# **M. Tech. COMPUTATIONAL BIOLOGY**

## **REGULATIONS AND SYLLABI**

(Effective from 2023-2024)



# DEPARTMENT OF BIOINFORMATICS SCHOOL OF LIFE SCIENCES PONDICHERRY UNIVERSITY PUDUCHERRY

## **Pondicherry University** School of Life Sciences Department of Bioinformatics

## Master of Technology in Computational Biology

Supported byDBT, Govt of India.

## **Program Objectives**

The main objective of the program is to make the student to develop and apply data-analytic mathematical modelling and computational simulation techniques to biological systems. To train the students in developing the algorithms, computer programing and experimental techniques to solve the biological problems,

## Program Outcomes

By end of the program, the students will be able:

- To use the experimental methods to solve the biological problem using computational algorithms including database design and implementation,
- To implement the computational methods to analyse large collections of complex biological data to make new predictions or discover new concepts in biological Sciences
- Capable of using critical thinking and research methods to be applied on computational biology problems.
- Gain an opportunity to participate in cutting edge research by the assignment of research project that spans over two semesters

## **Pondicherry University** School of Life Sciences Department of Bioinformatics

#### Eligibility for M. Tech. Computational Biology

Minimum of 55% of marks in Master's degree in Bioinformatics/computational biology/Physics/Chemistry/ Mathematics/ Statistics/ Computer Science/ all branches in Life sciences (Biotechnology/ Biochemistry/ Microbiology/ Plant Biology/ Botany/ Animal Biology/ Zoology)/ Agricultural sciences.

B.Tech /B.E degree in Industrial Biotechnology, Biotechnology, Pharmaceutical Technology, Food Technology, Bioinformatics, Chemical Engineering, Bioengineering, Information Technology, Information Science, Computer Science and Engineering, Biomedical Engineering, Agricultural sciences / B.Pharm.

#### Minimum number of credits required to be earned by students

The minimum number of credits required to be earned by students of M.Sc. Programmes

Sl.No.	Programme	Credits for Hard Core Courses	Credits for Soft Core Courses	Minimum credits required for award of degree
1	M.A./M.Sc./M.Tech. (except M.Tech ECE) / Any other 2 year P.G. Programme not mentioned below	48 to 60	12 to 24	72

A candidate who has passed in all the Hard-Core courses and Project Work (if any) and accumulated not less than the minimum number of Credits prescribed shall be eligible to receive the Degree

#### PONDICHERRY UNIVERSITY SCHOOL OF LIFE SCIENCES DEPARTMENT OF BIOINFORMATICS

### Syllabus For M. Tech. Computational Biology

(Academic Year 2023-2024)

#### List of Hard-Core Courses for M. Tech. Computational Biology

<b>Course Code</b>	Course Title	H/S	Credits	Pg. No.
Semester I			L	
CBIO 611	Bioinformatics and Sequence Analysis		3	8
CBIO 612	Fundamentals of Biostatistics		3	10
CBIO 618	Basics of Cell and Molecular Biology		3	12
CBIO 619	Design and Analysis of Algorithm	Н	3	14
CBIO 658 Introduction to Programming with C++ and JAVA		Н	3	16
	Lab	•		
CBIO 653	Bioinformatics And Sequence Analysis	Н	1	22
CBIO 657	Cell and Molecular Biology	Н	1	23
CBIO 659	Programming in C++ and JAVA	Н	1	24
	Total Credits		18	
Semester II			L	
CBIO 621	Algorithms in Computational Biology	Н	3	26
CBIO 623	Drug Discovery and IPR	Н	3	28
CBIO 624	Genomics and Proteomics	Н	3	30
CBIO 625	Structural Biology	Н	3	32
CBIO 631	Python programming	Н	3	34
	Lab		1	
CBIO 654	Structural Biology	Н	1	43
CBIO 632	Python programming lab			44
	Total Credits		17	
Semester III			L	
CBIO 711	Biomolecular Simulations <sup>s</sup>	Н	3	46
CBIO 712	Systems Biology	Н	3	48
CBIO 713	Data Mining and Data Warehousing	Н	3	50
CBIO 714	Metabolism and Immunology	Н	3	52
CBIO 751	<b>Project</b> (Phase – I)	Н	2	58
	Lab	•		
CBIO 752	Biomolecular Simulations	Н	1	57
CBIO 753	Data Mining and Data Warehousing	Н	1	58
	Total Credits		16	
Semester IV		•		
CBIO 721	Genetic Engineering (rDNA Technology)	Н	2	61
CBIO 722	Molecular evolution	Н	3	63
CBIO 756	Genetic Engineering Lab	Н	1	64
CBIO 755	<b>Project</b> (Phase – II)	Н	6	68

\*30 Hrs for 2 Credit paper (24 Lectures + 6 Tutorials)

\*45 Hrs for 3 Credit paper (36 Lectures + 9 Tutorials)

#### PONDICHERRY UNIVERSITY SCHOOL OF LIFE SCIENCES DEPARTMENT OF BIOINFORMATICS

#### List of Soft-Core Courses for M. Tech. Computational Biology

(Academic Year 2023-2024)

Course Code	Course Title	S	Credits	Pg. No
Semester I				
CBIO 620	Physical Sciences for Biologists		3	18
CBIO 617	Introductory Biology *		2	20
Semester II				
CBIO 630	Mathematics for Biosciences	S	3	36
CBIO 628	Big Data Analytics		2	37
CBIO 629	Bioethics and Research methodology	S	2	39
CBIO 724	Next Generation Sequencing using R	S	2	41
Semester III				
CBIO 715	Biophysical Techniques	S	2	54
CBIO 716	Perl Programming for Biologists	S	2	55
Lab				
CBIO-754	Perl Programming for Biologists	S	1	59
Semester IV				
CBIO 723	Biomedical Informatics and Translational Research	S	2	65
CBIO 725	Functional Plant Genomics	S	2	67

\*Students with Mathematical and Physical Science background are expected to choose CBIO-617 as compulsory papers.

- 30 Hrs for 2 Credit paper (24 Lectures + 6 Tutorials)
- 45 Hrs for 3 Credit paper (36 Lectures + 9 Tutorials)

# Semester-I

#### **CBIO 611- BIOINFORMATICS AND SEQUENCE ANALYSIS**

**<u>COURSE OBJECTIVES</u>**: The process of subjecting a DNA, RNA or peptide sequence to any of the wide range of analytical methods to understand its features, function, structure, or evolution will be explored by sequence alignment and searches against biological databases.

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

#### Unit I

**Introduction to Primary Databases:** Types of Biological data- Genomic DNA, cDNA, rDNA, ESTs, GSSs; Primary Databases -Nucleotide sequence databases-GenBank, EMBL, DDBJ, Protein Sequence Databases- UniProtKB, UniProt, TrEMBL, Swiss-Prot, UniProt Archive-UniParc, UniProt Reference Clusters-UniRef, UniProt Metagenomic and Environmental Sequences-UniMES. Literature Databases- PubMed, PLos, BioMed Central.

#### Unit II

Introduction to Secondary or Derived Databases- PDB, CSD, MMDB, SCOP, CATH, FSSP, CSA, KEGG ENZYME, BRENDA; Sequence motifs Databases:-Prosite, ProDom, Pfam, InterPro; Composite Databases-NRDB, Genome Databases- Viral genome database (ICTV db), Bacterial Genome database (GOLD, MBGD), Organism specific database (OMIM/OMIA, SGD, WormBase, PlasmoDB, FlyBase, TAIR), Genome Browsers (Ensembl, VEGA, NCBI map viewer, UCSC Genome Browse). Bioinformatics Database search engines:-Text-based search engines (Entrez, DBGET/LinkDB).

#### Unit III

**File formats, sequence patterns and profiles:** Sequence file formats – GenBank, FASTA, ALN/ClustalW2, PIR; Basic concept and definition of sequence patterns, motifs and profiles, various types of pattern representations viz. consensus, regular expression (Prosite-type)and sequence profiles; Sequence similarity based search engines (BLAST and FASTA); Pattern based search using MeMe and PRATT); Motif-based search using ScanProsite and eMOTIF; Profile-based database searches using PSI- BLAST and HMMer.

#### Unit IV

**Sequence Analysis and predictions:** Nucleic acid sequence analysis-Reading frames; Codon Usage analysis; Translational and transcriptional signals, Splice site identification, Gene prediction methods and RNA fold analysis; Protein sequence analysis-Compositional analysis, Hydrophobicity profiles, Amphiphilicity detection, Moment analysis, Transmembrane prediction methods, Secondary structure prediction methods.

#### Unit V

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

#### 9 Lectures

Total: 45 Hrs.

9 Lectures

9 Lectures

9 Lectures

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

#### Text books:

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

#### **References:**

- 1. Near real-time processing of proteomics data using HADOOP by Hillman et al., (2014) Mary ann Liebert, Inc- Big Data. 2 (1): BD44- BD49.
- 2. Curating Big Data Made Simple: Perspectives from Scientific Communities by SoweSulayman K. and ZettsuKoji(2014).Big Data. 2 (1): 23-33.
- 3. The quantified self: Fundamental Disruption in Big Data Science and Biological Discovery by Melanie Swan (2013) Mary ann Liebert, Inc. Big data , 1(2): BD85-99.

<u>COURSE OUTCOME</u>: The development of high-throughput production of gene and protein sequences have exponentially increased and therefore students will gain knowledge on the databases and tools available today for understanding the structure and functions of these sequences.

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#### **CBIO 612- FUNDAMENTALS OF BIOSTATISTICS**

**<u>COURSE OBJECTIVES</u>**: To understand the basic principles of statistical theory and methods and to apply them for analyzing the data related to biological system and draw the conclusions

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

Unit I Review of Basic statistical measures: Numerical description of data, Measures of central tendency, Measuring variations in data, Standard deviation and its significance, Percentiles, Quartiles, Box Plots. Correlation and regression Models with their applications in biological data analysis

#### Unit II

**Probability theory:** Classical and modern definition of probability, Sample space and events, Axioms of probability, Sample space having equally likely outcomes, Conditional probability, Independent events, Bayes formula and its application to Biology, RandomVariables- Types of Variables, Expected Value, Variance.

#### Unit III

Discrete and Continuous Distribution: Binomial distribution, Poisson distribution, Poisson approximation to Binomial distribution, Hypergeometric distribution, Joint distribution of two variables, Normal and Standard normal distribution, Normal approximation to Binomial (Poisson).

#### Unit IV

Sampling Distributions and Estimation: Statistic, Distribution of sample mean, sample variance, central limit theory, Biased and unbiased estimator, Confidence interval, Population mean, Population variance.

#### Unit V

**Tests of Hypotheses:** Formulation of Hypothesis- Simple and Composite, Type I and Type II errors, Power of a test, Significance of a test, P-value, Testing for Normality, Parametric and non-parametric tests- t-test, Analysis of Variance (ANOVA), Chi-square test, Mann-Whitney U test, Wilcoxon signed-rank test, Kruskal-Wallis test,

#### **Text Books:**

- 1. Biostatistics (9th Ed.), Wayne W. Daniel, John Wiley & Sons, 2018.
- 2. Biostatistical Analysis (5<sup>th</sup> edition), Jerrold H. Zar, Pearson, 2018

#### **Reference Books:**

1. Statistical Methods (1<sup>st</sup> Ed.), N. G. Das, Tata McGraw-Hill, 2017.

2. Fundamentals of Biostatistics (6th Ed.), Bernard Rosner, Thomson Brooks/Cole, 2015.

## 9 Lectures

Total: 45 Hrs.\*

9 Lectures

#### 9 Lectures

9 Lectures

#### COURSE OUTCOME

Have better understanding about the principles of biostatistics Knowledge about the applications of various statistical methods Ability to perform and interpret statistical analyses with real biological data.

