

## BI. HCT-1.3 C-Programming and C++

Total : 60 hrs

**C programming****Unit I – C- Language**

Introduction: History Of C Language, Getting Started With C, The Character Set – Alphabets, Digits And Special Symbols, Constants – Primary & Secondary Constants, Variables, Standard C Keywords, Data Types – Int, Float, Double, Char. C Instructions: Type Declaration Instruction, Arithmetic Instruction, Input/ Output Instruction, Control Instructions. Hierarchy of Operations, Priority, Operators Like Int to Float, Float to Int, Double to Int, etc., Type Conversions, Structure of a C Program

10 hrs

**Unit II - Operators**

Operators: Arithmetic, Relational, Logical, Assignment, Increment and Decrement, Conditional, Bitwise, Special Operators. Decision-Making, Branching And Looping: *If*, Multiple Statements Within *If*, *If-Else*, Nested *If-Else* Statement, Use of Logical Operators Like *&&*, *||* And! Conditional Operator *While*, *Do*, *Do-While* and *For* Loop Control Structures, Nesting of Loops *Break* And *Continue* Statements, *Switch*, Case Control Structure, *Goto* Control.

8 hrs

**Unit III – Pointers and Arrays Functions**

Pointers and Arrays Functions: Definition, Declaration, Initialization, Accessing elements of an Array, reading & entering data into an Array, Pointers and 2D And 3D Arrays  
Understanding Pointers, Accessing Address of a Variable, Declaring and Initializing Pointers, Accessing variables through Pointers, Pointer expressions, Pointers and Arrays, Pointers and Character Strings, Pointers and Functions, Pointers and Structures, Points on Pointers. Functions: Need for User Defined Functions, Multifunction Program, C Function Forms, Return Values and their types, Calling a Function, No arguments and No return values, Argument but no return values, Argument with return values, Handling of Non Integer Functions, Nesting of Functions, Recursions, Function with Arrays,

12 hrs

**Unit IV – Strings, Structures, Unions**

Strings, Structures, Unions Files In C : Definition, Declaring and Initialization of Strings, Reading Strings From Terminal, Writing Strings to Screen, Arithmetic operations on Characters, Putting Strings together, Comparison of two Strings, Strings-Handling Functions, Table of Strings.

Structures and Unions: Introduction, Structure Initialization and Giving Values to Members, Arrays of Structures, Arrays within Structures, Structures within Structures, Structures and Functions. Size of the Structures, Unions and Case Studies.

8 hrs

**Unit V**

Files In C: Defining a File and Opening a File, Closing a File, Input/Output Operation on a File, Error Handling During I/O Operations, Random access to Files, Command Line Arguments.

4 hrs

C++

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### Unit VI

Introduction: Procedural Oriented Programming, Object Oriented Programming, Basic Concepts Object Oriented Programming (OOP) - Objects, Classes, Data Abstraction and Encapsulation, Inheritance, Reusability, Polymorphism, Overloading, Dynamic binding. Benefits of OOP, O Languages.

Objects and Classes: Declaring the class, private and public, member functions, using the class, defining objects, calling member functions, C++ objects as data types, Objects as function arguments, member functions.

8 h

### Unit VII

Constructors: Introduction parameterized constructors, multiple constructors in a class, copy constructors and destructors.

Operator Overloading: Overloading unary operators, overloading binary operators, concatenating strings

Inheritance: Introduction, types of inheritance, defining derived classes, accessing base class member derived class constructors, Overriding member functions, single Inheritance, making a private member inheritable, multilevel Inheritance, multiple Inheritance.

4 hr

### Unit VIII

Virtual functions and Polymorphism: Introduction, pointers to objects, pointers to derived classes, virtual functions.

Streams and Files: Stream Classes, Stream class hierarchy, ios class, istream class, ostream class, Stream errors.

6 hrs

### BI. HCP-1.4 Lab based on BI. HCT-1.3

#### C-Programming

1. Flow Charts, Algorithm Keywords Identifiers, Variables Constants, Scope of Life of Variables- Local and Global variables. Data types, Expressions, Operators- Arithmetic Operators, Logical Operators, Relational, Conditional, Bitwise Operators- Input/ Output Library Functions.
2. Declaration Statements, Control Statement: If Statement, If...Else Statement, Nesting of If...Else statement, Switch Statement- Iteration Statements- Arrays: Multiple Dimensional Arrays, Array Declaration and Initialization of Arrays.
3. Functions: User Defined and Library Functions- File Handling: Opening A File, Closing A File Reading and Writing into a File, Appending a File, Pointers

C++

1. I/O Statements- Escape Sequences- Comment Lines- Expressions and Statements- Standard Libraries- Prototypes of Main() Function - Data Types - Conditional Statements
2. Functions and Variables- Classes and Objects- Constructors and Destructors- Inheritance, Operator Overloading, Virtual Functions and Polymorphism.

## BI. HCT-1.5 Fundamentals of Bioinformatics

Total: 60 hrs

**Unit I**

Generations of Computer; Computer Organization, Fundamentals of Computers, Block Diagram of Computer, Functions of the Different Units Input unit, Output unit, Memory unit, CPU (ALU+CU), Input & Output Devices Input Devices: a) Keyboard, b) Point and draw devices mouse, joystick, track ball, light pen c) Data Scanning d) Projector, Advantages and Limitations of Computers.

8 hrs

**Unit II**

Basics of operating system DOS, Windows, Unix, Linux Application Software. Storage devices (RAM, ROM, Hard Drives etc).

Communication Technology- Networking- LAN, WAN And MAN, Internet- Wireless Communication- Internet, Network Topologies- Types And Application, Internet Technologies: Web Services- Wwww, URL, DNS- Servers E Mail Server, WEB Servers, Browsers- IP Addressing.

8 hrs

**Unit III**

Bioinformatics: An Overview- Introduction to Computational Biology and Bioinformatics, scope and applications; Emergence of Bioinformatics as a Separate Discipline; Some of the biological problems that require computational methods.

8 hrs

**Unit IV**

Biologically Data Acquisition- DNA Sequencing Methods- Basics of DNA Sequencing, Automated DNA Sequencing, DNA Sequencing by Capillary Array and Electrophoresis; Types Of DNA Sequences- Genomic DNA, cDNA, Recombinant DNA, Expressed Sequence Tags(ESTS), Genomic Survey Sequences(GSS); RNA Sequencing Methods; Protein Structure Determination Methods; Gene Expression Data.

12 hrs

**Unit V**

Biological databases – types of databases, literature databases, sequence databases, structure database, functional databases and chemical databases.

Nucleotide Sequence Database – GenBank, EMBL-EBI, DDBJ and INSDC.

Protein sequence database – Swiss-Prot, TrEMBL, Uniprot KB, PIR, CDD.

Structure Databases (PDB, MMDB)

8 hrs

**Unit VI**

Genome databases – Bacterial genome database – GOLD, MBGD, Viral genome databases – ICTVDB, VirGen, Human genome databases – MapViewer, Ensembl, UCSC, Vista-genome Browser, OMIM/OMIA.

Organisms Specific Databases (Wormbase, Ecogene, SGD, TAIR, Flybase etc).

8 hrs

**Unit VII**

## References:

1. The C Programming Language B.W. Kjernighan and D.M.Ritchie 2<sup>nd</sup> ed. Prentice Hall, India
2. Yashavant Kanetkar, 2002. Let Us C, 4<sup>th</sup> Ed, BPB Publications, New Delhi.
3. Yashavant Kanetkar, 1998. Graphics Under C, BPB Publications, New Delhi.
4. Schildt, Herbert, 2000. C: The Complete Reference, 4<sup>th</sup> Ed. Tata Mc Graw – Hill Publishing Co Ltd. New Delhi.
5. Rajaraman, V. 1994, Computer Programming In C. Printice-Hall Of India Pvt. Ltd., New Delhi.
6. Sudha G Purohit et al, Statistics using R , Narosa publishing house, New Delhi
7. Lafore, R. (2002) "Object Oriented Programming Using C++", Fourth Edition, Sams Publishers.

Pending  
Value Added  
Basics of Clinical  
Research

Employability

M.Sc Bioinformatics (CBCS) Syllabus-2020-21

BI. SCT-1.7.1 Biostatistics and R-Programming

Total: 60 hrs

**Unit I**

Introduction and scope of statistics-Role of statistics in Bio-informatics, scientific method, experiments and observational, population statistics, protocol writing, Aims and objectives Organization and collection of data - Data units population vs sample-Standardization of terms variables-Levels of measurement -Dealing with response and non response

8 h

**Unit II**

Classification (Objectives and Methods-Quantitative and qualitative) Tabulation-Graphical and Diagrammatical representation-Spatial Data Analysis-summarization. Measures of central tendencies-Arithmetic mean, Median, Mode, Percentages, Proportion, Harmonic mean, Geometric mean, Rates, Ratios, Percentiles, Indicators and Indices.

8 h

**Unit III**

Measures of Dispersion-Range, Standard deviation, standard errors and co-efficient of variation and use of normal distributions, skewness and kurtosis.

6 h

**Unit IV**

Bivariate statistical methods-Pearson's correlation coefficient-specific measures-Measures of association-Spearman rank correlation coefficient-contingency coefficient. Regression-Linear regression-Logistic regression-Prediction-Applications in Bioinformatics-validity Reliability.

8

**Unit V**

Time variable-Survival Analysis-Life table-Life expectancy measures-Time series Data analysis-Correlation square test, t-test, F-test and Z-test, ANOVA and its types.

8

**Unit VI**

Concept of probability-A priori & posterior Probabilities - Laws of probability-Additive multiplicative and complementary probabilities conditional probability.

6

**R-language**

**Unit VII**

Introduction to R, R as statistical software and language, R as calculator, graphics with R. Getting into R and R objectives, extracting subsets of data-frames by value, sorting data, merging data, exporting data, simple functions (t-apply, s-apply, summary and table).

8

**Unit VIII**

Basic plotting tools, revisiting the plot functions, loops, functions and if statements. ANOVA and its significances. Management of biological data with R.

Common Sequencing File Formats- GenBank flatfile format, Fasta file format, NBRF/PIR, GDE; Multiple Sequence Format (MSA), ALN Format, Files from Structural Data -PDB flatfile format,

## Unit VIII

4 hrs

Data: Access, retrieval and submission of sequences to GenBank and structures to PDB.

Standard Search Engines Data Retrieval Tools- ENTREZ, DBGET and SRS.

4 hrs

## BI. HCP-1.6 Lab based on BI. HCT-1.5

## Biological databases

1. Entrez and Literature Searches.
  - a. Pubmed
  - b. Pubmed Central
  - c. OMIM/OMIA
  - d. Citation Matcher.
2. SRS of Biological Databases.
  - a. Nucleotide/ Genome Databases
  - b. Protein Sequence Database.
  - c. Structure Database
  - d. Protein Pattern Databases.
3. Sequence Analysis
  - a. Dotplot
  - b. Pairwise Alignment
  - c. Multiple Sequence Alignment
4. Softwares.
  - a. Bioedit
  - b. Clustalw/X, MEGA, MEME
5. Visualization Tools.
  - a. Rasmol
  - b. Cn3D
  - c. Molmol

## References:

1. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata Mcgraw Hill Publishing Co Ltd., India.
2. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2<sup>nd</sup> ed. Wiley Inter-science, New York.
3. Pennington, S.R. and Dunn, M.J. 2002. Proteomics, from Protein Sequence to Functions. Viva Books Pvt Ltd., New Delhi.
4. Rastogi, S. C, Mendiratta, N & Rastogi, P. 2004. Bioinformatics Methods and Applications, Genomics, Proteomics and Drug Discovery. PHI private limited, NewDelhi.
5. Rajan, S.S. and Balaji R. 2002. Introduction to Bioinformatics. Himalaya Publishing House, Mumbai.
6. Rastogi, S. C., Mendiratta, N. and Rastogi, P. 2003. Bioinformatics: Concept Skill and Applications. CBS Publisher and distributors, New Delhi.
7. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2<sup>nd</sup> ed. Wiley Inter-science, New York.
8. Attwood and Parry-Smith, D.J. 1999. Introduction of Bioinformatics. Pearson Eduaction Ltd, Delhi

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BI. SCT-1.7.2 Structural Bioinformatics

Total: (

**Unit I**

Structural features of Biomolecules; techniques used to determine the structure of Biomolecules; r for single crystal X-ray diffraction of macromolecules: molecular replacement method and direct Fiber diffraction; analysis of structures and correctness of structures; submission of data to PDB coordinates and electron density maps

**Unit II**

Proteins: Principles and Analysis of proteins; Hierarchical organization of protein structure- Secondary, motif, domains, Tertiary, Quaternary structure, internal co-ordinates of Proteins- Derivation and significance of Ramachandran Plot.

