# **M.Sc. BIOINFORMATICS**

**REGULATIONS AND SYLLABI** 

(Effective from 2010-2011)



Centre for Bioinformatics SCHOOL OF LIFE SCIENCES PONDICHERRY UNIVERSITY PUDUCHERRY

# **Eligibility for M. Sc. Bioinformatics**

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

• B. Sc Degree in Bioinformatics / Physical Sciences / Chemical Sciences / Mathematical Sciences / Life Sciences / Computer Sciences and Information Technology with mathematics at +2 level.

#### **PONDICHERRY UNIVERSITY** SCHOOL OF LIFE SCIENCES

### **Centre for Bioinformatics**

# SYLLABUS FOR M. Sc. BIOINFORMATICS (Academic Year 2010-2011 onwards)

Course Code	Course Title	H/S	Credits	Pg. No
Semester I				
BINF 411	Cell and Molecular Biology	Н	3	4
BINF 412	Bioinformatics Databases	Н	3	5
BINF 413	C and Data Structures	Н	3	6
BINF 414	General Physics	S	2	7
BINF 415	General Chemistry	S	2	8
BINF 416	General Mathematics	S	2	9
BINF 417	General Biology	S	2	10
BINF 418	Basics of Computer	S	2	11
<b>BINF 419</b>	Introduction to Bioinformatics <sup>*</sup>	S	3	12
BINF 461	Lab - Cell and Molecular Biology	Н	1	13
BINF 462	Lab - Biological Databases	Н	1	14
BINF 463	Lab - Basics of Computer & Operating Systems	Н	1	15
BINF 464	Lab - Programming in C/ C++	Н	1	16
<b>BINF 465</b>	Lab - Bioinformatics databases and tools <sup>*</sup>	S	1	17
Semester II				
BINF 431	Genomics and Proteomics	Н	3	18
BINF 432	Bioinformatics: Sequence Analysis	Н	3	19
BINF 433	Probability and Statistics	S	2	20
BINF 434	Programming in Java	Н	3	21
BINF 435	Database Management System	Н	3	22
BINF 436	Fundamentals of Algorithms	S	2	23
BINF 466	Lab - Programming in Java	Н	1	24
BINF 467	Lab – Programming in DBMS	Н	1	25
BINF 468	Lab - Biosequence Analysis	Н	1	26
Semester III				
BINF 511	Structural Biology	Н	3	27
BINF 512	Molecular Modeling and Drug Design	Н	3	28
BINF 513	Programming in Perl	Н	3	29
BINF 514	Systems Biology	Н	3	30
BINF 515	Fundamentals of Spectroscopy	S	2	31
BINF 516	Data Communication and Networks	Н	2	32
BINF 517	Finishing School	Н	2	33
BINF 561	Lab - Structural Biology	Н	1	34
BINF 562	Lab - Molecular Modeling and Drug Design	Н	1	35
BINF 563	Lab - Programming in Perl	Н	1	36
Semester IV				
BINF 531	Analytical Biophysics	S	2	37
BINF 532	Bioethics, Biodiversity and Intellectual Property Rights	Н	3	38
BINF 533	Scientific Presentation	Н	2	39
BINF 534	Project	Н	8	40

\* for other department students

#### **BINF 411 - CELL AND MOLECULAR BIOLOGY**

#### **Total Credits: 3**

#### Unit 1

**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

**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

**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

**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

**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, 2008, Wiley International Student Version

#### **Reference Books:**

- 1. Genes VIII (8<sup>th</sup> Ed.) by Lewin, B, 2004, Pearson Education International.
- 2. Cell and Molecular Biology by De Robertes and De Robertis, 2002, Saunders College, Philadelphia, USA.

# 6 Lectures

Total: 36 Hrs.

# 7 Lectures

7 Lectures

#### 9 Lectures

#### **BINF 412 - BIOINFORMATICS DATABASES**

#### **Total Credits: 3**

#### Unit 1

**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

**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. **Bioinformatics Resources at the species level,** ICTV Database, AVIS, VirGen, Viral genomes at NCBI, VBRC, VBCA, PBRC and Subviral RNA database, Species 2000, TreeBASE etc

#### Unit 3

Sequence databases: Nucleic acid sequence databases: GenBank, EMBL, DDBJ; Protein sequence databases: Uniprot-KB: SWISS-PROT, TrEMBL, UniParc; Repositories for high throughput genomic sequences: EST, STS GSS, etc.; Genome Databases at NCBI, EBI, TIGR, SANGER – Viral Genomes; Archeal and Bacterial Genomes; Eukaryotic genomes w.r.t model organisms (Yeast, Drosophila, C. elegans, Rat, Mouse, Human, Arabidopsis thaliana, Rice, etc.). Querying and retrieval;

#### Unit 4

**Structure and Derived Databases: Structure Databases**: PDB, NDB, PubChem, ChemBank. **Derived Databases:** Basic concept of derived databases, sources of primary data and basic principles of the method for deriving the secondary data, organization of data, contents and formats of database entries, identification of patterns in given sequences and interpretation w.r.t the Sequence databases: InterPro, Prosite, Pfam, ProDom; Structure databases: FSSP, DSSP

#### Unit 5

**Sequence file formats:** Various file formats for bio-molecular sequences: GenBank, FASTA, GCG, MSF etc. **Extraction of knowledge from resources:** Immunology, Plant, animal and infectious diseases: databases and servers published in the NAR Database and Web server Issues and other Bioinformatics journals viz. BMC Bioinformatics etc. **Protein and nucleic acid properties:** Proteomics tools at the ExPASy server, GCG utilities and EMBOSS, Computation of various parameters

#### **Text Books:**

- 1. Bioinformatics: Sequence and Genome Analysis by Mount D., 2004, Cold Spring Harbor Laboratory Press, New York.
- 2. Bioinformatics- a practical guide to the analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellellette, B.F., 1998, John Wiley & Sons, UK.
- 3. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith, 1999, Pearson Education.

