

ANNA UNIVERSITY: CHENNAI 600 025
UNIVERSITY DEPARTMENTS
REGULATIONS - 2015
CHOICE BASED CREDIT SYSTEM
M.TECH. COMPUTATIONAL BIOLOGY

Program Educational Objectives (PEOs):

The M.Tech Computational Biology program has been designed to develop interdisciplinary skills required in the area of Computational Biology. In recent years, due to advancements in experimental techniques, there has been a phenomenal increase in the volume of biological data. In order to organize, analyze and make use of this data, there is a need to impart training in a multidisciplinary way.

The program has a strong component of experimental techniques, high throughput data handling using *in silico* approaches, systems approaches involving strong foundations in physics, chemistry and mathematics. The curriculum includes subjects which cover computational biology, mathematics and statistics, programming languages, high performance computing, algorithms in computational biology, machine learning and data mining, molecular simulations, Systems Biology etc. The professional electives are designed to develop skills in specialized areas in Computational Biology and related disciplines. Since the program is interdisciplinary, courses for theory and lab which cover fundamental experimental techniques are part of the program. The program educational objectives are as follows:

1. To provide foundation in fundamental concepts, tools and resources in Computational Biology.
2. To provide a sound foundation in Mathematics and Statistics, essential for analysis of biological data.
3. To develop programming skills in languages like C++, PERL, Python and Java: both theory and lab. To introduce high performance computing.
4. To introduce algorithms for analysis of biological data.
5. To introduce machine learning and data mining concepts and techniques relevant to biological data along with practical implementation of machine learning techniques.
6. To impart training in experimental techniques, molecular modeling and simulations, structural biology, whole cell modelling and systems biology.
7. To develop skills in specialized areas related to Computational Biology which will enable high throughput data processing and analysis.
8. To equip students with the skills to design and implement a real time research oriented problem through their project work.

Program Outcomes (POs):

At the end of the program the student

1. Will be familiar with resources, biological data, its analysis and interpretation.
2. Will develop programming skills in object oriented languages like C++ and JAVA and languages like Python and PERL. Will be exposed to high performance computing.
3. Will be able to analyze high-throughput biological data and perform statistical analysis / develop mathematical models.
4. Will be familiar with the theory and practical aspects of important experimental techniques.
5. Will be familiar with the design and implementation of algorithms which may help them design their own.
6. Will be able to use data mining and apply machine learning techniques like ANN, SVM and HMM for any data classification and prediction problem.
7. Will develop skills in molecular modeling and simulation, whole cell modeling, drug discovery, Systems Biology and other emerging areas.
8. Will develop analytical skills and expertise to formulate and implement a research oriented real time problem. Will be trained in major areas related to Computational Biology. The experimental component will help them undertake interdisciplinary work. The program equips them with skills to pursue a career either in academia or industry.

	Program Objectives							
Program Educational Objectives (PEOs)	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
I	✓							✓
II			✓					✓
III		✓	✓					✓
IV					✓			✓
V						✓		✓
VI			✓	✓			✓	✓
VII			✓			✓		✓
VIII								✓

	Courses	Program Objectives							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Sem I	Programming Techniques		✓						✓
	Computational Biology	✓							✓
	Applied Statistics for Biologists		✓						✓
	Analytical Techniques and Methods				✓				✓
	Preparative and Analytical Techniques in Biotechnology				✓				✓
	Elective I								
	Elective II Elective III								

	Courses	Program Objectives							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Sem II	Algorithms in Computational Biology					✓			✓
	Biomolecular Simulations							✓	✓
	Structural Biology							✓	✓
	Machine Learning and Data Mining						✓		✓
	Programming Languages		✓						✓
	Elective IV Elective V								

	Courses	Program Objectives							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Sem III	Computational Systems Biology							✓	✓
	High Performance Computing		✓	✓					✓
	Elective VI								
	Project Work- Phase I								✓

		PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8
Sem IV	Project Work – Phase II								✓

ANNA UNIVERSITY: CHENNAI 600 025
UNIVERSITY DEPARTMENTS
REGULATIONS – 2015
I – IV SEMESTERS CURRICULUM AND SYLLABUS
M. TECH. COMPUTATIONAL BIOLOGY

SEMESTER I

S.n.	Course Code	Course Title	Category	Contact Periods	L	T	P	C
THEORY								
1	BC7102	Programming Techniques	PC	4	2	0	2	3
2	BT7153	Computational Biology	FC	4	2	0	2	3
3	BT7152	Applied Statistics for Biologists	FC	4	4	0	0	4
4	BC7101	Analytical Techniques and Methods	PC	4	2	0	2	3
5		Elective I	PE	3	3	0	0	3
6		Elective II	PE	3	3	0	0	3
7		Elective III	PE	3	3	0	0	3
PRACTICALS								
8	BT7161	Preparative and Analytical Techniques in Biotechnology	PC	6	0	0	6	3
TOTAL				31	19	0	12	25

SEMESTER II

S.n.	Course Code	Course Title	Category	Contact Periods	L	T	P	C
THEORY								
1	BC7201	Algorithms in Computational Biology	PC	3	3	0	0	3
2	BC7202	Biomolecular Simulations	PC	4	2	0	2	3
3	BC7203	Machine Learning and Data Mining	PC	4	2	0	2	3
4	BC7204	Programming Languages	PC	3	3	0	0	3
5	BC7205	Structural Biology	PC	3	3	0	0	3
6		Elective IV	PE	3	3	0	0	3
7		Elective V	PE	3	3	0	0	3
PRACTICALS								
8	BC7211	Programming Languages Lab	PC	4	0	0	4	2
TOTAL				27	19	0	8	23

SEMESTER III

S.n.	Course Code	Course Title	Category	Contact Periods	L	T	P	C
THEORY								
1	BC7301	Computational Systems Biology	PC	3	3	0	0	3
2	BC7302	High Performance Computing	PC	3	3	0	0	3
3		Elective VI	PE	3	3	0	0	3
PRACTICALS								
4	BC7311	Project Work Phase I	EEC	12	0	0	12	6
TOTAL				21	9	0	12	15

SEMESTER IV

S.n.	Course Code	Course Title	Category	Contact Periods	L	T	P	C
1	BC7411	Project Work Phase II	EEC	24	0	0	24	12
TOTAL				24	0	0	24	12

TOTAL CREDITS : 75

FOUNDATION COURSES (FC)

Sl.No	Course Code	Course Title	Category	Contact Hours	L	T	P	C
1.	BT....	Computational Biology	FC	4	2	0	2	3
2.	BT....	Applied Statistics for Biologists	FC	4	4	0	0	4

PROFESSIONAL CORE (PC)

Sl.No	Course Code	Course Title	Category	Contact Hours	L	T	P	C
1.	BC	Programming Techniques	PC	4	2	0	2	3
2.	BC	Analytical Techniques and Methods	PC	4	2	0	2	3
3.	BT....	Preparative and Analytical Techniques in Biotechnology	PC	6	0	0	6	3
4.	BC	Algorithms in Computational Biology	PC	3	3	0	0	3
5.	BC	Biomolecular Simulations	PC	4	2	0	2	3
6.	BC	Structural Biology	PC	3	3	0	0	3
7.	BC	Machine Learning and Data Mining	PC	4	2	0	2	3
8.	BC	Programming Languages	PC	3	3	0	0	3
9.	BC	Computational Systems Biology	PC	3	3	0	0	3
10.	BC	High Performance Computing	PC	3	3	0	0	3

EMPLOYABILITY ENHANCEMENT COURSES (EEC)

Sl.No	Course Code	Course Title	Category	Contact Hours	L	T	P	C
1.	BC	Project Work- Phase I	EEC	12	0	0	12	6
2.	BC	Project Work – Phase II	EEC	24	0	0	24	12

PROFESSIONAL ELECTIVES (PE)

Sl.No	Course Code	Course Title	Category	Contact Hours	L	T	P	C
1.	BT7071	Advanced Genomics and Proteomics	PE	3	3	0	0	3
2.	BT7073	Advances in Molecular Pathogenesis	PE	3	3	0	0	3
3.	BT7074	Biocatalysts and Enzyme Technology	PE	3	3	0	0	3
4.	BT7075	Communication Skill development	PE	3	2	0	2	3
5.	BT7076	Metabolic Process and Engineering	PE	3	3	0	0	3
6.	BT7077	Nanobiotechnology	PE	3	2	0	2	3
7.	BT7078	Research and Research Methodology in Biotechnology	PE	3	3	0	0	3
8.	BT7079	Tissue Engineering and Regenerative Medicine	PE	3	3	0	0	3
9.	BC7003	General Biology	PE	3	3	0	0	3
10.	BC7002	Drug Discovery	PE	3	3	0	0	3
11.	BC7004	Molecular Evolution and Phylogeny	PE	3	3	0	0	3
12.	BC7005	Next Generation Sequencing	PE	3	2	0	2	3
13.	BC7006	Signal Processing in Biotechnology	PE	3	3	0	0	3
14.	BP7071	Pharmacogenomics	PE	3	3	0	0	3
15.	BT7072	Advanced Technologies in Omics Sciences	PE	3	3	0	0	3
16.	BC7001	Big Data Analytics	PE	3	3	0	0	3

OBJECTIVES

This course will introduce C++ programming language and basics of Python.

UNIT I INTRODUCTION TO C++**12**

An Overview of Computers and Programming Languages, Programming methodologies- Introduction to Object Oriented Programming and Procedural Programming, Basics of C++ environment, Data types, Control Flow Constructs, Library functions, Arrays

UNIT II CLASSES**12**

Definition- Data members- Function members – Access specifiers, Constructors – Default constructors-Copy constructors-Destructors, Static members- This pointer- Constant members- Free store operators

UNIT III INHERITANCE AND POLYMORPHISM**12**

Overloading operators- Functions- Friends- Class derivation-Virtual functions-Abstract base classes- Multiple inheritance.

