

**Vels Institute of Science, Technology and Advanced Studies**

**Pallavaram, Chennai 600 117**

**School of Life Sciences**

**Department of Bioinformatics**

**M.Sc.,**

**BIOINFORMATICS**

**Program outcome:**

**PO-1:** He / She can gain the base path to the research work in the area of genetic diseases and medical genomics is rapidly increasing and the future of personalized medicine depends on bioinformatics approaches.

**PO-2:** He / She acquired the ability to do current biological approaches and methods that produce extremely large data sets, which cannot be analyzed by hand - for instance sequencing human genomes.

**PO-3:** He / She may able to analyze software for data studies and comparisons.

**PO-4:** He / She have the stable aptitude to carry out the project works relevant to future applications in biology, chemistry, pharmaceuticals, medicine, and agriculture.

**PO-5:** He / She acquire the base step to become an enterpreunar, consultant, medical coder and research analyst in modern biological and medical research and development which cannot be done without bioinformatics.

**PO-6:** He / She is gaining the capacity to accesses and do application research in web-based programs and databases.

**PO-7:** He / She have obtained knowledge to write competitive exams in Life Sciences.

**PO-8:** He / She is getting basic acquaintance in copyright and patent issues.

## **PROGRAM SPECIFIC OUTCOME**

**PSO-1:** The syllabus addresses the need to introduce students to new tools and application in bioinformatics.

**PSO-2:** To understand the basic technique in biological sciences and implement in the application oriented fields.

**PSO-3:** The PG course helps every candidate to analyze the software for data studies and comparisons and provides tools for modelling, visualizing, exploring and interpreting data.

**PSO-4:** This course focuses on employing existing bioinformatics resources - mainly web-based programs and databases.

**PSO-5:** To access the wealth of data to answer questions relevant to the average biologist, and is highly hands-on.

**PSO-6:** The main goal of the M.sc Bioinformatics is to convert multitude of complex data into useful information and knowledge.

**PSO-7:** The course is intended to describe not only with the programming languages but it covers the proteomics, genomics, cell and molecular biology, genetic engineering, biochemical pathways etc., relevant to the improvement and development of mankind and industrial application purposes.

**PSO-8:** The Research work in the area like genetic diseases and medical genomics is increasing rapidly and resulting in the future development of personalized medicine depends only on bioinformatics approaches.

## Department of Bioinformatics

### Board of Studies Members

#### M.Sc Bioinformatics

S.No	Name	Post	Contact address	Designation
1.	Dr.Radha Mahendran	Associate Professor/ Head Dept of Bioinformatics	VISTAS P.V. Vaithiyalingam Road Pallavaram Chennai - 600 117 Mobile no: 09003237145	Chairman
2.	Mrs. Suganya.J	Asst Professor/ Dept of Bioinformatics	VISTAS P.V. Vaithiyalingam Road Pallavaram Chennai - 600 117 Mobile no: 09042112221	Internal Members
3.	Dr. D. Velmurugan	Professor, Dept of Crystallography and Biophysics	University of Madras, Guindy Campus, Chennai 600 025 Phone: 044 – 22351367: 044- 22300122 Email: d_velu@yahoo.com	External Members
4.	Dr.P.Gautam	Professor, Centre for Biotechnology.	Anna University Chennai – 600 025 Phone: 044 –22350772 E.Mail: pgautam@annauniv.edu	External Members
5.	Dr. M.N Ponnusamy	Emeritus professor, dept of crystallography and biophysics	University of Madras, Guindy Campus, Chennai 600 025 Phone: 044 – 22300122 Email: mspy@hotmail.com	External expert

**M.Sc.,  
BIOINFORMATICS**

**Curriculum and Syllabus**

**(Based on Choice Based Credit System)**

**Effective from the Academic year**

**2015-2016**

**Department of Bioinformatics**

**School of Life Sciences**

## School of Life Sciences

### MSc. BIOINFORMATICS

### CURRICULUM

Total No. of Credits: 90

SEMESTER I						
Category	Code	Course	Hours / Week			Credits
			Lecture	Tutorial	Practical	
Core	15MBI001	INTRODUCTION TO BIOINFORMATICS	5	0	0	4
Core	15MBI002	BIOLOGICAL DATABANK AND SEQUENCE ANALYSIS – PRACTICAL	0	0	5	3
Core	15MBI003	COMPUTER PROGRAMMING IN C AND C++	5	0	0	4
Core	15MBI004	BIOPROGRAMMING IN C AND C++ - PRACTICAL	0	0	5	3
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE I	4	0	0	4
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE II	4	0	0	4
GE	-----	GENERIC ELECTIVE I	2	0	0	2
		<b>Total</b>	<b>20</b>	<b>0</b>	<b>10</b>	<b>24</b>

<b>SEMESTER II</b>						
<b>Category</b>	<b>Code</b>	<b>Course</b>	<b>Hours / Week</b>			<b>Credits</b>
			<b>Lecture</b>	<b>Tutorial</b>	<b>Practical</b>	
Core	15MBI005	PROGRAMMING IN VB AND RDBMS	5	0	0	4
Core	15MBI006	PROGRAMMING IN VB AND RDBMS - PRACTICAL	0	0	3	2
Core	15MBI007	PROGRAMMING IN PERL AND BIOPERL	5	0	0	4
Core	15MBI008	PROGRAMMING IN PERL AND BIOPERL - PRACTICAL	0	0	3	2
Core	15MBI009	MINI PROJECT	0	0	4	2
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE III	4	0	0	4
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE IV	4	0	0	4
GE	-----	GENERIC ELECTIVE II	2	0	0	2
		<b>Total</b>	<b>20</b>	<b>0</b>	<b>10</b>	<b>24</b>

SEMESTER III						
Category	Code	Course	Hours / Week			Credits
			Lecture	Tutorial	Practical	
Core	15MBI010	MOLECULAR MODELING AND DRUG DESIGNING	5	0	0	4
Core	15MBI011	COMPUTER AIDED DRUG DESIGNING - PRACTICAL	0	0	5	3
Core	15MBI012	ADVANCED PROGRAMMING IN JAVA	5	0	0	4
Core	15MBI013	PROGRAMMING IN JAVA AND BIOJAVA - PRACTICAL	0	0	5	3
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE V	4	0	0	4
DSE	-----	DISCIPLINE SPECIFIC ELECTIVE VI	4	0	0	4
GE	-----	GENERIC ELECTIVE III	2	0	0	2
		<b>Total</b>	<b>20</b>	<b>0</b>	<b>10</b>	<b>24</b>

SEMESTER IV						
Category	Code	Course	Hours / Week			Credits
			Lecture	Tutorial	Practical	
Core	15MBI014	OPERATING SYSTEMS	5	0	0	4
Core	15MBI015	CLINICAL RESEARCH	5	0	0	4
Core	15MBI016	MAIN PROJECT	0	0	20	10
		<b>Total</b>	<b>10</b>	<b>0</b>	<b>20</b>	<b>18</b>

### **DISCIPLINE SPECIFIC ELECTIVE COURSES**

1. 15MBI101 GENOMICS AND PROTEOMICS
2. 15MBI102 MOLECULAR CELL BIOLOGY AND BIOCHEMISTRY
3. 15MBI103 BIOENERGETICS
4. 15MBI104 CHEMINFORMATICS
5. 15MBI105 BIOPHYSICAL CHEMISTRY
6. 15MBI106 STRUCTURAL BIOINFORMATICS
7. 15MBI107 ENZYMES AND METABOLISM
8. 15MBI108 VIROLOGY
9. 15MBI109 DATA WAREHOUSING AND DATA MINING
10. 15MBI110 PYTHON FOR BIOINFORMATICS
11. 15MBI111 CLOUD COMPUTING
12. 15MBI112 GENETIC ENGINEERING

### **GENERIC ELECTIVE COURSES**

1. 15MBI151 INTRODUCTION TO BIOINFORMATICS
2. 15MBI152 CHEMINFORMATICS
3. 15MBI153 MOLECULAR MODELING AND DRUG DESIGNING
4. 15MBI154 STRUCTURAL BIOINFORMATICS
5. 15MBI155 PROGRAMMING IN PERL AND BIOPERL
6. 15MBI156 PYTHON FOR BIOINFORMATICS



## **MSc. BIOINFORMATICS**

### **SYLLABUS**

**15MBI001**

**INTRODUCTION TO BIOINFORMATICS**

**5 0 0 4**

#### **Course Outcome:**

- CO-1: To acquire the skill of in basics of computing including operating systems, Use of internet, visualization techniques, computing networks, softwares and hardwares.
- CO-2: To provide the necessary biological (Gene and protein) background which are required solve the problem that arise during the designing of algorithm.
- CO-3: To know about the biological concepts and relevant database workout for research entries.
- CO-4: To gain knowledge in biopolymer, synthetic polymer and basics in genome anatomy, structures of genomes in both prokaryotes and eukaryotes.
- CO-5: To understand generation of co-ordinates of biopolymers in Cartesian and cylindrical polar co-ordinate system.
- CO-6: To retrieve and analyze the biological sequences by using tools and software's.
- CO-7: To know about Similarity, Identity and Homology, Global Alignment, Local Alignment, Sequence assembly, Gene prediction, Protein Structure Prediction, Methodologies.
- CO-8: To prove an algorithm for the given biological problem is often necessary to replace the original problem with a more complicated problem in order to initialize the recursion.
- CO-9: Mathematical approach to solving certain types of biological problem like sequence alignment, gene detection, structure prediction, data-mining literature.
- CO-10: The problem is not directly noticeable, but the output of the problem dependent on the result predicted by the probability distribution.



## UNIT V      STRUCTURAL ANALYSIS

15

Analysis of structures and correctness of structures, Submission of data to PDB: atomic coordinates and electron density maps; Anatomy of Proteins - Ramachandran plot, Secondary structures, Motifs, Domains, Tertiary and quaternary structures; Calculation of conformational energy for bio-macromolecules; Methods for Prediction of Secondary and Tertiary structures of Proteins.

**Total: 75 Hours**

### **Text Book:**

1. Baxevanis A.D., Davison D.B., Page R. D. M. & Petsko G.A. Current Protocols in Bioinformatics. New York, John Wiley & Sons Inc., 2004. ISBN: 0555015254.

### **References:**

1. Korf Ian, Yandell Mark, Bedell Joseph. BLAST: an essential guide to the basic local alignment search tool. Shroff Publishers and Distributors Pvt. Ltd., 2003. ISBN: 8173665125.
2. Baxevanis Andreas D. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, 3rd Edition. Publisher: New York, John Wiley & Sons, Inc. 2002, ISBN: 9814126756
3. Lesk, A.M. (2002) "Introduction to Bioinformatics:", 1st Edition, Oxford University Press, Oxford, UK , , ISBN: 9042112221
4. Teresa Attwood, Parry-Smith David J. Introduction to Bioinformatics. Publisher: Pearson Education (Singapore) Pte.Ltd., 2001. ISBN:8178085070
5. Mount David W.. Bioinformatics: Sequence and Genome Analysis. Publisher: Cold Spring Harbor Laboratory Press; 1st edition 2001. ISBN: 0879695978
6. Gibas Cynthia, Jambeck Per. Developing Bioinformatics Computer Skills. Publisher: Shroff Publishers and distributors O'Reilly Media, Inc., 2001. ISBN: 8173662428

**Course Outcome:**

CO-1: To acquire skills to use different approaches for Retrieval of DNA Sequence.

CO-2: To develop the skills to Retrieval of protein Sequence from the protein databases. .

CO-3: To determine the three dimensional structure of protein

CO-4: To develop the knowledge to retrieve the particular information from the specialized databases.

CO-5: To achieve knowledge for the visualization of the Protein 3D Structure.

CO-6: To determine the functional information of the protein using functional databases

CO-7: To predict the classification of the protein based on its structural alignment.