**Unit III**

Structure of Nucleic Acids: DNA and RNA; Base pairing- Watson crick and Hoogestein; Type A,B,Z and their geometrical as well as structural features, DNA bending; Types of RNA and g parameters of each and their composition, Structure of ribosome.

**Unit IV**

Molecular Interactions: Protein-Protein interaction, Structural Analysis of domain interaction DNA interactions, Types of interactions of DNA with proteins and small molecules.

**Unit V**

Methods for prediction of secondary and tertiary structures of proteins- knowledge- based prediction; fold recognition; ab initio methods for structure prediction, comparative protein r

**Unit VI**

Methods for comparison of 3D structure of proteins; methods to predict three dimensional nucleic acids, rRNA; electrostatic energy surface generation.

**Unit VII**

Molecular mechanics and molecular dynamics of oligopeptides, proteins, nucleotic molecules- mechanism of dynamics of bio- macromolecules, simulation of molecular dynamics, simulations of free energy changes; force fields. Molecular interactions of p protein-DNA, protein-carbohydrate and DNA- small molecules.

## BI. SCP-1.8.1 Lab based on BI. SCT-1.7.1

1. Diagrammatical and graphical representation of data.
2. Examples on measures of central tendency.
3. Examples on measures of dispersion.
4. Co relation and regression. Examples on pearson correlation coefficient spearman rank coefficient, regression coefficient and equations
5. Time series analysis: examples on methods of finding measuring trend seasonal and cyclic variations
6. R- Software: Based on theory discuss all concept using R software, exercises the statistical problems with R.
7. Descriptive statistics in R- Diagrammatic and Graphical representation of data with R, measure of central tendency and dispersion, with example using R software.
8. Using R - Probability and probability distribution and Correlation and regression analysis.

## References:

1. Statistics concepts and Applications Author: Harry Frank & Steven.c.Athoen Publications: Cambridge University Press
2. Introduction to Statistics Author: Hog and Caraig Publications: Wiley Eastern
3. Mathematical Statistics Author: S.C.Gupta and V.K.Kapoor Publications: Sultan Chand publications
4. Basic Statistics Author: Dunn.O.J Publications: John Wiley & Sons
5. Principles of Statistics Author: Khan and khanamm Publications: Himalaya Publications
6. Robert G., 2008. "R-programming in Bioinformatics" CRC press, Taylor and Francis Group, USA.
7. Own J., Robert M., and Andrew R. 2014. Introduction to scientific and simulation using R. CRC press, Taylor and Francis Group, USA.



## BI. SCT-1.7.3 Bioinstrumentation

Total: 60 hrs

**Unit I - Chromatographic Techniques and Mass spectrometry**

Introduction to chromatography, Planar chromatography (paper and thin layer chromatography), Column chromatography, Ion exchange chromatography, Gel-exclusion chromatography, Affinity chromatography, High performance liquid chromatography (HPLC), Mass spectrometry, Gas chromatography mass spectrometry (GC-MS), Liquid chromatography mass spectrometry (LC-MS).

10 hrs

**Unit II - Electrophoresis**

Introduction to electrophoresis, sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), Discontinuous gel electrophoresis, Agarose gel electrophoresis, Pulsed field gel electrophoresis, 2-Dimensional Electrophoresis, Capillary electrophoresis, Immunoelectrophoresis.

10 hrs

**Unit III – Flowcytometry**

Introduction, basic components of a flow cytometer, sample preparation, limitations of the flow cytometer.

10 hrs

**Unit IV – Microscopy**

Principle, design and application of light microscope, phase contrast microscope, fluorescence microscope, scanning electron microscope, transmission electron microscope, scanning tunneling microscope, atomic force microscope, confocal microscope,

10 hrs

**Unit V – Spectroscopy**

Nuclear Magnetic Resonance Spectroscopy, Ultraviolet-Visible Absorption Spectrometry, Fluorescence Spectrometry, X-Ray Crystallography, Infrared Spectroscopy, Atomic absorption spectrometry, plasma emission spectroscopy and Electron spin resonance spectroscopy

10 hrs

**Unit VI: Omics technologies:**

Conventional PCR, Real Time PCR, Sequencing Technologies (DNA and Protein) Microarray etc.

10 hrs

## Reference

1. Andrew R. Leach (2001) "Molecular Modelling- Principles And Applications"; Secod Edition, Prentice Hall, USA.
2. Creighton, T.E. (1983) "Proteins: Structure And Molecular Properties:: Second Edition, W.H. Freeman And Company, New York, USA
3. Protein Structure, stability and folding Ed. K.P. Murphy (2001) Humana Press.
4. Introduction to protein architecture Arthur M. Lesk (2001) Oxford University Press.
5. Introduction of Macromolecular Crystallography - A. Mcpherson (2003) John Wiley Publications.
6. Introduction to protein structure, Branden, Carl and Tooze, John Garland Publ. Inc., 1991
7. Introduction to bioinformatics-attwood and parrysmith, pearson education.
8. Bioinformatics-A Beginner's guide by gena-michelclaverie,johnwiley&sons.
9. Structural bioinformatics by Philip.e.bourne and helgeweissing, wiley.
10. Structure and mechanism in protein science-Fresh W H freeman and co.

**BI. SCP-1.8.2 Lab based on BI. SCT-1.7.2**

Practicals are designed based on the BI. SCT-1.7.2 syllabus

**Semester II****BI. HCT-2.1 Biophysics, Biochemistry and Immunology**

Total: 60 hrs

**Unit I**

Mechanics: Newton's Law of Motion- Mechanics of Particle- Work Energy Principle- Relational Dynamics- Static and Dynamic Equilibrium – Conservation Laws. Thermodynamics- Concept of Temperatures- Thermodynamic Equilibrium; Zeroth Law- Conservation of Energy; First Law- Concept of Entropy; Second Law- Absolute Law of Temperature; Third Law of Thermodynamics.

6 hrs

**Unit II**

Nucleic Acids: Structure Of Nucleic Acids: Structures of Purines and Pyrimidines, Structure of DNA; Type of DNA and their structures, A, B and Z DNA, Supercoiled DNA, T<sub>m</sub> and Cot Curve for Dissociation of DNA. Motifs of DNA - Promoters, Enhancers and Attenuators.

DNA Protein Interaction: Recognition of DNA in Prokaryotes and Eukaryotes. Interaction of Specific Proteins with references to Trp-Repressors, CAP Proteins, Zinc Finger Proteins, Lac-Repressors, Phage Repressor and Cro Protein.

8 hrs

**Unit III**

Amino Acids: General Properties, Classification of Amino Acids; Based On Polarity, Based On Functional Groups, Essential and Non-Essential Amino Acids, Acid Base Properties, Stereo Chemistry, Non Standard Amino Acids.

Proteins: Salient Features of Peptide Bond; Conformation and its properties, Structural Hierarchy of the Protein, Primary, Secondary, Tertiary and Quaternary Structures with Examples.

8 hrs

**Unit IV**

Motifs of Proteins: Alpha Structures: Coiled Coil, Four Helix Bundles, and Globin Motifs with Examples, Beta Structures: Up And Down Beta Barrel, Greek Key Motif, and Jelly Roll Motifs with Examples Alpha/Beta Structures: Horse Shoe Motifs, TIM Barrel Motifs, Rosmann Fold, Beta Alpha Beta Motifs with Examples and Other Motifs.

6 hrs

**Unit V**

Folding And Flexibility: Concept of Protein Folding; Christian Anfinsen Reaction on Bovine Pancreatic RNase, Lavinthal Paradox, Thermodynamics Of Protein Folding, Steps Involved In Protein Folding, Structure And Molecular Mechanism Of Chaperon Mediated Protein Folding.

Structure and Structure Based Mechanism of Protein Action. Membrane proteins and Signal Transduction. Proteins of the Immune Systems, Structure of Viral Capsomeres, and Importance of Structure Based Drug Designing.

8 hrs

BI. SCP-1.8.3 Lab based on BI, SCT-1.7.3

Practicals are designed based on the BI, SCT-1.7.3 syllabus

Practicals:

1. Column Chromatography
2. Estimation of Nucleic Acid and Protein through spectrophotometer
3. Electrophoresis of DNA and Protein
4. Observation of Cell Morphology and Cell division under inverted microscope
5. Demonstration of Conventional and Real time PCR for gene amplification

REFERENCES

1. Biochemistry Laboratory: Modern theory and techniques, 2<sup>nd</sup> Edition - Rodney Boyer.
2. Bioinstrumentation. Student edition. John Wiley and Sons, Ltd - John G Webster.
3. Bioinstrumentation: Tools for understanding life, Published by National Association of Biology Teachers - James, Dennis and Lange.
4. Instrumental method of chemical analysis -Shrama BK
5. Instrumental methods of analysis- DA Skoog
6. An introduction to practical Biochemistry -Plummer
7. Instrumentation - Chatwal and Anand
8. Modern experimental Biology - Boyer

#BI-OE -1.9 offered by Women's Studies Department, K.S.A.W.U-Vijayapura

**BI-SCT-2.7.1 - JAVA and Python.**

Total: 60 hrs

**JAVA****Unit I**

An overview of Java: Object oriented programming, two paradigms, Abstraction, the three OOP principals, a first simple program. Data Types, Variables and Arrays: Integers, Floating point numbers, Characters, Boolean one dimensional array, Multidimensional arrays.

8 hrs

**Unit II**

Operators: Arithmetic operators, Module operator, Assignment operator, Increment and decrement operator, Bit-wise operator, Relational operator, Logical operator, Operator precedence.

Control Statements: Selection statement, Switch, While, Do-Whole, For, Nested loops, Break and Continue.

8 hrs

**Unit III**

Introducing Classes: Class fundamentals, declaring objects, Introducing methods, Constructors.

4 hrs

**Unit IV**

Inheritance: Inheritance basics, Using Super, Creating a multilevel hierarchy, when constructors as called, Method overriding, dynamic method dispatch using abstract class.

8 hrs

**Unit V**

Exception Handling: Exception handling fundamentals, Exception types, uncaught exceptions, Using Try and catch, multiple catch clauses, Nested try statements.

Multithreaded Program: The Java thread model, Thread priorities, Synchronization, Mastering, The main thread, creating a thread.

8 hrs

**Unit VI**

I/O Applets: I/O basics, Reading console inputs, Applet fundamentals, the applet class, Applet architecture, Simple applet, Display methods, Using the status window, The HTML applet tag.

6 hrs

**Python****Unit VII**

Basics of python, installing, writing python programming, python values and variables.

8 hrs

**Unit VIII**

Working with sequences, parsing sequence file formats, connecting with biological databases, sequence objectives, sequence input and outputs, accessing biological database resources.

