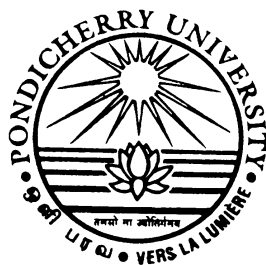


M.Sc. BIOINFORMATICS

REGULATIONS AND SYLLABI

(Effective from 2011-2012)



**Centre for Bioinformatics
SCHOOL OF LIFE SCIENCES
PONDICHERY UNIVERSITY
PUDUCHERRY**

Eligibility for M. Sc. Bioinformatics

Students from any of the below listed Bachelor degrees with minimum 55% of marks are eligible.

- Bachelor's degree in any relevant area of Physics/Chemistry/Computers Science/Life Science/with a minimum of 55% of marks

PONDICHERY UNIVERSITY
SCHOOL OF LIFE SCIENCES
Centre for Bioinformatics
SYLLABUS FOR M. Sc. BIOINFORMATICS
(Academic Year 2011-2012 onwards)

Course Code	Course Title	H / S	Credits	Pg. No
Semester I				
BINF 421	Cell and Molecular Biology	H	3	4
BINF 422	Bioinformatics Databases	H	3	5
BINF 423	C and Data Structures	H	3	6
BINF 424	Physics	S	2	7
BINF 425	Chemistry	S	2	8
BINF 426	Mathematics	S	2	9
BINF 427	Biology	S	2	10
BINF 428	Basics of Computer	S	2	11
BINF 419	Introduction to Bioinformatics*	S	3	12
BINF 471	Lab - Cell and Molecular Biology	H	1	13
BINF 472	Lab - Biological Databases	H	1	14
BINF 473	Lab - Basics of Computer & Operating Systems	H	1	15
BINF 474	Lab - Programming in C/ C++	H	1	16
BINF 465	Lab - Bioinformatics databases and tools*	S	1	17
Semester II				
BINF 451	Genomics and Proteomics	H	3	18
BINF 452	Bioinformatics: Sequence Analysis	H	3	19
BINF 453	Probability and Statistics	S	2	20
BINF 454	Programming in Java	H	3	21
BINF 455	Database Management System	H	3	22
BINF 456	Fundamentals of Algorithms	S	2	23
BINF 457	Microscopic Techniques For Image Processing	S	2	24
BINF 475	Lab - Programming in Java	H	1	25
BINF 476	Lab – Programming in DBMS	H	1	26
BINF 477	Lab - Biosequence Analysis	H	1	27
Semester III				
BINF 521	Structural Biology	H	3	28
BINF 522	Molecular Modeling and Drug Design	H	3	29
BINF 523	Programming in Perl	H	3	30
BINF 524	Systems Biology	H	3	31
BINF 525	Biological Spectroscopy	S	2	32
BINF 526	Data Communication and Networks	H	2	33
BINF 527	Scientific Presentation and Finishing School	H	3	34
BINF 571	Lab - Structural Biology	H	1	35
BINF 572	Lab - Molecular Modeling and Drug Design	H	1	36
BINF 573	Lab - Programming in Perl	H	1	37
Semester IV				
BINF 551	Analytical Techniques	S	3	38
BINF 552	Bioethics, Biodiversity and Intellectual Property Rights	H	3	39
BINF 553	R language and Bioconductor	S	3	40
BINF 554	Project	H	8	41

* for other department students

BINF 421 - CELL AND MOLECULAR BIOLOGY

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 Lectures

Molecules of life - structural organization of prokaryotic and eukaryotic cells- Concept of a composite cell and Molecular composition of cells. Biomembranes- Structural organization - Models of a plasma membrane, Membrane permeability - Transport across cell membranes - Transmembrane signals - Artificial membranes - liposome.

Unit 2

7 Lectures

Mitochondrial Genome, Structure and Function – Oxidative Metabolism in the Mitochondrion – The Role of Mitochondria in the formation of ATP – Translocation of Protons and the Establishment of a proton-motive force – The Machinery for ATP formation – Peroxisomes. Genome studies of Mitochondria.

Unit 3

7 Lectures

Chloroplast structure and function – An overview of photosynthetic Metabolism – The absorption of light – Photosynthetic units and reaction centers – Photophosphorylation – Carbondioxide fixation and the synthesis of carbohydrates. Chloroplast and its genome study.

Unit 4

7 Lectures

Cellular Organelles – Cytoskeleton – components of Cytoskeleton, Microtubules, Intermediate filaments – Microfilaments, Endoplasmic reticulum, Golgi complex, Types of m.\vesicles - transport and their functions, Lysosomes. Nucleus - Internal organization, Nuclear pore complex, Nucleosomes, Chromatin.

Unit 5

9 Lectures

DNA and Protein Synthesis - Structure of DNA - evidence for DNA as genetic material. Gene transfer in microorganisms – conjugation, transformation, transduction - protoplasmic fusion. The genomes of bacteria, viruses, plasmids. DNA Structural organization - DNA replication, Transcription – mRNA processing, Translation. Protein synthesis – Ribosomes, enzymes, Protein processing, Introduction to the methods of DNA sequencing

Text Book:

1. Cell and Molecular Biology – Concepts and Experiments by Gerald Karp. Wiley International Student Version. 2008

Reference Books:

1. Genes VIII by Lewin, B, Pearson Education International. 2004
2. Cell and Molecular Biology by De Robertes and De Robertis. Saunders College, Philadelphia, USA. 2002

BINF 422 - BIOINFORMATICS DATABASES

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 lectures

Introduction to Bioinformatics data and databases:- Types of Biological data:- Genomic DNA, Complementary DNA (cDNA), Recombinant DNA (rDNA), Expressed sequence tags (ESTs), Genomic survey sequences (GSSs). Primary Databases:- GenBank, EMBL, DDBJ, Composite Databases:-NRDB, UniProt, Literature Databases:- Open access and open sources, PubMed, PLoS, Biomed CentralCentral.

Unit 2

8 lectures

Genome Databases:- Viral genome database (ICTVdb, VirGen), Bacterial Genomes database (Genomes OnLine Database –GOLD, Microbial Genome Database-MBGD), Organism specific Genome database (OMIM / OMIA, SGD, WormBase, PlasmoDB, FlyBase, TAIR), and Genome Browsers (Ensembl, VEGA genome browser, NCBI-NCBI map viewer, KEGG, MIPS, UCSC Genome Browser)

Unit 3:

8 lectures

Sequence Databases :- Nucleotide sequence Databases (GenBank, EMBL, DDBJ). Protein sequences Databases (Swiss-ProtProt, TrEMBL, UniProt, UniProt Knowledgebase – UniProtKB, UniProt Archive –UniParc, UniProt Reference Clusters –UniRef, UniProt Metagenomic and Environmental Sequences –UniMES. Sequence motifs Databases:-Prosite, ProDom, Pfam, InterPro. Sequence file formats:- GenBank, FASTA, PIR, ALN/ClustalW2, GCG/MSF.

Unit 4:

8 lectures

Structure and derived databases:- The primary structure databases (Protein Data Bank –PDB, Cambridge Structural Database –CSD, Molecular Modeling Database -MMDB). The secondary structure databases (Structural Classification of Proteins –SCOP, Class Architecture Topology Homology –CATH, Families of Structurally Similar Proteins –FSSP, Catalytic Site Atlas –CSA. Molecular functions/Enzymatic catalysis databases (KEGG ENZYME database, BRENDA)

Unit 5

6 lectures

Bioinformatics Database search engines:-Text-based search engines (Entrez, SRS, DBGET / LinkDB). Sequence similarity based search engines (BLASTBLAST and FASTA). Motif-based search engines (ScanPrositeScanProsite and eMOTIF). Structure similarity based search engines (VAST and DALI). Proteomics tools at the ExPASy server, GCG utilities and EMBOSS..

Text Books:

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 Ouellette, B.F., Wiley India Pvt Ltd. 2009
3. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith. Pearson Education. 1999

BINF 423 – C AND DATA STRUCTURES

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 lectures

Introduction to programming languages: Introduction – Programming languages – Problem solving Technique: Algorithm, Flowchart, Compilation, Testing and Debugging, Documentation – Data structures – Array, Stack, Queue, Linked List concepts

Unit 2

10 lectures

Programming in C:

C language Introduction – Tokens – Keywords, Identifier , Variables, Constants, Operators – Expression – Data types –Operator precedence - Statement: Input statement, Output statement, Conditional and Unconditional Control Statement – Looping Statement: while, do-while, for – nested loop – Arrays.