CO-8: To perform multiple sequence alignment and phylogenetic analysis.

CO-9: To identified the gene coding region from the prediction servers.

CO-10: To develop the skill for calculating potential energy of the regular structure.

1. Biological Databanks, Sequence Databases, Structure Databases, Specialized Databases.8
2. Data retrieval tools and methods. 8
3. Database file formats. 8
4. Molecular visualization. 8
5. Gene structure and function prediction (using GenScan, Gene Mark). 8
6. Sequence similarity searching (NCBI BLAST). 5
7. Protein sequence analysis (ExpASy proteomics tools). 5
8. Multiple sequence alignment (Clustal). 2
9. Molecular phylogeny (PHYLP). 3

- |   |    |
|---|----|
| 10. Analysis of protein and nucleic acids sequences.  | 2  |
| 11. Sequence analysis using EMBOSS or GCG Wisconsin Package.  | 3  |
| 12. Development of programs in the analysis of nucleic acid sequences – such as protein coding regions in prokaryotes.  | 5  |
| 13. Programs to calculate potential energy of regular structures such as Collagen triple helix, DNA double helix, and their visualization in wire and stick model as well as space filling model. | 10 |

**Total: 75 Hours**

**Text Books:**

1. Epstein Richard J. Human molecular biology: an introduction to the molecular basis of health and disease. Publisher: Cambridge, UK ; Cambridge University Press, 2003.ISBN: 052164481X.

**References:**

1. Russell Peter J. Genetics: A Molecular Approach 3rd ed.: Pearson International Edition. Publisher : New York, Pearson ISBN: 9780321610225.
2. Brown, T.A. Genomes 2 Publisher: New York, BIOS Scientific Publishers Ltd. 2002, ISBN: 1859960294

**Course Outcome:**

CO-1: To understand the fundamentals of C and C++ programming.

CO-2: To understand the basic terminology used in computer programming.

CO-3: To write, compile and debug programs in C and C++ language.

CO-4: To use different data types in a computer program.

CO-5: To design programs involving decision structures, loops and functions.

CO-6: To choose the loops and decision making statements to solve the problem.

CO-7: To implement different operations on arrays.

CO-8: To use functions to solve the given problem and to understand the dynamics of memory by the use of pointers.

CO-9: To understand how to apply the major object-oriented concepts to implement object oriented programs in C++, encapsulation, inheritance and polymorphism.

CO-10: To gain a better understanding of Object Oriented design and program implementation using OOPS language features.

**UNIT I      C PROGRAMMING****15**

Concept of variables and constants, structure of a C program. Operators & Expressions: Arithmetic, Unary, Logical, Bit-wise, Assignment & Conditional Operators, Library Functions, Control Statements: while, do While, for statements, Nested loops, if..else, switch, break, continue and go to statements, Comma operator.

**UNIT II      FUNCTION, STRING, POINTERS****20**

Functions: Defining & Accessing : Passing arguments, Function Prototype, Recursion, Use of Library Functions, Storage Classes: Automatic, External and Static Variables (Register), Arrays:



**References:**

1. Kanetkar Yashavant. Let Us C 9th Edition. Publisher: New Delhi BPB Publications. 2009. ISBN: 9788183331630.
2. Jonassen Inge, Kim Junhyong. Algorithms in Bioinformatics: 4th International Workshop, WABI 2004 Bergen, Norway, September 2004 Proceedings. Publisher: New York Springer. 2004. ISBN: 3540230181.
3. Kernighan Brian W. Ritchie Dennis M. The C Programming Language 2nd Edition. Publisher: USA, Prentice-Hall, Inc. 1988. ISBN: 0876925964.

**15MBI004****BIOPROGRAMMING IN C AND C++****0 0 5 3****Course Outcome:**

CO-1: To learn about the operators arithmetic and logical.

CO-2: To gain knowledge in identify branching and looping in C.

CO-3: To enlighten about classes and objects in C++.

CO-4: To learn the program of inheritance in C++.

CO-5: To execute comparisons and translation of DNA sequence to protein sequence in C and C++.

CO-6: Analyze the functional blocks, handling default reference arguments.

CO-7: To run the handling inline and overload function in C++.

CO-8: To understand arrays and objects in C++.

CO-9: Learn to rectify the errors Insertion and deletions programs in C++.

CO-10: To know about reversal sorting of elements using C++.



1) Operators and Expressions, Branching and Looping in C.	8
2) Classes and Objects in C++.	8
3) Program to demonstrate Inheritance in C++.	8
4) Translate DNA sequence to Protein in C & C++.	10
5) Comparing two Sequences.	8
6) Calculate the true length of a Sequence.	8
7) Function Blocks: a. Handling default reference arguments b. Handling inline and overloaded function C++.	10
8) Arrays and String as objects: Insertion, Deletion, reversal sorting of elements into a single in C++.	15

**Total: 75 Hours**

**Text Book:**

1. Balagurusamy E. Programming In ANSI C. Publisher: New Delhi Tata McGraw Hill Publishing Company Ltd. 2007. ISBN: 9780070648227

**References:**

1. Kanetkar Yashavant. Let Us C 9th Edition. Publisher: New Delhi BPB Publications. 2009. ISBN: 9788183331630.
2. Jonassen Inge, Kim Junhyong. Algorithms in Bioinformatics: 4th International Workshop, WABI 2004 Bergen, Norway, September 2004 Proceedings. Publisher: New York Springer. 2004. ISBN: 3540230181.
3. Kernighan Brian W. Ritchie Dennis M. The C Programming Language 2nd Edition. Publisher: USA, Prentice-Hall, Inc. 1988. ISBN: 0876925964.

**Course Outcome:**

CO-1: To gain basic knowledge on VB and RDMS programming.

CO-2: To be well versed with the VB forms, its controls and ODBC concepts.

CO-3: To acquire knowledge on creating user interface by events and dialog boxes.

CO-4: To perform graphical application and multiple document interfacing.

CO-5: To understand the concepts of VB classes and objects.

CO-6: To create modules in the classes and objects.

CO-7: To understand the usage of menu events and Flex Grid control.

CO-8: To gain knowledge on advantages of RDMS and data types.

CO-9: To be well versed with the database creation using VB with RDMS.

CO-10: To create database using ORACLE and SQL concepts.

**UNIT I INTRODUCTION TO VISUAL BASIC****15**

Introduction to Visual Basic: IDE, working with forms, developing an application, variables, datatypes and modules, procedures and control structures, arrays in VB. Working with VB Controls: Creating and using controls, working with control arrays - ODBC and Data Access Objects.

**UNIT II USER INTERFACES****15**

Menus Events and Dialog Boxes: Menu and Events definition, Event model in VB, Menu Interfaces, Mouse Events, Dialog Boxes: Definition, Types of Dialog Boxes, Applying dialog. Graphics, MDI and FlexGrid: Graphics for application, Multiple Document Interface and Using the FlexGrid Control



**Course Outcome:**

CO-1: To gain basic knowledge on VB and RDMS programming.

CO-2: To create simple forms for arithmetic calculations and biological functions.

CO-3: To acquire knowledge on creating applications using variables, control structures and data types.

CO-4: To perform calculations for GC content in the given DNA sequence.

CO-5: To understand the concepts of objects in VB and create applications.

CO-6: To create graphics using VB.

CO-7: To understand the usage of oracle and PL/SQL.

CO-8: To create table that related to simple biological functions.

CO-9: To be well versed with the database creation using VB with RDMS.

CO-10: To create database for library information system and railway reservation system.

**VB**

1. Creating Simple application forms in Visual Basic. **5**
  - a) Creating a form for simple Arithmetic Calculations
  - b) Creating a form for simple Biological applications
2. Creating application forms using Variables, Data Types and Control structures. **5**
  - a) Creating Factorial Calculator
  - b) Creating GC – Content Calculator
3. Creating application forms using different types of “Objects” in VB. **5**
  - a) Creating form to find,

- i) Leap Year,
- ii) Currency Exchange,
- iii) Octal, Decimal, Hexadecimal Calculation
- iv) Scroll Bar

b) Creating form to find

- i) The Complement of given sequence
- ii) The reverse of given sequence
- iii) The frequency of Nucleotides.

- 4. Creating application forms using Menus, Mouse Events. **5**
- 5. Creating applications forms using Graphics in VB. **5**

**Oracle, PL/SQL**

- 1. a) Creation of student information records containing Roll number, Name, Subject Code Marks etc.,
- b) Finding the total and average marks, result for each student table. **5**
- c) Record Manipulations such as Deletion, Modification, Addition and Counting the Record.
- 2. Creating table that demonstrates simple biological applications. **5**
- 3. Creating table to demonstrate applications with biological sequences. **5**

**Database Creation using VB with RDBMS**

- 1. a) Create a database that demonstrates “Library Information System” with VB forms and Query language.(User Interface with VB) **3**
- b) Create a database that stores and retrieves simple biological applications. (User Interface with VB). **5**
- 2. a) Create a database for “Railway Reservation System”. (User Interface with VB) **3**

- b) Create a database that stores and retrieves biological sequences and to find the similarities between two sequences. (User Interface with VB) 4

**Total: 75 Hours**

**Text Book:**

3. Steven Holzner, “Visual Basic 6 Programming: Black Book”, Dreamtech Press, 2000.  
ISBN:13: 9788177220537
4. C. J. Date, A. Kannan, “Database Systems”, Pearson Education Publication, 2006

**References:**

4. Noel Jerke, “Visual Basic 6: The Complete Reference”, Tata McGraw Hill, 1999.  
ISBN:139780074636664
5. Kevin Loney, George Kuch, “Oracle – The complete Reference”, Tata McGraw Hill Publication, 2005
6. C. J. Date, “Database Systems”, Addison Wesley Publication, 1990.

**15MBI007**

**PROGRAMMING IN PERL AND BIOPERL**

**5 0 0 4**

**Course Outcome:**

- CO-1: To acquire sound knowledge on basics in perl and more on usage of scalar, arrays and hashes.
- CO-2: To understand the concepts of subroutines in perl.
- CO-3: To acquire knowledge on file handling and file management in perl.
- CO-4: To understand the role of regular expressions concepts in perl and its major role in bioinformatics.
- CO-5: To understand the basics of control structures in perl.
- CO-6: To understand the importance of perl modules in the advance programming skills.
- CO-7: To acquire the knowledge on BioPerl and its modules.
- CO-8: To understand the usage of BioPerl in Bioinformatics research.







CO-4: To perform concatenation of the given sequence by using dot operator.

CO-5: To find the complement and reverse complement of the given sequence by using Tr operator.

CO-6: To know the GC content of the given DNA sequence in order to evaluate the stability of DNA. .

CO-7: To convert DNA to protein sequence by using perl program and be used in the translation process.

CO-8: To know the basics and implement bioperl modules in the perl program.

CO-9: To retrieve DNA sequence from the database and translate it using bioperl modules.

CO-10: To parse PDB and FASTA file using bioperl.

1. Write a Perl program to find the length of the given sequence? 3
2. Write a Perl program to reverse and concatenation of the given sequence? 3
3. Write a Perl program to complement and reverse complement of DNA sequence? 3
4. Write a Perl program to calculate GC content in the given DNA sequence? 3
5. Write a Perl program to translate DNA into Protein Sequence? 3
6. Operators and Expressions. 3
7. Branching and Looping. 3
8. Formatting Data. 3
9. Sort an Array of Strings in Reverse Order. 3
10. Splitting DNA sequence into Pieces by Using split(). 3
11. How do I read or write Fasta files using BioPerl? 3
12. Comparing two Sequences. 3
13. How do I calculate the true length of a Sequence? 3

14. How can I parse a PDB file using BioPerl? 3
15. Translating DNA sequence into Protein Sequence . 3

**Total: 75 Hours**

**Text Book:**

Martin C Brown, “Perl The Complete Reference”, Tata McGraw Hill, 2001

**References:**

1. Erick Storm, “Perl CGI Programming”, BPB Publication, 1998.
2. Steven Holzner, “Perl: Black Book”, Second Edition, Dreamtech Publication, 2007.
3. Ed Peschko & Michele Dewolf, “Perl Developer’s Guide”, Tata McGraw Hill, 2000.

