Ramanand Teerth Marathwada University
Nanded

(NAAC Re-accredited with 'A' Grade)

School of Technology
Sub Centre, Latur

Syllabus of

M.Sc. Bioinformatics(2 years)

(Revised CBCS pattern)

Introduced from Academic Year 2015-16

School of Technology,
SRTMUN Sub-Centre, Latur

M.Sc. Bioinformatics

M.Sc. Bioinformatics (2years) degree builds the student on higher studies in Life Science and to become competent in the current race and development of new computational technologies. The duration of the study is of four semesters, which is normally completed in two years. The primary goal of this M.Sc. program is to increase the understanding of life science . What sets it apart from others is its approach and focus on developing and applying computationally intensive techniques to achieve higher goals in life science. Major inputs given in the curriculum are from the field of Structure analysis,Functional genomics,Structural genomics, Microarray,Genetic algorithm, Artificial neural network,Metabolic engineering

CBCS pattern and CGPA system

The School newly introduces its M.Sc. Bioinformatics program as per CBCS (Choice based credit system) pattern, in which choice, is given to the students under open electives and subject electives. The students can choose open electives from the same course or from other course of the same school or from other courses of other schools.

The Evaluation of performances of students for the course under Choice based Credit system (CBCS) is based on CGPA (Cumulative Grade Point Average) formulae. A Cumulative Grade Point Average is the mean Grade Point Average (GPA) from all academic terms within a given academic year, whereas the GPA may only refer to one term.

Eligibility and Fees

The eligibility of a candidate to take admission to M.Sc. (Bioinformatics) 2 years program is B.Sc. with any one subject from Physics, Chemistry, Botany, Agriculture, life science .More details on admission procedure and fee structure can be seen from the prospectus of the University.

Features of CBCS pattern

[1] Master Degree would be of 100 Credits

[2] Each semester shall consists of four theory courses and two practical courses and one foundation Course or seminar

[3] Four theory courses = 16 Credits

[4] two practical courses= 8 Credits

[5] one seminar=1 credit

[6] Total credits per semester= 25

[7] Total Credits of Four Semesters= 100

[8] Total marks per semester= 625

[9] Total marks for Master Degree program =2500

[10] One Credit = 25 marks

[11] Two Credits = 50 Marks

[12] Four Credits = 100 Marks

[13] Each Theory Course/Practical course = 100 Marks

Internal Exam evaluation	External Exam evaluation
50 Marks = 2 Credits	50 Marks = 2 Credits

[14] Break up of internal marks evaluation for each Theory course

Home Assignments /Seminar / Mini Project/ E – Content Development / Examination/ Skill based activity or Concerned Teacher can adopt any other internal evaluation method	Total Marks 50 Marks = 2 Credits

[15] Practical Course = 100 Marks

Internal Exam evaluation	External Exam evaluation
50 Marks = 2 Credit	50 Marks = 2 Credits

[16] Break up of internal exam marks for Practical

Internal Exam	Total Marks
Record Book /Experiments / Mini Project/ E – Content Development / Examination/ Skill based activity / Concern Teacher can adopt any other internal evaluation method	50 marks = 2 Credits

Passing rules: As per the CGPA system of the University

Outline of M.Sc. Bioinformatics Syllabus (As per CBCS Pattern)

Sr. No	**Course category**	**Paper code**	**Paper Title**	**Internal credits**	**External credits**	**Total credits**
First Semester						
1.	Core Subjects	BIM 1-1	Introduction to Bioinformatics	2	2	4
2		BIM 1-2	Biological Databases and data analysis	2	2	4
3		BIM 1-3	Biological Databases and data analysis	2	2	4
Choose any one from BIM 1-4 A and 1-4 B						
4	Subject Elective	BIM 1-4 A	Biological Chemistry	2	2	4
5		BIM 1-4 B	Advances in Operating System	2	2	4
6		BIM 1-5	Advances in Operating System	2	2	4
7	Open Elective	BIM 1-6	Genetic Information Flow and Processing	2	2	4
8						
9	Seminar	BIM 1-7	Seminar	1	-	1
						25
Second Semester						
10	Core Subjects	BIM 2-1	Structural Biology and Bioinformatics	2	2	4
11		BIM 2-2	Chemoinformatics	2	2	4
12		BIM 2-3	Chemoinformatics	2	2	4
Choose any one from BIM 2-4 A and 2-4 B						
13	Elective Subjects	BIM 2-4 A	Cell Biology Genetics and Genomics	2	2	4
14		BIM 2-4 B	Immunology and Bioinformatics	2	2	4
15		BIM 2-5	Immunology and Bioinformatics	2	2	4
16	Open Elective	BIM 2-6	Perl Programming	2	2	4
17						
18	Seminar	BIM 2-7	Seminar	1	-	1
						25

Sr. No	Course category	Paper code	Paper Title	Internal credits	External credits	Total credits
			Third Semester			
19	Core Subjects	BIM 3-1	Genome to Drug and Vaccine	2	2	4
20		BIM 3-2	Comparative Genomics and Proteomics	2	2	4
21		BIM 3-3	Plant Genomics	2	2	4
22		BIM 3-4	Comparative Genomics and Proteomics	2	2	4
			Choose any two from BIM 3-5 A and CS 3-5 B			
23	Subject Elective					
		BIM 3-5 A	Molecular Phylogenetics	2	2	4
		BIM 3-5 B	Molecular Modelling and Simulation	2	2	4
		BIM 3-6	Molecular Modelling and Simulation	2	2	4
24	Seminar	BIM 3-7	Seminar	1	-	1
						25
			Fourth Semester			
25	Core Subjects	BIM 4-1	Advanced Techniques for sequence and Structure Analysis	2	2	4
26		BIM 4-2	Metabolic Engineering	2	2	4
27		BIM 4-3	Project	-	4	4
28		BIM 4-4	Metabolic Engineering	2	2	4
			Choose any one from BIM 4-5 A and 4-5 B			
29	Elective Subjects	BIM 4-5 A	Introduction to database system	2	2	4
30		BIM 4-5 B	Computational Structural Biology	2	2	4
31		BIM 4-6	Computational Structural Biology	2	2	4
32	Seminar	BIM 4-7	Seminar	1	-	1
						25

Course Title :- INTRODUCTION TO BIOINFORMATICS
Course Code :-BIM 1-1 **40L**
Objective :- Students will understand the scope and importance of Bioinformatics

MODULE I Introduction

Introduction: Aim and branches of Bioinformatics, Application of Bioinformatics, Role of internetand www in bioinformatics. Basic biomolecular concepts: Protein and amino acid, DNA & RNA,Sequence, structure and function. Forms of biological information, Types of Nucleotide Sequence:Genomic DNA, Complementary DNA (cDNA), Recombinant DNA (rDNA), Expressed sequence tags (ESTs), Genomic survey sequences (GSSs). DNA sequencing methods: Basic and Automated DNA sequencing, DNA sequencing by capillary array and electrophoresis, Gene expression data.

MODULE II Bioinformatics Resources

Bioinformatics Resources: NCBI, EBI, ExPASy, RCSB, DDBJ: The knowledge of databases andbioinformatics tools available at these resources, organization of databases: data contents, purpose andutility. Open access bibliographic resources and literature databases: PubMed, BioMed Central,Public Library of Sciences (PloS), CiteXplore.

MODULE III Sequence databases

Sequence databases: Nucleic acid sequence databases: GenBank, EMBL, DDBJ; Protein sequence
databases: Uniprot-KB: SWISS-PROT, TrEMBL, UniParc; Structure Databases: PDB, NDB, PubChem, ChemBank. Sequence file formats: Various file formats for bio-molecular sequences:
GenBank, FASTA, GCG, MSF etc. Protein and nucleic acid properties: Proteomics tools at the ExPASy server, GCG utilities and EMBOSS, Computation of various parameters

MODULE IV Sequence analysis

Sequence Analysis: Basic concepts of sequence similarity, identity and homology, definitions of homologues, orthologues, paralogues and xenologues Scoring matrices: basic concept of a scoring matrix, Matrices for nucleic acid and proteins sequences, PAM and BLOSUM series, matrix derivation methods and principles.

