -Frames, Repeating Frames, Fields, Boiler Plate, Anchor; Interface Components; Report Formats; Example Reports; Single Query, Multi Query, Matrix, Master-Detail etc.; User Defined Columns; PL/SQL Interface/ Triggers; Packaged Procedure; Calling Report from a Form

Menu -Default Menus; Custom Menus; Menu Objects; Menu Module, Main Menu, Individual Menus, Sub Menus, Menu Items; Menu Editor, PL/SQL in Menu Modules, Menu Security

SQL

Select Statements, Data Definition Statements, Data Manipulation Statements, Data Control Statements, Other Database Objects, Views, Sequences, Synonyms, Introduction to Application Development using Visual Basic, Working with Code, Variables, Procedures and Controlling Program Executor, Standard Controls, Data Access Using Data Control, Connecting to Oracle Database using Visual Basic

References:

Database System Concepts; Hanery Korth and Abraham Silberschatz; Tata Mac-Graw Hill Publications

Parallel and Distributed Databases; Wilteach et.al. .

Introduction to Database Systems C.J.Date

Database system organization; J.M. Martin; Princeton-Hall .

Introduction to Database systems; J.M. Martin; Princeton-Hall

ORACLE: Power Objects Handbook; Bruce Kolste; David Peterson

BI 404: Biological Databases and Data Analysis

Objectives:

Understand the nature of biological data and need for Biological databases Understand and explore the major bimolecular sequence databases (organization and contents) and their respective search engines and database searches Understand and appreciate the need and significance of sequence analysis and the bioinformatics approaches for the same application of software analysis tools to sequence data

Syllabus:

Overview of available Bioinformatics resources on the web NCBI/EBI/EXPASYetc Biological Databases: Nucleic acid sequence databases GenBank/EMBUDDBJ Biological Databases: Protein sequence databases NBRF-PIR SwissProt Database search engines Entrez SRS Overview/concepts in sequence analysis Scoring matrices for Nucleic acids and proteins MDM, BLOSUM Pair wise sequence alignment algorithms Needleman & Wunsch Smith & waterman Database Similarity Searches BLAST FASTA Multiple sequence alignment PRAS CLUSTALW Derived databases Prosite BLOCKS Pfam/Prodom

BI 451: Practical based on BI 401

Practical based the use of the following statistical methods

Basic concept of statistical models & use of samples;

Statistical measures;

Mean, mode median variance, covariance, correlation& handling of data sets.

Distributions;

Tests of significance;

Analysis of variance, multivariate analysis;

Regression & correlation;

Chi-square test;

Testing of hypothesis, nonparametric methods, Bayesian methods, likelihood ratio, and maximum likelihood estimate.

Statistical methods on Markov chain: tests for stationary, mounte Carlo methods.

Hidden markov models.

Phylogenetics tree analysis

Cluster analysis. Probabilistic modeling Program the UPGMA and EM algorithm for Clustering. Estimator of transition probabilities for Marko models based on various sample sizes.

BI 452 Programming in C

Objectives

To be able to conceptualize and formulate the logic and flow for the implementation of a computational task and to code the same using the structured programming approach as provided by the 'c' programming language. Finally the implementation is to be made to various applications in the area of Bioinformatics.

Syllabus:

Concepts of flowcharting, algorithm development, pseudo codes etc.

Laboratory assignments based on the following topics in 'c' programming:

Data types, operators and expressions, Hierarchy of operators, control statements including decision (if, if-else), loops (while, do-while, for), branching (switch, break, continue), functions, arrays (1 D, 2D- all matrix operations including inverse of a matrix), strings, file handling, data structures etc.

Applications in Bioinformatics:

Extract a protein or nucleic acid sequence from any of the databank files (GenBank entry, Swiss-Prot, EMBL entry etc.)

Interconverting the sequence from one databank format to the other ego GenBank format to FAST a format, FAST A to PIR format etc.

Determining the base composition in a nucleic acid sequence and amino acid composition in a protein sequence.

Generating the complimentary sequence of a DNA sequence

Pattern search algorithms

Search for a specific oligonucleotide pattern (e.g. GAACATCC) in a given DNA sequence. .Find the position where a specific sequence say "GGTCCCGAC" will hybridize a given

DNA sequence.

Find the restriction enzyme cleavage sites ego where PVUZ, ECORI etc. will cut the DNA.

Locate palindromic sequence stretches in a DNA sequence.

Count the number of Open Reading frames (ORF's) in a DNA sequence.

Calculate the codon usage in a nucleic acid sequence.

Translate a DNA sequence into protein sequence in the forward and reverse frames. Implementation of the Needleman-Wunsch algorithm for pair wise alignment and testing alignment, score with randomized pairs of sequences also.

BI 453: Practical based on BI 403

Assignment based on "Data Definition Language"

A set of SQL commands used to create table, modify table structure, drop table, rename table. Assignment based on "Data Manipulation Language A set of SQL commands used to change the data within the database. It consists of inserting of records in the tables, updation of all or specific set of records in tables, viewing the attributes of table's column. Assignment based on "Data Query Language

It allows getting the data out of the database and doing things with it. Selecting the data from table using computation

Arithmetic and logical operators.