# Total: 36 Hrs.

#### 8 lectures

# 8 lectures

8 lectures

**6** lectures

# 6 lectures

### **BINF 413 – C AND DATA STRUCTURES**

## **Total Credits: 3**

#### Unit 1

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

### Unit 2

### **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

### **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

#### **String Handling & Sorting:**

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

### Unit 5

### **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 (4th Ed.) by E. Balagurusamy, 2007, Tata McGrawHill Publishing Company Limited.
- 2. Object Oriented Programming using C++ by Lafore, R. (4th Ed.), 2002. Sams Publishers.

# **6** lectures

7 lectures

#### 7 lectures

# **6** lectures

**10 lectures** 

Total: 36 Hrs.

#### **BINF 414 - GENERAL PHYSICS**

#### **Total Credits: 2**

#### Total: 24 Hrs.

b

#### Unit 1

**4** lectures Mechanics: Motion in 1D: Position, Velocity, and Speed. Instantaneous Velocity and Speed. Acceleration. Motion Diagrams. 1D Motion with Constant Acceleration. Freely Falling Objects. Kinematic Equations Derived from Calculus. Motion in 2D: The Position, Velocity, and Acceleration Vectors. 2D Motion with Constant Acceleration. Projectile Motion. Uniform Circular Motion. Relative Velocity and Relative Acceleration. The Newton's Laws of Motion and applications: Newton's First Law and Inertial Frames. Mass. Newton's Second Law. The Gravitational Force and Weight. Newton's Third Law. Forces of Friction. Newton's Second Law Applied to Uniform Circular Motion. Nonuniform Circular Motion. Motion in Accelerated Frames. Motion in the Presence of Resistive Forces.

#### Unit 2

Thermodynamics: Zeroth Law of thermodynamics: Equilibrium, State functions, temperature, Equations of State, First law of thermodynamics: Work, Heat, Internal Energy, Heat Capacity, Internal Energy, First Law of thermodynamics, Concept of Enthalpy. Second law of thermodynamics: Reversible and Irreversible Processes, Heat Engines, Carnot Cycle, Second Law statements, Spontaneous change, Entropy, Free Energy and Standard States: Free Energies and Thermodynamic potentials, Equilibrium, concepts of pH, pK, Chemical Potentials, Third Law of thermodynamics, Standard States, Reaction Thermodynamics, Equilibrium constant.

#### Unit 3

Electricity: Electric Fields: Properties of Electric Charges. Coulomb's Law. The Electric Field. Electric Field of a Continuous Charge Distribution. Motion of Charged Particles in a Uniform Electric Field. Gauss's Law: Electric Flux. Gauss's Law and its application to various charge distributions. Conductors in Electrostatic Equilibrium. Electric Potential: Potential Difference and Electric Potential. Potential Differences in a Uniform Electric Field. Electric Potential and Potential Energy Due to Point Charges. Electric Field from the Electric Potential. Electric Potential Due to Continuous Charge Distributions, Charged Conductor.

#### Unit 4

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. Motion of a Charged Particle in a Uniform Magnetic Field. Charged Particles Moving in a 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's Law. Displacement Current and Ampere's Law. Faraday's Law: Faraday's Law of Induction. Motional emf. Lenz's Law. Induced emf and Electric Fields. Generators and Motors/ Eddy Currents.

#### Unit 5

**5** lectures Optics: The Nature of Light: Reflection. Refraction. Huygens's Principle. Dispersion and Prisms. Total Internal Reflection. Fermat's Principle. Images Formed by Flat Mirrors, Spherical Mirrors, Refraction. Interference: Conditions for Interference. Young's Double-Slit Experiment. Intensity Distribution of the Double-Slit Interference Pattern. Phasor Addition of Wayes, Change of Phase Due to Reflection. Interference in Thin Films. Diffraction Patterns and Polarization: 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. Polarization of Light Waves.

#### **Text Books:**

- 1. Physics for Scientists and Engineers (6<sup>th</sup> Ed.) by Raymond A. Serway, John W. Jewett, 2004, Thomson Brooks/Cole.
- 2. Physics for Scientists and Engineers (6<sup>th</sup> Ed.) by Paul A. Tipler, Gene P. Mosca, 2007, Freeman Company
- 3. Fundamentals of Physics (6<sup>th</sup> Ed.), Resnick, Halliday and Walker, 2001, John Wiley and Sons, USA

#### **5** lectures

**5** lectures

**5** lectures

#### **BINF 415 - GENRAL CHEMISTRY**

**Total Credits: 2** 

#### Unit 1

#### 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  $\sigma$  and  $\pi$  bond with example. Meaning and Difference between  $\sigma$  and  $\pi$  bonds – hybridization, resonance. Bond properties. Molecular geometry. Intermolecular forces

#### Unit 2

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

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

Stereochemistry: Concept of isomerism, types of isomerism, optical isomerism, elements of symmetry, molecular chirallity, 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

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 (6<sup>th</sup> Ed.) by Paula Yurkanis Bruice, 2010, Prentice Hall
- 2. Virtual textbook of Organic chemistry, http://www.cem.msu.edu/~reusch/VirtTxtJml/intro1.htm

#### 8

# **5** Lectures

**5** Lectures

### 4 Lectures

# **5** Lectures

# **5** Lectures

Total: 24 Hrs.

#### **BINF 416 - GENERAL MATHEMATICS**

#### **Total Credits: 2**

Unit I Determinants and 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 II

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**

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

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

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

#### **Text Books:**

- **1.** Algebra (3<sup>rd</sup> Ed.) by Serge A. Lang, 2003, Pearson education.
- 2. Introduction to Calculus & Analysis, Vol I and II by Richard Courant & Fritz John, 1999, Springer publisher.
- 3. Trignometry, Algebra and Calculus (3<sup>rd</sup> Ed.) by Veerarajan, T., 2003, Tata McGraw Hill Publishing Co. Ltd, New Delhi.

#### **Reference Books:**

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

# **5** lectures

# 4 lectures

#### 9

### **5** lectures

# **6** lectures

# **4** lectures

Total: 24 Hrs.

