



INSTITUTE OF SCIENCE, TECHNOLOGY & ADVANCED STUDIES (VISTAS)
(Deemed to be University Estd. u/s 3 of the UGC Act, 1956)

PALLAVARAM - CHENNAI

NAAC ACCREDITED WITH 'A' GRADE

Marching Beyond 25 Years Successfully

M.Sc.

BIOINFORMATICS

Curriculum and Syllabus

(Based on choice based credit system)

Effective from the Academic year

2018 - 2019

Department of Bioinformatics

School of Life Science

PROGRAM EDUCATIONAL OBJECTIVES (PEO)

PEO-1:

Describe the basis of biology, computer science and information technology and develop as a key expertise in applications of bioinformatics.

PEO-2:

An extra-ordinary ability to gain practical knowledge and keen in developing a successful career in academia, R&D institutes and industrial sector.

PEO-3:

Possess a high level knowledge in comparing and analyze the best programming language, database and software to implement and support the critical biological challenges.

PEO-4:

Promoting the bioinformatics hardcore research and support the experimental scientist in the hypothesis and mechanism related to biology.

PEO-5:

Will address the increasing need for skilled computer expert in maintaining and analyze the biological resource and big data and contribute globally.

PROGRAM OUTCOME (PO)

The M.Sc. programme (Biochemistry/Biotechnology/Bioinformatics/microbiology) at VISTAS has documented measurable outcomes that are based on the needs of the programme's stakeholders. The programme outcomes that the department presently adapts to are as follows:

PO-1: Life Sciences knowledge:

Successful candidates will acquire current/recent specific knowledge in the respective discipline with proficiency in practical skills and leadership skills for a successful career.

PO-2: Problem analysis:

Successful candidates will be able to analyse, design standards, resolve and troubleshoot problems in implementation or standardization of Life sciences protocols.

PO-3: Design/development of solutions:

Successful candidates will develop creative and cognitive thinking and cooperate with each other to solve problems in the field of Life sciences.

PO-4: Conduct investigations of complex problems:

Successful candidates will acquire capabilities to plan and design protocols and utilizes practical skills to validate hypothesis by executing experimental techniques independently coupled with the ability to assimilate, analyse, interpret and accurately evaluate subsequent data.

PO-5: Modern tool usage:

Successful candidates will effectively be able to manage resources and time using ICT and other computer enabled devices.

PO-6: Ethics:

Successful candidates will be aware of their role and responsibility in handling and use of microbes including genetically modified microorganisms.

PO-7: Communication:

Successful candidates will have the ability to understand and communicate all ideas and concepts effectively.

PO-8: Environment sustainability:

Successful candidates will get adequate knowledge to use information and implement solutions for environmental protection, safeguards and remediation. PO-9: Lifelong learning: Successful candidates will carry on learning, adapting and disseminating knowledge in a world of constantly evolving technology.

PROGRAMME SPECIFIC OUTCOME (PSO)

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.

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.	Dr. 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, 9841075847 Email: shirai2011@gmail.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
6.	Ms M.Kannika	Process Associate	Dell International Ambattur, Chennai. Phone : 9840431667	Alumni Member
7.	Ms.Abinaya	II Year M.Sc., Bioinformatics	VISTAS P.V. vaithiyalingam Road, pallavaram, Chennai -117	Student Member

VISTAS
SCHOOL OF LIFE SCIENCES DEPARTMENT OF BIOINFORMATICS
M.Sc. BIOINFORMATICS
REGULATIONS

Eligibility for the award of degree:

A candidate with a Bachelor's Degree in Science in the disciplinary of Genetics, Biochemistry, Biotechnology, Physics, Chemistry, Computer Science, Botany, Zoology, Microbiology, Mathematics, Statistics, Nutrition, Foodservice and Management & Dietetics, Agriculture, B.E./B. Tech (Biotech), B. V.Sc, MBBS, BDS, B. Pharm, BPT & BCA from the University, or an examination of some other University, accepted by the Syndicate as equivalent thereto, shall be permitted to appear and qualify for the M.Sc. Bioinformatics Degree examination of this University after a course of two academic years in an affiliated college of this University.

Duration of the course:

The duration of the course is for two academic years consisting of four semesters.

Examinations:

There shall be four examinations, the odd semester examination at the middle of the academic year and even semester examination at the end of the academic year.

Practical examinations:

Practical examinations for practical I & II will be conducted at the end of first semester. Examinations for practical III & IV will be conducted at the end of second semester. Examinations for practical V & VI will be conducted at the end of third semester.

Registration for exams:

All candidates shall register their name for the first semester examination and will be permitted to proceed up to final year irrespective of the failure in any of the semester examinations. The candidates should register for all the arrear subjects of earlier semesters along with the current semester subjects.