#### **CBIO 618 -BASICS OF CELL AND MOLECULAR BIOLOGY**

**<u>COURSE OBJECTIVES:</u>** Students will understand the structure and purpose of basic components of different cells with their functions in detail.

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

#### Unit 1

**Structural organization of cells:** Cell theories, properties and classes of cells- Prokaryotes and eukaryotes, Cell specialization- cell types, totipotency, Origin of multicellularity, evolution of life. Biomolecular composition of cells- Macromolecules: Lipids, Carbohydrates, Nucleic Acid and water. Structures outside the cell membrane- cell wall, capsule, flagella, fimbria and their motility.

#### Unit 2

**Structure and functions of Biomembranes:** Structures (Models) and functions- properties, thermodynamics and transport types-passive, active and co-transport, pumps, membrane selectivity, liposomes. Signal transduction mechanisms- stimuli (ligands, mechanical forces, osmolarity, temperature and light), receptors (GPCRs, tyrosine kinases, acetylcholinesterase) and second messengers (calcium, lipid messengers and nitric oxide) with reference to major pathways.

#### Unit 3

**Structure and functions of Mitochondria and Chloroplast:** Ultra-structure, origin and replication, Functions- cellular respiration (Glycolysis, oxidation of pyruvic acid, Fate of pyruvate under aerobic and anaerobic conditions, TCA cycle and energy conversion- Electron transport and oxidative phosphorylation (Translocation of Protons and the Establishment of a proton-motive force; machinery for ATP formation (Chemiosmotic theory). Regulation and dysfunctions of mitochondrial intermediary products. An overview of photosynthetic Metabolism, Absorption of light, Photosynthetic units and reaction centers, Photophosphorylation, Carbon-dioxide fixation.

#### Unit 4

**Cytoskeleton and their functions:** Peroxisomes, Lysosomes, Cytoskeleton – components of Cytoskeleton, Microtubules, Intermediate filaments, Microfilaments. Endoplasmic reticulum, Golgi complex, Types of vesicles.

#### Unit 5

**Flow of genetic information:** Structure of DNA, Experimental evidence to prove DNA as genetic material. Mechanism of DNA replication, transcription and translation in both prokaryotes and eukaryotes. Protein synthesis – Ribosomes, enzymes, Protein processing. Cell cycle and regulation.

#### **Text Book:**

- 1. Cell and Molecular Biology Concepts and Experiments by Gerald Karp. Wiley International Student Version. 2008
- 2. Cell and Molecular Biology by De Robertis and De Robertis. Saunders College, Philadelphia, USA. 2002
- 3. Molecular Biology of the cell (4<sup>th</sup> Ed.) by Bruce Alberts. Garland publishing Inc. 2002

#### Total: 45 Hrs.\*

#### 9 Lectures

#### 9 Lectures

## 9 Lectures

9 Lectures

#### **Reference materials:**

- 1. Genes VIII (8<sup>th</sup>Ed.) by Lewin, B. Pearson Education International. 2004
- 2. Concepts of Biology (2<sup>nd</sup> Ed.) by Sylvia S. Mader. McGraw Hill Publishers, 2011.
- Principles of Gene Manipulation (7<sup>th</sup> Ed.) An Introduction to Genetic Engineering by S.B. Primrose, university of California Press. 2006

<u>COURSE OUTCOME:</u> At the end of the course, the students will be able to explain the purpose of the structural organization and functional differences between the prokaryotic and eukaryotic cells along with explaining the mechanism of DNA replication and theprocess of synthesis and regulation of genetic elements.

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#### **CBIO 619 - DESIGN AND ANALYSIS OF ALGORITHM**

**COURSE OBJECTIVES:** This course concentrates on studying algorithmic designtechniques and methods for analyzing algorithms. To design and implement the appropriate algorithm on biological domain.

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

#### Unit 1

Algorithm Analysis: Analyzing algorithms-Designing algorithms-Asymptotic notation-Standard notations and common functions-The substitution method-The recursion tree method-The master method -Basics of time complexity estimates, General norms for running time calculation.

#### Unit 2

Divide and Conquer: General method, applications-Binary search, Quick sort, Merge sort, Strassen's Matrix Multiplication. Greedy method: General method, applications-Job sequencing with deadlines, 0/1 knapsack problem, Minimum cost spanning trees, Single source shortest path problem.

#### Unit 3

#### Dynamic Programming: General method, applications-Matrix chain multiplication, Optimal binary search trees, 0/1 knapsack problem, All pairs shortest path problem, Traveling sales person problem.

#### Unit 4

Searching and Traversal Techniques: Efficient non-recursive Tree Traversal Algorithms, DFS, BFS of Graphs, AND/OR graphs, game trees, Bi-Connected components, Search Trees-Balanced search trees-AVL trees, representation, Operations-insertion, deletion and searching, B-Trees-B-Tree of order m, Operations- insertion, deletion and searching.

#### Unit 5

Backtracking and Branch and Bound: General method (Backtracking), Applications-nqueen problem, sum of subsets problem, graph coloring, Hamiltonian cycles. General method (Branch and Bound), Applications - Traveling sales person problem.

#### **Text Books:**

- 1. Computer Algorithms/C++, E.Horowitz, S.Sahani and S.Rajasekharan, Galgotia Publishers pvt. Limited.1998
- 2. Data Structures and Algorithm Analysis in C++, 2nd Edition, Mark Allen Weiss, Pearson Education. 1997
- 3. Introduction to Algorithms, 2nd Edition, T.H.Cormen, C.E.Leiserson, R.L.Rivest, and C.Stein. PHI Pvt.Ltd./ Pearson Education. 2001

9 lectures

## 9 lectures

#### 9 lectures

9 lectures

## Total: 45 Hrs\*

9 lectures

#### **Reference Books:**

- 1. Design and Analysis of algorithms, Aho, Ullman and Hopcroft, Pearson Education, 2<sup>nd</sup> edition, 2013.
- 2. Introduction to the Design and Analysis of Algorithms, A.Levitin, Pearson Education, 2<sup>nd</sup> edition, 2011.
- 3. Data Structures And Algorithms in C++, 3rd Edition, Adam Drozdek, Thomson, 3<sup>rd</sup> edition, 2011.
- 4. Algorithm Design: Foundations, Analysis and Internet examples, M.T.Goodrich and R.Tomassia, John Wiley and sons, 2<sup>nd</sup> edition, 2006

**<u>COURSE OUTCOME:</u>** Learn to apply divide and conquer strategy, greedy methods, dynamic programming and backtracking for design of various algorithms. Analyze the running time of algorithms using asymptotic notations and using Recursion.

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#### CBIO 655 - INTRODUCTION TO PROGRAMMING WITH C++ AND JAVA

<u>COURSE OBJECTIVES:</u>  $T_{o}$  introduce students to the modern object-oriented programming paradigm and *To train them in writing programs in C++ and JAVA languages* 

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

#### Unit 1

C++ programming basics: Compilation of C++ programs – Input and output statements – integer, float, and character variables – arithmetic operations and built-in library functions. **Decision making, functions and structures-** Loops and decision-making statements – structures and unions – arrays and strings.

#### Unit 2

**Features of Object-Oriented Programming:** Object oriented concepts – working with objects and classes in C++ – scope resolution operator – constructors – destructors – overloading of constructors and operators – string class. Concept of inheritance- levels of inheritance. **Pointers and file handling-** Pointer concept – pointers and arrays – pointers and functions - File handling – Reading and Writing the data from file.

#### Unit 3

**Java Basics and java packages:** Installing Java, Importance and features of JAVA, Lexical elements of JAVA, Data types and Control structure, Program structure, Arrays, Command line input handling, OOPS, String Handling. Packages in java- working with util package (Scanner, StringTokenizer, etc).

#### UNIT-4-

JAVA Swing: Introduction to Swing, Swing Features, Heirarchy of Java Swing Classes, Swing GUI Components, Packages Used in Swing, AWT v/s Swing, Event Handling In Swing.

#### UNIT-5

**JDBC & Applets:** JDBC: Steps to connect database, Classes and Methods for Database connectivity and Data Manipulation, Applets: Importance of applets, Steps to build an applet, creation and execution of applets. Biojava - Concepts, Installation, Symbols & SymbolList, DNA to RNA conversion and proteomics classes

#### **Text Books:**

- 1. E.Balaguruswamy "Object Oriented Programming with C++", 6th edition, Tata McGraw Hill Education, 2015
- 2. C++: The Complete Reference, 4th Edition by Herbert Schildt, McGraw Hill Education (2017)
- 3. Herbert Schildt, 2017. Java A Beginner's Guide, 7th Edition, MCGRAW HILL
- 4. Andreas Prlic, Andrew Yates, Spencer E. Bliven, et al., BioJava: on open-source framework for bioinformatics in 2012. Bioinformatics. 28(20): 2693-2695. https://www.biojava.org

## 9 lectures

10 lectures

## 9 lectures

## 9 lectures

8 lectures

# Total: 45 Hrs\*.

#### **Reference Books:**

- 1. Stanley Lippman, JoseeLajoie, Barbara E. Moo ,"C++ Primer", 5th Edition, Addison Wesley, 2015
- 2. Sams Teach yourself C++ in 24 Hours by J Liberty and R Cadenhead, Pearson publisher (2012)
- 3. Herbert Schildt, 2018, JAVA: The complete reference, 11th Edition, TATA MCGRAW HILL Edition, Kindle Edition.
- 4. Yakov Fain. 2015, Java Programming: 24 Hour Trainer, 2<sup>nd</sup> Edition, Wileypublication

<u>COURSE OUTCOME</u>: On successful completion of the course students will get themselves familiarize with the concepts and coding in C++ and JAVA languages and their implementation in biological data analysis.

#### **CBIO 620- PHYSICAL SCIENCES FOR BIOLOGISTS**

**<u>COURSE OBJECTIVES:</u>** The main objective of this course is to help the students to understand the basic concept of fundamental physics and their applications in biology.

#### Total Credits: 3

#### Unit 1:

**Classical Mechanics:** Types of Motion:-Uniform, projectile, circular and relative motions, Newton's Laws of Motion, Law of Gravitation, **Work and energy**:- work energy theorem, conservative / non-conservative forces, energy conservation, power, Linear momentum and collisions (elastic and inelastic), impulse, momentum theorem, **Rigid body rotation**:angular velocity and acceleration, rotational kinetic energy, inertia, torque, dynamics of rotation, **Angular Momentum**:- conservation of angular momentum, translation and rotation, Statics Oscillatory motion.