#### **BINF 417 - GENERAL BIOLOGY**

#### **Total Credits: 2**

#### Unit 1

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) classification, viruses, viroids, lichens Botanical gardens, herbaria, zoological parks and museums.

#### Unit 2

Structural Organisation in Animals and Plants : Tissues 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

Cell: Structure and Function: Cell: Discovery of the cells - Cell theory; Prokaryotic and eukaryotic cell, cell wall, cell membrane and cell organelles' (plastids, mitochondria, endoplasmic reticulum, Golgi bodies/dictyosomes, ribosomes, lysosomes, vacuoles, centrioles) and nuclear organization. Mitosis, meiosis, cell cycle.Basic chemical constituents of living bodies.Structure and functions of carbohydrates, proteins, lipids and nucleic acids.Enzymes: types, properties and function.

#### Unit 4

Genetics and Evolution: 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 and RNA, search for genetic material, replication, transcription, genetic code, translation. Gene expression and regulation. Genome and Human Genome Project. DNA fingerprinting. Evolution: Origin of life, theories and evidences, adaptive radiation, mechanism of Evolution, origin and evolution of man.

#### Unit 5

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 (4<sup>th</sup> Ed.) by Bruce Alberts, 2002, Garland publishing Inc.

#### **Reference Books:**

- 1. Cell A molecular approach (2<sup>nd</sup> Ed.) by Cooper. G. M., 2000, Oxford University Press
- 2. Cell and Molecular Biology by De Robertes and De Robertis, 2002 Saunders College, Philadelphia, USA.

Total: 24 Hrs.

### **6** Lectures

# **4** Lectures

**5** Lectures

### **5** Lectures

### **BINF 418 - BASICS OF COMPUTER**

# **Total Credits: 2**

# Unit 1

# **Computer Organization**

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

#### Unit 2 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

# 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

# **Programming Language**

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

# Unit 5

### **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., 2001 Butterworth-Heinemann Ltd, USA
- 2. Computer Fundamentals and Applications (2<sup>nd</sup> Ed.) by Balaguruswamy, E., 1985, Tata McGraw-Hill Publishing Co. Ltd., India.
- 3. Microsoft Office Manual

# 5 Lectures

# 5 Lectures

**4** Lectures

### **5** Lectures

# 5 Lectures

Total: 24 Hrs.

#### - Lectures

#### **BINF 419 - INTRODUCTION TO BIOINFORMATICS**

#### **Total Credits: 3**

#### Unit 1

**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

**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

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

**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

**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., 2004 Cold Spring Harbor Laboratory Press, New York.
- 2. Bioinformatics- a practical guide to the analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellellette, B.F., 1998, John Wiley & Sons, UK.

#### **Reference Book:**

1. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith, 1999, Pearson Education.

# 6 lectures

7 lectures

7 lectures

Total: 36 Hrs.

# 8 lectures

### 8 lectures

# 12

#### **BINF 461 - 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

#### **BINF 462 - 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, VBRC, VBCA, PBRC and Subviral RNA database, Species 2000, TreeBASE etc
- 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, etc.;
  - 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 etc.
- 8. Protein and nucleic acid properties: Proteomics tools at the ExPASy server, GCG utilities and EMBOSS

#### **BINF 463 - LAB – BASICS OF COMPUTER & OPERATING SYSTEMS**

#### **Total Credits: 1**

#### **Exercises:**

- 1. DOS Commands Internal Commands: Viewing a directory, Changing Directory, Renaming a Directory - File operations: Creating files, removing a file, renaming files, viewing a file - External commands: Copying a disk, Comparing disks
- 2. Overview of different versions of Windows –Working with Windows- Desktop Basic Layout, Icons, Opening Windows, Window Characteristics, Window Controls, Resize Windows, Arrange Windows, Taskbar.
- 3. Working with Programs: Basic Program Layout, WordPad Program, Scrolling in Documents, Moving Insertion Point, Delete & Insert Key, Selecting Text, Cut, Copy & Paste, Working with Multiple Programs.
- 4. Files & Folders: Organization, View Folder Structure, Working with Folders Search for Files, Organizing Workspace - Personal Desktop, Shortcuts, Start Menu, Start Properties, Display as Menu, Taskbar, Quick Launch.
- 5. Windows Properties Navigating Control Panel, Changing Theme, Desktop Settings, Screen Saver Settings, Appearance Settings, Display Settings, Mouse Settings
- 6. Working with documents: Creating a document, Manage files and folders for documents, working with icons, editing documents Text formatting and alignment, Indentation.
- 7. Paragraph formatting Margins, tabs and page numbering.
- 8. Working with tables and borders Printing Working with Images and Text Find and replace text Mail merge.
- 9. Creating and formatting a presentation –Creation of a new Presentation, Adding Slides and Text to a Presentation, Editing Slide Text, Saving a Presentation, and Running a Slide Show- Adding Tables and charting data – Modifying objects and adding Images, Preparing to deliver a presentation.
- 10. Creating and modifying a worksheet- Formatting Worksheets Working with multiple worksheets Performing Calculations
- 11. Surfing information using Search Engines, Saving web pages to a disk, Composing Email, Sending E-mail.

#### BINF 464 - LAB - PROGRAMMING IN C/ C++

#### **Total Credits: 1**

**LINUX Operating System:** Overview of Linux Architecture, Installation, Booting and Shutdown Process, System Processes(an overview), User Management-Types of users, Creating Users, Granting Rights, File System management

#### С

- 1. Working with the Escape sequence
- 2. Program that illustrate operator precedence
- 3. working with Switch case construct
- 4. Working with looping construct (print n sequences)
- 5. Program for character manipulation ( count the number of codons )
- 6. Matrix manipulation
- 7. Program for pointer manipulation in a function
- 8. Program for String Handling (Find the longest sequence among the n sequences)
- 9. Sorting and Binary search (Check the presence of sequence in the list)
- 10. Read and write a sequence in a file

#### C++

- 1. Create a class which shows the various form 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 431 - GENOMICS AND PROTEOMICS**

#### **Total Credits: 3**

#### Unit 1

**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

**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

**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

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

# Total: 36 Hrs.

8 Lectures

7 Lectures

7 Lectures

7 Lectures

#### 18

#### **BINF 432 - BIOINFORMATICS: SEQUENCE ANALYSIS**

#### **Total Credits: 3**

#### Unit 1

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

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

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

Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, various types of pattern representations viz. consensus, regular expression (Prositetype) 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., 2004 Cold Spring Harbor Laboratory Press, New York.
- 2. Bioinformatics- a practical guide to the analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellellette, B.F., 1998, John Wiley & Sons, UK.