Range searching and pattern matching.

Function. group function. scalar function.-

Assignment based on defining Constraints.

Types: I/O constraints like Primary Key, Foreign key, Null and Unique constraints. Business constraints like check constraints.

Levels: Table level constraints, column level constraints, creating and deletion of constraints using the Alter Table clause.

Assignment based on using Joins.

Joining multiple tables, joining a table to it.

Assignment based on using Indexes, Sequences

Security Management using SQL

Granting rights on user objects such as Tables, Views, and Sequences.

Revoking rights on user objects such as Tables, Views, and Sequences.

PL/SQL

Writing PL/SQL blocks by using power of SQL with procedural statements Writing Database triggers.

Writing PL/SQL blocks using Built-in and User-defined function.

Writing PL/SQL blocks using procedure and package to organize PUSQL code into logical groups for maintenance and implementation.

Writing PUSQL blocks using expressions with operators such as Arithmetic operators,

Comparison operators, Logical operators, String operators.

Handling with cursors in PUSQL blocks

Types of cursors: Implicit and Explicit cursors.

Visual Basic

Exploring various windows in Visual Basic Environment to create the Visual Basic project. .Form window

Project. Explorer window

Properties window

Form layout window

Toolbox window

Toolbar window

Exploring the MSDN library, which contains several books, technical articles, frequently asked questions and their answers? Writing the Visual Basic application, that evolves the three steps process.

Defining the user interface.

Setting the properties.

Writing the Basic code.

Writing the various Visual Basic application using controls such as:

Text Box.

Frames.

Check Boxes.

Option Buttons.

Images.

Exploring various techniques for connecting Visual Basic application to the database.

Writing the GUI interface using Visual Basic to Database application.

Making use of list box, combo box as data bound controls.

Writing the Visual Basic application using ADO data control.

BI 454 : Practical based on BI 404

Objectives

To understand the application of methods for analysis of the bimolecular sequence data.

Syllabus

Exploring the integrated database system at NCBI server and querying the PUBMED and GenBank databases using the ENTREZ search engine

Exploring the integrated database system at EBI server and searching the EMBL Nucleotide database using the SRS search engine

Exploring and querying the SWISSPROT database

Exploring and querying the PIR database

Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteinsIDNA) with the database sequences

Database (homology) searches using different versions of FASTA and interpretation of the results to derive the biologically significant relationships of the query sequences (proteinsIDNA) with the database sequences Pair-wise local alignments of protein and DNA sequences using Smith-Waterman algorithm and interpretation of results. Pair-wise global alignments of protein and DNA sequences using Needleman-Wunsch algorithm and interpretation of results to deduce homology between the sequences

Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLOST AL. Interpretation of results to identify conserved and variable regions and correlate them with physico-chemical and structural properties Exploring and using the derived databases: PRO SITE, PRINTS, BLOCKS, Pfam and Prodom for pattern searching, domain searches etc.

References

Introduction to Bioinformatics; Attwood Bioinformatics; C,V. Murthy Bioinformatics;Baxvanis.

Semester II

BI 405 Cell Biology, Genetics and Immunology

Objectives:

The objective is to expose the student to the principles of structure and function of cells, membranes and organelles, laws of inheritance and population genetics as well as the elements of the immune system and their functioning.

Syllabus:

Cell Biology

Prokaryotic and eukaryotic cells; membranes and cellular comp art mentation; an overview of organelles, (mitochondria, chloroplasts, ER, *Golgi,* lysosomes and peroxisomes; nucleus and nucleolus) and organelle genetic systems.

Cellular membranes: Structure, transport, channels, carriers, receptors, endocytosis, and membrane potentials.

Cell motility and shape: cytoskeletal elements, cilia and flagella; motor proteins.

Cell-cell interactions and signal transduction: Intercellular junctions, signaling by hormones and neurotransmitters; receptors, G-proteins, proteinkinases and second messengers

Protein traffic in cells: Protein sorting and signal sequences; protein translocation in ER and vesicular transport to Golgi, lysosmes and plasma membrane; protein import into nuclei, mitochondria, chloroplasts and peroxisomes.

Cell cycle and its regulation; events during mitosis and meiosis

Genetics

Science of genetics -objectives, terminologies, methods

Mendelian principles of inheritance, sex linked inheritance

Concept of linkage, linkage maps and recombination

Mutations -molecular, gene/point and chromosomal

Phenotype and genotype relationships, role of environment, from gene to phenotype, gene interactions

Study of quantitative traits

Genetics of populations, genetics and evolution Genetics and diseases, cancer

Immunology

Overview of immune system, innate and acquired immune system Structure and function of antibody molecule and TCR Genetics of antibody diversity

MHC I & II, Polymorphism

Characteristics of B Cell and T Cell antigens

MHC Peptide interaction

Affinity maturation

Autoimmunity and molecular mimicry

Ligand- receptor interaction in the light of protein structure in immune system Use of bioinformatics in immunology and vaccine development References: <mark>Immunology; Roit</mark> Immunology; Rechard Coico 5th edi

BI 406: Structural Biology

Objectives:

The students should be able to understand and appreciate:

Physicochemical principles underlying the structure and function of biomolecules (DNA,

RNA, Proteins, Carbohydrates)

Various levels of structural organizations in biomolecules

Representation of the 2D and 3D structures: coordinate systems, modeling

Bioinformatics approaches for structure analysis and structure predictions

Structure-function correlations

Syllabus:

Internal and external co-ordinate system

Generation of co-ordinates of biopolymers in Cartesian and cylindrical polar co-ordinate System.

