## **M.Sc. COMPUTATIONAL BIOLOGY**

## **REGULATIONS AND SYLLABI**

(Effective from 2011-2012)



## Centre for Bioinformatics SCHOOL OF LIFE SCIENCES PONDICHERRY UNIVERSITY PUDUCHERRY

#### Eligibility for M. Sc. Computational Biology

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

- 1. B. Sc. Bioinformatics
  - B. Sc. Physics
  - B. Sc. Chemistry
  - B. Sc. Mathematics
- 2. B. Sc. Biotechnology
  - B. Sc. Biochemistry
  - B. Sc. Microbiology
  - B. Sc. Plant Biology and Biotechnology / Botany
  - B. Sc. Animal Biology and Biotechnology / Zoology

With Mathematics at +2 level Compulsory

- 3. B. Tech. Bioinformatics
  - B. Tech. Biotechnology
  - B. Tech. Industrial Biotechnology
  - B. Tech. Pharmaceutical Technology
  - B. Tech. Food Technology
  - B. Tech. Chemical Engineering
- 4. B. E. Information Technology
  - B. E. Computer Science and Engineering
  - B. E. Electrical and Electronics Engineering
  - B. E. Electronics and Instrumentation
  - B. E. Electronics and Communication Engineering
  - B. E. Mechanical Engineering
  - B. E. Biomedical Engineering

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

#### **Centre for Bioinformatics**

## SYLLABUS FOR M. Sc. Computational Biology (Academic Year 2011-2012 onwards)

<b>Course Code</b>	Course Title	H/S	Credits	Pg. No.
Semester I				
CBIO 403	Probability and Statistics	Н	3	4
CBIO 404	Communication Skills in Science & Technology	Η	3	5
CBIO 406	Programming Language – Introduction to C and	Н	3	6
	PERL			
CBIO 411	Cell & Molecular Biology	Н	3	7
CBIO 412	Biochemistry	Н	3	8
CBIO 413	Analytical Methods in Biotechnology	Н	3	9
CBIO 414	Biology	S	2	10
CBIO 415	Mathematics	S	2	11
	Lab			
CBIO 450	Analytical Techniques in Biotechnology	Н	1	12
	Laboratory			
CBIO 452	Programming Language – Introduction to C and	Н	1	13
	PERL			
Semester II				
CBIO 421	Algorithms in Computational Biology	Н	3	14
CBIO 423	Database Management Systems	Н	3	15
CBIO 425	Structural Biology	Н	3	16
CBIO 426	Biodiversity and IPR	S	2	17
CBIO 427	Biomedical Informatics	S	2	18
CBIO 431	Sequence Analysis	Н	3	19
CBIO 432	Molecular Evolution	Н	3	20
	Lab			
CBIO 454	Database Management Systems	Н	1	21
CBIO 455	Sequence Analysis	Η	1	22
Semester III				
CBIO 502	Data Mining and Machine Learning	Η	3	23
CBIO 503	Advanced Programming Language	Н	3	24
CBIO 505	Genomics and Proteomics	Н	3	25
CBIO 506	Systems Biology	S	2	26
CBIO 507	Immunology & Pharmacology	Н	3	27
CBIO 508	Molecular Modeling and Molecular Dynamics	Η	3	28
	Lab			
CBIO 550	Molecular Modeling and Molecular Dynamics	Н	1	29
CBIO 551	Advanced Programming Language	Η	1	30
Semester IV				
CBIO 521	Project Work	Η	12	31

### **CBIO 403 - Probability and Statistics**

### **Total Credits: 3**

#### Unit 1

Numerical descriptive techniques: Measures of central tendency: mean, median, mode, relation between mean, median and mode. **Partition values**: guartiles, 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

**8** Lectures 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<sup>th</sup> Ed.) by Wayne W. Daniel. John Wiley. 2004
- 2. Schaum's Outline series Introduction to Probability and Statistics by Seymour Lipschutz and John Schiller. TATA McGraw-Hill edition. 199,

### **Reference Books:**

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

#### 7 Lectures

7 Lectures

#### 7 Lectures

### 7 Lectures

Total: 36 Hrs.

#### **CBIO 404 - Communication Skills for Science and Technology**

## **Total Credits: 3**

#### Unit 1

Basics of Technical Communication: Introduction and Structure of Communication, The Process of Communication, Language as a Tool of Communication, Levels of communication, The Flow of Communication, Communication Networks, The Importance of Technical Communication.