Unit 3

7 lectures

Procedural Concept:

Structured Programming – Built-in library function – User defined functions – Pointer introduction – Passing pointer in a function – Structure – Union – File handle: Read and Write character from a file

Unit 4

6 lectures

String Handling & Sorting:

String declaration – String library functions - String Manipulation - Sorting: Bubble sort, Selection sort, Insertion sort – Searching: Linear search, Binary search

Unit 5

7 lectures

Object Oriented Programming: Programming in C++:

C++ programming – Object Oriented Concept: Encapsulation, Inheritance, Polymorphism – Different forms of Constructor – Destructor – Abstract class – Virtual function

Text Books:

1. Programming in ANSI C by E. Balagurusamy. Tata McGrawHill Publishing Company Limited. 2007
2. Object Oriented Programming using C++ by Lafore, R. Galgotia Publishers. 2006

BINF 424 – PHYSICS

Total Credits: 2

Total: 24 Hrs.

Unit 1

Mechanics: Motion in 1D:

6 lectures

Displacement velocity and Acceleration... Relative Velocity and Relative Acceleration. **The Newton's Laws of Motion and applications:** Newton's First Law . Newton's Second Law. Third Law. Derivations of Equation of motions. The gravitational force (the Newton's law of universal gravitation), and Relation between mass and weight. Work- energy theorem. Quantum Mechanics: Black body radiation, photoelectric effect, Crompton effect. The Heisenberg uncertainty principle, Time dependent Schrodinger equation.

Unit 2

6 lectures

Thermodynamics: Laws of thermodynamics: Heat Capacity, First Law of thermodynamics, Concept of Enthalpy. **Second law of thermodynamics:** Heat Engines, Carnot Cycle, Second Law statements, concept of Entropy. **Free Energy:** Gibbs and Helmholtz free energy. thermodynamic potentials, Third Law of thermodynamics. Materials: Stress, Strain, Elastic deformation, Plastic deformation, The Young's Modules. Deformation and Dislocation: Elastic Strain, Plastic Strain, Strengthening Metals: Grain boundaries. Cracks and fractures: Brittle fractures, Ductile fractures. Elastic Moduli: Bulk modulus, Young modulus, sheer modulus, bulk modulus.

Unit 3

4 lectures

Electricity: Electric Fields: Coulomb's Law. Motion **Gauss's Law:** Gauss's Law and its application to various charge distributions. Conductors in electrostatic equilibrium. **Electric Potential:** Potential Difference, Electric Field of Point Charge, Electric Field of Line of charges, Electric Field of conducting sphere. Electric Field: sheet of charge, Electric Field: parallel plates, Work and Voltage: Constant Electric Field, voltage and voltage difference in an electric field.

Unit 4

4 lectures

Magnetism: Magnetic Fields: Magnetic Field and Forces. Magnetic force acting on a current-carrying conductor. Torque on a current loop in a Uniform Magnetic Field. The Hall Effect. **Sources of Magnetic Field:** The Biot-Savart Law. Magnetic Force between two parallel conductors. Ampere's Law. Magnetic Field of a solenoid. Magnetic Flux. Gauss' Law. Displacement current and Ampere's Law. **Faraday's Law:** Faraday's Law of induction. Motional emf. Lenz's Law and electric fields.

Unit 5

4 lectures

Electromagnetic waves: Electromagnetic spectrum - and **Diffraction: Classification of diffraction, Fresnel diffraction: rectangular aperture, single narrow slit, circular aperture Fraunhofer diffraction : Single slit, rectangular aperture and circular aperture, double slit.** Introduction to diffraction patterns. Diffraction patterns from narrow slits. Resolution of single-slit and circular apertures. The diffraction grating. Diffraction of X-rays by crystals.

Text Books:

1. Physics for Scientists and Engineers (6th Ed.) by Raymond A. Serway, John W. Jewett, Thomson Brooks/Cole. 2004

Reference Books:

1. Physics for Scientists and Engineers by Paul A. Tipler, Gene P. Mosca. Freeman Company. 2007
2. Fundamentals of Physics by Resnick, Halliday and Walker. 2001

BINF 425 – CHEMISTRY

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Atomic and Molecular Structure:

Atomic Structure - Elements and compounds, atoms and molecules-definition, Classical atomic models - J. J. Thomson, E. Rutherford, N. Bohr. Quantum mechanical model. Electronic configuration - aufbau principle - Pauli exclusion principle - Hund's rule Modern periodic table, periodicity. **Chemical bonds** - ionic bonding - covalent bonding - Coordinate covalent bonding. Overlapping of atomic orbital to form σ and π bond with example. Meaning and Difference between σ and π bonds – hybridization, resonance. Bond properties. Molecular geometry. Intermolecular forces

Unit 2

5 Lectures

Symmetry and Principles: Definitions and theorems of group theory, subgroups, Classes. Molecular symmetry and symmetry groups – symmetry elements and operations. Symmetry planes, reflections, inversion centre, proper/ improper axes of rotation, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups.

Unit 3

5 Lectures

Introduction to Organic chemistry: Carbon and its compounds, Position of Carbon in periodic table, tetra covalency of carbon, catenation, functional groups, formal charge, oxidation number, aromaticity, electrophiles and nucleophiles, organic acids and bases, types of organic reactions.

Unit 4

5 Lectures

Stereochemistry: Concept of isomerism, types of isomerism, optical isomerism, elements of symmetry, molecular chirality, enantiomers, stereogenic centres, optical activity, properties of enantiomers, chiral and achiral molecules with two stereogenic centres, distereoisomers, mesocompounds, resolution of enantiomers. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature.

Unit 5

4 Lectures

Heteroaromatics: Five membered and six membered hetero aromatics with one and two hetero atoms and their benannulated analogues, Nucleic acid bases, Structure, name and properties like acid base property, electron rich electron deficient heterocycles, hydrogen bonding etc. (Synthesis and reactions not necessary).

Text Books:

1. Organic Chemistry by Paula Yurkanis Bruice, Prentice Hall. 2010

BINF 426 – MATHEMATICS

Total Credits: 2

Total: 24 Hrs.

Unit I

Matrices and Linear Algebra

4 lectures

Matrices- Properties of Determinants, Minors and Cofactors, Multiplication of Determinants, Adjoint, Reciprocal, Symmetric Determinants, Cramer's rule, Different types of matrices, Matrix Operations, Transpose of a matrix, Adjoint of a square matrix, Inverse of a matrix, Eigen values and eigen vector

Linear Algebra - Definition of vector space, Subspaces, Linear independence and Bases.

Unit II

4 lectures

Vector Analysis: The concept of a Vector, Vector addition and subtraction, Products of two vectors- Dot product and Cross product, Products of three vectors- scalar triple product and vector triple product, Gradient, Divergence and Curl.

Unit III

5 lectures

Trigonometry and Analytical Geometry: Trigonometric ratios, De Moivre's theorem, The general equation of a Straight line, slope of a line, intercepts of a line, Angle between two lines, Intersection of two lines, The general equation of a Circle.

Unit IV

6 lectures

Calculus: Differential Calculus- Derivative of a function, Concept of limit, Continuity, Differentiation, Maxima and Minima of a function, Introduction to Partial Differentiation, Integral Calculus: The Idea of the Integral, The Definite Integrals, Indefinite Integrals.

Unit 5

5 lectures

Numerical Methods: Solution of algebraic and transcendental equations: Bisection method, Method of false position / Regula-falsi method, Newton-Raphson method.

Text Books:

1. Algebra by Serge A. Lang, Pearson Education. 2003
2. Introduction to Calculus & Analysis, Vol I and II by Richard Courant & Fritz John, Springer publisher.1999

Reference Books:

1. Basic Mathematics by Serge A. Lang. Springer Publisher. 1988
2. A First Course in Calculus by Serge A. Lang. Springer publisher. 1986
3. Higher Engineering Mathematics (40th Ed), by B.S. Grewal and J.S. Grewal. Khanna Publishers, New Delhi. 2007

BINF 427 – BIOLOGY

Total Credits: 2

Total: 24 Hrs.