#### **Unit 2:**

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

#### Unit 3:

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

#### Unit 4:

**Introduction to Inorganic Chemistry:** Atomic Structure - Elements and compounds, atoms and molecules-definition, Classical atomic models - J. J. Thomson, E. Rutherford, N. Bohr. Electronic configuration- aufbau principle - Pauli exclusion principle - Hund's rule- Modern periodic table, periodicity. Chemical bonds - ionic bonding - covalent bonding - Coordinate covalent bonding. Overlap of  $\sigma$  and  $\pi$  orbitals – hybridization, resonance, Bond properties, Molecular geometry.

#### Unit 5:

**Introduction to Organic Chemistry:** Carbon and its compounds, Position of Carbon in periodic table, tetra covalency of carbon, functional groups. **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 & Ssystems of nomenclature. **Heteroaromatics:** Five / six membered hetero aromatics and analogues, Nucleic acid bases

### Total: 45 Hrs\*

9 Lectures

## 9 Lectures

9 Lectures

9 Lectures

9 Lectures

#### 18

#### **Text Books:**

- 1. Physics for Scientists and Engineers (6th Ed.) by Raymond A. Serway, John W. Jewett, Thomson Brooks/Cole. 2004
- 2. Fundamental Principles of Physical Chemistry (Prutton, Carl F.; Maron, Samuel H.),1949.
- 3. Organic Chemistry by Morrison and Boyd Sixth Edition. 1992

#### **Reference Books:**

- 1. Physics for Scientists and Engineers by Paul A. Tipler, Gene P. Mosca. Freeman Company. 2007
- 2. Fundamentals of Physics by Resnick, Halliday and Walker. 2013
- 3. Chemistry, The Central Science, 10th edition, Theodore L. Brown; H. Eugene LeMay, Jr.; and Bruce E. Bursten. 2006
- 4. Selected Topics in Inorganic Chemistry, Wahid U. Malik, G. D. Tuli and R.D. Madan .1993
- 5. Chemistry<sup>3</sup> Introducing inorganic, organic and physical chemistry, Andrew Burrows, John Holman, Andrew Parsons, Gwen Pilling, Gareth. 2013
- 6. Organic Chemistry by Paula Yurkanis Bruice, Prentice Hall. 2010 Heterocyclic chemistry at a glance, John A. Joule and Keith Mills.2007

**<u>COURSE OUTCOME</u>**: Students gained the knowledge of concept of fundamental physics and their application s in biology.

#### **CBIO 617 - INTRODUCTORY BIOLOGY**

**<u>COURSE OBJECTIVES</u>**: Biology is the study of organic life, through the complex evolutionary and regulatory processes of cells, organisms, populations, communities, and ecosystems. Students must be comfortable considering the fundamental concepts that weave through these levels of organization.

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

#### Unit I

**Diversity of Life forms:** 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 - Linnaeus) classification.

#### Unit II

**Inheritance biology:** Mendelian principles- Dominance, segregation, independentassortment, Codominance, incomplete dominance, genomic imprinting, linkage and crossing over; extra chromosomal inheritance, microbial genetics, mutations, recombination, structural and numerical alterations of chromosomes.

#### Unit III

**Developmental Biology:** Basic concepts of development, gametogenesis, fertilization and early development, morphogenesis and organogenesis in animals and plants, programmed cell death, aging and senescence.

#### Unit IV

**Ecology & Evolution:** Habitat and niche, population growth curves, Ecosystems stability-species interactions, competition, conservation methods (both in situ and ex situ); Origin of life, theories and evidences.

#### Unit V

**Applied Biology:** Microbial fermentation and production of micro and macro molecules, Tissue and cell culture methods for plants and animals, transgenic animals and plants, Genomics and its application to health and agriculture, Bioremediation and phytoremediation.

#### Text books:

- 1. Concepts of Biology (2<sup>nd</sup> Ed.) by Sylvia S. Mader. McGraw Hill Publishers, 2011.
- Molecular Biology of the cell (4<sup>th</sup> Ed.) by Bruce Alberts. Garland publishing Inc. 2002.
- **3.** Life: The Science of Biology, 10th Edition by David E. Sadava, David M. Hillis, H. Craig Heller and May Berenbaum-2012.

#### **References books:**

- 1. Genetics: A Conceptual Approach 6<sup>th</sup> ed by Benjamin A. Pierce-2017.
- 2. Fundamentals of Ecology Eugene P.ODUM 1971 (Third Edition): W. B. Saunders, Comp. Philadelphia London Toronto.

#### Total: 30 Hrs.\*

6 Lectures

6 Lectures

#### 6 Lectures

6 Lectures

- 3. Developmental biology by Scott F Gilbert (Ninth edition). 2010
- 4. Principles of Gene Manipulation (Seventh Edition) An Introduction to Genetic Engineering By S.B. Primrose, university of California Press. 2006

**<u>COURSE OUTCOME</u>**: The course will ensure to apply a basic core of scientific knowledge to enhance understanding of living organisms and function at the molecular level.

#### **CBIO 653- BIOINFORMATICS AND SEQUENCE ANALYSIS - LAB**

#### **COURSE OBJECTIVES:** To make the students familiarized with the Bioinformatics

databases and their applications

#### Total Credits: 1 Exercises:

- 1. Sequence Databases: EMBOSS, NCBI ToolKit, ExPASy tools
- 2. Search tools against Databases:
  - i. BLAST
  - ii. FASTA
- 3. Pair wise alignment:
  - a. Dot Plot
  - b. Global and Local alignment methods
- 4. Multiple sequence alignment:
  - a. Clustal
  - b. Dialign
  - c. Multalign
- 5. Primary and secondary structure prediction methods
  - a. GOR Method
  - b. PSI-pred
  - c. Chou-Fasman method
- 6. Sequence patterns and profiles:
  - a. generation of sequence profiles
    - i. PSI-BLAST
  - b. derivation of and searching sequence patterns:
    - i. PHI-BLAST
    - ii. SCanProsite
    - iii. PRATT
- 7. Protein motif and domain analysis:
  - a. MEME/MAST
  - b. eMotif
  - c. InterproScan
  - d. ProSite
  - e. ProDom
  - f. Pfam

8. Tools in sequence assembly and annotation

<u>COURSE OUTCOME:</u> Students will understand the information's available in Bioinformatics databases and their applications in research

#### CBIO 657-CELL AND MOLECULAR BIOLOGY – LAB

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

<u>COURSE OBJECTIVES:</u> Students will gain hands on experience of various instruments used in experimental techniques to understand the basic experimental procedures and techniques in cell and molecular biology.

- 1. Microscopic analysis of different stages of mitosis and meosis from onion root tip.
- 2. Enumeration of microbes (bacteria and fungi) from different samples through serial dilution.
- 3. Staining and isolation of the colony of interest from the bacteria and fungus-culture techniques.
- 4. Spore counting using Haemocytometer.
- 5. Estimation of chlorophyll and pigment profiling through Paper chromatography.
- 6. Determination of anti-oxidants by enzymatic methods.
- 7. Isolation, extraction and separation of genomic DNA from plant/fungi samples.
- 8. Restriction digestion of genomic DNA.
- 9. Ligation of DNA fragments.
- 10. Amplification of DNA fragments through PCR and gDNA agarose gel electrophoresis.
- 11. Total proteome extraction and spectrophotometric estimation using Bradford reagent from plant/fungi sample.
- 12. Isolation of total microsomal proteome from the plant/fungi sample.
- 13. Separation and quantification of total and microsomal proteins through SDS-PAGE.
- 14. Spectrometric estimation of the microsomal proteins

**<u>COURSE OUTCOME</u>**: The course will help student to understand about various experimental techniques, usage of laboratory instruments, learn the principles of laboratory usage and its guidelines.

#### **CBIO 656– PROGRAMMING IN C++ and JAVA LAB**

#### **COURSE OBJECTIVES**

To give practical training in writing codes in C++ and JAVA programming languages

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

- 1. Simple C++ programs to demonstrate various decision making and loop constructs.
- 2. Demonstration of switch construct.
- 3. Working with pointers.
- 4. File handling
- 5. Illustration of constructors and destructors.
- 6. Demonstration of scope resolution operator.
- 7. Simple and multiple inheritance
- 8. Simple java programs to demonstrate decision making, and loops.
- 9. Working with Classes and objects in java.
- 10. Interface and abstract class implementation
- 11. Exception handling
- 12. Reading and writing files.
- 13. JDBC, Animation and threads

#### COURSE OUTCOME:

At the end of the course, students will be able to write, compile and run the programs in c++ and JAVA

# **Semester II**

#### 26

#### **CBIO 621 - ALGORITHMS IN COMPUTATIONAL BIOLOGY**

**COURSE OBJECTIVES:** To make the students understand the application of Artificial Intelligence in Biocomputing.

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

#### Unit 1

Unit 2

Unit 3

**DNA computing**: Motivation, DNA structure, processing and computational operations, steps involved in DNA computation, Filtering models: Adleman's experiment, Lipton's solution, Scope and Applications of DNA computing. Search Algorithms: Hill climbing, Simulated annealing:-introduction, Simulated annealing algorithm,

Combinatorial Pattern Matching: Hash Tables, Repeat Finding, Exact Pattern Matching; Genetic Algorithm: Basic Concepts, Reproduction, Cross over, Mutation, Fitness Value, Optimization using GAs; Applications of GA in bioinformatics.

Hidden Markov Model: Markov processes and Markov Models, Hidden Markov Models. Forward and Backward Algorithms, Most probable state path: Viterbi algorithm, Parameter Estimation for HMMs:-Baum-Welch Algorithm, Applications of profile HMMs for multiple alignment of proteins and for finding genes in the DNA.

Unit 4

Support Vector Machines: Introduction, hyperplane separation (maximum and soft margin hyperplanes), linear classifier, Kernel functions, Large Margin Classification, Optimization problem with SVM, Applications of SVM in bioinformatics. Bayesian network: Bayes Theorem, Inference and learning of Bayesian network, BN and Other Probabilistic Models.

#### Unit 5

**Artificial Neural Network:** Historic evolution – Perceptron, characteristics of neural networks terminology, models of neuron Mc Culloch – Pitts model, Perceptron, Adaline model, Basic learning laws, Topology of neural network architecture, single layer ANN, multilayer perceptron, back propagation learning, input - hidden and output layer computation, back propagation algorithm, Applications of ANN.

#### **Text Books:**

- 1. An introduction to bioinformatics algorithms by Neil C. Jones, Pavel Pevzner. MIT Press.2004
- 2. Biological sequence analysis: Probabilistic models of proteins and nucleic acids by Richard Durbin, Eddy, Anders Krogh, 1998
- 3. Algorithms for Molecular Biology by Ron Shamir Lecture, Fall Semester, 2001
- 4. Neural Networks: A Systematic Introduction by Raul Rojas. Springer. 1996

# 9 lectures

## 9 lectures

9 Lectures

## 9 lectures

Total: 45 Hrs\*.

# 9 lectures

5. Artificial Intelligence and Games by Georgios N. Yannakakis and Julian Togelius, Springer 2018

#### **Reference Books:**

1. Bioinformatics: the machine learning approach by Pierre Baldi, Søren Brunak. MIT Press.2001.

2. Bioinformatics: Sequence and Genome Analysis: by David Mount, University of Arizona, Tucson. 2005

3. Fundamentals of natural computing : Basic concepts, Algorithms and Applications, Chapman & Hall / CRC, Taylor & Francis group, 2006

**<u>COURSE OUTCOME</u>**: Students are trained in the application of Artificial Intelligence in Biocomputing.

#### **CBIO 623 – DRUG DISCOVERY AND IPR**

**<u>COURSE OBJECTIVES</u>**: To provide a detailed background about the science behind drug discovery process along with various forms of Intellectual property protection and their importance.