10 hrs

BI. SCP-2.8.1 Lab based on BI. SCT-2.7.1

**Java**

1. Concepts of Flowcharting, Algorithm Development.
2. Writing Pseudo Codes
3. Working With Objects, Arrays, Conditional Statements And Loops
4. Creating Classes And Applications In Java
5. Java Applets Basics, Graphics, Fonts and Colors.
6. Simple Animation And Threads, Advanced Animation, Images And Sound'
7. Managing Simple Events and Interactivity.
8. Creating User Interfaces with, Modifiers.
9. Packages and Interfaces, Exception, Multithreading.
10. Stream and I/O, Using Native Methods and Libraries.
11. Java Programming Tools Working With Data Structures

**Python**

1. Programming to store a DNA sequence, concatenation, reverse complement.
2. Writing sequence files (converting between sequence file formats, converting a file of sequences to their reverse complements)
3. Getting your sequence record objects as formatted strings
4. Sequence alignment using python programming

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**References**

1. Balaguruswamy, E.(1985) "Fundamentals Of Java", Second Edition, Tata McGraw Publishing Co. Ltd., India .
2. Joseph, O. N.2000. Teach Yourself Java, Tata McGraw Hill Publishing Company Ltd., New Delhi.
3. King, K.N.2000.Java Programming, From the Beginning, W.W. Norton & Company, New York.
4. Patrick Naughton.1997. Java Handbook, Tata McGraw Hill Publishing Company Ltd., New Delhi.
5. Richard L., Halterman, 2011 Learning to program with Python.

## BI. SCT-2.7.2 Immunology and Systems Biology

Total: 60 hrs

**Immunology****Unit I**

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

10 hrs

**Unit II**

Antibody generation: structure and function –clonal selection theory-different types of immunoglobulins, effectors, receptors and antibody diversity. Complement system activation, pathways and biological effects.

10 hrs

**Unit III**

Major Histochemical molecules/peptide complexes Structure and Function and production of MHC Locus in Mice and Human. t-lymphocytes and cytokine network, receptors, production from TH1 and TH2 CD4+ T- cells.

10 hrs

**Systems Biology****Unit IV**

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

10 hrs

**Unit V**

Simulation of pathways: Whole cell: Principle and levels of simulation – Virtual Erythrocytes. Pathological analysis. Flux Balance Analysis. Biochemical metabolic pathways, metabolomics and enzymes. Interconnection of pathways, metabolic regulation. Cellular models. Networks and Motifs: Gene Networks: basic concepts, computational models. Lambda receptor and Lac operon as an example. – all types of networks and its uses.

10 hrs

**Unit VI**

Design of Circuits and Databases: Introduction- databases KEGG, EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, Expression databases and various databases related to systems biology.

10 hrs

## BI. SCP-2.8.2 Lab based on BI. SCT-2.7.2

## Practical:

1. Immuno-diffusion - Rocket immunoelectrophoresis, Agarose Gel Immunodiffusion,
2. RIA, ELISA.
3. PAGE
4. Immunoblotting
5. Import and simulate models from different databases
6. To Import and simulate a model from the repository
7. SBML-A markup language for mathematical models in systems biology using cell designer
8. Creating and Visualizing a Simple Network Model
9. Analysis of biological networks for feature detection
10. Integrating Biological Networks and Microarray Expression data
11. Analyzing the network by finding sub modules

## Reference:

1. Essentials of Immunology by Riott I .M. 1998. ELBS, Blackwell Scientific Publishers, London.
2. Immunology 2 nd Edition by Kuby J. 1994. W.H. Freeman and Co. New York.
3. Immunology - Understanding of Immune System by Claus D. Elgert. 1996. Wiley -Liss, New York.
4. Fundamentals of Immunology by William Paul.
5. Cellular and Molecular Immunology. 3rd Edition by Abbas.
6. Immunobiology: The Immune System in Health and Disease. 3rd Edition by Travers.
7. Immunology- A short Course. 2 nd Edition by Benjamin.
8. Manual of Clinical Laboratory and Immunology 6th Edition. 2002 by Noel R. Rose, Chief Editor: Robert G. Hamilton and Barbara Detrick (Eds.) , ASM Publications.
9. Systems Biology in practice: Concepts, Implementation and applications by E.Klipp R.Herwig, A.Kowlad, C.Wierling and H.Lehrach, Wiley InterScience. 2005
10. Systems Biology and Synthetic Biology by Pengcheng Fu, Sven Panke, Wiley InterScience. 2009
11. System Biology: Computational Systems Biology (Hardcover) by Andres Kriete (Editor), Roland Eils (Editor)
12. Stochastic Modelling for Systems Biology. ISBN-10 1-58488-540-8 and ISBN-13 978-158488-540-5
13. Uri Alon, An Introduction to Systems Biology: Design Principles of Biological Circuits, Chapman & Hall/CRC Press, A Mathematical and Computational Biology, 2nd edition, 2006.
14. Systems Biology: Definitions and perspectives by L.Alberghina H.V.westerhoff, Springer. 2005
15. Synthetic Biology, A New Paradigm for Biological Discovery, a report by Beachhead Consulting, 2006



## BI. SCT-2.7.3 IMAGE PROCESSING

Total: 60 hrs

## Unit I

**Digital Image and its properties:** Basic concepts, Image digitization, Digital image properties. 8 hrs.

## Unit II

**Image Pre-Processing:** Brightness and geometric transformations, local preprocessing. 3 hrs.

## Unit III

**Segmentation:** Thresholding, Edge-based segmentation, Region based segmentation, Matching. 10 hrs.

## Unit IV

**Image enhancement in the spatial domain:** Background, Some basic gray level transformations, Histogram processing, Enhancement using arithmetic/logic operations, Basics of spatial filtering, Smoothing spatial filters, Sharpening spatial filters. 8 hrs.

## Unit V

**Image enhancement in the frequency domain:** Background, Introduction to the Fourier transform and the frequency domain, Smoothing, Frequency-Domain filters, Sharpening Frequency Domain filters, Homomorphic filtering. 8 hrs.

## Unit VI

**Image compression:** Fundamental, Image compression models, Elements of information theory, Error-Free Compression, Lossy compression. 8 hrs.

## Unit VII

**Region identification, Contour-based shape representation and description Region based shape representation and description, Shape classes.** 5 hrs.

## Unit VIII

**Morphology:** Basic morphological concepts, Morphology principles, Binary dilation and erosion, Gray-scale dilation and erosion, Morphological segmentation and watersheds. 5 hrs.

**TEXT BOOK:**

1. *Milan Sonka, Vaclav Hlavac and Roger Boyle*, "Image Processing, Analysis and Machine Vision", Thomson Learning, Brooks/Cole, 2<sup>nd</sup> Edition. 2001. [Chapters 2,4 (4.1 to 4.3), 5 (5.1 to 5.4), 6, 11 (11.1 to 11.4, 11.7)].
2. *Rafel C Gonzalez and Richard E Woods*, "Digital Image Processing", Pearson Education, 2<sup>nd</sup> Edition, 2003. [Chapters 3 (3.1 to 3.7), 4 (4.1 to 4.5), 8 (8.1 to 8.5)]

**REFERENCE BOOKS:**

1. *Anil K Jain*, "Fundamentals of Digital Image Processing", 1997, Pearson Education / Prentice-Hall of India Pvt., Ltd.
2. *B. Chanda D Dutta Majumder*, "Digital Image Processing and Analysis", 2002, Prentice-Hall, India.

BI. SCP-2.8.3 Lab based on BI. SCT-2.7.3

**PRACTICALS**

MATLAB based practical image processing.

**Semester III****BI. HCT-3.1 Genomics, Proteomics and System Biology**

Total: 60 hrs

**GENOMICS****Unit I**

Introduction – Genomes, Omics and its importance, general features, C-value paradox, gene identification, annotation of a genome, genome diversity, taxonomy and significance of genome, structural and comparative genomics, transcriptomics, proteomics and metabolomics, HAP-MAP project, 1000 genome project, ENCODE project, Genome structure predictions of prokaryotes and eukaryotes. Integrated genomic maps, gene expression profiling.

10 hrs

**Unit II**

Functional genomics of microbes, plants and animals: Sequencing technologies - shotgun approach, sanger sequencing, pyro-sequencing, de-novo sequencing of whole genomes, assembly of sequence reads, concept of base calling; annotation and other methods of genome alignments; EST, STS and SNPs sequence analysis.

Transcriptome analysis methods: Serial Analysis of Gene Expression (SAGE) and its application. Databases of expressed sequence tag (ESTs) and data mining.

8 hrs

**Unit III**

Micro arrays protocol and its application - gene expression analysis; DNA array for global expression profile; Types of DNA array, Array database; Applications of DNA microarray – analysis of gene expression, differential gene expression under different conditions and during development of organisms. Comparative genomics, steps involved in comparative genomics, Implications of comparative genomics

8 hrs

**PROTEOMICS****Unit IV**

Definition and scope: methods of proteome analysis, 2D-PAGE, DIGE, Mass spectrometry and analysis (ESI, MALDI TOF and hybrid), LC-MS, Tandem Mass spectrometry, Peptide mass finger printing – MASCOT, SALSA. Multidimensional chromatography and MuDPIT.

8 hrs

**Unit V**

Protein interaction analysis: Principle, strategy and applications of tandem affinity purification (TAP), Yeast two hybrid (Y2H) systems and analysis of selective interacting domains in proteome mapping, protein structure determination and structural proteomic tools, concepts of protein engineering, proteomic databases (PRIDE, NEXTPRO), Shotgun proteomics approach for isolation and study of whole cell interactome, and interactome analysis.

8 hrs

**SYSTEMS BIOLOGY****Unit VI**

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

4 hrs

**Unit VII**

Simulation of pathways: Whole cell: Principle and levels of simulation – Virtual Erythrocytes. Pathological analysis. Flux Balance Analysis. Biochemical metabolic pathways, metabolomics and enzymes. Interconnection of pathways, metabolic regulation. Cellular models. Networks and Motifs: Gene Networks: basic concepts, computational models. Lambda receptor and Lac operon as an example. – all types of networks and its uses.

8 hrs

**Unit VIII**

Design of Circuits and Databases: Introduction- databases KEGG, EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, Expression databases and various databases related to systems biology.

6 hrs

**BI. HCP-3.2 Lab based on BI. HCT-3.1**

1. TM-HMM
2. Plasmid construction
3. Gene tool
4. Pept tool
5. Split tree
6. Detection of recombination event in viral genome using RDP software
7. Protein scope- protein structure viewer and Propred.
8. Comparative proteomics analysis 2D-PAGE gel profile to study differentially expressed proteins.
9. Mass spectrometry data analysis - Peptide mass finger printing using MASCOT.
10. Study of databases - EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, PRIDE, NEXTPRO.
11. Mathematical modeling and simulating of Biochemical network
12. Import and simulate models from different databases
13. To Import and simulate a model from the repository
14. SBML-A markup language for mathematical models in systems biology using cell designer
15. Creating and Visualizing a Simple Network Model
16. Analysis of biological networks for feature detection
17. Integrating Biological Networks and Microarray Expression data
18. Analyzing the network by finding sub modules

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BI. SCT-3.5.2 Molecular Modeling and Dynamics

**Unit I**

Computational Chemistry: concepts of computational chemistry-Born-Oppenheimer approximation. Application of Hartree-Fock equations to molecular systems, approximate molecular orbital theory, semi-empirical methods. Macro-molecular force fields, salvation, long range forces.

8hrs

**Unit II**

Molecular Mechanics: Introduction, The Morse Potential, The Harmonic Oscillator Model for Molecules. Comparison of Morse and Harmonic Potential, Two atoms connected by a bond, Poly atomic Molecules, Energy due to Stretch, Bend, Stretch-Bend, Torsional strain, van der Waals and Dipole Dipole interactions. Types of Potentials: Lennard-Jones, Truncated Lennard-jones, Exponential-6, Ionic and Polar potentials. Types of Force Fields: AMBER, CHARMM, Merck Molecular Force Field, Consistent Force Field, MM2, MM3 and MM4 force fields.

10 hrs

**Unit III**

Potential Energy Surface: - Convergence Criteria, Characterizing Stationary Points, Search for Transition States. Optimization: - multivariable Optimization Algorithms, level Sets, Level Curves, Gradients, Optimization Criteria, Unidirectional Search, Finding Minimum Point, and Gradient based Methods- Steepest Descent and Conjugate Gradient Methods

8 hrs

**Unit IV**

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

8 hrs

**Unit V**

Simulation methods : Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, Solvent access, Equilibration, cutoffs, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation software's. Various methods of MD, Monte Carlo, systematic and random search methods.