MODULE V Sequence alignment

Sequence alignment: Measurement of sequence similarity; Similarity and homology. Pairwise sequence alignment: Basic concepts of sequence alignment, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments, gap penalties, use of pairwise alignments for analysisof Nucleic acid and protein sequences and interpretation of results.

Reference

1. . Bioinformatics: Sequence and Genome Analysis by Mount D., Cold Spring Harbor Laboratory Press, New York. 2004
2. Bioinformatics- a Practical Guide to the Analysis of Genes and Proteins by Baxevanis, A.D.and Francis Ouellellette, B.F., Wiley India Pvt Ltd. 2009
3. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith, Pearson Education. 1999
4. . Bioinformatics for Dummies by Jean-michel Claverie Cedric Notredame. Publisher: Dummies

(Jan 2007)

Course Title :- BIOLOGICAL DATABASES AND DATA ANALYSIS 40L
Course Code:- BIM 1-2
Objectives:

This course will enable the students to:

1. Understand the nature of biological data and need for biological databases
2. To understand and explore major biomolecular sequence databases (organization and contents); search and retrieve data from the databases using their respective search engines
3. Understand and appreciate the need and significance of sequence analysis and the bioinformatics approaches for the same
4. Understand algorithms for sequence analysis
5. Understand the application of methods for analysis of the biomolecular sequence data

MODULE I Biological data

- Introduction to Bioinformatics , Nature of biological data

MODULE II Biological Databases

- Overview of Bioinformatics resources on the web , NCBI/EBI/EXPASY etc, Biological Databases: Nucleic acid sequence databases ,EMBL/DDBJ

MODULE III Uniprot

- Biological Databases: Protein sequence databases , UniProtKB , Overview of concepts in sequence analysis

MODULE IV Sequence alignment

- Pairwise sequence alignment algorithms ,Needleman & Wunsch, Smith & waterman: Scoring matrices for Nucleic acids and proteins,MDM, BLOSUM, CSW, Database Similarity Searches, BLAST, FASTA

MODULE V Multiple sequence alignment

Multiple sequence alignment, PRAS, CLUSTALW, Derived databases, Prosite, BLOCKS, Pfam/Prodom, Recent derived database (To be decided by faculty member), Biological databases: structural databases, PDB, NDB CCSD

References:

1. Baxevanis A.D., Davison D.B., Page R. D. M. & Petsko G.A. Current Protocols in
2. Bioinformatics. New York, John Wiley & Sons Inc., 2004. ISBN: 0555015254

3. Korf Ian, Yandell Mark, Bedell Joseph. BLAST: an essential guide to the basic local alignment search tool. Shroff Publishers and Distributors Pvt. Ltd., 2003. ISBN:8173665125.
4. Baxevanis Andreas D. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, 3rd Edition. Publisher: New York, John Wiley & Sons, Inc. 2002, ISBN: 9814126756
5. Teresa Attwood, Parry-Smith David J. Introduction to Bioinformatics. Publisher: Pearson Education (Singapore) Pte.Ltd., 2001. ISBN:8178085070.
6. Mount David W.. Bioinformatics: Sequence and Genome Analysis. Publisher: Cold
7. Spring Harbor Laboratory Press; 1st edition 2001. ISBN: 0879695978
8. Gibas Cynthia, Jambeck Per. Developing Bioinformatics Computer Skills. Publisher: Shroff Publishers and distributors O'Reilly Media, Inc., 2001. ISBN: 8173662428

Course Title:- BIOLOGICAL DATABASES AND DATA ANALYSIS
Course Code :- BIM 1-3 **40L**

Objectives:

This course will enable the students to:

- to understand and explore major biomolecular sequence databases (organization and contents); search and retrieve data from the databases using their respective search engines
- apply bioinformatics methods for analysis and interpretation of biomolecular sequence data

1. Exploring the integrated database system at NCBI server and querying the PUBMEDand GenBank databases using the ENTREZ search engine
   Use of operators (AND, OR & NOT)Use of limits,Exporting GI list
2. Batch retrieval
   a. Exploring the integrated database system at EBI server and searching the EMBL Nucleotide database using the SRS search engine
   b. Exploring & querying SWISSPROT & UniProtKB
   c. Sequence Formats & Format converters
   d. Exploring tools on ExPASY
3. Exploring utilities in EMBOSS packages

4. Pair-wise global alignments of protein and DNA sequences using Needleman-Wunsch algorithm & interpretation of results to deduce homology between the sequences, use of scoring matrices

5. Pair-wise local alignments of protein and DNA sequences using Smith-Waterman algorithm and interpretation of results

6. Database (homology) searches using different versions of BLAST and interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences

7. Database (homology) searches using different versions of FASTA & interpretation of the results to derive the biologically significant relationships of the query sequences (proteins/DNA) with the database sequences

8. Multiple sequence alignments of sets of sequences using web-based and stand-alone version of CLUSTAL. Interpretation of results to identify conserved and variable regions and correlate them with physico-chemical & structural properties

9. Exploring and using the derived databases: PROSITE, PRINTS, BLOCKS, Pfam and

10. Prodom for pattern searching, domain searches etc.

11. Studying the format & content of structural databases & visualization of structures using Rasmol, Cn3D and other utilities

References:

1. Baxevanis Andreas D. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, 3rd Edition. Publisher: New York, John Wiley & Sons, Inc. 2002, ISBN: 9814126756

1. Teresa Attwood, Parry-Smith David J. Introduction to Bioinformatics. Publisher: Pearson Education (Singapore) Pte.Ltd., 2001. ISBN:8178085070.

2. Mount David W.. Bioinformatics: Sequence and Genome Analysis. Publisher: Cold

3. Spring Harbor Laboratory Press; 1st edition 2001. ISBN: 0879695978

4. Gibas Cynthia, Jambeck Per. Developing Bioinformatics Computer Skills. Publisher: Shroff Publishers and distributors O'Reilly Media, Inc., 2001. ISBN: 8173662428

Course Title:-BIOLOGICAL CHEMISTRY **40L**

Course Code :-BIM 1-4A

Objectives*:*

This course will enable the students to:

- be familiar with the chemistry of different classes of biomolecules and their interactions in an aqueous environment
- understand the structure-function relationships of macromolecules, the principles of enzyme catalysis and regulation,
- understand organization of metabolic systems with an in-depth account of the pathways for the complete oxidation of glucose.

MODULE I Carbohydrates

- Water as the universal biological solvent; concepts of pH, buffer and osmolarity , Carbohydrates: monosaccharides, glycoproteins

MODULE II Nucleic acid and Lipids

- Lipids: fatty acids, acylglycerols; phospholipids, sphingolipids, cholesterol and membranes; Isoprenoids, icosanoids and their biological importance., Nucleic acids: bases, nucleotides, RNA and DNA; different structural forms of DNA; different types of RNA.

MODULE III Proteins and Enzymes

•Proteins: amino acids and peptides; primary, secondary, tertiary and quaternary structures; structure, function and evolutionary relationships; protein – protein interactions, protein folding; allosteric proteins.Enzymes: enzyme nomenclature and classification; Modules of enzyme activity; specificity; 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.

MODULE IV Metabolic pathways

- 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.

MODULE V Glycolysis

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

References:

1. Nelson David L., Cox Michale. Lehninger Principles of Biochemistry 5th Edition.
2. Publisher: New York. W. H. Freeman. 2008. ISBN 978 0716771081.
3. Berg, Jeremy M, Tymoczko, John L. Stryer, Lubert. Biochemistry 6th Edition.
4. Publisher: New York : W.H. Freeman. 2007.ISBN: 071676766X.Hames David, Hooper Nigel. Instant Notes in Biochemistry 3rd Edition. Publisher .
5. Nodia, Taylor & Francis. 2007. ISBN: 185996 2491.
6. Voet, Donald, Voe Judith, Pratt, Charlotte W. Fundamentals of Biochemistry: Life at the molecular Level 2nd Edition. Publisher: Asia, John Wiley & Sons. 2006. ISBN:0471753416.Horton, Robert, Moran, Laurence A, Scrimgeour, Perry Gray Marc, Rawn.David.
7. Principles of biochemistry. Publisher: New Jersey, Pearson Prentice Hall, 2006. ISBN: 0131453068.
8. Mathews, Christopher K. van Holde, K. E., Ahern Kevin G. Biochemistry. Publisher: San Francisco, Pearson Education 2000.ISBN: 81 29702150.
9. Zubay,Geoffrey.Biochemistry 4th Edition, Publisher: Boston,Wm C. Brown, 1998, ISBN 0697219003.
10. Garrett, Reginald H. , Grisham, Charles M. Principles of biochemistry: with a human focus. Publisher: Australia Brooks/Cole, Thomson Learning, 1997. ISBN:0030973694.

