

M.Sc. BIOINFORMATICS

Proposed modifications

REGULATIONS AND SYLLABI

(Effective from 2015-2016)



**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
LIST OF COMPULSORY HARD-CORE COURSES FOR M.Sc. BIOINFORMATICS
(Academic Year 2015-2016 onwards)

Course Code	Course Title	H	Credits	Pg. No
Semester I				
BINF 441	Cell and Molecular Biology	H	3	5
BINF 442	Bioinformatics Databases	H	3	6
BINF 443	C, C++ and Data Structures	H	3	7
BINF 481	Lab - Cell and Molecular Biology	H	1	15
BINF 482	Lab - Biological Databases	H	1	16
BINF 483	Lab - Basics of Computer & Operating Systems	H	1	17
BINF 484	Lab - Programming in C/ C++	H	1	18
Semester II				
BINF 491	Genomics and Proteomics	H	3	20
BINF 492	Bioinformatics: Sequence Analysis	H	3	21
BINF 494	Programming in Java	H	3	23
BINF 495	Database Management System	H	3	24
BINF 496	Fundamentals of Algorithms	H	3	25
BINF 486	Lab - Programming in Java	H	1	27
BINF 487	Lab - Programming in DBMS	H	1	28
BINF 488	Lab - Biosequence Analysis	H	1	29
Semester III				
BINF 541	Structural Biology	H	3	30
BINF 542	Molecular Modeling and Drug Design	H	3	31
BINF 543	Programming in Perl	H	3	32
BINF 544	Systems Biology	H	3	33
BINF 546	Data Mining and Machine Learning	H	3	35
BINF 547	Research Methodology and Finishing School	H	3	36
BINF 581	Lab - Structural Biology	H	1	38
BINF 582	Lab - Molecular Modeling and Drug Design	H	1	39
BINF 583	Lab - Programming in Perl	H	1	40
Semester IV				
BINF 592	Bioethics, Biodiversity and Intellectual Property Rights	H	3	42
BINF 599	Project	H	5	44

PONDICHERY UNIVERSITY
SCHOOL OF LIFE SCIENCES
Centre for Bioinformatics
LIST OF SOFT-CORE COURSES FOR M.Sc. BIOINFORMATICS
(Academic Year 2015-2016 onwards)

Course Code	Course Title	S	Credits	Pg. No
Semester I				
BINF 444	Physics ⁺	S	3	8
BINF 445	Chemistry ⁺	S	3	10
BINF 446	Mathematics ⁺	S	3	11
BINF 447	Biology	S	2	12
BINF 448	Basics of Computer [#]	S	2	13
BINF 449	Introduction to Bioinformatics [*]	S	3	14
BINF 485	Lab - Bioinformatics databases and tools [*]	S	1	19
Semester II				
BINF 493	Probability and Statistics [#]	S	2	22
BINF 497	Microscopic Techniques For Image Processing	S	2	26
Semester III				
BINF 545	Biological Spectroscopy	S	2	34
Semester IV				
BINF 591	Analytical Techniques	S	3	41
BINF 593	R language and Bioconductor	S	3	43

+ Physics, Chemistry and Mathematics are compulsory for students having UG degree in Biological Sciences.

Essential Soft core for all students of the Centre.

* Exclusively for students from sister departments.

BINF 441 - 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, Eukaryotic Cell Cycle : mitosis and meiosis.

Unit 2

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 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

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 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 – Gene Regulation

Text Books:

1. Cell and Molecular Biology – Concepts and Experiments by Gerald Karp. Wiley International Student Version. 2008
2. Genes VIII by Lewin, B, Pearson Education International. 2004
3. Cell and Molecular Biology by De Robertes and De Robertis. Saunders College, Philadelphia, USA. 2002

BINF 442 - 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, Recombinant DNA, Expressed sequence tags, Sequence-Tagged Sites, Genomic survey sequences; Primary Databases:- GenBank, EMBL, DDBJ; Composite Databases:- NRDB, UniProt; Literature Databases:- Open access and open sources, PubMed, PLoS, Biomed Central, NAR databases; Bioinformatic Resources:- NCBI, EBI, ExPASy, RCSB.