**15MBI010**

**MOLECULAR MODELING AND DRUG DESIGNIN**

**5 0 0 4**

**Course Outcome:**

CO-1: To understand the molecular geometry information, basic concepts of a molecule.

CO-2: To explore the molecular geometry information to determine the stability of small molecule interactions with the proteins.

CO-3: To perceive the knowledge on the activities of a molecule inside the biological system through simulation studies.

CO-4: To understand the algorithms used to develop software to predict the molecular activities through computational approach.

CO-5: To get knowledge on pharmacophore, its features, applications and to get access to the sources exist at present.

CO-6: To determine a significant pharmacophore model in order to identify the most promising candidates.

CO-7: To understand the algorithms used in the molecular docking concepts and its types.



**UNIT IV MOLECULAR DOCKING****15**

Molecular Docking - Introduction to molecular docking, Rigid docking, Flexible docking, manual docking, Advantage and disadvantage of Flex-X, Flex-S, AUTODOCK and other docking software, Scoring Functions, Simple Interaction Energies, GB/SA scoring (implicit solvation), CScore (consensus scoring algorithms).

**UNIT V MOLECULAR AND STRUCTURAL DATABASE****15**

Library and Database- Molecular Database - Swiss-model, ModBase , Protein Model Portal and Structural Database - Protein Data Bank, (SCOP) Structural Classification of Proteins, (CATH) Protein Structure Classification, PDBsum, Bioactivity Databases, Gene and Protein Sequence Databases, Cambridge Crystallographic Database, Compound Storage and Management.

**Total: 75 Hours****Text Book:**

1. Andrew R. Leach. Molecular Modelling: Principles and Applications, second edition. Pearson Education EMA, January 2001 ISBN 0-582-38210-6

**References:**

1. D. C. Rapaport, The Art of Molecular Dynamics Simulation, 2004, ISBN 0-521-82568-7
2. M. P. Allen, D. J. Tildesley, Computer simulation of liquids, 1989, Oxford University Press, ISBN 0-19-855645-4.
3. R. J. Sadus, Molecular Simulation of Fluids: Theory, Algorithms and Object-Orientation, 2002, ISBN 0-444-51082-6
4. J.M.Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
5. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
6. Guy H. Grant and W. Graham Richards. Computational Chemistry Oxford Chemistry Primers, 29 1995. 9780198557401

**Course Outcome:**

CO-1: To understand the basic concepts includes in computer aided drug designing.

CO-2: To draw small molecule building using drawing tools.

CO-3: To perform homology modeling using SPDBV and Modeller.

CO-4: To be well versed in structure refinement of protein model.

CO-5: To understand the validation steps in the protein model using What If and Pro Check.

CO-6: To perform protein-rigid docking using HEX.

CO-7: To perform molecular docking using AutoDock.

CO-8: To implement molecular dynamics concepts in AMBER.

CO-9: To do docking in Arguslab.

CO-10: To do virtual screening in NCI database for lead identification.

1. Small molecule building, using ISIS Draw.	7
2. Small molecule building, using CHEM SKETCH.	7
3. Homology Modeling using SPDBV.	7
4. Homology Modeling using Modeller.	7
5. Model structure refinement using SPDBV.	7
6. Model validation using What Check.	8
7. Model validation using Pro Check.	8
8. Docking using Hex.	4
9. Docking using AUTODOCK.	5
10. Molecular dynamics using AMBER.	5
11. Docking using ARGUSLAB.	5
12. Virtual screening using NCI database.	5

**Total :75 Hours**

**Text Book:**

Andrew R. Leach. Molecular Modelling: Principles and Applications, second edition. Pearson Education EMA, January 2001 ISBN 0-582-38210-6

**References:**

1. D. C. Rapaport, The Art of Molecular Dynamics Simulation, 2004, ISBN 0-521-82568-7
2. M. P. Allen, D. J. Tildesley, Computer simulation of liquids, 1989, Oxford University Press, ISBN 0-19-855645-4.
3. R. J. Sadus, Molecular Simulation of Fluids: Theory, Algorithms and Object-Orientation, 2002, ISBN 0-444-51082-6
4. J.M.Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
5. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

**15MBI012****ADVANCED PROGRAMMING IN JAVA****5 0 0 4****Course Outcome:**

- CO-1: To understand the java fundamentals including expression, operators, logicals, control structures and packages and interfaces.
- CO-2: To learn dynamic HTML with java script, XML document and DOM & SAX for WWW.
- CO-3: To improve the ability to solve computational problems using basic constructs like if-else, and control structures.
- CO-4: To gain knowledge in array and strings.
- CO-5: To learn swing controls and developing a home page using applet and swing.
- CO-6: To understand parameters including reading servlet and initialization.
- CO-7: To study the anatomy of a JSP page, processing and application design.

CO-8: To understand installing the java software development kit, tomcat server & testing tomcat.

CO-9: to gain knowledge in introduction to Biojava, installing biojava, symbols and symbol list.

CO-10: To understand the theoretical views in error handling, sharing data and sessions.

## **UNIT I                      FUNDAMENTAL OF JAVA                      15**

Java features – Java Platform – Java Fundamentals – Expressions, Operators – Arithmetic – Logical - Comparison – Bitwise operators, Control Structures – Looping : while, do while, for, Branching: if, if else, elseif ladder, nested if, Classes, Packages and Interfaces – Exception Handling.

## **UNIT II                      JAVA FOR WWW                      15**

Introduction to Java Scripts, Objects in Java Script, Dynamic HTML with Java Script. XML: Document type definition, XML Schemas, Document Object model, Presenting XML, Using XML Processors: DOM and SAX Review of Applets, Class, Event Handling, AWT Programming.

## **UNIT III                      INTRODUCTION TO SWING                      15**

JApplet, Handling Swing Controls like Icons – Labels – Buttons – Text Boxes – Combo – Boxes – Tabbed Pains – Scroll Pains – Trees – Tables Differences between AWT Controls & Swing Controls Developing a Home page using Applet & Swing. Java Beans: Introduction to Java Beans, Advantages of Java Beans, JDK Introspection, Using Bound properties, Bean Info Interface, Constrained properties Persistence, Customizers, Java Beans API.

## **UNIT IV                      INTRODUCTION TO SERVELETS                      15**

Lifecycle of a Servlet, JSDK The Servlet API, The javax.servelet Package, Reading Servlet parameters, Reading Initialization parameters. The javax.servelet HTTP package, Handling Http Request & Responses, Using Cookies- Session Tracking, Security Issues Introduction to JSP, The Problem with Servlet. The Anatomy of a JSP Page, JSP Processing. JSP Application

Design with MVC Setting Up and JSP Environment: Installing the Java Software Development Kit, Tomcat Server & Testing Tomcat

## **UNIT V      JAVA APPLICATION**

**15**

Biojava: Introduction to Biojava, Installing Biojava, Symbols and SymbolLists, Sequence and Features, Sequence I/O Basics, viewing molecule structures through BioJava. JSP Application Development: Generating Dynamic Content, Using Scripting Elements Implicit JSP Objects, Conditional Processing – Displaying Values Using an Expression to Set an Attribute, Declaring Variables and Methods Error Handling and Debugging Sharing Data Between JSP pages, Requests, and Users Passing Control and Date between Pages – Sharing Session and Application Data – Memory Usage Considerations.

**Total :75 Hours**

### **Text Book:**

1. E Balagurusamy, “Programming with Java: A Primer”, Fourth Edition, Tata McGraw Hill, 2010

### **References:**

1. P. Naughton and H.Schildt- Java2 (The Complete Reference) - Third Edn.TMH 1999.
2. Deital & Deital, “How to Program Java”, Pearson Education, 1999.
3. Cays Horstmann, Gary Cornell, “Core Java 2: Advanced Features”, Sun Micro System, 2007

**15MBI013**

**PROGRAMMING IN JAVA AND BIOJAVA**

**0 0 5 3**

### **Course Outcome:**

CO-1: To understand the operators and objects.

CO-2: To learn basics of Java such as branching and looping.

CO-3: To able to solve computational problems using basic constructs like classes and objects.

CO-4: To be well versed in array, and strings.

CO-5: To understand how to define class and create objects.



- CO-6: To able to implement multiple inheritance through interfaces and develop packages.
- CO-7: To understand the exception handling mechanism and will be able to handle exceptions while programming.
- CO-8: To overcome all the errors while executing programs.
- CO-9: To able to demonstrate programs on multithreading.
- CO-10: To able to demonstrate programs using applets.

- |   |   |
|---|---|
| 1) Operators and Expressions,                           |   |
| 2) Branching and Looping.                               | 8 |
| 3) Classes and Objects.                                 | 7 |
| 4) Packages.  | 5 |
| 5) Formatting Data.                                     | 5 |
| 6) Sort an Array of Strings in Reverse Order.           | 5 |
| 7) Implementing Case Differences Ignorance.             | 5 |
| 8) Splitting DNA sequence into Pieces by Using split(). | 5 |
| 9) Applet Example.                                      | 5 |
| 10) Drawing Circle, rectangle using Java Graphics.      | 5 |
| 11) How do I read or write Fasta files using Biojava?   | 5 |
| 12) Comparing two Sequences.                            | 5 |
| 13) How do I calculate the true length of a Sequence?   | 5 |
| 14) How can I parse a PDB file using Biojava?           | 5 |
| 15) Creating web page using JSP.                        | 5 |

**Total: 75 Hours**

**Text Book:**

1. E Balagurusamy, “Programming with Java: A Primer”, Fourth Edition, Tata McGraw Hill, 2010

**References:**

1. P. Naughton and H.Schildt- Java2 (The Complete Reference) - Third Edn.TMH 1999.
2. Deital & Deital, “How to Program Java”, Pearson Education, 1999.
3. Cays Horstmann, Gary Cornell, “Core Java 2: Advanced Features”, Sun Micro System, 2007

**15MBI014****OPERATING SYSTEMS****5 0 0 4****Course Outcome:**

CO-1: To acquire sound knowledge on operating system and architecture.

CO-2: To understand the basics of operating system types and uses.

CO-3: To acquire knowledge on process management and various concepts.

CO-4: To understand the basis of scheduling, algorithm and types.

CO-5: To understand the memory management and the concepts related to allocation, paging and segmentation.

CO-6: To understand the virtual memory management and related to allocation and assessment.

CO-7: To acquire the knowledge on file system, mounting, allocation and protection.

CO-8: To understand the usage of Linux and Unix.

CO-9: To be well versed with the I/O systems.

CO-10: To acquire knowledge on storage devices and concepts related to storage.

**UNIT I****OPERATING SYSTEMS INTRODUCTION****15**

Introduction - Views- Goals - types of operating systems – Operating System Structure – Components of Operating System - Operating System services - system calls and system

programs, Development of Operating Systems, Uses of Operating Systems, Types of Operating Systems, .

## **UNIT II                      PROCESS MANAGEMENT AND PROCESS SCHEDULING                      15**

Process management - Process concepts - process scheduling - operation on process Inter process communication - CPU Scheduling: Scheduling criteria – Scheduling algorithms – Multiple-processor scheduling – Real time scheduling – Algorithm Evaluation. Case study: Process scheduling in Linux.

## **UNIT III                      STORAGE MANAGEMENT                      15**

Memory Management - Single and multiple partitioned allocation – paging - segmentation - internal & External Fragmentation. Non-Contiguous Allocation: Paging and Segmentation Schemes - Implementation - Hardware-Protection - Sharing – Fragmentation. Virtual Memory Management - Demand paging and Page Replacement Algorithms, Information management - File concept - Access methods - Directory structure - allocation methods - free space management - disk scheduling.