Course title :-Advances in Operating System

Course Code:- **BIM 1-4 B** **40L**

Objective:

- To introduce Advanced Operating Systems Concepts
- Introduction of Multiprocessor and Distributed Operating system.
- Finally Unix/Linux and Windows as representative examples

Unit1: Overview of OS

Operating System Concepts, Operating System Structure, Process and Thread Management, Memory Management, File System, deadlocks.

Unit 2: Multimedia Operating Systems

Introduction to Multimedia, Multimedia Files, Video Encoding, Audio Encoding, The JPEG Standard The MPEG Standard, Multimedia Process Scheduling, Scheduling Homogeneous Processes, General Real-Time Scheduling, Rate Monotonic Scheduling, Earliest Deadline First Scheduling, Placing a File on a Single Disk, Two Alternative File Organization Strategies, Placing Files for Near Video on Demand, Placing Multiple Files on a Single Disk, Placing Files on Multiple Disks, Static Disk Scheduling, Dynamic Disk Scheduling.

Unit3: Multiple Processor System

Multiprocessor, Multiprocessor Hardware, Multiprocessor Operating System Types, Multiprocessor Synchronization, Multiprocessor Scheduling, MULTICOMPUTERS, Multicomputer Hardware, Low-Level Communication Software, User-Level Communication Software, Remote Procedure Call, VIRTUALIZATION, Requirements for Virtualization, Type I Hypervisors, Type 2 Hypervisors, Para virtualization

Unit 4: Distributed Operating System

Motivation, Types of Network based Operating Systems, Network Structure, Network Topology, Communication Structure, Communication Protocols, Robustness, Design Issues An Example: Networking, Introduction to distributed file system.

Unit 5: Case study: Linux

Linux History, Design Principles, Kernel Modules, Process Management, Scheduling, Memory Management, File Systems, Input and Output, Inter process Communication, Network Structure, Security Summary.

Suggested Readings:

1. Abraham Silberschatz, Peter B. Galvin, G. Gagne, “Operating System Concepts”, Sixth Edition, Addison Wesley Publishing Co., 2003.
2. Andrew S. Tanenbaum, “Modern Operating Systems”, Second Edition, Addison Wesley, 2001
3. Pradeep K.Sinha, "Distributed operating system-Concepts and design", PHI, 2003.

4. Andrew S.Tanenbaum, "Distributed operating system", Pearson education, 2003
5. Mukesh Singhal and N. G. Shivaratri, “Advanced Concepts in Operating Systems”, McGraw- Hill, 2000

Course Title :-Advances in Operating System **40L**
Course Code :- BIM 1-5
Practical based on Advanced Operating System

1. Processor Management
2. Memory Management
3. Scheduling Algorithm
4. Multimedia based operations
5. Demo of distributed operating System
6. Linux Commands
7. Shell programming Ten programs based on shell programming

Apart from the above list concern teacher can conduct different kinds of programs for the better understanding of concept.

Course Title:-GENETIC INFORMATION FLOW AND PROCESSING **40L**
Course Code:- BIM 1-6

Objectives:

This course will enable the students to:

- understand the current concepts in gene organization, transcription, translation and regulation of gene function
- know biotechnological implications of recent developments in cloning and genome sequencing.

MODULE I: DNA as genetic material

Introduction: DNA as a genetic material – Experiments done to prove this

Nucleic acid structure: single stranded & double stranded; denaturation, renaturation and hybridization of DNA; secondary structures in single stranded molecules; alternative double helical structures in double stranded DNA; Closed DNA as supercoiled molecule

MODULE II Genome organisation

Genome organization: Prokaryotic and eukaryotic genomes – C value paradox, repetitive and non-repetitive DNA., transposons and retroposons; Exons and introns – organization of interrupted genes, one DNA sequence may code for multiple proteins; Gene numbers – essential genes and total gene number, gene clusters, pseudogenes; Gene families – globin and rDNA gene families; Organelle genome – mitochondrial and chloroplast Packaging of genome – Bacterial genome as nucleoid; Eukaryotic genome – nucleosomes, chromatin, solenoids, loops, domains, scaffolds, chromosomes. .

MODULE III Replication and DNA repair

- Perpetuation of DNA: Prokaryotic DNA replication – DNA polymerases, origin of replication, initiation, elongation and termination of replication. Rolling circle model of replication; Eukaryotic DNA polymerases – multiple origins of replication, process of replication; Regulation of replication in both prokaryotes and eukaryotes. (5)

- DNA damage, repair and recombination: Different types of DNA damages; Variety of DNA repair systems in prokaryotes and eukaryotes – Base excision repair system, Nucleotide excision repair system, Mismatch repair system, Recombination repair system; Recombination – homologous and non-homologous recombination. (3)

MODULE IV Operon Concept

- Gene Expression – Transcription and Translation: Transcription in prokaryotes – RNA polymerase, initiation, elongation and termination of transcription; regulation of transcription – operon concept, lactose and tryptophan operons (6)

- Transcription in eukaryotes: Different RNA polymerases – requirement of promoters by these RNA polymerases, initiation, elongation and termination by these polymerases; Processing of transcripts – 5’ capping, 3’ polyadenylation, splicing and editing; Regulation of transcription – response elements, enhancers and silencers,protein-nucleic acid interaction, HLH, leucine zipper proteins, noncoding RNA

MODULE V Translation

- Translation in prokaryotes: protein synthesis machinery – mRNA, tRNA and rRNA molecules; initiation, elongation and termination of translation; Genetic code – interpreting genetic code; Accuracy of translation.

- Eukaryotic translation: protein synthesis – initiation, elongation and termination; Post- translational modifications of proteins; protein degradation; Regulation of translation - mRNA stability, 5’ and 3’ UTRs, mRNA localization

- Gene regulation by post-translational modifications of proteins (acetylation, methylation, ribosylation, phosphorylation etc.) and different intermediate RNAs (ribozymes, miRNAs, siRNAs etc.)

References*:*

1. Krebs, Jocelyn E. Goldstein, Elliott S. Kilpatrick, Stephen T. Lewin's Essential GENES 2nd Ed. Publisher: Boston, Jones & Bartlett. 2010. ISBN: 978-0763759155.

2 Krebs Jocelyn E., Goldstein Elliott S., Kilpatrick Stephen T. Lewin's Genes X Publisher: Jones & Bartlett 2009. ISBN: 9780763766320.

3.Hood Leroy, Goldberg Michael L., Reynolds Ann E., Reynolds Lee M., Veres Ruth

    a. C. Hartwell Leland H. Genetics: From Genes to Genomes Publisher: McGraw/Hill,

    .

2. Watson James D., Baker Tania A., Bell Stephen P., Alexander Gann, Levine, Michael Losick Richard. Molecular Biology of the Gene 6th Edition. Publisher: New York, Cold Spring Harbor Laboratory Press. 2008. ISBN: 9780321507815

3. Weaver Robert F. Molecular Biology, 3rd Edition. Publisher : Boston McGraw-Hill's

4. Epstein Richard J. Human molecular biology: an introduction to the molecular basis of health and disease. Publisher: Cambridge, UK ; Cambridge University Press, 2003. ISBN: 052164481X.