#### Unit 2

Barriers to Communication: Definition of Noise, Classification of Barriers

#### Unit 3

Oral/visual Communication: Active Listening, Speech Structure, The Art of Delivery, Effective Presentation Strategies, Use of audio visual Aids, ICTs, Handling the Audience, Body Language, Conducting Meetings, Interviews, Group Discussion, Negotiation, Small Talk

#### Unit 4

Written Communication: Letter, Memos and E-mails/ discussion groups, Business Letters, Memos, Reports-Informal and Formal: Characteristics of a Report, Types of Reports, The Importance of Reports, Formats, Prewriting, Structure of Reports, Writing the Report, Revising, Editing and Proofreading.

Writing Journal Articles: Word choice and Syntax style, Number use, References, Plagiarism

#### Unit 5

#### **Technical Proposal and Thesis Writing Methodology**

#### **Text Book:**

- 1. Technical Communication, Principles and Practice by Meenakshi Raman, Sangeetha Sharma, Oxford University Press. 2004
- 2. More Effective Communication: A Manual for Professionals by Vilanilam J V., Saga Publications. 2000.

#### **Reference Books:**

- 1. Principles of Technical Writing by Robert Hays. Addison-Wesley, 1965
- 2. Writing for Engineers by Joan van Emden. Palgrave Macmillan. 2005
- 3. Improving Writing Skills by Arthur Asa Berger. Sage Publications. 1993
- 4. The Art of Communication by K.C. Verma. Associated Publishing Company.2001

### 7 Lectures

Total: 36 Hrs.

## **5** Lectures

## 7 Lectures

9 Lectures

### **CBIO 406 - Programming Language - Introduction to C and PERL**

## **Total Credits: 3**

#### Unit 1

#### Introduction to programming languages:

Introduction – Programming languages – Problem solving Technique: Algorithm, Flowchart, Compiling, Testing and Debugging, 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

#### **Object Oriented Programming:**

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

## Unit 5

**PERL:** 

Basic Perl Data Types, References, Matrices, Complex/Nested Data Structures, Scope: my, local, our - Function/Subroutines, System and User Function, File handle and File Tests - stat and lstat Functions - Perl Modules

### **Text Books:**

1. Programming in ANSI C (4<sup>th</sup> Ed.) by E. Balagurusamy. Tata McGrawHill Publishing Company Limited. 2007

#### **Reference Books:**

- 1. Object Oriented Programming using C++ (4<sup>th</sup> Ed.) by Lafore, R. Sams Publishers. 2002
- 2. Beginning PERL for Bioinformatics by James Tisdall. O'Reilly publications.2001

#### 7 lectures

#### 9 lectures

### **6** lectures

7 lectures

Total: 36 Hrs.

#### 7 lectures

### **CBIO 411 - Cell and Molecular Biology**

### Unit 1

**Total Credits: 3** 

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 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.

### 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

### Unit 4

7 Lectures Cellular Components – Cytoskeleton – components of Cytoskeleton, Microtubules, Intermediate filaments – Microfilaments, Cell cycle, Endoplasmic reticulum, Golgi complex, Types of vesicles - transport and their functions, Lysosomes.

### Unit 5

9 Lectures DNA and Protein Synthesis - Structure of DNA - evidence for DNA as genetic material. Gene transfer in microorganisms - conjugation, transformation, transduction - DNA replication, Transcription – mRNA processing, Translation. Protein synthesis – Ribosomes, enzymes, Protein processing.

#### **Text Book:**

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

#### **Reference Books:**

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

#### **6** Lectures

Total: 36 Hrs.

#### 7 Lectures

#### **CBIO 412 – Biochemistry**

#### Total Credits: 3

#### Total: 36 Hrs.

#### Unit 1

Basic enzymology: Enzyme nomenclature and classification of enzymes according to I.U.B. convention, General properties of enzymes, substrate specificity and active site. Fundamentals of enzyme assay-enzyme units, enzyme coupled kinetics assay. Enzyme kinetics of single substrate reactions, study state assumption, Michales-Menten, Lineweavar Burk, Eadie Hofstee, Hanes plots. Pre-study state kinetics, effect of temperature and pH.

#### Unit 2

Overview of metabolism, high energy compounds, oxidation-reduction reactions, experimental approaches to the study of metabolism, the reactions of glycolysis, fermentation, the anaerobic fate of pyruvate, control of glycolysis, metabolism of hexoses other than glucose. The pentose phosphate pathway, glycogen breakdown and synthesis, control of glycogen metabolism, gluconeogenesis and other carbohydrate biosynthetic pathways.

#### Unit 3

Overview of citric acid cycle. Synthesis of acetyl coenzyme A, enzymes of the citric acid cycle, regulation of the citric acid cycle, reactions related to the citric acid cycle, protein degradation, amino acid deamination, the urea cycle, breakdown of amino acids, amino acid biosynthesis, heme biosynthesis and degradation, chemical synthesis of peptides, oligonucleotides and oligosachharides.