UNIT IV TEMPLATES AND FILE HANDLING**12**

Class templates-Function templates-Exception handling- File Handling

UNIT V INTRODUCTION TO PYTHON**12**

Introduction to Python, Data Types, Expressions, tuples, lists, dictionaries, and sets, Functions, Control Statements-Loops-Iterations, Pattern Matching- Fixed length and Variable length matching

TOTAL : 60 PERIODS**Lab: Exercises for all the topics****OUTCOME**

This course will enable students to understand object oriented programming concepts and enable them to write programs in C++ and Python

REFERENCES

1. Lippman S.B., The C++ Primer, 4e, Addison Wesley,p- 2007.
2. Deitel and Deitel, C++ How to Program, 8e, Prentice Hall, 2011.
3. Balagurasamy E. , Object-Oriented Programming using C++, Tata McGraw- Hill, 2008.
4. Sebastian Bassi, Python for Bioinformatics (Chapman & Hall, CRC Mathematical and Computational Biology), CRC Press, 2009
5. Mitchell L Model, Bioinformatics Programming Using Python- Practical Programming for Biological Data, O'Reilly Media, 2009

OBJECTIVES

The course introduces students to biological data, tools and analysis. PERL programming language is introduced to provide skills in generating user defined scripts.

UNIT I INTRODUCTION TO COMPUTATIONAL BIOLOGY AND SEQUENCE**ANALYSIS****12**

Molecular sequences, Genome sequencing: pipeline and data, Next generation sequencing data, Biological databases: Protein and Nucleotide databases, Sequence Alignment, Dynamic Programming for computing edit distance and string similarity, Local and Global Alignment, Needleman Wunsch Algorithm, Smith Waterman Algorithm, BLAST family of programs, FASTA algorithm, Functional Annotation, Progressive and Iterative Methods for Multiple sequence alignment, Applications.

UNIT II PHYLOGENETICS**12**

Introduction to Phylogenetics, Distance and Character based methods for phylogenetic tree construction: UPGMA, Neighbour joining, Ultrametric and Min ultrametric trees, Parsimonous trees, Additive trees, Bootstrapping.

UNIT III PROTEIN STRUCTURE, MODELLING AND SIMULATIONS**12**

Protein Structure Basics, Visualization, Prediction of Secondary Structure and Tertiary Structure, Homology Modeling, Structural Genomics, Molecular Docking principles and applications, Molecular dynamics simulations.

UNIT IV MACHINE LEARNING, SYSTEMS BIOLOGY AND OTHER ADVANCED TOPICS**12**

Machine learning techniques: Artificial Neural Networks and Hidden Markov Models: Applications in Protein Secondary Structure Prediction and Gene Finding, Introduction to Systems Biology and its applications in whole cell modelling, Microarrays and Clustering techniques for microarray data analysis, informatics in Genomics and Proteomics, DNA computing.

UNIT V PERL FOR BIOINFORMATICS**12**

Variables, Data types, control flow constructs, Pattern Matching, String manipulation, arrays, lists and hashes, File handling, Programs to handle biological data and parse output files for interpretation

Laboratory Demonstrations for

Biological Databases, Sequence alignment: BLAST family of programs, FASTA, ClustalW for multiple sequence alignment, Phylogenetics software, Homology Modeling and Model evaluation, AutoDock, GROMACS, Prokaryotic and Eukaryotic Gene finding software, Programs in PERL.

TOTAL: 60 PERIODS**OUTCOME**

At the end of the course, the student will acquire skills required for analysis of biological data and interpretation of results. The skills acquired will help in interdisciplinary research.

REFERENCES

1. Dan Gusfield. Algorithms on Strings Trees and Sequences, Cambridge University Press.
2. David W. Mount Bioinformatics: Sequence and Genome Analysis, Cold Spring Harbor Laboratory Press, Second Edition, 2004.
3. Arthur M. Lesk, Introduction to Bioinformatics by Oxford University Press, 2008.

4. Tisdall, James, Beginning PERL for Bioinformatics, O'Reilley Publications, 2001.
5. Andrew R. Leach, Molecular Modeling Principles And Applications, Second Edition, Prentice Hall.
6. Baldi, P., Brunak, S. Bioinformatics: The Machine Learning Approach, 2nd ed., East West Press, 2003
7. Baxevanis A.D. and Oullette, B.F.F. A Practical Guide to the Analysis of Genes and Proteins, 2nd ed., John Wiley, 2002
8. Durbin, R. Eddy S., Krogh A., Mitchison G. Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids. Cambridge University Press, 1998.
9. Proteomics from protein sequence to function: Edited by S.R.Pennington and M.J.Dunn, Taylor and Francis Group, 2001.

BT7152

APPLIED STATISTICS FOR BIOLOGISTS

L T P C

4 0 0 4

OBJECTIVES

This subject will facilitate the students to understand the fundamentals of statistics for biologists.

UNIT I

12

Random variable-sample spaces-Events-Axiomatic approach to probability- conditional probability-additional theorem, Multiplication theorem - Baye's theorem problems-continuous and discrete random variables, Distribution function-Expectation with properties-Moments, mean, Variance problems-for continuous and discrete distributions.

UNIT II

12

Bivariate distribution-conditional and marginal distribution-Discrete distribution-Binomial, Poisson, geometric distribution-Continuous distribution, Normal, exponential and negative exponential, gamma distributions-simple problems-properties

UNIT III

12

Correlation coefficient, properties-problems-Rank correlation-Regression equations-problems curve fitting by the method of least squares-fitting curves of the form $ax+b$, ax^2+bx+c , abx and axb -Bivariate correlation application to biological problems

UNIT IV

12

Concept of sampling-Methods of sampling-sampling distributions and Standard Error-Small samples and large samples-Test of hypothesis-Type I, Type II Errors-Critical region-Large sample tests for proportion, mean-Exact test based on normal, t , f and chi-square distribution problems- Test of goodness of fit.

UNIT V

12

Basic principles of experimentation-Analysis of variance-one-way, Two-way classifications-Randomised block design, Latin square design-problems.

TOTAL: 60 PERIODS

OUTCOME

On the completion of the course the students are expected to have learnt, Understanding and applying Statistical methods of analysis for Biological applications

TEXT BOOKS

1. Kapoor, V. C. "Elements of Mathematical statistics".
2. Vittal, P.R. and V.Malini."Statistical and Numerical Methods". Margham Publications.

3. Veerarajan, T. "Probability, Statistics and Random Processes". 3rd Edition., Tata Mc Graw-Hill, 2008.

REFERENCES

1. Johnson, R. A. "Miller & Freund's Probability and Statistics for Engineers". 6th ed. PHI, 2003.
2. Arora, P. N. Smeet Arora, and Arora, S. "Comprehensive Statistical Methods". S. Chand & Co,
3. Spiegel, Murray R., J. Schiller and R. Alu Srinivasan. "Schaum's Outlines Probability and Statistics". 2nd Edition. Tata Mc Graw-Hill 2000.
4. Kandasamy, P. K. Thilagavathi & K. Gunavathi. "Probability Statistics and Queuing Theory". S. Chand & C

BC7101

ANALYTICAL TECHNIQUES AND METHODS

L T P C

2 0 2 3

OBJECTIVES

The course intends to familiarize students with the basic concepts and analytical techniques and methods in microscopy, spectroscopy, separation methods, electrochemistry and Biochemistry

UNIT I MICROSCOPY

12

Identification of microorganisms using light and compound microscopy, Phase Contrast Microscopy, Fluorescence Microscopy, Confocal Microscopy, Microscopy with Light and Electrons, Electrons and Their Interactions with the Specimen, Electron Diffraction, The Transmission Electron Microscope, The Scanning Electron Microscope, Atomic Force Microscopy.

UNIT II SPECTROSCOPY

12

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

UNIT III SEPARATION METHODS

12

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

UNIT IV ELECTROANALYTICAL TECHNIQUES

12

Fundamentals of Electrochemistry, Electrodes, Potentiometry, Electrolysis, Electrogravimetric Analysis, Coulometry, Voltammetry- Polarography, Faradaic and Charging Currents, Square Wave Voltammetry, Microelectrodes

UNIT V BIOCHEMICAL TECHNIQUES

12

Estimation of Carbohydrates, Estimation of Lipids, Estimation of Proteins and Nucleic Acids

TOTAL : 60 PERIODS

OUTCOME

The student will gain knowledge in the working and principles of various analytical techniques. It will help them design their experiments and analyze the data obtained.

REFERENCES

1. Skoog, Holler, Crouch, Instrumental Analysis Brooks/Cole 2007 ISBN-13: 978-81-315-0542-7.
2. Robert D. Braun, Introduction to Instrumental Analysis Pharma Book Syndicate. ISBN 891-88449-15-6

OBJECTIVE

To prepare the student in all the latest preparative and analytical techniques required in research or Industry.

1. Preparation of Acetate, Tris and Phosphate Buffer systems and validation of Henderson-Hasselbach equation.
2. Reactions of amino acids – Ninhydrin, Pthaldehyde, Dansyl chloride – measurement using colorimetric and fluorimetric methods.
3. Differential estimations of carbohydrates – reducing vs non-reducing, polymeric vs oligomeric, hexose vs pentose
4. Estimation of protein concentration using Lowrys' method, Dye-binding method
5. DNA determination by UV-Vis Spectrophotometer – hyperchromic effect Separation of lipids by TLC.
6. Enzyme Kinetics: Direct and indirect assays – determination of Km, Vmax and Kcat, Kcat/Km
7. Restriction enzyme – Enrichment and unit calculation
8. Ion-exchange Chromatography – Purification of IgG and Albumin
9. Gel filtration – Size based separation of proteins
10. Affinity chromatography – IMAC purification of His-tagged recombinant protein
11. Assessing purity by SDS-PAGE Gel Electrophoresis
12. Chemical modification of proteins – PITC modification of IgG and Protein immobilization

TOTAL : 90 PERIODS

OUTCOME

Having learned all the techniques in this lab, the student will become capable in enzymology, techniques required in the quantitation of biomolecules, downstream processing and the chemical modification of proteins, which will prepare him for a career in research or employment in the biotech Industry.

REFERENCES

1. Biochemical Methods: A Concise Guide for Students and Researchers, Alfred Pingoud, Claus Urbanke, Jim Hoggett, Albert Jeltsch, 2002 John Wiley & Sons Publishers, Inc,
2. Biochemical Calculations: How to Solve Mathematical Problems in General Biochemistry, 2nd Edition, Irwin H. Segel, 1976 John Wiley & Sons Publishers, Inc,
3. Principles and Techniques of Practical Biochemistry- Wilson, K. and Walker, J. Cambridge Press.

OBJECTIVES

The course introduces the student to algorithms used in computational biology relating to protein, DNA and RNA.

UNIT I INTRODUCTION TO ALGORITHMS 9

Algorithms-Complexity of algorithms and running time, Polynomial, NP complete problems, Recursion, Linear, Exhaustive search, Branch and Bound, divide and conquer algorithms, sorting.