#### Total: 36 Hrs.

7 Lectures

# **6** Lectures

# 7 Lectures

**5** Lectures

#### **BINF 433 - PROBABILITY AND STATISTICS**

### **Total Credits: 2**

#### Unit 1

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

**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

**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, Bernoulli trials, binomial distribution, normal distributions, Poisson distribution

#### Unit 4

**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

**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 ISBN: 978-0-471-45654-4
- 2. Schaum's Outlines Introduction to Probability and Statistics by Seymour Lipschutz and John Schiller, 1998, TATA McGraw-Hill edition.

#### **Reference Books:**

- 1. Statistical Methods by N. G. Das, Vol: I and II, 2009, The McGraw-Hill Companies
- 2. Fundamentals of Biostatistics (6<sup>th</sup> Ed.), Bernard Rosner, 2006, Thomson Brooks/Cole ISBN: 0-534-41820-1

# Total: 24 Hrs.

**5** Lectures

# 4 Lectures

**5** Lectures

#### **BINF 434 - PROGRAMMING IN JAVA**

### **Total Credits: 3**

#### Unit 1

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

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

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 Layouts, Image Processing, Delegation Event Model, Event Classes, Event Listener Interfaces, Adapter and Inner Classes

### Unit 5

**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 (4<sup>th</sup> Ed.), 2007, Tata Mc-Graw-Hill publication

#### **Reference Books:**

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

# **6** Lectures

Total: 36 Hrs.

7 Lectures

8 Lectures

# 22

# **BINF 435 - DATABASE MANAGEMENT SYSTEM**

# **Total Credits: 3**

# Unit 1

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

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

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

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

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 (4<sup>th</sup> Ed.) by Silberschatz, A., Korth, H.F. and Sudarshan, S., 2002, McGraw Hill Publishers.

# **Text Books:**

- 1. An introduction to Database systems (7<sup>th</sup> Ed.) by Date, C.J., 2000, Addison Wesley Publishers.
- 2. Fundamentals of Database systems (4<sup>th</sup> Ed.) by Elmasri and Navathe, 2004, Addison Weslev Publishers.
- 3. Principles of Database systems (2<sup>nd</sup> Ed.) by Ullman, J. D., 2001, Galgotia Publications.

**6** Lectures

# **8** Lectures

# 7 Lectures

Total: 36 Hrs.

# 8 Lectures

#### **BINF 436 - FUNDAMENTALS OF ALGORITHMS**

#### **Total Credits: 2**

#### Unit 1

#### **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

#### Sorting, Searching & Strings Matching

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

#### Unit 3

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

#### 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

### 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, 1999, Galgotia Book source Pvt. Ltd.
- 2. Data Structures by Seymour Lipschutz, 2007, Tata Mc-Graw-Hill publication
- 3. Introduction to Algorithms (3<sup>rd</sup> Ed.) by T .H. Cormen, C. E. Leiserson, R .L. Rivest, 2007, The MIT Press

**4** lectures

**5** lectures

**5** lectures

Total: 24 Hrs.

#### **5** lectures

#### **5** lectures

#### 23

#### BINF 466 - 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 467 - 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 468 - LAB - BIOSEQUENCE ANALYSIS**

#### **Total Credits: 1**

#### **Exercices:**

- 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
- 8. Genome annotation Artemis.
- 9. Hypothetical Protein analysis
- 10. Genome Comparison

#### **BINF 511 - STRUCTURAL BIOLOGY**

#### **Total Credits: 3**

#### Unit 1

**DNA and RNA**: types of base pairing – Watson-Crick and Hoogstein; 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

#### Unit 2

Proteins: Principles of protein structure; anatomy of proteins – Hierarchical organization of protein structure - Primary. Secondary, Super secondary, Tertiary and Quaternary structure; Hydrophobicity of amino acids, Pacing of protein structure, van der Waal and Solvent accessible surface, Internal coordinates of proteins; Derivation, significance and applications of Ramachandran Map.

#### Unit 3

Carbohydrates: The various building blocks (monosaccharides), configurations and conformations of the building blocks; formations of polysaccharides and structural diversity due to the different types of linkages. Glyco-conjugates: various types of glycolipids and glycoproteins

#### Unit 4

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

Tertiary Structure prediction: Fundamentals of the methods for 3D structure prediction (sequence similarity/identity of target proteins of known structure, fundamental principles of protein folding etc.) Homology Modeling, fold recognition, threading approaches, and ab-initio structure prediction methods - protocols/algorithms. Prediction of protein structure: PHD and **PSI-PRED** methods

#### Unit 6

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

# **5** Lectures

Total: 36 Hrs.

# **6** Lectures

# **6** Lectures

7 Lectures

6 Lectures

#### **BINF 512 – MOLECULAR MODELING AND DRUG DESIGN**

#### **Total Credits: 3**

#### Unit 1

Introduction to molecular force fields: General features- bond stretching, angle bending, improper torsions, out of plane bending, cross terms, non-bonded interactions, point charges, calculation of atomic charges, polarization, van der waals interactions, hydrogen bond interactions, Water models. Types of force field - all atoms force field, united atom force field, etc.

#### Unit 2

Molecular Energy minization: Steepest descent, conjugate gradient – Derivatives, First order steepest decent and conjugate gradients. Second order derivatices Newton-Raphson, Minima, maxima saddle points and convergence criteria.-non derivatives minimization methods, the simplex, sequential univariative.