Unit 1

4 Lectures

Diversity in Living World: Diversity of living organisms-Classification of the living organisms (five kingdom classification, major groups and principles of classification within each kingdom). Systematics and binomial System of nomenclature - Salient features of animal (non-chordates up to phylum level and chordates up to class level) and plant (major groups; Angiosperms up to class)) linnaean classification.

Unit 2

4 Lectures

Structural Organisation in Animals and Plants : Morphology, anatomy and functions of different parts of flowering plants: Root, stem, leaf, inflorescence, flower, fruit and seed. Morphology, anatomy and functions of different systems of an annelid (earthworm), an insect (cockroach) and an amphibian (frog).

Unit 3

6 Lectures

Genetics: Mendelian inheritance. Chromosome theory of inheritance, deviations from Mendelian ratio (gene interaction- incomplete dominance, co-dominance, multiple alleles). Sex determination in human beings: XX, XY. Linkage and crossing over. Inheritance pattern : Mendelian disorders and chromosomal disorders in humans. DNA fingerprinting.

Unit 4

5 Lectures

Ecology & Evolution: Ecological niche, population growth curves, Ecosystems stability, competition, conservation methods (both in situ and ex situ) Origin of life, theories and evidences, adaptive radiation, mechanism of Evolution, origin and evolution of man.

Unit 5

5 Lectures

Methods in Biology: Light Microscope – Transmission Electron Microscopy – Scanning Electron and Atomic Force Microscopy – Fractionation of Cell contents by Differential Centrifugation – Purification of Nucleic Acids – Enzymatic amplification of DNA by PCR – DNA Sequencing.

Text Book:

1. Molecular Biology of the cell by Bruce Alberts, Garland publishing Inc. 2002

Reference Books:

1. Cell - A molecular approach by Cooper. G. M., Oxford University Press. 2000
2. Cell and Molecular Biology by De Robertes and De Robertis. Saunders College, Philadelphia, USA. 2002

BINF 428 - BASICS OF COMPUTER

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Computer Organization

Fundamentals of computers – Block diagram of computer (input and output devices) – **History** - Generations – **Memory devices** - Advantages and Limitations of Computers – **Comparison** of different operating systems DOS, Windows NT & XP, Application Softwares.

Unit 2

5 Lectures

Network Basics

Communication Technology – Networking Elements: Networking Hardware, Networking services: Types of Networks – LAN, WAN & MAN, Intranet–Wireless communication – Internet services, Uses of Internet

Unit 3

4 Lectures

Introduction to Database systems

Fundamentals of database - Database models (Hierarchical, Network, Relational and Object-Oriented Models) – RDBMS: Relational Database Management systems - Database System Applications and Security.

Unit 4

5 Lectures

Programming Language

Algorithm – Flowchart – Programming language – Compiling and Linking – Testing and Debugging – Documentation – Maintenance - Utility programs.

Unit 5

5 Lectures

Internet Technologies

Web Services – WWW, URL, Servers: Client/ Server essentials - Domain Name Server, FTP server, E-mail server, WEB servers, Web publishing-Browsers-IP Addressing, IPV6

Text Books:

1. Basic Computer Skills made easy, by Sherman, J., Butterworth-Heinemann Ltd, USA. 2001
2. Computer Fundamentals and Applications (2nd Ed.) by Balaguruswamy, E., Tata McGraw-Hill Publishing Co. Ltd., India. 1985
3. Microsoft Office 2003: WITH Lab Manual (Microsoft Official Academic Course)

BINF 419 - INTRODUCTION TO BIOINFORMATICS

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 lectures

Introduction: Aim and branches of Bioinformatics, Application of Bioinformatics, Role of internet and 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.

Unit 2

7 lectures

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

Unit 3

7 lectures

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

Unit 4

8 lectures

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.

Unit 5

8 lectures

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 analysis of Nucleic acid and protein sequences and interpretation of results.

Text Books:

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 Ouellette, B.F., Wiley India Pvt Ltd. 2009

Reference Book:

1. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith, Pearson Education. 1999
2. Bioinformatics for Dummies by Jean-michel Claverie Cedric Notredame. Publisher: Dummies (Jan 2007)

BINF 471 - LAB - CELL AND MOLECULAR BIOLOGY

Total Credits: 1

Exercises in Cell Biology

Paper Chromatography of Chlorophyll pigments

Estimation of Chlorophyll

Ascorbic acid estimation in different tissues of plants and animals.

Growth curve of Bacteria.

Estimation of cell mass of bacteria.

Exercises in Molecular Biology

Isolation & Purification of genomic DNA from bacteria

Isolation & Purification of plasmid DNA

Agarose gel electrophoresis of chromosomal & plasmid DNA

Restriction Digestion of chromosomal & plasmid DNA

Isolation of DNA fragment from agarose gel

PCR for DNA amplification

Protein separation using HPLC (demo)

Protein separation using SDS-PAGE

BINF 472 - LAB - BIOLOGICAL DATABASES

Total Credits: 1

Exercises:

1. Bioinformatics Resources : NCBI, EBI, DDBJ, RCSB, ExPASy
2. Open access bibliographic resources and literature databases
 - a. PubMed
 - b. BioMed Central
 - c. Public Library of Sciences (PloS)
 - d. CiteXplore.
3. Bioinformatics Resources at the species level
 - a. ICTV Database
 - b. AVIS
 - c. VirGen
 - d. Viral genomes at NCBI
4. Sequence databases:
 - a. Nucleic acid sequence databases: GenBank, EMBL, DDBJ;
 - b. Protein sequence databases: Uniprot-KB: SWISS-PROT, TrEMBL, UniParc;
 - c. Repositories for high throughput genomic sequences: EST, STS, GSS.
 - d. Genome Databases at NCBI, EBI, TIGR, SANGER
5. Structure Databases: PDB, NDB, PubChem, ChemBank, FSSP, DSSP
6. Derived Databases: InterPro, Prosite, Pfam, ProDom
7. Sequence file formats: GenBank, FASTA, GCG, MSF.
8. Protein and nucleic acid properties: Proteomics tools at the ExPASy server, GCG utilities and EMBOSS

BINF 473 - LAB – BASICS OF COMPUTER & OPERATING SYSTEMS

Total Credits: 1

Exercises:

1. Command Line Interface - Internal Commands- External commands
2. Graphical User Interface: Peer-to-Peer Operating System
3. Client- Server Operating System
4. Software Package:
 - a. Create a manuscript using ms-word by applying relevant font styles, margins, bullets and tables.
 - b. Prepare a call letter for the admission of MSC bioinformatics to all the selected students by using mail merge.
 - c. Prepare a student's fee table for four semesters in a excel sheet. Calculate the consolidated payment using links.
 - d. Create all types of charts using excel for any clinical data.
5. Create a web page for an educational institution using HTML tags.
6. Create a web page to display your details by creating a model web site.

BINF 474 - LAB - PROGRAMMING IN C/ C++

Total Credits: 1

LINUX Operating System: Overview of Linux Architecture and Basic commands

C

1. Display a protein details using escape sequence
2. Calculate rotations per minute [$\text{rpm} = 1000 \sqrt{\text{RCF}} / 11.17r$]
3. Create amino acid dictionary using switch construct
4. Identify the glucose level in a blood using if - else if construct
[The glucose level is identified by
<70 – hypoglycemia, 70-180 hyperglycemia, > 180 diabetics]
5. Identify the type of two peptides using nested if
[peptide length is < 8 small, poly otherwise]
6. Count the number of base characters entered among n characters using loop
7. Implement stack operation
8. Count the number of positive, negative and zero energy molecules stored in an array
9. Find the transpose of the given matrix using two dimensional array
10. To calculate pH value for a given [OH⁻] concentration [$\text{pH} = -\log_{10}(\text{OH}^-)$]
11. Draw a line in different pattern using user defined function
12. Write a user defined function to illustrate the storage class of the variables
13. Determine the percentage of a,t,g,c in the given sequence
14. Count the number of gaps in the given sequence using user defined function
15. Sort n names
16. Align two sequences
17. Count the number of motif in the given sequence
18. Swap two numbers using pointers
19. Process the organism details using structure
20. Convert the RNA sequence into DNA sequence using text file

C++

1. Create a class which shows the various forms of constructors
2. Inheritance implementation
3. Function overloading example
4. Operator overloading example
5. Dynamic polymorphism implementation

BINF 465 - LAB - BIOINFORMATICS DATABASES AND TOOLS

Total Credits: 1

Exercises:

1. Entrez and Literature Searches.
 - a. PubMed
 - b. PubMed central
 - c. OMIM / OMIA
 - d. Citation matcher
2. SRS of Biological Databases
 - a. Nucleotide/ Genome Databases.
 - b. Protein Sequence Database.
 - c. Structure databases.
 - d. Protein Pattern Databases
3. File format conversion
 - a. FmtSeq
 - b. ReadSeq
 - c. Sequence manipulation Suite
4. Sequence Analysis
 - a. Dot Plot
 - b. Pairwise alignment
 - c. Multiple Sequence Alignment
5. Softwares
 - a. BioEdit.
 - b. GeneDoc
 - c. ClustalW / X, MEGA, MEME
6. Visualization Tool
 - a. RasMol
 - b. Cn3D
 - c. MolMol

BINF 451 - GENOMICS AND PROTEOMICS

Total Credits: 3

Total: 36 Hrs.