#### Unit 4

# Lipid digestion, adsorption and transport, fatty acid oxidation, ketone bodies, fatty acid biosynthesis, regulation of fatty acid metabolism. Lipid bilayers and membranes. Membrane transport.

#### Unit 5

#### 7 lectures

Synthesis of purine ribonucleotides, synthesis of pyrimidiine ribonucleotides, formation of deoxyribonucleotides. nucleotide degradation integration and regulation of mammalian fuel metabolism.

#### Text book:

1. Biochemistry by Voet and Voet. Wiley. 2011

#### **Reference Books:**

- 2. Principles of Biochemistry by Nelson and Cox, Lehninger. W H Freeman & Co. 2009
- 3. Biochemistry by Berg, Tymoczko & Stryer. W.H.Freeman and Co New York. 2007

#### 7 lectures

## 8 lectures

7 lectures

#### 7 lectures

## **CBIO 413 - Analytical Methods in Biotechnology**

### **Total Credits: 3**

#### Unit 1

Microscopy

Light Microscopy: Identification of microorganisms using light and compound microscopes, Phase Contrast Microscopy, Fluorescence Microscopy, Confocal Microscopy.

**Electron Microscopy**, Electrons and Their Interactions with the Specimen, Electron Diffraction, Transmission Electron Microscope, Scanning Electron Microscope, Atomic Force Microscopy.

### Unit 2

8 Lectures Spectroscopy: Introduction to Spectroscopic Methods, Ultraviolet-Visible Molecular Absorption Spectrometry, Fluorescence Spectrometry, Infrared Spectrometry, Raman Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Molecular Mass Spectroscopy.

#### Unit 3

Separation Methods: Introduction to Chromatographic Separation, Column Chromatography, Thin Layer Chromatography, Gas Chromatography, High Performance Liquid Chromatography.

#### Unit 4

Biochemical Techniques: Protein and DNA isolation and purification; PCR amplification. Estimation of Carbohydrates, Lipids, Proteins and Nucleic Acids.

#### Unit 5

#### 7 Lectures

7 Lectures

7 Lectures

Sequencing methods: Basic DNA sequencing: Maxam-Gilbert method, Sanger method, Pyrosequencing, automated DNA sequencing, DNA sequencing by capillary array and electrophoresis. RNA sequencing, Protein sequencing: Edman degradation, Peptide mass fingerprinting, Protease digests. Genome sequencing: High-throughput sequencing, shot-gun sequencing.

#### **Text Books:**

- 1. Instrumental Analysis by Skoog, Holler, Crouch, 2007, Brooks/Cole,
- 2. Analytical Biochemistry by David. J. Holme & Hazel Peck, 3<sup>rd</sup> ed, Prentice Hall 1998.

#### **Reference Books:**

1. Introduction to Instrumental Analysis by Robert D. Braun, 2006, Pharma Book Syndicate. ISBN 891- 88449-15-6 Genome (2nd Ed.) by, T.A Brown, 2002, BIOS Scientific Publishers Ltd.

#### Total: 36 Hrs.

### **CBIO 414- 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 (nonchordates up to phylum level and chordates up to class level) and plant (major groups; Angiosperms up to class - linnaeus) classification.

#### Unit 2

7 Lectures Structural Organization in Plants: Morphology, anatomy and functions of different parts of flowering plants: Root, stem, leaf, inflorescence, flower, fruit and seed.

#### Unit 3

#### 7 Lectures

Structural Organization in Animals: Morphology, anatomy and functions of different systems of an annelid (earthworm), an insect (cockroach) and an amphibian (frog).

#### Unit 4

**8** 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 5

#### **8** 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.

#### **Text Books:**

1. Molecular Biology of the cell (4<sup>th</sup> Ed.) by Bruce Alberts. Garland publishing Inc. 2002

#### **Reference Books:**

1. Cell - A molecular approach (2<sup>nd</sup> Ed.) by Cooper. G. M., Oxford University Press. 2000 2. Cell And Molecular Biology. Wolter Kluwer. 2011.

Total: 24 Hrs.

10

## **CBIO 415 – Mathematics**

### **Total Credits: 2**

#### Unit I

#### **Matrices and Linear Algebra**

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

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

#### Unit II

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.

### **Text Books:**

- 1. Algebra (3<sup>rd</sup> Ed.) 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 (40<sup>th</sup> Ed.) by B.S. Grewal and J.S. Grewal, 2007, Khanna Publishers, New Delhi.