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

#### Unit 1

**Introduction to Drugs:** Drug nomenclature, Routes of drug administration and dosageforms, Principles of Pharmacokinetics and Pharmacodynamics: ADME, Bioavailability of drugs - Lipinski's rule; How drugs work - Drug targets, drug-target interaction and dose- response relationships.

#### Unit 2

**New Drug Discovery & Development:** Overview of new drug discovery, development, cost and time lines. **Target Identification & Validation**. **Lead Discovery**: Rational and irrational approaches - Drug repurposing, Natural products, High-throughput screening (HTS), Combinatorial chemistry and computer aided drug design (CADD).

#### Unit 3

**Preclinical trails of New Drugs**: Pharmacology - In vitro/in vivo Pharmacokinetics and Pharmacodynamics; Toxicology - Acute, chronic, carcinogenicity and reproductive toxicity; Drug formulation. **Clinical Trial of New Drugs**: Phase I, Phase II and Phase III; Good clinical practice (GCP) guidelines - Investigators brochures, Clinical trial protocols and trial design; Ethical issues in clinical trials - How are patient rights protected?

#### Unit 4

**Drug Regulatory Agencies**: US Food & Drug Administration (US FDA) and Central Drugs Standard Control Organization (CDSCO), India. **Regulatory Applications & New Drug Approval**: Investigational new drug (IND) application & New drug application (NDA); Regulatory review and approval process. **Regulatory Requirements for Drug Manufacturing**: Current Good manufacturing practice (cGMP) and GMP manufacturing facility inspection & approval.

#### Unit 5

**Intellectual Property Rights (IPR):** IPR Definition and implications for discovery & development. Forms of IPR Protection - Copyright, Trademark and Patents. International organization and treaties for IPR protection – World Trade Organization (WTO) & Trade Related Aspects of Intellectual Property Rights (TRIPS) Agreements. Importance of IPR in Indian Scenario & Indian laws for IPR protection. **Patents**: National and international agencies for patenting - US Patent & Trademark office (USPTO), Controller General of Patents, Designs & Trade Marks, India (CGPDTM), World Intellectual Property organization(WIPO)-Patent Cooperation Treaty (PCT); Requirements for patentability, Composition of a patent, How to apply and get patents – US, Indian and PCT.

#### Total: 45 Hrs\*

8 Lectures

#### 9 Lectures

#### **10 Lectures**

## 9 Lectures

#### **Text Books:**

- 1. Drugs: From discovery to approval 3<sup>rd</sup> Ed by Rick N.G, Wiley-Blackwell (2015), ISBN-10: 1118907272.
- Intellectual Property: The Law of Trademarks, Copyrights, Patents, and Trade Secrets, 4<sup>th</sup> Ed by Deborah E. Bouchoux, CENGAGE Learning Custom Publishing (2013).

#### **Reference books:**

- 1. Burger's Medicinal Chemistry and Drug discovery. Volume 2, Drug Discovery and development. 7<sup>th</sup> Ed by Donald J. Abraham and David P. Rotella (Eds), Wiley-Interscience (2010), ISBN-10: 0470278153.
- 2. Essentials of Medical Pharmacology, 8<sup>th</sup> Ed by K.D. Tripathi, Publisher: Jaypee Brothers Medical (2018), ISBN-10: 9789352704996.
- 3. Laws of Patents: Concepts and Cases Edited by A. V. Narasimha Rao, The ICFAI University Press (2005).
- 4. Intellectual Property Rights In India: General Issues And Implications by Prankrishna Pal. Publisher: Deep & Deep Publications Pvt. Ltd (2008).

**<u>COURSE OUTCOME</u>**: A detailed knowledge on how drugs work and how they are discovered from bench to bedside. Also students will be aware of the concept and forms of Intellectual property and national/international laws for their protection.

#### **CBIO 624 – GENOMICS AND PROTEOMICS**

**<u>COURSE OBJECTIVES</u>**: To train the students to understand the Role of Pharmacogenomics and Pharmacogenetics in the field of personalized medicine and the role of various data bases related to proteomics and genomics.

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

#### Unit 1

**Genomics**: Large scale genome sequencing strategies. 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, Metagenomics.

#### Unit 2

**Transcriptome Analysis**: Databases 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), RNA Sequencing.

#### Unit 3

**Functional genomics**: Application of sequence based and structure-based approaches to assignment of gene functions – e.g. sequence comparison, structure analysis (especiallyactive 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 4

**Evolution from protein chemistry to proteomics:** The proteomics workflow - Basic of separation sciences: Protein and peptides; Two-dimensional electrophoresis (2-DE), Advancement in solubilization of hydrophobic proteins, development of immobilized pH gradient strips, gel casting, staining of gels and image analysis. Two-dimensionalfluorescence difference in-gel electrophoresis (DIGE), Blue native PAGE (BN-PAGE), gel free proteomics methods.

#### Unit 5

**Quantitative Proteomics:** Protein MS applications – identifying unknown proteins bypeptide mass fingerprinting; de novo sequencing of peptides from fragment ion spectraobtained by tandem MS; Protein arrays: basic principles. Bioinformatics tools for proteomics (SEQUEST, MASCOT etc.).

## 9 Lectures

## 9 Lectures

9 Lectures

## 9 Lectures

30

## Total: 45 Hrs.

#### **Text Books:**

- 1. Discovering Genomics, Proteomics and Bioinformatics 2nd edition by A. Malcolm Campbell and Laurie J. Heyer. by Cold Spring Harbor Laboratory Press 2006.
- 2. Principles of Genome Analysis and Genomics (3rd 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 (1st Ed.) by Liebler, D.C., Humana Press Inc., New Jersey, USA. 2002
- 2. Bioinformatics and Functional Genomics (3rd Ed.) by Pevsner, J., John Wiley and Sons, New Jersey, USA. 2015
- 3. Bioinformatics: Sequence and Genome Analysis (2<sup>nd</sup> Ed.) by Mount, D., Cold Spring Harbor Laboratory Press, New York. 2004

**<u>COURSE OUTCOME</u>**: The subject is designed to impart knowledge on the current state of the art techniques involved in Genomics and Proteomics

#### **CBIO 625-STRUCTURAL BIOLOGY**

<u>COURSE OBJECTIVES</u>: The main objective of this course is to make the students to thorough understanding of structural biology of biological macromolecules

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

#### Unit 1

**Fundamentals of protein structure:** amino acids fundamental building blocks, Peptide bond, rigid planar peptide unit, *cis* and *trans* configuration. **Structural Hierarchy**: Primary, Secondary, Tertiary, Quaternary structures. **Motifs and domains**:  $\alpha$  - domain structures,  $\beta$  - domain structures,  $\alpha$  / $\beta$  (alpha/beta) - structures. **Principles of nucleic acid structure:** Chemical structure of nucleic acids, Watson and Crick's base-pairings and their implications. Non Watson and Crick pairing schemes - base stacking interactions - DNA polymorphism - structure of ADNA, BDNA and ZDNA - helical transitions.

#### Unit 2

**Protein Crystallization**: Principles of protein crystallization, Preparation of crystal for X- ray experiment. **Crystallization techniques**: Batch method, liquid-liquid diffusion method, vapour diffusion method- hanging drop, sitting drop, dialysis. **Seeding Method**-macroseeding, microseeding, other seeding methods.

#### Unit 3

**Elementary crystallography: Introduction**: symmetry in crystals, lattices and unit cells, crystal systems, Bravais lattices, **Elements of symmetry** - rotation axis, mirror planes and center of inversion, proper/ improper axes of rotation, translational symmetry- screw axis and glide planes. **Symmetry operation:** classes of symmetry operations, classification of symmetry point groups and molecular space groups and equivalent points. X-ray diffraction - Laue equations - Bragg's law - reciprocal lattice and its application to geometrical Crystallography.

#### Unit 4

**X-ray scattering:** Atomic scattering factor - diffraction by a space lattice - structure factor equation - electron density and Fourier series - Fourier Transform and crystal diffraction - **Phase Problem** – Direct methods, molecular replacement method, Patterson function, heavy atom method.

#### Unit 5

**Nuclear Magnetic Resonance:** Introduction, Nuclear spin, NMR sensitivity, shielding and deshielding effects of NMR, nuclear Over hauser effect. Spectral parameters: chemical shift, spin-spin splitting, coupling, non-equivalent proton. Carbon-13 NMR spectra of protein, FTNMR, spin-spin splitting, proton spin decoupling, off-resonance decoupling, Spin-lattice relaxation time. Multidimensional NMR, COSY, NOSEY, MRI, ESR. Application of NMR to biology- Regulation of DNA transcription, Protein-DNA interaction.

#### **Text Books:**

- 1. Introduction to protein structure, C. Branden and J. Tooze.1999
- 2. X-Ray Structure Determination: A Practical Guide, 2nd Edition, by George H. Stout, Lyle H. Jensen.1989.

#### Total: 45 Hrs\*

**10 Lectures** 

#### **9 Lectures** stal for X- ra

9 Lectures

## 8 Lectures

3. Principles of Protein Structure by G. E. Schulz., Springer 2009

#### **Reference Books:**

- 1. Structural Bioinformatics, Philip E. Bourne, Helge Weissig, Wiley Publication.2009
- 2. Crystallization of Biological Macromolecules, A. McPherson, Cold Spring Harbor Laboratory Press.1999.

**<u>COURSE OUTCOME:</u>** Students gained the knowledge of structural biology of biological macromolecules.

## **CBIO-631- PYTHON PROGRAMMING**

**COURSE OBJECTIVES:** To introduce the effectiveness of scripting language concepts with biological applications.

Total Credits: 3

#### UNIT 1

Introduction and Control structure: A brief history of python – Unique features –Installation of Python and IDE - Lexical structure of python – Introduction of variables and data types with examples. Introduction to python interpreter and interactive mode -Statement Read and Print commands – Evaluating expressions

#### Unit 2

Functions and Regular expressions: Defining and Calling a function - Fruitful functions (return value, parameters, local and global scope, function composition, recursion) - Examples in sequence analysis using function - Introduction to Modules. Regular Expression: Importance of patterns in biology - String manipulation using regular expressions (Extraction, splitting and matching).

#### UNIT 3

Lists, Tuples and Dictionaries: Introduction to Lists – List slicing – Finding items in Lists with operator - Copying and Processing Lists - List built-in methods - Two Dimensional lists. Tuples: Basic tuple operations - creation, concatenation, repetition, slicing, immutable and deletion. Dictionaries: creation, accessing and processing - Dictionary methods.

#### UNIT 4

Files and Exception Handling: File objects - File built-in methods and attributes - Reading and writing files - command line arguments. Exception Handling: Errors and exceptions, Detecting and Handling Exceptions.