5. Russell Peter J. iGenetics: A Molecular Approach 3rd edt.: Pearson International

6. Brown, T.A. Genomes 2 Publisher: New York, BIOS Scientific Publishers Ltd. 2002, ISBN: 1859960294

BIM 1-7

Seminar

Course Title:-STRUCTURAL BIOLOGY AND BIOINFORMATICS 40L
Course Code:- BIM 2-1
Objectives*:*

This course will enable the students to:

- o understand the levels of structural organization of macromolecules and experimental methods of structure determination
- know the approaches for structure analysis
- acquire knowledge of various algorithms & methods of structure prediction
- understand the principles of macromolecular interactions

MODULE I*: Ramachnadran Plot*

Macromolecular Structure
(14) Protein - Primary, Secondary, Supersecondary, Tertiary and Quaternary structure, Potential energy maps, Ramachandran map, Nucleic acid – DNA and RNA, Carbohydrates ,Co-ordinate systems , Overview of experimental techniques to study macromolecular structures ,Methods to study 3D structure: X-ray, NMR, Cryo-electronmicroscopy ,Validation using Procheck, ProsaII

MODULE II Protin folding

Principles of protein folding and methods to study protein folding ,Macromolecular interactions ,Protein – Protein ,Protein – Nucleic acids Protein - carbohydrates

MODULE III protein structure prediction

Structure of Ribosome ,Prediction of protein structure

MODULE IV Tertiary structure prediction

o secondary structure prediction methods , First, second and third generation methods ,Tertiary structure prediction

MODULE V Homology modeling

Homology modeling, fold recognition and *ab initio* methods

References*:*

1 Bourne Philip E., Weissig Helge. Structural Bioinformatics (Methods of BiochemicalAnalysis, V. 44), 2003. Publisher: Wiley-Liss. ISBN: 0471202002.
2 Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890.
3 Leach, Andrew. Molecular Modelling: Principles and Applications. Publisher: PrenticeHall. 2001. ISBN: 0582239338.

4 Friesner Richard A. Computational Methods for Protein Folding:advances in Chemical Physics Volume 120 Kindle Edition. Publisher: New York, John Wiley & Sons. 2002. ISBN: 0471209554.
5 Heilmeyer L., Friedrich P. Protein Modules in Cellular Signalling. Publisher: Amsterdam, IOS Press. 2001. ISBN: 1586031805.
6 Rhodes Gale.Crystallography Made Crystal Clear, Third Edition: A Guide for Users ofMacromolecular Models. Publisher: USA, Academic Press 2000 ISBN: 0125870728.
7 Branden ,Tooze John. Introduction to Protein Structure. Publisher: New York, Garland Publishing Inc. 1999. ISBN: 0815323050.

Course Title:- CHEMOINFORMAITCS **40L**
Course Code:- BIM 2-2

Objectives:

This course will enable the students to:

- understand the fundamentals of chemoinformatics
- appreciate complementary aspects of chemoinformatics and bioinformatics for design of bioactive molecules.
- get hands-on experience in chemical structure representation, storage and analysis of small molecular data.

MODULE I Introduction

- Introduction to Chemoinformatics: aims, scope. Role of Chemoinformatics in pharmaceutical/chemical research Chemical Structure representation: 1D, 2D and 3D structures , Molecular file formats (SMILES, WLN, SDF, MOL)

MODULE II Molecular fingerprints

- o Molecular patterns- SMARTS, Fragment based Molecular Fingerprints (ChemAxon, Daylight, MDL and BCI ,SMIRKS fingerprints- Daylight fingerprints). Molecular Descriptors (1D, 2D and 3D) and MACCS Keys Topological, electrotoplogical and shape indices.

MODULE III Chemical databases

- Molecular Similarity and Molecular Diversity Analysis. Similarity metrics: Tanimoto Coefficient, Euclidean distance and Tversky Index
  Chemical Databases – Design, Storage and Retrieval methods

MODULE IV Molecular informatics

- Molecular Database Screening: (Lipinski Rule: Drug/Lead like molecules Chemical Structure based Search techniques: Exact, Sub-structure and similar structure searches Clustering and Statistical methods for Molecular Informatics (PLS, PCA, PCR, kNN, ANN, Correlation and regression analysis Modeling of small molecules ,Generation of lowest energy conformations from2D structures using Molecular Mechanics and Quantum mechanics methods

MODULE V QSAR and Docking

Quantitative Structure Activity/Property/Toxicity Relationship Studies

Introduction to Molecular Properties, Activities and Toxicities,o Training Data, Test Data and External validation Data, Applicability domain in QSAR Cross validation techniques

Pubchem BioAssay data for QSAR Studies, Ligand based design of compounds ,In-silico ADMET Studies , Design & Analysis of combinatorial libraries Molecular Scaffolds, Linkers and Functional groups,Reagents and products based combinatorial library generation ,Pharmacophore Modeling , Pharmocophore: Definition and classes (HBA, HBD, Aromatic etc.) o Identification of pharmacophore features 2D/3D pharmacophore hypothesis Searching databases using pharmocophores o Application in HTS Analysis,Docking Studies

References:.

1 Creighton T. E. Editor. Protein Structure: A Practical Approach. Publisher: IRL Press at Oxford University Press. 1989. ISBN: 0199630011.

2 Bunin Barry A. Siesel Brian,Morales Guillermo,Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher:New York, Springer. 2006. ISBN: 1402050003.

3 Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: Wiley- VCH; 1st edition. 2003. ISBN: 3527306811.

4 Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic , 2003. ISBN: 1402013477.

5 Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4Volumes), 2003. Publisher: Wiley-VCH. ISBN:3527306803.

Course Tile :- CHEMOINFORMATICS **40L**
Course Code:- BIM 2-3

Objectives:

This course will enable the students to:

- use chemical databases and storage systems
- retrieve and analyse data using physicochemical properties
- understand and model structure-activity activity

1. Practical session for chemical structure representation and storage in special file formats (SMILES,WLN, sd and mol
2. Importance of 3D structures and method of generation from 1D & 2D representations. MODULE II
3. A brief introduction to building molecular databases with special emphasis on retrieval using structure input.
4. Substructure/Exact/similar structure based searching
5. Property based search of molecular databases
6. Quantitative Structure Activity/Property/Toxicity Relationship Studies
7. Pharmacophore hypothesis and searching
8. Docking studies (Rigid, Flexible & library based)
9. Design and analysis of focused combinatorial library

References:

1. Bunin Barry A. Siesel Brian,Morales Guillermo,Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher:New York, Springer. 2006. ISBN:
2. 1402050003.
3. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: Wiley- VCH; 1st edition. 2003. ISBN: 3527306811.
4. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic , 2003. ISBN: 1402013477.
5. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4
6. Volumes), 2003. Publisher: Wiley-VCH. ISBN:3527306803..

Course Tile:- CELL BIOLOGY GENETICS AND GENOMICS 45L
Course Code :- BIM 2-4 A

Objectives:

This course will enable the students to:

- study the principles of structure and function of cells, membranes and organelles
- understand the laws of inheritance and principles of population genetics
- understand genome sequencing and related technologies

MODULE I Cell Biology

- Prokaryotic and eukaryotic cells; membranes and cellular compartmentation; An overview of organelles, (chloroplasts, ER, Golgi, lysosomes and peroxisomes; nucleus) Cellular membranes: Structure, transport, channels, carriers, receptors, membrane potentials Cell motility and shape: cytoskeletal elements, motor proteins

MODULE II Signal transduction

- Signal transduction: signaling by hormones and neurotransmitters; receptors,G-proteins, protein kinases and second messengers Cell cycle and its regulation; events during mitosis and meiosis

MODULE III Genetics

- Science of genetics – objectives, terminologies, methods Mendelian principles of inheritance, sex linked Chromosomes, linkage, linkage maps and recombination inheritance Mutations – molecular, gene/point and chromosomal

MODULE IV Genetics of Population

- Phenotype and genotype relationships, role of environment,from gene to phenotype, gene interactions Study of quantitative Genetics of populations, genetics and evolution

MODULE V Recombinant DNA technology

- Recombinant DNA technology: cloning strategies, vectors Genome projects – importance and strategies Genome markers and mapping: STS, EST, RFLP, SNP, Genome sequencing – first, second and third generation, Functional genomics-Transcriptomics & Proteomics

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Cell Biology

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Genetics

1 Russell P. J. iGenetics: A molecular approach, Pearson International Edition 3rd.

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5 Klug William S., Cummings Michael R., Spencer Charlotte, Palladino Michael A.