#### **5** lectures

#### **4** lectures

**5** lectures

### **6** lectures

### 4 lectures

Total: 24 Hrs.

#### CBIO 450 – Lab- Analytical Techniques in Biotechnology Laboratory

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

#### **Analytical Techniques**

- 1. Optical Microscopy Gram's Staining
- 2. Visible Spectroscopy Verification of Beer Lambert's law using KMnO<sub>4</sub> & determination of unknown sample concentration using calibration curve.
- 3. Fluorescence Microscopy (Demonstration)
- 4. Protein purification using HPLC (Demonstration)
- 5. Thin Layer Chromatography Separation of Chlorophyll / Amino acids
- 6. Interpretation of NMR, Mass spectra and FTIR data.

#### Cell & Molecular Biology

- 7. Isolation & Purification of genomic DNA from bacteria
- 8. Isolation & Purification of plasmid DNA
- 9. Restriction Digestion, Agarose gel electrophoresis of chromosomal & plasmid DNA
- 10. Separation of protein on SDS PAGE
- 11. DNA amplification using PCR

#### CBIO 452 - Lab - Programming Language - Introduction to C and PERL

#### **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 C tokens
- 2. Program that illustrate operator precedence
- 3. Sample program for Switch case construct
- 4. Sample program for looping construct
- 5. Program for creating user defined function
- 6. Program for passing pointer in a function
- 7. Program for String Handling ( Sequence alignment , Pattern match)
- 8. Sorting and Binary search
- 9. Read and write a sequence in a file

#### C++

- 1. Create a class which shows the various form of constructors
- 2. Implement any one form of Inheritance
- 3. Implement static and dynamic Polymorphism

#### PERL

- 1. Read and Print Matrix
- 2. Program to find the longest sequence
- 3. Implementing complex data structure
- 4. Procedure creation example
- 5. Reading / Writing Protein / DNA sequences in files.

## **CBIO 421 - Algorithms in Computational Biology**

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

#### Unit 1

**Introduction:** Algorithms in Computing; Analyzing algorithms-Asymptotic notation, Standard notations, Big 'O' notations; Algorithm design techniques- Exhaustive Search, Branch-and-Bound Algorithms, Greedy Algorithms, Dynamic Programming, Divide-and-Conquer Algorithms, Machine Learning, Randomized Algorithms; Time and space complexity of algorithms, common Sort and Search algorithms.

#### Unit 2

**Exhaustive Search**- Restriction Mapping, Finding Motifs; **Greedy Algorithms**- Genome Rearrangements, Sorting by Reversals, Finding Motifs; **Dynamic Programming Algorithms**-Edit Distance and Alignments, Global and local Sequence Alignment, Scoring Alignments, Alignment with Gap Penalties, Gene Prediction, Multiple Alignment; **Divide-and-Conquer Algorithms**- Divide-and-Conquer Approach to Sorting, Space-Efficient Sequence Alignment, Block Alignment;

#### Unit 3

**Combinatorial Pattern Matching**- Hash Tables, Repeat Finding, Exact Pattern Matching; **Expectation and Maximation** (EM) with forward and backward algorithms, discriminative learning; **Genetic Algorithm:** Basic Concepts, Reproduction, Cross over, Mutation, Fitness Value, Optimization using GAs; Applications in bioinformatics

#### Unit 4

**Hidden Markov Models:** Markov processes and Markov Models, Hidden Markov Models, Parameter estimation for HMMs, Optimal model construction, Applications of HMMs

Artificial Neural Networks: Historic evolution – Perceptron, NN Architecture, supervised and unsupervised learning, Back Propagation Algorithm, Training and Testing, Self-organizing Feature Map and Radial Basis Function Network; Overview of Support Vector Machines, Bayesian network

#### Unit 5

**Clustering and Trees:** Hierarchical Clustering, k-Means Clustering, Evolutionary Trees, Distance-Based Tree Reconstruction, Reconstructing Trees from Additive Matrices, Character-Based Tree Reconstruction, Small and large Parsimony Problem.

#### **Text Books:**

- 1. Fundamentals of Computer Algorithms by Horowitz, S. Sahini, and Rajasekharan. Galgotia Publications.1984
- 2. An introduction to bioinformatics algorithms by Neil C. Jones, Pavel Pevzner. MIT Press. 2004

#### **Reference Books:**

- 1. Bioinformatics: the machine learning approach by Pierre Baldi, Søren Brunak. MIT Press. 2001
- 2. Probabilistic Methods for Bioinformatics: With an Introduction to Bayesian Networks by Richard E. Neapolitan. Morgan Kaufmann Publishers. 2009
- 3. Hand book for Hidden Markov model for Bioinformatics by Martin Gollery. CPC Press. 2008.
- 4. Neural Networks: A Systematic Introduction by Raul Rojas. Springer. 1996

#### Total: 36 Hrs.

#### 7 Lectures

**8** Lectures

#### 9 Lectures

7 Lectures

#### **CBIO 423 - Database Management Systems**

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

#### 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

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

#### **Reference Books:**

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

Total: 36 Hrs.