Unit 2

8 lectures

Genome Databases – Viral genome database:-ICTVdb; Bacterial Genomes database:-Genomes OnLine Database –GOLD, Microbial Genome Database-MBGD; Genome Browsers:- Ensembl, VEGA genome browser, NCBI-NCBI map viewer, KEGG, MIPS, UCSC Genome Browser; Archeal Genomics, Eukaryotic genomes with special reference to model organisms:- Yeast(SGD), Drosophila (FlyBase), C.elegans (WormBase), Rat, Mouse, Human (OMIM / OMIA), plants – Arabidopsis thaliana (TAIR), Rice, PlasmodiumDB, etc.

Unit 3

8 lectures

Sequence Databases – Nucleotide sequence Databases:- GenBank, EMBL, DDBJ; Protein sequences Databases:- Swiss-Prot, TrEMBL, UniProt, UniProtKB, UniParc, UniRef, UniMES; Sequence motifs Databases:- Prosite, ProDom, Pfam, InterPro, Gene Ontology; Sequence file formats:- GenBank, FASTA, PIR, ALN/ClustalW2.

Unit 4

8 lectures

Structure and derived databases – Primary structure databases:- PDB, NDB, MMDB; 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; Protein-Protein interaction database:- STRING; Chemical Structure database:- Pubchem; Gene Expression database:- GEO, SAGE.

Unit 5

6 lectures

Bioinformatics Database search engines – Text-based search engines (Entrez, DBGET / LinkDB). **Sequence** similarity based search engines (BLAST and FASTA). Motif-based search engines (ScanProsite and eMOTIF). Structure similarity based search engines (Combinatorial Extension, VAST and DALI). Proteomics tools:- ExPASy server, 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 443 – C, C++ AND DATA STRUCTURES

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 lectures

Introduction to C – C language Introduction – Tokens – Keywords, Identifier, Variables, Constants, Operators – Expression – Data types – Operator precedence - Statement: Input statement, Output statement

Unit 2

6 lectures

Controls and loops – Conditional and Unconditional Control Statement – Looping Statement: while, do-while, for – nested loop – Arrays.

Unit 3

8 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, Clustering.

Unit 5

9 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 444 – PHYSICS

Total Credits: 3

Total: 36 Hrs.

Unit 1

10 lectures

Classical Mechanics – Motion in 1D:- displacement, velocity, acceleration, motion with constant acceleration, freely falling bodies. **Motion in 2D**:- projectile motion, circular motion, relative motion, **Newton's Laws of Motion**:- forces, equilibrium, three laws of motion, inertial frames, free body diagrams, friction, gravitation, **Work and energy**:- work, kinetic energy, work energy theorem, conservative and non-conservative forces, potential energy, energy conservation, power, **Linear momentum and collisions**:- momentum and its conservation, complex bodies, center of mass, elastic and inelastic collisions, impulse, momentum theorem, **Rigid body rotation**:- angular velocity and acceleration, rotational kinetic energy, and inertia, torque, dynamics of rotation, **Angular Momentum**:- conservation of angular momentum, translation and rotation, **Statics Oscillatory motion**:- simple harmonic motion. **Mechanics: Motions** – Newtonian mechanics: laws and Derivations of Equation of motions. The gravitational force, work energy theorem, keplers law of planetary motions, lagrangian mechanics: Euler- lagrangian equations Quantum Mechanics: Black body radiation, photoelectric effect, Crompton effect. The Heisenberg uncertainty principle, Time dependent Schrodinger equation.