Methods of single crystal X-ray Diffraction of macromolecules:

Analysis of structures and correctness of structures

Submission of data to PDB: atomic coordinates and electron density maps

Anatomy of Proteins

Ramachandran plot

Secondary structures

Motifs

Domains

Tertiary and quaternary structures

Anatomy of DNA: A, B, Z DNA, DNA bending etc.

RNA structure

Structure of Ribosome

Principles of Protein Folding

Structural data banks -Protein Data Bank, Cambridge small molecular crystal structure data bank

Calculation of conformational energy for bio-macromolecules

Hidden Markov models: Theory & Applications

Classification of Proteins

Identification of Protein Domains

Prediction of Secondary and Tertiary Structures of Proteins

Neural networks: Theory & Applications

Classification of proteins

Prediction of Secondary Structure

Prediction of Para topes

Methods for Prediction of Secondary and Tertiary structures of Proteins

Knowledge-based structure prediction

Approaches based on machine learning methods

Fold recognition

Methods to predict three-dimensional structures of nucleic acids, rRNA

Molecular Mechanics & Molecular Dynamics of Oligopeptides, Proteins, Nucleotides and

small Molecules

Mechanics and dynamics of bio-macromolecules

Simulation of molecular mechanics and dynamics

Simulations of Free Energy changes

Force fields

Molecular interactions of

Protein -Protein

Protein -DNA

Protein -carbohydrate

DNA -small molecules etc.

References

Creighton, T. E. Ed.: Protein Structure: A Practical Approach. 1989.

Creighton, T.E.: Proteins: Structure And Molecular Properties. Second Edition. New

York. W. H. Freeman and Company, 1993.

Creighton, T.: Protein Folding, 1992. .

Sternberg, M.I.E.: Protein structure prediction: a practical approach, 1996 Pain, R.G.: Mechanisms of protein folding, 1994 Leach.A.R: Molecular modeling: principles and applications Immunology; Roit Immunology; Rechard Coico.

BI 407 Chemo Informatics and Biodiversity Informatics

Objective:

Introduction to the application of informatics in chemical enumeration, creation of databases & analysis of chemicals.

Syllabus:

Chemo Informatics

Role of Chemo informatics in pharmaceutical/chemical research Structure representation systems, 2D and 3D structures Chemical Databases -Design, Storage & Retrieval methods Search techniques, similarity searches & clustering Modeling of small molecules & methods for interaction mapping Characterization of chemicals by Class & by Pharmacophore, application in HTS analysis . Quantitative Structure Activity Relationship & application to Hit to lead optimization. Design & Analysis of combinatorial libraries 2 Chemo informatics tools for drug discovery.

Biodiversity Informatics Biological information Biological diversity of life Species diversity: taxonomic information on plants, animals, microbes and viruses Genetic diversity Ecological/ Ecosystem diversity Urban biodiversity Methods for species identification & classification **Biodiversity Databases** Organizing biological species information Datasets in biodiversity informatics: Species 2000, Tree of life, A TCC, NBII, Species analyst collaboration, ICTV, Animal Virus Information System etc. Software for identification Accessing existing databases on the World-wide Web Software for identification of species Probabilistic and deterministic identification Delta, MicroIS, AVIS, ICTV. Biocomplexity issues in biodiversity Need of metadata standards & ontology Reference: Medicinal Chemistry; Wilson Gisvold Principles of Medical Chemistry; William O Foye Organic and Medical Chemistry; Kadam Mahadik Bothara

Textbook of Pharmacognasy; T.E Walis

Pharmacology and Pharmacothearupetics; Satoskar and Bhandarker

- PANKHURST, R.I.: Practical taxonomic computing. 1991
- Biodiversity, Conservation Environment pollution, Ecology; B.N. Pandey

Protein Evolution; Laszlo Pathy

BI 408: Programming in object oriented languages, Computer Graphics, Networking and data security

Objectives:

To introduce the basic concepts in computer graphics as applied to Biomolecules.

Syllabus

Computer Graphics:

Introduction,Scientific	&	Engineering	Opportunities,Visualizati	on teo	chniques,
Software,Hardware,Gra	phics	,Interactive	Graphics, Interaction	device	s &

techniques,Geometric Transformations,Viewing in three dimensions,Raster algorithms,Frame buffer techniques,Surface and solid modeling,Rendering,Standards - CGI, GKS, PlliGS,Animation,Image Processing with stress on biological systems,3-D image reconstruction,User Interface Studies

Network Security:

Introduction to Information & Network Security

General security fundamentals

Network Security Fundamentals

Network Defense

Incident Response

Elements of security. With terminology

Risk Assessment Auditing

Security Policies

Introduction to security services & Attacks

IDS/Firewalls (Introduction and types)

Tools and techniques involved in info. & Network security

Types of attacks (General information)

Encryption/decryptions

Current & future technologies (like wireless, biometric etc.) and security concerns.