Attendance:

All candidates shall proceed to subsequent semesters only if they earn sufficient attendance, as prescribed by the University. Candidates earning less than 50% of attendance under extra ordinary circumstances shall be permitted to proceed the next semester provided he/she produces a relevant certificated authorized by the concerning authority and certified by the Principal of the college.

Candidate, otherwise, has to repeat the semester after paying the penalty prescribed by the University,

QUESTION PAPER PATTERN

Maximum marks: 100

Section A: 10 X 3 = 30

Each question carries 3 marks (Any 10 out of 12)

Section B: 5 X 8 = 40

Each question carries 8 marks (Any 5 out of 8)

Section C: 2 X 15 = 30

Each question carries 15 marks (Answer all either or pattern)

M.Sc. BIOINFORMATICS

CURRICULUM

Total No. of Credits: 90

SEMESTER I

Category	Course	Hours / Week			Credits
		Lecture	Tutorial	Practical	
Core	Introduction to bioinformatics	5	0	0	4
Core	Biological databank and Sequence analysis – practical	0	0	5	3
Core	Computer Programming in c & c++	5	0	0	4
Core	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
	Total	20	0	10	24

SEMESTER II

Category	Course	Hours / Week			Credits
		Lecture	Tutorial	Practical	
Core	Programming in VB and RDBMS	5	0	0	4
Core	Programming in VB and RDBMS - Practical	0	0	3	2
Core	Programming in Perl and Bioperl	5	0	0	4
Core	Programming in Perl and Bioperl - practical	0	0	3	2
Core	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
	Total	20	0	10	24

SEMESTER III

Category	Course	Hours / Week			Credits
		Lecture	Tutorial	Practical	
Core	MOLECULAR MODELING AND DRUG DESIGNING	5	0	0	4
Core	COMPUTER AIDED DRUG DESIGNING - PRACTICAL	0	0	5	3
Core	ADVANCED PROGRAMMING IN JAVA	5	0	0	4
Core	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
	Total	20	0	10	24

SEMESTER IV

Category	Course	Hours / Week			Credits
		Lecture	Tutorial	Practical	
Core	OPERATING SYSTEMS	5	0	0	4
Core	CLINICAL RESEARCH	5	0	0	4
Core	MAIN PROJECT	0	0	20	10
	Total	10	0	20	18

DISCIPLINE SPECIFIC ELECTIVE COURSES

1. GENOMICS AND PROTEOMICS
2. MOLECULAR CELL BIOLOGY AND BIOCHEMISTRY
3. BIOENERGETICS
4. CHEMINFORMATICS
5. BIOPHYSICAL CHEMISTRY
6. STRUCTURAL BIOINFORMATICS
7. ENZYMES AND METABOLISMS
8. VIROLOGY
9. DATA WAREHOUSING AND DATA MINING
10. PYTHON FOR BIOINFORMATICS
11. CLOUD COMPUTING
12. GENETIC ENGINEERING AND NANOTECHNOLOGY

GENERIC ELECTIVE COURSES

1. INTRODUCTION TO BIOINFORMATICS
2. CHEMINFORMATICS
3. MOLECULAR MODELING AND DRUG DESIGNING
4. STRUCTURAL BIOINFORMATICS
5. PROGRAMMING IN PERL AND BIOPERL
6. PYTHON FOR BIOINFORMATICS

Course Objective:

This course will enable the students to understand the nature of biological data and need for biological databases and also to explore major biomolecular sequence databases (organization and contents); search and retrieve data from the databases using their respective search engines. To understand and appreciate the need and significance of sequence analysis and the bioinformatics approaches, algorithms for sequence analysis, the application of methods for analysis of the biomolecular sequence data

Course Outcome:

- CO-1: To acquire the skill of constructing algorithms and there by determining the computational complexity of algorithms by knowing the basic biological information.
- 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 map an unknown segment of DNA by breaking it into pieces and then by identifying the locations of the breakpoints in the gene.
- CO-4: To follow the problem solving heuristic of making the locally optimal choice at each stages with the hope of finding a global optimum.
- CO-5: To solve many different types of complex problem by breaking down into a collection of simpler sub biological problems and by solving each of those biological problems one by one until expected solutions arrived.
- CO-6: To analyze the previously solved sub problems and combine their solutions along with the achieved result to give the best solution for the given biological problem.
- CO-7: To divide the given problem, at least into 2 sub-problems and the combination of the results arrived by sub problem is much easier than finding the solution of the initial problem directly.
- 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 I INTRODUCTION TO COMPUTERS 15

Basics of computing: Introduction to operating systems – WINDOWS, UNIX, LINUX; Advantages of security installation; Use of internet; Graphics – visualization techniques; softwares and hardwares; Computer networking – LAN, WAN, MODEM, Optical vs electronic networking, firewalls; Ethernet and TCP/IP family of protocols.