#### **6** Lectures

7 Lectures

#### **8** Lectures

### **CBIO 425 - Structural Biology**

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

#### Unit 1

Basic structural principles, building blocks of proteins, motifs of protein structures, alpha domain structures, alpha/beta structures, Macromolecular crystallography-concepts

#### Unit2

DNA structures, DNA recognition in prokaryotes and eukaryotes, specific transcription factors, enzyme catalysis and structure. Membrane proteins signal transduction, proteins of the immune system. Structure of Spherical viruses.

#### Unit 3

Folding and flexibility, Prediction, engineering and design of protein structures. Methods to identify secondary structural elements

#### Unit 4

8 Lectures Determination of protein structures by X-ray and NMR methods. Prediction of secondary structure- PHD and PSI-PRED methods. Tertiary Structure: homology modeling, fold recognition and ab-initio approaches. Structures of oligomeric proteins and study of interaction interfaces.

#### Unit 5

In silico study of biological structures. Structural genomics- concepts and significance. Structural databases.

#### **Text Books:**

- 1. Protein structure, stability and folding Ed KP.Murphy, Humana press. 2001.
- 2. Introduction to Macromolecular Crystallography- A. McPherson., John Wiley Publications. 2003.

#### **Reference Books:**

- 1. Introduction to protein architexcture Arthur M.Lesk., Oxford University Press. 2001.
- 2. Introduction to Protein Structure, Branden, Carl and Tooze. John Garland, Publication Inc. 1991

#### 7 Lectures

Total: 36 Hrs.

#### 7 Lectures

#### 7 Lectures

## **CBIO 426 - Biodiversity and IPR**

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

Unit 1 Introduction to biological diversity- What is biodiversity: genetic, species and ecosystem diversity. Conservation of biodiversity. National legal frameworks for biodiversity conservation: Wildlife Protection Act (1972). Types of protected area, landed trusts, community forests. Biodiversity inventories and monitoring. Introduction to software such as Distance, Estimate S to assess densities and species diversity. DNA barcoding for rapid assessment of genetic diversity.

#### Unit 2

Biodiversity and species extinction: impact of deforestation, hunting, wildlife trade, diseases and climate change on species extinction. Case studies on Amazonian deforestation, amphibian extinction through diseases, REDD, CITES. IUCN Red lists and other legal framework for biodiversity conservation.

#### Unit 3

Convention on biological diversity (CBD), Rio Summit, Intergovernmental Committee for the Cartagena Protocol on Biosafety (ICCP). Case study: has the CDB achieved its 2010 target.

#### Unit 4

Laws and agreements: IPR- patents, trade secrets, copyrights, trademarks - Plant genetic resources Agreement - GATT (General Agreement on Tariffs and Trade) and TRIPS (Agreement on Trade-Related Aspects of Intellectual Property Rights) Cooperation and implications - Patents of Higher plants, Transgenic organisms, Isolated genes and DNA sequences

#### Unit 5

SUI-GENESIS system and its uses - Plant variety protection and UPOV - Terminator and Traitor technologies for seed protection, uses and implications.

#### **Text Books:**

- 1. Intellectual Property Rights by Deborah E. Bouchoux, Delmar Cenage Learning. 2005
- 2. Biodiversity and Conservation (2<sup>nd</sup> Ed) by Jeffries, M. J., Routledge. 2006

#### **Reference Books:**

- 1. Conservation of Genetic Resources by Virchow, Detlef. Springer 1999
- 2. Biodiversity, conservation law and livelihoods by Jeffrey, M. J., Firestone, J., Bubna-Litic, K., Cambridge University Press. 2008
- 3. Intellectual Property Rights on Biotechnology by Singh, KC, BCIL, New Delhi

17

#### **6** Lectures

Total: 24 Hrs.

#### **4** Lectures

**5** Lectures

#### **5** Lectures

#### **CBIO 427 - Biomedical Informatics**

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

#### Unit 1

Introduction: Biomedical data,-Clinical and life sciences -standards and databases. Principles and its uses

#### Unit 2

**Electronic health records (EMR)** and health Information exchanges—including information retrieval, medical decision making, evaluation and evidence. Patient monitoring systems-ethics in informatics - bayesian networks-learning and decision-data structure in algorithm design and analysis.