Unit 2

4 lectures

Quantum Mechanics – Black body radiation, photoelectric effect, Bohr's Model of Hydrogen atom, De Broglie's Hypothesis, Harmonic wave function, wave packets, Heisenberg uncertainty principle, eigen states and eigen values, Pauli's exclusion principle, Schrodinger equation

Unit 3

10 lectures

Thermodynamics – Definitions and Fundamental Ideas of Thermodynamics :- Continuum Model, System (closed, isolated), State functions & variables, Adiabatic & diathermal boundary walls, Equilibrium, Process, equation of state. Heat, Zeroth Law of Thermodynamics, Heat Conduction Equation, **The First Law of Thermodynamics** :- The First Law of Thermodynamics, Work, Entropy, **The Second Law of Thermodynamics**:- reversibility and irreversibility, free and isothermal expansions, **Heat Capacity**:- Heat Capacity, ratio of the heat capacities of a Gas, Isothermal and reversible-adiabatic expansion of an Ideal Gas , **Enthalpy**:- Enthalpy, Change of state, Latent heat and Enthalpy, **Heat engines**:- Carnot cycle, **Free Energy**:- Gibbs and Helmholtz free energy, Young's Modulus, The Third Law of Thermodynamics.

Unit 4

6 lectures

Electricity – Electrostatic Field:- Electric charge, Coulomb's Law, Electrostatic Field, Electric Field of a point charge, Electric Field from Charge Distribution, forces on charges in electric fields, electric flux, Gauss's law, Electric field and conductor, **The Electric Potential**:- Electrical Potential Energy, Electric potential, equipotential surface, finding E from V, Potential of a Point Charge and Groups of Points Charges, Potential Due to a Continuous Charge Distribution.

Unit 5

6 lectures

Electromagnetic waves:-Electromagnetic spectrum - and Diffraction, Classification of diffraction, **Fresnel diffraction**:- single narrow slit, **Fraunhofer diffraction**:- Single slit, double slit. **Diffraction patterns**:-Diffraction patterns from narrow slits, Resolution of single-slit and 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.
2. Physics of the Life Sciences by Jay Newman, Springer, 2008.

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 445 - CHEMISTRY

Total Credits: 3

Total: 36 Hrs.

Unit 1

8 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

8 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

6 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

8 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

6 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 446 - MATHEMATICS

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 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

Unit 2

6 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 3

8 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 4

10 lectures

Fourier Transformations – Properties of Fourier Transformations – Fourier Transformation of a convolution – Inverse Fourier Transformations.

Unit 5

6 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 447 - 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 448 - 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 449 - 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 481 - 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 482 - LAB - BIOLOGICAL DATABASES

Total Credits: 1

Exercises:

1. Bioinformatics Resources: NCBI, EBI, DDBJ, RCSB, ExPASy
2. Database search engines: EntrezDBGET
3. Open access bibliographic resources and literature databases
 - a. PubMed
 - b. BioMed Central
 - c. Public Library of Sciences (PloS)
 - d. CiteXplore.
4. Bioinformatics Resources at the species level
 - a. ICTV Database
 - b. AVIS
 - c. Viral genomes at NCBI
5. 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
6. Structure Databases: PDB, NDB, PubChem, ChemBank, FSSP, DSSP
7. Derived Databases: InterPro, Prosite, Pfam, ProDom
8. Sequence file formats: GenBank, FASTA
9. Protein and nucleic acid properties: Proteomics tools at the ExPASy server, EMBOSS

BINF 483 - 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 484 - 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 $[\text{OH}^-]$ 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 485 - 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 491 - 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 492 - 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. Repeats: Tandem and Interspersed repeat finding, Motifs, consensus, position weight matrices

Unit 2

6 Lectures

Pairwise sequence alignment – Basic concepts of sequence alignment, gap penalties, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments and application in Nucleic acid and protein sequences alignments.

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 application, concept of dendrogram and its interpretation, Use of HMM-based Algorithm for MSA (e.g. SAM method)

Unit 3

7 Lectures

Comparative Genomics – Basic concepts, Applications of Comparative Genomics: Identifications of Protein coding genes, Regulatory Regions, virulence factors / pathogeneity islands; Reconstruction of metabolic pathways, Genome analysis tools : Artemis, MegaBLAST, Geneplot

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 493 - PROBABILITY AND STATISTICS

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 Lectures

Numerical descriptive techniques – Measures of central tendency: mean, median, 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.