UNIT II INTRODUCTION TO BIOLOGICAL DATABASES 20

Nucleotide databases (Genbank, EMBL, DDBJ); Protein databases (Swiss-Prot, Tr-EMBL, PIR_PSD, Expasy); Derived Databases (Prosite, PRODOM, Pfam, PRINTS) Specialized Genome databases: (NCBI, EBI, TIGR, SANGER).

UNIT III BIOLOGICAL DATABASES II 10

Sequence submission Methods and tools (Sequin, Sakura, Bankit); Sequence retrieval systems (Entrez& SRS); Sequence File Formats and Conversion tools; Metabolic Pathway database (KEGG, EMP, EcoCyc, BioCyc and MetaCyc); Specialized database (IMG, Rebase, COG, LIGAND, BRENDA); Structural database (CATH, SCOP, and PDBsum).

UNIT IV SEQUENCE ANALYSIS 15

Analysis of protein and nucleic acid sequences, multiple alignment programs, Development of programs for analysis of nucleic acid sequences, Pair wise Sequence Alignment - Similarity, Identity and Homology, Global Alignment, Local Alignment; database search methods- Multiple Sequence Alignment - Multiple alignment programs, Development of programs for analysis of nucleic acid sequences, Conversion of various file formats; Phylogenetic Analysis - Concept of dendrograms; Strings and Evolutionary trees.

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 Syllabus draft: BoS April 26, 2010 Dr. Urmila Kulkarni-Kale 15

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 Objective: This course will enable the students to understand the nature of biological data and need for biological databases and also to explore major biomolecular sequence databases (organization and contents); search and retrieve data from the databases using their respective search engines. To understand and appreciate the need and significance of sequence analysis and the bioinformatics approaches, algorithms for sequence analysis, the application of methods for analysis of the biomolecular sequence data

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

Program:

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 (PHYLIP). Analysis of protein and nucleic acids sequences.	2
10. Sequence analysis using EMBOSS or GCG Wisconsin Package.	3
11. Development of programs in the analysis of nucleic acid sequences – such as protein coding regions in prokaryotes.	5
12. 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:

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 Objective: This course will enable the students to conceptualize and formulate logic and flow for the implementation of a computational task and develop codes using the structured programming approach of 'C' & c++ programming language and also to develop and implement programs to analyze biological data.

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: Defining & Processing, Passing to a function, Multidimensional Arrays. String: Operations of

Strings (String handling through built-in & UDF: Length, Compare Concatenate, Reverse, Copy, Character Search using array) Pointers: Declarations, Passing to a function, Operations on Pointers, Pointers & Arrays, Array of Pointer, Pointer Arithmetic, Array accessing through pointers, Pointer to structure, Pointer to functions, Function returning pointers, Dynamic Memory Allocations.

UNIT III STRUCTURES AND FILES

20

Structures: Defining & Processing, Passing to a function, Unions (Array within structure, Array of structure, Nesting of structure, Passing structure and its pointer to UDF, Introduction to Unions and its Utilities) Data Files: Open, Close, Create, Process Unformatted Data Files. (Formatted Console I/O functions, Unformatted Console I/O functions, Modes Of Files, Use Of fopen(), fclose(), fgetc(), fputc(), fgets(), fprintf(), fscanf(), fread(), fwrite(), Command Line Arguments). Documentation, debugging, C Processors, Macros. Examples illustrating structured program development methodology and use of a block structured algorithmic language to solve specific problems.

UNIT IV INTRODUCTION TO OBJECT ORIENTED PROGRAM

10

Introduction to object oriented programming, user defined types, polymorphism, and encapsulation. Getting started with C++ - syntax, data-type, variables, strings, functions, exceptions and statements, namespaces and exceptions, operators. Flow control, functions, recursion. Arrays and pointers, structures.

UNIT V ABSTRACTION MECHANISMS, INHERITANCE

10

Abstraction Mechanisms: Classes, private, public, constructors, destructors, member functions, static members, references etc. Class hierarchy, derived classes. Inheritance: simple inheritance, polymorphism, object slicing, base initialization, virtual functions.

Total: 75 Hours

Text Book

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 Objectives: This course will enable the students to conceptualize and formulate logic and flow for the implementation of a computational task and develop codes using the structured programming approach of 'C' & c++programming language and also to develop and implement programs to analyze biological data.

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++

Program:

- | | |
|---|----|
| 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:

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.

Course Objective: Identify the differences between the procedural languages and event – driven languages. Define and modify the properties and methods associated with an object. To load, modify, and save changes made to forms and projects in the Visual Basic Environment. Make clear understand on RDBMS concepts and Database languages such as Oracle and PL/SQL.

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 FlexGrid 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.