## **UNIT IV                      FILE SYSTEM                      20**

File-System Interface: File concept – Access methods – Directory structure – File system mounting – Protection. File-System Implementation: Directory implementation – Allocation methods – Free-space management – efficiency and performance – recovery – log-structured file systems. Case studies: File system in Linux – file system in Windows.

## **UNIT V                      I / O SYSTEMS                      10**

I/O Systems – I/O Hardware – Application I/O interface – kernel I/O subsystem – streams – performance. Mass-Storage Structure: Disk scheduling – Disk management – Swap-space management – RAID – disk attachment – stable storage – tertiary storage.

**Total: 75 Hours**

**Text Book:**

1. Andrew S. Tanenbaum, "Modern Operating Systems", Second Edition, Pearson Education, 2004

**References:**

1. Davis Rajkumar, "Operating System: A Systematic View", Pearson Education, 2007
2. H. M. Deitel, "Operating System", Second Edition, Pearson Education, 1990.
3. Harvery M. Deitel, Paul J. Deitel, "Operating System", Third Education, Pearson Education, 2004

**15MBI015****CLINICAL RESEARCH****5 0 0 4****Course Outcome:**

CO-1: To know the basics of clinical research and its advantages.

CO-2: To understand the key trail activities in clinical research.

CO-3: To acquire knowledge on research training and review board.

CO-4: To acquire knowledge on clinical trials and role in drug development.

CO-5: To understand the ethical aspects in the clinical trial.

CO-6: To do good clinical research practice using standard operating procedures.

CO-7: To know the steps in ethics committee review and authoroties.

CO-8: To know more on WHO principles in clinical research.

CO-9: To get skills on presentation in clinical research.

CO-10: To acquire knowledge on main elements of presentation skills.



## **UNIT V      PRESENTATION SKILLS**

**20**

Continuing review, investigator and staff qualifications, records confidentiality, Ethical conduct, protocol, risk identification, benefit risk assessment, review, protocol compliance, and informed consent GMP, and quality systems. 6 main Elements of Presentation skills - Be Prepared , Give of Yourself, Stay Relaxed, Use Natural Humor, Plan Your Body & Hand Positions, Pay attention to all details How to present research result (Presentation).

**Total: 75 Hours**

### **Text Book:**

1. Glasser, Stephen P. Essentials of Clinical Research springer 2014 ISBN 9783319054704

### **References:**

1. John I. Gallin. Principles and Practice of Clinical Research (Third Edition). Elsevier Inc 2012. ISBN: 978-0-12-382167-6
2. Gupta SK. Basic Principles of Clinical Research and Methodology. Institute of Clinical research.2007 ISBN 9788184480863
3. Friedman, L.M., Furberg, C.D., DeMets, D., Reboussin, D.M.,Granger, C.B. Fundamentals of Clinical Trials springer 2015 ISBN 978-3-319-18539-2.
4. Dr. Arun Bhatt, Clinical Trials And Good Clinical Practice In India Career Publication ISBN10: 8188513210

# DISCIPLINE SPECIFIC ELECTIVES

15MBI101

GENOMICS AND PROTEOMICS

4 0 0 3

CO-1: To learn about the overview of genome, composition and evolution.

CO-2: To gain knowledge in gene predictions.

CO-3: To understand the location of genes in the chromosomes using mapping techniques.

CO-4: To learn the markers and types of maps in locating the genes in the chromosome.

CO-5: To know about the fundamentals of proteomics.

CO-6: To enlighten about gene expression, codon bias and protein levels.

CO-7: To learn the analytical techniques and instrumentations for protein identification, separation.

CO-8: To know about the algorithms for mining specific features of tandem MS data.

CO-9: To enrich the knowledge on Proteomic tools.

CO-10: To learn about the mining proteomes with its applications.

## UNIT I

### INTRODUCTION TO GENES

12

Introduction to genetics, Definition of gene, History of genetics genome and genome sequencing overview of genome,, genome composition & genome evolution. Inheritance in biology - Genes and inheritance, Inherited diseases, Working of gene - Genes make proteins, Genes are copied. Finding Specific Genes. Gene prediction in prokaryotes, Gene prediction in eukaryotes.

## UNIT II

### TYPES OF MAPPING

12

Genetic Mapping, Physical Mapping, Types of Genome maps and their uses, Genetic linkage mapping,, High and low-resolution map, Polymorphic markers, Line, sine, Restriction Fragment





**References:**

1. Ann Gibbons, "Comparative genetics", *Science*. 281: 1432 – 1434, 1998
2. Baxevanis A.D., "The Molecular Biology Database Collection: updated compilations of Biological database resources", *Nucleic Acids Research*. 29 p 1-10, 2001
3. Jeremy D. Peterson et.al.. The Comprehensive Microbial Resource. *Nucleic Acids Research*. 29: 123 – 125, 2001
4. S.R.Pennigton and M.J.Dunn, "Proteomics", Viva Books Private Limited. New Delhi, 2002

**15MBI102      MOLECULAR CELL BIOLOGY AND BIOCHEMISTRY      4 0 0 4**

**Course Outcome:**

- CO-1: To develop the knowledge towards functional accept of the cells present in our body.
- CO-2: To understand the working of the different types of tissues present in the human body.
- CO-3: To determine biological importance of carbohydrates in living organisms.
- CO-4: To acquire the basic information about the structure, function of DNA and RNA.
- CO-5: To obtained the overall information about the vitamins especially its metabolic function and daily requirement.
- CO-6: To develop the knowledge towards the amino acid plays an important role in protein formation.
- CO-7: To understand the biological importance of protein responsible for some biological processes.
- CO-8: To achieve knowledge about metabolic pathways involved for the production of energy



## **UNIT V      PROTEIN IDENTIFICATION TECHNIQUE**

**12**

Electrophoresis – Basic techniques of Electrophoresis, Types, Working & Application, Advantages and disadvantages. Centrifugation- Basic principles, Types, Molecular weight determination. & Application, Advantages and disadvantages Chromatography- Overview of Centrifugation, Types, Principles, Working & Application, Advantages and disadvantages

**Total : 60 Hours**

### **Text Book:**

1. Albert's, B; Johnson, A; Lewis, J; Raff, M; Bray.D; Hopkin,K; Roberts, K; Walter, P, "Essential Cell Biology" ,2<sup>nd</sup> edition, Garland Science, Taylor & Francis Group,USA, 2003

### **Reference:**

1. Becker WM, Kleinsmith LJ, Hardin J "World of the Cell" 6Th edition, Benjamin Cummings, 2005.
2. Voet, D., and J.G. Voet. "Biochemistry" 3<sup>rd</sup> edition. Hoboken, NJ: Wiley. 2004.
3. Horton, R, Moran, L, Scrimgeour, G, Perry, M, Ravon, D "Principles of Biochemistry", 4<sup>th</sup> edition, Prentice-Hall of India. 2005.

**Course Outcome:**

- CO-1: To acquire knowledge on fundamentals of energy aspects in the field of biology.
- CO-2: To understand the basics of free energy concepts and its measurement.
- CO-3: To gain knowledge on nitrogen fixation and symbiotic-non symbiotic fixation.
- CO-4: To understand the important of nitrogenase enzyme complex.
- CO-5: To observe the architecture and role of mitochondria in energy metabolism.
- CO-6: To be clear with the different theoretical concepts and respiratory control in mitochondria.
- CO-7: To gain knowledge on chloroplast and its architecture.
- CO-8: To obtain knowledge on photosystem pathway and protein complexes.
- CO-9: To know the features of hormones, synthesis, its classification and structure.
- CO-10: To be well versed with hormonal control mechanism and plant growth hormones.

**UNIT I      FREE ENERGY CONCEPT      10**

Free energy concept: Molecular basis of entropy, concept of free energy, standard free energy and measurement of free energy, significance in metabolism. Application of first and second law of thermodynamics to biological systems. Energy rich bonds - ATP and interconversions of nucleotide phosphates. Phosphorylation potential.

**UNIT II      NITROGEN FIXATION      10**

Nitrogen fixation: Biological fixation of nitrogen, symbiotic and non-symbiotic nitrogen fixation. Nitrogenase enzyme complex - azoferredoxin and molybdoferredoxin. Physiological electron donors and mechanism of nitrogen reduction, assimilation of ammonia, nitrogen cycle. Nif genes and its regulation.

**UNIT III      MITOCHONDRIA      15**

Mitochondria - Architecture, chemical activity of mitochondria. Sequence of electron carriers and sites of oxidative phosphorylation, ATP generation, heme and non-heme iron proteins. Thermodynamic considerations, oxidation – reduction electrodes, standard electrode potential, redox couples, phosphate group transfer potential. Respiratory controls. Theories of oxidative phosphorylation, uncouplers and inhibitors of energy transfer. ATP synthetase complex.

**UNIT IV      CHLOROPLAST      15**

Chloroplast - Architecture - light harvesting complexes, bacteriorhodopsin, plastocyanin, carotenoids and other pigments. Hill reaction, photosystem I and II - location and mechanism of energy transfer, photophosphorylation and reduction of carbon dioxide. Calvin cycle , quantitative efficiency, photorespiration, C4 - metabolism. Chemiosmotic theory and evidence for its occurrence, ion transport through membranes, proton circuit and electro-chemical gradient, ionophores, Q cycle and stoichiometry of proton extrusion and uptake, P/O and H/P ratios, reverse electron transfer. Fractionation and reconstitution of respiratory chain complexes.

**UNIT V      HORMONES      10**

Hormones - General classification of hormones - synthesis, structure, secretion, transport, metabolism and mechanism of action of pancreatic, thyroid, parathyroid, hypothalamus, pituitary, adrenal and prostaglandins. Hormonal control of spermatogenesis, menstrual cycle, pregnancy and lactation. Cell membrane and intracellular receptors for hormones. Secondary messengers. Plant growth hormones - auxins, gibberellins, abscisic acid, cytokinins. Phytohormones.

**Total : 60 Hours**

**Text Books:**

1. Krebs, Jocelyn E. Goldstein, Elliott S. Kilpatrick, Stephen T. Lewin's Essential Genes 2nd Ed. Publisher: Boston, Jones & Bartlett. 2010. ISBN: 978-0763759155.
2. Krebs Jocelyn E., Goldstein Elliott S., Kilpatrick Stephen T. Lewin's Genes X Publisher: Jones & Bartlett 2009. ISBN: 9780763766320.

**References:**

1. Clark David P. Molecular Biology. Publisher: Boston Academic Press, Elsevier. 2009. ISBN: 9780123785893.
2. Hood Leroy, Goldberg Michael L., Reynolds Ann E., Reynolds Lee M., Veres Ruth C. Hartwell Leland H. Genetics: From Genes to Genomes Publisher: McGraw/Hill, 2008. ASIN: B00210THP6.
3. Watson James D., Baker Tania A., Bell Stephen P., Alexander Gann, Levine, Michael Losick Richard. Molecular Biology of the Gene 6th Edition. Publisher: New York, Cold Spring Harbor Laboratory Press. 2008. ISBN: 9780321507815
4. Weaver Robert F. Molecular Biology, 3rd Edition. Publisher : Boston McGraw-Hill's 2005. ISBN:0071243445.
5. Epstein Richard J. Human molecular biology: an introduction to the molecular basis of health and disease. Publisher: Cambridge, UK ; Cambridge University Press, 2003. ISBN: 052164481X.
6. Russell Peter J. iGenetics: A Molecular Approach 3rd ed.: Pearson International Edition. Publisher : New York, Pearson ISBN: 9780321610225.
7. Brown, T.A. Genomes 2 Publisher: New York, BIOS Scientific Publishers Ltd. 2002, ISBN: 1859960294

**15MBI104****CHEMINFORMATICS****4 0 0 4****Course Outcome:**

- CO-1: To acquire knowledge on the basic representation and file formats of chemical molecules.
- CO-2: To understand the applications of chemical information in various fields.
- CO-3: To gain knowledge on different descriptor formats available for the molecules.
- CO-4: To understand the important properties of small molecules and its application in the similarity and diversity analysis.
- CO-5: To observe the infrastructure of chemical databases, information stored and its types.