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8 Hartwell Leland, Leroy Hood, Michael L. Goldberg, Ann E. Reynolds, Lee M.

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Genomes

a. Dale Jeremy, Schantz Malcolm Von. From genes to genomes: concepts and applications of DNA technology. Publisher: John Wiley & Sons Ltd., 2007. ISBN: 9780470017340.

b. Brown, T.A., Genomes, 3rd edition Garland Science publishers, 2006. ISBN: 1859960294.

c. Primrose Sandy B., Twyman Richard. Principles of Gene Manipulation and Genomics. Publisher: Wiley-Blackwell. 7th edition 2006. ISBN: 1405135441.

Course Title:- IMMUNOLOGY AND BIOINFORMATICS 40L
Course Code:- BIM 2-4B

Objectives:
This course will enable the students to:

- understand the immune system, its components and their functions
- study informatics-based approaches for prediction of epitopes, design of vaccines and immuno-diagnostic tools

MODULE I : Introduction

Immune systems:

Innate and adaptive immModuley in vertebrates,Antigen processing and presentation Contemporary challenges to the immune system Infectious diseases Autoimmune diseases Categories of vaccines

MODULE II Antibodies

o Immunoglobulin classes and subclasses DR and LDR regions and sequence numbering ,Immunogenetics & immunogenomics ,o Hybridoma technology: applications, Humanization of antibodies by design, Membrane receptors for antigen,

o The B-cell surface receptor for antigen (BCR) o The T-cell surface receptor for antigen (TCR) o The major histocompatibility complex (MHC) MHC polymorphism,o Causes of MHC polymorphism, MHC supertypes, Epitopes ,

o Affinity Maturation, Recognition of Antigen by B cells , Neutralizing Antibody

MODULE III Immunoinformatics overview

o Reverse ccinology ,rational vaccine designo Evolution and escape due to variations ,Immunoinformatics databases & tools IMGT & IEDB BciPep, Epitome, CED, AgAbDb:

MODULE IV Molecular interactions

MHC- peptide, Specificity,characterization,Ag-Ab: Sequential and conformational epitopes ,HLA: nomenclature, HLA-peptide interactions & matrices ,Epitope prediction algorithms: B-cell epitope predictions using sequence-based approaches ,B-cell epitope predictions using structure-based approacheso T-cell epitope prediction methods

MODULE V Vaccine design:

o Pipeline & workflows , Prediction of immunogenicity,o Case studies: JEV, Mumps etc

References:

1. Flower Darren R. Bioinformatics for Vaccinology Publisher: UK, John Wiley & Sons Inc. 2008. ISBN: 9780470027110.
2. Flower Darren R. Immunoinformatics: Predicting Immunogenicity In Silico Publisher: New Jersey,Humana Press. 2007. ISBN: 9781603271189.
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Course Title :- IMMUNOLOGY AND BIOINFORMATICS **40L**
Course Code:- BIM 2-5

Objectives :-

This course will enable the students to:

- understand and explore sequence and structural databases relevant in the area of immunology
- explore sequence and structural features of antibodies using computational tools
- characterize and understand principles of antigen-antibody interactions
- understand algorithms and methods for prediction of epitopes
- explore and use approaches for vaccine design

Browsing and searching sequence & structure databases to retrieve data

1. Immunoglobulin: sequence and structure
2. Study of Antibody sequence and structure
3. Antibody numbering: Kabat & Chothia methods
4. Equivalence between different numbering schemes & PDB numbering
5. Visualisation of structure & mapping CDRs on structure
6. Study of variable and constant domains
7. Searching for Ag-Ab complexes
8. Use of molsurfer, explorer etc
9. Charaterisation of binding sites
10. Ab-protein complex
11. Ab-peptide complex
12. Geometric and molecular interaction
13. Alignments: antibody sequences
14. Alignments: antigen sequences, molecular evolution, variability analysis and phylogeny
15. Prediction of sequential epitopes
16. Prediction of conformational epitopes
17. Estimation of accuracy of predicted epitopes: use of experimental data

18. Prediction of cytotoxic and helper T cell epitopes
19. MHC Class I epitopes
20. MHC Class II epitopes
21. Web-based tools for vaccine design
22. Predicting immunogenicity
23. Combination of MHC and Proteasome predictions
24. Combination of MHC, TAP, and Proteasome predictions

References:

1. Flower Darren R. Bioinformatics for Vaccinology Publisher: UK, John Wiley & Sons Inc. 2008. ISBN: 9780470027110.
2. Flower Darren R. Immunoinformatics: Predicting Immunogenicity In SilicoPublisher: New Jersey,Humana Press. 2007. ISBN: 9781603271189.
3. Kindt, Thomas J.,Osborne Barbara A.Goldsby Richard A. Kuby Immunology 6th Edition. Publisher:New York, W. H. Freeman. 2007. ISBN: 9780716785903.
4. Lund Ole , Nielsen Morten , Lundegaard Claus, Kesmir Can, Brunak SÃ¸ren.Immunological Bioinformatics. Publishesr: London, MIT PRess 2005 ISBN: 0262122804.
5. Foundation Novartis.Immunoinformatics: Bioinformatic Strategies for Better
6. Understanding of Immune Function. Publisher: Chichester,John Wiley & Sons Inc.2003. ISBN: 0470853565.
7. Roitt Ivan, Delves Peter. Roitt's Essential Immunology 10th Edition.Publisher: Canada,Blackwell. 2001, ISBN: 0632059028.
8. Ellis Ronald W. Vaccines: New Approaches to Immunological Problems. Publisher: Stoneham, Butterworth-Heinemann 1992. ISBN: 0750692650

Course Title:- PERL PROGRAMMING **45L**

Course Code:- BIM 2-6

Objectives:

This course will enable the students to:

- know basic concepts in programming
- develop Perl scripts to solve biological problems

MODULE I: Introduction

- Concepts of flowcharting, algorithm development, pseudo codes etc, 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

MODULE II Control statement

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, HashFunctions, Hash Slices Basic I/O

MODULE III Subroutines

•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:

MODULE IV File handling

•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, Globbing, Directory Handles, Opening and Closing a Directory Handle, Reading a Directory Handle File and Directory Manipulation , Process Management: Using system and exec, Using Backquotes, Other Data Transformation: Finding a Substring, Extracting and Replacing a Substring

MODULE V Hashes

- 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 , Object oriented perl: Introduction to modules, Creating Objects , Bioperl: Introduction, Installation procedures, Architecture, Uses of bioperl,,A tutorial to be developed to include the numerical techniques/algorithms as part of the programs.

References:

1. Moorhouse Michael, Barry Paul. Bioinformatics, Biocomputing and Perl: an introduction to bioinformatics computing skills and practice. Publisher: John Wiley and Sons, 2004. ISBN:047085331X.

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Bal, H.P. Perl programming for Bioinformatics. Publisher: Tata McGraw-Hill New

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4. Tisdall James D. Beginning Perl for bioinformatics. Publisher: Shroff Publishers and distributors O'Reilly Media, Inc. 2001 ISBN: 8173663955.

5. Gibas Cynthia, Jambeck Per. Developing Bioinformatics Computer Skills. Publisher: Shroff Publishers and distributors O'Reilly Media, Inc., 2001. ISBN: 8173662428

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Wall Larry, Christiansen Tom, Orwant Jon. Programming Perl. Publisher: Shroff

Publishers and distributors O'Reilly Media, Inc. 1998. ISBN: 8173660328.