10hrs

**Unit VI**

Drug design: Drug discovery process. Target identification and validation, lead optimization and validation. Methods and Tools in Computer-aided molecular Design, Analog Based drug design:- Pharmacophores (3D database searching, conformation searches, deriving and using 3D Pharmacophore, constrained systematic search, Genetic Algorithm, clique detection techniques, maximum likelihood method) and QSAR. Structure based drug design: - Docking, De Novo Drug Design (Fragment Placements, Connection Methods, and Sequential Grow), Virtual screening

8 hrs

**Unit VII**

## BI. HCP-3.6.1 Lab based on BI. HCT-3.5.1

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- 1. Data definition language (DDL) statements
    - Creating database, selecting database, deleting database, creating database, creating table, modifying table, deleting table
  - 2. Data manipulation statements: inserting and deleting records, retrieving records retrieving specific rows and columns
  - 3. Use of MySQL operators- arithmetic operators, comparison operators, logical operators and math function, aggregate functions string operations limiting, sorting and grouping query results handling null values
  - 5. Renaming or aliasing table and column names
  - 6. Using subqueries
  - 7. Using joins-joining a table to itself, joining multiple tables
  - 8. Using indexes
  - 9. Security management
  - 10. Granting and revoking rights on the tables

## References

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1. Elmascori and Navathe. 2002. Fundamentals of Database Concepts, McGraw Hills.
  2. Ramakrishnan, R. 2003. Database management System, McGraw Hills, Boston.
  3. Palinski, J. A. 2003. Oracle SQL and PL/SQL Handbook. Pearson education Asia.
  4. Alexis Leon and Mathews leon. 2003. SQL, A Complete Reference. Tata McGraw-Hill publishing company limited, New Delhi.
  5. Robert Sheldon. 2003. SQL, A Beginner's Guide, 2<sup>nd</sup> ed., Tata McGraw-Hill publishing company limited, New Delhi.
  6. Silberschatz, A.,Korth, H & Sudarshan, S. 2002. Database system concepts, 4<sup>th</sup> ed., McGraw-Hill, Boston.

## BI. SCT-3.5.3 IPR, Entrepreneurship and Bioethics

Total: 60 hrs

**Unit I**

Intellectual Property Rights: Introduction to IPR, Types of IP - Patents, Trademarks, Copyright & Related Rights, Industrial Design, Traditional Knowledge and Geographical Indications. Importance of IPR - patentable and non patentables, patenting life, legal protection of Biotechnological inventions. Agreements and Treaties - History of GATT & TRIPS Agreement; Madrid Agreement; Hague Agreement; WIPO Treaties; Budapest Treaty; PCT; Indian Patent Act 1970 & recent amendments. IPR and WTO regime - Consumer protection and plant genetic resources.

10 Hrs

**Unit II**

Patents And Patent Laws: Objectives of the patent system - Basic, principles and general requirements of patent law. Biotechnological inventions and patent law - Legal development - Patentable subjects and protection in Biotechnology. Patent Filing Procedures - National & PCT filing procedure, Time frame and cost, Status of the patent applications, Precautions while patenting, disclosure/ nondisclosure, financial assistance for patenting, introduction to existing schemes. Patent licensing and agreement. Patent infringement - meaning, scope, litigation, case studies.

10 Hrs

**Unit III**

Entrepreneurship, objectives, qualities of an entrepreneur, market need and business strategies, steps to establish a business, developing a business plan, managing the human resource, management of finance, employee and employer relationships. Product Innovation, competing the global industry, technology up gradation. Knowing the successful entrepreneur, SWOC analysis.

10 Hrs

**Unit IV**

Bioethics: Introduction to ethics and bioethics, framework for ethical decision making. Ethical, legal and socioeconomic aspects of gene therapy, germ line, somatic, embryonic and adult stem cell research.

10 Hrs

**Unit V**

Ethical implications of GM crops, GMO's, human genome project, human cloning, designer babies, biopiracy and biowarfare. Eugenics and its possible approaches. Animal right activities - Blue cross in India- society for prevention of cruelty against animals. Ethical limits of Animal use. Green peace - Human Rights and Responsibilities.

10 Hrs

**Unit VI**

Ethical issues in clinical research: Preclinical studies ethical issues, Introduction to clinical research guidelines (Nuremberg code, Declaration of Helsinki, Belmont report, ICH GCP, FDA (21 CFR Part 11) and EMEA guidelines. Informed consent issues and clinical studies ethical issues, Regulatory control of clinical research: FDA, US, Indian clinical research, global scenario of clinical research, Regulatory agency.

10 Hrs

Structure Activity Relationship: Introduction to QSAR, QSPR, Various Descriptors used in QSARs: Electronics; Topology; Quantum Chemical based Descriptors. Regression Analysis, the Significance and Validity of QSAR Regression Equations, Partial Least Squares (PLS) Analysis, Multi Linear Regression Analysis. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations.

8 hrs

**References**

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

**BI. HCP-3.6.2 Lab based on BI. HCT-3.5.2**

**Practicals are designed based on the BI.HCT-3.5.2 syllabus**



## BI. SCT-4.3.2 Medical Bioinformatics and Big Data Analytics

Total: 60 hrs

**Unit I**

MEDICAL INFORMATICS: Introduction – Medical Informatics, Bioinformatics, Health Informatics, Structure of Medical Informatics, Functional capabilities of Hospital Information System, On-line services and Off line services, Dialogue with the computer.

10 hrs

**Unit II**

MEDICAL STANDARDS: Evolution of Medical Standards, IEEE 11073, HL7, DICOM, IRMA, LOINC, HIPPA, Electronics Patient Records, Healthcare Standard Organizations, JCAHO (Joint Commission on Accreditation of Healthcare Organization), JCIA (Joint Commission International Accreditation), Evidence Based Medicine, Bioethics.

20 hrs

**Unit III**

MEDICAL DATA STORAGE AND AUTOMATION: Representation of Data, Data modeling Techniques, Relational Hierarchical and network Approach, Normalization techniques for Data handling - Plug-in Data Acquisition and Control Boards, Data Acquisition using Serial Interface, Medical Data formats, Signal, Image and Video Formats, Medical Databases, Automation in clinical laboratories, Intelligent Laboratory Information System, PACS.

10 hrs

**Unit IV**

HEALTH INFORMATICS: Bioinformatics Databases, Bio-information technologies, Semantic web and Bioinformatics, Genome projects, Clinical informatics, Nursing informatics, Public health informatics, Education and Training.

10 hrs

**Unit V**

RECENT TRENDS IN MEDICAL INFORMATICS: Medical Expert Systems, Virtual reality applications in medicine, Virtual Environment, Surgical simulation, Radiation therapy and planning, Telemedicine, virtual Hospitals, Smart Medical Homes, Personalized e-health services, Biometrics, GRID and Cloud Computing in Medicine.

10 hrs

**References:**

1. R.D.Lele, "Computers in medicine progress in medical informatics", Tata McGraw Hill Publishing Ltd, 2005.
2. Mohan Bansal, "Medical informatics", Tata McGraw Hill Publishing Ltd, 2003.
3. Orpita Bosu and Simminder Kaur Thukral, "Bioinformatics Databases, Tools and Algorithms", Oxford University press, 2007.
4. Yi Ping Phoebe Chen, "Bioinformatics Technologies", Springer International Edition, New Delhi

## BI. SCP-4.4.1 Lab based on BI. SCT-4.3.1

1. Basic operators and control flow, basic perl data types, references, matrices, complex/nested data structures, scope(my, local, our), function/subroutines, system and user function, the local operator, variable-length parameter lists, notes on lexical variable, file handle and file tests, stat and isstat functions, formats, directory access & manipulation, process management, formatting data, system information.
2. Uses of regular expressions, patterns, single-character patterns, grouping patterns (sequence, multipliers, parentheses as memory, alternation) anchoring patterns, precedence, matching operators, ignoring case, different delimiters, variable interpolation, special read-only variables, substitutions split and join functions, dynamic programming, approximate string matching.
3. URL encoding, CGI environment variables, handling forms, accessing form input, extra path information, CGI.pm module, passing parameters via CGI, less typing, server side includes, debugging CGI programs, stepping through programs, breakpoints, line action

## Bioperl

4. Installing bioperl, general bioperl classes sequences (Bio::seq class, sequence manipulation), features and location classes (extracting CDS), alignments (AlignIO), analysis (BLAST, GenScan), Databases (database classes, accessing a local database), implementing REBASE.

## References:

1. Perl CookBook – T.Christainsen and N.Torkington 2<sup>nd</sup> ed. 2003 O'Reilly
2. <http://zoic.org/training/nothtml/perl/db.pdf>
3. <http://doc.bioperl.org/>
4. Programming Perl + Larry Wall, Tom Christiansen & John Orwant 3ed 2000- O' Reilly
5. James Tisdall. D. 2002. Beginning Perl for Bioinformatics, O'Reilly, Shroff Publishers and Distributors Pvt. Ltd., New Delhi.
6. Schwartz, R.T. and Tomphoenix. 2004. Learning Perl, O'Reilly, Shroff Publishers and Distributors Pvt. Ltd., New Delhi.
7. Programming Web Graphics with Perl and GNU Software – S.Wallace, 1st ed. 1999 XML and Perl 1st ed, M. Riehl and L. Sterin Pearson Education 2002

## BI. SCT-4.3.3 Molecular Simulation

Total: 60 hrs

**Unit I**

Introduction: Model systems and interaction potentials, Basics of Monte Carlo and Molecular Dynamics simulation techniques.

10 Hrs

**Unit II**

Monte Carlo simulations in various ensembles: Micro-canonical, Canonical and Grand-Canonical. Molecular dynamics in various ensembles: Constant temperature, constant pressure ensembles.

20 Hrs

**Unit III**

Free energy and phase equilibria: Methods of free energy calculations, The Gibb's ensemble, Coexistence, Free energy of solids.

15 Hrs

**Unit IV**

Molecular simulation software's: GROMACS, CHARMM, AMBER, NAMD, LAMMPS AND Desmond.

15 Hrs

**Reference**

1. D. Frenkel and B. Smit: Understanding Molecular Simulation, Academic Press.
2. M.P. Allen and D.J. Tildesley: Computer Simulation of Liquids, Oxford University Press, USA.
3. A. Hinchliffe: Molecular Modeling for Beginners, John Wiley & Sons.
4. A. Leach: Molecular Modeling: Principles and applications, Prentice Hall.

**BI. SCP-4.4.3 Lab based on BI. SCT-4.3.3**

Practicals Designed based on the BI. SCT-4.3.3 syllabus

## BI. SCP-4.4.2 Lab based on BI. SCT-4.3.2

## PRACTICAL

1. Study of different Medical data formats.
2. Study of disease mechanism using KEGG
3. Study of human genome and various gene locations using Ensembl.
4. Variant analysis in the genome of cancer patient.
5. Study of virtual hospital
6. Study on e-health care services

**Semester IV****BI. HCT-4.1 Chemo-informatics and Drug Designing**

Total: 60 hrs

**Chemoinformatics****Unit I**

Introduction and evolution of chemoinformatics, medicinal chemistry, high throughput synthesis and screening of compounds, prospects of chemoinformatics, chemical structure design (2D and 3D structure), physiochemical properties of compounds, chemical databases. Computational chemistry, classical, potential energy methods, quantum chemistry, geometry optimization, molecular mechanics and force fields, primary, secondary and tertiary chemical information, chemical indexing.

10 hrs

**Unit II**

Functional Groups and their biological properties of drugs

Alkylene groups, alkylating and acylating groups, sulfonic acids and derivatives, aldehyde and ketone groups, hydroxy groups, nitroso and nitro compounds, amines, effect of methyl groups on bioactivity and biotransformation.

8 hrs

**Unit III**

Action, Administration, Toxicity and Efficacy of drugs, pharmacodynamics and pharmacokinetics, drug action, drug interactions, Adverse drug reactions and remedial measures, effectiveness and safety, drug abuse.

Routs of drug administration, merits & demerits, distributions, Toxicity: acute, sub-acute and chronic toxicity. Management of acute toxicity and excretion, ADMET property prediction, selectivity of drug action, receptors potency and efficacy, tolerance & intolerance.