References:

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

Course Objective: Identify the differences between the procedural languages and event – driven languages. Define and modify the properties and methods associated with an object. To load, modify, and save changes made to forms and projects in the Visual Basic Environment. Make clear understand on RDBMS concepts and Database languages such as Oracle and PL/SQL.

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:

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

References:

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

Course Objective: To learn the fundamentals of the Perl programming language and how it can be used to write data reporting and systems administration applications. To discover how to use of the DBI.pm module and related DBD (driver) files with Perl to build database-driven applications.

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 V COMMON GATEWAY INTERFACE (CGI)

15

Common Gateway Interface:- Web Servers and Browsers, HTML tags, table, frames, form elements, GET, POST & HEAD Method, URL Encoding, CGI Environment Variables, Handling forms, Accessing form Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action

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, “Per: Black Book”, Second Edition, Dreamtech Publication, 2007.
3. Ed Peschko & Michele Dewolf, “Perl Developer’s Guide”, Tata McGraw Hill, 2000.

PROGRAMMING IN PERL AND BIOPERL – PRACTICAL

Course Objective: To learn the fundamentals of the Perl programming language and how it can be used to write data reporting and systems administration applications. To discover how to use of the DBI.pm module and related DBD (driver) files with Perl to build database-driven applications.

Course Outcome:

- CO-1: To gain basic knowledge on programming skills in PERL.
- CO-2: To know how to calculate the length of the sequence using perl program.
- CO-3: To perform the reverse of the given sequence using Rev List.
- 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.

Course Objective: This course will enable the students to understand the critical relationship among biomolecular structure, function and force field models. To utilize basic modeling techniques to explore biological phenomena at the molecular level. To emphasize Modelling drug/receptor interactions in detail by molecular mechanics, molecular dynamics simulations and homology modeling.

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 data available.

UNIT I Molecular Modeling and Mechanics 15

Basic Concepts of Molecular Structure: Bond Length, Bond Angle, Torsion Angle, Non-Covalent Interactions and force field parametrisation and transferability – Molecular Structure and Internal Energy – Energy Minimization, Derivative and Non-Derivative Methods, Local and Global Minima.

UNIT II Quantum Mechanics 10

Introduction to Computational Quantum Mechanics: One Electron Atom, Poly Electronic Atoms and Molecules, Hartree Fock Equations, Molecular Properties calculation using Ab initio and Semi Empirical Methods, Density Functional Theory, Moller and Plesset Perturbation Theory.

UNIT III Molecular Modeling and Docking 20

Molecular Modeling in Drug Discovery, Sequence Analysis, Secondary structure prediction, Tertiary Structure prediction- Homology Modeling, Threading and *ab-initio* methods, Structure validation, Molecular Docking – Introduction, Approaches (Simulation and Shape complementarity approach), Molecular Docking Algorithm, Docking Optimization- Scoring functions, Molecular Docking Application.

UNIT IV Pharmacophore 15

Pharmacophore – Historical Perspective and Features, Viewpoint of Pharmacophore, Pharmacophore modeling- Molecular alignments, handling flexibility, alignment techniques, scoring and optimization, conformational expansion, validation and usage, Applications of pharmacophore model in medicinal chemistry.

UNIT V Molecular Dynamics 15

Molecular Dynamics- Introduction, MD using simple models, MD with continuous potentials, setting up and running a molecular dynamics simulation, Constraint Dynamics, Monte Carlo Simulation Methods- Monte Carlo simulation of molecules, Simulation Analysis.

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

Referen

ces:

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-Oriented, 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 Objective: This course will enable the students to understand the critical relationship among biomolecular structure, function and force field models. To utilize basic modeling techniques to explore biological phenomena at the molecular level. To emphasize Modelling drug/receptor interactions in detail by molecular mechanics, molecular dynamics simulations and homology modeling.

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.

Course Objectives: Understand fundamentals of programming such as variables, conditional and iterative execution, methods, etc. Understand fundamentals of object-oriented programming in Java, including defining classes, invoking methods, using class libraries, etc. Be aware of the important topics and principles of software development. Have the ability to write a computer program to solve specified problems.

Course Outcome:

- CO-1: To understand the object oriented programming concepts.
- CO-2: To learn basics of Java such as tokens, data types and expressions.
- CO-3: To able to solve computational problems using basic constructs like if-else, and control structures.
- 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.

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. servlet 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 Symbol Lists, 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

Course Objective: Understand fundamentals of programming such as variables, conditional and iterative execution, methods, etc. Understand fundamentals of object-oriented programming in Java, including defining classes, invoking methods, using class libraries, etc. Be aware of the important topics and principles of software development. Have the ability to write a computer program to solve specified problems

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

Total: 75 Hours

Text Book:

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.

Course Objectives: Aims to give clear view of operating system structure, Processing and its memory. Also to make the student to clear understand on OS memory management system and its implementations on computer programming structures.