Unit 4

4 Lectures

Sampling Theory – Meaning and objective of sampling, Sampling Error, Types of Sampling, Sampling Distribution and Sampling Distribution of Sample Mean.

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 494 - 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 495 - 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 496 - FUNDAMENTALS OF ALGORITHMS

Total Credits: 3

Total: 36 Hrs.

Unit 1

5 lectures

Computing Algorithms – 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

9 lectures

Sorting, Searching & Strings Matching – 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

8 lectures

Graphs – 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

7 lectures

Trees – 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

7 lectures

Algorithm Design and Analysis – 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 497 - 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 486 - 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 487 - 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 488 - LAB - BIOSEQUENCE ANALYSIS

Total Credits: 1

Exercises:

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

BINF 541 - 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 542 - 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 543 - PROGRAMMING IN PERL

Total Credit: 3

Total: 36 Hrs.

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 Perl Special Variables – 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 544 - SYSTEMS BIOLOGY

Total Credits: 3

Total: 36 Hrs.

Unit 1

5 lectures

Introduction & Biological Networks – Systems Biology: Emergent property, Applications in health and diseases. Microarrays and its applications in systems biology. Self-organizing maps and Connectivity maps-definition and its uses. Biological Networks: Degree distribution, Clustering coefficient, Random networks, Scale-free networks, small-world effect.

Unit 2

5 lectures

Simulation of pathways – Metabolic network, Metabolic reconstruction, Flux Balance Analysis (FBA): Translating biochemical networks into linear algebra, Stoichiometric matrix, Elementary mode, Extreme pathways, Objective function, Optimization using linear programming. Genome-scale cellular models: Virtual Erythrocytes, Global human metabolic model (Recon 1).

Unit 3

5 lectures

Signalling & Experimental methods in systems biology – slow and auto-regulation The coherent FFL and incoherent FFL, single-input module (SIM): LIFO and FIFO, DOR, signaling networks and neuronal circuits.

Robustness and optimality in Biological complex systems – Biological Robustness: System control, modularity, decoupling. Optimal design of gene circuits I- cost and benefit: gene circuits II- selection of regulation. Stochasticity in gene expression.

Unit 4

4 lectures

Databases and softwares for Systems Biology – Introduction- databases: KEGG, EMP, MetaCyc. Expression databases and other databases related to systems biology. Cytoscape, visANT & CellDesigner.

Unit 5

5 lectures

Synthetic Biology – Introduction, definition and Basics, Synthetic Oligonucleotide/DNA-based, RNA-based, Peptide-based Technologies and Applications, Technologies and Applications of Directed Evolution and Microbial Engineering, Potential Hazards of Synthetic Biology, iGEM.

Text Books:

1. Introduction to Systems Biology: Design Principles of Biological Circuits by Uri Alon, Chapman & Hall/CRC, 2007.
2. Synthetic Biology: A Primer by P.S. Freemont & R.I. Kitney, Imperial College Press, 2012.

Reference Books:

1. Introduction to Systems Biology, S. Choi, Humana Press, 2007.
2. Linked – The New Science of Networks, Albert-László Barabási, Perseus Publishing, 2002.
3. Networks – an Introduction, Mark Newman, Oxford University Press, 2010.

BINF 545 - BIOLOGICAL SPECTROSCOPY

Total Credits: 2

Total: 24 Hrs.

Unit 1

5 lectures

UV- Visible spectroscopy – Absorption laws - calculations involving Beer - Lambert's law - instrumentation - photocolimeter 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 – Raleigh 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. Levins, Wiley Interscience. 1975
2. Fundamentals of molecular spectroscopy by C. N. Banwell, and Colin. 2000

BINF 546 - DATA MINING AND MACHINE LEARNING

Total Credits: 3

Total: 36 Hrs.

Unit 1

7 lectures

Introduction – Introduction, Importance of Data Mining, Relational Databases, Data Warehouses, Transactional Databases, Advance Database Systems and Applications, Data Mining Functionalities, Classification of Data Mining Systems, Major issues in Data Mining.