**UNIT IV      QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP      12**

Quantitative Structure Activity/Property/Toxicity Relationship Studies. SAR and the SAR paradox, Types- Fragment based (group contribution), 3D-QSAR, Chemical descriptor based, Modeling – Data mining approach, Matched molecular pair analysis, Evaluation of the quality of QSAR models, Application- Chemical, Biological, Applications. Introduction to Molecular Properties, Activities and Toxicities. Training Data, Test Data and External validation Data.

**UNIT V      PHARMACOPHORE      12**

Historical Perspective And Features Design & Analysis Of Combinatorial Libraries. Molecular Scaffolds, Linkers And Functional groups. Reagents and products based combinatorial library generation. Identification of pharmacophore features. Searching databases using pharmacophores Docking Studies. Pharmacophore Model, Viewpoint of Pharmacophore

**Total : 60 hours**

**Text Books:**

1. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: Wiley-VCH; 1<sup>st</sup> edition. 2003. ISBN: 3527306811.

**Reference Books:**

1. Bunin Barry A. Siesel Brian, Morales Guillermo, Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher: New York, Springer. 2006. ISBN: 1402050003.
2. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic, 2003. ISBN: 1402013477.
3. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4 Volumes), 2003. Publisher: Wiley-VCH. ISBN: 3527306803
4. Dr. Thomas Engel. Chemoinformatics – A Textbook Publisher: Kluwer academic, 2005 ISBN 3-527-30681-1.
5. Jones Neil C., Pevzner Pavel A. An Introduction to Bioinformatics Algorithms Publisher: New Delhi, Ane Books 2005. ISBN: 8180520781



6. Baxevanis Andreas D., Ouellette B. F. Francis. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins 2<sup>nd</sup> Edition. Publisher: Singapore, John Wiley & Sons, 2002. ISBN: 9814126756.

**15MBI105**

**BIOPHYSICAL CHEMISTRY**

**4 0 0 4**

**Course Outcome:**

CO-1: To know the nature of quantum particles and its mechanics.

CO-2: To understand the molecular basics of quantum particles.

CO-3: To acquire knowledge on thermodynamics of particles and the importance of various laws in computing energies.

CO-4: To understand the concepts of energy contributions in biological systems.

CO-5: To understand the theoretical basics of atoms and biological systems.

CO-6: To gain knowledge on various bond interactions and its dynamic behavior in biology.

CO-7: To acquire the knowledge on basics of physical concepts of X-ray and crystallization.

CO-8: To understand the usage of X-ray crystallography and macromolecular structure.

CO-9: To be well versed with the spectroscopy techniques and its uses.

CO-10: To acquire knowledge on NMR technique and its uses in macromolecular structure.

**UNIT I CLASSICAL AND QUANTUM MECHANICS**

**15**

Classical mechanics: History, Description of the theory, Limits of validity. Quantum mechanics- History, Interactions with other scientific theories, Philosophical implications, Applications, Examples. Elementary introduction to Lagrangian and Hamiltonian formulation of mechanics — Planck theory of blackbody radiation – photoelectric effect – Bohr model of the atom – atomic spectra – De Broglie theory of matter waves – Schrodinger wave equation – interpretation of wave function .

**UNIT II THERMODYNAMICS 10**

Thermodynamics And Energetics: Thermodynamics Systems – Laws Of Thermodynamics First Law Of Thermodynamics, Second Law Of Thermodynamics, Third Law Of Thermodynamics – Statement And Applications – Concepts Of Entropy And Enthalpy – Chemical Potentials – Free Energy – Gibbs And Helmholtz Free Energy – ATP (Adenosine triphosphate) As Energy Currency In Biological Systems.

**UNIT III MOLECULAR MECHANICS AND DYNAMICS 15**

Molecular Mechanics – Functional form, Areas of application, Environment and Validation, Software packages Molecular Dynamics: History, Areas of application and limitations, Basic Principles – Molecular Representations – Force Fields – Atom-Atom Pair Potentials – Bond Length And Bond Angle And Torsion Angle Potential – Van Der Waals And Electrostatic Potential – Hydrogen Bonding Terms.

**UNIT IV X-RAY CRYSTALLOGRAPHY 10**

X-ray crystallography – History, Contributions to chemistry and material science, Relationship to other scattering techniques, Methods – Procedure, Limitations, Crystallization, Data collection, Data analysis, Diffraction theory, Advantages of a crystal, Elementary description of crystallography- Unit cell – Miller indices – Crystal growth, X-ray diffraction- Refinement and interpretation- Concept of resolution.

**UNIT V SPECTROSCOPY TECHNIQUES 10**

IR spectroscopy – Theory, Practical IR spectroscopy, Absorption bands, Uses and applications UV-Visible spectroscopy – Principle of ultraviolet-visible absorption, Applications, Beer-Lambert law, Ultraviolet-visible spectrophotometer, Microspectrophotometry, Additional applications Raman spectroscopy – Theoretical basis, History, Raman shift, Applications, Microspectroscopy, Polarized analysis, Variations. NMR (Nuclear magnetic resonance) spectroscopy. History, Basic NMR techniques, Correlation spectroscopy, Biomolecular NMR spectroscopy

**Total: 60 Hours**

**Text Books:**

1. Vasantha Pattabhi and N.Gautham. 'Biophysics' Narosa Publishing Company, New Delhi. (2001)
2. P.Narayanan. 'Introductory Biophysics' New Age Publishing Co., Mumbai, India(1999)

**Reference books:**

1. C.R.Cantor and P.Schimmel. Biophysical Chemistry, Vol.I, II and III' W.H.Freeman and Company, New York, USA. (1985)
2. D.Freifelder. 'Physical Biochemistry' W.H.Freeman and Company, New York, USA. (1982)
3. E.Ackerman, L.B.M.Ellis and L.E.Williams' 'Biophysical Science' Prentice Hall Inc., New Jersey, USA. (1979)
4. F.W.Sears, M.W.Zemansky and H.D.Young. 'College Physics' Addison Wesley Publishing Company, Massachusetts, USA (1985).

**15MBI106****STRUCTURAL BIOINFORMATICS****4 0 0 4****Course Outcome:**

CO-1: To learn about the introduction to bioinformatics, structural bioinformatics, molecular structure and internal energy.

CO-2: To gain knowledge in energy minimization of small molecules.

CO-3: To enlighten about bioinformatics databases applied in protein structure prediction.

CO-4: To learn the protein structural terminology, protein classification and modelling.

CO-5: To know about the protein structures.

CO-6: To enrich the knowledge on Proteomic tools.

CO-7: To learn about the protein stability and fold, protein function prediction methods and approaches to protein structural genomics.

CO-8: To understand protein function predictions- sequence based and network based methods.

CO-9: To learn secondary structure predictions homology modelling, fold recognition and *ab initio* 3D structure predictions.

CO-10: To know about protein sequence and structure analysis tools.

## **UNIT I ENERGY MINIMIZATION 12**

Introduction to bioinformatics-structural bioinformatics-molecular structure and internal energy. Application of molecular graphics. Energy minimization of small molecules: empirical representation of molecular energies. Use of force fields and the molecular mechanics method. Discussion of local and global energy minima.

## **UNIT II COMPARATIVE FEATURES 12**

Protein structure evolution and the SCOP database- CATH domain structure databases- Structural quality assurance – Structure comparison alignment, Protein structure terminology, Protein classification, Comparative protein modeling – Homology modeling and Protein threading.

## **UNIT III STRUCTURE AND FUNCTIONAL ASSIGNMENT 12**

Protein structure: - Primary, Secondary, Tertiary structure and Quaternary structure, Secondary structure assignment-identifying structural domains in proteins-Inferring protein function from structure, Evaluation of automatic structure prediction servers.

## **UNIT IV DETERMINATION OF FUNCTION 12**

Protein stability and folding-SCOP-DALI-assignment of protein structures to genomes-determining gene function through conserved protein structure-prediction of protein function-approaches to protein structural genomics, Protein function prediction:- Homology Based Methods, Sequence motif – based methods, Structure based methods, network based methods,

## **UNIT V STRUCTURE PREDICTION 12**

Structure prediction – secondary structure – homology modeling, fold recognition and *ab initio* 3D structure prediction – structure comparison and alignment, Structural information of protein – ExPasy, protein sequence analysis, De Novo Protein Structure prediction.

**Total: 60 Hours**

**Text Book:**

1. Webster David (Editor). Protein Structure Prediction: Methods and Protocols (Methods in Molecular Biology) Volume 143. Publisher: New Jersey Humana Press. 2000. ISBN: 0896036375.

**References:**

1. Cesareni Giovanni, Gimona Mario, Sudol Marius, Yaffe Michael (Editors). Modular Protein Domains. Publisher: Weinheim Wiley-VCH. 2005. ISBN: 352730813X.
2. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890.

**15MBI107**

**ENZYMES AND METABOLISM**

**4 0 0 4**

**Course Outcome:**

CO-1: To acquire sound knowledge on fundamentals and regulation of enzymes with its activities, chemical kinetics, and inhibition of enzyme reactions.

CO-2: To understand the basics of regulatory enzymes and immobilized enzymes.

CO-3: To know the introduction to metabolism with overview of anabolic and catabolic pathways of carbohydrates, proteins and lipids.

CO-4: To understand the Clinical correlation of purine and pyrimidine metabolism.

CO-5: To understand the steps involve in the Digestion and absorption of carbohydrates.

CO-6: To acquire knowledge about the biochemical pathways involved in metabolism function.



**UNIT IV LIPID METABOLISM****15**

Digestion and absorption of lipids. Introduction to lipid metabolism,  $\beta$ -Oxidation of fatty acids, Ketogenesis. Biosynthesis of fatty acids, Triacylglycerols and prostaglandins. Metabolism of phospholipids, glycolipids and cholesterol. Lipoproteins: Metabolism of HDL, Disorder of Plasma Lipoproteins, Fatty liver, Obesity, Atherosclerosis, Tay – Sachs disease, Gaucher's disease, Niemann – Pick disease.

**UNIT V PROTEIN METABOLISM****10**

Digestion and absorption of proteins. General aspects of amino acids metabolism; deamination, transamination, transmethylation, transpeptidation, and decarboxylation. Metabolism of ammonia: urea cycle and its regulation, Nitrogen balance, biosynthesis of non-essential amino acids. Metabolic breakdown of individual amino acids. Clinical correlations of protein metabolism. Integration of metabolism.

**Total: 60 hours****Text Book**

1. Shanmughavel P, "Principles of Bioinformatics", Pointer Publishers, Jaipur, India. 2005.

**Reference:**

1. C. K. Mathews, K. E. Van Holde, & K.G. Ahern, "Biochemistry", Third Edition, Prentice Hall, 1999.
2. Cesareni Giovanni, Gimona Mario, Sudol Marius, Yaffe Michael (Editors). Modular Protein Domains. Publisher: Weinheim Wiley-VCH. 2005..

**Course Outcome:**

CO-1: To understand the basic structures, morphology and taxonomy of virus.

CO-2: To acquire knowledge on bio-safety measures to maintain and handle virus in the laboratorial conditions.

CO-3: To obtain a clear knowledge on basic cellular functions and the cell receptors involved in interactions.

CO-4: To get a clear understanding in the cell organelles and its role in regular cellular functions.

CO-5: To acquire knowledge on viral cell morphogenesis and transport of proteins, replications.