Data security:

Classification of data security threats, protection mechanism (authentication, access control, access rules)

Data accuracy:

General issues regarding Biological Databases; Representation of errors due to (machines, 3D structural and sequence data of proteins and nucleic acid, Proteomics and Micro array data)

JAVA An introduction to *JA* VA programming Object-oriented programming and Java Java Basics Working with objects Arrays, Conditionals and I-oops Creating Classes and Applications in Java More about methods Java Applets Basics Graphics, Fonts and Color Simple Animation and Threads Advanced Animation, Images and Sound Managing Simple Events and Interactivity Creating User Interfaces with A WT Windows, Networking and other Tidbits Modifiers, Access Control and Class Design Packages and Interfaces Exception Multithreading Streams and I/O Using Native Methods and Libraries Under the Hood Java Programming Tools Working with Data Structures and Java Image Filters References:

Fundamentals of Interactive Computer Graphics -J.D.Foley, A.Van Dam
Procedural Elements for Computer Graphics -David F. Rogers.
Mathematical Elements for Computer Graphics -David F. Rogers, J.A.Adams
Graphics Gems -Andrew S. Glassner
IEEE Computer Graphics & applications (monthly journal)
ACM SIGGRAPH Computer Graphics

Exploring the PDB & NDB: Database searches, understanding entry contents and file formats, etc.

Visualization of tertiary structures, quaternary structures, architectures and topologies of proteins and DNA using molecular visualization software such as RasMol, Cn3D, SPDBV, Chime etc.

Prediction of secondary structures of proteins using at least 5 different methods with analysis and interpretation of the results. Comparison of the performance of the different methods for various classes of proteins.

Prediction of tertiary structures of proteins using Homology Modeling approach: SWISSMODEL, SWISS-PDB Viewer.

Prediction of tertiary structures of proteins using at least 3 methods for fold recognition along with analysis and interpretation of results.

Calculation of binding energy of inhibitors and analysis of active sites of enzymes using appropriate software.

BI 456: Practical based on BI 407

Objectives:

This course aims at giving hands-on experience to the students with some of the laboratory techniques necessary to understudy genomic and proteomics.

BI 457 Practical based on BI 408

JAVA

An introduction to JAVA programming Object-oriented programming and Java Java Basics Working with objects Arrays, Conditionals and loops Creating Classes and Applications in Java

More about methods

Java Applets Basics

Graphics, Fonts and Color Simple Animation and Threads Advanced Animation, Images and Sound Managing Simple Events and Interactivity Creating User Interfaces with A WT Windows, Networking and other Tidbits Modifiers, Access Control and Class Design Packages and Interfaces Exception Multithreading Streams and I/O Using Native Methods and Libraries Under the Hood Java Programming Tools Working with Data Structures and Java Image Filters

BI 458: Computer graphics and structure visualization

Objectives:

To be aware of the various algorithmic approaches that is implemented for graphical applications. To appreciate visualization packages used in Bioinformatics and are able to develop better graphical and visualization aids for ones own requirement and application. Standard functions in the 'c' graphics module -Introduction to pixels, drawing various geometric objects, filling polygons, images etc.

Implementation of the basic line drawing algorithm and the Circle drawing algorithm using DDA, Midpoint algorithm, Bresenham's algorithm etc.

Polygon filling using seed fill, scan line algorithm etc.

Clipping algorithms -Cohen-Sutherland algorithm, Liang-Barsky algorithm etc.

2D and 3D Transformations -Translation, scaling, rotation etc.

Projections -Parallel and perspective projections and their types.

Curve fitting -Cubic curves (Bezier curves, spline curves etc.) Lighting and Shading -Implementing Phong illumination model, Gouraud and Phong shading, Animation Image processing demonstration

Semester III:

BI 501 Taxonomy & Phylogeny

Objectives:

Understand the concepts in Systematics, Classical Taxonomy and Phylogeny in the viral, microbial, animal and plant universe: basis for classification, nature of characteristic properties used for the same

Understand the concepts of molecular evolution and the nature of data for deriving molecular phylogeny

Understand the statistical approaches and models that can be used for Phylogenetic analysis and tree reconstruction

Understand the computational approaches for Phylogenetic analysis and their applications

Syllabus:

Basic concepts in Systematics, Taxonomy and Phylogeny

Concepts in Classical Taxonomy

Concepts in Molecular Evolution

Nature of data used in Taxonomy and Phylogeny

Morphological and molecular character data

Phylogenetic trees: Definition and description, various types of trees

Phylogenetic analysis algorithms

Maximum Parsimony

Distance-based: UPGMA, Transformed Distance, Neighbors-Relation, Neighbor-Joining

Probabilistic models and associated algorithms

Probabilistic models of evolution

Maximum likelihood algorithm

Approaches for tree reconstruction

Character optimization; delayed and accelerated transformation. Reliability of trees. Bootstrap, jackknife, decay, randomization tests.