Unit 1

8 Lectures

Genomics and Metagenomics: Large scale genome sequencing strategies. Genome assembly and annotation. Genome databases of Plants, animals and pathogens. **Metagenomics:** Gene networks: basic concepts, computational model such as Lambda receptor and lac operon. Prediction of genes, promoters, splice sites, regulatory regions: basic principles, application of methods to prokaryotic and eukaryotic genomes and interpretation of results. Basic concepts on identification of disease genes, role of bioinformatics-OMIM database, reference genome sequence, integrated genomic maps, gene expression profiling; identification of SNPs, SNP database (DbSNP). Role of SNP in Pharmacogenomics, SNP arrays. Basic concepts in identification of Drought stress response genes, insect resistant genes, nutrition enhancing genes

Unit 2

7 Lectures

Epigenetics: DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), ArrayExpress, SAGE databases DNA microarray: understanding of microarray data, normalizing microarray data, detecting differential gene expression, correlation of gene expression data to biological process and computational analysis tools (especially clustering approaches)

Unit 3

7 Lectures

Comparative genomics: Basic concepts and applications, whole genome alignments: understanding the significance; Artemis, BLAST2, MegaBlast algorithms, PipMaker, AVID, Vista, MUMmer, applications of suffix tree in comparative genomics, synteny and gene order comparisons Comparative genomics databases: COG, VOG

Unit 4

7 Lectures

Functional genomics: Application of sequence based and structure-based approaches to assignment of gene functions – e.g. sequence comparison, structure analysis (especially active sites, binding sites) and comparison, pattern identification, etc. Use of various derived databases in function assignment, use of SNPs for identification of genetic traits. Gene/Protein function prediction using Machine learning tools viz. Neural network, SVM etc

Unit 5

7 Lectures

Proteomics: Protein arrays: basic principles. Computational methods for identification of polypeptides from mass spectrometry. Protein arrays: bioinformatics-based tools for analysis of proteomics data (Tools available at ExPASy Proteomics server); databases (such as InterPro) and analysis tools. Protein-protein interactions: databases such as DIP, PPI server and tools for analysis of protein-protein interactions

Text Books:

1. Discovering Genomics, Proteomics and Bioinformatics 2nd edition - by A. Malcolm Campbell and Laurie J. Heyer. by Cold Spring Harbor Laboratory Press 2006.

Reference books:

1. Principles of Genome Analysis and Genomics (3rd Ed.) by Primrose, S.B. and Twyman, R.M., Blackwell Publishing Company, Oxford, UK. 2003
2. Introduction to Proteomics – Tools for the new biology (1st Ed.) by Liebler, D.C., Humana Press Inc., New Jersey, USA. 2002
3. Bioinformatics and Functional Genomics by Pevsner, J., John Wiley and Sons, New Jersey, USA. 2003
4. Bioinformatics: Sequence and Genome Analysis by Mount, D., Cold Spring Harbor Laboratory Press, New York. 2004

BINF 452 - BIOINFORMATICS: SEQUENCE ANALYSIS

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 Lectures

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. **Database Searches:** Keyword-based Entrez and SRS; Sequence-based: BLAST & FASTA; Use of these methods for sequence analysis including the on-line use of the tools and interpretation of results from various sequence and structural as well as bibliographic databases

Unit 2

6 Lectures

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 analysis of Nucleic acid and protein sequences and interpretation of results

Unit 3

7 Lectures

Multiple sequence alignments (MSA): The need for MSA, basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW and PileUp and their application for sequence analysis (including interpretation of results), concept of dendrogram and its interpretation, Use of HMM-based Algorithm for MSA (e.g. SAM method)

Unit 4

8 Lectures

Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, various types of pattern representations viz. consensus, regular expression (Prosite-type) and sequence profiles; profile-based database searches using PSI-BLAST, analysis and interpretation of profile-based searches.

Algorithms for derivation and searching sequence patterns: MeMe, PHI-BLAST, SCanProsite and PRATT. Algorithms for generation of sequence profiles: Profile Analysis method of Gribskov, HMMer, PSI-BLAST

Unit 5

8 Lectures

Taxonomy and phylogeny: Basic concepts in systematics, taxonomy and phylogeny; molecular evolution; nature of data used in Taxonomy and Phylogeny, Definition and description of phylogenetic trees and various types of trees, Phylogenetic analysis algorithms such as maximum Parsimony, UPGMA, Transformed Distance, Neighbors-Relation, Neighbor-Joining, Probabilistic models and associated algorithms such as Probabilistic models of evolution and maximum likelihood algorithm, Bootstrapping methods, use of tools such as Phylip, Mega, PAUP

Text Books:

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 Ouellette, B.F., Wiley India Pvt Ltd. 2009

BINF 453 - PROBABILITY AND STATISTICS

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Numerical descriptive techniques: Measures of central tendency: mean, median, mode, relation between mean, median and mode. **Partition values:** quartiles, deciles, percentiles; **Measures of dispersion:** Absolute and Relative Measures, Moments, skewness and kurtosis

Unit 2

5 Lectures

Correlation and Regression: Principles of least squares, scatter diagram, correlation, covariance, correlation coefficient, properties of correlation coefficient, regression, properties of linear regression, rank correlation, multiple correlation

Unit 3

5 Lectures

Probability Theory: Concept of probability: sample space and events, independent events, mutually exclusive events. axioms of probability, conditional probability, additional and multiplication theorem of probability, Baye's theorem, Introduction to Markov Chain Model.

Unit 4

4 Lectures

Sampling Theory: Meaning and objective of sampling, Sampling Error, Types of Sampling, Sampling Distribution, Sampling Distribution of Sample Mean and Sample Proportion, Standard Error

Unit 5

5 Lectures

Probability Distribution: Bernoulli trials, binomial distribution, normal distributions, Poisson distribution, Test of Hypothesis of Small and Large Samples- Standard Normal distribution, Chi-square distribution, Student's t distribution, F distribution, Analysis of Variance

Text Books:

1. Biostatistics (9 Ed.) by Wayne W. Daniel, Wiley 2004
2. Schaum's Outlines - Introduction to Probability and Statistics by Seymour Lipschutz and John Schiller., TATA McGraw-Hill edition. 1998

Reference Books:

1. Statistical Methods by N. G. Das, Vol: I and II., The McGraw-Hill Companies. 2009
2. Fundamentals of Biostatistics (6th Ed.), Bernard Rosner., Thomson Brooks/Cole. 2006

BINF 454 - PROGRAMMING IN JAVA

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 Lectures

Java Basics - Importance and features of java, Modifiers, Access Controls, Data types, Expressions, Declarations, Statements & Control Structures, Program Structures, String handling, Packages, Interfaces, Working with java util Package, Garbage Collection

Unit 2

8 Lectures

Exception Handling, I/O & JDBC – Exception Handling: built in exception, creating your own exceptions, Input Stream & Output Stream: Streams, Byte and Character stream, Predefined streams, Reading and Writing from Console and Files, Buffered Reader & Writer, Serialization, Database: JDBC Basics

Unit 3

7 Lectures

Multithreading and Communication – Java Thread Model: Life Cycle of Thread, Thread class, Runnable interface, Interthread Communication, Suspending, Resuming and Stopping threads, Synchronization, Scheduling and Priority of Threads.