CO-6: To attain clear knowledge on signaling pathways and cytoskeletal interactions as well as the host-parasite relations.

CO-7: To figure out the strategies of replication in both RNA and DNA molecules.

CO-8: To be aware of mechanisms involved in host viral infection in order to develop effective antiviral medicines.

CO-9: To perceive knowledge on antiviral and viral vaccines combating viral infections in the host.

CO-10: To implement modern approaches and computational techniques to get rid of viral infections.

**UNIT I INTRODUCTION OF VIRUS****15**

Introduction of virus, History and principles of virology, virus taxonomy, introduction to replication strategies. Virus structure and morphology, viruses of veterinary importance and plant viruses. Principles of bio-safety, containment facilities, maintenance and handling of laboratory animals and requirements of virological laboratory.



**UNIT II      CELLULAR RECEPTORS      10**

Cellular receptors and virus entry – Definition, structure and methods of discovery of viral receptors (polio, herpes, VSV, HIV). Kinetics of receptor binding. Cellular interactions—clathrin coated pits, lipid rafts, caveolae, endocytosis and virus uncoating mechanisms Nuclear localization signals and nuclear pore transit, virus –cytoskeletal interactions, chaperons.

**UNIT III      VIRUS MORPHOGENESIS      10**

Virus morphogenesis Replication sites and their characterization, IRES, replicones, transport of viral proteins.Mechanism of host cell damage- Host cell ‘shut off’, apoptosis, necrosis, stress response, alteration of signaling pathways, cellular basis of transformation, types of centrophic effects, ultrastructural cytopathology.

**UNIT IV      VIRUS REPLICATION      15**

Virus Replication: RNA viruses: General strategies, replication of plus stranded RNA virus (polio), negative strand. RNA viruses (VSV and influenza). Other RNA viruses. Replication of double stranded RNA virus (rota), ambisense RNA (LCM) and retroviruses (HIV and HTLV). DNA viruses Replication of double stranded DNA viruses (SV40, pox), ssDNA virus (AAV). Miscellaneous(Prion proteins, replication of plant virus (Poty))

**UNIT V      ANTIVIRALS AND VIRAL VACCINES      10**

Antivirals and Viral Vaccines: Viral Vaccines – Conventional vaccines –killed and attenuated, modern vaccines—recombinant proteins, subunits, DNA vaccines, peptides, immunomodulators (cytokines), vaccinedelivery and adjuvants. Antivirals- Interferons, designing and screening for antivirals, mechanisms of action, antivirallibraries, antiretrovirals—mechanism of action and drug resistance.Modern approaches of virus control Anti-sense RNA, siRNA, ribozymes, in silico approaches for drug designing.

**Total : 60 hours**

**Text Book:**

1. P.saravanan, “Virology”, Neha Publishers & Distributors, 2009, ISBN13: 9788180940170.

**References:**

1. Antiviral Agents, Vaccines, and Immunotherapies. Stephen K. Tying. Latest edition / Pub. Date: October 2004. Publisher: Marcel Dekker.
2. Antiviral Drug Discovery for Emerging Diseases and Bioterrorism Threats. Paul F. Torrence (Editor). Latest edition / Pub. Date: July 2005. Publisher: Wiley, John & Sons, Incorporated
3. Principles of Virology: Molecular Biology, Pathogenesis, and Control of Animal Viruses. S. J. Flint, V. R. Racaniello, L. W. Enquist, V. R. Rancaniello, A. M. Skalka Latest edition / Pub. Date: December 2003 Publisher: American Society Microbiology.
4. DNA Virus Replication. Alan J. Cann. Latest edition / Pub. Date: March 2000. Publisher: Oxford University Press.

**15MBI109****DATA WAREHOUSING AND DATA MINING****4 0 0 4****Course Outcome:**

CO-1: To learn about the components in data ware housing.

CO-2: To gain knowledge in identify the subject area for which a data warehouse is to be built.

CO-3: To enlighten about query tools and Applications.

CO-4: To learn the Dimensional model for data warehouse.

CO-5: To know about introduction and types of data mining.

CO-6: Analyze the market needs by applying suitable OLAP operations.

CO-7: CO-7: Identify the patterns that can be extracted on application of data mining techniques in various domains.

CO-8: To Understand several different data mining techniques such as market basket analysis, Clustering, classification.

CO-9: To develop an application by using various data mining techniques to identify patterns that evolves in various business domains.

CO-10: To know about clustering and applications and trends in data mining.

### **UNIT I                          INTRODUCTION TO DATA WAREHOUSING                          12**

Data Warehousing:- Data warehousing Components –Building a Data warehouse -- Mapping the Data Warehouse to a Multiprocessor Architecture – DBMS Schemas for Decision Support – Data Extraction, Cleanup, and Transformation Tools –Metadata.

### **UNIT II                          BUSINESS ANALYSIS                          12**

Business Analysis:- Reporting and Query tools and Applications – Tool Categories – The Need for Applications – Online Analytical Processing (OLAP) – Need –Multidimensional Data Model – OLAP Guidelines – Multidimensional versus Multi relational OLAP – Categories of Tools – OLAP Tools and the Internet.

### **UNIT III                          DATA MINING                          12**

Data Mining:- Introduction – Data – Types of Data – Data Mining Functionalities – Interestingness of patterns – Classification of Data Mining Systems – Data Mining Task Primitives –Integration of a Data Mining System with a Data Warehouse – Issues –Data Preprocessing.

### **UNIT IV                          ASSOCIATION RULE MINING                          12**

Association Rule Mining and Classification:- Mining Frequent Patterns, Associations and Correlations – Mining Methods – Mining Various Kinds of Association Rules – Correlation

Analysis – Constraint Based Association Mining – Classification and Prediction – Basic Concepts.

**UNIT V CLUSTERING AND ITS APPLICATIONS 12**

Clustering and Applications and Trends in Data Mining:- Cluster Analysis – Types of Data – Categorization of Major Clustering Methods – K means – Partitioning Methods – Hierarchical Methods – Density-Based Methods – Grid Based Methods – Model-Based Clustering Methods – Clustering High Dimensional Data – Constraint – Based Cluster Analysis.

**Total: 60 Hours**

**Text Book:**

1. Alex Berson and Stephen J. Smith, “ Data Warehousing, Data Mining & OLAP”, Tata McGraw – Hill Edition, Tenth Reprint 2007.

**References:**

1. Jiawei Han and Micheline Kamber, “Data Mining Concepts and Techniques”, Second Edition, Elsevier, 2007.
2. Pang-Ning Tan, Michael Steinbach and Vipin Kumar, “Introduction To Data Mining”, Person Education, 2007.
3. G. K. Gupta, “Introduction to Data Mining with Case Studies”, Easter Economy Edition, Prentice Hall of India, 2006.
4. Data Mining Data Warehousing And Olap S K Kataria Paperback 2010

**Course outcome:**

CO-1: To understand script and the contributions of scripting languages.

CO-2: To understand Python especially toward object-oriented concepts.

CO-3: To understanding of the built-in objects of Python.

CO-4: To implement a given biological algorithm as a computer program using Python.

CO-5: To adapt and combine standard python algorithms to solve a given biological problem (includes numerical as well as non-numerical algorithms).

CO-6: To use standard python programming for biological constructs of algorithm using repetition, selection, functions, composition, modules, aggregated data (arrays, lists, etc.)

CO--7: To identify and to repair coding errors in a biological program.

CO-8: To understand and use object based software concepts to solve the gene coding problem.

CO-9: To use library software for building a graphical user interface, web application, mathematical software.

CO-10: To build new Python software tools for life science research.

**UNIT I INTRODUCTION TO PYTHON****12**

Introduction to Python, History of Python, Python Features, Python Development Tools, Writing Python Program, Values and Variables:- Numeric Values, Variables and Assignment, Identifiers, Control codes within Structure, Controlling the print Function

**UNIT II EXPRESSION****12**

Expressions and Arithmetic:- Operator Precedence and Associativity, Comments, Errors (Syntax, Run-time errors, Logic Errors), Arithmetic Examples, Conditional Execution:- Simple if

Statement, if/else statement, Compound Boolean Expressions, Nested Conditionals, Multi-way Decision Statements, Conditional Expressions.

**UNIT III      CONDITIONAL EXECUTION      12**

Conditional Execution:- What is conditional statement in Python, Simple if Statement, if/else statement, nested if condition, else – if ladder, Compound Boolean Expressions, Nested Conditionals, Multi-way Decision Statements, Conditional Expressions.

**UNIT IV      ITERATION      12**

Iteration:- While Statement, For Statement, Nested Loops, the break statement, the continue statement, Infinite Loops, Computing Square roots, Drawing a Tree, Using Functions – mathematical functions – time Functions, reading the files from existing database using Python.

**UNIT V      SEQUENCE ANALYSIS THROUGH PYTHON      12**

Sequence Alignment:- Alphabets, Matching Sequences – Perfect Matches – Insertions and Deletions – Rearrangements – Global Versus Local Alignments – Sequence Length, Simple Alignment (Direct Alignment), Statistics:- Simple Statistics, Distributions, Normalizations, Multivariate Statistics, Probabilities, Odds.

**Total : 60 hours**

**Text Book:**

1. Jason Kinser, “Python for Bioinformatics”, Jones and Bartlett Publishers, Sudbury, Massachusetts 2009

**References:**

1. Richard L., Halterman, “Learning to Program With Python”, 2011
2. Kent D. Lee, “Python Programming Fundamentals: Second Edition”, Springer, 2010
3. Cody Jackson, “Learning to Program Using Python”, Second Edition, 2013
4. Mark Lutz, “Learning Python”, Third Edition, O’Reilly, 2007

**Course Outcome:**

CO-1: To acquire sound knowledge on cloud and its architecture in computing.

CO-2: To understand the business values of cloud computing.

CO-3: To know the concepts of cloud computing applied in various field.

CO-4: To understand the basis of service administration of cloud computing.

CO-5: To know the steps involve in cloud computing technology.

CO-6: To understand the usage of cloud computing in web applications.

CO-7: To acquire the knowledge on cloud computing data management, security and protection.

CO-8: To understand the concepts of data storage in cloud computing.

CO-9: To be well versed with the private cloud computing concepts.

CO-10: To acquire knowledge on accessing the novel hybrid clouds.

**UNIT I INTRODUCTION TO CLOUD COMPUTING****12**

Introduction to cloud computing: Collaborative to Cloud – A Short History, Functioning of Cloud computing, Cloud Architecture, Cloud Storage and Cloud Services, Industrial Applications, Business Values :- Introduction, Service Modeling, Infrastructure as a Service, Platform as a Service.

**UNIT II SERVICE ADMINISTRATION****12**

Inside Cloud Computing: Introduction, Sensational Feeling about Organization, Deciding on Strategy, Governance Issues, Monitoring Business Process, IT Cost Management, Cloud Service Administration:- Introduction, Service Level Agreements and Monitoring, Support Services, Resource Management, Service Management.

**UNIT III      COMPUTING TECHNOLOGY      12**

Cloud Computing Technology: Introduction, Clients – Hardware clients, software clients, cloud clients, Security, Network – Basic public internet, The accelerated internet, Site-to-Site VPN, cloud providers, Cloud consumers, Pipe size, Redundancy, Services – Identity, Integration, Mapping, Payments, Search, Accessing the Cloud:- Introduction, Platforms – Web application frame work, web hosting service, propriety methods, Web applications, API in cloud computing, browsers for cloud computing.

**UNIT IV      DATA MANAGEMENT      12**

Cloud Data Management: Data Security, Data Location, Data Control, Securing data for Transport, Scalability and cloud services – Large scale data processing, Databases and data stores and data archival, Storage as a Service, Information Storage in Cloud computing – Storage Providers, Storage Security, Merits and Demerits of Cloud Storage.