#### Unit 3

**Networking:** TCP/IP Sockets and DNS clinical database concepts-design of the clinical information systems/Clinical Decision support systems--Synchornization, concurrency, deadlock, full-text databases, distributed database services and architexture on one of the database.any clinical database structure as one example.

#### Unit 4

**Methods and Evaluation**: Sampling, appropriate use of controls, data collection including human-testing of statiscal significance, sensitivity and specificity.ROC plots. Methods and issues specific to healthcare.

#### Unit 5

**Healthcare informatics**: Understanding and interaction Health organization especially academic health centers, understanding the health care environment, understanding the organization informatics- Interaction between these three units-machine learning approaches to make decision making and discovery. Human factors in clinical systems –use of machine learning to make modeling, datamining, policy design and law. Translation research and its uses and implications Evidence based medicines.

#### **Text Books:**

- 1. Biomedical Informatics: First edition, By Jules J. Berman. Jones & Bartlett, 2010
- 2. Biomedical Informatics: computer applications in Health care and Biomedicine (3<sup>rd</sup> ed), by Shortliffe EH, Ciminio JJ., New York Springer-Verlag. 2000

#### **Reference Books:**

1. Evaluation methods in medical Informatics by Friedman CP. Wyatt JC, New York Springer-Verlag-1996.

## Total: 24 Hrs. 4 Lectures

#### 5 Lectures

## 5 Lectures

**5** Lectures

## 19

#### **CBIO 431 - Sequence Analysis**

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

#### Unit 1

Overview: Biological Literature Information access, storage and retrieval systems- Primary and secondary databases of genomics, trascriptomics, proteomics and metabolomics. Knowledge on freeware and commercial software. Importance of hardware and software creations.

#### Unit 2

**Data- alignment and applications:** Collecting and Storing Sequence Data: Sequence assembly; Submission of Sequences; Sequence accuracy; Sequence databases; Sequence formats; Conversion between formats; EST databases; SNP databases; Annotation and Archival .Sequence alignment and applications: Uses: Choice to be made for alignment; Scoring matrices; Homology and related concepts; Dot Matrix methods; Dynamic programming methods for global and local alignments tools- FASTA, BLAST, statistical and Biological significance.

#### Unit 3

Nucleic acid sequence analysis: Reading frames; Codon Usage analysis; Translational and transcriptional signals; Splice site identification; Gene prediction methods; RNA fold analysis

#### Unit 4

Multiple Sequence alignment and applications: Uses; Methods available- Iterative alignment, Progressive alignment - ClustalW, T-Coffee; Profile Methods - Gribskov profile, PSI-BLAST, HMM ; Clustering and Phylogeny; Methods for Phylogeny analysis: Distance and Character based methods; Motif detection ; Protein family databases; Use of Structure based sequence alignment

#### Unit 5

#### 7 Lectures

**Protein sequence analysis:** Compositional analysis; Hydrophobicity profiles; Amphiphilicity detection; Moment analysis; Transmembrane prediction methods; Secondary structure prediction methods

#### **Text Book:**

1) Computational Molecular Biology by P. A. Pevzner, Prentice Hall of India Ltd. 2004

#### **Reference Books:**

- 1. Current Protocols in Bioinformatics, Edited by A.D. Baxevanis et al, Wiley Publishers. 2005
- 2. Bioinformatics by David W. Mount, Cold Spring Harbor Laboratory Press. 2001
- 3. Fundamental concepts of Bioinformatics by D.E. Krane and M.L Raymer, Pearson Education. 2003

#### Total: 36 Hrs.

**8** Lectures

## **6** Lectures

#### 8 Lectures

#### **CBIO 432 - Molecular Evolution**

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

#### Unit 1

History of evolution of life on earth: elements, molecules to species. Mendelian inhereitance. Hardy-Weinberg equilibrium: stability of gene (allele) frequencies under five conditions. Evolution of DNA, RNA and proteins, origin of the genetic code: chemical basis of evolution.

#### Unit 2

Evolutionary change by mutation, gene flow, genetic drift, natural selection and non-random mating. Role of gene duplication, transitions and transversions- chromosomal deletions and insertions, in evolution. Role of repetitive DNA, transposable elements and junk DNA in evolution. Homology of proteins and DNA in evolution

#### Unit 3

Theoretical aspects: Darwin Wallace theory of evolution by natural selection, Neutral theory of molecular evolution (Kimura). Role of Mutation in evolution. Divergence rates as a function of heterozygosity and gene functionality. Computation of phyogenetic trees using distance matrix methods, Maximum Parsimony method, Maximum likelihood and Bayesian inference.