UNIT II EXACT MATCH AND HIDDEN MARKOV MODELS 9

Knuth-Morris-Pratt and Boyer-Moore algorithm for exact match and graph and maximum likelihood algorithm, Hidden Markov Model: Forward and Backward Algorithms, Most probable state path: Viterbi algorithm, Parameter Estimation for HMMs:-Baum-Welch Algorithm, EM Algorithm, Applications of profile HMMs for multiple alignment of proteins and for finding genes in the DNA.

UNIT III DNA AND RNA RELATED ALGORITHMS 9

Finding regulatory motifs in DNA, Genome alignment, Suffix Trees, RNA secondary structure prediction: Base pair maximization and the Nussinov folding algorithm, Energy minimization and the Zuker folding algorithm, Design of covariance models, Application of RNA Fold.

UNIT IV DYNAMIC PROGRAMMING AND SEQUENCE BASED ALGORITHMS 7

Dynamic programming Principles and its uses. Local and Global alignment principles, Finding longest common subsequences, Statistical and Similarity based methods for gene prediction, Models of evolution.

UNIT V SEQUENCE ASSEMBLY AND PROTEIN STRUCTURE 11

DNA sequencing, shortest super-string problem, Sequencing by Hybridization as a Hamiltonian Path Problem, Consecutive ones problem (CIP) for aligning clones based on SNPs, Randomized algorithms: Gibbs Sampling, Protein sequencing and identification, spectral graphs and spectral alignment, Protein structure prediction- Secondary structure prediction algorithms, Threading, Comparative Modeling.

TOTAL : 45 PERIODS**OUTCOME**

At the end of the course, students will be able to appreciate the design and implementation of algorithms used in Computational Biology. This will enable them to make more effective choices and interpretations while using tools based on these algorithms.

REFERENCES

1. Neil C. Jones and Pavel A. Pevzner An introduction to Bioinformatics Algorithms.(computational Molecular Biology) (2004) MIT press. ISBN-10: 0262101068
2. R. Durbin, S.Eddy, A.Krogh, G.Mitchison Biological sequence analysis : Probabilistic models of Proteins and Nucleic acids (2005) Cambridge University Press 0521540798
3. Michael.S.Waterman Introduction to Computational Biology : Maps, Sequences and Genomes . Waterman. Edition 2 (2012) Chapman and Hall/ CRC Press ISBN: 1439861315
4. Dan Gusfield Algorithms on Strings, Trees and Sequences : Computer Science and Computational Biology (1997) Cambridge University Press. ISBN-10: 0521585198
5. Horowitz, S. Sahini, and Rajasekharan : Fundamentals of Computer Algorithms (2004) , Galgotia Publications. ISBN-10: 81-7515-257-5

BC7202**BIOMOLECULAR SIMULATIONS****L T P C
2 0 2 3****OBJECTIVES**

This course will introduce the principles and practices on Molecular Modeling, in particular simulation of biological macromolecules and it will provide demos on MD Simulation and Docking Software.

UNIT I INTRODUCTION	12
Introduction-Molecular Modeling, Statistical Mechanics, Thermodynamics Basics, Introduction to Quantum Mechanics- Black body radiation, Harmonic Wave Function, Schrodinger equation	
UNIT II MOLECULAR MECHANICS	12
Force Fields, General features of Molecular Mechanics Force Fields, Types of Force Fields, Bond Stretching, Angel bending, Torsional terms, Non bonded interactions- Electrostatic and , van der Waals interactions, Types of Potentials, Lennard-Jones Potential	
UNIT III MOLECULAR DYNAMICS SIMULATION METHODS	12
Molecular Dynamics Simulation-Introduction, Molecular units and timescales, Energies, Equations of motion, trajectories, phase space, Temperature, velocity distributions, elements of an MD simulation, Setting up and Running a Molecular Dynamics Simulation, Visualization and Analysis	
UNIT IV MOLECULAR DYNAMICS SIMULATION PARAMETERS	12
Potential Energy Surface, Energy minimization, constraints, Cutoffs and long-range electrostatics, Integration algorithms, Entropy, Properties of water, Water models, Hydrogen bonds, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations	
UNIT V MOLECULAR MODELLING	12
Introduction - Homology Modeling, Drug discovery process, Introduction - Methods and Tools in Computer-aided molecular Design, Docking, De Novo Drug Design, Virtual screening.	

Note: For Lab sessions tutorials on Gromacs, and Autodock will be given.

TOTAL : 45 PERIODS

OUTCOME

At the end of the course, students would be expected to learn Molecular Dynamics Simulation and Docking

REFERENCES

1. Andrew R. Leach Molecular Modeling Principles and Applications (2nd Ed.). Prentice Hall USA. 2001ISBN-13: 978-0582382107
2. Ramachandran, Deepa and Namboori Computational Chemistry and Molecular Modeling- Principles and Applications, Springer_Verlag2008 Reference for Unit 1 and 2.ISBN-13 978-3-540-77302-3.
3. Alan Hinchliffe, Molecular Modelling for Beginners, (2nd Edition) John Wiley & Sons Ltd. 2008ISBN: 978-0-470-51314-9
4. Tamar Schlick Molecular Modeling and Simulation – An interdisciplinary Guide Springerverlag 2000ISBN 978-1-4419-6350-5
5. Patrick Bultinck, Marcel Dekker Computational medicinal chemistry for drug discovery CRC Press 2004ISBN 9780824747749

OBJECTIVES

This course is designed to introduce concepts in Machine learning and Data Mining. The Data Mining modules will help students appreciate the power of Data Mining Query Language and the utility of data mining in extracting interesting associations. The lab demos are intended to show how the concepts learnt in machine learning can be implemented.

UNIT I MACHINE LEARNING 12

Machine learning Introduction: goals and applications, Supervised and Unsupervised learning - Inductive Classification concepts and Learning aspects. Clustering : k-means, Outlier analysis, Techniques of machine learning – Artificial Neural Networks: Feed Forward Networks, Error correction and Back propagation algorithm, Genetic algorithms, operators, crossover and mutation rates, fitness functions. Decision trees, Computing average disorder of trees, noisy data and pruning.

UNIT II MODELS AND METHODS 12

Bayesian Classification, Bayes theorem, Naive Bayes classification, Support Vector Machines, Concept of Hyperplanes and Support Vectors. Reinforcement Learning, Ensemble Learning - Bagging and Boosting. Graphical models.

UNIT III DATA MINING 12

Data Mining Introduction, Relational databases and Data warehouses, Data Mining functionalities, Concept/Class Description, Data mining Task primitives, Data Preprocessing: Descriptive Data Summarization: Statistical measures, measuring central tendency, dispersion of data, box plots. Data cleaning, integration, transformation and reduction.

UNIT IV DMQL AND MULTIDIMENSIONAL DATA MODELS 12

Use of Data mining Query Language DMQL, Multidimensional Data Models: Tables, Stars, Snowflakes and Fact Constellations. Data cubes, Curse of dimensionality, Data Warehouse and Online Analytical Processing Technologies: OLAP, Data visualization.

UNIT V ASSOCIATION MINING AND CORRELATION ANALYSIS 12

Frequent itemsets, Interestingness measures: Support, Confidence. Frequent Itemset Mining methods- Apriori algorithm, Frequent Pattern tree algorithm, Association mining-correlation analysis.

TOTAL : 60 PERIODS**OUTCOME**

The students will acquire skills required for data mining. It will enable them to utilize machine learning techniques for training and classification of biological data and prediction.

REFERENCES

1. Jiawei Han, Micheline Kamber "Data Mining: Concepts and Techniques", Third Edition (2011) Morgan Kaufmann Publishers. ISBN-13: 978-0123814791
2. Ian H. Witten, Eibe Frank "Data Mining : "Practical machine learning tools and Techniques with java implementation" (2005) ISBN 1-55864-552-5
3. Tom Mitchell "Machine Learning" McGraw-Hill (1997) ISBN-13: 978-0070428072
4. Petra Perner, Azriel Rosenfeld "Machine Learning and data mining in pattern recognition in third International conference MLDM (2003) Springer ISBN 978-3-540-40504-7.

OBJECTIVES

This course will introduce Java programming language and BioPython.

UNIT I INTRODUCTION TO JAVA 9

Introduction to Java: Compilation of java programs – Java Development Kit – Java Data Types – Operators – Operator precedence Keywords, Constants, Variables, Operators, Expressions, Decision Making, Branching and Looping

UNIT II JAVA CLASSES 9

Working with java classes: Declaring classes – super and sub classes – Objects – Methods, Arrays, Strings and Vectors, Constructors – Inheritance – Overloading – Exception handling – Managing Inputs/Output Files in Java

UNIT III MULTI-THREAD PROGRAMMING 9

Multi-thread programming: Life cycle of a thread – Creating a thread– Thread priorities – Synchronization – Deadlock, Event handling mechanisms

UNIT IV JAVA APPLETS 9

Graphics - Applet basics – passing parameters to applets – applet display methods – drawing lines, ovals, rectangles and polygons – Threads and Animation, Java and Database connection

UNIT V PYTHON AND BIOPYTHON 9

Python Packages, Modules, Files, Python Classes-Objects-Methods, Inheritance, Biopython – Introduction- Biopython Components – Alphabet, Seq, MutableSeq, SeqRecord, Align, ClustalW, SeqIO, AlignIO, Blast, PDB

TOTAL : 45 PERIODS

OUTCOME

This course will enable the students to understand the Java programming concepts and enable them to do programs in Java, Python and BioPython

REFERENCES

1. Herbert Schildt, Java:The completer Reference. (7th Ed.) by TMH. 2012
2. E. Balagurusamy, Programming with Java: A Primer, Tata McGraw-Hill Education, 2010
3. Sebastian Bassi, Python for Bioinformatics (Chapman & Hall, CRC Mathematical and Computational Biology), CRC Press, 2009
4. Mitchell L Model, Bioinformatics Programming Using Python-Practical Programming for Biological Data, O'Reilly Media, 2009
5. John Zelle , Python Programming: An Introduction to Computer Science, 2nd Ed. Paperback , Franklin Beddle and Associates Inc 2010

OBJECTIVES

To familiarize students with structural aspects of protein and DNA, biophysical techniques for structure determination.