Unit 4

7 Lectures

AWT & Event Handling – Creating User interface with AWT, Applets, Applet Life Cycle, Simple Graphics, Fonts and Colors, Events, Listeners, Components, Containers, Working with LayoutsEvent Classes, Event Listener Interfaces, Adapter and Inner Classes

Unit 5

8 Lectures

BioJava - Installing BioJava, Symbols, Basic Sequence Manipulation (DNA to RNA, Reverse Complement, motif as regular expression), Translation (DNA to Protein, Codon to amino acid, Six frame translation), Proteomics (Calculate the mass and pI of a peptide), Sequence I/O (File Formats conversions), Locations and Features (PointLocation, RangeLocation, Feature modifications), BLAST and FASTA (Blast and FastA Parser, extract information from parsed results), Counts and Distributions, Weight Matrices and Dynamic Programming, User Interfaces.

Text Books:

1. Herbert Schildt, Java- A Beginners Guide (4th Ed.), Tata Mc-Graw-Hill publication. 2007

Reference Books:

1. Computing Concepts with Java 2 Essentials (2nd Ed.) by Horstmann, C.S., John Wiley Publishers. 2000
2. Object Oriented Design and Applications (2nd Ed.) by Benjamin, Cummings and Booch, G., Addison Wesley Publishers. 1994

BINF 455 - DATABASE MANAGEMENT SYSTEM

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 Lectures

Introduction –, Database System Versus File Systems, Characteristics of Database, Database Concepts, Schemas & Instances, DBMS architecture and Data Independence, Data Models, Database Languages & Interfaces, View of Data, Database users and Administrators, Database System Structure, Database System Applications

Unit 2

7 Lectures

Data models – ER Model: Keys, Constraints, Design Issues, Extended ER features, Reductions of ER Schema to Tables. Relational Model: Structure, Relational Algebra; Hierarchical Model, Network Model, Object Oriented Model

Unit 3

6 Lectures

Structured Query Language – Basic Structure, Set Operations, Aggregate Functions, Null Values, Nested Sub queries, Views, Integrity: Domain constraints, Joined Relations, Data-Definition Language

Unit 4

8 Lectures

Relational Database and Storage – Pitfalls in Relational Design Database, Functional dependencies, Decomposition Normal Forms – 1NF, 2NF, 3NF & Boyce-Codd NF, Data Storage – Ordered indices, Hashing concepts - Security and Authorization.

Unit 5

8 Lectures

Concurrency control techniques & Information retrieval – Transactions: Properties of transactions: Concurrency problems, Serialisability and Locking techniques, Granularity of Data Items – Database System Architecture and Information retrieval: Centralized and Client-Server Architecture

Text Books:

1. Database System Concepts (4th Ed.) by Silberschatz, A., Korth, H.F. and Sudarshan, S., 2002, McGraw Hill Publishers.

Reference books:

1. An Introduction to Database Systems (7th Ed.) by Date, C.J., Addison Wesley Publishers. 2000
2. Fundamentals of Database Systems (4th Ed.) by Elmasri and Navathe, Addison Wesley Publishers. 2004
3. Principles of Database Systems (2nd Ed.) by Ullman, J. D., Galgotia Publications. 2001

BINF 456 - FUNDAMENTALS OF ALGORITHMS

Total Credits: 2

Total: 24 Hrs.

Unit 1

Computing Algorithms

4 lectures

Algorithms in Computing, Analyzing algorithms, Designing algorithms, Asymptotic notation, Standard notations, Big 'O' notations, Time and space complexity of algorithms and common functions.

Unit 2

Sorting, Searching & Strings Matching

5 lectures

Sorting: Bubble sort, Insertion sort, Selection sort, Merge Sort, Quick Sort, External sort: K-way mergesort, balanced mergesort, Searching: Binary Search, Fibonacci Search. String Matching: Naïve algorithm, Boyer Moore algorithm.

Unit 3

Graphs

5 lectures

Representation of Graphs, Breadth First Search, Depth First Search, Topological Sort, Connected Components, Minimum Spanning Tree, Single-Source Shortest Path: Dijkstra's Algorithm, All-Pairs Shortest Paths, Coloring of Graphs

Unit 4

Trees

5 lectures

Forests, DAGs, Ancestors, and Descendants, Binary Search Trees, Querying a Binary search tree, Insertion and Deletion, Tree Traversals, AVL-Trees, Rotations, Insertion, Deletion, B-trees.

Unit 5

Algorithm Design and Analysis

5 lectures

The substitution method, The iteration method, Divide and Conquer, Greedy Algorithms, Dynamic Programming: Traveling Sales Person Problem Backtracking Algorithms: 8-queens Problem.

Text Books:

1. Fundamentals of Algorithms by E. Horowitz and S. Sahani., Galgotia Book source Pvt. Ltd. 1999

Reference Books:

1. Data Structures by Seymour Lipschutz., Tata Mc-Graw-Hill publication. 2007
2. Introduction to Algorithms (3rd Ed.) by T .H. Cormen, C. E. Leiserson, R .L. Rivest., The MIT Press. 2007

BINF 457 – Microscopic Techniques For Image Processing

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Transmission electron microscopy:

Wave nature of electrons – Electromagnetic lenses – Basic components of Transmission Electron Microscope – Alignment of TEM – Major operational modes of TEM.

Unit 2

5 Lectures

Scanning electron microscopy:

Basic systems of the SEM – Contrast and three-dimensionality of the SEM image – Stereo imaging with the SEM

Unit 3

8 Lectures

Specimen preparation for EM:

TEM : Specimen preparation for TEM – Fixation – Washing – Dehydration – Embedding – Specimen staining for TEM – Positive staining and negative staining – Metal shadowing techniques – CryoEM.

Ultramicrotomy: Shaping the specimen block – Types of ultramicrotome knives – EM grids – Support films for grids – Ultramicrotome and section processing.

SEM: Surface cleaning – Rinsing and dehydration – Specimen drying techniques – Specimen fracture procedures – Replication procedures – Specimen mounting – Specimen coating for conductivity.

Unit 4

4 Lectures

Image processing and image analysis by computer

Capturing the image – Conventional vs. digital – Image processing – Controlling contrast, brightness and gamma – Removing noise – Fast Fourier Transform – images for publication and presentation – Three dimensional imaging.

Unit 5

2 Lectures

Atomic Force microscopy and Confocal Microscopy

Atomic force microscopy (AFM) including contact-mode, tapping-mode and lateral-force AFM

Confocal Microscopy: Basics of Confocal Microscopy, Sample Preparation, Confocal Optics, Resolution.

Text Book:

1. Electron Microscopy: Principles and techniques for biologists by John J Bozzola, and Lonnie Dee Russell., Jones & Bartlett Learning. 1999

Reference Books:

1. Principles and Techniques of Electron Microscopy: Biological Applications by M.A.Hayat., Cambridge University Press. 2000
2. Handbook of Biological Confocal Microscopy, by Pawley, J.B., Springer-verlag. 2006

BINF 475 - LAB - PROGRAMMING IN JAVA

Total Credits: 1

Exercise in JAVA

1. Working with Objects, Arrays, Conditionals and Loops.
2. Creating Classes and Applications in Java.
3. Java Exception handling
4. Streams and I/O, Using Native Methods and Libraries
5. Simple Animation and Threads, Advanced Animation, Images and Sound.
6. Managing Simple Events and Interactivity.
7. Local and global alignment of sequences
8. Creating User Interfaces with AWT, Modifiers.
9. Multithreading example
10. Java Programming Tools, Working with Data Structures.

BINF 476 - LAB – PROGRAMMING IN DBMS

Total Credits: 1

Exercise in DBMS (MYSQL)

Data Definition Language (DDL) statements:

Creating database, Selecting database, Deleting database, Creating table, Modifying Table, Deleting table

Data Manipulation statements:

Inserting, updating and deleting records

Retrieving Records

Retrieving specific rows and columns

Use of MySQL operators – Arithmetic operators, Comparison

Operators, Logical operators

Math functions, Aggregate functions

String operations

Limiting, Sorting and grouping query results

Handling null values

Renaming or aliasing table and column names

Using subqueries

Using Joins – joining a table to itself, joining multiple tables

Use of Indexes

Security Management

Granting and Revoking rights on tables

BINF 477 - LAB - BIOSEQUENCE ANALYSIS

Total Credits: 1

Exercises:

1. Sequence Analysis Packages: EMBOSS, NCBI ToolKit, SMS
2. Database search engines: Entrez, SRS, DBGET
3. Pair wise alignment:
 - a. Search tools against Databases:
 - i. BLAST
 - ii. FASTA
4. Multiple sequence alignment:
 - a. Clustal
 - b. Dialign
 - c. Multalign
5. Sequence patterns and profiles:
 - a. generation of sequence profiles
 - i. PSI-BLAST
 - b. derivation of and searching sequence patterns:
 - i. MeMe,
 - ii. PHI-BLAST
 - iii. SCanProsite
 - iv. PRATT
6. Protein motif and domain analysis:
 - a. MEME/MAST
 - b. eMotif
 - c. InterproScan
 - d. ProSite
 - e. ProDom
 - f. Pfam
7. Phylogenetic analysis – MEGA, PAUP, PHYLIP

BINF 521 - STRUCTURAL BIOLOGY

Total Credits: 3

Total: 36 Hrs.