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:

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

Course Objective: This course will enable the students to understand the key concepts of research in responsible to the conduct of research and able to conduct research that conforms to the highest standards for the protection of human research subjects.

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 I INTRODUCTION TO CLINICAL RESEARCH 10

Introduction to clinical research, History of clinical research, Clinical Research Degree, Clinical Research Training and an overview of the common research designs. Safety- Sponsor, Local site investigators, Institutional review boards (IRBs), Regulatory agencies. Economics - Sponsor, Investigators, Subjects, Participation as labor. Participating in a clinical trial - Locating trials, Steps for volunteers, Research. an overview of key trial activities in clinical research, clinical research and media.

UNIT II INTRODUCTION TO CLINICAL TRIALS 10

Introduction to clinical trials, Trials of drugs, Trials of devices. History - Development, Modern trials. Types - different phases of clinical trials,. Trial design - Active comparator studies, Master protocol, Clinical trial protocol, Design features, Placebo groups, Duration. Administration – Marketing, Information technology. Ethical aspects - Conflicts of interest and unfavorable studies. Ethical principles that govern clinical trials.

UNIT III GOOD CLINICAL RESEARCH PRACTICE (GCP), 15

Introduction to Good clinical research practice – Background, Objectives, Scope, Overview of the clinical research process, Key trial activities include -Development of the trial protocol, . Development of standard operating procedures (SOPs), Development of support systems and tools, Generation and approval of trial-related documents, Selection of trial sites and the selection of properly qualified, trained, and experienced investigators and study personnel, Ethics committee review and approval of the protocol, Review by regulatory authorities. Enrollment of subjects into the study: recruitment, eligibility, and informed consent

UNIT IV WHO PRINCIPLES 20

WHO principles of GCP- Principle 1: Ethical Conduct, Principle 2: Protocol, Principle 3: Risk Identification, Principle 4: Benefit-Risk Assessment, Principle 5: Review by IEC/IRB, Principle 6: Protocol Compliance, Principle 7: Informed Consent, Principle 8: Continuing Review/ Ongoing Benefit-Risk Assessment, Principle 9: Investigator Qualifications, Principle 10: Staff Qualifications, Principle 11: Records. Principle 12: Confidentiality/Privacy, Principle 13: Good Manufacturing Practice, Principle 14: Quality Systems

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:

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

Course Objective:

This course will enable the students to appreciate the importance and understanding of full genome and to explore the genomics databases & various algorithms used for comparisons of full genome and gene order. It also useful for understanding the concepts of SNPs and their significance with increase in value of proteomics concepts and technology.

Course Outcome:

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 Length Polymorphism,(RFLP), single nucleotide polymorphism(SNP). Types of maps: Cytogenetic, Transcript map, Comparative map, integrated map. Completing Maps and Sequences

UNIT III PROTEOME 12

Proteomics and new biology: The New Biology, Protein Chemistry, Gene Expression, Proteomics :an analytical challenge, Proteome and the Genome, The Life and Death of a Protein life cycle of protein, protein as the modullar structure, functional protein families, deducing proteome from genome, Gene Expression, Codon Bias, and Protein Levels, Significance and overview of analytical proteomics.

UNIT IV PROTEOMICS TOOLS 12

Analytical protein and peptide separation - Extracting Proteins from Biological Samples, Protein Separations Before Digestion, After Digestion, One-Dimensional & Two-Dimensional SDS-PAGE, Protein digestion techniques, Mass spectrometers for protein and peptide analysis- MALDI-TOF MS Instruments, Protein identification by peptide mass fingerprinting - Analytical Approach, An Algorithm for Mining Specific Features of Tandem MS Data - SALSA.

UNIT V PROTEOMIC APPLICATIONS 12

Mining Proteomes - 2D-SDS-PAGE & MALDI-TOF MS, Multidimensional Peptide Chromatography and LC-Tandem MS Analysis. Protein Expression Profiling - Comparative Proteomics with 2D Gels, LC-MS and Isotope Tags, , Identifying Protein – Protein Interaction and Protein complexes, Mapping protein modifications - Mining MS-MS Data, New Direction in Proteomics- Automation and Robotics, Micro- and Nanoscale Instrumentation, Protein Arrays.

Total: 60 Hours

Text Book:

David W. Mount, "Bioinformatics Sequence and Genome Analysis", Cold Spring Harbor Laboratory Press. 2001.

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

FUNDAMENTALS OF MOLECULAR CELL BIOLOGY AND BIOCHEMISTRY 4004

Course Objective:

This course covers basic properties of cells and cell organelles. It also examines properties of differentiated cell systems and tissues. The Principal aim of the course is to equip students with a basic knowledge of the structural and functional properties of cells and also understanding of biological principles, and the ability to make connections across different levels of biological organization, from molecules to cells, to whole organisms, populations and ecosystems.