UNIT I STRUCTURE OF PROTEIN AND DNA 9

Fundamentals of protein structure, Structural Hierarchy, Motifs and domains: domain structures, Types of proteins, Complex proteins, Principles of nucleic acid structure - 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. Non-uniform helical DNA Structure. Unusual DNA structures - hairpins, bulges, cruciform, triplexes, tetraplexes

UNIT II PROTEIN STRUCTURE AND FUNCTION 9

Enzyme catalysis and structure. Membrane proteins, signal transduction, proteins of the immune system. Structure of Spherical viruses, Folding and flexibility, Prediction, engineering and design of protein structures. Methods to identify secondary structural elements

UNIT III CRYSTALLOGRAPHY 9

Elementary crystallography: Introduction: symmetry in crystals, lattices and unit cells, crystal systems, Bravais lattices, Elements of symmetry, 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 IV X-RAY SCATTERING 9

X-ray scattering: Atomic scattering factor - diffraction by a space lattice - structure factor equation - electron density and Fourier series - Fourier Transform and crystal diffraction - diffraction by real crystals - Lorentz and polarization factor - primary and secondary extinctions.

UNIT V NUCLEAR MAGNETIC RESONANCE 9

Nuclear Magnetic Resonance:- Introduction, Nuclear spin, NMR sensitivity, shielding and deshielding effects of NMR, nuclear Overhauser 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. 1D- NMR spectra, 2D- NMR spectroscopy.

TOTAL : 45 PERIODS

OUTCOME

The student will be able to understand biophysical techniques and principles of macromolecular structure determination.

REFERENCES

1. K.P.Murphy. Protein structure, stability and folding (2001) Humana press. ISBN 0-89603682-0
2. Arthur M.LeskiIntroduction to protein architecture (2001) Oxford University Press. ISBN 0198504748
3. A.McPherson, Introduction to Macromolecular Crystallography. 2nd edition (2009)., John Wiley Co.
4. Carl Branden and John Tooze and Carl Brandon Introduction to Protein Structure, (1999)

John Garland, Publication Inc. ISBN 0815323050

5. N.Gautham Bioinformatics (2006) Narosa publications. ISBN-13: 9781842653005
6. VasanthaPattabhai and N.Gautham Biophysics (2002) Narosa Publishers ISBN 1-4020-0218-1
7. George H. Stout , Lyle H. Jensen ,X-Ray Structure Determination: A Practical Guide, 2nd Edition.ISBN 0471607118.
8. G. E. Schulz. Principles of Protein Structure. Springer 2009
9. Rick NG, Wiley Blackwell. Drugs: From discovery to approval 2nd edition (2009)
10. Ed Donald J AbrahamWiley-Interscience. Burger's Medicinal Chemistry and Drug discovery. Volume 2, Drug Discovery and development.6th Edition (2003). ISBN 0471370282
11. TripathiKd. Essentials of Medical Pharmacology, 6th Edition. Publisher: Jaypee Brothers (2008). ISBN 978-9350259375

BC7211

PROGRAMMING LANGUAGES LAB

L T P C
0 0 4 2

OBJECTIVES

This Lab course will provide hands on sessions to the students to do programs in Java and Python.

LIST OF EXPERIMENTS

1. Java programs to demonstrate decision making, and loops
2. Working with Arrays
3. Working with Classes and objects in java, Use of constructor
4. Simple, multiple and multilevel inheritances.
5. Operator Overloading, Exception handling,
6. Multithreading
7. Applets.
8. Animation and Threads
9. Java and Database connection
10. Python – Simple Programs, Control statements
11. Python - Tuples, Lists
12. Dictionaries, Modules
13. Python Classes
14. Reading/Writing Protein/DNA sequences using Biopython
15. BiopythonClustalW and other components

TOTAL : 60 PERIODS

OUTCOME

At the end of this lab course the students will be able to do programs in Java and Python.

OBJECTIVES

To introduce concepts of system biology and familiarize students with kinetic modeling, flux balance analysis, genome scale modeling, tools and resources.

UNIT I INTRODUCTION TO NETWORKS 9

Introduction to Systems Biology, Systems level understanding of biological systems. Basic concepts in Systems modeling, Networks and graph theory: Basic properties of Network: Degree, average degree and degree distribution. Adjacency matrix, weighted and unweighted networks, Bipartite network, Paths and distances, Random Networks: Erdos-Renyi model, Small-world effect, clustering coefficient, Scale-free networks: Power laws, Hubs, ultra-small property, degree exponent, The Barabasi-Albert Model. Degree correlations: assortativity and disassortativity.

UNIT II KINETIC MODELING 9

Kinetic modeling of biochemical reactions, describing dynamics with ODEs, rate equations, deriving a rate equation, incorporating regulation of enzyme activity by effectors, E-cell platform and erythrocyte modeling

UNIT III FLUX BALANCE ANALYSIS 9

Introduction to Flux balance analysis, Construction of stoichiometric matrices, Constraint based models. Network basics, examples of mathematical reconstruction of transcriptional networks and signal transduction networks.

UNIT IV NETWORK MOTIFS AND MODELS 9

Network motifs, Feed forward loop network motif. Gene circuits, robustness of models, Chemotaxis model, Integration of data from multiple sources: Building genome scale models.

UNIT V RESOURCES AND SBML 9

Tools and databases for modeling: Pathway databases KEGG, EMP, Metacyc, Enzymekinetiks database BRENDA, Gene expression databases, Biomodels database, Basics of Systems Biology Markup Language (SBML), SBML editors.

TOTAL : 45 PERIODS**OUTCOME**

Students will be able to appreciate the design, implementation and working of system biology models.

REFERENCES

1. Systems Biology a Textbook by Edda Klipp, Wolfram Liebermeister, Christoph Wierling Wiley-BlackWell Publications (2009 Edition).
2. An introduction to Systems Biology: Design Principles of Biological Circuits by Uri Alon (Chapman and Hall / CRC 2007 Edition)
3. Systems Biology in practice : concepts, implementation and application by Edda Klipp, Ralf Herwig, Axel Kowald, Christoph Wierling, Hans Lehrach. (Wiley – VCH 2005)
4. Foundations of Systems Biology Edited by Hiroaki Kitano (MIT Press)
5. Systems Biology: Definitions and perspectives by Lilia Albergina (Springer Publications 2008)

OBJECTIVES

This course will facilitate students to understand parallel processing, parallel programming and languages.

UNIT I PARALLEL PROCESSING FUNDAMENTALS 9

Parallel Processing Concepts - Levels of parallelism - task, thread, memory, function; Models (SIMD, MIMD, Dataflow Models etc), Architectures- multi-core, multi-threaded.

UNIT II PARALLEL PROGRAMMING MODELS 9

Parallel Programming and Multiprogramming, Programming Models in high performance computing architectures – Shared memory and Message passing paradigms - Fundamental Design Issues in Parallel Computing – Synchronization - Interconnect, Communication, Memory Organization Memory hierarchy and transaction specific memory design - Thread Organization.

UNIT III PARALLEL PROGRAMMING LANGUAGES 9

Parallel Programming Languages – Overview, OpenMP, History of GPUs leading to their use and design for HPC, Introduction to the GPU programming model and CUDA, host and device memories, Basic CUDA program structure, kernel calls, threads, blocks, grid, thread addressing, predefined variables

UNIT IV CUDA 9

CUDA - example code: vector and matrix addition, matrix multiplication, Using Windows and Linux environments to compile and execute simple CUDA programs, Linux make files, Timing execution time, CUDA events, Host synchronization

UNIT V BIOINFORMATICS AND PARALLEL COMPUTING 9

Bioinformatics and Parallel Computing- Bioinformatics Applications, Recent developments in Computational Biology and Nanotechnology and its impact on HPC

TOTAL : 45 PERIODS**OUTCOME**

At the end of this course students would be expected to learn parallel computing

REFERENCES

1. Highly Parallel Computing", by George S. Almasi and Alan Gottlieb
2. Advanced Computer Architecture: Parallelism, Scalability, Programmability, by Kai Hwang, McGraw Hill 1993
3. CUDA by Example- An Introduction to General-Purpose GPU Programming by Jason Sanders and Edwards Kandrot Addison-Wesley, 2011.
4. "Parallel Computer Architecture: A hardware/Software Approach", by David Culler Jaswinder Pal Singh, Morgan Kaufmann, 1999.
5. Jeffrey S. Vetter (Editor), Contemporary High Performance Computing: From Petascale toward Exascale (Chapman & Hall/CRC Computational Science) CRC Press, 2013
6. Georg Hager, Gerhard Wellein, Introduction to High Performance Computing, CRC Press, 2011
7. Wagner, S., Steinmetz, M., Bode, A., Müller, M.M. (Eds.), High Performance Computing in Science and Engineering, Garching/Munich, Springer Verlag, 2010

OBJECTIVES

The course intends to provide advanced theoretical knowledge on the organization and function of genomes, functional genomic analyses, and advanced methods and approaches in proteomics.

UNIT I STRUCTURE OF GENOMES, MAPPING AND SEQUENCING 9

Organization and structure of genomes in prokaryotes, eukaryotes, and organelles (chloroplast, mitochondrion); Genome mapping methods (genetic and physical); RAPD, RFLP, SNP analyses; Fluorescence In-Situ Hybridization (FISH) techniques; Advances in gene finding and functional prediction; Chain termination and chemical degradation sequencing methods.

UNIT II LARGE SCALE GENOMICS/ FUNCTIONAL GENOMICS ANALYSES 9

Genome-wide association (GWA) analysis; Comparative Genomic Hybridization (CGH); Massively parallel Signature Sequencing (MPSS); Whole genome shot-gun sequencing and its applications. Introduction of Next Generation Sequencing (NGS).

UNIT III TRANSCRIPTOMICS ANALYSES 9

Gene expression analysis by cDNA and oligonucleotide arrays; Micro array experimental analysis and data analysis. Methylome analysis using microarray; ChIP-on-Chip analysis. Bioinformatic analysis of large-scale microarray data for comparative transcriptomics.

UNIT IV SEPARATION AND PROCESSING OF PROTEINS FOR PROTEOMICS 9

Over-view of strategies used for the identification and analysis of proteins; Protein extraction from biological samples (Mammalian Tissues, Yeast, Bacteria, and Plant Tissues); 2-DE of proteins for proteome analysis; Liquid chromatography separations in proteomics (Affinity, Ion Exchange, Reversed-phase, and size exclusion); Enzymatic cleavage of proteins. Analysis of complex protein mixtures using Nano-liquid chromatography (Nano-LC) coupled to Mass-spectrometry analysis.