Unit 1

8 Lectures

Macromolecules: DNA and RNA: types of base pairing – Watson-Crick and Hoogsteen; types of double helices A, B, Z and their geometrical as well as structural features; structural and geometrical parameters of each form and their comparison; various types of interactions of DNA with proteins, small molecules. RNA secondary and tertiary structures, t-RNA tertiary structure. **Proteins:** Principles of protein structure; anatomy of proteins – Hierarchical organization of protein structure – Primary, Secondary, Super secondary, Tertiary and Quaternary structure; Ramachandran Map.

Unit 2

6 Lectures

Xray Crystallography: Electromagnetic radiation, X-rays, principles, Bragg's Law, Types of solids: Crystal and amorphous, solids, Crystal Systems: Seven crystal system, Bravais Lattices, Space group, Symmetry. Crystallization Techniques: Small and Protein Molecules.

Unit 3

9 Lectures

Phase Problem, What is phase problem, How to solve the phase problem, Patterson function, Direct methods, Isomorphism replacement method, heavy atom method. Nuclear Magnetic Resonance: Chemical Shift, Coupling constant, spin-spin relaxation, spin-lattice relaxation, COSY, NOESY and NOE.

Unit 4

7 Lectures

Structure Prediction Strategies: Secondary structure prediction: Algorithms viz. Chou Fasman, GOR methods; analysis of results and measuring the accuracy of predictions using Q3, Segment overlap, Mathew's correlation coefficient Identification/assignment of secondary structural elements from the knowledge of 3-D structure of macromolecule using DSSP and STRIDE methods

Unit 5

6 Lectures

Classification and comparison of protein 3D structures: Purpose of 3-D structure comparison and concepts; Algorithms such as FSSP, CE, VAST and DALI, Fold Classes. Databases of structure-based classification: CATH and SCOP. Structures of oligomeric proteins and study of interaction interfaces

Text Books:

1. Molecular Modeling Principles and Applications (2nd Ed.) by Andrew R. Leach., Prentice Hall, USA. 2001
2. Principles of Protein Structure by G. E. Schulz., Springer 2009
3. Lehninger Principles of Biochemistry by David L. Nelson and Michael M. Cox, W. H. Freeman. 2005

BINF 522 – MOLECULAR MODELING AND DRUG DESIGN

Total Credits: 3

Total: 36 Hrs.

Unit 1

8 Lectures

Molecular Mechanics: Introduction, The Morse Potential, The Harmonic Oscillator Model for Molecules, Comparison of Morse and Harmonic Potential, Two atoms connected by a bond, Poly atomic Molecules, Energy due to Stretch, Bend, Stretch-Bend, Torsional strain, van der Waals and Dipole-Dipole interactions. Types of Potentials: Lennard-Jones, Truncated Lennard-jones, Exponential-6, Ionic and Polar potentials. Types of Force Fields: AMBER, CHARMM, Merck Molecular Force Field, Consistent Force Field, MM2, MM3 and MM4 force fields.

Unit 2

5 Lectures

Potential Energy Surface:- Convergence Criteria, Characterizing Stationary Points, Search for Transition States. Optimization:- multivariable Optimization Algorithms, level Sets, Level Curves, Gradients, Optimization Criteria, Unidirectional Search, Finding Minimum Point, Gradient based Methods-Steepest Descent and Conjugate Gradient Methods

Unit 3

8 Lectures

Molecular Dynamics Simulation: Introduction, Radial distribution functions, Pair Correlation function, Newtonian dynamics, Integrators- Leapfrog and Verlet algorithm, Potential truncation and shifted-force potentials, Implicit and explicit Solvation models, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations

Unit 4

8 Lectures

Drug design: Drug discovery process. Target identification and validation, lead optimization and validation. Methods and Tools in Computer-aided molecular Design, Analog Based drug design:- Pharmacophores (3D database searching, conformation searches, deriving and using 3D Pharmacophore, constrained systematic search, Genetic Algorithm, clique detection techniques, maximum likelihood method) and QSAR. Structure based drug design:- Docking, De Novo Drug Design (Fragment Placements, Connection Methods, Sequential Grow), Virtual screening.

Unit 5

7 Lectures

Structure Activity Relationship: Introduction to QSAR, QSPR, Various Descriptors used in QSARs: Electronics; Topology; Quantum Chemical based Descriptors. Regression Analysis, The Significance and Validity of QSAR Regression Equations, Partial Least Squares (PLS) Analysis, Multi Linear Regression Analysis. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations.

Text Books:

1. Computational Chemistry and Molecular Modeling-Principles and Applications by Ramachandran, Deepa and Namboori., 2008, Springer_Verlag. Reference for Unit 1 and 2.
2. Molecular Modeling Principles and Applications (2nd Ed.) by Andrew R. Leach., Prentice Hall, USA. 2001

Reference:

1. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe., John Wiley & Sons Ltd.2008
2. Molecular Modeling and Simulation – An Interdisciplinary Guide by Tamar Schlick., Springer-verlag 2000
3. Computational Medicinal Chemistry for Drug Discovery, edited by Patrick Bultinck., Marcel Dekker Inc. 2004

BINF 523 - PROGRAMMING IN PERL

Total Credit: 3

Total hrs: 36

Unit 1

7 lectures

Data Structure : Scalar Variables, Scalar Operations and Functions, Array Variables Literal Representation of Array, Array Operations and Functions, Scalar and List Context, Hash Variables, Literal Representation of a Hash, Hash Functions, Using Hashes for the Genetic Code, Gene Expression Data Using Hashes

Unit 2

7 lectures

Modular Programming: Subroutines, Advantage of Subroutines, Scoping and Subroutines, Arguments, Passing Data to Subroutines, Modules and Libraries of Subroutines, Concept about File handle, Opening and Closing a File handle, Opening and Closing a Directory Handle, Reading a Directory Handle, File and Directory Manipulation.

Unit 3

7 lectures

Regular Expression and Pattern Matching: Concepts about Regular Expressions, Simple uses of Regular Expressions, Patterns, Matching Operator, Substitutions, Split and Join functions.

Unit 4

7 lectures

Common Gateway Interface (CGI) Programming: The CGI.pm Module, CGI program in Context, Simple CGI programs, Passing Parameters via CGI, Perl and the Web

Unit 5

8 lectures

Bioperl: Introduction to Bioperl, Installing procedures, Architectures, General Bioperl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local database), Implementing REBASE

Text Books:

1. Beginning Perl for Bioinformatics (1st Edition) by Tisdall, J., O'Reilly Publishers. 2004
2. Learning Perl (5th Edition) by Randal L. Schwartz, Tom Phoenix and Brain d Foy, O'Reilly Publishers. 2008
3. Programming Perl (3rd Edition) by Wall, W., Christiansen, T. and Orwant, J., O'Reilly Publishers. 2000

BINF 524 - SYSTEMS BIOLOGY

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 lectures

Introduction: Systems Biology Networks- basics of computer networks, Biological uses and Integration. Micro array – definition, Applications of Micro Arrays in systems biology. Self-organizing maps and Connectivity maps - definition and its uses. Networks and Pathways – Types and methods. Metabolic networks.

Unit 2

8 lectures

Simulation of pathways: Whole cell: Principle and levels of simulation – E-cell and v-cell, Virtual Erythrocytes. Pathological analysis. Flux Balance Analysis. Biochemical metabolic pathways, Metabolomics and enzymes. Interconnection of pathways, metabolic regulation. Translating biochemical networks into linear algebra. Cellular models.