8 hrs

**Drug Designing****Unit IV**

Drug Discovery: Basics, technologies and strategies.

Historical perspective, objectives and strategies of drug discovery, animal models in drug discovery, management and regulatory issues, important parameters in drug discovery, process of drug discovery, computational techniques, areas influencing drug discovery, modeling, simulation and algorithms in drug discovery.

8 hrs

**Unit V**

Peptide combinatorial library technology, use of chemical databases in identifying drug targets, G-protein coupled receptors as drug targets, structure of GPCRs, GPCR modeling and screening, Orphan GPCRs (OGPCRs).

4 hrs

**Unit VI**

Drug Designing techniques and approaches. Preclinical Pharmacology, Pharmacological screening of Candidate molecules, Clinical trials.

## Unit VIII

Gene structure prediction tools – GenScan, Genome Scan, GRAIL, GLIMMER, ORF finder.

Drug designing softwares: ArgusLab, Hex, Autodock, GOLD, Schrodinger, Molegro, Discovery Studio, Hyperchem, Dragon, Avegado.

10 hrs

## References:

9. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata McGraw Hill Publishing Co Ltd., India.
10. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2<sup>nd</sup> ed. Wiley Inter-science, New York.
11. Pennington, S.R. and Dunn, M.J. 2002. Proteomics, from Protein Sequence to Functions. Viva Books Pvt Lrt., New Delhi.
12. Rastogi, S. C, Mendiratta, N & Rastogi, P. 2004. Bioinformatics Methods and Applications, Genomics, Proteomics and Drug Discovery. PHI private limited, NewDelhi.
13. Rajan, S.S. and Balaji R. 2002. Introduction to Bioinformatics. Himalaya Publishing House, Mumbai.
14. Rastogi, S. C., Mendiratta, N. and Rastogi, P. 2003. Bioinformatics: Concept Skill and Applications. CBS Publisher and distributors, New Delhi.
15. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2<sup>nd</sup> ed. Wiley Inter-science, New York.
16. Attwood and Parry-Smith, D.J. 1999. Introduction of Bioinformatics. Pearson Eduaction Ltd, Delhi.

BI. HCP-3.6.3 Lab based on BI. HCT-3.5.3

Practicals are designed based on the BI.HCT-3.5.3 syllabus

Practicals:

1. Problem based exercise
2. Process of patenting
3. Preparing Business Plan
4. Case based study on patent and its violation
5. Clinical Trials

### #BI-ESS-3.7 Entrepreneurship and Start up Studies

#ESS- Entrepreneurship and Start-up Studies \* Entrepreneurship and Startup Studies Report is mandatory in 3<sup>rd</sup> Semester, \*\*In C3 evaluation 70 marks is been distributed as 50 marks for report submission and 20 marks for presentation and Viva-Voce

## BI. OET-3.8 Biological databases and Tools

Total: 60 hrs

**Unit I**

Bioinformatics: An Overview- Introduction to Computational Biology and Bioinformatics, scope and applications; Emergence of Bioinformatics as a Separate Discipline; Some of the biological problems that require computational methods.

6 hrs

**Unit II**

Biologically Data Acquisition- DNA Sequencing Methods- Basics of DNA Sequencing, Automated DNA Sequencing, DNA Sequencing by Capillary Array and Electrophoresis; Types Of DNA Sequences- Genomic DNA, cDNA, Recombinant DNA, Expressed Sequence Tags(ESTS), Genomic Survey Sequences(GSS); RNA Sequencing Methods; Protein Structure Determination Methods; Gene Expression Data.

12 hrs

**Unit III**

Biological databases – types of databases, literature databases, sequence databases, structure database, functional databases and chemical databases.

Nucleotide Sequence Database – GenBank, EMBL-EBI, DDBJ and INSDC.

Protein sequence data – Swiss-Prot, TrEMBL, Uniprot KB, PIR, CDD.

Structure Databases (PDB, MMDB)

8 hrs

**Unit IV**

Genome databases – Bacterial genome database – GOLD, MBGD, Viral genome databases – ICTVDB, VirGen, Human genome databases – MapViewer, Ensembl, UCSC, Vista-genome Browser, OMIM/OMIA.

Organisms Specific Databases (Wormbase, Ecogene, SGD, TAIR, Flybase etc).

8 hrs

**Unit V**

Common Sequencing File Formats- GenBank flatfile format, Fasta file format, NBRF/PIR, GDE; Multiple Sequence Format (MSA), ALN Format, Files from Structural Data –PDB flatfile format,

4 hrs

**Unit VI**

Data: Access, retrieval and submission of sequences to GenBank and structures to PDB.

Standard Search Engines Data Retrieval Tools- ENTREZ, DBGET and SRS.

4 hrs

**Unit VII**

Design of Circuits and Databases: Introduction- databases KEGG, EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, Expression databases and various databases related to systems biology.

8 hrs



## BI. SCT-4.3 Perl and CGI

Total: 60 hrs

**Unit I**

Getting Started with Perl: Overview, perl benefits, installation, interpreter, documentation, Edit-run-reverse, open sources, Comprehensive Perl Active Network.

4 hrs

**Unit II**

Data Structures – Command interpretations, commands, scalar strings, values, numbers and variables, assignments, scalar operations, and functions, statements and blocks, array variables, literal representation of arrays, array operations and functions, scalar and list context, hash variables, literal representation of hash variables, hash functions, using hashes for genetic code, gene expression data using hashes.

10 hrs

**Unit III**

Operators – arithmetic operators, bitwise operators, string operators, file test operators, conditional and logical operators (true and false), logical operators, binding operators, loops, i/o functions.

8 hrs

**Unit IV**

Programming with PERL – Representing sequence data, a program to store a DNA sequence, concatenation of strings, transcription, translation, flow control, finding motifs, counting nucleosides, conversion of sequences into FASTA format.

8 hrs

**Unit V**

Subroutines, advantages of subroutines, scoping and subroutines, arguments, passing data to subroutines, modules and libraries of subroutines, concept about file handling, open and closing of file handle, opening and closing a directory handle, directory manipulations, Perl debugger, regular expressions and pattern matching, simple uses of regular expressions, matching operators, substitutions, split and join function.

10 hrs

**CGI Programming****Unit VI**

Introduction on CGI, Applications of CGI, Some Working CGI Applications, Internal Workings of CGI, Configuring the Server, Programming in CGI, CGI Considerations, Input to the Common Gateway Interface: Using Environment Variables,

Accessing Form Input, Extra Path Information, Other Languages Under UNIX, Other Languages Under Microsoft Windows, Other Languages on Macintosh Servers, Examining Environment Variables;

Output from the Common Gateway Interface, Forms and CGI, HTML Tags, Sending Data to the Server, Designing Applications Using Forms in Perl, Decoding Forms in Other Languages, Environment Variables, Including Boilerplates, File Statistics, Executing External Programs, Executing CGI Programs.

20 hrs

Target identification and Target validation - Molecular modelling and simulation.

8 hrs

**Unit VII**

Concept of lead, lead identification and lead optimization, Computer Aided Drug Design (CADD) Structure based drug design (SBDD) and Ligand Based Drug Design (LBDD); Specific activity relationship (SAR), Quantitative Structure Activity Relationship (QSAR) methods and applications. Combinatorial chemistry and virtual screening.

Drug designing softwares: ArgusLab, Hex, Autodock, GOLD, Schrodinger, Molegro, Discovery Studio, Hyperchem, Dragon, Avegado.

10 hrs

**Unit VIII**

Pharmacogenomics: Hereditary basis for differences in population, Examples of pharmacogenetic traits. Enzymes involved in the metabolism of drugs. Pharmacological Technology.

Association between Genome data and drug response pattern. Analysis of variation among the population by polymorphism. Pharmacogenetic and Pharmacogenomics applications.

4 hrs

**BI. HCP-4.2 Lab based on BI. HCT-4.1**

1. Chemical databases
2. Pharmacophore identification
3. Protein structure database
4. Homology modelling
5. Binding site/active site identification
6. Computational Toxicity and druggability studies
7. Computational pharmacokinetics studies
8. Computed atlas of surface topography of protein (cast p).
9. Software - V-Life, Marvin sketch, Chems sketch, etc
10. Molecular Docking studies (Autodock)
11. QSAR studies
12. *In silico* Protein-protein interaction studies

**References**

1. Molecular Modelling, Principles and Applications, IInd Edition, A.R. Leach, 2001, Prentice Hall
2. Proteine Research: New Frontiers in Functional Genomics (1997). Edited by M.R. Wilkins, K.L. Williams, R.D.Appel and D.F. Hochstrasser, Springer – Verlag, New York.
3. Expression Genetics: Acclerated and High Throughput Methods (1999) Edited by M.McClelland and A. Pardee, Eaton Publishing, MA.
4. 2-D Proteome Analysis Protocols (1998). Edited by A.L. Link, Humana Press, Totowa, NJ.
5. Proteins and Proteomics. 2002. R.J. Simpson. Cold Spring Harbor Lab. Press. New York.

## PGDBI-T1.1 Cell and Molecular Biology

Total : 60 hrs

### Unit I

Architecture of prokaryotic and eukaryotic cells and tissues, Dynamics of eukaryotic cell, Molecules of life, cellular evolution, Concept of Macromolecular assembly and structure and function of cell organelles. chemical organization of cell, comparison of cells, Cell division- mitosis and meiosis, eukaryotic cell cycle and its regulation. Cellular Physiology – electron transport system in mitochondria and chloroplast.

12 hrs

### Unit II

DNA replication- prokaryotic and eukaryotic DNA replication, mechanism of replication. Enzymes and necessary proteins in DNA replication. Telomeres, telomerase and end replication. Role of telomerase in aging and cancer.

8 hrs

### Unit III

Transcription-prokaryotic and eukaryotic transcription- RNA polymerases- general and specific transcription factors- regulation- Transcription termination; post transcriptional modification. Translation: prokaryotic and eukaryotic translation and regulation.

8 hrs

### Unit IV

Organization of prokaryotic and eukaryotic genomes, components of eukaryotic chromatin and chromosome structure, DNA super coiling, Gene expression in prokaryotes- Lac operon, Gal operon- role of promoters, Arabinose operon- positive control and trp operon – attenuation control. Gene expression in eukaryotes. Role of histones, histone acetyltransferases and histone deacetylases, transcription factors, NFkB, DNA binding protein motifs.

8 hrs

### Unit V

Mutations - Introduction and Types of Gene mutations, Base substitution, Frame shift mutation (insertion, deletion, missense, nonsense mutation). Mutagens - Physical and chemical, Reverse mutation in bacteria, DNA damage and repair mechanism (Mismatch repair photoreactivation, excision and SOS repair). Beneficial and harmful effects of mutations. Transposable elements.

8 hrs

### Unit VI

Cell Communication – Membrane Transport Principles, Active Transport, Ion Channel; Protein Sorting- An Overview Of Targeting Proteins To Mitochondria, Nucleus, Endoplasmic Reticulum, Lysosome And Plasma Membrane. Cell-Cell Communication.

8 hrs

### Unit VII

Cell signaling mechanism, K<sup>+</sup> channel, cell signaling through receptors and messengers, cell signaling through growth factors, Apoptosis, Necrosis and Autophagy.