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 which play an important role in protein formation.

CO-7: To understand the biological importance of protein that are responsible for some biological processes.

CO-8: To achieve knowledge about metabolic pathways that are involved for the production of energy

CO-9: To acquire the skill to separate and purify the biomolecules by three key analytical and purification methods (electrophoresis chromatography centrifugation).

CO-10: To develop the skill for detecting and characterizing biomolecules using electrophoresis chromatography centrifugation techniques.

– Location, Pathway, Energy Produced, Function. Gluconeogenesis – Location, Pathway, Energy Produced, Function, Urea Cycle- Location, Pathway, Energy Produced, Function.

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:

Albert's, B; Johnson, A; Lewis, J; Raff, M; Bray,D; Hopkin,K; Roberts, K; Walter, P, "Essential Cell Biology" ,2nd 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" 3rd edition. Hoboken, NJ: Wiley. 2004.
3. Horton, R, Moran, L, Scrimgeour, G, Perry, M, Ravon, D "Principles of Biocehmistry", 4th edition, Prentice-Hall of India. 2005.

BIOENERGETICS

4004

Course Objectives: This course will enable the students to understand the fundamentals and complementary aspects of energy involved in bioinformatics for designing of bioactive molecules. To get hands-on experience in storage and analysis of small molecular data.

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, abscissic acid, cytokinins. Phenomones.

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. 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

Course Objectives:

This course will enable the students to understand the fundamentals and complementary aspects of chemo informatics and bioinformatics for design of bioactive molecules. To get hands-on experience in chemical structure representation, storage and analysis of small molecular data.

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 CHEMO INFORMATICS 12

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 12

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 12

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 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: WileyVCH; 1st edition. 2003. ISBN: 3527306811.

Reference Books:

1. Bunin Barry A. SieselBrian, MoralesGuillermo, 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 2nd Edition. Publisher: Singapore, John Wiley & Sons, 2002. ISBN: 9814126756.

Course Objectives: This course will enable the students to be familiar with the Physics, chemistry of different classes of biomolecules and their interactions in an aqueous environment and also understand the structure-function relationships of macromolecules, the principles of enzyme catalysis and regulation.

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 MOLECULARMECHANICSAND DYNAMICS 15

Molecular Mechanics – Functional form, Areas of application, Environment and solvation, 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).

Course Objective:

This course will enable the students to explore primary and derived databases in the field of computational structural biology and to visualize macromolecular structures using various visualization tools. Finally acquire skills to use different approaches for prediction of protein structure.

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.

Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN:
3527305890.

Course Objective: This course will enable the students to understand the fundamentals and complementary aspects of enzyme and metabolism action involved in bioinformatics and wide range of enzymatic activities of different protein classes and their metabolism's which responsible for causing Disorder.

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.
- CO-7: To acquire the knowledge in introduction to lipid metabolism, β -Oxidation of fatty acids, Ketogenesis. Biosynthesis of fatty acids, Triacylglycerols and prostaglandins. Metabolism of phospholipids, glycolipids and cholesterol its uses.
- CO-8: To understand the transport channel and its importance in addition about Triacylglycerols and prostaglandins.
- CO-9: To be well metabolism of lipids and its uses.
- CO-10: To acquire sound knowledge on basic protein metabolism, clinical correlation of proteins and integration of metabolisms.

UNIT I INTRODUCTION TO ENZYMES 10

Introduction to enzymes, nomenclature, classification, riboenzyme, general characteristics of theories of enzyme catalysis, substrate specificity, isozymes, coenzymes, cofactors, regulation of enzyme activity, chemical kinetics and enzyme kinetics, Michaelis-Menten equation, effect of various factors on rate of reactions, inhibition of enzymatic reactions and kinetics, multienzyme system and bisubstrate reactions, catalytic mechanisms, regulatory enzymes and immobilised enzyme.

UNIT II INTRODUCTION TO METABOLISM 10

Introduction to metabolism- Overview of anabolic and catabolic pathways of carbohydrates, proteins and lipids. Role of ATP, NAD, FAD and CoA in metabolism. Nucleic Acid Metabolism: Biosynthesis and degradation of purines and pyrimidines, nucleosides and nucleotides. Clinical correlation of purine and pyrimidine metabolism. Nucleotides as coenzymes.