#### **UNIT-5**

Python libraries and Biopython: using standard modules and creating a new module. Introduction to Biopython, installation, important components like seq, seqIO, alignIO, etc. Working with biological data. **RDKit in python**- general molecular functionality- drawing small molecules and other major applications in drug designing.

#### **Text Books:**

- 1. Michael T Goodrich, Micheal S Goldwasser and RoberttoThamassia, 2016. Data Structures and Algorithms in Python. Wiley Publisher.
- 2. Martin Jones. 2013. Python for Biologist A programming course for complete beginners. http://pythonforbiologists.com.
- 3. Kenneth A. Lambert. 2011. Fundamentals of Python: First Programs. CENGAGE Learning.(ISBN: 978-1111822705).
- Guido van Rossum and Fred L. Drake Jr. 2011. An Introduction to Python Revised 4. and updated for Python 3.2, Network Theory Ltd.

#### 8 lectures

**10 lectures** 

#### 9 lectures

9 lectures

## 9 lectures

Total: 45 Hrs\*.

#### **Reference Books:**

- 1. Leonard Eddison. 2018. Python Machine Learning, A Guide for Beginners. 2<sup>nd</sup>Edition. Kindle Edition.
- 2. Timothy A. Budd. 2011. Exploring Python. 1<sup>st</sup> Edition. Mc-Graw Hill Education (India) Private Ltd.
- 3. https://www.rdkit.org/docs/GettingStartedInPython.html
- 4. Martin C. Brown. 2001. Python The Complete Reference. Osbome/McGraw-Hill Companies

<u>COURSE OUTCOME</u>: To understand the pros and cons on scripting languages vs. classical programming languages (at a high level) and able to write script in python language for sequence, statistical data manipulation and analysis.

#### **CBIO 630 - MATHEMATICS FOR BIOSCIENCES**

**COURSE OBJECTIVES:** The objective of this course is to impart knowledge on the application of Mathematics in the field of Computational Biology

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

Unit 1 Limits and Differentiation: Limits of Functions, Continuity of Functions; Basics of Differentiation-Differentiability, Derivatives, Interpretations of Derivatives, General Rules of Differentiations.

#### Unit 2

Integration: Review of Definite Integrals, Double (Surface) Integrals - Definition, Iterated Integrals (Fubini's Theorem), Properties; Triple (Volume) Integrals- Definition, Properties, Geometric Interpretation of Double and Triple Integrals.

#### Unit 3

Differential Equation: Ordinary Differential Equation- Definitions, Order and Degree; Equations of the first order and first degree:Variables separable, Homogeneous equations, Linear equations, Bernoulli's equation and Exact equations.

#### Unit 4

Linear Differential Equations: Definitions, Complete solution, Opeator D, Rules of finding Complementary function, Inverse operator, Rules of finding particular integral, Procedure to solve the equations.

#### Unit5

Introduction to Laplace and Fourier Transform: Definition of Laplace Transform, Elementary Functions and their Laplace Transforms, Piecewise Continuity, Sufficient Conditions for Existence and Important Properties of Laplace Transform, Convolution of Laplace Transform, Inverse Laplace Transform. Definition of Fourier Series, Fourier Transform, Fourier Transform Properties, Fourier Transforms-The convolution theorem and its applications.

#### **Text Books:**

1. Fundamentals of University Mathematics (3<sup>rd</sup> Ed.), Colin McGregor, Woodhead Publishing in Mathematics, 2010.

2. Introduction to Mathematics for Life Scientists, Edward Batschelet, Springer, 1979.

#### **Reference Books :**

- 1. Higher Engineering Mathematics (40th Ed), B.S. Grewal and J.S. Grewal, Khanna Publishers, 2007.
- 2. Mathematical Techniques (4<sup>th</sup> Edition), Jordan & Smith, Oxford University Press, 2008
- 3. Fourier and Laplace Transforms, RJ Beerends and JC van den Berg, Cambridge University Press, 2012

**COURSE OUTCOME:** After completion of this course, it is expected that the student will be able to implement different mathematical methods to analyze complex biological system.

#### 9 Lectures

Total: 45 Hrs.\*

# 8 Lectures

9 Lectures

#### **10 Lectures**

## Unit 1

**Total Credits: 2** 

analyze the huge data set.

**Fundamentals of Big Data:** Overview of Big Data, Evolution of Big data - Best Practices for Big data Analytics - Big data characteristics - Validating - The Promotion of the Value of Big Data - Big Data Use Cases.

## Unit 2

**Understanding of Big Data** - Characteristics of Big Data - Four V's, Basic operations of in big data, Datasets, Data Analytics, different data types of big data, Awareness of Architecture.

## Unit 3

**Data Analytics with R:** R basics, Data Types, Data Structure: Vectors and Factors, Vector operations, Arrays & Matrices, Lists, and Dataframes. Conditions and loops, Handling Files, Data visualization, Regression Analysis and Correlation analysis.

#### Unit 4

**Big Data Tools**: Big Data–Platforms, Big Data with Hadoop, Introduction to Hadoop, Hadoop ecosystem, Hadoop components: HDFS - MapReduce - Pig - Hive, Handling files, Data Analysis.

#### Unit 5

**HDFS**: Architecture, Components: Namenode, file system, Data Node, Secondary Namenode. Replication Management, Rack Awareness, Handling files in HDFS, Case Studies.

#### **Text Books**

 Big Data Fundamentals, Concepts, Drivers & Techniques Concepts, Drivers & Techniques by Thomas Erl, Wajid Khattak, and Paul Buhler, PRENTICE HALL, 2012.
Analytics in a Big Data World: The Essential Guide to Data Science and its Applications (WILEY Big Data Series) – Bart Baysen, 2014

#### **Reference Books**

 Big Data Now, O'Reilly Radar, O'Reilly Media, 2012
Big Data for Dummies, Wiley, Judith Hurwitz, Alan Nugent, Fern Halper, Marcia Kaufman, 2012
<u>COURSE OUTCOME:</u> Able to analyze the data using R language. Able to work in NO SQL databases. Able to find hidden patterns in Big data

## 6 lectures

#### 6 lectures

6 lectures

37

## **CBIO 628- BIG DATA ANALYTICS**

**COURSE OBJECTIVES:** To understand R language, Big data tools and commands to

# Total: 30 Hrs\*.

**6** lectures

# 6 lectures

## followed by a Q&A sessions). **Text Books:**

- 1. Bioethics and Biosafety in Biotechnology by Sree Krishna V., New Age International (P) Ltd., Publ., Mumbai. 2007
- 2. Scientific Writing: Easy When You Know How by Jennifer Peat, BMJ books. 2002
- 3. Successful Scientific Writing: A step-by-step Guide for Biomedical Scientists (3<sup>rd</sup> Ed.) by J.R. Matthews and R.W. Matthews, Cambridge University Press. 2008

#### **References:**

- 1. Rules for manufacture, use/import/export and storage of hazardous microorganisms or cells Act. 1989.
- 2. From Research to Manuscript: A Guide to Scientific Writing by Michael Jay Katz, by Springer. 2006

#### **CBIO 629 – BIOETHICS AND RESEARCH METHODOLOGY**

**COURSE OBJECTIVES:** To provide overview of how to identify research problem and *conduct research ethically* 

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

Unit 1 8 Lectures Regulatory Procedures for research and manufacturing of biotechnology products: Good laboratory practice, Good manufacturing practice and National and International regulations -Regulations for recombinant DNA research and manufacturing process - Bio-safety and Bioethics -Regulations for clinical trials, Documentation and Compliance, in India and selected countries - Rules for import and export of biological materials.

#### Unit 2

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

#### Unit 3

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

#### Unit 4

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

poster- Individual Poster presentation (Students select a research project/topic and prepare posters

#### Unit 5

#### **5** Lectures **Poster Presentation** – Elements and Significance of poster presentations- Planning and designing a

6 Lectures

Total: 30 Hrs\*.

#### 5 Lectures

- 3. Writing and Presenting Scientific Papers, 2<sup>nd</sup> Edition by Brigitta Malmfors, Phil Garnsworthy and Michel Grossman, Nottingham University Press, 2004, Viva Books Pvt. Ltd. 2011
- 4. Scientific Writing- A Reader and Writer's Guide, by Jean Luc- Lebrun, World Scientific Publishers, 2007

**<u>COURSE OUTCOME</u>**: Students can understand the basics of how to design, conduct research, analyze and communicate the results to research community. Also team work ethos and stress management strategies would help to cope-up with their day-to-day life in a competitive world.

## **CBIO 724 - NEXT GENERATION SEQUENCING USING R**

**<u>COURSE OBJECTIVES</u>**: The main goal of this course is to help students in learning the various next-generation sequencing platforms and computational methods involved in the reference-based and de novo assembly of short reads for genome mapping and gene expression analysis.

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

#### Unit 1

**NGS Platforms:** Introduction to NGS, Second-generation DNA sequencing: Pyrosequencing, Reversible Dye-Terminator Sequencing, Emulsion PCR approach with small magnetic beads, Ion semiconductor sequencing, Ion torrent, Third-generation DNA sequencing: Single molecule real time (SMRT) sequencing, Fourth-generation nanopore- based sequencing.

#### Unit 2

**Genome assembly algorithms:** Alignment of short-reads to reference genome using spaced seed (ELAND, SOAP), FM-index (Bowtie, BWA, SOAP2), and suffix tree (MUMmer). Sequence Alignment formats: Sequence Alignment/Map (SAM) format, Binary Alignment/Map (BAM) format, Tools for conversion (SAMtools), Alignment viewers (IGV, MGAviewer).

#### Unit 3

**De-novo assemblies:** Overlap-layout-consensus (OLC) approach (Arachne, Phusion), de Bruijn and Euler path approach (Euler, SOAPdenovo), string graph assembler (SGA). Scaffolding: Supercontig, contig orientation, contig ordering, contig distancing and gap closing.

#### Unit 4

**Big Data and R language in NGS analysis:** Elements of Big data and R, Introduction to Bioconductor, Reading of RNA-seq data (ShortRead, Rsamtools, GenomicRanges), annotation (biomaRt, genomeIntervals), reads coverage and assign counts (IRanges, GenomicFeatures), differential expression (DESeq).

#### Unit-V

**Biological applications of NGS:** Whole-genome sequencing, Exome sequencing, Transcriptome sequencing, DNA-Protein Interactions (CHIP-Seq), Epigenomics and DNA methylation analysis, Metagenome analysis.

#### **Text Books:**

1. Next-generation DNA sequencing Informatics by Stuart M. Brown, Cold Spring Harbor Laboratory, 2013.

2. Big Data Analysis for Bioinformatics and Biomedical Discoveries by Shui Quing Ye. Chapman and Hall/<u>CRC Press</u>, 2016.

#### **Reference Books:**

1. Next generation sequencing: Translation to Clinical Diagnostics by Wong Lee-Jun C. (ed.), Springer, 2013.

2. Next-generation genome sequencing: Towards Personalized Medicine by Michal Janitz,

## Total: 30 Hrs\*.

## 6 Lectures

#### 6 Lectures

# 6 Lectures

6 Lectures

Wiley-VCH, 2008

3. Network Medicine: Complex Systems in Human Disease and Therapeutics by Joseph Loscalzo, Albert-Laszlo Barabasi, and Edwin K. Silverman, 2017, Harvard University Press.