8 hrs

## PGDBI-P1.1 Lab based on PGDBI 1.1

### Cell biology

1. Paper chromatography/Thin Layer chromatography of chlorophyll pigments
2. Mitosis and Meiosis
3. Chromosomal analysis and Karyotyping
4. Bacterial Growth curve study
5. Human Bar Body study
6. Study of mutants of *Drosophila*
7. Study of polytene chromosome

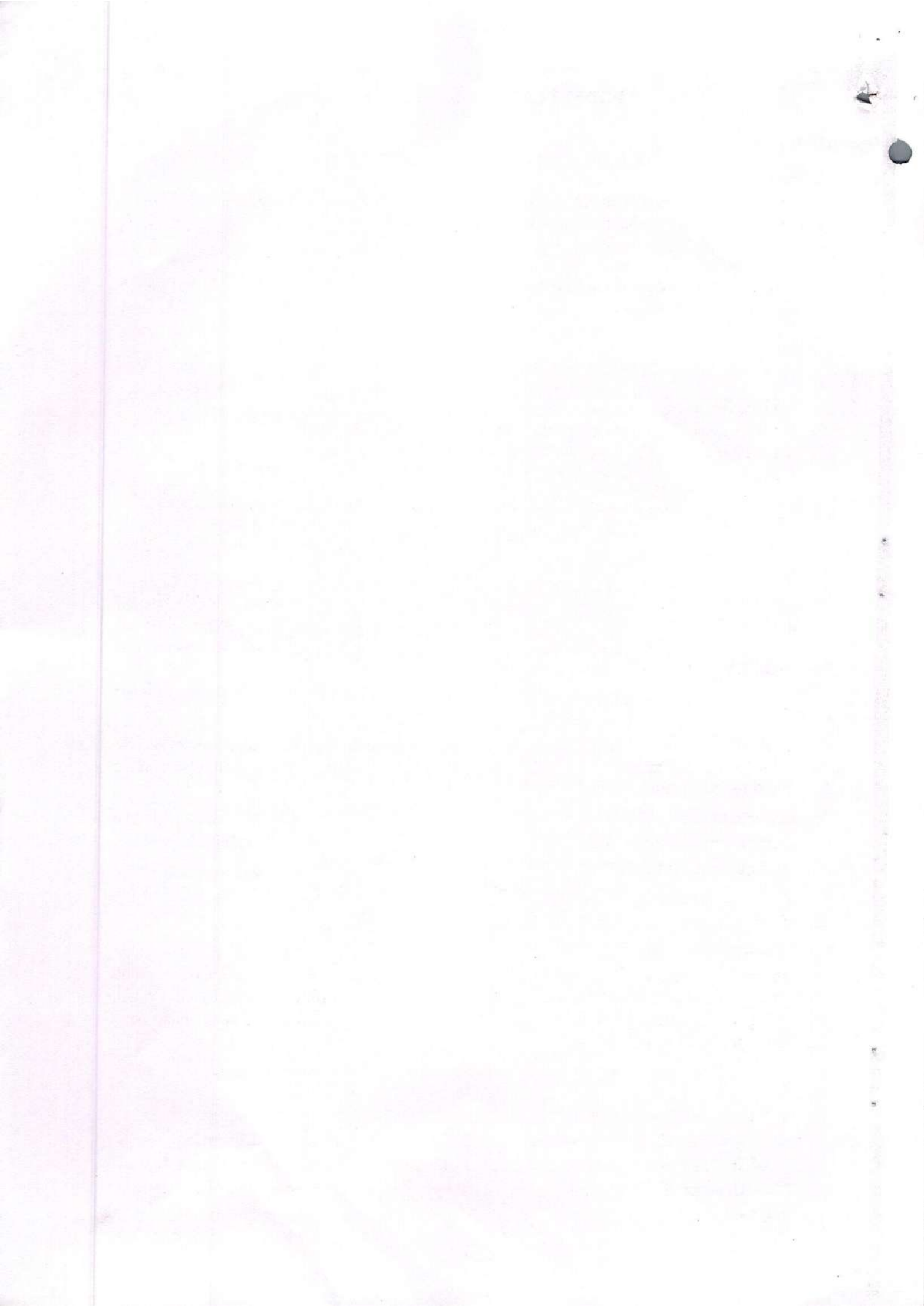
### Molecular biology

1. Quantitative estimation of DNA and RNA.
2. Isolation & purification of genomic DNA from bacteria
3. Isolation & purification of plasmid DNA.
4. Agarose gel electrophoresis of chromosomal & plasmid DNA.
5. Restriction digestion of chromosomal & plasmid DNA
6. Isolation of DNA fragments from agarose gel.
7. Transformation studies

Note: Including the above experiment, teachers can design additional experiment if needed.

### References:

1. Karp, G. (2005) "Cell and Molecular Biology: Concepts and Experiments"; Fourth Edition, Wiley Publishing Co. USA.
2. Lodish, H., Scott, M.P., Matsudaira, P., Darnell, J., Zipursky, L., Kaiser, C.A., Berk, A. and Krieger, M. (2003) "Molecular Cell Biology"; Fifth Edition, W. H. Freeman and Co., New York.
3. De Robertes and DE Robertes (2002) "Cell and Molecular Biology". Saunders College, Philadelphia, USA.
4. Brown, T.A.(Ed). 1998. Molecular Biology I: Recombinant DNA. Academic press, New York.
5. Brown, T.A.(Ed). 1998. Molecular Biology II: Gene Analysis, Academic press, New York.
6. Watson, J.D. *et al.* 1987. Molecular Biology of the Genes, 4<sup>th</sup> ed. The Benjamin Cunnings Pub. Inc., California.
7. Lewin, B. 1997. Gene VI. John Wiley and Sons, New York.
8. Freifelder and G.M. Malacinski. 1996. Essentials of Molecular Biology Panim, New Delhi.



## PGDBI-T1.2 Biochemistry and Biophysics

Total: 60 hrs

### Unit I

Nucleic Acids: Structure Of Nucleic Acids: Structures of Purines and Pyrimidines, Structure of DNA; Type of DNA and their structures, A, B and Z DNA, Supercoiled DNA, T<sub>m</sub> and C<sub>ot</sub> Curve for Dissociation of DNA. Motifs of DNA - Promoters, Enhancers and Attenuators.

DNA Protein Interaction: Recognition of DNA in Prokaryotes and Eukaryotes. Interaction of Specific Proteins with references to Trp-Repressors, CAP Proteins, Zinc Finger Proteins, Lac-Repressors, Phage Repressor and Cro Protein.

8 hrs

### Unit II

Amino Acids: General Properties, Classification of Amino Acids; Based On Polarity, Based On Functional Groups, Essential and Non-Essential Amino Acids, Acid Base Properties, Stereo Chemistry. Non Standard Amino Acids.

Proteins: Salient Features of Peptide Bond; Conformation and its properties, Structural Hierarchy of the Protein, Primary, Secondary, Tertiary and Quaternary Structures with Examples.

8 hrs

### Unit III

Motifs of Proteins: Alpha Structures: Coiled Coil, Four Helix Bundles. and Globin Motifs with Examples, Beta Structures: Up And Down Beta Barrel, Greek Key Motif, and Jelly Roll Motifs with Examples Alpha/Beta Structures: Horse Shoe Motifs, TIM Barrel Motifs, Rosmann Fold, Beta Alpha Beta Motifs with Examples and Other Motifs.

8 hrs

### Unit IV

Folding And Flexibility: Concept of Protein Folding; Christian Anfinsen Reaction on Bovine Pancreatic RNase, Lavinthal Paradox, Thermodynamics Of Protein Folding, Steps Involved In Protein Folding, Structure And Molecular Mechanism Of Chaperon Mediated Protein Folding.

Structure and Structure Based Mechanism of Protein Action. Membrane proteins and Signal Transduction. Proteins of the Immune Systems, Structure of Viral Capsomeres, and Importance of Structure Based Drug Designing.

8 hrs

### Unit V

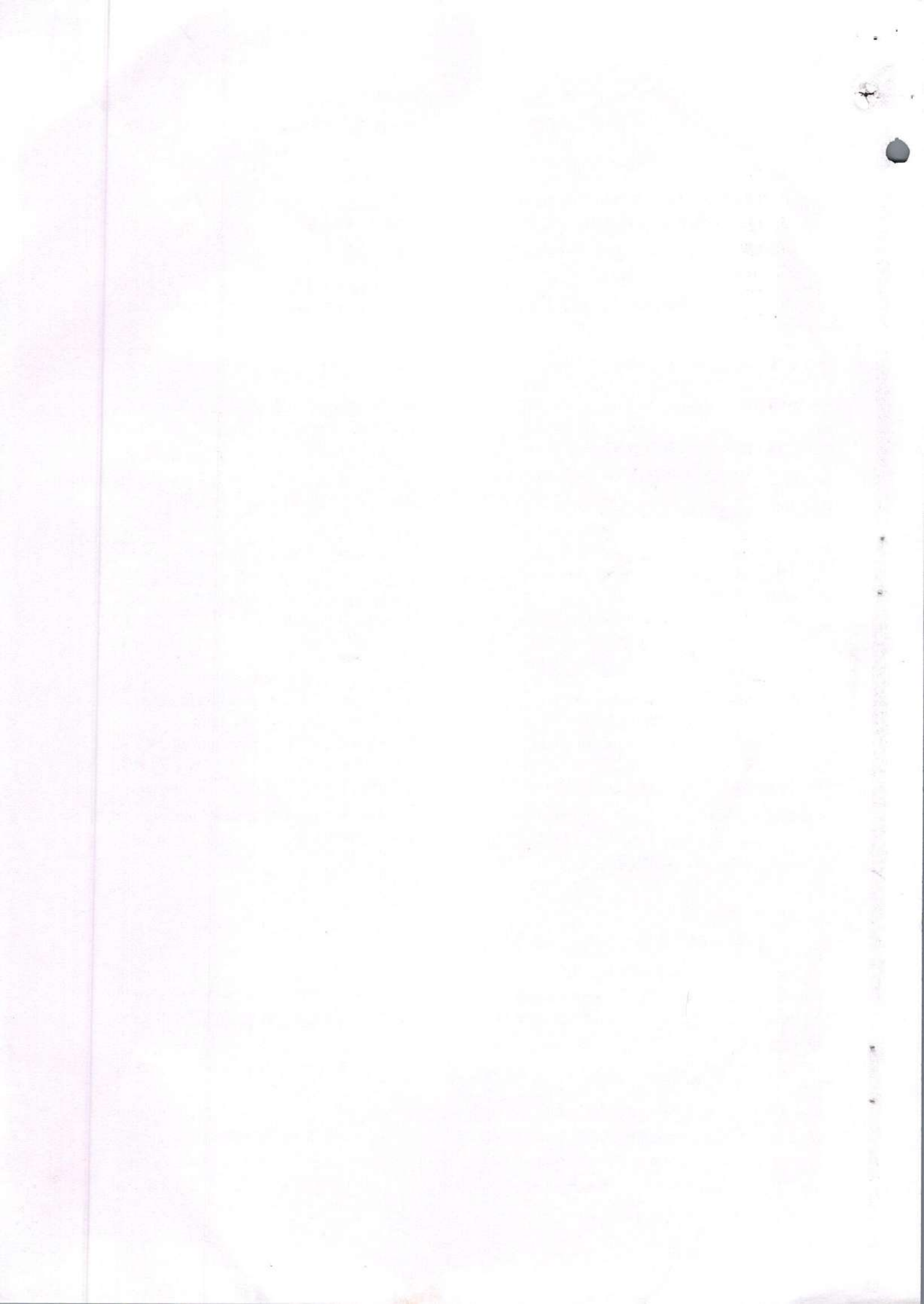
Protein Purification and Sequencing Techniques: General Approaches: Chromatography, Electrophoresis, Different types of PAGE, Western Blotting. Protein Sequencing-Steps and Strategies Involved In Protein Sequencing, Chemistry of Different Methods of Protein Sequencing and Sequence Assembly. Determination of Protein Structures by NMR and X-ray Crystallography

8 hrs

### Unit VI

Mechanics: Newton's Law of Motion- Mechanics of Particle- Work Energy Principle- Relational Dynamics- Static and Dynamic Equilibrium – Conservation Laws. Thermodynamics- Concept of Temperatures- Thermodynamic Equilibrium; Zeroth Law- Conservation of Energy; First Law- Concept of Entropy; Second Law- Absolute Law of Temperature; Third Law of Thermodynamics.

12 hrs



## PGDBI-P1.2 Lab based on PGDBI 1.2

1. Qualitative and Quantitative Analysis of Carbohydrates.
2. Qualitative and Quantitative Analysis of Proteins.
3. Qualitative and Quantitative Analysis of Amino Acids.
4. Qualitative Analysis of Nucleic Acids.
5. Study of Protein Motifs.
6. Bioinstrumentation - Thin layer chromatography, Column chromatography, HPLC, AGE, PAGE.