#### Unit 4

The concept of the Molecular Clock. Calibration. Limitation of molecular clock models. Human molecular clock: deducing evolutionary histories through mitrochondrial DNA and Y chromosome.

#### Unit 5

Evolution of the genome: Genomic sequencing and mapping: Genome databases Human Genome Project.

#### **Text Books:**

- 1) Molecular Evolution by Wen Hsiung-Li, Sinauer Associates, Sunderland, MA. 1997
- 2) Evolution (3<sup>rd</sup> Edition) by Ridley, M., Blackwell Science. 2004

#### **6** Lectures

#### **10 Lectures**

**10 Lectures** 

#### **6** Lectures

#### **4** Lectures

Total: 36 Hrs.

#### **CBIO 454 - Lab-Database Management Systems**

**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

#### CBIO 455 - Lab - Sequence Analysis

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

- 1. Accessing Biological databases:
- 2. Retrieving protein and nucleic acid sequences, structures, ESTsequences, SNP data using database browsers and genome browsers.
- 3. converting sequences between different formats. Using sequence editors. sequence assembly.
- 4. **Nucleic acid sequence analysis** : detecting ORF's, identification of translational and transcriptional signals, gene predictions, codon usage, RNA fold analysis.
- 5. **sequence alignment and applications** : pairwise alignment-dot matrix comparisons, global and local alignment, Database searching-different pairwise methods. Use of scoring matrices and gap penalities.
- 6. **Multiple sequence alignment and applications**: Use of multiple sequence editors. Progressive alignment and iterative alignment approaches. Use of profile methods for motif detection. Clustering and Phylogeny approaches.
- 7. **Protein Sequence analysis:** Composition, Hydrophobicity and amphilicity. *Predictions:* transmembrane and secondary.

## **CBIO 502 - Data Mining and Machine Learning**

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

#### Unit 1

#### 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

#### **Primitives and System Architectures**

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

#### Unit 3

#### **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

#### **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

#### **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 Kambler, Academic Press Morgan Kaufman Publishers. 2006

#### **Reference Books:**

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

#### 7 lectures

Total: 36 Hrs.

#### 7 lectures

7 lectures

#### 7 lectures

#### 8 lectures

#### **CBIO 503 - Advanced Programming Language**

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

#### Unit 1

Perl & Bioperl : Uses of Regular expressions: Patterns, Single-character Patterns, Grouping Patterns (Sequence, Multipliers, Parantheses as Memory, Alternation) Anchoring patterns, Precedence, Matching operators, Ignoring case, Different Delimiter, Split and Join functions-Bioperl: Installation, architecture and uses.

#### Unit 2

#### **Object Oriented Language II:**

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 3

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 4

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

#### Unit 5

#### **HTML:** Introduction – Formatting tags for creating a web page

AWT & Event Handling in java – 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

#### **Text Books:**

1. Advanced Perl Programming by Sriram Srinivasan, O-Reilly, 1997

#### **Reference Books:**

2. Patrick Naughton and Herbertz Schildt, "Java2 The Complete Reference", TMH, 1999.

#### Total: 36 Hrs.

#### 7 Lectures

### 8 Lectures

**6** Lectures

## 7 Lectures

### **CBIO 505 - Genomics and Proteomics**

#### Unit 1

**Total Credits: 3** 

Genomics and Metagenomics: Genome databases of Plants, animals and pathogens; Gene networks: basic concepts on identification of disease genes, drought stress response genes, insect resistant genes and nutrition enhancing genes.

**Epigenetics:** DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), ArrayExpress, SAGE databases: 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)

**6** Lectures

7Lectures

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

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

Proteomics: Protein arrays: basic principles, 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. Bioinformatics and Functional Genomics by Pevsner, J., John Wiley and Sons, New Jersey, USA. 2003
- 2. Principles of Genome Analysis and Genomics (3<sup>rd</sup> Ed.) by Primrose, S.B. and Twyman, R.M., Blackwell Publishing Company, Oxford, UK. 2003

#### **Reference Books:**

- 1. Introduction to proteomics Tools for the new biology (1<sup>st</sup> Ed.) by Liebler, D.C., 2002, Human Press Inc., New Jersey, USA.
- 2. Bioinformatics: Sequence and Genome Analysis by Mount, D., Cold Spring Harbor Laboratory Press, New York. 2004

#### Unit 4

Unit 3

## Unit 2

**8** Lectures

### 8 Lectures

7 Lectures

Total: 36 Hrs.