Networks and Motifs: Gene Networks: basic concepts, computational models. Lambda receptor and lac operon as an example. All types of networks and its uses.

Unit 3

7 lectures

Signalling & Experimental methods in systems biology: slow and auto-regulation The coherent FFL- temporal order, FIFO, DOR, Global, Development, memory and irreversibility- signaling networks and neuron circuits-robust adaptation-any model.

Robustness and optimality in Biology: model and integral feedback-signaling/bifunctional enzymes. Perfect robustness- Role and its measurement. Linking models and measurement, concepts, calibration and identification, data Vs metadata

Unit 4

6 lectures

Design of Circuits and Databases: Introduction- databases KEGG, EMP, MetaCyc, AraCyc etc., Expression databases and various databases related to systems biology, introduction to iGEM. Optional design of gene circuits I- cost and benefit: gene circuits II- selection of regulation. Stochasticity in gene expression.

Unit 5

8 lectures

Synthetic Biology:

Introduction, definition and Basics, Synthetic Oligonucleotide/DNA-based, RNA-based, Peptide-based and polyketide Technologies and Applications, Technologies and Applications of Directed Evolution and Microbial Engineering.

Text Books:

1. Systems Biology: Definitions and Perspectives by L. Alberghina H.V. Westerhoff., Springer.2005
2. Synthetic Biology, A New Paradigm for Biological Discovery, a report by Beachhead Consulting. 2006

Reference Books:

1. Computational Systems Biology by A.Kriete, R. Eils, Academic Press. 2005
2. Systems Biology in practice: Concepts, Implementation and applications by E.Klipp R.Herwig, A.Kowlad, C.Wierling and H.Lehrach, Wiley InterScience. 2005
3. Systems Biology and Synthetic Biology by Pengcheng Fu, Sven Panke., Wiley InterScience .2009

BINF 525 BIOLOGICAL SPECTROSCOPY

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 lectures

UV- Visible spectroscopy - Absorption laws - calculations involving Beer - Lambert's law - instrumentation - photocolormeter and spectrophotometer - block diagrams with description of components - theory - types of electronic transitions - chromophore and auxochromes - absorption bands and intensity - factors governing absorption maximum and intensity.

Unit 2

5 lectures

Infrared spectroscopy - principle - types of stretching and bending vibrations - vibrational frequencies - instrumentation - block diagram - source - monochromator - cell sampling techniques - detector and recorders - identification of organic molecules from characteristic absorption bands. FTIR and its advantages

Unit 3

4 lectures

Raman spectroscopy - Rayleigh and Raman scattering - Stokes' and anti Stokes lines - instrumentation - block diagram - differences between IR and Raman spectroscopy - mutual exclusion principle - applications - structural diagnosis.

Unit 4

5 lectures

Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance Spectroscopy- Nuclear spin magnetic moment, Interaction of nuclear magnet with external magnetic field, NMR spectrometer, relaxation and dynamic processes, chemical shift, Heteronuclear NMR experiments.

Electron Spin Resonance Spectroscopy: Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value, applications of ESR.

Unit 5

5 lectures

X-ray Spectroscopy: Production and properties of X-rays. The Bragg's Law – X-ray Spectroscopy – Diffraction Directions – Diffraction Methods – Powder Method – Particle size Calculation – X-ray scattering by electrons.

Text books:

1. Fundamentals of molecular spectroscopy by C. N. Banwell., McGraw-Hill.1983
2. Introduction to molecular spectroscopy by G. M. Barrow., McGraw-Hill.1962

Reference Books:

1. Molecular spectroscopy by I. N. Levine, Wiley Interscience. 1975
2. Fundamentals of molecular spectroscopy by C. N. Banwell, and Colin. 2000

BINF 526 – DATA COMMUNICATION AND NETWORKS

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Nuts & Bolts in Networks

Reference Model, Network Topologies and Protocols, Types of Networks: Local Area Network (LAN), Wide Area Network (WAN), Metropolitan Area Network (MAN), Network Security (Firewall, Packet Filtering, VPN), Uses of Computer Networks

Unit 2

6 Lectures

Network Architecture

OSI & Internet Architecture, IEEE 802 standards, Physical Layer - Transmission Media, Switching. Data Link Layer - Design Issues, Example Data Link Protocols, Data Link layer in the Internet, **Media Access Sub layer:** Static and Dynamic channel allocation –ALOHA – CSMA – CSMA / CD.

Unit 3

4 Lectures

Network Layer

Network Layer - Design Issues, Routing Algorithms, Congestion Control algorithm, Router Operation, Router Configuration, Internetworking, IP Addressing, IP Subnet Mask, IPv6 (an overview)

Unit 4

4 Lectures

Transport Layer

Transport Layer – Transport Service, Elements of Transport protocols – Internet Transport Protocols (UDP) - Internet Transport Protocols (TCP) –Related issues

Unit 5

5 Lectures

Application Layer

Design Issues, Conventional Encryption, Classical and Modern Techniques, Encryption and Decryption Algorithms (RSA), Confidentiality, DNS, SNMP, RMON, WWW, E-mail, Digital Signatures

Text Book:

1. Computer Networks (3rd Ed.) by Tananbaum A.S., PHI. 1999

Reference Books:

1. Computer Networks-Protocols, Standards and Interfaces by Black U., PHI. 1996
2. Distributed Systems Concepts & Design (3rd Ed) by George Coulouris, Jean Dollimore, Tim Kindsberg., Addison Wesley. 2000

BINF 527 – SCIENTIFIC PRESENTATION AND FINISHING SCHOOL

Total Credits: 3

Total: 36 Hrs.

Unit 1

9 Lectures

Scientific writing – Introduction- Types of scientific writings- Thesis or dissertation- Popular science writing- Types of publications- Open Access Resources- Choosing a journal- Instructions to authors - Scientific paper writing – Structure and Style- Authorships –figures tables with legends - References and citations - Acknowledgements- Conflict of interest - Peer review mechanism- Scientometric Analyses of a paper/ journal- Plagiarism issues

Unit 2

8 Lectures

Dissertation writing and grammar - Thesis: Format- Writing style; Grammar - Nouns - Adjectives - Verbs - Adverbs - Pronouns and determiners - Conjunctions and prepositions - Phrases – Clauses- spellings- Word choice -Punctuation.

Unit 3

7 Lectures

Oral presentation- Planning the oral presentations and visuals- In-class discussion (Students in small groups or individually will take up the assignments or select a research project/ topic and prepare oral presentations followed by a Q&A sessions)

Unit 4

5 Lectures

Poster Presentation- Elements and Significance of poster presentations- Planning and designing a poster- Individual Poster presentation (Students select a research project/topic and prepare posters followed by a Q&A sessions)

Unit 5

7 Lectures

Personality development, Ethics and values - elements of recruitment, selection, interview techniques- Personality Development - team work- inter personal and intra-personal interactions – human behavior at work- Time and human resources management- planning and scheduling, stress at work- work-life balance- Culture and cultural ethos- cultural diversity-diversity in organizations.

Text Books:

1. Scientific Writing: Easy When You Know How by Jennifer Peat, BMJ books. 2002
2. Successful Scientific Writing: A step-by-step Guide for Biomedical Scientists (3rd Ed.) by J.R. Matthews and R.W. Matthews, Cambridge University Press. 2008

References:

1. From Research to Manuscript: A Guide to Scientific Writing by Michael Jay Katz, by Springer. 2006,
2. Writing and Presenting Scientific Papers, 2nd Edition by Brigitta Malmfors, Phil Garnsworthy and Michel Grossman, Nottingham University Press, 2004, Viva Books Pvt. Ltd. 2011
3. Scientific Writing- A Reader and Writer's Guide, by Jean Luc- Lebrun, World Scientific Publishers, 2007

BINF 571 – LAB: STRUCTURAL BIOLOGY

Total Credits: 1

1. Advanced Visualization Software and 3D representations.
2. Small Molecule Structure determination
 - a) Structure Solution: SHELXS
 - b) Structure Refinement: SHELXL
3. Thermal Ellipsoid Plot:
 - a) ORTEP
4. Structure analysis
 - a) PARST
 - b) Platon
 - c) Mercury
5. Protein Structure Determination:
 - a) Exploration of CCP4 website
 - b) Protein Model building: COOT
 - c) Structure Solution: AMoRe
6. Structure Validation
Procheck, WHATIF, VERIFY 3D