Note: Including the above experiment, teachers can design additional experiment if needed.

### References

1. Resnick, R., Halliday, D And Walker (2001) "Fundamentals Of Physics". Sixth Edition, John Wiley And Sons, USA
2. Tipler, P. A (1999) "Physics for Engineers and Scientists: Fourth Edition, W.H. Freeman And Company, USA
3. Essentials of Immunology by Riott I .M. 1998. ELBS, Blackwell Scientific Publishers, London.
4. Immunology 2 nd Edition by Kuby J. 1994. W.H. Freeman and Co. New York.
5. Immunology - Understanding of Immune System by Claus D. Elgert. 1996. Wiley - Liss, New York.
6. Fundamentals of Immunology by William Paul.
7. Cellular and Molecular Immunology. 3rd Edition by Abbas.
8. Immunobiology: The Immune System in Health and Disease. 3rd Edition by Travers.
9. Immunology- A short Course. 2 nd Edition by Benjamin.
10. Manual of Clinical Laboratory and Immunology 6th Edition. 2002 by Noel R. Rose, Chief Editor: Robert G. Hamilton and Barbara Detrick (Eds.) , ASM Publications.



## PGDBI-T1.3 : Fundamentals of computers and C-programming

Total: 60 hrs

### Unit I

Generations of Computer, Computer Organization, Fundamentals of Computers, Block Diagram of Computer, Functions of the Different Units Input unit, Output unit, Memory unit, CPU (ALU+CU), Input & Output Devices Input Devices: a) Keyboard, b) Point and draw devices mouse, joystick, track ball, light pen c) Data Scanning d) Projector, Advantages and Limitations of Computers.

8 hrs

### Unit II

Basics of operating system DOS, Windows, Unix, Linux Application Software. Storage devices (RAM, ROM, Hard Drives etc).

Communication Technology- Networking- LAN, WAN And MAN, Internet- Wireless Communication- Internet, Network Topologies- Types And Application, Internet Technologies: Web Services- Www, URL, DNS- Servers E Mail Server, WEB Servers, Browsers- IP Addressing.

8 hrs

### C-Programming

#### Unit III

**Introduction:** History Of C Language, Getting Started With C, The Character Set – Alphabets, Digits And Special Symbols, Constants – Primary & Secondary Constants, Variables, Standard C Keywords, Data Types – Int, Float, Double, Char. C Instructions: Type Declaration Instruction, Arithmetic Instruction, Input/ Output Instruction, Control Instructions. Hierarchy of Operations, Priority, Operators Like Int to Float, Float to Int, Double to Int, etc., Type Conversions, Structure of a C Program

10 hrs

#### Unit IV

**Operators:** Arithmetic, Relational, Logical, Assignment, Increment and Decrement, Conditional, Bitwise, Special Operators. Decision-Making, Branching And Looping: *If*, Multiple Statements Within *If*, *If-Else*, Nested *If-Else* Statement, Use of Logical Operators Like *&&*, *||* And! Conditional Operator *While*, *Do*, *Do-While* and *For* Loop Control Structures, Nesting of Loops *Break* And *Continue* Statements, *Switch*, Case Control Structure, *Goto* Control.

8 hrs

#### Unit V

**Pointers and Arrays Functions:** Definition, Declaration, Initialization, Accessing elements of an Array, reading & entering data into an Array, Pointers and 2D And 3D Arrays

Understanding Pointers, Accessing Address of a Variable, Declaring and Initializing Pointers, Accessing variables through Pointers, Pointer expressions, Pointers and Arrays, Pointers and Character Strings, Pointers and Functions, Pointers and Structures, Points on Pointers. Functions: Need for User Defined Functions, Multifunction Program, C Function Forms, Return Values and their types, Calling a Function, No arguments and No return values, Argument but no return values, Argument with return values, Handling of Non Integer Functions, Nesting of Functions, Recursions, Function with Arrays,



**Unit VI**

**Strings:** Definition, Declaring and Initialization of Strings, Reading Strings From Terminal, Writing Strings to Screen, Arithmetic operations on Characters, Putting Strings together, Comparison of two Strings, Strings-Handling Functions, Table of Strings.

6 hrs

**Unit VII**

**Structures and Unions:** Introduction, Structure Initialization and Giving Values to Members, Arrays of Structures, Arrays within Structures, Structures within Structures, Structures and Functions. Size of the Structures, Unions and Case Studies.

**Files In C:** Defining a File and Opening a File, Closing a File, Input/Output Operation on a File, Error Handling During I/O Operations, Random access to Files, Command Line Arguments.

8 hrs

**PGDBI-P1.3 Lab based on PGDBI 1.3****C-Programming**

1. Flow Charts, Algorithm Keywords Identifiers, Variables Constants, Scope of Life of Variables- Local and Global variables. Data types, Expressions, Operators- Arithmetic Operators, Logical Operators, Relational, Conditional, Bitwise Operators- Input/ Output Library Functions.
2. Declaration Statements, Control Statement: If Statement, If...Else Statement, Nesting of If...Else statement, Switch Statement- Iteration Statements- Arrays: Multiple Dimensional Arrays, Array Declaration and Initialization of Arrays.
3. Functions: User Defined and Library Functions- File Handling: Opening A File, Closing A File Reading and Writing into a File, Appending a File, Pointers

Note: Including the above experiment, teachers can design additional experiment if needed.

**References:**

1. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata Mcgraw Hill Publishing Co Ltd., India.
2. The C Programming Language B.W. Kjernighan and D.M.Ritchie 2<sup>nd</sup> ed. Prentice Hall, India
3. Yashavant Kanetkar, 2002. Let Us C, 4<sup>th</sup> Ed, BPB Publications, New Delhi.
4. Yashavant Kanetkar, 1998. Graphics Under C, BPB Publications, New Delhi.
5. Schildt, Herbert, 2000. C: The Complete Reference, 4<sup>th</sup> Ed. Tata Mc Graw – Hill Publishing Co. Ltd., New Delhi.
6. Rajaraman, V. 1994, Computer Programming In C. Printice-Hall Of India Pvt. Ltd., New Delhi.
7. Sudha G Purohit et al, Statistics using R , Narosa publishing house, New Delhi
8. Lafore, R. (2002) "Object Oriented Programming Using C++", Fourth Edition, Sams Publishers.



## PGDBI-T1.4 Biological Databases and Tools

Total: 60 hrs

### Unit I

**Bioinformatics:** An Overview- Introduction to Computational Biology and Bioinformatics, scope and applications; Emergence of Bioinformatics as a Separate Discipline; Some of the biological problems that require computational methods.

6 hrs

### Unit II

**Biologically Data Acquisition-** DNA Sequencing Methods- Basics of DNA Sequencing, Automated DNA Sequencing, DNA Sequencing by Capillary Array and Electrophoresis; Types Of DNA Sequences- Genomic DNA, cDNA, Recombinant DNA, Expressed Sequence Tags(ESTS), Genomic Survey Sequences(GSS); RNA Sequencing Methods; Protein Structure Determination Methods; Gene Expression Data.

12 hrs

### Unit III

**Biological databases** – types of databases, literature databases, sequence databases, structure database, functional databases and chemical databases.

Nucleotide Sequence Database – GenBank, EMBL-EBI, DDBJ and INSDC. Protein sequence data – Swiss-Prot, TrEMBL, Uniprot KB, PIR, CDD. Structure Databases (PDB, MMDB)

8 hrs

### Unit IV

**Genome databases** – Bacterial genome database – GOLD, MGBD, Viral genome databases – ICTVDB, VirGen, Human genome databases – MapViewer, Ensembl, UCSC, Vista-genome Browser, OMIM/OMIA.

Organisms Specific Databases (Wormbase, Ecogene, SGD, TAIR, Flybase etc).

8 hrs

### Unit V

Common Sequencing File Formats- GenBank flatfile format, Fasta file format, NBRF/PIR, GDE; Multiple Sequence Format (MSA), ALN Format, Files from Structural Data –PDB flatfile format,

**Data:** Access, retrieval and submission of sequences to GenBank and structures to PDB. Standard Search Engines Data Retrieval Tools- ENTREZ, DBGET and SRS.

8 hrs

### Unit VI

**Design of Circuits and Databases:** Introduction- databases KEGG, EcoCyc, MetaCyc and BioCyc, PantherDB, Reactome, Biocarta, StringDB, Expression databases and various databases related to systems biology.

8 hrs

### Unit VII

**Gene structure prediction tools** – GenScan, Genome Scan, GRAIL, GLIMMER, ORF finder.

Drug designing softwares: ArgusLab, Hex, Autodock, GOLD, Schrodinger, Molegro, Discovery Studio, Hyperchem, Dragon, Avegado.

10 hrs

## PGDBI-P1.4 Lab based on PGDBI 1.4

### Biological databases:

- Nucleotide database
- Genome databases
- Protein Databases ..etc.

Note: Including the above experiment, teachers can design additional experiment if needed.

### References:

1. Balaguruswamy, E. (1985) "Computer Fundamentals And Applications ", Second Edition, Tata Mcgraw Hill Publishing Co Ltd., India.
2. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
3. Pennington, S.R. and Dunn, M.J. 2002. Proteomics, from Protein Sequence to Functions. Viva Books Pvt Lrt., New Delhi.
4. Rastogi, S. C, Mendiratta, N & Rastogi, P. 2004. Bioinformatics Methods and Applications, Genomics, Proteomics and Drug Discovery. PHI private limited, NewDelhi.
5. Rajan, S.S. and Balaji R. 2002. Introduction to Bioinformatics. Himalaya Publishing House, Mumbai.
6. Rastogi, S. C., Mendiratta, N. and Rastogi, P. 2003. Bioinformatics: Concept Skill and Applications. CBS Publisher and distributors, New Delhi.
7. Baxevanis, A.D. and Ouellette, B.F.F. 2001. Bioinformatics, A Practical Guide to the Analysis of Genes and Proteins, 2nd ed. Wiley Inter-science, New York.
8. Attwood and Parry-Smith, D.J. 1999. Introduction of Bioinformatics. Pearson Eduaction Ltd, Delhi.



## PGDBI-T2.1 High Through Technologies

Total: 60 hrs

### Unit-I

#### High-throughput sequencing technology

Introduction to Omic's technologies, Next-generation sequencing; Genome Alignment, Genome Visualization, De Novo Assembly Genome Variation

10 hrs

### Unit-II

**Quantitative transcriptomics:** qRT-PCR; Advanced transcriptomics: gene expression microarrays, Next-generation sequencing in transcriptomics: RNA-seq experiments; Analysis of transcription factor binding sites

10 hrs

### Unit-III

#### Information processing from Sequence data

Organizing high throughput data; Analysis of Genome, Transcriptome, Metagenome, miRNA and Epigenomics data; Multiple testing and false discovery rate; Quality control of raw reads: FASTQC and fastx toolkit; Read alignment to a reference genome: Bowtie and Tophat; Peak calling: MACS, USeq and SISSR

10 hrs

### Unit-IV

Statistical Modeling; Hierarchical Models and the basics of Bayesian Statistics; Exploratory Data Analysis for High throughput data; Analysis of Metagenomic Data; QIIME, PICRUST; High-Throughput Sequencing Data Informatics

10 hrs

### Unit-V

#### RNA sequencing and analysis

Introduction to R; Informatics for RNA-seq Analysis and ChIP-seq; Experiment design for ChIP-seq and RNA-seq; Small non-coding RNA analysis: R, Reaper; Exploratory Analysis of Biological Data using R; Pathway and Network Analysis of -omic Data; Microbiome projects; Proteogenomics

10 hrs

### Unit-VI

#### Gene Expression Analysis and Network Analysis

Microarray Expression Analysis - Quantification of expression and differential expression analysis and differential exon usage: R, DESeq, DEXSeq; Normalisation and experimental design models for microarray data. Metabolomics - Informatics and Statistics for Metabolomics; Expression and Differential Expression, Isoform Discovery and Alternate Expression, Regulatory Network Analysis

10 hrs





## PGDBI-P2.1 Lab based on PGDBI 2.1

### NGS sequencing data analysis tools

- FastQC
- BWA
- Bowtie
- Fastx tool kit
- Samtools

### Microarray Data analysis tools

- R and bioconductor

Note: Including the above experiment, teachers can design additional experiment if needed.