Comparisons of Trees

Consensus (Strict, semi strict, Adams, majority rule, Nelson). Data partitioning and combination. Tree to tree distances, similarity.

Applications of phylogeny analyses

Comparison of Phylogenetic Trees obtained using DNA seq. Vs. protein. Seq. Vs. Full Genomes. Need for addition of other properties towards total Phylogenetic analysis Comparative methods for detection of species / organism relationships Gene duplication, Horizontal transfer, Domain evolution

Study of co-evolution: Plant-insect interactions. Host-parasite interactions Viral evolution.

Books

Crystallographic and modelling methods in molecular designing; C.E. Bugg,S.F.Ealick

.D. Graur and W-H Li, Fundamentals of Molecular Evolution, 2nd Edition. Sinauer Associates. ISBN 0-87893-266-6

.R.D.M. Page and E.C. Holmes, Molecular Evolution a Phylogenetic Approach, 1998. Blackwell Scientific. ISBN 0-86542-889-1

.L. Patthy, Protein Evolution, 1999. Blackwell Scientific. SBN 0-63204-774-7

BI 502 Object Oriented and Relation Databases

Part 1: Basic Concepts Introduction Database System Concepts and Architecture Entity-Relationship Model EER and Object Modeling Part 2: Relational Databases Relational Model, Algebra, Calculus ER- and EER-to-Relational Mapping Relational languages SQL and QBE RDBMS Systems: SQL server and MS Access Part 3: Object-Oriented Database Systems Object-oriented concepts Object Modeling **Object-Oriented Databases**

Object Database Languages

Object Database Design

Object-Relational and Extended Relational Database Systems

Part 4: Database Design

Functional Dependencies

Normalization

Design Algorithms and Further Dependencies

Part 5: System Implementation Techniques

Query Processing and Optimization

Transaction Processing

Concurrency Control

Recovery

Security and Authorization

Selected Advanced Topics

Distributed Databases and Client-Server Architecture

Distributed Database Architecture

Data Fragmentation, Replication, and Allocation

Distributed Query Processing

Distributed Concurrency Control

Client-Server Architecture

Active Databases

Event Languages, Event Detection and Delivery

Rule Processing

Applications of Active Databases

Data Management in Mobile Computing

Caching and Prefetching

Data Replication

Speculative Data Dissemination and Broadcast Disk

Mobile and Distributed Query Processing

Mobile Transactions

Logic and Deductive Databases

Rule Interpretation

Inference Mechanisms

Program Evaluation

Deductive Databases

Multimedia Databases.

Multimedia Networking

Multimedia Storage and Indexing

Content-based Multimedia Information Retrieval

Data Warehousing and Data Mining

Data Warehousing

Data Mining

OLAP

Database Systems and the World-Wide-Web

Connecting Database to the Web

Web Search

XML and the New Generation Web

Reference

Database Management and Design by G. W. Hansen and J. V. Hansen, Prentice-Hall of India, Eastern Economy Edition, Latest Edition.

Database System Concepts by A. Silberschatz, H.F. Korth and S. Sudarshan, 3rd edition, McGraw-Hill, Latest International Edition.

Database Systems: The Complete Book by Garcia-Molina, J. D. Ullman, and J. Widom., Prentice Hall, Latest Edition.

Fundamentals of Database Systems by Ramez Elmasri and Shamkant B. Navathe, Addison-Wesley. Latest Edition

Database Management Systems by R. Ramakrishnan and J. Gehrke., McGraw-Hill, Latest Edition.

Database Systems by T. Connolly and C. Begg. , Addison-Wesley, Latest Edition.

BI 503 Genomics, Proteomics and Genome to Drug and Vaccine

Objectives:

Appreciate and understand the changes in the approaches for computational analysis between the pre- and post-genomic era. Understand the role of Bioinformatics in the genome sequencing process and post genomic analyses for gene identification, full genome comparison, structural and functional elucidation of genomes, drug target identification etc.

Appreciate the role of Bioinformatics in post-genomic technologies and areas such as DNA micro-array experiments, Proteomics, protein-protein interactions, pharmacogenetics, identification of disease genes, drug and vaccine design etc.

Appreciate the importance of full genome comparisons, Understand the various algorithms used for comparisons of full genome and gene order. Understand and appreciate the full genome comparative studies viruses, microbes, pathogens and eukaryotes ,Understand and explore the comparative genomic databases,Understand the concepts of SNPs and their significance, Understand and appreciate the proteomics concepts and technology,Understand the basis and nature of protein-protein interactions and related databases

Syllabus:

Genomics and Proteomics

Objective and Overview of Genome Comparisons

Genome Alignments

BLAST2

Mummer

Pip Maker

VISTA

Comparison of Gene Order

Gene Order

Comparative Genomic

Viruses

Microbes

Pathogens

Eukaryotes

Comparative Genomic Databases

COG

VirGen

CORG

HOBACGEN

Homophila

XREFdb

Gramene

Single Nucleotide Polymorphism, dbSNP and other SNP-related databases

Overview of Proteomics. Experimental Techniques

Bioinformatics Approaches

Protein-Protein Interaction Networks, databases and software

DIP (Database of Interacting Proteins)

PPI Server

BIND -Biomolecular Interaction Network Database

PIM -Hybrigenics

Path Calling Yeast Interaction Database

MINT -a Molecular Interactions Database\GRID -The General Repository for Interaction Datasets

Interprets -protein interaction prediction through tertiary structure

Genome to Drug and Vaccine

Genome Assembly

Genome Databases and related data resources (EST, STS, GSS, HSS etc.)