**<u>COURSE OUTCOME</u>**: The student will have an understanding of different generations of sequencing platforms. He/she will be able to analyse and assemble the short reads using different reference-based methods and de novo assembly methods especially in the R environment.

#### CBIO 654 – STRUCTURAL BIOLOGY – LAB

**<u>COURSE OBJECTIVE</u>**: to train the students both dry and wet lab techniques in structural biology

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

- 1. Learning the protein folding problem :
  - 1. Denature and re-nature the protein chromatography
  - 2. UV study of denatured and renatured proteins
  - 3. IR study of amide bond stretching
- 4. Secondary structure analysis :
  - 1. In silico tools
  - 2. CD study of protein
- 5. Torsion angle calculation. Model the protein from given torsion angle
- 6. DNA melting point and intercalation study
- 7. Purification of protein from tissue or milk
- 8. Crystallization of lysozyme
- 9. Structure solution using molecular replacement CCP4 suit
- 10. Structure based alignment and structural Blast VAST, DALI
- 11. Exploration of PDB tools

**<u>COURSE OUTCOME</u>**: students gain the knowledge of both dry and wet lab techniques in structural biology

#### **CBIO632-PYTHON PROGRAMMING LABORATORY**

#### **Course Objectives:**

- To make students aware of the role of python programing in proteomics and genomics to understand the relevance of multidisciplinary research
- To equip the students with the fundamental concepts of python programing and understand the implementation of Bio-libraires in computer aided drug designing

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

- 1. Installation of Python and IDE
- 2. Variables and data types
- 3. Statement read and print commands
- 4. Boolean logic, statements blocks and conditional statement
- 5. Conditional loop statement
- 6. Regular expression
- 7. List, Tuple, Dictionaries
- 8. Read a file and write to a File in python
- 9. Exception handling
- 10. Bio-python libraries
- 11. RDKit
- 12. Chemical structure analysis
- 13. Python in computer aided drug designing

#### **COURSE OUTCOME:**

Students will be able to

Apply their knowledge of Python in Biological and health sciences create simple python program and implement biopython libraries Asses various basic programming applications for multidisciplinary research domains

# **Semester III**

#### **CBIO 711 - BIOMOLECULAR SIMULATIONS**

**COURSE OBJECTIVES:** To make the students understand the principles of Molecular Modeling, Dynamics and Drug design.

#### **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, TruncatedLennardjones, 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 and optimization techniques: Convergence Criteria, Characterizing Stationary Points, Search for Transition States. Optimization:- multivariable Optimization Algorithms, 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, Time Integrators- Leapfrog and Verlet algorithm, Potential truncation and shifted-force potentials, Implicit and explicit Solvation models, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations .(discuss with expert)

#### Unit 4

Computer-aided drug Design (CADD): Structure based drug design - Homology modeling - Prediction of 3D structure of proteins (Template identification, alignment, Backbone generation, Loop modeling, Side-chain modelling) and validation of structure for use in docking. Basis of Docking (pose prediction and scoring algorithms) and its application in lead identification and optimization, De Novo Drug Design concepts (Fragment Placements, Connection Methods, Sequential Grow) and application. Virtual screening strategies for lead identification.

#### Unit 5

Computer-aided drug Design (CADD): Ligand based drug design - Chemoinformatics analysis of large database of ligands using similarity, rule of five and sub-structure based methods. Pharmacophore generation (3D database searching, conformation searches, deriving and using 3D Pharmacophore, constrained systematic search, Genetic Algorithm, clique detection techniques, maximum likelihood method) and application for virtual screening. Introduction to QSAR, descriptors used in QSAR study, model building, model validation methods and applications.

## 45

#### 9 Lectures

#### 9 Lectures

## 9 Lectures

9 Lectures

Total: 45Hrs\*.

#### **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
- 3. Computational Drug Design: A Guide for Computational and Medicinal Chemists, by David C. Young, Wiley, 2009.

#### **Reference Books:**

- 1. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe, John Wiley & Sons Ltd. 2008
- 2. Molecular Modeling and Simulation An interdisciplinary Guide by Tamar Schlick, Springer-Verlag. 2000
- 3. Computational medicinal chemistry for drug discovery edited by Patrick Bultinck, Hans De Winter, Wilfried Langenaeker, Jan P. Tollenare, CRC press, 2003
- 4. The art of molecular dynamics simulation, second edition by D. C. Rapaport, Cambridge University Press, 2004
- 5. Homology Modeling Methods and Protocols by Andrew J.W. Orry., University of California, USA.2012.

**<u>COURSE OUTCOME</u>**: Students are trained to understand the theories behind macromolecular simulations and also to perform research work in the area of computational drug design.

## CBIO 712 SYSTEMS BIOLOGY

**COURSE OBJECTIVES:** The main goal of this course is to help students in learning the fundamental concepts of network biology and computational methods involved in the computational modelling of the biological systems.

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

#### Unit-I

Networks and graph theory: Basic properties of biological networks: Degree, average degree and degree distribution. Adjacency matrix, weighted and unweighted networks, Bipartite network, Paths and distances.

#### Unit-II

Random Networks: Erdos-Renyi model, Small-world effect, clustering coefficient. Scalefree networks: Power laws, Hubs, ultra-small property, degree exponent, The Barabasi-Albert Model. Degree correlations: assortativity and disassortativity.

#### **Unit-III**

Biological networks: Complex Biological Systems, Types of Biological networks, Intracellular networks: Gene-regulatory network, Protein-interaction network, Metabolic networks and Signalling network; Inter-cellular networks: Neuronal networks, Network motifs, Computational medicine.

#### Unit-IV

Modularity: Motifs and sub-graphs, Feed-forward loops, Single-input modules: LIFO, FIFO. Dense overlapping regulons (DORs). Optimal gene design circuits: fitness function and optimal expression of a protein in bacteria, Robustness of complex systems.

#### Unit-V

**Constraint-based modelling** – Metabolic reconstruction, Flux Balance Analysis (FBA): Translating biochemical networks into linear algebra, Stoichiometric matrix, Elementarymode, Extreme pathways, Objective function, Optimization using linear programming. Genome-scale cellular models: Virtual Erythrocytes, Global human metabolic model (Recon 3D).

#### Text Books:

- 1. Networks: An Introduction by M.E.J. Newman, Oxford University Press, 2010.
- 2. Introduction to Systems Biology: Design Principles of Biological Circuits by Uri Alon, Chapman & Hall/CRC, 2007.

# Total: 45 Hrs\*.

### 8 Lectures

8 Lectures

#### **10 Lectures**

9Lectures

#### **Reference Books:**

- 1. Introduction to Systems Biology, S. Choi, Humana Press, 2007.
- Linked The New Science of Networks, Albert-László Barabási, Perseus Publishing, 2002.
- 3. Systems and Synthetic Biology by Vikram Singh and Pavan K. Dhar, 2014, Springer.

**<u>COURSE OUTCOME</u>**: The student will have a system-level understanding of the biological systems. He/she will be able to develop and analyse the properties of in silico models of genegene interactions and protein-protein interactions.

#### **CBIO 713-DATA MINING AND DATA WAREHOUSING**

**<u>COURSE OBJECTIVES</u>**: To provide an understanding of the concepts of data warehousing and to explain the data mining tasks and to study different data mining techniques in the diverse intelligent systems.

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

#### Unit 1

**Introduction:** Need for data warehouse, definition, goals of data warehouse, Data Mart, Data warehouse architecture, extract and load process, clean and transform data, Designing fact tables, partitioning, Data warehouse and OLAP technology.

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

#### Unit 3

**Concept Description and Association Rules:** Concept Description, Characterization and comparison, Data Generalization and Summarization - Analytical Characterization, Mining Class Comparisons, Association Rule Mining, Mining Association Rules in Large Databases, Mining Single-Dimensional Boolean Association Rules from Transactional Databases, Mining descriptive statistical measures in large data bases, multidimensional association rules from relational DBS and DWS, Correlation analysis, Constraint based association mining.

#### Unit 4

**Classification and Prediction Issues:** Data preparation for classification and Prediction, Comparing classification Methods, Classification by Decision Tree Induction, Back propagation, Bayesian classification.

#### 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, 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

- 2. Building Data Ware House by W.H.Inmon, John Wiley & Sons. 2005
- 3. Data warehousing by S. Anahory and D.Murray, Pearson Education, ASIA.1997.

#### Total: 45 Hrs\*.

#### 9 lectures

#### 9 lectures

#### 9 lectures

9 lectures

9 lectures

#### **Reference Books:**

**1.** SumeetDua, Pradeep Chowriappa. 2012. Data Mining for Bioinformatics. First edition. CRC Press. ISBN 9780849328015.

**2.** Jiawei Hen, Micheline Kambler, 2006, Data Mining Concepts and Techniques –, Academic Press Morgan Kaufman Publishers.

**3.** Yonghua Cen and Yanchang Zhao, 2013, Data Mining Applications with R, Academic Press, ISBN: 9780124115118.

<u>COURSE OUTCOME</u>: Able to describe the concepts, benefits, of architectures and main components of a data warehouse. Compare and evaluate different data mining techniques. . Inculcated the research interest to apply data mining techniques on biological data.

#### Unit 2

Overview of metabolism, high energy compounds, the reactions of glycolysis, fermentation, control of glycolysis. The pentose phosphate pathway, gluconeogenesis, glycogen breakdown and synthesis, control of glycogen metabolism. Citric acid cycle: enzymes of the citric acid cycle, regulation of the citric acid cycle.

#### Unit 3

Protein metabolism: amino acid deamination, the urea cycle, breakdown of amino acids, amino acid biosynthesis. Fatty acid metabolism Lipid digestion, adsorption and transport, fatty acid oxidation, ketone bodies, Nucleic acid metabolism: Synthesis of purineribonucleotides, synthesis of pyrimidiine ribonucleotides, formation of deoxyribonucleotides.

#### Unit 4

Introduction to Immunology: Innate and acquired immunity, active and passive immunity, natural and artificial immunity and humoral. Lymphoid system- primary or secondary organ. Antibody generation: structure and function -clonal selection theory-different types of immunoglobulins, antibody diversity. Complement system- activation, pathways and biological effects. Major Histochemical molecules/peptide complexes- Structure and Function. Antigen and antibody reaction/interaction: Precipitation, Haemagglutination, direct and indirect immunofluorescence.

#### Unit 5

Vaccine development and Immunoinformatics: hybridoma technology for mass production. Chimeric antibodies, antibody engineering; large scale manufacture of antibodies. Recombinant vaccines, combined vaccines, polyvalent vaccines. Immunoinformatics, databases in immunology, DNA, Plant and protein based recombinant antigens as vaccines.

#### **Text books:**

- 1. Biochemistry by Voet and Voet. Wiley. 2011
- 2. Text book of Immunology by Kuby, 2008

#### **Reference Books:**

- 1. Principles of Biochemistry by Nelson and Cox, Lehninger. W H Freeman & Co. 2009
- 2. Biochemistry by Berg, Tymoczko & Stryer. W.H.Freeman and Co New York. 2007
- 3. Text book of Immunology by Riott, 2006

#### **CBIO 714 - METABOLISM AND IMMUNOLOGY**

**<u>COURSE OBJECTIVES:</u>** To provide an overview of cellular metabolism, organization of metabolic networks and to understand the basic concepts in Immunology and also techniques used in Immunology

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

Unit 1

Basic enzymology: Enzyme nomenclature and classification of enzymes according to I.U.B. Convention, General properties of enzymes. Enzyme kinetics, Michales-Menten, Lineweavar Burk, Factors effect Enzyme activity, Enzyme Inhibition, allosteric enzymes.