UNIT V MASS SPECTROMETRY AND COMPARATIVE PROTEOMICS 9

Common ionization methods for peptide/protein analysis; Introduction to Mass spectrometers; MALDI-TOF and LC-MS analyses; Comparative proteomics based on global in-vitro and in-vivo labeling of proteins/peptides followed by Mass-spectrometry. Analysis of post translational modification (PTM) of proteins; Characterization of protein interactions using yeast two-hybrid system and Protein microarrays; Proteomics informatics and analysis of protein functions.

TOTAL: 45 PERIODS**OUTCOME**

The students will acquire in-depth knowledge on the methods and approaches in genomics and proteomics areas which help them to carry out cutting edge academic and industrial research.

TEXTS/REFERENCES

1. S.P. Hunt and F. J. Livesey, (2000) Functional Genomics
2. N. K. Spur, B. D. Young, and S. P. Bryant (1998) ICRF Handbook of Genome Analysis Volume 1 & 2.
3. G. Gibson and S. V. Muse (2002) A primer of Genome Science
4. R. J. Reece (2004) Analysis of Genes and Genomes
5. Rinaldis E. D. and Lahm A (2007) DNA Microarrays. Horizon bioscience.
6. Simpson R. J. "Proteins and Proteomics - A Laboratory Manual". Cold Spring Harbour Laboratory Press, 2002.
7. Twyman R. M. "Principles of Proteomics". Taylor & Francis. 2004
8. O'Connor C. D. and Hames B. D. "Proteomics". Scion, 2008.
9. Schena M. "Protein Microarrays". Jones and Bartlett, 2005.
10. Smejkal G. B. and Lazarev A. V. "Separation methods in Proteomics". CRC Press, 2006.

OBJECTIVES

The course will provide advanced information on molecular pathogenesis of infectious diseases

UNIT I INTRODUCTION**5**

Discovery of microscope, Molecular Koch's postulates, Concepts of disease, Virulence, Pathogenic cycle, Vaccines and its historical perspective, Biofilms, quorum sensing, multidrug resistance.

UNIT II HOST DEFENSE AGAINST PATHOGENS AND BACTERIAL DEFENSE STRATEGIES**10**

Skin, mucosa, cilia secretions, physical movements, physical and chemical barriers to bacterial colonisation, Mechanism of killing by humoral and cellular defenses, Complement, Inflammatory process, Phagocytosis, Colonization, Adherence, Iron acquisition mechanisms, Bacterial defense strategies.

UNIT III MOLECULAR MECHANISMS OF VIRULENCE**10**

Virulence, Colonization factors, Microbial toxins, Secretion systems: General secretory pathway, Two-step secretion, Contact dependent secretion, Conjugal transfer system and Autotransporters.

UNIT IV MECHANISMS UNDERLYING MOLECULAR PATHOGENESIS (COMMON ENTERIC PATHOGENS)**10**

Shigella: Entry, Induction of macropinocytosis, Invasion of epithelial cells, Intracellular motility and spread, Apoptotic killing of macrophages, Virulence factors involved. **E.coli:** Enterotoxigenic *E.coli* (ETEC), labile & stable toxins, Enteropathogenic *E.coli* (EPEC), type III secretion, Cytoskeletal changes, intimate attachment; Enterohaemorrhagic *E.coli* (EHEC), Mechanism of bloody diarrhea and Hemolytic Uremic Syndrome, Enteraggregative *E.coli* (EAEC). **Vibrio Cholerae:** Cholera toxin, Co-regulated pili, filamentous phage, survival.

UNIT V MECHANISMS UNDERLYING MOLECULAR PATHOGENESIS (COMMON NON-ENTERIC PATHOGENS)**10**

Mycobacterium tuberculosis: The Mycobacterial cell envelope, Route of entry, Uptake by macrophages, Latency and persistence, Entry into and survival in phagocytes, Immune response against MTB, MTB virulence factors, Emergence of resistance. **Influenza virus:** Intracellular stages, Neuraminidase and Haemagglutinin in entry, M1 & M2 proteins in assembly and disassembly, action of amantadine. **Plasmodium:** Lifecycle, erythrocyte stages, transport mechanism and processes to support the rapidly growing schizont, parasitophorous vacuoles and knob protein transport, Antimalarials based on transport processes.

TOTAL: 45 PERIODS**OUTCOME**

The subject will help the student towards understanding the virulence of the pathogen and Host-parasite interactions for advanced academic and industrial research in molecular pathogenesis.

TEXTS/REFERENCES

1. Salyers, Abigail A. "Bacterial Pathogenesis: A Molecular Approach"
2. Groisman, "Principles of Bacterial Pathogenesis".
3. Waksman, Gabriel and Michael Caparon "Structural Biology of Bacterial Pathogenesis".
4. Clark, Virginia L. "Bacterial Pathogenesis"
5. Williams, Peter "Bacterial Pathogenesis" (Methods in Microbiology)
6. Mc Clane, Bruce A. "Microbial Pathogenesis"

7. Madigan, Michael T. "Biology of Microorganisms"
8. Stanley, "Genetic analysis of Pathogenic Bacteria".
9. Hacker, Jorg "Molecular Infection Biology"

BT7074

BIOCATALYSTS AND ENZYME TECHNOLOGY

**L T P C
3 0 0 3**

OBJECTIVES

The course intends to give advanced knowledge about Biocatalysts, Enzyme kinetics, immobilization and enzymatic biotransformation of drugs

UNIT I BASICS OF ENZYMES AS BIOCATALYSIS

9

Introduction to enzymes, Classification, Sources, Mechanism of enzyme action. Strategies of purification of enzymes, criteria of purity, molecular weight determination and characterization of enzymes, Enzymes of biological importance - Acetylcholinesterase, angiotensin converting enzyme (ACE), ACE Inhibitors, HMG Co A reductase inhibitors, pseudocholinesterase, 5 nucleotidase (5NT), glucose-6-phosphate dehydrogenase (GPD), CKisoforms, immunoreactive trypsinogen (IRT) and chymotrypsin; amylase isoenzymes

UNIT II KINETICS OF ENZYME ACTION

9

Methods for investigating the kinetics of Enzyme catalysed reactions – Initial velocity Studies, Estimation of Michaelis Menten parameters, Effect of pH and temperature on enzyme activity, kinetics of inhibition. Modeling of rate equations for single and multiple substrate reactions.

UNIT III IMMOBILIZED ENZYMES

9

Techniques of enzyme immobilization; kinetics of immobilized enzymes, effect of solute, partition & diffusion on the kinetics of immobilized enzymes, design and configuration of immobilized enzyme reactors; applications of immobilized enzyme technology, Economic argument for immobilization

UNIT IV ENZYMES IN FUNCTIONAL GROUP TRANSFORMATION

9

Functional group interconversion using enzymes (hydrolysis reaction, oxidation/reduction reactions, C-C bond formations), Retrosynthetic biocatalysis, Chemoenzymatic synthesis of natural products. Industrial process using enzymes for production of drugs, fine chemicals and chiral intermediates.

UNIT V ENZYMATIC TRANSFORMATION

9

Reaction engineering for enzyme-catalyzed biotransformations. Catalytic antibodies. Biocatalysts from extreme Thermophilic and Hyperthermophilic microorganisms (extremozymes). The design and construction of novel enzymes, artificial enzymes, Biotransformation of drugs (hydroxylation of Steroids), Host Guest Complexation chemistry, enzyme design using steroid templates, enzymes for production of drugs, fine chemicals and chiral intermediates.

TOTAL : 45 PERIODS

OUTCOME

The students will acquire knowledge in all aspect of Biocatalysis, enzyme kinetics and immobilization. The enzymatic transformation will give theoretical idea about drug biotransformation.

TEXTS/REFERENCES

1. Blanch, H.W., Clark, D.S. Biochemical Engineering, Marcel Dekker, 1997
2. Lee, James M. Biochemical Engineering, PHI, USA, 1982.

3. Bailey J.E. & Ollis, D.F. Biochemical Engineering Fundamentals, 2nd Ed., McGraw Hill, 1986
4. Faber, Kurt "Biotransformations in organic chemistry : A Textbook" 5th Edition. Springer 2008.
5. Enzyme catalysis in organic synthesis (Vol I-III); Eds by K.Drauz and H. Waldmann. Willey-VCH (ISBN: 3-527-29949-1)
6. Hydrolases in organic synthesis (regio and stereoselective biotransformations). U. T. Bornscheuer and R. J. Kazlauskas. Willey-VCH. (ISBN: 3-527-30104-6).
7. Stereoselective biocatalysis. Ed. R.N. Patel. Marcel Dekker. (ISBN: 0-8247- 8282-8)

BT7075

COMMUNICATION SKILL DEVELOPMENT

**L T P C
2 0 2 3**

OBJECTIVES

To enhance the overall capability of students and to equip them with the necessary communication and soft skills to enable them to excel in their profession

UNIT I PROCESS OF COMMUNICATION

12

Concept of effective communication- Setting clear goals for communication; Determining outcomes and results; Initiating communication; Avoiding breakdowns while communicating; Creating value in conversation; Barriers to effective communication; Non verbal communication- Interpreting non verbal cues; Importance of body language, Power of effective listening; recognizing cultural differences

UNIT II PRESENTATION SKILLS

12

Formal presentation skills; Preparing and presenting using Over Head Projector, Power Point; Defending Interrogation; Scientific poster preparation & presentation; Participating in group discussions

UNIT III TECHNICAL WRITING SKILLS

12

Types of reports; Layout of a formal report; Scientific writing skills: Importance of communicating Science; Problems while writing a scientific document; Plagiarism; Scientific Publication Writing: Elements of a Scientific paper including Abstract, Introduction, Materials & Methods, Results, Discussion, References; Drafting titles and framing abstracts

UNIT IV COMPUTING SKILLS FOR SCIENTIFIC RESEARCH

12

Web browsing for information search; search engines and their mechanism of searching; Hidden Web and its importance in Scientific research; Internet as a medium of interaction between scientists; Effective email strategy using the right tone and conciseness

UNIT V RESUME / REPORT PREPARATION / LETTER WRITING

12

Students prepare their own resume and report, Presentation- Students make presentations on given topics, Group Discussion- Students participate in group discussions, and Interview Skills- Students participate in Mock Interviews

TOTAL: 60 PERIODS

OUTCOME

The course will enhance soft skills and interpersonal skills, which will make their transition from college to work place smoother and help them excel in their job.