BINF 572 - LAB – MOLECULAR MODELING AND DRUG DESIGN

Total Credits: 1

Exercises

1. Molecular Visualization Softwares: Pymol and Rasmol
2. Geometry Optimization
3. Tutorial on Molecular Dynamics: Gromacs
4. Binding Site Identification
5. Structure based Drug Design:- Molecular Docking
6. Ligand based Drug Design:- QSAR

BINF 573 - LAB - PROGRAMMING IN PERL

Total Credits: 1

1. Uses of Scalar and Array Variables to manipulate DNA/RNA/Protein sequence data
2. Concatenation DNA fragments, Transcribing DNA into RNA
3. Calculating the Reverse complement of a DNA strand
4. Uses of common Array Operators
5. Uses of Do-Until Loops
6. Uses of 'substr' function to look into the string
7. Reading a sequence data from a file and writing the results to a file
8. Opening and closing a Directory Handle, Reading a Directory and other directory manipulation functions.
9. Uses of Subroutines
10. Uses of Hashes for the genetic code: translating codons into amino acids
11. Uses of subroutine to read FASTA files
12. Translate a DNA sequence in all six reading frames
13. Uses of Regular Expressions
14. Extract annotation and sequence from GenBank file
15. Parsing GenBank annotation using arrays
16. Extract sequence chains from PDB file
17. Uses of CGI.pm Module and Passing Parameters via CGI, Debugging CGI programs
18. Installing Bioperl, Uses of Bioperl modules for sequence manipulation, accessing local database

BINF 551- ANALYTICAL TECHNIQUES

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 lectures

Electrophoresis: Theory and types; moving boundary electrophoresis, zone electrophoresis, paper, cellulose acetate gel electrophoresis, Native PAGE, disc PAGE, Gradient PAGE, SDS PAGE, DNA agarose gel electrophoresis, Southern, Northern, Western blotting techniques, Isoelectric focusing, finger printing, DNA sequencing, Pulsed - field Electrophoresis, Capillary Electrophoresis.

Unit 2

7 lectures

Chromatography: Principles, methodology and applications of chromatography using paper, thin layer, column (gel filtration, ion exchange, affinity), gas and types of HPLC.

Unit 3

6 lectures

Centrifugation: Principles, types and applications. Ultracentrifugation- types, optical methods used and applications of preparative and analytical ultracentrifuges.

Unit 4

8 lectures

Enzyme kinetics: Membrane potential, Active site, Cofactors, apo-enzymes, Enzyme specificity, Factor affecting enzyme activity, Michaelis-Menten equation, LB Plot, Determination of K_m , Types of inhibition, Allosteric enzymes.

Unit 5

8 lectures

Various Biophysical techniques to study interactions caused by the macromolecules: **Isothermal Titration Calorimetry**- instrumentation. Protocol and application in the study of Protein-ligand interactions. **Optical and magnetic tweezers**- principle, Instrumentation and modern developments. Role of Optical tweezers in studying the molecular motors and the properties of DNA. Fluorescence Resonance Energy Transfer: Principle, Instrumentation, Protocol and application in analyzing the macromolecular interactions. **Dual Polarisation Interferometry [DPI]**- Principle, Instrumentation and protocol. Application of DPI in one dimensional determination of protein structures and in studying the interactions and activity of biomolecules. ORD and CD, DLS

Text Books:

1. Principles and Techniques of Practical Biochemistry (5th Ed) by Keith Wilson and John Walker, Cambridge University Press. 2001

Reference Books:

1. Physical Biochemistry (2nd Ed) by D. Freifelder., Freeman. 1982
 2. Biochemical calculation (5th Ed.) by I.H. Segal., Cambridge University Press. 2000
 3. Protein Purification - Principles & Practices (3rd Ed.) by R. Scopes., Springer Verlag. 1994
- Biophysical Chemistry: Techniques for the study of biological structure and functions by Charles C. R. & Paul. S. R., W.H. Freeman & Co. New York. 2004

BINF 552 – BIOETHICS, BIODIVERSITY AND INTELLECTUAL PROPERTY RIGHTS

Total Credits: 3

Total: 36 Hrs.

Unit 1

8 Lectures

Regulatory Procedures: Good laboratory practice, Good manufacturing practice and FDA regulations - Regulations for recombinant DNA research and manufacturing process - Bio-safety and Bioethics - Regulations for clinical trials, Documentation and Compliance, in India and selected countries - Rules for import and export of biological materials.

Unit 2

8 Lectures

Biotechnology Processes and Products : Techniques used in Biotechnology, with special emphasis on molecular and recombinant DNA techniques - Cloning Strategies and Tissue culture procedures for plant cells, animal and stem cells - Transgenic plants, animals, genetically modified organisms (GMO) and GM food etc. - Large scale production of recombinant proteins, Processes for separation and purification - Medical Biotechnology: gene therapy, tissue engineering and xenotransplantations - Biotechnology Products: Health care products – Vaccines – Diagnostics - Recombinant therapeutic proteins - Agricultural : Hybrid and modified seeds - Bio-pesticides - Bio-fertilizers

Unit 3

6 Lectures

IPR - Definition - Forms of IPR Protection, WTO - Definition — Functions- International treaties for IPR Protection

Unit 4

7 Lectures

Patents - Definition - conditions for patentability - test of novelty of patents – composition of a patent - Patenting of Biotechnological discoveries

Unit 5

7 Lectures

Other forms of IPR protection: Copyright - Trademark - Designs - Importance in Indian Scenario & laws in India for IPR protection.

Text Books:

1. Bioethics and Biosafety in Biotechnology by Sree Krishna V., New Age International (P) Ltd., Publ., Mumbai. 2007
2. Intellectual Property Rights by Deborah E. Bouchoux., Delmar Cenage Learning. 2005

Reference Books:

1. The Indian Environmental Protection Act (EPA), 1986
2. Rules for manufacture, use/import/export and storage of hazardous microorganisms or cells Act, 1989
3. Food Safety and Standards act (Government of India), 2006
4. Intellectual Property Rights on Biotechnology by Singh, KC, BCIL, New Delhi

BINF 553 – R Language and Bioconductor

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 Lectures

Overview of the R language: Defining the R project, Obtaining R, Generating R codes, Scripts, Text editors for R, Graphical User Interfaces (GUIs) for R, Packages.

Unit 2

7 Lectures

R Objects and data structures: Variable classes, Vectors and matrices, Data frames and lists, Data sets included in R packages, Summarizing and exploring data, Reading data from external files, Storing data to external files, Creating and storing R workspaces.

Unit 3

8 Lectures

Manipulating objects in R: Mathematical operations (recycling rules, propagation of names, dimensional attributes, NA handling), Basic matrix computation (element-wise multiplication, matrix multiplication, outer product, transpose, eigenvalues, eigenvectors), Textual operations, Basic graphics (high-level plotting, low-level plotting, interacting with graphics).

Unit 4

7 Lectures

Hypothesis testing and data handling: Parametric and nonparametric tests, Chi-square test, t-tests, ANOVA, Correlation and regression, Principal component Analysis

Unit 5

8 Lectures

Bioconductor: Introduction, Bioconductor packages, ExpressionSet Class, Data annotation, biomaRt, Network analysis.

Text Books:

1. Alain F. Zuur, Elena N. Ieno, and Erik Meesters. **A Beginner's Guide to R**. Use R. Springer, 2009.
2. Florian Hahne, Wolfgang Huber, Robert Gentleman, Seth Falcon. Bioconductor case studies. Springer, 2008

Reference books:

1. Robert Gentleman. **Bioinformatics with R**. Chapman & Hall/CRC, Boca Raton, FL, 2008.
2. Robert Gentleman. **R Programming for Bioinformatics**. Computer Science & Data Analysis. Chapman & Hall/CRC, Boca Raton, FL, 2008.
3. Peter Dalgaard. **Introductory Statistics with R**. Springer, 2nd edition, 2008.

BINF 554 - PROJECT

Total Credits: 8

The course is designed to result in the satisfactory completion and defense of the Masters dissertation.

This process includes

- a) the conceptualization of the independent research that will comprise the dissertation,
- b) the preparation of and satisfactory defense of the dissertation proposal,
- c) the collection, analysis, and interpretation of data,
- d) presentation of findings in the dissertation format, and
- e) oral defense of the dissertation.

Dissertation activity must be completed within prescribed time frame for the semester.