Unit 3

Molecular Dynamics Simulation methods: Classical Molecular Dynamics: Newtonian dynamics, Integration algorithm, Periodic boundary conditions and minimum image convention, Potential truncation and shifted-force potentials, Neighbor list, Force calculations, Long range interactions, MD code for liquid Argon. Classical Monte Carlo: Random numbers, Evaluating integrals using random numbers, Importance sampling, Metropolis algorithm, Smart MC techniques. Analysis of simulated trajectories: Radial distribution functions, Self diffusion coefficient, Time correlation functions

#### Unit 4

Drug and Vaccine design: Drug discovery process. Role of Bioinformatics in drug design. Target identification and validation, lead optimization and validation. Structure-based drug design and ligand based drug design. Modeling of target-small molecule interactions. Fundamentals of docking small and macromolecules to proteins and nucleic acids. Vaccine design: Reverse vaccinology and immunoinformatics. Databases in Immunology. B-cell epitope prediction methods. T-cell epitope prediction methods. Resources to study antibodies, antigen-antibody interactions

#### Unit 5

Structure Activity Relationship: QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronics; Topology; Quantum Chemical based Descriptors. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations

#### **Text Books**:

- 1. Molecular Modeling Principles and Applications (2<sup>nd</sup> Ed.) by Andrew R. Leach, 2001, Prentice Hall, USA.
- 2. Molecular Modeling and Simulation An interdisciplinary Guide by Tamar Schlick, 2000, Springer-verlag
- 3. Computational medicinal chemistry for drug discovery edited by Patrick Bultinck, 2004, Marcel Dekker Inc.

# Total: 36 Hrs.

**4** lectures

### **10 Lectures**

# **5** lectures

# **10 Lectures**

#### **BINF 513 - PROGRAMMING IN PERL**

#### **Total Credit: 3**

#### Unit 1

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

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

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

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

## 7 lectures

### 7 lectures

**8** lectures

7 lectures

Total hrs: 36

#### **BINF 514 - SYSTEMS BIOLOGY**

#### **Total Credits: 3**

#### Unit 1

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

#### Unit 2

Simulation of pathways: Whole cell: Principle and levels of simulation – 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

**5** lectures Signalling & Experimental methods in systems biology: slow and auto-regulation The coherent FFL- temporal order, FIFO, DOR, Global, Development, memory and irreversibilitysignaling 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

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

### Unit 5

#### **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, Potential Hazards of Synthetic Biology

### **Text Books:**

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

#### **Reference Books:**

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

### **5** lectures

5 lectures

Total: 24 Hrs.

# **5** lectures

4 lectures

### 30

#### **BINF 515 - FUNDAMENTALS OF SPECTROSCOPY**

#### **Total Credits: 2**

#### Unit 1

**UV- Visible spectroscopy** - Absorption laws - calculations involving Beer - lambert's law - instrumentation - photocolonmeter 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

**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

**Raman spectroscopy** - Raleigh and Raman scattering - stoke's and anti stokes lines - instrumentation block diagram - differences between IR and Raman spectroscopy - mutual exclusion principle - applications - structural diagnosis.

#### Unit 4

**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

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

#### **Reference Books:**

- 1. Atomic spectra & atomic structure by Gerhard Hertzberg, 1944, Dover publication, New york Recent edition.
- 2. Fundamentals of molecular spectroscopy by C. N. Banwell, 1983, McGraw-Hill
- 3. Physical chemistry by P. W. Atkins. ELBS. 1986
- 4. Introduction to molecular spectroscopy by G. M. Barrow, 1962, McGraw-Hill
- 5. Molecular spectroscopy by I. N. Levins, 1975, Wiley interscience.
- 6. Nuclear magnetic Resonance by J. D. Roberts, McGraw-Hill.
- 7. Introduction to Magnetic resonance by A. Carrrington and A. D. McLachlan. Harper and Row, 1967
- 8. Electron Spin Resonance , Elemenatry theory and practical applications by J. E. Wetz and J. R. Boulton , 1972, McGrew Hill .
- 9. Introduction to Magnetochemistry by Earnst Shaw., 1968, Academic Press
- 10. Electrical and optical properties of molecular behavior by M. Davies, pergman press.

#### 31

### Total: 24 Hrs.

### 4 lectures

#### **5** lectures

**5** lectures

### 5 lectures

**5** lectures

# **BINF 516 – DATA COMMUNICATION AND NETWORKS**

# **Total Credits: 2**

# Unit 1

# **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

# **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

# **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

# **Transport Layer**

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

# Unit 5

# **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 (3<sup>rd</sup> Ed.) by Tananbaum A.S., 1999, PHI

# **Reference Books:**

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

### **4** Lectures

### **6** Lectures

# **4** Lectures

# **5** Lectures

Total: 24 Hrs.

#### **BINF 517 – FINISHING SCHOOL**

#### **Total Credits: 2**

#### Unit 1

**5** Lectures Organizations- their meaning, formations, establishments- individuals and organizations- their inter connections- elements of recruitment, selection, interview techniques, induction, training and development, promotions, transfers, retirement, retrenchment, rehabilitation. Teams- team works- need for inter personal and intra-personal interactions - human behavior at workpersonnel issues- human resources management issues.

#### Unit 2

Personality Development - role of health in personality development - a healthy mind and a healthy body for greater productivity- role of productivity for the individual and organizationgoals setting for individuals and organizations

#### Unit 3

Human behavior in organizations- elementary aspects

#### Unit 4

Time management- planning and scheduling, stress in work- work-life balance

#### Unit 5

Ethics and values, Indian culture and cultural ethos- cultural diversity-diversity in organizations

# Total: 24 Hrs.

#### **4** Lectures

**5** Lectures

### **5** Lectures

#### **BINF 561 – LAB: STRUCTURAL BIOLOGY**

#### **Total Credits: 1**

- 1. Advanced Visualization Software and 3D representations.
- 2. Coordinate generations and inter-conversions.
- 3. Secondary Structure Prediction
- 4. Fold Recognition, ab initio (Rosetta Server)
- 5. Homology based comparative protein modeling.
- 6. Energy minimizations.
- 7. Validation of models.
  - PDB Goodies, Procheck, ProsaII, PDBsum, WHATIF, VERIFY 3D
- 8. Protein 3D Structure Alignment.
- 9. Modeller
- 10. Geno-3D
- 11. Discovery Studio Server.