REFERENCE

1. 1 Mohan Krishna and N.P. Singh, Speaking English effectively, Macmillan, 2003.

OBJECTIVES

To familiarize the student with quantitative approaches for analyzing cellular metabolism and the use of theoretical and experimental tools that can give insights into the structure and regulation of metabolic networks. A central aspect of the course is to identify the optimal strategy for introducing directed genetic changes in the microorganisms with the aim of obtaining better production strains. Case studies will be taken up on metabolically-engineered products and processes in various expression systems.

UNIT I METABOLIC FLUX ANALYSIS**9**

Introduction to metabolic engineering, comprehensive models of cellular reactions with stoichiometry and reaction rates; metabolic flux analysis of exactly/over/under determined systems. Shadow price, sensitivity analysis.

UNIT II TOOLS FOR EXPERIMENTALLY DETERMINING FLUX THROUGH PATHWAYS**9**

Monitoring and measuring the metabolome, Methods for the experimental determination of metabolic fluxes by isotope labeling metabolic fluxes using various separation-analytical techniques. GC-MS for metabolic flux analysis, genome wide technologies: DNA /phenotypic microarrays and proteomics.

UNIT III CONSTRAINT BASED GENOMIC SCALE METABOLIC MODEL**9**

Development of Genomic scale metabolic model, Insilico Cells:studying genotype-phenotype relationships using constraint-based models, case studies in *E. coli*, *S.cerevisiae* metabolic network reconstruction methods, optimization of metabolic network, Identification of targets for metabolic engineering; software and databases for genome scale modeling

UNIT IV METABOLIC CONTROL ANALYSIS AND KINETIC MODELING**9**

Fundamental of Metabolic Control Analysis, control coefficients and the summation theorems, Determination of flux control coefficients. Multi-substrate enzyme kinetics, engineering multifunctional enzyme systems for optimal conversion, and a multi scale approach for the predictive modeling of metabolic regulation.

UNIT V CASE STUDIES IN METABOLIC ENGINEERING**9**

Metabolic engineering examples for bio-fuel, bio-plastic and green chemical synthesis. Study of genome scale model in various systems for the production of green chemicals using software tools. Validation of the model with experimental parameters.

TOTAL : 45 PERIODS**OUTCOME**

This course work will provide essential knowledge for the students to make their career in bioprocess Industries.

TEXT BOOKS

1. Stephanopoulos, G.N. "Metabolic Engineering: Principles and Methodologies". Academic Press / Elsevier, 1998.
2. Lee, S.Y. and Papoutsakis, E.T. "Metabolic Engineering". Marcel Dekker, 1998.
3. Nielsen, J. and Villadsen, J. "Bioreaction Engineering Principles". Springer, 2007.
4. Smolke, Christiana D., "The Metabolic Pathway Engineering Handbook Fundamentals", CRC Press Taylor & Francis, 2010.

REFERENCES

1. Voit, E.O. "Computational Analysis of Biochemical Systems : A Practical Guide for Biochemists and Molecular Biologists". Cambridge University Press, 2000.
2. Scheper, T. "Metabolic Engineering" Vol 73 (Advances in Biochemical Engineering Biotechnology) Springer, 2001.
3. Cortassa, S. et al, " An Introduction to Metabolic and Cellular Engineering", World Scientific Publishing, 2002.
4. Kholodenko, Boris N and H. V. Westerhoff "Metabolic Engineering in the Post Genomic Era", Horizon Bioscience, 2004.

BT7077

NANOBIOTECHNOLOGY

L T P C
2 0 2 3

OBJECTIVES

The course will provide advanced knowledge in field of Nanobiology and Nano medicine

UNIT I NANOSCALES

12

What is meant by Nanoscale – Nanoscale Processes – Physical and Chemical Properties of Materials in the Nanoscales - Nanoscale Measurements.

UNIT II PROPERTIES AND MEASUREMENTS OF NANOMATERIALS

12

Optical Properties – Absorption and Fluorescence – Microscopy measurements – SEM – TEM - AFM and STM. Confocal and TIRF. Imaging

UNIT III NANOBIOLOGY

12

Properties of DNA and motor proteins – Measurements of Conductivity of DNA nanowires and angular properties of motor - Lessons from Nature on making nanodevices.

UNIT IV BIOCONJUGATION OF NANOMATERIALS TO BIOLOGICAL MOLECULES

12

Reactive Groups on biomolecules (DNA & Proteins) - Conjugation to nanoparticles (ZnSFe₃O₄) - Uses of Bioconjugated Nanoparticles

UNIT V NANO DRUG DELIVERY

12

Various Drug Delivery Systems – aerosol - Inhalants - Injectibles – Properties of Nanocarriers – Efficiency of the Systems.

PRACTICALS

15

1. Preparation of Silver Nanoparticles by Chemical Methods
2. Characterization of ZnS nanoparticles by Optical Methods.
3. Templated Synthesis of Fe₃O₄ Nanoparticles
4. AFM of ZnS nanoparticles.
5. SEM & HRTEM Analysis of silver and Fe₃O₄ Nanoparticles
6. Bacterial Synthesis of ZnS Nanoparticles.
7. Confocal & TIRF Microscopy of ZnS particles Interaction with Cell lines

TOTAL : 60 PERIODS

OUTCOME

After the completion of course, the students would have learnt advanced theoretical knowledge in nano science and its application in new bioconjugation and nano delivery system to carry out cutting edge research in future.

TEXTS/REFERENCES

1. Niemeyer, Cristof M and Mirkiu, Chad A. "Nanobiotechnology: Concepts, Applications and Perspectives" Wiley-VCH, 2004.
2. Shoseyov, Oded and Ilan Levy "NanoBioTechnology: BioInspired Devices and Materials of the Future", Humana Press, 2007.
3. Rosenthal, Sandra J and D. W. Wright "NanoBiotechnology Protocols" Humana Press, 2005.

BT7078 RESEARCH AND RESEARCH METHODOLOGY IN BIOTECHNOLOGY L T P C 3 0 0 3

OBJECTIVES

The course will provide knowledge about the objectives to perform research and for interpretation of data from experimental results and presenting technical publications.

UNIT I RESEARCH AND ITS METHODOLOGIES (WITH EXAMPLES) 9

Objectives of research; research process – observation, analysis, inference, hypothesis, axiom, theory, experimentation; Types of research (basic, applied, qualitative, quantitative, analytical etc); Features of translational research, the concept of laboratory to market (bench to public) and Industrial R&D.

UNIT II RESEARCH IN BIOTECHNOLOGY – AN OVERVIEW 9

Biological systems and their characteristics that influence the type and outcome of research; Exploratory and product-oriented research in various fields of biotechnology (health, agri, food, industrial etc). Types of expertise and facilities required; Interdisciplinary nature of biotech research; Sources of literature for biotech research

UNIT III EXPERIMENTAL RESEARCH: BASIC CONCEPTS IN DESIGN AND METHODOLOGY 9

Precision, accuracy, sensitivity and specificity; major experimental variables, biochemical measurements, types of measurements, enzymes and enzymatic analysis, antibodies and immunoassays, instrumental methods, bioinformatics and computation, experimental planning general guidelines

UNIT IV RESULTS AND ANALYSIS 9

Importance and scientific methodology in recording results, importance of negative results, different ways of recording, industrial requirement, artifacts versus true results, types of analysis (analytical, objective, subjective) and cross verification, correlation with published results, discussion, outcome as new idea, hypothesis, concept, theory, model etc.

UNIT V SCIENTIFIC AND TECHNICAL PUBLICATION 9

Different types of scientific and technical publications in the area of biotechnology, and their specifications, Ways to protect intellectual property – Patents, technical writing skills, definition and importance of impact factor and citation index; Assignment in technical writing

TOTAL : 45 PERIODS

OUTCOME

After the completion of course, students will able to design, conduct, and interpret research outcomes for academic and industrial research needs.

TEXT/REFERENCES

1. Essentials of Research Design and Methodology Geoffrey R. Marczyk, David DeMatteo, David Festinger, 2005 John Wiley & Sons Publishers, Inc
2. Biochemical Calculations: How to Solve Mathematical Problems in General Biochemistry, 2nd Edition, Irwin H. Segel, 1976 John Wiley & Sons Publishers, Inc
3. Guide to Publishing a Scientific paper, Ann M. Korner, 2004, Bioscript Press.

BT7079 TISSUE ENGINEERING AND REGENERATIVE MEDICINE

**L T P C
3 0 0 3**

OBJECTIVES

The course intends to give advanced theoretical knowledge on tissue engineering, Stem cells and its biological applications

UNIT I INTRODUCTION

9

Introduction to tissue engineering: Basic definition; current scope of development; use in therapeutics, cells as therapeutic agents, cell numbers and growth rates, measurement of cell characteristics morphology, number viability, motility and functions. Measurement of tissue characteristics, appearance, cellular component, ECM component, mechanical measurements and physical properties.

UNIT II TISSUE ARCHITECTURE

9

Tissue types and Tissue components, Tissue repair, Basic wound healing events, Applications of growth factors: Role of VEGF. Angiogenesis, Basic properties, Cell-Matrix & Cell-Cell Interactions, Control of cell migration in tissue engineering.

UNIT III BIOMATERIALS

9

Biomaterials: Properties of Biomaterials, Surface, bulk, mechanical and biological properties. Scaffolds & tissue engineering, Types of Biomaterials, biological and synthetic materials, Biopolymers, Applications of biomaterials, Modifications of Biomaterials, Role of Nanotechnology.

UNIT IV BASIC BIOLOGY OF STEM CELLS

9

Stem Cells : Introduction, Types & sources of stem cell with characteristics: hematopoietic differentiation pathway, Potency and plasticity of stem cells, sources, embryonic stem cells, hematopoietic and mesenchymal stem cells, Stem Cell markers, FACS analysis, Differentiation, Stem cell systems- Liver, neuronal stem cells, cancer stem cells, induced pluripotent stem cells.

UNIT V CLINICAL APPLICATIONS

9

Stem cell therapy, Molecular therapy, In vitro organogenesis, Neurodegenerative diseases, spinal cord injury, heart disease, diabetes, burns and skin ulcers, muscular dystrophy, orthopaedic applications, Stem cells and Gene therapy, Physiological models, tissue engineering therapies, product characterization, components, safety, efficacy. Preservation –freezing and drying. Patent protection and regulation of tissue-engineered products, ethical issues.