Course Title :- Seminar

Course Code:- BIM 2-7

Course Title:- GENOME TO DRUG AND VACCINE 40L
Course Code:- BIM3-1

Objectives:
This course will enable the students to:

- appreciate and understand the changes in the approaches for computational analysis between the pre- and post-genomic era
- understand the role of Bioinformatics in sequence assembly and annotation
- appreciate the role of Bioinformatics in post-genomics technologies and areas such as DNA micro-array experiments, proteomics, protein-protein interactions, pharmacogenetics, identification of disease genes, drug and vaccine design etc.

MODULE I: Genome sequencing

- Genome sequencing, Raw data & Assembly Genome Databases and related data resources (EST, STS, GSS, HSS etc.) Organization of data in databases; Genome Data Visualization (With emphasis on Human Genome)
    - Ensembl
    - MapViewer

Biology of the following:

- M. tuberculosis, Plasmodium, Leishmania, Entamoeba histolytica, Mosquito

MODULE II Genome databases

Genome databases of the following (To be explored by the students for presentation in a seminar)

- E. coli
- M. tuberculosis
- Yeast
- Entamoeba histolytica
- Leishmania
- Plasmodium
- C. elegans
- Drosophila
- Anopheles gambae
- Zebra fish

- Fugu
- Human
- Mouse
- Arabidopsis thaliana
- Rice
- Any other

Tools for Genomic Data Mining

- Basic Aspects of Genome Annotation
- Prediction of ORFs
- Prediction of Promoters, splice sites, UTRs etc
- Algorithms for gene prediction gene modeling

MODULE III Functional and structural genomics

- Identification of Disease Genes & Drug Targets , (in the context of Human Genetics and Genetics of Model organisms),OMIM,Metabolic diseases and Pathogenic diseases,High throughput data & its analysis ,Gene Expression Analysis,Structural Genomics,Functional Genomics,Host-Parasite and Host-Vector-Parasite Interactions,Multi-Drug Resistance , Mechanism of MDR: genomic, molecular, cellular,Identification of genes responsible for MDR

MODULE IV ADMET Introduction

- Pharmacokinetics ,Classification, Case study,Comparative screening ,ADMET: Drug metabolism; Elimination half-life, Toxicity screening

MODULE V Protein interaction

- Pharmacogenetics, The genetics of drug metabolism,The genetics of therapeutic targets, Interactions of small molecules and gene-based drug targets

References*:*

1. Meyers Robert A. Genomics and Genetics: From Molecular Details to Analysis and
2. Techniques. Volume 1 & 2.. Publisher: Wiley-VCH, 2007; ISBN: 9783527316090.
3. Falciani Francesco. Microarray Technology Through Applications. Publisher: New
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5. Primrose Sandy B., Twyman Richard. Principles of Genome Analysis and Genomics
6. 3rd Edition. Publisher: Wiley-Blackwell, 2003. ISBN: 9781405101202.
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13. Individualized Therapies. Publisher: Germany, Wiley-VCH. 2002. ISBN:
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17. Aspects. Publisher: New York, W H Freeman & Co. 1990. ISBN: 0716720388.

Course Title:- COMPARATIVE GENOMICS AND PROTEOMICS 40L

Course Code :- BIM 3-2

Objectives:

This course will enable the students to:

- appreciate the importance of full genome comparisons
- understand and explore the comparative genomics databases
- understand various algorithms used for comparisons of full genome and gene order
- understand the concepts of SNPs and their significance
- understand and appreciate the proteomics concepts and technology

MODULE I: Introduction

• Objective and Overview of Genome Comparisons , Genome Alignments, BLAST2 MUMmer, PipMaker, VISTA, Comparison of Gene Order, GeneOrder

MODULE II Comparative Genomics

o Viruses, Microbes, Pathogens, Eukaryotes, Comparative Genomics Databases ,CORG
o HOBACGEN , Homophila, XREFdb, Gramene

MODULE III SNP

• Single Nucleotide Polymorphism, dbSNP and other SNP-related databases , Overview of Proteomics ,Experimental Techniques, Bioinformatics Approaches

MODULE IV BIND DIP

Protein-Protein Interaction Networks, databases and software ,o DIP (Database of Interacting Proteins), PPI Server, BIND - Biomolecular Interaction Network Database
o PIM –Hybrigenics

MODULE V GRID MINT

o PathCalling Yeast Interaction Database, MINT - a Molecular Interactions Database, GRID - The General Repository for Interaction Datasetso InterPreTS - protein interaction prediction through tertiary structure

References:

1. Choudhuri Supratim & Carlson David B. Genomics fundamentals and applications.Publisher: New York. Informa healthcare, 2009. 9781420067057.

2. Primrose Sandy B., Twyman Richard. Principles of Gene Manipulation andGenomics, 7th edition. Publisher: Australia, Wiley-Blackwell. 2006. ISBN:1405135441.
3. Mount David W. Bioinformatics: Sequence and Genome Analysis, Second EditionPublisher: New York, Cold Spring Harbor Laboratory Press, 2004. ISBN10:0879697121.
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7. Sankoff D., Nadeau J.H., Comparative Genomics: Empirical and Analytical Approaches to Gene Order Dynamics, Map Alignment and the Evolution of Gene Families. Publisher: Netherlands, Kluwer Academic Publishers, 2000. ISBN:0792365836.

Course Title :-PLANT GENOMICS 40L

Course Code:- BIM 3-3

Course Objectives: To enable the students to gain knowledge about Plant Genomics

Module-I: introduction

- Plant Genome Databases ,Nucleotide database- NCBI (GenBank), DDBJ, EMBL, Protein structure Databank - PDB, Search Engine - SRS, Entrez Enzyme databases- BRENDA, , KEGG Protein database - TrEMBL, UniProt, PIR Index to Plant Chromosome Numbers database - IPCN

Module-II: Genome project

- The Arabidopsis Genome ,History of Plant, Arabidopsis Genome study, Entrez Records, Phylogenetic relationship, Model Plant Arabidopsis Thaliana, TAIR, TIGR,Cytogenetics - A cytogenetic resource of FISH-mapped, sequence-tagged clones; dbSNP- Database of SNPs and other genetic variation; Entrez- Gene Focal point for genes and associated information; RefSeq - Reference Sequence collection: genomic DNA, transcripts, and proteins;

Module-III: Genome organization and evolution

- Plant genomics and ProteomicsTransmission of genetic information – Mapping, High resolution maps, Horizontal gene transfer,Genome Analysis,Eukaryotic Genome- Arabidopsis, Soybean, Mungbean, Rice, Cotton, Withania, Maize,Plant viruses study – Coat protein study, TMV, PMV, PAMV

Module-IV: Protein function and biochemical pathways

- BRITE- Biomolecular Relations in Information Transmission and Expression EcoCyc/MetaCyc- Encyclopedia of E. coli genes and metabolism; Metabolic encyclopedia ,EMP- Metabolic pathways ,KEGG -Kyoto encyclopedia of genes and genomes ,Biochemical Pathways -Enzyme database and link to biochemical pathway map

Module-V:

Application of Plant Genomics (9L)

- Transgenic Plants,Metabolomics,Functional genomics- Arabidopsis thaliana,Metabolic profiling and fingerprinting,New drug developments, Phylogenetic analysis

REFERENCES :

1. Plant Biotechnology: Green Revolution, Virendra Gomase and Anant Sherkhane, VDM Verlag Dr. Müller, Germany, ISBN:978-3-639-03208-6, (2010).

2. Encyclopedia of Agricultural Sciences (5 Vol. Set), Virendra Gomase, Shruti Gomase, Serial Publication, India, ISBN:978-8-183-87339-0, (2010).

3. Toxicogenomics, Virendra Gomase and Shruti Gomase, VDM Verlag Dr. Müller, Germany, ISBN:978-3639249958, (2010).

4. Plant Genomics: Methods and Protocols (Methods in Molecular Biology), Daryl J. Somers, Peter Langridge, J.P. Gustafson, Humana Press; 1 edition, ISBN-13: 978-1588299970, (2009).

5. Principles and Practices of Plant Genomics, Volume 3: Advanced Genomics, Chittaranjan Kole, Albert G. Abbott, Science Publishers; 1 edition, ISBN-13: 978-1578086832, (2010).