UNIT III CARBOHYDRATE METABOLISM 15

Digestion and absorption of carbohydrates. Glycolysis and its significance, Fermentation, Fate of pyruvate, Citric acid cycle, Gluconeogenesis, Cori cycle, Glycogenesis, Glycogenolysis Glycogen storage diseases. HMP shunt, Uronic acid pathway, Metabolism of hexoses other than glucose, Regulation of glycogen metabolism, Glyoxylate pathway, Biosynthesis of oligosaccharides and glycoproteins,

UNIT IV LIPID METABOLISM 15

Digestion and absorption of lipids. Introduction to lipid metabolism, β -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

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 Objectives: This course will enable the students to describe at the molecular level the replication strategies of representative DNA and RNA viruses and the effects of virus infection on cell growth control and survival. To elucidate individual steps in virus life cycles and their interactions with host cells and their vaccine.

Course Outcome:

CO-1: To understand the basics 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 involve 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 mechanism involve 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 cytopathic 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), vaccine delivery and adjuvants. Antivirals- Interferons, designing and screening for antivirals, mechanisms of action, antiviral libraries, 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:

P.S aravanan, “Virology”, Neha Publishers & Distributors, 2009, ISBN13: 9788180940170.

References:

1. Antiviral Agents, Vaccines, and Immunotherapies. Stephen K. Tyring. 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.

Course Objective: Students will be enabled to understand and implement classical models and algorithms in data warehousing and data mining. They will learn how to analyze the data, identify the problems, and choose the relevant models and algorithms to apply. They will further be able to assess the strengths and weaknesses of various methods and algorithms and to analyze their behavior.

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:

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 Objective: Read and understand the Python syntax. Be familiar with Python's fundamentals and develop simple applications. Apply the principles and techniques of object-oriented programming. Use sophisticated techniques and Python modules that are particularly useful for bioinformatics programming. Build new Python software tools for life science research. Summarize text patterns using regular expressions.

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 Objective: World-leading IT technology with high international standard of service. Implementation service with a quality control from project imitation to production. A commitment of quality of work delivered to the public 5. Continuously strengthen our business rapport among IT vendors, manufacturers, resellers, and distributors, is also our main focusing area in running the business.

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. Dr. 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 Objective:

This course will enable the students to understand the knowledge in genetic information, vectors in gene cloning, transformation in higher organisms and its applications and to introduce the Bioinformatians for the application of Genetic Engineering.

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, λDASH, λgt10/11, λZAP 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.

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.

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. 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.

UNIT V PCR AND ITS APPLICATIONS 10

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, 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:

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

Course Objective: This course will enable the students to understand the nature of biological data and need for biological databases and also to explore major biomolecular sequence databases (organization and contents); search and retrieve data from the databases using their respective search engines. To understand and appreciate the need and significance of sequence analysis and the bioinformatics approaches, algorithms for sequence analysis, the application of methods for analysis of the biomolecular sequence data

Course Outcome:

- CO-1: To acquire the skill of constructing algorithms and there by determining the computational complexity of algorithms by knowing the basic biological information.
- 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 map an unknown segment of DNA by breaking it into pieces and then by identifying the locations of the breakpoints in the gene.
- CO-4: To follow the problem solving heuristic of making the locally optimal choice at each stages with the hope of finding a global optimum.
- CO-5: To solve many different types of complex problem by breaking down into a collection of simpler sub biological problems and by solving each of those biological problems one by one until expected solutions arrived.
- CO-6: To analyze the previously solved sub problems and combine their solutions along with the achieved result to give the best solution for the given biological problem.
- CO-7: To divide the given problem, at least into 2 sub-problems and the combination of the results arrived by sub problem is much more easier than finding the solution of the initial problem directly.
- 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 I INTRODUCTION TO COMPUTERS 6

Basics of computing: Introduction to operating systems – WINDOWS, UNIX, LINUX; Advantages of security installation; Use of internet; Graphics – visualization techniques; softwares and hardwares; Computer networking – LAN, WAN, MODEM, Optical vs electronic networking, firewalls; Ethernet and TCP/IP family of protocols.

UNIT II INTRODUCTION TO BIOLOGICAL DATABASES 6

Nucleotide databases (Genbank, EMBL, DDBJ); Protein databases (Swiss-Prot, Tr-EMBL, PIR_PSD, Expsy); Derived Databases (Prosite, PRODOM, Pfam, PRINTS) Specialized Genome databases: (NCBI, EBI, TIGR, SANGER).

UNIT III BIOLOGICAL DATABASES II 6

Sequence submission Methods and tools (Sequin, Sakura, Bankit); Sequence retrieval systems (Entrez& SRS); Sequence File Formats and Conversion tools; Metabolic Pathway database (KEGG, EMP, EcoCyc, BioCyc and MetaCyc); Specialized database (IMGT, Rebase, COG, LIGAND, BRENDA); Structural database (CATH, SCOP, and PDBsum).

UNIT IV SEQUENCE ANALYSIS 6

Analysis of protein and nucleic acid sequences, multiple alignment programs, Development of programs for analysis of nucleic acid sequences, Pair wise Sequence Alignment - Similarity, Identity and Homology, Global Alignment, Local Alignment; database search methods-Multiple Sequence Alignment - Multiple alignment programs, Development of programs for analysis of nucleic acid sequences, Conversion of various file formats; Phylogenetic Analysis - Concept of dendrograms; Strings and Evolutionary trees.