Nature and types of data

Organization of data in databases

Genome Data Visualization (With emphasis on Human Genome)

Tools for Genomic Data Mining

Basic Aspects of Genome Annotation

Database Search Engines: Special tools for searching genomic data

Prediction of ORFs and Genes; Gene Modeling

Prediction of Signal sequences (Promoters, Primers, splice sites, UTRs etc.), Operons

Identification of Disease Genes in the context of Human Genetics and Genetics of Model Animals

Identification of Drug Targets

Gene Expression Analysis

Structural Genomic

Functional Genomic

Pharmacogenetics.

The genetics of drug metabolism

The genetics of therapeutic targets

Interactions of small molecules and gene-based drug targets

Protein Sequence Analysis and Prediction of epitomes on Genomic scale

Interactions of epitomes with Antibodies, MHC molecules and TCR

Approaches for designing vaccines

Peptide/DNA vaccines

Polytope vaccines

Recombinant vaccines References Bio informatics from Genome to drugs (ed.) Vol., I &II ;Thomas Lengaure Microcomputer in physiology : a practical approach ;P.J. Frasre

BI 504 Parasite Bioinformatics

Objectives:

Understanding of life cycles and biology of select parasites as well as their interactions with the host and vector

Understanding the role of Bioinformatics in combating parasitic diseases through parasite- specific databases and analysis of genomic, proteomic data

Appreciating the need and approaches for novel drugs/vaccines for parasitic diseases in the context of multidrug resistance

Syllabus:

Biology of Parasites: Life Cycle, Infectivity, Demographic distribution of strains
Parasite Genome and Proteome Databases
Vectors of parasites
Biology of vectors
Genome & Proteome databases
Application of Bioinformatics Data Mining tools for Identification of Parasite-specific genes / gene products (e.g. house-keeping genes, genes essential for survival)
Resistant Genes

Tools: Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis Microarray and Proteomics Data Analysis, Structural genomic of parasites. Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases

Multi-Drug Resistance.

Mechanism of MDR: genomic, molecular, cellular

Identification of genes responsible for MDR Approaches to novel drug discovery Challenges and opportunities in vaccine development Plant Parasites and diseases Disease resistance genes of plants Plant-pathogen interactions

References Parasitology: protozoology, Helminthology; K.D Chatargee

BI 551 Practical based on BI501

Use Phylip to derive Phylogenetic relationships of DNA, RNA and protein sequences using the various methods such as .Parsimony .Maximum likelihood Distance-based methods .Using bootstrapping tool to generate multiple datasets from the original input data .Plotting and visualizing Phylogenetic trees and interpretation (Tree View and other tools)

BI 552 Practical based on BI502

Objectives:

To be able to understand the exiting data structures in various databanks and databases in terms of the data model, relationships between entities etc., attempts being made to create relational databases, object oriented relational databases and the tools for data integration. The student should be able to use the knowledge gained in the various computational courses such as Database systems (Oracle, SQL, VB etc), Perl, CORBA etc for the development of value added databases.

Syllabus

Drawing ER diagrams for the primary sequence databanks to convert them into relational models (swiss-prot, PIR, GenBank, EMBL, DDBJ)

Parse .the 'records from various entries of the primary databank. Create tables with

appropriate relationships using a RDBMS tool, populate tables and query them using SQL.

In-depth study of the PDB relational model as in the EBI Macromolecular structure database. Compare with the PDB flat file and study the various fields.

Study the secondary / derived databases and create suitable relational models for the same. (Prosite, ProDom, Profiles, PRINTS, Pfam, BLOCKS etc.)

Assignment on InterPro as a model for Data Integration.

PlasmoDB, ICTV DB, Species 2000, VirGen, MPE (Metabolic pathway engineering) etc. as other models for Data Integration.

BI 553 Practical based on BI503

Comparison of full / partial genomic sequences using following methods to identify conserved genes and map/compare the annotations of the two sequences

BLAST2, MUMmer, Pip Maker, VISTA .Compare gene order of given genomic sequences using the Gene Order tool.

Explore and query the comparative genomics databases: COG, VirGen, CORG, HOBACGEN, Homophila, XREFdb, Gramene etc.