Unit 2

7 lectures

Primitives and System Architectures – Data Mining Primitives, Data Mining Query Language, Designing Graphical User, Interfaces Based on a Data Mining Query Language, Architectures of Data Mining Systems.

Unit 3

7 lectures

Concept Description and Association Rules – Concept Description, Characterization and comparison, Data Generalization and Summarization-Based Characterization, Analytical Characterization, Mining Class Comparisons, Mining Association Rules in Large Databases, Association Rule Mining, Mining Single-Dimensional Boolean Association Rules from Transactional Databases.

Unit 4

7 lectures

Classification and Prediction – Classification and Prediction, Issues: Data preparation for classification and Prediction, Comparing classification Methods, Classification by Decision Tree Induction: Decision Trees and Decision Tress induction

Unit 5

8 lectures

Clustering Methods – Clustering Analysis, Types data in clustering analysis: Scaled variable, Binary variables, Variables of Mixed Types, Partitioning Methods: K-means and K-Medoids, Model-Based Methods, Data Mining Applications: Data mining for Biomedical and DNA Data Analysis

Text Books:

1. Data Mining Concepts and Techniques – Jiawei Hen, Micheline Kamblar, Academic Press Morgan Kaufman Publishers. 2006

Reference Books:

1. Data Mining: Practical machine learning tools Techniques with java implementation by Ian H.Witten, Eibe Frank, 2005.
2. Machine Learning and data mining in pattern recognition in third International conference MLDM, by Petra Perner and Azriel Rosenfield, Springer.2003

BINF 547 – RESEARCH METHODOLOGY AND FINISHING SCHOOL

Total Credits: 3

Total: 36 Hrs.

Unit 1

6 Lectures

Research Methodology Objectives of research and motivation; Problem Identification & Formulation – Research Question - Hypothesis and Hypothesis Testing; Types of research - Qualitative vs Quantitative Research - Applied vs. Fundamental Research; Features of good research design; Data Collection - Data Analysis - Interpretation of results and Report writing.

Unit 2

10 Lectures

Scientific writing – Introduction - Types of scientific writings - Thesis or dissertation writing – Research paper writing; Types of publications - Open access and subscription based resources; Scientific paper writing - Choosing a journal- Instructions to authors - Structure and Style- Authorships –figures tables with legends - References and citations - Acknowledgements- Conflict of interest; Peer review mechanism and publication process; Scientometric Analyses of a paper/journal; Ethics in publishing and Plagiarism issues. Use of software for Reference Management – (Mendeley/endnote) and detection of Plagiarism (turnitin).

Unit 3

8 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 & team building – Recruitment process and interview techniques, Team work - Personality development - Interpersonal skills, Time and human resources management - Goal setting - planning and scheduling work, 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 581 - 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 582 - 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 583 - 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 591 - 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 592 - 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 Cengage Learning. 2005
3. Biodiversity and Conservation by G. Melchias, Oxford & IBH Publishing Co. Pvt. Ltd., New Delhi, 2001
4. An Advanced textbook on Biodiversity: Principles and Practice by K.V. Krishnamurthy, Oxford & IBH Publishing Co. Pvt. Ltd., New Delhi, 2003.

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 593 - 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, and 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, Applications of R in phylogenetics, microarray data analysis, next-generation sequencing (NGS) data (RNA-Seq) analysis and network analysis.

Text Books:

1. Robert Gentleman. **Bioinformatics with R**. Chapman & Hall/CRC, Boca Raton, FL, 2008. ISBN 1-420-06367-7.
2. Robert Gentleman. **R Programming for Bioinformatics**. Computer Science & Data Analysis. Chapman & Hall/CRC, Boca Raton, FL, 2008. ISBN 978-1-420-06367-7.

Reference Books:

1. Florian Hahne, Wolfgang Huber, Robert Gentleman, Seth Falcon. *Bioconductor case studies*. Springer, 2008.
2. Paul D. Lewis, R for Medicine and Biology, Jones and Bartlett Series, 2010.

BINF 599 - PROJECT

Total Credits: 5

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.