**UNIT V      PRIVATE AND HYBRID CLOUDS      12**

Discovery of Private and Hybrid clouds: Need for privacy, comparing public, private and hybrid, Examining the economics of the private cloud, The Up Key Vendors, Cloud Computing Standards – Best Practices and Standards, Practical Issues, Standards Organizations and Groups.

**Total : 60 hours**

**Text Book:**

1. Kumar Saurabh, “Cloud Computing”, Second Edition, Wiley India Private Limited; 2012

**References:**

1. Anthony T. Velte, Toby J. Velte, Robert Elsenpeter, “Cloud Computing: A Practical Approach”, Tata McGrah Hill, 2014



**Course Outcome:**

- CO-1: To learn about the fundamentals and role of biomolecules in Recombinant DNA technology.
- CO-2: To gain knowledge about the hybridization technique, fluorescence in situ hybridization, restriction maps and mapping techniques.
- CO-3: To understand the basic techniques and applications in Genetic engineering.
- CO-4: To enrich the quest on applications including cloning vectors and expression vectors.
- CO-5: To know about the concepts of cell transformation due to the changes in genetic material, and cell cloning.
- CO-6: To bring into the light about the creation of gene libraries, advances in genetic engineering and applications in gene expression analysis.
- CO-7: To learn about the beginning of transformation and transfection methods.
- CO-8: To bring abundant knowledge in cloning methodologies.
- CO-9: To learn about the advent of Polymerase Chain Reaction and tremendous impact on molecular biology.
- CO-10: To understand the Polymerase Chain Reaction based mutagenesis and gene silencing techniques.

**UNIT I      DNA & RECOMBINANT DNA TECHNOLOGY****15**

Structure of DNA: A-,B-,Z-, and triplex DNA, Measurement of properties, spectrophotometric, CD, AFM, and electron microscope analysis of DNA structure. Restriction analysis: Types of restriction enzyme, Type I, II and III, restriction modification systems, type II restriction endonucleases and properties, isoschizomers and neoschizomers, mcr/mrr genotypes, Cohesive and blunt end ligation, linkers, adaptors, homopolymeric tailing. Labeling of DNA: Nick translation, random priming, radioactive and non-radioactive probes, use of Klenow enzyme, T4 DNA polymerase, bacterial alkaline phosphatase, polynucleotide kinase. Hybridization

techniques: Northern, Southern and Colony hybridization, Fluorescence in situ hybridization, Restriction maps and mapping techniques,

## **UNIT II APPLICATION 15**

DNA fingerprinting, chromosome walking & chromosome jumping. DNA-Protein interactions: - Electro mobility shift assay, DNaseI footprinting, methyl interference assay. Cloning vectors - Gene Cloning Vectors: Plasmids, bacteriophages, Cloning in M13 mp vectors, phagemids, Lambda vectors. Insertion and replacement vectors, EMBL,  $\lambda$ DASH,  $\lambda$ gt10/11,  $\lambda$ ZAP etc. Cosmid vectors. Artificial chromosome vectors (YACs, BACs), Animal Virus derived vectors- SV-40, vaccinia/baculo& retroviral vectors, Expression vectors; pMal, GST, pET-based vectors , Protein purification; His-tag, GST-tag, MBP-tag etc. Restriction proteases, intein-based vectors. Inclusion bodies, methodologies to reduce formation of inclusion bodies. Baculovirus and pichia vectors system.

## **UNIT III CLONING METHODOLOGIES 10**

Cloning methodologies - Insertion of Foreign DNA into Host Cells: Transformation, Transfection. Chemical and physical methods, liposomes, microinjection, macroinjection, electroporation, biolistics, somatic cell fusion, gene transfer by pronuclear microinjection. Plant transformation technology: Basis of tumor formation, hairy root, features of Ti and Ri plasmids, mechanism of DNA transfer, role of virulence genes, use of Ti and Ri as vectors. Cloning and expression in yeasts (Saccharomyces, Pichia etc.).

## **UNIT IV SCREENING OF ANIMAL AND PLANTS CELLS 10**

Animal and plants cells. methods of selection and screening, cDNA and genomic cloning, expression cloning, jumping and hopping libraries, southwestern and far western cloning, yeast two hybrid system, phage display, Construction of cDNA libraries in plasmids and screening methodologies, Construction of cDNA and genomic DNA libraries in lambda vector. Principles in maximizing gene expression, Site-directed mutagenesis. Gene knockouts and Gene Therapy: Creation of knockout mice, disease model, somatic and germ-line therapy in vivo and ex-vivo, suicide gene therapy, gene replacement, gene targeting Other applications: Transgenics, Genome projects and their implications, application in global gene expression analysis.

PCR and its applications - Primer design, Fidelity of thermostable enzymes, DNA polymerases, multiplex, nested, reverse transcriptase, real time PCR, touchdown PCR, hot start PCR, colony PCR, cloning of PCR products, T-vectors, proof reading enzymes, PCR in gene recombination, deletion, addition, overlap extension, and SOEing, site specific mutagenesis, PCR in molecular diagnostics, viral and bacterial detection, PCR based mutagenesis. Applications:-Sequencing methods: Enzymatic DNA sequencing, Chemical sequencing of DNA, principle of automated DNA sequencing, RNA sequencing. Chemical Synthesis of oligonucleotides. Gene silencing techniques: Introduction to siRNA and siRNA technology, micro RNA

**Total : 60 hours**

**Text Book:**

1. Watson James D., Baker Tania A., Bell Stephen P., Alexander Gann, Levine, Michael Losick Richard. Molecular Biology of the Gene 6th Edition. Publisher: New York, Cold Spring Harbor Laboratory Press. 2008. ISBN: 9780321507815

**References:**

1. Clark David P. Molecular Biology. Publisher: Boston Academic Press, Elsevier. 2009. ISBN: 9780123785893.
2. Hood Leroy, Goldberg Michael L., Reynolds Ann E., Reynolds Lee M., Veres Ruth C. Hartwell Leland H. Genetics: From Genes to Genomes Publisher: McGraw/Hill, 2008. ASIN: B00210THP6.
3. Krebs Jocelyn E., Goldstein Elliott S., Kilpatrick Stephen T. Lewin's Genes X Publisher: Jones & Bartlett 2009. ISBN: 9780763766320
4. Weaver Robert F. Molecular Biology, 3rd Edition. Publisher : Boston McGraw-Hill's 2005. ISBN: 0071243445.

## GENERIC ELECTIVES

15MBI151

INTRODUCTION TO BIOINFORMATICS

2 0 0 2

### Course Outcome:

- CO-1: To acquire the skill of in basics of computing including operating systems, Use of internet, visualization techniques, computing networks, softwares and hardwares.
- CO-2: To provide the necessary biological (Gene and protein) background which are required solve the problem that arise during the designing of algorithm.
- CO-3: To know about the biological concepts and relevant database workout for research entries.
- CO-4: To gain knowledge in biopolymer, synthetic polymer and basics in genome anatomy, structures of genomes in both prokaryotes and eukaryotes.
- CO-5: To understand generation of co-ordinates of biopolymers in Cartesian and cylindrical polar co-ordinate system.
- CO-6: To retrieve and analyze the biological sequences by using tools and software's.
- CO-7: To know about similarity, identity and homology, global alignment, local alignment, sequence assembly, gene prediction, protein structure prediction, methodologies.
- CO-8: To prove an algorithm for the given biological problem is often necessary to replace the original problem with a more complicated problem in order to initialize the recursion.
- CO-9: Mathematical approach to solving certain types of biological problem like sequence alignment, gene detection, structure prediction, data-mining literature.
- CO-10: The problem is not directly noticeable, but the output of the problem dependent on the result predicted by the probability distribution.



Of Structures And Correctness Of Structures, Submission Of Data To PDB: Atomic Coordinates And Electron Density Maps; Methods For Prediction Of Secondary And Tertiary Structures Of Proteins.

**Total : 30 hours.**

**Text Book:**

Baxevanis A.D., Davison D.B., Page R. D. M. & Petsko G.A. Current Protocols in Bioinformatics. New York, John Wiley & Sons Inc., 2004. ISBN: 0555015254 Syllabus draft: BoS April 26, 2010 Dr. Urmila Kulkarni-Kale 15

**Reference :**

1. N. Gautham, "Bioinformatics", Narosa Publishing Company, New Delhi, 2006.
2. Lesk, A.M., "Introduction to Bioinformatics", 1<sup>st</sup> Edition, Oxford University Press, Oxford, UK, 2002.

**15MBI152**

**CHEMINFORMATICS**

**2 0 0 2**

**Course Outcome:**

CO-1: To acquire knowledge on the basic representation and file formats of chemical molecules.

CO-2: To understand the applications of chemical information in various fields.

CO-3: To gain knowledge on different descriptor formats available for the molecules.

CO-4: To understand the important properties of small molecules and its application in the similarity and diversity analysis.

CO-5: To observe the infrastructure of chemical databases, information stored and its types.

CO-6: To be clear with the different search techniques and its importance in acquiring required data.

CO-7: To perceive the molecular relationships based on physical and chemical properties with the biological properties.

CO-8: To obtain knowledge on the molecular properties and to develop tools for predicting the specific properties.

CO-9: To observe the features of pharmacophore and to access the combinatorial libraries for pharmacophore designing.

CO-10: To be clear with identification, accession and application of pharmacophores in drug designing process.

### **Unit I: Introduction to Cheminformatics (6)**

Introduction To Chemo Informatics: Aims, Scope. History, Basics, Role Of Chemo Informatics In Pharmaceutical/Chemical Research. Chemical Structure Representation: 1D, 2D And 3D Structures. Molecular File Formats (SMILES, WLN, SDF, And MOL). Applications – Storage And Retrieval, Virtual Libraries, Virtual Screening, Quantitative Structure-Activity Relationship (QSAR)

### **Unit II: Molecular Descriptors (6)**

Introduction, Invariance Properties Of Molecular Descriptors , Degeneracy Of Molecular Descriptors, Basic Requirements For Optimal Descriptors, Molecular Descriptors (1dimension, 2dimension And 3dimension) And MACCS Keys Topological, Electrotopological And Shape Indices. Molecular Similarity And Molecular Diversity Analysis.

### **Unit III: Molecular Database Screening (6)**

Introduction To Molecular Database Screening, Methods- Ligand-Based, Structure-Based, Computing Infrastructure – Ligand-Based, Structure-Based, Accuracy, Lipinski Rule: Drug/Lead

Like Molecules,. Chemical Structure Representation – Substructure, Conformation. Chemical Structure Based Search Techniques: Exact, Sub-Structure And Similar Structure Searches.

**Unit IV: Quantitative Structure Activity Relationship (6)**

Quantitative Structure Activity/Property/Toxicity Relationship Studies. SAR and the SAR paradox, Types- Fragment based (group contribution), 3D-QSAR, Chemical descriptor based, Modeling – Data mining approach, Matched molecular pair analysis, Evaluation of the quality of QSAR models, Application- Chemical, Biological, Applications. Introduction to Molecular Properties, Activities and Toxicities. Training Data, Test Data and External validation Data.

**Unit V: Pharmacophore (6)**

Historical Perspective And Features Design & Analysis Of Combinatorial Libraries. Molecular Scaffolds, Linkers And Functional groups. Reagents and products based combinatorial library generation. Identification of pharmacophore features. Searching databases using pharmacophores Docking Studies. Pharmacophore Model, Viewpoint of Pharmacophore

**Total : 30 hours.**

**Text Books:**

1. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: WileyVCH; 1<sup>st</sup> edition. 2003. ISBN: 3527306811.