6. Plant Stress Biology: From Genomics to Systems Biology, Heribert Hirt, Wiley-VCH, ISBN-13: 978-3527322909, (2009).

7. Genetics and Genomics of Soybean (Plant Genetics and Genomics: Crops and Models), Gary Stacey, B. Goldberg, Springer; 1 edition, ISBN-13: 978-0387722986, (2008).

8. Plant Pathogenic Bacteria: Genomics and Molecular Biology, Robert W. Jackson, Caister Academic Press; illustrated edition edition, ISBN-13: 978-1904455370, (2009).

Course Title :- COMPARATIVE GENOMICS AND PROTEOMICS 40L

Course Code:- BIM 3-4

Objectives*:*

This course will enable the students to:

- browse and search the comparative genomics & proteomics databases
- use the methods in comparative genomics and interpret the results.
- learn and apply methods in characterization of protein-protein interactions

Explore comparative genomics resources and NCBI and EBI,Comparison of full / partial genomic sequences using following methods to identify conserved genes and map/compare the annotations of the two sequences,BLAST2 MegaBLAST and Discontiguous MegaBLAST ,MUMmer o PipMaker ,VISTA ,Compare gene order of given genomic sequences using the GeneOrder tool , Explore and query the comparative genomics databases: COG, VirGen,CORG, HOBACGEN, Homophila, XREFdb, Gramene etc.Explore and query SNP and SNP-related databases Explore and query the protein-protein interaction databases: DIP, PPI Server, BIND, PIM, PathCalling, MINT, GRID, InterPreTS

Course Title :-MOLECULAR PHYLOGENETICS **40L**

Course Code:- BIM 3-5A

Objectives:

This course will enable the students to:
•understand concepts of molecular evolution and the nature of data for deriving molecular phylogeny
•learn and apply the statistical approaches and models for phylogenetic analysis and tree reconstruction

MODULE I: Introduction

- Molecular Evolution ,overview & protocols, Nature of data used

MODULE II Evolution models

- Probabilistic models and associated algorithms, Probabilistic models of evolution , Maximum likelihood algorithm

MODULE III Phyogentic algorithms

- Phylogenetic analysis algorithms, Distance-based: UPGMA, Transformed Distance, Neighbors-Relation,Neighbor-Joining

MODULE IV Maximum parsimony

Character optimization; delayed and accelerated transformation, Maximum Parsimony , Reliability of trees: Bootstrap, jackknife, decay, randomization tests. Phylogenetic trees and their comparison:
, Definition and description, various types of trees;

MODULE V Tree construction

Consensus (strict, semi-strict, Adams, majority rule, Nelson)., Data partitioning and combination Tree to tree distances, similarity, Case studies , Numerical taxonomy & bacterial identification

References:

1 Bromham Lindell. Reading the Story in DNA: A Beginner's Guide to Molecular

2 Evolution. Publisher: USA, Oxford University Press. 2008. ISBN: 9780199290918.

3 Bernardi Giorgio. Structural and Evolutionary Genomics, Volume 37: Natural Selection in Genome Evolution (New Comprehensive Biochemistry). Publisher: Netherlands, Elsevier Science.2005. ISBN: 9780444521361.

4 Marco Salemi, Anne-Mieke Vandamme. The phylogenetic handbook: a practical approach to DNA and protein phylogeny. Publisher: Cambridge University Press,2003. ISBN: 052180390X.Patthy Laszlo. Protein Evolution. Publisher: London, Blackwell Science Ltd. 1999. ISBN: 0632047747.

5 Takahata Naoyuki, Clark Andrew G.(Editor). Mechanisms of Molecular Evolution: Introduction to Molecular Paleopopulation Biology. Publisher: Japan, Japan Scientific Socities Press and Sinauer Associates, Inc. 1993. ISBN: 476226718X.

6 Graur Dan, Wen-Hsiung Li. Fundamentals of molecular evolution Publisher: SinauerAssociates, 1991. ISBN: 0878932666.

Course Title:- MOLECULAR MODELING AND SIMULATION 40L

Course Code:- BIM3-5B

Objectives:

This course will enable the students to:

- understand basic concepts in molecular mechanics, modeling & simulations
- understand application of classical mechanics for biomolecules
- understand application of simulation techniques to study molecular dynamics & derive properties of thereof
- understand principles of docking simulations

MODULE I Introduction

- Overview of molecular modeling ,Molecular modelling methods,Semi-empirical methods, Empirical methods,Molecular Mechanics ,Conformations: global vs. local

MODULE II Molecular dynamics

- Force fields: expressions for stretch, bond, torsion, etc. Description of various force fields: MM3, Dreiding, AMBER, CHARMM Mechanics of Bio-macromolecules ,Molecular Dynamics , Newton's equations for many particles,Verlet and related algorithms

MODULE III Energy minimization

- Types of dynamics simulations: adiabatic, constant T, simulated annealing, etc. Conformational searching using MD and other methods,Free energy calculations,Dynamics of Bio-macromolecules,Electrostatics of biomolecules,Energy Minimisation
  Golden section,derivative based method (SD, CG, Newton-Raphson)

MODULE IV Docking and simulation

Docking simulation,Rigid docking,Flexible docking

MODULE V scoring methods

Different Scoring schemes ,

References:

1. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH.2003. ISBN: 3527305890.
2. •Friesner Richard A. Computational Methods for Protein Folding:advances in Chemical Physics Volume 120 Kindle Edition. Publisher: New York, John Wiley & Sons. 2002 ISBN: 0471209554
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5. • McCammon Andrew J., Harvey Stephen C. Dynamics of Proteins and Nucleic Acids
6. Publisher: New York, Cambridge University Press, 1987. ISBN: 0521356520

Course Title:- MOLECULAR MODELING AND SIMULATION 40L

Course Code :- BIM3-6

Objectives:

This course will enable the students to:

- Use energy minimization methods for optimization of geometry
- Use molecular dynamics methods to sample conformational space/predict structures of oligopeptides

1. Use methods of molecular docking & its applications
2. Use of SD and CG for energy minimization of biomolecule
3. Oligopeptide/oligonucleotide model building (PYMOL / DStools)
4. MD using any one of the SW (GROMACS, AMBER & CHARMM):
5. MD in vaccuo
6. MD using implicit solvent
7. MD using explicit solvent with PBC/layer of solvent
8. Visualisation and analysis of MD trajectory data (Dstools & VMD)
9. Docking simulations

References:

1. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular
2. Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH.
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Course Title :- SEMINAR

Course Code :-BIM 3-7

Course Title:- ADVANCED TECHNIQUES FOR SEQUENCE AND STRUCTURE ANALYSIS

Course Code:-BIM4-1

Objectives:

This course will enable the students to:

•understand and implement various advanced level techniques for mining biomolecular sequence and structure data.

MODULE I Introduction

- Advanced Techniques for Sequence Analysis , Sequence Profiles: Derivation, Databases, Application

MODULE II Data mining techniques

o PSI-BLAST, PHI-BLAST , Advanced data mining Techniques

MODULE III Ligand active site prediction

o Random forest : ligand binding site prediction, Decision trees: prediction of post-translational modifications

MODULE IV Advance sequence analysis

- Advanced sequence analysis ,QTL, CNV, LoH

MODULE V Graph theory

- Image analysis , Graph theory

References*:*

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11. Davies E. R. Machine Vision: Theory, Algorithms, Practicalities. Publisher: New
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    a. 1990. ISBN: 0122861655.
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Course Tile :-METABOLIC ENGINEERING **40L**

Course Code:- BIM 4-2

Objectives:

This course will enable the students to:

- learn the basic biochemical concepts of metabolic pathways
- understand the role of Bioinformatics in the study of metabolic pathways & pathway databases
- learn the Bioinformatics-based approaches for predicting and engineering metabolic pathways

MODULE I Introduction

- Major Metabolic Pathways

o Gluconeogenesis, Pentose phosphate pathway, Glycogen synthesis and degradation, Fatty acid oxidation and synthesis, Amino acid catabolism, Purine and pyrimidine nucleotide synthesis etc, Enzyme Nomenclature and Classification (5)

MODULE II Metabolic pathway databases

- Metabolic Pathways databases, KEGG, EcoCyc and MetaCyc,, EMP, Malaria Parasite Metabolic Pathways, Boehringer Mannheim -Biochemical Pathways

MODULE III BRENDA

- Enzymes, Compounds and Reactions databases , LIGAND - Biochemical Compounds and Reactions ,ENZYME – Enzymes,o BRENDA - Comprehensive Enzyme Information System

MODULE IV Modeling metabolic pathways

Mathematical modeling of metabolic pathways ,Prokaryotes Vs Eukaryotes – single cell Vs multi cell species biology from a modeling perspective,Systems approach to Metabolism and integration of different data types,Properties of biochemical networks: structural, topological and dynamic,Determining Optimal states and applications

MODULE V Metabolic Engineering

Metabolic Engineering- Basics,E. coli as a Host for metabolic engineering,Rational Metabolic engineering design.