Explore and query the protein-protein interaction databases: DIP, PPI Server, BIND, PIM, Path Calling, MINT, GRID, and Interprets

BI 554 Programming in Perl

-Perl

Introduction: What is Perl? Why use Perl in Bioinformatics? history of Perl, Availability, Support, Basic Concepts

Scalar Data: What Is Scalar Data?, Numbers, Strings, Scalar Operators, Scalar Variables, Scalar Operators and Functions

Arrays and List Data: What Is a List or Array? Literal Representation, Variables, Array

Operators and Functions, Scalar and List Context

Control Structures: Statement Blocks

Hashes: What Is a Hash? Hash Variables, Literal Representation of a Hash, Hash Functions,

Hash Slices

Basic VO

Regular Expressions: Concepts About Regular Expressions, Simple Uses of Regular

Expressions, Patterns, More on the Matching Operator, Substitutions, The split and join Functions

Subroutines: System and User Functions, The local Operator, Variable-length Parameter Lists, Notes on Lexical Variables

Miscellaneous Control Structures:

File handles and File Tests: What Is a File handle? Opening and Closing a File handle, Using Pathnames and Filenames, A Slight Diversion: die, Using File handles, The -x File Tests, The stat

Function

Formats: What Is a Format? Defining a Format, Invoking a Format

Directory Access: Moving Around the Directory Tree, Globing, Directory Handles, and Opening and Closing 'a Directory Handle, Reading a Directory Handle

File and Directory Manipulation

Process Management: Using system and exec1 Using Back quotes,

Other Data Transformation: Finding a Sub string, Extracting and Replacing a Sub string Formatting Data: Sorting, Transliteration

System Information: Getting User and Machine Information, Packing and Unpacking Binary

Data

Getting Network Information

Database Manipulation: DBM Databases and DBM Hashes, Opening and Closing DBM Hashes, Fixed-Length Random-Access Databases, Variable-Length (Text) Databases, Win32 Database Interfaces ~':

CGI programming: The CGI. pm Module, Your CGI Program in Context, Simplest CGI Program,

Passing Parameters via CGI, Perl and the Web ~5':

Object oriented perl: Introduction to modules, Creating Objects .. .Bioperl: Introduction, Installation procedures, Architecture, Uses of bioperl --

CORBA

Common Object Request Broker Architecture: Distributed computing, Introduction to CORDA,

About Object management group, CORBA architecture, architectural similarities, CORBA versus Java RMI, CORBA services, CORBA facilities- (Vertical and Horizontal facilities) CORBA domains. IDL (Interface definition language): compiler, stubs, skeletons, Repositories, ORB (Object request broker); naming service;

Inter-ORB communication: Creating CORBA objects; L modules and interfaces, data members and methods; Java; Simple server class, helper class, holder class, client and server stubs;

Initializing ORB, Registering with a naming service; Adding objects to a naming context; Finding remote objects; Initial ORB references; Getting objects from other remote objects, Springfield object references; Dynamic invocation interface.

RECOMMENDED BOOKS

Perl

Beginning Perl for Bioinformatics by James Tisdall, a-Reilly Developing Bioinformatics Computer Skills by Cynthia Gibas, Per Jambeck, a-Reilly Learning Perl by Randal L. Schwartz, Tom Phoenix, a-Reilly Programming Perl by Larry Wall, Tom Christiansen, Jon Orwant, a-Reilly Programming the Perl DBI by Alligator Descartes, Tim Bunce, a-Reilly Advanced Perl Programming by Sriram Srinivasan, a-Reilly

CORBA

The *Essential Distributed Objects Survival Guide* by Orfali and Harkey, Wiley *Client/Server Programming with JA V A and CORBA* by Orfali and Harkey, Wiley *CORBA Fundamentals and Programming* by Siegel, Wiley *Teach Yourself CORBA in* 14 *Days by* Jeremy L. Rosenberger, SAMS. *CORBA: A Guide to Common Object Request Broker Architecture* by Ron Ben-Natan, McGraw-Hill

Understanding Corba by Randy Otte, Paul Patrick, Mark Roy, Prentice Hall

SEMESTER IV

BI 505 Advanced Techniques for Sequence and Structure Analysis and Data Mining

Objectives:

To be able to understand and implement various advanced mathematical, physical and statistical techniques that are being applied for analyzing information at sequence and structure level.

Syllabus

Advanced Techniques for Sequence Analysis .Sequence Profiles: Derivation, Databases, Application Gapped BLAST, PSI-BLAST, PHi-BLAST, **Epitope Prediction Methods** Advanced Techniques for Structure Analysis .Molecular replacement method, direct method & Fiber diffraction, .Methods for Comparison of 3D structures Dynamic Programming .Sequence Alignments, .Structure Alignments Genetic Algorithms .Sequence Alignments Prediction of Protein Structure, .Docking Simulations t1 Ab initio methods for structure prediction . Lattice, SOM, etc. Information theory, entropy and relative entropy **Stochastic Grammars & Linguistics** Electrostatics of biomolecules .Molecular Dynamics Simulations & Monte Carlo Methods Simulations of Bio-macromolecular Structures, Biomolecular Structure Prediction, Conformational Searches, Free energy perturbation method Simulated Annealing .Multiple Sequence Alignments Simulations of Bio-macromolecular Structures, .Docking and Scoring Ant colony optimization .Multiple Sequence Alignments **Biomolecular Structure Prediction** Optimization Techniques .Steepest Descent, Conjugate Gradient, Newton-Raphson Biomolecular Structure Optimization Clustering Algorithms .Hierarchical and non-hierarchical Clustering Rossetta Stone