#### **BINF 562 - LAB – MOLECULAR MODELING AND DRUG DESIGN**

#### **Total Credits: 1**

#### **Exercise:**

#### Software packages:

- 1. Discovery Studio
- 2. Gold
- 3. Autodock
- 4. Schrodinger maestro
- 5. Sybyl CoMFA
- 6. Gromacs
- 7. VMD

The above tools are to be used for the following analysis

- 1. Conformational Analysis
- 2. BABEL, MOPAC
- 3. Binding Site Identification.
- 4. Pharmacophore Identification
- 5. Receptor and Ligand Optimization
- 6. Docking
- 7. QSAR
- 8. Molecular dynamics simulations
- 9. Molecular Dynamics Visualization

#### **BINF 563 - 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

**4** 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

Unit 2

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

#### Unit 4

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

#### Unit 5

Various Biophsical techniques to study interactions caused by the macromolecules: Isothermal Titration Calorimetry- instrumentation. Protocol and application in the study of Proteinligand 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.

#### **Text Books:**

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

#### **Reference Books:**

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

#### **BINF 531- ANALYTICAL BIOPHYSICS**

paper, cellulose acetate gel electrophoresis, Native PAGE, disc PAGE, Gradient PAGE, SDS

# **5** lectures

# **4** lectures

#### **6** lectures

#### **5** lectures Electrophoresis: Theory and types; moving boundary electrophoresis, zone electrophoresis,

Total: 24 Hrs.

#### PAGE, DNA agarose gel electrophoresis, Southern, Northern, Western blotting techniques, Isoelectric focusing, finger printing, DNA sequencing, Pulsed - field Electrophoresis, Capillary

Unit 1

**Total Credits: 2** 

Electrophoresis.

#### **BINF 532 – BIOETHICS, BIODIVERSITY AND INTELLECTUAL PROPERTY RIGHTS**

#### **Total Credits: 3**

#### Unit 1

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

#### Unit 2

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 xeno-transplantations - Biotechnology Products: Health care products - Vaccines - Diagnostics - Recombinant therapeutic proteins - Agricultural : Hybrid and modified seeds - Bio-pesticides - Bio-fertilizers

#### Unit 3

IPR - Definition - WTO - Definition - Functions - Forms of IPR Protection

#### Unit 4

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

### Unit 5

7 Lectures Other forms of IPR - Copyright - Trademark - Designs - Importance in Indian Scenario & forthcoming laws in India.

### **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. Bioethics and Biosafety in Biotechnology by Sree Krishna V., 2007, New Age International (P) Ltd., Publ., Mumbai (ISBN: 81-224-2085-0)
- 5. Intellectual Property Rights on Biotechnology by Singh, KC, BCIL, New Delhi

# 7 Lectures

# 8 Lectures

# 38

6 Lectures

# Total: 36 Hrs.

#### **BINF 533 – SCIENTIFIC PRESENTATION**

### **Total Credits: 2**

#### Unit 1

Scientific writing - Reasons to publish - being a good writer - Making it happen - Achieving creativity -Thought, structure and style - Getting started - Forming a plan - Choosing a journal -Uniform requirements - Instructions to authors - Standardised reporting guidelines - Authorship Contributions - Writing your paper - Abstract - Introduction - Methods - Results - Discussion -Finishing your paper - Choosing a title - Title page - References and citations - Peer review.

#### Unit 2

Post-graduate theses - Writing style - Plain English - Topic sentences - Subjects, verbs and objects -Eliminating fog - Say what you mean - Word order - Creating flow - Tight writing -Chopping up snakes - Parallel structures - Style matters - Grammar - Nouns - Adjectives -Verbs - Adverbs - Pronouns and determiners - Conjunctions and prepositions - Phrases -Clauses - Which and that - Grammar matters - Word choice - Label consistently.

#### Unit 3

Readings, writing exercises and in-class discussion - Students (in small groups) will lead inclass discussions on assigned readings and writing exercises.

#### Unit 4

Individual oral presentation - Students select a research project/topic and present results as an oral presentation followed by a Q&A session.

#### Unit 5

Individual Poster presentation - Students select a research project/topic and present results as a poster followed by a Q&A session

#### **Text Books:**

- 1. Scientific Writing Easy when you know how by Jennifer Peat, 2002, BMJ books
- 2. Successful Scientific Writing: A step-by-step Guide for Biomedical Scientists (2<sup>nd</sup> Ed.) by Mathews, 2001, Cambridge University Press

#### **Reference Book:**

1. From Research to Manuscript: A Guide to Scientific Writing by MICHAEL JAY KATZ, 2006, Published by Springer.

#### 39

# **3** Lectures

# **5** Lectures

6 Lectures

# **4** Lectures

# **6** Lectures

Total: 24 Hrs.

#### **BINF 534 - 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.

# **Requirements for Starting M.Sc., Bioinformatics**

1. Faculty Requirement :	6 Nos.	
I year 4 Nos.		
Area of Specialization		
Cell and Molecular Biology, Genomics and Proteomics, Bioinformatics	:	1
Physics, Chemistry and Biophysical Chemistry	:	1
Mathematics, Statistics	:	1
Computer Science	:	1
II year 2 Nos.		
Structural Biology / Molecular Modeling	:	2

# 2. Infrastructure Requirement

### Hardware Requirement

PDB server	<i>Processor:</i> Intel Xeon quard core@1.6 Ghz; <i>RAM</i> - 4 GB; <i>HDD</i> - 876 GB; <i>OS</i> : Red Hat Linux advanced server 4	1
Linux clustering	<i>Processor:</i> Xeon@3.7 Ghz (dual processor); <i>RAM-</i> 4 GB; <i>HDD</i> -900 GB; Rack mountable; <i>OS</i> : Red Hat Linux 9	1
	<i>Processor:</i> Xeon@3.7 Ghz (dual processor); <i>RAM-</i> 4 GB; <i>HDD</i> -288 GB; Rack mountable,	2
DSM Modeling Server	Processor: Pentium IV@2.8 Ghz.; RAM: 512+256; HDD:40 GB; OS:Windows XP; CD-RW; DVD-RW	1
Workstation	Intel Pentium Core 2 Duo with dual OS (windows XP and Red Hat Linus 9) MS windows 7 certification, Red Hat Linux enterprise edition, Linux advanced server	20
Color Printer		1

#### **Software Requirement**

Schrodinger Maestro – For Docking studies, Structure based drug design.