## 9 Lectures

9 lectures

Total: 45 Hrs.\*

9 Lectures

#### 9 Lectures

#### 9 Lectures

#### 51

**<u>COURSE OUTCOME</u>**: Students will learn the basics of immune-surveillance mechanisms by both humoral and cell mediated immunity at molecular and cellular level. Students will also acquire knowledge on immunological techniques, immunotherapy, different regulatory mechanisms in metabolic pathways, the key regulatory points in metabolic pathways and molecular mechanisms underlying major inherited diseases of metabolism

#### 53

#### **CBIO 715 - BIOPHYSICAL TECHNIQUES**

**COURSE OBJECTIVES:** To train and understand the students in the concept of biophysical techniques applied in biology.

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

#### Unit 1

Introduction to Spectroscopy: Basic principles, instrumentation and applications of UV- VIS absorption, infrared, Raman, fluorescence spectroscopy.

#### Unit 2

Application of Spectroscopy to macromolecules: Amino acid, Protein absorption at UV spectra, DNA absorption spectrum, Protein-DNA interaction study using UV spectra. CD and ORD introduction, linear and circular Dichroism for biological molecules, secondary structure prediction using CD. NMR application to macromolecules. Mass spectroscopy and application to macromolecules.

#### Unit 3

Scattering from Solutions of Macromolecules: Principles of light scattering, Rayleigh scattering, scattering from particles comparable to wavelength of radiation, static light scattering, dynamic light scattering, low angle X-ray scattering. Small angle X-ray.

#### Unit 4

Separation techniques: Chromatography- column chromatography, TLC. paper chromatography, adsorption chromatography, partition chromatography, Gas liquid chromatography, Ion exchange chromatography, Molecular exclusion chromatography, affinity chromatography, Hydrophobic interaction chromatography. Electrophoresis: Moving boundary electrophoresis, zone electrophoresis, low voltage electrophoresis, high voltage electrophoresis, gel electrophoresis, SDS, Isoelectric focusing, continuous flow electrophoresis, capillary electrophoresis in DNA sequencing. Centrifugation, Ultra centrifugation.

#### Unit 5

Membrane Biophysics and Neurobiophysics: Membrane Constituents: Review of chemistry and biochemistry of constituents of membranes - lipids, phospholipids, lipoproteins, models of membrane structure. Nervous System: Organization of the nervous system -Membrane potentials - origins of membrane potential - electrochemical potentials - Donnan equilibrium - Nernst equation - Goldman equation.

#### **Text Books:**

- 1. Principles of Biochemistry by Nelson and Cox, Lehninger. W H Freeman & Co. 2009
- 2. Biophysics, V. Pattabhi, N. Gautham, 2002, Narosa Publishing House

#### **Reference Books:**

- 1. Guide to protein purification, 2<sup>nd</sup> edition, Methods in enzymology V463, JN. Abelson and Melvin I. Simon. 2006
- 2. Spectroscopy for the biological sciences, Gordon G. Hammes, John Wiley & Sons, Inc., Publication. 2005
- 3. Introduction to biological membrane, Second Edition, Jain RK. 2016
- Biomembrane structure and function, Chapman D. 1983 4.

**6** Lectures

**6** Lectures

#### **6Lectures**

#### 6 Lectures

**6** Lectures

Total: 30 Hrs\*

**<u>COURSE OUTCOME:</u>** Students gained the knowledge of biophysical methods applied in biology.

#### 55

#### **CBIO 716 - PERL PROGRAMMING FOR BIOLOGISTS**

**COURSE OBJECTIVES:** To provide an introduction to Perl programming, CGI and Bioperl modules for designing tools related to biological data handling

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

Unit 1 Perl Basic Data types: Scalar Variables, Scalar Operations and Functions, Array Variables, Literal Representation of an Array, Array Operations and Functions, Scalar and List Context, Hash Variables, Literal Representation of a Hash, Hash Functions.

#### Unit 2

Perl Regular Expression: Concepts on Regular Expressions, Uses of Regular Expressions in biological data handling, metacharacters, quantifiers, Pattern-matching, Substitutions, Transliteration, Split and join functions.

#### Unit 3

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

#### Unit 4

Common Gateway Interface (CGI): Introduction to HTML and its tags, The CGI.pm Module, CGI program in Context, Simple CGI programs, Passing Parameters via CGI, Perl and the Web, User interface design for sequence manipulation.

#### 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, Databases- Database Classes, Accessing a Local Database.

#### **Text Books**

1. Mastering Perl for Bioinformatics (1<sup>st</sup> Ed.), J. Tisdall, O'Reilly, 2010

2. Mastering Perl: Creating Professional Programs with Perl (2<sup>nd</sup> Ed.), Brian d foy, O'Reilly, 2014

#### **Reference Books**

1. Programming Perl (3rd Ed), L.Wall, T. Christiansen and J. Orwant, O'Reilly, 2007

2. Beginning Perl for Bioinformatics (1st Ed.), J. Tisdall, O'Reilly, 2004

#### **COURSE OUTCOME**

Have good knowledge about the syntax and structure of Perl language *Able to write Perl codes to develop bioinformatics toolkit for internet computing* 

# 6 Lectures

Total: 30 Hrs.\*

## 6 Lectures

6 Lectures

## 6 Lectures

#### CBIO - 751 PROJECT (PHASE - I)

**COURSE OBJECTIVE:** To enable the students to identify a research problem, perform review of literature, plan a study to address the same and frame a research proposal and defend the same.

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

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) preliminary report should be submitted and presentation for evaluation.

#### **COURSE OUTCOME:**

The students will learn to -

• Identify research gaps through study of scientific literature and device ways to address the same.

• Write a Project Proposal along with a Literature Review.

• Gain the experience of presenting a research proposal before an evaluating committee.

#### **CBIO 752 - BIO-MOLECULAR SIMULATIONS – LAB**

**<u>COURSE OBJECTIVES</u>**: To train the students in molecular Modelling, Dynamics and Drug design approaches.

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

#### Exercises

1. Molecular Visualization: PYMOL and Chimera

- Pdb file format and Parsing
- Visualizing a molecule in different representations
- Identifying interacting residues (protein and ligand interactions)
- Measuring distances between atoms
- B-factor visualization
- Image tracing and preparation
- 2. Small Molecule sketching using Marvin sketch and bond optimization in 2D & 3D format
  - SDF, MOL2 file formats

3. Geometry Optimization using SwissPdb Viewer

- Energy Minimization of protein molecule
- Determining Maxima and Minima energy points
- 4. Homology modeling of protein 3D structure
  - Model building using Modeller
  - Model validation

#### 5. Binding Site Identification

- Different approaches for binding site identification
- Tools Cast-P, POCASA, 3D ligand site, Metapocket, Ghecom
- 6. Structure based Drug design
  - Molecular docking using AutoDock
  - Virtual Screening using AutoDock Vina
- 7. Molecular Dynamics Simulation
  - Protein dynamics using Gromacs
  - Protein-ligand complex MD simulation

**<u>COURSE OUTCOME</u>**: Students will be skilled to perform macromolecular simulations and drug design, which will be useful for their research/project work.

#### CBIO 753 - DATA MINING AND DATA WAREHOUSING -LAB

**COURSE OBJECTIVES:** Implementation of various data mining tools and tests the real data sets using popular data mining tools such as WEKA

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

#### Exercises :

- 1. Demonstration of Data mining tools: Weka, Tanagra, Rapid miner, Keel, Orange
- 2. Introduction, Data pre-processing on dataset
- 3. Association rule process on dataset using apriori algorithm
- 4. Classification rule process on dataset using j48 algorithm
- 5. Classification rule process on dataset using id3 algorithm
- 6. Classification rule process on dataset using naïve bayes algorithm
- 7. Clustering rule process on dataset using simple k-means

#### **CBIO 754 - PERL PROGRAMMING FOR BIOLOGISTS -LAB**

<u>COURSE OBJECTIVES</u>: To practice and implement perl data structures, control statements, file & database access and bio-perl modules for sequence manipulations and database handling

#### **Total Credit: 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

#### COURSE OUTCOME

Able to design tools and web pages for various biological applications

# **Semester IV**

# **CBIO 721 – GENETIC ENGINEERING**

**COURSE OBJECTIVES**: To provide understanding of genetic manipulation and gene transfer in addition to providing insights into its success in living systems.

## **Total Credits: 2**

#### Unit 1

Scope of Genetic Engineering, Milestones in Genetic Engineering, Genetic engineering guidelines, Regulatory Procedures: Good laboratory practice, Good manufacturing practice and FDA regulations - Regulations for recombinant DNA research and manufacturing process -Bio-safety and Bioethics.

#### Unit 2

Nucleic Acid cloning and amplification methods: Molecular Tools in genetic engineering: Restriction enzymes, Restriction Map Construction. Ligases, S1 nuclease, terminal deoxynucleotides, transferases, polymerases, Reverse Transcriptase and Alkaline phosphatase. Gene Cloning Vectors- Plasmids, bacteriophages, phagemids, cosmids, artificial chromosomes. Ligation - transformation methods, Gene amplification: Polymerase chain reaction, Primers, Real Time PCR and applications.

#### Unit 3

cDNA Synthesis and cDNA library preparations: Cloning mRNA enrichment, reverse transcription, Linkers, adaptors, Library construction and screening. Alternative Strategies of Gene Cloning Cloning interacting genes- screening for genes of interest – Labeling of DNA: Nick translation, Random priming, Radioactive and non- radioactive probes, Hybridization techniques: Northern, Southern and Colony hybridization, Fluorescence in situ hybridization.

#### Unit 4

Gene Regulation methods: S1 mapping, RNase protection assay, Reporter assays. Transgenic and Gene Knockout Technologies including CRISPR Cas, Targeted gene replacement, Strategies of gene delivery, gene regulation silencing and transcription factors.

#### Unit 5

Expression Strategies for Heterologous Genes, Vector engineering and codon optimization, host engineering, In-vitro transcription and translation, expression in bacteria, expression in Yeast, expression in insects and insect cells, expression in mammalian cells, expression in plants. Processing of Recombinant Proteins Purification, Characterization of recombinant proteins. Transgenic plants, genetically modified organisms (GMO) and GM food.