TOTAL : 45 PERIODS

OUTCOME

The students will acquire knowledge in advanced methods to carry out cutting edge academic and industrial research.

TEXTS/REFERENCES

1. Bernhard O.Palsson, Sangeeta N.Bhatia, "Tissue Engineering" Pearson Publishers 2009.
2. Meyer, U.; Meyer, Th.; Handschel, J.; Wiesmann, H.P. Fundamentals of Tissue Engineering and Regenerative Medicine. 2009.
3. Bernard N. Kennedy (editor). New York : Nova Science Publishers, c2008. Stem cell transplantation, tissue engineering, and cancer applications
4. Raphael Gorodetsky, Richard Schäfer. Cambridge : RSC Publishing, c2011. Stem cell-based tissue repair.
5. R. Lanza, I. Weissman, J. Thomson, and R. Pedersen, Handbook of Stem Cells, Two-Volume, Volume 1-2: Volume 1-Embryonic Stem Cells; Volume 2-Adult & Fetal Stem Cells, 2004, Academic Press.
6. R. Lanza, J. Gearhart et al (Eds), Essential of Stem Cell Biology, 2006, Elsevier Academic press.
7. J. J. Mao, G. Vunjak-Novakovic et al (Eds), Translational Approaches In Tissue Engineering & Regenerative Medicine" 2008, Artech House, INC Publications. Naggy N. Habib, M.Y. Levicar, , L. G. Jiao,., , and N. Fisk, Stem Cell.
8. Repair and Regeneration, volume-2, 2007, Imperial College Press.

BC7003

GENERAL BIOLOGY

L T P C
3 0 0 3

OBJECTIVES

The course intends to introduce general concepts in Biology. It serves as a primer to the more advanced courses in Biology.

UNIT I CELL BIOLOGY

9

Structural organization of prokaryotic and eukaryotic cells, Cellular Components – Cytoskeleton – components of Cytoskeleton, Microtubules, Intermediate filaments – Microfilaments, Endoplasmic reticulum, Golgi complex, Types of vesicles - transport and their functions, Lysosomes. Cell cycle, Biomembranes- Structural organization- Models of a plasma membrane, Membrane permeability- Transport across cell membranes

UNIT II INTRODUCTION TO BIOMOLECULES

9

Amino Acids, Nucleic Acids, Covalent Structures of Proteins and Nucleic Acids , Tertiary and Quaternary structures of Proteins, Introduction to Carbohydrates and Lipids.

UNIT III ENZYMES AND METABOLISM

9

Introduction to Enzymes. Rates of Enzymatic Reactions. Enzymatic Catalysis. Introduction to Metabolism, Glycolysis, Glycogen Metabolism, Citric Acid Cycle, Electron Transport and Oxidative Phosphorylation, Introduction to Lipid Metabolism, Amino Acid Metabolism and Nucleotide Metabolism.

UNIT IV GENES AND REGULATION

9

Genes and Chromosomes, DNA replication and recombination, transcription, translation, prokaryotic and eukaryotic gene regulation

UNIT V GENETIC ENGINEERING

9

Restriction enzymes, DNA modifying enzymes, Gene manipulation, Host cells and vectors, PCR, Applications of Genetic engineering in biotechnology: production of enzymes, therapeutic proteins.

OUTCOME

At the end of the course, the student will be familiar with organization of the cell, bio-molecules and basic principles of biochemistry and molecular biology.

REFERENCES

1. Voet and Voet, Biochemistry 3e Wiley 2004 ISBN: 978-0-471-19350-0
2. Nelson and Cox, Lehninger Principles of Biochemistry 5e W H Freeman & Co 2009 ISBN: 978-0-716-77108-1
3. Jocelyn, E. Krebs., Stephen, T. Kilpatrick., Elliott S Goldstein, Lewin's Gene X, 10th Edition 2011, Jones and Bartlett Publishers.
4. An introduction to Genetic engineering, Desmond S.T. Nicholl., Cambridge University Press, 3rd Edition., 2008

BC7002

DRUG DISCOVERY

**L T P C
3 0 0 3**

OBJECTIVES

To introduce drug discovery pipeline, high throughput screening, testing and regulatory affairs.

UNIT I DRUGS AND THEIR INTERACTIONS 9

Introduction to Drugs: Drug nomenclature, Routes of drug administration and dosage forms, 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 II DRUG DISCOVERY PIPELINE AND CADD 9

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 III DRUG TOXICITY, ASSAYS AND TESTING 9

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

UNIT IV DRUG REGULATORY AFFAIRS 9

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 V INTELLECTUAL PROPERTY RIGHTS AND PATENTS 9

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 PERIODS

OUTCOME

Students will gain knowledge on different aspects of drug discovery process and regulatory affairs. This will be useful for industrial and academic research.

REFERENCES

1. Drugs: From discovery to approval 2nd ed by Rick NG. Wiley Blackwell (2009)
2. Intellectual Property Rights by Deborah E. Bouchoux,. Delmar Cenage Learning. 2005
3. Burger's Medicinal Chemistry and Drug discovery. Volume 2, Drug Discovery and development.6th Edition. Ed Donald J AbrahamWiley-Interscience.
4. Essentials of Medical Pharmacology, 6the Edition (Hardcover) by TripathiKd. Publisher: Jaypee Brothers (2008)
5. Laws of Patents: Concepts and Cases Edited by A. V. Narasimha Rao © 2005 The ICFAI University Press
6. Intellectual Property Rights In India: General Issues And Implications by Prankrishna Pal. Publisher: Deep & Deep Publications Pvt.ltd (2008)

BC7004

MOLECULAR EVOLUTION AND PHYLOGENY

**L T P C
3 0 0 3**

OBJECTIVES

To enable students to understand molecular aspects of evolution, models of evolution, genome evolution

UNIT I INTRODUCTION TO EVOLUTION

9

History of evolution of life on earth: Chemical basis of evolution, Evolution of DNA, RNA and proteins, origin of the genetic code. Hardy-Weinberg equilibrium; Evolutionary changes by mutation, gene flow, genetic drift and natural selection.

UNIT II MOLECULAR EVOLUTION AND INSERTION ELEMENTS

9

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

UNIT III MODELS OF EVOLUTION

9

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

UNIT IV MOLECULAR CLOCK, MITOCHONDRIA IN EVOLUTION

9

9

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 V GENOME EVOLUTION, HUMAN GENOME PROJECT 9

Evolution of the genome: Human Genome Project, ENCODE, Genome 10 K, Genome duplication (Ohno's hypothesis), Gene duplication, Exon Shuffling, Concerted evolution.

TOTAL : 45 PERIODS

OUTCOME

The student will be able to appreciate the molecular basis of evolution, phylogeny and different models of evolution.

REFERENCES

1. Molecular Evolution by Wen Hsiung-Li, 1997, Sinauer Associates, Sunderland, MA. ISBN 0878934634.
2. Evolution (3rd Edition) by Ridley, M., 2004, Blackwell Science. ISBN 1-4051-0345-0

BC7005

NEXT GENERATION SEQUENCING

**L T P C
2 0 2 3**

OBJECTIVES

To introduce students to the emerging area of next generation sequencing. To familiarize them with NGS platforms, big data analysis and applications of R package.

UNIT I NGS PLATFORMS, SEQUENCING AND ALIGNMENT 9

NGS Platforms: Introduction to NGS, Roche/454 FLX, Illumina/Solexa Genome Analyzer, Applied Biosystems SOLiD system, Helicos Heliscope, Pacific Biosciences/single molecule real time (SMRT) sequencing, Genome assembly algorithms: Alignment of short-reads to reference genome using spaced seed (ELAND, SOAP), index-filtering algorithm (SeqMap), quality-score (RMAP), q-filter algorithm (SHRiMP), FM-index (Bowtie, BWA, SOAP2), 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 II ASSEMBLY AND CONTIG GENERATION 9

De-novo assembly: 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 using SOAPdenovo, ABySS, OPERA and RACA.

UNIT III R PACKAGE IN NGS ANALYSIS 9

Application of R in NGS analysis: 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 IV APPLICATIONS OF NGS 9

Biological applications of NGS: Whole-genome sequencing, Exome sequencing, Transcriptome sequencing, Epigenome sequencing, Interactome sequencing, methylome sequencing.

UNIT V BIG DATA AND HIGH PERFORMANCE COMPUTING IN OMICS 9

BIG DATA in OMICS: Big data industry standards, Data acquisition, cleaning, distribution, and best practices, Visualization and design principles of big data infrastructures, Biological

databases for big data management, High Performance Computing, grid, and cloud computing for omics sciences, Real-Time Processing of Proteomics Data Using Hadoop.

TOTAL : 45 PERIODS

OUTCOME

The student will be able to understand NGS data, its applications and usage of R package for analysis.

REFERENCES

1. Stuart M. Brown Next-generation DNA sequencing Informatics Cold Spring Harbor Laboratory 2013 ISBN 1936113872
2. Eija Korpelainen, Jarno Tuimala, Panu Somervuo, Mikael Huss, Garry Wong. RNA-seq Data Analysis: A Practical Approach. Chapman & Hall/CRC, 2014. ISBN-13: 978-1466595002
3. Hillman Chris, Ahmad Yasmeen, Whitehorn Mark, and Cobley Andy Near real-time processing of proteomics data using HADOOP Mary ann Liebert, Inc- Big Data. 2014 2 (1): BD44- BD49.
4. Sowe Sulayman K. and Zettsu Koji Curating Big Data Made Simple: Perspectives from Scientific Communities Big Data. 2014 2 (1): 23-33
5. Melanie Swan The quantified self: Fundamental Disruption in Big Data Science and Biological Discovery Mary ann Liebert, Inc. Big data ,2013, 1(2): BD85-99
6. Wong Lee-Jun C. (ed.) Next generation sequencing: Translation to Clinical Diagnostics Springer 2013 ISBN 978-1-4614-7001-4
7. Michal Janitz Next-generation genome sequencing: Towards Personalized Medicine Wiley-VCH, 2008 ISBN 3527644733

BC7006

SIGNAL PROCESSING IN BIOTECHNOLOGY

**L T P C
3 0 0 3**

UNIT I SIGNALS AND SYSTEMS

9

Signals and Systems -Example Signals: Sinusoids, complex exponentials, impulse and step signals, - LTI Systems and properties: impulse response, convolution, Eigenfunctions of LTI systems-Example: Biological time series signals from gene expression microarrays

UNIT II TRANSFORMS

9

Transforms-Discrete time fourier transform-Fast fourier transform-Sampling theorems-Biological example: Fourier transform of DNA sequences reveal inherent periodicities

UNIT III DETECTION THEORY (NON-BAYESIAN)

9

Detection theory (Non-Bayesian)-Hypothesis testing-Neyman-Pearson lemma-Likelihood ratio test-Matched filter-Metrics: ROC curve, area-under-the-ROC curve, sensitivity, specificity

UNIT IV ESTIMATION THEORY (NON-BAYESIAN)

9

Estimation theory (Non-Bayesian)-Sufficient statistic-Bias and Minimum Variance unbiased estimators-Maximum likelihood estimators-Efficient estimation

UNIT V BAYESIAN DETECTION AND ESTIMATION

9

Bayesian Detection and Estimation-Bayesian statistics: Incorporating prior knowledge-Minimum mean square error -Linear MMSE estimator-Maximum A Posteriori Probability detection

TOTAL : 45 PERIODS

REFERENCES

1. Oppenheim and A. Willsky, "Signals and Systems," Prentice Hall
2. S. M. Kay, "Fundamentals of Statistical Signal Processing: Estimation Theory", Prentice Hall PTR, 1993.
3. S. M. Kay, "Fundamentals of Statistical Signal Processing: Detection Theory", Prentice Hall PTR, 1998.