Tripos Sybyl - For ComFA (comparative molecular field analysis) QSAR (Quantitative Structure activity relationship) studies

Discovery Studio 2.1 - For Protein Modeling, To check ADMET property

VLife – 2D QSAR

Academic License Software

- Amber 10
- GROMOS
- GROMACS
- HMMER
- AutoDock
- PyMoL

#### 3. Wet Lab Requirement

- 1. Water Purifier 1
- 2. pH meters 3
- 3. Vertical Gel apparatus 10
- 4. Horizontal Gel apparatus 10
- 5. Western blot apparatus 3
- 6. -20°C Freezer -1
- 7. UV illuminator portable 3
- 8. High Speed Refrigerated Centrifuge -1
- 9. Thermal Cyclers 2
- 10. Gel Documentation System 1
- 11. UV-Visible Spectrophotometer 1
- 12. Colorimeters 5
- 13. High performance Liquid Chromatography (HPLC) 1
- 14. ELISA Reader 1
- 15. Biosafety Cabinet 1
- 16. Ultrasonic Homogenizer 1
- 17. Freeze Dryer 1
- 18. Heating Block 5
- 19. Water Bath 3
- 20. Magnetic Stirrer 10
- 21. Gel Rocker 5
- 22. Chemical Balances 5

#### 4. Books

- 1. Cell and Molecular Biology Concepts and Experiments by Gerald Karp, 2008, Wiley International Student Version
- 2. Genes VIII by Lewin, B, 2004 Eighth edition, Pearson Education International.
- 3. Cell and Molecular Biology, De Robertes and De Robertis, 2002, Saunders College, Philadelphia, USA.
- 4. Bioinformatics: Sequence and Genome Analysis by Mount D., 2004 Cold Spring Harbor Laboratory Press, New York.
- 5. Bioinformatics- a practical guide to the analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellellette, B.F., 1998, John Wiley & Sons, UK.
- 6. Introduction to bioinformatics by Teresa K. Attwood, David J. Parry-Smith, 1999, Pearson Education.
- 7. Fundamentals of Data Structures, E. Horowitz and S. Sahani, 1999, Galgotia Booksource Pvt. Ltd.
- 8. Programming in ANSI C 4E , Balaguruswamy, E. , 2007 Tata McGraw-Hill publication
- 9. Object Oriented Programming with C++, Balagurusamy, 2007, McGraw-Hill publication
- 10. An Introduction to Thermodynamics, Y.V.C. Rao, 2004, University Press (India) Private Limited, Revised Edition.
- 11. Fundamentals of Classical Thermodynamics, G.VanWylen, R.Sonntag and C.Borgnakke, John Willey & Sons (Fourth edition).
- 12. Fundamentals of Physics, Resnick, R., Halliday, D. and Walker, 2001 Sixth edition, John Wiley and Sons, USA.
- 13. Statistical Thermodynamics, L.K. Nash.
- 14. Chemical application and group Theory: F.A. Cotton, 1999, 3rd edition
- 15. A Text book of Quantum Mechanics, P.M.Mathews and K.Venkatesan, Tata McGraw Hill
- 16. Organic Chemistry (6th Edition) by Paula Yurkanis Bruice, 2010
- 17. Virtual textbook of Organic chemistry,
- 18. Higher Engineering Mathematics by B.S. Grewal, Khanna Publishers, New Delhi
- 19. Basic mathematics By Serge Lang
- 20. Molecular Biology of the cell by Bruce Alberts 4th ed. 2002, Garland publishing Inc.
- 21. Cell A molecular approach by Cooper. G. M.. 2nd ed. Oxford University Press, 2000
- 22. Basic Computer Skills made easy, by Sherman, J., 2001 Butterworth-Heinemann Ltd, USA
- 23. Computer Fundamentals and Applications, Balaguruswamy, E., 1985, Second Edition, Tata McGraw-Hill Publishing Co. Ltd., India.
- 24. Microsoft Office Manual
- 25. Principles of Genome Analysis and Genomics by Primrose, S.B. and Twyman, R.M., 2003, Third edition, Blackwell Publishing Company, Oxford, UK.
- 26. Introduction to proteomics Tools for the new biology by Liebler, D.C., 2002, First edition, Human Press Inc., New Jersey, USA.
- 27. Bioinformatics and Functional Genomics by Pevsner, J., 2003, John Wiley and Sons, New Jersey, USA.
- 28. Bioinformatics: Sequence and Genome Analysis by Mount, D., 2004, Cold Spring Harbor Laboratory Press, New York.