References

a. Klipp Edda, Liebermeister Wolfram, Wierling Christoph, Kowald Axel, Lehrach,Hans, Herwig Ralf. Systems Biology: A Textbook. Publisher: Germany, Wiley-VCH.2009. ISBN: 9783527318742.Nelson David L., Cox Michale. Lehninger Principles of Biochemistry 5th Edition.Publisher: New York. W. H. Freeman. 2008. ISBN: 9780716771081.

b. Alterovitz Gil, Ramoni Marco F. Systems Bioinformatics: An Engineering Case- Based Approach. Publisher: Boston, Artech House Publishers. 2007. ISBN:9781596931244.•

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h. Anton Howard. Elementary Linear Algebra 5th Edition. Publisher: New York, John Wiley & Sons. 1987. ISBN: 0471852236.

Course Ttile:- PROJECT

Course Code:- BIM4-3

Course Title :-METABOLIC ENGINEERING

Course Code:- BIM4-4

Objectives:

This course will enable the students to:

- use metabolic pathway databases and associated tools
- use advanced methodologies to model pathways

1. Browse & search metabolic pathway databases
2. MATLAB introduction
3. Structural and topological properties of biochemical networks
4. Setting up Genome scale models
5. Mini project

References

1. Hans, Herwig Ralf. Systems Biology: A Textbook. Publisher: Germany, Wiley-VCH. 2009. ISBN: 9783527318742.
2. Nelson David L., Cox Michale. Lehninger Principles of Biochemistry 5th Edition.Publisher: New York. W. H. Freeman. 2008. ISBN: 9780716771081.
3. Alterovitz Gil, Ramoni Marco F. Systems Bioinformatics: An Engineering Case- Based Approach. Publisher: Boston, Artech House Publishers. 2007. ISBN:9781596931244.
4. Palsson Bernhard O. Systems Biology: Properties of Reconstructed Networks.Publisher: New York, Cambridge University Press. 2007. ISBN: 9780521859035.
5. Voet, Donald, Voe Judith, Pratt, Charlotte W. Fundamentals of Biochemistry: Life at the molecular Level 2nd Edition. Publisher: Asia, John Wiley & Sons. 2006. ISBN:0471753416.
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7. Purich Daniel L., Allison R. Donald. The Enzyme Reference: A Comprehensive Guidebook to Enzyme Nomenclature, Reactions, and Methods. Publisher: California, Academic Press. 2002. ISBN: 0125680414.

Course Title :-INTRODUCTION TO DATABASE SYSTEM 40L

Ourse Code:- BIM4-5A

Objectives*:*

This course will enable the students to:

- understand the concepts of data, data models and relationships
- be aware of various data representation techniques and various types of databases
- appreciate and implement relational database design
    - create the database systems with user-friendly front-ends for fast and efficient data retrieval and storage
    - acquire the skills of using MySQL, SQL and basic skills in creating front end applications

MODULE I ER diagram

- Database designing, data acquisition , Data Abstraction, Data Models, Instances & SchemesE-R Model , Entity and entity sets , E-R diagrams, Reducing E-R Diagrams to tables

MODULE II Indexing and Hashing

- Relational Algebra and relational Calculus,Data Normalization ,Basic concepts and applications of Network Data Model, Hierarchical Data,Model, Multimedia Databases ,Basic concepts of Indexing and Hashing Textual Databases ,Introduction to Distributed Database Processing,Data warehousing and Data mining , biological species information using various database techniques.

MODULE III My SQL

- MySQL Architecture,objects - Tables, Views, Indexes, Sequences; Synonyms, Snapshots, ClustersDatabase - Table space, Data files, Blocks, Extents, Segments; SQL *DBA - Export-Import/SQL Monitor Backup & Recovery (Archiving); Physical Storage & Logical Storage

MODULE IV Reports

Reports - Reports Features; Full Integration with Forms and Graphics; Data Model and layout editors

MODULE V Layout

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

References

1. Bayross Ivan. SQL, PL/SQL The Programming Language of Oracle. 2nd revised edition. Publisher: BPB New Delhi. 2003. ISBN: 8176560723.
2. Kevin Loney, George Koch and experts at TUSC. Oracle9i: The Complete
3. Reference. 2002. Publisher: Tata McGraw-Hill. ISBN: 0070499020.
4. Silberschatz, A, Korth, H F & Sudarshan, S. Database system concepts; (4th Edition) Boston. McGraw-Hill higher education, 2002. ISBN: 007120413X.
5. Date C. J. An Introduction to Database Systems. 1999. Publisher: Addison Wesley;

Course Title :-COMPUTATIONAL STRUCTRAL BIOLOGY 40L

Course Code:- BIM 4-5B

Objectives:

This course will enable the students to:

- explore primary and derived databases databases in the field of computational structural biology

- visualize macromolecular structures using various visualization tools

- acquire skills to use different approaches for prediction of protein structure

MODULE I : Structure analysis

- Structural data, databases and structure analysis Exploring the Database & searches on PDB and CSD, WHATIF

- Molecular visualization tools

Visualization of tertiary structures, quaternary structures, architectures and topologies of proteins and DNA using molecular visualization softwares such as RasMol, Cn3D, SPDBV, Chime, Mol4D, PyMOL etc.

MODULE II : Secondary structure

- Methods for prediction of secondary structure of proteins ,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.
- Methods for prediction tertiary structure of proteins along with analysis and interpretation of results

MODULE III: Swiss PDB

Homology modeling: InsightII, Discovery Studio, SWISSMODEL, SWISS- PDB Viewer

MODULE IV Fold recognition methods

o Fold recognition methods: PHYRE, TOPITS, GenThreader (or other equivalent methods)

MODULE V Structure analysis

Annotation of the structure

References:

1. Cesareni Giovanni, Gimona Mario, Sudol Marius, Yaffe Michael (Editors). Modular Protein Domains. Publisher: Weinheim Wiley-VCH. 2005. ISBN: 352730813X.
2. Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH.2003. ISBN: 3527305890.
3. Webster David (Editor). Protein Structure Prediction: Methods and Protocols
4. (Methods in Molecular Biology) Volume 143. Publisher: New Jersey Humana Press.2000. ISBN: 0896036375.
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Course Tile :- COMPUTATIONAL STRUCTURAL BIOLOGY 40L

Course Code:- BIM 4-6

Objective :- students will explore the different techniques of protein structure annotation

1. Introduction, Interaction in biology systems
2. Structure of Biomolecules: and confirmations of protein and nucleic acid
3. . Secondary, tertiary and quaternary structure of protein
4. . Primary and secondary structure of RNA and DNA
5. Method of conformational analysis and prediction of conformation
6. Thermodynamics and kinetics of conformational transition of proteins
7. Protein folding, techniques for studying Macromolecular structure
8. Ultra centrifugation Sedimentation velocity and equilibrium- determinat
9. ion of molecular weights
10. Electron microscopy
11. UV Visible Spectroscopy, Fluorescence Spectroscopy

References

1. Biophysical Chemistry by Cantor & P. Schimmel. Vol. I & II
2. Physical Biochemistry by David I reifelder
3. Protein: Structure 7 molecular Properties by TE Creighton

Course Title:- Seminar

Course Code:- BIM 4-7