#### **Text Books:**

- 1. Lewin's GENES XI by Jocelyn E. Krebs, Elliott S. Goldstein and Stephen T. Kilpatrick (Dec 31, 2012)
- 2. DNA Cloning- a Practical Approach, .M. Glover and B.D. Hames, IRL Press, Oxford, 1st edition, 1995

# Total:30 Hrs\*

#### 6 Lectures

# 6 Lectures

6 Lectures

#### 6 Lectures

#### **Reference Books:**

- 1. Molecular and Cellular Methods in Biology and Medicine, P.B. Kaufman, W. Wu. D. Kim and L.J; Cseke, CRC Press, Florida, 6<sup>th</sup> edition,2006.
- 2. Molecular Cloning, a Laboratory Manual, J. Sambrook, E.F. Fritsch and T. Maniatis, Cold Spring Harbor Laboratory Press, New York. 1<sup>st</sup> Edition-2000
- 3. Methods in Enzymology vol. 152, *Guide to Molecular Cloning Techniques*, S.L. Berger and A.R. Kimmel, Academic Press, Inc. San Diego, 2<sup>nd</sup> edition,1998,
- 4. DNA Science. A First Course in Recombinant Technology, D,A. Mickloss and G.A. Froyer. Cold Spring Harbor Laboratory Press, New York, 1<sup>st</sup> edition, 1990.
- Molecular Biotechnology, S.B. Primrose. Blackwell Scientific Publishers, Oxford, 2<sup>nd</sup> Edition, 1994.
- 6. Milestones in Biotechnology. Classic papers on Genetic Engineering, J.A. Davies and W.S. Reznikoff, Butterworth-Heinemann, Boston, 2<sup>nd</sup> edition, 1992.

**<u>COURSE OUTCOME</u>**: Understanding of basic cloning, gene transfer techniques and methods of identifying the successful clones and expression of the desired protein, concepts of knock-in, knock-out and gene therapy.

#### **CBIO 722 – MOLECULAR EVOLUTION**

**<u>COURSE OBJECTIVES</u>**: The main goal of this course is to help students in learning the basic concepts and computational methods involved in the molecular evolutionary analysis of genes and proteins.

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

#### Unit 1

Evolution of DNA and proteins, origin of the genetic code. Hardy-Weinberg equilibrium; Evolutionary changes by mutation, gene flow, natural selection and genetic drift.

#### Unit 2

The concept of homology in molecular evolution. Role of transitions and transversions; chromosomal deletions and insertions in evolution. Role of pseudogenes, repetitive DNA, transposable elements and junk DNA in evolution.

#### Unit 3

Neutral theory (Kimura) and nearly neutral theory (Ohta) of molecular evolution.Phylogenetic tree. Reconstruction of phyogenetic trees using distance matrix methods, the Maximum Parsimony method, Maximum likelihood and Bayesian inference. Estimation of selection at the molecular level.

#### Unit 4

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

#### Unit 5

**Evolution of the genome:** Human Genome Project, ENCODE, Genome duplication (Ohno's hypothesis), Exon Shuffling, Concerted evolution. Evolutionary Medicine.

#### **Text Books:**

1. An Introduction to Molecular Evolution and Phylogenetics by Lindell Bromham, 2016, Oxford University Press.

2. Molecular Evolution by Wen Hsiung-Li, 1997, Sinauer Associates, Sunderland, MA. **Reference Books:** 

1. Molecular Evolution and Phylogenetics by Masatoshi Nei and Sudhir Kumar, 2000, Oxford University Press.

2. Neutral Theory of Molecular Evolution by Motoo Kimura, 1985, Cambridge University Press.

3. Bioinformatics and Molecular Evolution by Paul G. Higgs and Teresa K. Attwood, 2013, Willey-Blackwell.

**<u>COURSE OUTCOME</u>**: The student will be able to understand the molecular basis of the evolution of the genome. He/she will be able to analyse the genomic data using phylogenetics and infer the evolutionary explanation of a biological phenomenon

#### Total: 45 Hrs\*.

9 Lectures

9 Lectures

# 9 Lectures

#### 9 Lectures

#### **BIO 756- GENETIC ENGINEERING LAB**

**Objective:** To explain the various tools that are used in genetic engineering to create recombinants and its applications in biological research as well as in biotechnology industries.

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

- 1. Sterilization of media and instruments (Biosafety cabinet, solutions, media, cell sample etc.).
- 2. Online tools for PCR primer generation and restriction analysis
- 3. Preparations of media for bacterial culture
- 4. Extraction of total RNA and quantification by spectrophotometer
- 5. Reverse-transcription cDNA synthesis -polymerase chain reaction.
- 6. Cloning of PCR product in vector using T/A cloning strategy.
- 7. Preparation of competent cells and Bacterial transformation
- 8. Screening of recombinant transformants using blue white selection and confirmation of clone
- 9. Antigen-antibody interactions in vitro-double immunodiffusion
- 10. Study of gene expression using RT-PCR or blotting.
- 11. Blotting technique- Western Blot of proteins-Sothern Bolt of genomic DNA

**Outcome:** Given the impact of genetic engineering in modern society, students should be endowed with strong theoretical knowledge of this technology. In conjunction with the practicals in molecular biology & genetic engineering, the students should be able to take up biological research as well as placement in the relevant biotech industry.

#### **Text and Reference Books**:

1. Molecular Cloning: a laboratory manual, Sambrook J., Fritsch EF. and Maniatis T, Cold Spring harbor Laboratory Press, (2000)

- 2. Practical Biochemistry, Plummer L, Tata McGraw-Hill, (1990).
- 3. Biochemistry, Stryer I., H.Freeman and Company, (2000).
- 4. Roitt's essential Immunology, Roitt IM and Delves PJ, Blackwell Science Ltd., (2001).
- 5. Immunology 6th Edition, Roitt I, Brostoff J. and Male D, Mosby Harcourt Publishers, (2001).
- 6. Bioinformatics: A practical guide to the analysis of genes and proteins. Baxevanis A.D and

Ovellette B.F.F., Wiley-Interscience, (2002).

#### **CBIO 723 - BIOMEDICAL INFORMATICS AND TRANSLATIONAL RESEARCH**

**COURSE OBJECTIVES:** To introduce biomedical data, their acquisition, storage and analysis for better healthcare. Concepts of translational research from bench to bed side.

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

#### Unit 1

6 Lectures **Overview of Medical Informatics:** Healthcare functions and information technology, Key Players in Health Information technology (HIT), Organizations involved with HIT, Barriers to HIT Adoption. Public Health Informatics - Information systems in public health - National Health Information Infrastructure (NHII). Internet based consumer health information telehealth and telemedicine.

#### Unit 2

Biomedical data: Their acquisition, storage and use, Electronic health records (EHR), Information Retrieval from Digital Libraries, Imaging Systems in Radiology and Picture archiving. Genomics and Proteomics data - Human Genome project, HapMap and 1000 genomes projects, Genetic profiling of individuals and large populations, Creation and use of Bioinformatics databases - gene, metabolic pathways of diseases.

#### Unit 3

Managing Information Security and Privacy in Health Care Data. General approaches to assuring appropriate use of data, data tracking and deidentifying data. Methods and Evaluation in biomedical decision making: Sampling, appropriate use of controls, data collection, testing of statistical significance, sensitivity and specificity, ROC plots. Standards in Biomedical informatics; Ethics, legal and regulatory matters in health informatics.

#### Unit 4

Clinical Decision-Support Systems - The Nature of clinical decision making, types of decisions, The role of computers in decision support, Historical perspectives- Leeds abdominal pain system, MYCIN, HELP; Ilustrative examples of clinical decision-support systems-Internist-1, DXplain system. Patient monitoring system and information management in intensive care unit.

#### Unit 5

Translational Research - Concepts and Principles. Therapeutic discovery in an academic setting, Technology Transfer and Commercialization process of a product. Bringing drugs from bench to bedside for cancer therapy - Molecular basis of cancer, strategies for developing therapeutic treatments, how imatinib and dasatinib were developed. Principles of Clinical Trials: Genetics/-Omics in Clinical Investigation, Principles of biomarker development and utility, pharmacogenomics including utilization of key knowledge from the human genome projects for personalized medicine. Regulatory and ethical issues involved in translational clinical research.

#### **Text Books:**

- 1. Biomedical Informatics: computer applications in Health care and Biomedicine (Health Informatics), 4<sup>th</sup> Ed by Shortliffe EH and Ciminio JJ., Springer-Verlag London (2014), ISBN 978-1-4471-4473-1.
- 2. Translational Research in Genetics and Genomics, by Moyra Smith, Oxford University press (2008), ISBN: 978-0-19-531376-5.

#### Total :30\* Hrs\*

6 Lectures

#### 6 Lectures

6 Lectures

#### **Reference Books:**

- 1. Evaluation methods in medical Informatics by Friedman CP. Wyatt JC, New York Springer-Verlag (1996), ISBN 0-387-25899-2.
- 2. Biomedical Informatics in Translational Research, by Hai Hu, Richard J. Mural and Michael N. Liebman, Artech House, INC (2008), ISBN-13: 978-1-59693-038-4.

**COURSE OUTCOME:** Students will be capable of applying informatics theories, methods and tools related to health care and biomedical research in academic as well as industrial research setting in an ethical manner. Also they will be knowledgeable to translate basic research findings to clinics with help of omics technologies for personalized medicine.

## **CBIO 725 – FUNCTIONAL PLANT GENOMICS**

**COURSE OBJECTIVES:** Students will learn about the general the relationships between the structure and functions of plants co-ordinating the process of overall development along with the economic values and their advances.

#### **Total credits: 2**

6 Lectures Plant Interactions: Modes- Competitive, Non-competitive and Complementary. Types- plant to microbe interactions, plant to fungus interactions, plant to pollinators interactions.

#### Unit 2

Unit 1

Molecular mechanism in plant adaptation: Plant secondary metabolism, Biosynthetic and regulatory pathway. Plant defensins- defensive phenyl propanoids, jasmonates, aromatic alkaloids. Abiotic stress tolerance-induced peptides, small signaling peptides and role of small RNAs.

#### Unit 3

Plant Genomics: Overview on the genetic engineering of plants, development in gene transformation technologies, methods to utilize these vectors for the direct transformation of regenerable explants and development of selectable markers.

#### Unit 4

Plant Pheromones and edible vaccines: Volatiles and secondary plant substances, Use of pheromones in pest management. Plant based edible vaccines, types and properties, Advantages and disadvantages.

#### Unit 5

Plant Synthetic Biology: Targeted plant genome editing - gene editing, ZFN, TALEN and CRISPR.

#### **Text Books:**

1. C. Neal Stewart Jr. (2016) Plant biotechnology and genetics principles, techniques, and applications- John Wiley & Sons Inc.

2. Gloria Coruzzi, Rodrigo Gutirrez (2009) Plant systems Biology Annual Plant Reviews, Volume 35, Wiley Blackwell

3. Heribert Hert (2009) Plant Stress Physiology From genomics to system biology, Wiley Blackwell

#### **Reference Books:**

1. Taiz & Zeiger Plant Physiology 5 ed. Sinauer Associates. 2010

2. Rob W. Brooker, Plant-plant interactions and environmental change, New Phytologist, 71 (2): 271-84. 2006.

**COURSE OUTCOME:** The course will enable the learners to explain the basic concepts of plant molecular and synthetic plant functional biology and help them understand the potential benefits of the plant canopy.

6 Lectures

6 Lectures

Total: 30Hrs\*

6 Lectures

#### CBIO- 755 PROJECT (PHASE – II)

**<u>COURSE OBJECTIVES:</u>** To enable the students to have hands-on research experience and write a comprehensive report, present and defend the same.

#### **Total Credits: 6**

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.

**<u>COURSE OUTCOME:</u>** The students will learn to execute a Research Proposal, prepare a Project report, present and defend the same.