- 29. Bioinformatics- a practical guide to the analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellellette, B.F., 1998, John Wiley & Sons, UK.
- 30. Biostatistics, Wayne W. Daniel, 9e Wiley 2004 ISBN: 978-0-471-45654-4
- **31. Introduction to Probability and Statistics ( Schaum's Outlines) by Seymour** Lipschutz and John Schiller, TATA McGraw-Hill edition.
- 32. Statistical Methods by N. G. Das, Vol: I and II, The McGraw-Hill Companies, 2009
- Fundamentals of Biostatistics, Bernard Rosner, 6e Thomson Brooks/Cole ISBN: 0-534-41820-1
- 34. Herbert Schildt, Java- A Beginners Guide, 2007, 4E, Tata Mc-Graw-Hill publication
- 35. Computing Concepts with Java 2 Essentials (2<sup>nd</sup> Ed.) by Horstmann, C.S., 2000, John Wiley Publishers.
- 36. Object Oriented Design and Applications (2<sup>nd</sup> Ed.) by Benjamin, Cummings and Booch, G., 1994, Addison Wesley Publishers.
- **37.** Database system Concepts by Silberschatz, A., Korth, H.F. and Sudarshan, S., 2002, Fourth Edition, McGraw Hill Publishers.
- 38. An introduction to Database systems (7<sup>th</sup> Ed.) by Date, C.J., 2000, Addison Wesley Publishers.
- 39. Fundamentals of Database systems (4<sup>th</sup> Ed.) by Elmasri and Navathe, 2004, Addison Wesley Publishers.
- 40. Principles of Database systems (2<sup>nd</sup> Ed.) by Ullman, J. D., 2001, Galgotia Publications.
- 41. Fundamentals of Data structures, E. Horowitz and S. Sahani, 1999, Galgotia Book source Pvt. Ltd.
- 42. Data Structures by Seymour Lipschutz, 2007, Tata Mc-Graw-Hill publication
- 43. Introduction to Algorithms (3<sup>rd</sup> Ed.) by T .H. Cormen, C. E. Leiserson, R .L. Rivest, 2007
- 44. Molecular Modeling Principles and Applications (2<sup>nd</sup> Ed.) by Andrew R. Leach, 2001, Prentice Hall, USA.
- 45. Principles of Protein Structure by G. E. Schulz, 2009
- 46. Principles of Biochemistry by Lehninger
- 47. Keith Wilson and John Walker, Principles and Techniques of Practical Biochemistry, 5<sup>th</sup> edition
- 48. Physical Biochemistry by D. Freifelder, 1982, 2<sup>nd</sup> Ed.
- 49. Biochemical calculation by I.H. Segal (5<sup>th</sup> Ed.), Cambridge University Press, 2000.
- 50. R. Scopes, Protein Purification Principles & Practices (3<sup>rd</sup> Ed.) Springer Verlag, 1994.
- 51. Biophysical Chemistry: Techniques for the study of biological structure and functions, Charles C. R. & Paul. S. R. W.H. Freeman & Co. New York, 2004.
- 52. Programming Perl (3<sup>rd</sup> Ed.) by Wall, W., Christiansen, T. and Orwant, J. (2000), O'Reilly Publishers.
- 53. Beginning Perl for Bioinformatics (1<sup>st</sup> Ed.) by Tisdall, J. (2004), O'Reilly Publishers.
- 54. HTML4 unleashed (2<sup>nd</sup> Ed.) by Dranell, R. (1994), Techmedia Publications.
- 55. Systems Biology: Definitions and perspectives by L.Alberghina H.V.westerhoff. Springer ISBN 978 3-540-74269-2
- 56. An Introduction to Systems Biology-Design principles of Biological circuits by Uri Alon Chapman and Hall/CRC Taylor francis group. ISBN 1-58488-642-0
- 57. Computational systems biology: A.Kriete, R.Eils Academic press. ISBN 0-12-088786-X
- 58. Systems Biology in practice: Concepts, Implementation and applications by E.Klipp R.Herwig, A.Kowlad, C.Wierling and H.Lehrach. ISBN 10-3-527-31078-9

- 59. Atomic spectra & atomic structure, Gerhard Hertzberg : Dover publication, New york Recent edition.
- 60. Fundamentals of molecular spectroscopy by C. N. Banwell.
- 61. Physical chemistry by P. W. Atkins . ELBS. 1986
- 62. Introduction to molecular spectroscopy by G. M. Barrow.
- 63. Molecular spectroscopy by I. N. Levins, Wiley interscience.
- 64. Nuclear magnetic Resonance by J. D. Roberts, Mcgrew Hill.
- 65. Introduction to Magnetic resonance by A. Carrrington and A. D. McLachlan. Harper and Row.
- 66. Electron Spin Resonance , Elemenatry theory and practical applications by J. E. Wetz and J. R. Boulton , McGrew Hill .
- 67. Introduction to Magnetochemistry by Earnst Shaw. Academic Press
- 68. Electrical and optical properties of molecular behavior by M. Davies, pergman press.
- 69. Computer Networks (3<sup>rd</sup> Ed.) by Tananbaum A.S.(1999) PHI
- 70. Computer Networks-Protocols, Standards and Interfaces by Black U. (1996) PHI
- 71. Distributed Systems Concepts & Design (3<sup>rd</sup> Ed) by George Coulouris, Jean Dollimore, Tim Kindsberg,(2000), Addison Wesley
- 72. Successful Scientific Writing: A step-by-step Guide for Biomedical Scientists (2<sup>nd</sup> Ed.) by Mathews, Cambridge University Press, 2001.
- 73. The Art of Molecular Dynamics Simulation by D. C. Rapaport
- 74. Computational medicinal chemistry for drug discovery edited by Patrick Bultinck
- 75. Biotechnologies and Development by Sasson, A. (1988) UNESCO Publications.
- 76. Biotechnologies in developing countries present and future by Sasson, A. (1993) UNESCO Publishers.
- 77. Intellectual Property Rights on Biotechnology by Singh, K, BCIL, New Delhi.
- 78. Current Protocols in Molecular Biology, January 25, 2010.
- 79. Current protocols in Protein Science, February 12, 2010.

#### \* Books Marked in Bold are Compulsory needed ( 5 copies each)

#### **5.** Journals

Science, Nature, Scientific American, Briefings in Bioinformatics, Bioinformatics, Nature Structural and Molecular Biology, Nature Chemical Biology, Cell, Bioinformatics Trends, Current Science, Chem informatics,

#### 6. E-Journals

PLos – Pathogen, BMC – Bioinformatics, BMC-Genomics, Nucleic Acid Research, Protein Science, Protein – Structure function and Bioinformatics, Journal of Virology, Journal of Molecular Recognition, Structure, Current opinion in Structural Biology, Biochemical Journal, Biochemistry, Journal of Molecular Biology, In Silico Biology.