Phylogenetic Analysis, .Analysis of MD trajectories
Micro array and Protein Array data Analysis
Foundations for Machine learning Techniques:
The probabilistic framework, .Bayesian modeling
The Cox-Jaynes Axiomes
Probabilistic modeling and Inference .Fuzzy Logic system & application

References

Preparation and analysis of protein crystal; Alexander McPherson

BI 506 Metabolomes and Metabolic Pathway Engineering.

Objectives:

Learning the basic biochemical concepts of metabolic pathways Understanding the role of Bioinfonnatics in the study of metabolic pathways Learning the Bioinformatics-based approaches for predicting and engineering metabolic pathways

Syllabus Classification of Enzymes Classification of Metabolic Pathways (with respect to enzymes) Metabolic Pathway databases KEGG EMP Malaria Parasite Metabolic Pathways Coccyx and MetaCyc **Boehringer Mannheim - Biochemical Pathways** Enzymes, Compounds and Reactions databases LIGAND -Biochemical Compounds and Reactions ENZYME - Enzymes BRENDA - Comprehensive Enzyme Information System Full Genome Annotation through knowledge of Metabolic Pathways **Organism Specific Metabolic Pathways** Comparison of Metabolic Pathways Engineering of Metabolic Pathways **Representation of Metabolic Pathways** Generation and Dynamic Representation of Metabolic Pathways Deriving Common Principles from the Metabolic Pathways Knowledge E.g. deriving sets of enzymes specific for various reactions (e.g. oxidation), alternative paths for synthesis of metabolites etc.

References

Protein- Protein Interaction; C.Frieden Biological chemistry: The molecular approach to biological system K.E.Suckling, C.J. Suckling

BI 507 Emerging Areas in Bioinformatics

Objective:

Recent developments in Life sciences in the context of Bioinformatics will be discussed

Syllabus:

Topics such as Linguistic modeling, chemical descriptors in QSAR, Clinical data management, Advanced clinical immunology, Epigenetics, Advanced Glycobiology.

BI 555 Practical based on 505

Objectives: To be able to understand and implement various advanced mathematical, physical and statistical techniques that are being applied for analyzing information at sequence and structure level.

Syllabus

Advanced techniques for Sequence analysis: .Exploring the Profiles databases Usage of profiles created from MSA for database searches: at least 2 different methods (e.g., Profile Analysis (Gribskov) and PSI-BLAST)

Study and application of pattern databases (prints, BLOCKS, Pfam). Developing codes in C/ Perl for deriving patterns using regular expression, consensus and profile.

Study of various epitope prediction algorithms and developing 'c' program for epitope prediction

Optimization Algorithms:

Programming in 'c' for implementation of Golden section algorithm, Steepest descent, Newton Raphson, Conjugate gradient etc for energy minimization applications.

Implementation of random walk and Monte Carlo algorithm.

Simulated Annealing algorithm for energy minimization.

Ant colony algorithm for the Traveling salesman problem (TSP)

Molecular dynamics simulation & docking: .Simulation of a peptide of about 4 amino acids length using appropriate force field in the

absence and presence of a box of water.

Ligand docking and virtual scoring

Neural networks: .Use of neural network tools like Brain Box, MA TLAB etc.

Program in 'c' for implementing the perception learning rule and the delta learning rule (adaline network) for say logic gate patterns.

Implementation of the Back propagation learning algorithm for the XOR gate and for an application such as protein secondary structure prediction, promoter prediction etc. Detenn1ne the entropy in. a DNA sequence, relative entropy in 2 sequences etc. Implement the moment estimator/ maximum likelihood estimator. Hidden Markov model implementation in C/ Java.

BI 556 Practical based on BI 506

As per theory syllabus conduct minimum eight practicals.

BI 557 Practical based on BI 507

Seminar report and Presentation.

Seminar on any one of the following:

- 1 Seminars on Applications of Bioinformatics in Agriculture
- 2 Seminars on Applications of Bioinformatics in Human Health
- 3 Seminars on Applications of Bioinformatics in Environment
- 4 Seminars on Applications of Bioinformatics in Biotechnology
- 5 Seminars on Applications of Bioinformatics in Molecular Biology
- 6 Seminars on Applications of Bioinformatics in Neurobiology
- 7 Seminars on Applications of Bioinformatics in Drug Designing
- 8 Seminars on Applications of Bioinformatics in Veterinary Sciences
- 9 Seminars on any recent advance topic

BI 558 Project

Project report and Presentation.

Project should be based on the following topics:

- 1 Parasite bioinformatics
- 2 Biodiversity informatics
- 3 Microbial informatics
- 4 Immunology bioinformatics
- 5 Plant bioinformatics
- 6 Molecular modeling
- 7 Any recent advance topic.

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