### References:

- Data Mining Techniques for the Life Sciences Oliviero Carugo (Editor), Frank Eisenhaber (Editor) Humana Press; 2010 edition. ISBN-13: 978-1603272407.
- An Introduction To High Content Screening: Imaging Technology, Assay Development, and Data Analysis in Biology and Drug Discovery - Steven A. Haney (Editor), Douglas Bowman (Editor), Arijit Chakravarty (Editor). Wiley-Blackwell (31 December 2014). ISBN-13: 978-0470624562.
- High Throughput Screening: Methods and Protocols (Methods in Molecular Biology) 29 Nov 2011 - William P. Janzen (Editor), Paul Bernasconi (Editor) ISBN-13: 978-1617794919.
- RNA Bioinformatics (Methods in Molecular Biology) Hardcover – 22 Jan 2015 - Ernesto Picardi (Editor) ISBN-13: 978-1493922901.

**Unit-I**

**An Introduction to Python Programming:** Working with Python, An interpreter for python, Relational operators, Logical operators, Bitwise operators, Variables and assignment Statements, Keywords, Script mode.

8 hrs

**Unit-II**

**Basic Concepts:** Control structures, if-else conditional statement, Looping statements, Nested loops, break, continue and pass, Debugging, Scope of variables, Strings, String manipulations, Regular Expressions, Built-in Functions, I/O Functions, Function Definition and Call, Importing user defined modules, Command-line arguments, Mutable and Immutable objects, Recursion.

8 hrs

**Unit-III**

**Advanced Concepts:** Lists, Accessing lists, Working with lists, Operations, related Functions and Methods, Tuples, Accessing tuples, Working with tuples, Operations, related Functions and Methods, Dictionary, Working with dictionary, Accessing values in dictionaries, Working with dictionaries, Operations, related Functions and Methods. Files and Exceptions: File Handling, Writing structures to a file, Errors and Exceptions, Handling exceptions using try-except, File processing examples.

8 hrs

**Unit IV**

**Biopython:** Basics of python, installing, writing python programming, python values and variables. working with sequences, parsing sequence file formats, connecting with biological databases, sequence objectives, sequence input and outputs, accessing biological database resources.

8 hrs

**Unit V**

**Introduction to Artificial Intelligence:** Introduction to Artificial Intelligence, Problems, Approaches and tools for Artificial Intelligence. Introduction to search, Search algorithms, Heuristic search methods, Optimal search strategies. Use of graphs in Bioinformatics. Grammers, Languages and Automata. Current Techniques of Artificial Intelligence: Probabilistic approaches: Introduction to probability, Bayes' theorem, Bayesian networks and Markov networks

8 hrs

**Unit VI**

**Classification Methods:** Linear Classifiers & Logistic Regression, Linear Classifiers, Overfitting & Regularization in Logistic Regression, Decision Trees, Preventing Overfitting in Decision Trees, Handling Missing Data, Clustering and retrieval of data, Nearest Neighbor Search, Clustering with kmeans, Hierarchical Clustering.

8 hrs

**Unit VII**

**Introduction –Agents– Problem formulation– uninformed search strategies – heuristics – informed search strategies – constraint satisfaction. Study of Ethical, legal and social issues associated with AI.**

Supervised learning (parametric/non-parametric algorithms, support vector machines, kernels, neural networks, Unsupervised learning (clustering, dimensionality reduction, recommender systems, deep learning, Best practices in machine learning (bias/variance theory; innovation process in machine learning and AI, Support vector machines (SVMs), case studies and applications.

12 hrs

## PGDBI-T2.3 Molecular Modeling and Drug Discovery

Total: 60 hrs

### Unit I

**Force field parameters and models:** Introduction:- Hooks law, Harmonic Oscillator Model for Molecules, Morse Potential and comparison with Harmonic Potential, Intra- and Inter- molecular forces and energies, Potentials: Lennard-Jones, Truncated Lennard-jones, Exponential-6, Ionic and Polar potentials. Types of Force Fields: Biomolecular force fields (AMBER, GROMOS, etc.), Molecular Mechanics potentials for small organic molecules (MM series), second generation force fields (UFF, CFF and MMFF)

8 hrs

### Unit II

**Potential Energy Surface and Energy Minimization:** PES and features, Convergence Criteria and Characterization. Minimization:- multivariable minimization Algorithms, level Sets and Curves, Gradients, Minimization Criteria, Unidirectional Search, Finding Minimum Point, First order methods:- Steepest Descent and Conjugate Gradient Methods.

8 hrs

### Unit III

**Molecular Dynamics Simulation:** Introduction, Newtonian dynamics, Integrators- Leapfrog and Verlet algorithm, Radial distribution functions, Pair Correlation function, Potential truncation and shifted-force potentials, solvation and models, Periodic boundary conditions, Temperature and pressure control in molecular dynamics simulations.

8 hrs

### Unit IV

**Basis of drug action:** How drugs work - Pharmacokinetics (ADME) and pharmacodynamics basis of drug action.

4 hrs

### Unit V

**New drug discovery process** - Target identification and validation, lead identification and optimization. Pre-clinical and clinical testing of new drugs.

4 hrs

### Unit VI

**Drug Design approaches:- Structure based drug design:** Prediction and validation of 3D structure of proteins using homology modeling for docking. Basis of Docking (pose prediction and scoring algorithms) and its application in lead identification and optimization, De Novo Drug Design (Fragment Placements, Connection Methods, Sequential Grow), Virtual screening strategies for lead identification.

8 hrs

### Unit VII

**Ligand based drug design** - 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 (regression Analysis, Partial Least Squares (PLS), Principle Components Analysis (PCA)), model validation methods and applications of QSAR.

12 hrs

### PGDBI-P2.3 Lab based on PGDBI 2.3

1. Chemical databases
2. Pharmacophore identification
3. Protein structure database
4. Homology modelling
5. Binding site/active site identification
6. Computational Toxicity and druggability studies
7. Computational pharmacokinetics studies
8. Computed atlas of surface topography of protein (cast p).
9. Software - V-Life, Marvin sketch, Chems sketch, etc
10. Molecular Docking studies (Autodock)
11. QSAR studies
12. *In silico* Protein-protein interaction studies

Note: Including the above experiment, teachers can design additional experiment if needed.

#### Reference:

1. Computational Chemistry and Molecular Modeling-Principles and Applications by Ramachandran, Deepa and Namboori., 2008, Springer-Verlag.
2. Molecular Modeling Principles and Applications (2nd Ed.) by Andrew R. Leach., Prentice Hall, USA. 2001 46
3. Computational Drug Design: A Guide for Computational and Medicinal Chemists, by David C. Young, Wiley, 2009.
4. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe., John Wiley & Sons Ltd.2008
5. Molecular Modeling and Simulation – An Interdisciplinary Guide by Tamar Schlick., Springer-Verlag 2000
6. Computational Medicinal Chemistry for Drug Discovery, edited by Patrick Bultinck., Hans De Winter, Wilfried Langenaeker, Jan P. Tollenare, CRC press, 2003.
7. The art of molecular dynamics simulation, second edition by D. C. Rapaport, Cambridge University Press, 2004
8. Homology Modeling Methods and Protocols by Andrew J.W. Orry.,University of California,USA.2012.

## PGDBI-T2.4 Biological data Analytics

Total: 60 hrs

### Unit I

**Introduction to Bioinformatics** : History of Bioinformatics, Role of Bioinformatics in biological sciences, scope of bioinformatics. Introduction to internet: WWW, network basics, LAN & WAN standards. Network topologies and protocols: ftp, http.

6 hrs

### Unit II

**Introduction to Database**: Types of database. Biological Database: Need of biological database, Sequence and Structure database – (NCBI, EMBL, DDBJ, and PDB), other databases - KEGG, PubMed, OMIM, PubChem, NCI, ZINC, Drug Bank, Ligand. Format of Databases: GenBank and PDB flat file. Protein Structure Visualization: RasMol, PyMol, Jmol, CN3D, Swiss PDB viewer, Chimera and Discovery Studio visualizer. Protein Structure Comparison: Intra-molecular Method, Intermolecular method, combined method. Protein Structure Comparison: SCOP and CATH.

8 hrs

### Unit III

**Sequence Alignment and Motif**, Domain Prediction Pairwise Alignment: Dot Matrix Method, Dynamic programming - (Local and Global Alignment) Gap Penalties, POA Alignment. Scoring Matrices: Amino acid scoring matrices, PAM, BLOSUM. Database Similarity Searching: BLAST. BLAST variants. BLAST output format. FASTA. Multiple Sequence Alignment: Scoring function, exhaustive algorithms, and Heuristic algorithms. PSSM, Markov Model and Hidden Markov Model. Protein Motif and Domain Prediction: Motif and Domain Databases PROSITE. Sequence Logos and Web-logo.

10 hrs

### Unit IV

**Gene and Promoter Prediction and Phylogenetic Gene Prediction** in Prokaryotes: Conventional determination of Open Reading Frames (ORF), Markov model and HMM. Gene Prediction in Eukaryotes: An Initio based program, Neural Networks. Promoter and Regulatory Element Prediction: Prokaryotes and Eukaryotes. Introduction to Phylogenetic: Phylogenetic Basics, Terminologies. Phylogenetic Tree construction Methods: Distant based method - (UPGMA, NJ) Character Based Method - (MP and ML), Phylogenetic Tree Evaluation: Bootstrapping.

10 hrs

### Unit V

**Protein Structure Prediction and Molecular Dynamics** Globular Proteins: Ab-Initio, Homology Based, Neural networks method. Transmembrane Proteins: Prediction of Helical membrane,  $\beta$ -barrel membrane proteins. RNA Structure Prediction: Ab Initio approach, dot matrices. Introduction to Homology modeling: Model refinement, model evaluation, homology model databases. Threading and fold recognition, CASP.

8 hrs

### Unit VI

**Introduction of Molecular Modeling**: Coordinate system, potential energy. Steps in Molecular Modeling: introduction to Quantum Mechanics, introduction to Molecular mechanics. Force Filed: Types of force fields: Amber force field, CHARMM force field. Introduction about molecular dynamics (GROMACS).

8 hrs

## Unit VII

Drug Discovery Process, Molecular Modeling in Drug Discovery, Quantitative Structure-Activity Relationship (QSAR). Chemoinformatics: Introduction, stereochemistry, origin of stereospecificity in molecular recognition, importance of design. Docking and Virtual Screening: Using different docking algorithms, Optimization of algorithms based on different target, Ligand - Receptor Interactions: Docking software's (AUTODOCK, LEAD IT), Post docking analysis. Pharmacokinetics: Absorption, Distribution, Metabolism, Excretion and Toxicity of drugs.

10 hrs

### PGDBI-P2.4 Lab based on PGDBI-P2.4

1. Entrez and Structure Searches. a. Pubmed  
b. Pubmed  
c. OMIM/ClinicalTrials.gov  
d. Citation
2. SRS of Biological Databases. a. Nucleotide/ Genome Databases  
b. Protein Structure Database.  
c. Structure Databases  
d. Protein PDB Databases.
3. Sequence Analysis a. Dotplot  
b. Pairwise Alignment  
c. Multiple Sequence Alignment
4. Software Tools a. BLAST  
b. ClustalW, GA, MEME
5. Visualization Tools. a. Rasmol  
b. Cn3D  
c. Molmol

Note: Including the above experiment, teachers can design additional experiment if needed.

### References

1. David W Moore "Bioinformatics sequence and Genome analysis", Second Edition, Cold Spring Harbor Laboratory Press, 2013.
2. Attwood T K, Doolittle-Rifkin-Smith, "Introduction to Bioinformatics", Pearson Education, 2005.
3. Neil C. Jones and Pavel A. Pevzner, "An Introduction to Bioinformatics Algorithms", MIT Press, 2005. 2. Steffen Schuster-Kremer, "Molecular Bioinformatics: Algorithms and Applications", Walter de Gruyter, 1996.

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