## **CBIO 506 - Systems Biology**

### **Total Credits: 2**

#### 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 adapation-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, Springer. 2005
- 2. Synthetic Biology, A New Paradigm for Biological Discovery, a report by Beachhead Consulting, 2006

#### **Reference Books:**

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

#### Total: 24 Hrs.

## **5** lectures

**4** lectures

## **5** lectures

**5** lectures

#### CBIO 507 - Immunology & Pharmacology

**Total Credits: 3** 

#### Unit 1

#### Total: 36 Hrs. 7 Lectures

**Introduction and Antibodies**: Innate and acquired immunity, active and passive immunity, natural and artificial immunity and humoral. Lymphoid system- primary or secondary organ. Cells- Lymphocytes, mononuclear, phagocytes, antigen presenting, polymorphs, mast cells, cluster designation (CD) and antigen specific receptors – Principles and its uses.

#### Unit 2

7 Lectures

**Antibody generation:** structure and function –clonal selection theory-different types of immunoglobulins, effectors, receptors and antibody diversity. complement system-activation, pathways and biological effects. Major Histochemical molecules/peptide complexes-Structure and Function and production of MHC Locus in Mice and Human. t-lymphocytes and cytokine network, receptors, production from TH1 and TH2 CD4+ T- cells.

#### Unit 3

#### 7 Lectures

9 Lectures

Antigen and antibody reaction/interaction: Haemagglutination, direct and indirect immunofluroescence, hybridoma technology for mass production.

**Vaccine design and development**: Reverse vaccinology and, immunoinformatics, databases in immunology, prediction methods-B-cell and T-cell resources to study antibodies. DNA, Plant and protein based recombinant antigens as vaccines.

#### Unit 4

**Introduction to Pharmacology:** Introduction to the principles of pharmacokinetics and pharmacodynamics. ADMET (Drug Absorption, Metabolism, distribution & toxicity of drugs) and bioavailability of drugs. General pathways of drug metabolism (Phase I and phase II metabolism), toxicity due to drug-drug interactions with one specific example.

**Receptor theory and mechanism of drug action (Pharmacodynamics):** How drugs work, receptor occupancy theory and characterization of drug action, including dose-response relationships, agonists and antagonists.

Autonomic nervous system: Outline of autonomic nervous system, Receptor systems, second messengers and location/specificity of action of alpha and beta receptor systems in the autonomic nervous system. Mechanism of action of antihypertensive drug – beta adrenergic antagonist with one example.

#### Unit 5

#### 6 Lectures

**Chemotherapy**: Antibiotics - antibacterial – antiviral and anticancer - drug types and mechanism of action with one example each.

**New drug discovery and approval:** Lead discovery process - Basis of preclinical and clinical trial testing of new drugs. Regulatory review: Investigational new drug & New drug application and approval process.

#### **Text Books:**

- 1. Text book of Immunology by Kuby, 2008
- 2. Rang and Dale's Pharamcology ed Churchill Livingstone, 2007,

#### **Reference books:**

- 1. Text book of Immunology by Riott, 2006
- 2. Lippincott's Illustrative Reviews of Pharmacology. Lippinncott. 2009
- 3. Burger's Medicinal Chemistry and Drug discovery. Volume 2, Drug Discovery and development.6th Edition. Ed Donald J AbrahamWiley-Interscience.

#### **CBIO 508 - Molecular Modeling and Molecular Dynamics**

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

#### Unit 1

**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-Diploe 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

**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

**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 simulationssimulations

#### Unit 4

**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

**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:**

- Molecular Modelling for Beginners, (2<sup>nd</sup> Edition) by Alan Hinchliffe, John Wiley & Sons Ltd. 2008
- 2. Molecular Modeling and Simulation An interdisciplinary Guide by Tamar Schlick, Springerverlag. 2000
- 3. Computational medicinal chemistry for drug discovery edited by Patrick Bultinck, Marcel Dekker Inc. 2004

#### Total: 36 Hrs.

#### **8** Lectures

#### 8 Lectures

5Lectures

#### 8 Lectures

#### 7 Lectures

#### 28

#### **CBIO 550 - LAB: Molecular Modeling and Molecular Dynamics**

#### **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

#### **CBIO 551 - Lab: Advanced Programming Language**

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

- 1. Reading/Writing Protein/DNA sequences in files.
- 2. Mutation and randomization in Bioperl.
- 3. DNA manipulation: Transcription DNA to RNA, Reverse complementing.
- 4. Passing Data to Subroutines
- 5. Local and Global alignment of sequences
- 6. Java Applets Basics, Graphics, Fonts and Color.
- 7. Simple Animation and Threads.
- 8. Creating simple JAVA graphical user interface

#### **Total Credits: 12**

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.