UNIT V STRUCTURAL ANALYSIS 6

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 : 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", 1st Edition, Oxford University Press, Oxford, UK, 2002.

Course Objective: This course will enable the students to understand the fundamentals and complementary aspects of chemo informatics and bioinformatics for design of bioactive molecules. To get hands-on experience in chemical structure representation, storage and analysis of small molecular data.

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:

Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: WileyVCH; 1st 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 Objective: This course will enable the students to understand the critical relationship among biomolecular structure, function and force field models. To utilize basic modeling techniques to explore biological phenomena at the molecular level. To emphasize Modelling drug/receptor interactions in detail by molecular mechanics, molecular dynamics simulations and homology modeling.

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 data available

Unit I Molecular Modeling and Mechanics 06

Basic Concepts of Molecular Structure: Bond Length, Bond Angle, Torsion Angle, Non-Covalent Interactions and force field parametrisation and transferability – Molecular Structure and Internal Energy – Energy Minimization, Derivative and Non-Derivative Methods, Local and Global Minima.

Unit II Quantum Mechanics 06

Introduction to Computational Quantum Mechanics: One Electron Atom, Poly Electronic Atoms and Molecules, Hartree Fock Equations, Molecular Properties calculation using Ab initio and Semi Empirical Methods, Density Functional Theory, Moller and Plesset Perturbation Theory.

Unit III Molecular Modeling and Docking 06

Molecular Modeling in Drug Discovery, Sequence Analysis, Secondary structure prediction, Tertiary Structure prediction- Homology Modeling, Threading and *ab-initio* methods, Structure validation, Molecular Docking – Introduction, Approaches (Simulation and Shape complementarity approach), Molecular Docking Algorithm, Docking Optimization- Scoring functions, Molecular Docking Application.

Unit IV Pharmacophore 06

Pharmacophore – Historical Perspective and Features, Viewpoint of Pharmacophore, Pharmacophore modeling- Molecular alignments, handling flexibility, alignment techniques, scoring and optimization, conformational expansion, validation and usage, Applications of pharmacophore model in medicinal chemistry.

Unit V Molecular Dynamics 06

Molecular Dynamics- Introduction, MD using simple models, MD with continuous potentials, setting up and running a molecular dynamics simulation, Constraint Dynamics, Monte Carlo Simulation Methods- Monte Carlo simulation of molecules, Simulation Analysis.

Total: 30 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.

Course Objective: This course will enable the students to explore primary and derived databases in the field of computational structural biology and to visualize macromolecular structures using various visualization tools. Finally acquire skills to use different approaches for prediction of protein structure.

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 **INTRODUCTION TO PROTEINS** **6**

Fundamentals of X-ray diffraction, NMR spectroscopy of macromolecules Protein Structure: Primary, Secondary, Super Secondary, Domains, Tertiary, Quaternary, Ramachandran plot.

Unit II **PROTEIN SECONDARY DATABASES** **6**

Protein secondary structure classification databases: HSSP, FSSP, CATH, SCOP. Protein secondary structure prediction methods: GOR, Chou-Fasman, PHD, PSI- PRED, J-Pred.

Unit III **PROTEIN TERTIARY DATABASES** **6**

Protein Tertiary structure prediction methods: Homology Modeling, Fold Recognition, Abintio Method. Protein folding, Molecular Dynamics of Protein, Molecular Docking of Protein, Small molecule and Nucleotide, Concepts of Force Field

Unit IV **INTRODUCTION TO HMM** **6**

Motif and Domain: Motif databases and analysis tools. Domain databases (CDD, SMART, ProDom) and Analysis tools. HMM (Hidden Markov Model): Introduction to HMM, its application in Sequence alignment and Structure prediction, HMM based Softwares (HMMER and HMMSTR)

Unit V **STRUCTURAL FEATURES OF RNA** **6**

Structural features of RNA: Primary, Secondary, Tertiary. Introduction to RNA Secondary structure prediction, Methods for RNA Secondary structure prediction, Limitation of RNA Secondary 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 Objective: To learn the fundamentals of the Perl programming language and how it can be used to write data reporting and systems administration applications. To discover how to use of the DBI.pm module and related DBD (driver) files with Perl to build database-driven applications.

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 V 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:

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 Objective: Read and understand the Python syntax. Be familiar with Python's fundamentals and develop simple applications. Apply the principles and techniques of object-oriented programming. Use sophisticated techniques and Python modules that are particularly useful for bioinformatics programming. Build new Python software tools for life science research. Summarize text patterns using regular expressions

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:

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