BP7071

PHARMACOGENOMICS

**L T P C
3 0 0 3**

OBJECTIVES:

The course intends to provide knowledge about Pharmacogenomics and drug design using genomic applications for drug action and toxicity.

UNIT I INTRODUCTION TO PHARMACOGENOMICS 9

Pharmacogenetics-The roots of pharmacogenomics, It is not just pharmacogenomics, Genetic drug response profiles, the effect of drugs on Gene expression, pharmacogenomics in drug discovery and drug development.

UNIT II THE HUMAN GENOME 9

Expressed sequence Tags (EST) and computational biology, Microbial genomics, computational analysis of whole genomes, computational genome analysis, Genomic differences that affect the outcome of host pathogen interactions: A template for the future of whole genome-based pharmacological science.

UNIT III ASSOCIATION STUDIES IN PHARMACOGENOMICS 9

Viability and ADR in drug response: contribution of genetic factor, Multiple inherited genetic factors influence the out come of drug treatments, Plasma binding proteins, Drug targets.

UNIT IV GENOMICS APPLICATIONS FOR DRUG ACTION AND TOXICITY 9

Genomics, Proteomics, Bioinformatics, The pharmaceutical process, applications of pharmaceutical industry, Understanding biology and diseases, Target identification and validation, Drug candidate identification and optimization.

UNIT V PHARMACOGENOMICS AND DRUG DESIGN 9

The need of protein structure information, protein structure and variation in drug targets-the scale of problem, Mutation of drug targets leading to change in the ligand binding pocket.

TOTAL: 45 PERIODS

OUTCOME:

At the completion of course, the student would have learnt advanced pharmacogenomics enabling him for cutting edge academic and industrial research.

TEXTS/REFERENCE:

1. Licinio, Julio and Ma-Li Wong, "Pharmacogenomics: The Search for the Individualized Therapies", Wiley-VCH, 2002
2. Chabrabarthy, Chiranjib and Bhattacharyya, Atane, "Pharmacogenomics: An Approach to New Drugs Development", 2004.
3. Othstein, Mark, A. "Pharmacogenomics: Social, Ethical and Clinical Dimensions", Wiley-Liss, 2003

UNIT I MICRO ARRAYS IN GENOMICS**9**

Designing and producing microarrays; types of microarrays; cDNA microarray technology; Oligonucleotide arrays; Sample preparation, labeling, hybridization, generation of microarray data. Transcriptomics using cDNA and oligonucleotide arrays.

UNIT II NEXT GENERATION SEQUENCING TECHNOLOGIES**9**

Over-view of Next Generation Sequencing (NGS) technologies; Principles of NGS by Roche/454, Illumina, Life Technologies, Pacific Biosciences, Ion Torrent technologies; Applications of NGS to disease diagnosis and personalized medicine.

UNIT III PROTEIN MICRO ARRAYS AND YEAST TWO-HYBRID SYSTEM**9**

Types of protein arrays; Protein microarray fabrication; Experimental analysis of proteins arrays. Data acquisition and processing; Applications of protein microarray types. Principles and methods in yeast two-hybrid system, Advances in yeast two hybrid system and its applications.

UNIT IV TWO-DIMENSIONAL GELECTRO PHORESIS OF PROTEINS**9**

Sample preparation, First-dimension IEF with IPG; Second dimensional separation of proteins; Image analysis of 2-DE gels; DIGE, Protein expression profiling and comparative proteomics of complex proteomes using 2-DE.

UNIT V MASS-SPECTROMETRY**9**

Basics of Mass-spectrometry (MS) and bimolecular analysis; Common ionization methods for peptide/protein analysis; Principles of Time of Flight (TOF), Ion Trap (IT), and Orbitrap mass analyzers; Mass spectrometry based proteomics: MALDI-TOF, Nano-LC-MS; Gas-chromatography coupled to Mass spectrometry; Mass-spectrometry analysis of Post-Translational Modifications of proteins.

TOTAL : 45 PERIODS**REFERENCES**

1. Schena M. (2000) DNA Microarrays _ A Practical Approach. Oxford University Press.
2. Rinaldis E. D. and Lahm A (2007) DNA Microarrays. Horizon bioscience. Causton,H.C
3. Muller H. J. and Roder T. (2006) Microarrays. Elsevier Academic Press
4. Causton H. C., Quackenbush J., and Brazma A. (2004) A Beginner's Guide
5. Microarray. Gene Expression Data Analysis. Blackwell Publishing.
6. Schena M. (2005) Protein Microarrays. Jones and Bartlett Publishers
7. O'Connor C. D. and Hames B. D. (2008) Proteomics. Scion Publishing Ltd.
8. Hoffman E. D. and Stroobant V. (2007) Mass Spectrometry – Principles and Applications. John Wiley & Sons Ltd.

OBJECTIVES:

- To understand big data analytics as the next wave for businesses looking for competitive advantage
- To understand the financial value of big data analytics
- To explore tools and practices for working with big data

- To understand how big data analytics can leverage into a key component
- To understand how to mine the data
- To learn about stream computing
- To know about the research that requires the integration of large amounts of data

UNIT I INTRODUCTION TO BIG DATA 9

Analytics – Nuances of big data – Value – Issues – Case for Big data – Big data options Team challenge – Big data sources – Acquisition – Nuts and Bolts of Big data. Features of Big Data - Security, Compliance, auditing and protection - Evolution of Big data – Best Practices for Big data Analytics - Big data characteristics - Volume, Veracity, Velocity, Variety – Data Appliance and Integration tools – Greenplum – Informatica

UNIT II DATA ANALYSIS 9

Evolution of analytic scalability – Convergence – parallel processing systems – Cloud computing – grid computing – map reduce – enterprise analytic sand box – analytic data sets – Analytic methods – analytic tools – Cognos – Microstrategy - Pentaho. Analysis approaches – Statistical significance – business approaches – Analytic innovation – Traditional approaches – Iterative

UNIT III STREAM COMPUTING 9

Introduction to Streams Concepts – Stream data model and architecture - Stream Computing, Sampling data in a stream – Filtering streams – Counting distinct elements in a stream – Estimating moments – Counting oneness in a window – Decaying window - Realtime Analytics Platform(RTAP) applications IBM Infosphere – Big data at rest – Infosphere streams – Data stage – Statistical analysis – Intelligent scheduler – Infosphere Streams

UNIT IV PREDICTIVE ANALYTICS AND VISUALIZATION 9

Predictive Analytics – Supervised – Unsupervised learning – Neural networks – Kohonen models – Normal – Deviations from normal patterns – Normal behaviours – Expert options – Variable entry - Mining Frequent itemsets - Market based model – Apriori Algorithm – Handling large data sets in Main memory – Limited Pass algorithm – Counting frequent itemsets in a stream – Clustering Techniques – Hierarchical – K- Means – Clustering high dimensional data Visualizations - Visual data analysis techniques, interaction techniques; Systems and applications:

UNIT V FRAMEWORKS AND APPLICATIONS 9

IBM for Big Data – Map Reduce Framework - Hadoop – Hive - – Sharding – NoSQL Databases - S3 - Hadoop Distributed file systems – Hbase – Impala – Analyzing big data with twitter – Big data for E-Commerce – Big data for blogs.

TOTAL : 45 PERIODS

OUTCOMES:

Upon Completion of the course, the students will be able to

- Identify the need for big data analytics for a domain
- Use Hadoop, Map Reduce Framework
- Apply big data analytics for a give problem
- Suggest areas to apply big data to increase business outcome
- Contextually integrate and correlate large amounts of information automatically to gain faster insights.

REFERENCES

1. Frank J Ohlhorst, “Big Data Analytics: Turning Big Data into Big Money”, Wiley and SAS Business Series, 2012.
2. Colleen Mccue, “Data Mining and Predictive Analysis: Intelligence Gathering and Crime Analysis”, Elsevier, 2007

3. Michael Berthold, David J. Hand, Intelligent Data Analysis, Springer, 2007.
4. Anand Rajaraman and Jeffrey David Ullman, Mining of Massive Datasets, Cambridge University Press, 2012.
5. Bill Franks, "Taming the Big Data Tidal Wave: Finding Opportunities in Huge Data Streams with Advanced Analytics", Wiley and SAS Business Series, 2012.
6. Paul Zikopoulos, Chris Eaton, Paul Zikopoulos, "Understanding Big Data: Analytics for Enterprise Class Hadoop and Streaming Data", McGraw Hill, 2011.
7. Paul Zikopoulos, Dirk deRoos, Krishnan Parasuraman, Thomas Deutsch , James Giles, David Corrigan, "Harness the Power of Big data – The big data platform", McGraw Hill, 2012.
8. Glenn J. Myatt, Making Sense of Data, John Wiley & Sons, 2007
9. Pete Warden, Big Data Glossary, O'Reilly, 2011.
10. Jiawei Han, Micheline Kamber "Data Mining Concepts and Techniques", Second Edition, Elsevier, Reprinted 2008.