**References:**

1. Bunin Barry A. Siesel Brian, Morales Guillermo, Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher: New York, Springer. 2006. ISBN: 1402050003.
2. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic, 2003. ISBN: 1402013477.
3. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4 Volumes), 2003. Publisher: Wiley-VCH. ISBN: 3527306803



**Course Outcome:**

- CO-1: To understand the molecular geometry information, basic concepts of a molecule.
- CO-2: To explore the molecular geometry information to determine the stability of small molecule interactions with the proteins.
- CO-3: To perceive the knowledge on the activities of a molecule inside the biological system through simulation studies.
- CO-4: To understand the algorithms used to develop software to predict the molecular activities through computational approach.
- CO-5: To get knowledge on pharmacophore, its features, applications and to get access to the sources exist at present
- CO-6: To determine a significant pharmacophore model in order to identify the most promising candidates.
- CO-7: To understand the algorithms used in the molecular docking concepts and its types.
- CO-8: To get an exposure to the existing docking software and to observe the result.
- CO-9: To be aware of molecular databases available at present to explore the biological molecules.
- CO-10: To understand the basic steps in querying database and to interpret information from the datas available.

**UNIT I MOLECULAR GEOMETRY**

**6**

Molecular Geometry – Introduction to Molecular Geometry, Electronic Spatial Extent and Molecular Volume, Electron Affinity and Ionization Potential, Hyperfine Coupling, Dielectric

Constant, Force Field Customization., The influence of thermal excitation, Bonding, Isomers, Types of molecular structure(VSEPR table), 3D representations, Molecular geometry determination.

**UNIT II      MOLECULAR DYNAMICS      6**

Molecular Dynamics- Introduction to Molecular Dynamics, History, Areas of application and limitations, Design constraints, Potentials in MD simulations, Examples of applications, Density Functional Theory, Linear Scaling Techniques, Ab initio Methods, Hartree-Fock Approximation, Mùller-Plesset Perturbation Theory, Quantum Monte Carlo Methods, Natural Orbitals and Monte Carlo Simulations.

**UNIT III      PHARMACOPHORE      6**

Pharmacophore – Historical Perspective and Features, Viewpoint of Pharmacophore, Functional Groups Considered as Pharmacophores, Molecular Alignments, Handling Flexibility, Alignment Techniques, Scoring and Optimization, Pharmacophores, Model development – Select a training set of ligands, Conformational analysis, Molecular superimposition, Abstraction, Validation. Applications

**UNIT IV      MOLECULAR DOCKING      6**

Molecular Docking – Introduction to molecular docking, Definition of problem, Docking approaches, Mechanics of docking, Applications, Types of docking – Rigid docking, Flexible docking, manual docking, Advantage and disadvantage of Flex-X, Flex-S, List of Protein-Ligand Docking Software AUTODOCK, Arguslab, Hex, PyRx.

**UNIT V      MOLECULAR AND STRUCTURAL DATABASE      6**

Library and Database- Molecular Database – Swiss-model, ModBase , Protein Model Portal and Structural Database - Protein Data Bank, (SCOP) Structural Classification of Proteins, (CATH) Protein Structure Classification, PDBsum, Bioactivity Databases, Gene and Protein Sequence Databases, Cambridge Crystallographic Database, Compound Storage and Management.

**Total : 30 hours.**

**Text Book:**

1. Andrew R. Leach. Molecular Modelling: Principles and Applications, second edition. Pearson Education EMA, January 2001 ISBN 0-582-38210-6

**References:**

2. D. C. Rapaport, The Art of Molecular Dynamics Simulation, 2004, ISBN 0-521-82568-7
3. M. P. Allen, D. J. Tildesley, Computer simulation of liquids, 1989, Oxford University Press, ISBN 0-19-855645-4.
4. R. J. Sadus, Molecular Simulation of Fluids: Theory, Algorithms and Object-Oriented, 2002, ISBN 0-444-51082-6
5. J.M.Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.

**Course Outcome:**

CO-1: To learn about the introduction to bioinformatics, structural bioinformatics, molecular structure and internal energy.

CO-2: To gain knowledge in energy minimization of small molecules.

CO-3: To enlighten about bioinformatics databases applied in protein structure prediction.

CO-4: To learn the protein structural terminology, protein classification and modelling.

CO-5: To know about the protein structures.

CO-6: To enrich the knowledge on Proteomic tools.

CO-7: To learn about the protein stability and fold, protein function prediction methods and approaches to protein structural genomics.

CO-8: To understand protein function predictions- sequence based and network based methods.

CO-9: To learn secondary structure predictions homology modelling, fold recognition and *ab initio* 3D structure predictions.

CO-10: To know about protein sequence and structure analysis tools.

**UNIT I ENERGY MINIMIZATION****6**

Introduction to bioinformatics-structural bioinformatics-molecular structure and internal energy. Application of molecular graphics. Energy minimization of small molecules: empirical representation of molecular energies. Use of force fields and the molecular mechanics method. Discussion of local and global energy minima.

**UNIT II COMPARATIVE FEATURES****6**

Protein structure evolution and the SCOP database- CATH domain structure databases- Structural quality assurance – Structure comparison alignment, Protein structure terminology,

Protein classification, Comparative protein modeling – Homology modeling and Protein threading.

### **UNIT III      STRUCTURE AND FUNCTIONAL ASSIGNMENT      6**

Protein structure: - Primary, Secondary, Tertiary structure and Quaternary structure, Secondary structure assignment-identifying structural domains in proteins-Inferring protein function from structure, Evaluation of automatic structure prediction servers.

### **UNIT IV      DETERMINATION OF FUNCTION      6**

Protein stability and folding-SCOP-DALI-assignment of protein structures to genomes-determining gene function through conserved protein structure-prediction of protein function-approaches to protein structural genomics, Protein function prediction:- Homology Based Methods, Sequence motif – based methods, Structure based methods, network based methods,

### **UNIT V      STRUCTURE PREDICTION      6**

Structure prediction – secondary structure – homology modeling, fold recognition and *ab initio* 3D structure prediction – structure comparison and alignment, Structural information of protein – ExPasy, protein sequence analysis, De Novo Protein Structure prediction.

**Total : 30 hours.**

#### **Text Book:**

Webster David (Editor). Protein Structure Prediction: Methods and Protocols (Methods in Molecular Biology) Volume 143. Publisher: New Jersey Humana Press. 2000. ISBN: 0896036375.

#### **References:**

1. Cesareni Giovanni, Gimona Mario, Sudol Marius, Yaffe Michael (Editors). Modular Protein Domains. Publisher: Weinheim Wiley-VCH. 2005. ISBN: 352730813X.
2. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890.

**Course Outcome:**

CO-1: To acquire sound knowledge on basics in perl and more on usage of scalar, arrays and hashes.

CO-2: To understand the concepts of subroutines in perl.

CO-3: To acquire knowledge on file handling and file management in perl.

CO-4: To understand the role of regular expressions concepts in perl and its major role in bioinformatics.

CO-5: To understand the basics of control structures in perl.

CO-6: To understand the importance of perl modules in the advance programming skills.

CO-7: To acquire the knowledge on BioPerl and its modules.

CO-8: To understand the usage of BioPerl in Bioinformatics research.

CO-9: To gain knowledge on common gateway interface (CGI) and methods.

CO-10: To acquire knowledge on CGI connecting HTML and webpages.

**UNIT I INTRODUCTION TO PERL.****6**

**Introduction:-** Scalar Data- Numbers, Strings, Scalar Variables, Output with print, Getting User Input, The chomp operator, undef Value, defined function, The if and while control structures,

**Lists and Arrays:-** Accessing elements of an array, Subroutines.

**UNIT II EXPRESSIONS****6**

Input and Output:- Input from Standard Input, Input from the diamond operator, Invocation arguments, Output to Standard Output, Filehandles, Opening a Filehandle, Expressions:- Matches with m//, Option Modifiers, Anchors, The Binding operator, =~, Interpolating into Patterns, The match Variables, General Quantifiers.

### **UNIT III CONTROL STRUCTURES**

**6**

Control Structures:- The unless Control Structure, The until Control Structure, Expression Modifiers, The Naked Block Control Structure, The elsif Clause, Autoincrement and Autodecrement, The for Control Structure, Loop Controls, Logical Operators,

### **UNIT IV FILES**

**6**

File Tests:- File Test Operators, The stat and lstat functions, The localtime function, Bitwise Operators, Using the Special Underscore Filehandle, Strings and Sorting:- Finding a Substring with index, Manipulating a Substring with substr, Formatting Data with sprintf, Advanced Sorting, Perl Modules:- Finding Modules, Installing Modules, Using Simple Modules.

### **UNIT IV INTRODUCTION TO BIOPERL.**

**6**

**Bioperl:-** Introduction, Installing Bioperl, General Bioperl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan). Application of BioPerl Module, uses of BioPerl Module in biological analysis.

**Total: 30 hours.**

#### **Text Book:**

1. Martin C Brown, "Perl The Complete Reference", Tata McGraw Hill, 2001

#### **References:**

1. Erick Storm, "Perl CGI Programming", BPB Publication, 1998.
2. Steven Holzner, "Perl: Black Book", Second Edition, Dreamtech Publication, 2007.
3. Ed Peschko & Michele Dewolf, "Perl Developer's Guide", Tata McGraw Hill, 2000.

**Course outcome:**

CO-1: To understand script and the contributions of scripting languages.

CO-2: To understand Python especially toward object-oriented concepts

CO-3: To understanding of the built-in objects of Python,

CO-4: To implement a given biological algorithm as a computer program using Python

CO-5: To adapt and combine standard python algorithms to solve a given biological problem  
(includes numerical as well as non-numerical algorithms)

CO-6: To use standard python programming for biological constructs of algorithm using  
repetition, selection, functions, composition, modules, aggregated data (arrays, lists, etc.)

CO--7: To identify and to repair coding errors in a biological program

CO-8: To understand and use object based software concepts to solve the gene coding problem

CO-9: To use library software for building a graphical user interface, web application,  
mathematical software

CO-10: To build new Python software tools for life science research.

**UNIT I INTRODUCTION TO PYTHON****6**

Introduction to Python, History of Python, Python Features, Python Development Tools, Writing Python Program, Values and Variables:- Numeric Values, Variables and Assignment, Identifiers, Control codes within Structure, Controlling the print Function

**UNIT II EXPRESSION****6**

Expressions and Arithmetic:- Operator Precedence and Associativity, Comments, Errors (Syntax, Run-time errors, Logic Errors), Arithmetic Examples, Conditional Execution:- Simple if



Statement, if/else statement, Compound Boolean Expressions, Nested Conditionals, Multi-way Decision Statements, Conditional Expressions.

**UNIT III                    CONDITIONAL EXECUTION                    6**

Conditional Execution:- What is conditional statement in Python, Simple if Statement, if/else statement, nested if condition, else – if ladder, Compound Boolean Expressions, Nested Conditionals, Multi-way Decision Statements, Conditional Expressions.

**UNIT IV                    ITERATION                    6**

Iteration:- While Statement, For Statement, Nested Loops, the break statement, the continue statement, Infinite Loops, Computing Square roots, Drawing a Tree, Using Functions – mathematical functions – time Functions, reading the files from existing database using Python.

**UNIT V                    SEQUENCE ANALYSIS THROUGH PYTHON                    6**

Sequence Alignment:- Alphabets, Matching Sequences – Perfect Matches – Insertions and Deletions – Rearrangements – Global Versus Local Alignments – Sequence Length, Simple Alignment (Direct Alignment), Statistics:- Simple Statistics, Distributions, Normalizations, Multivariate Statistics, Probabilities, Odds.

**Total: 30 hours.**

**Text Book:**

1. Jason Kinser, “Python for Bioinformatics”, Jones and Bartlett Publishers, Sudbury, Massachusetts 2009

**References:**

1. Richard L., Halterman, “Learning to Program With Python”, 2011
2. Kent D. Lee, “Python Programming Fundamentals: Second Edition”, Springer, 2010
3. Cody Jackson, “Learning to Program Using Python”, Second Edition, 2013
4. Mark Lutz, “Learning Python”, Third Edition, O’Reilly, 2007