

BHARATHIAR UNIVERSITY: COIMBATORE – 641046
M.Sc., BIOINFORMATICS (CBCS PATTERN)
Effective from Academic year 2019-2020 onwards

Duration of the course: 2 years

Eligibility:

A pass in any one of the following degree courses of UGC recognized universities.
B.Sc. / B.Tech. in all Science disciplines, B.V.Sc. / B,Pharm / M.B.B.S and B.D.S.

M.Sc., Bioinformatics – Semester Wise Syllabus and Scheme

Semester	Core / Elective / Supportive	Subject Code	Title of the Paper	Hours/ Week	Internal	External	Total Marks	Total Credits
I	CORE -I	13A	Cell & Molecular Biology	4	25	75	100	4
	CORE –II	13B	Computational Methods for Sequence Analysis	4	25	75	100	4
	CORE –III	13C	Programming in C And C++	4	25	75	100	4
	CORE -IV	13D	Recombinant DNA Technology	4	25	75	100	4
	CORE PRACTICAL– I	13P	Practical – I. Wet lab – Microbial and Phytochemical Techniques	6	40	60	100	4
	ELECTIVE – I	1EA	Mathematical &Statistical Applications in Bioinformatics	4	25	75	100	4
		1EB	Biostatistics					
	SUPPORTIVE – I	GS02	Supportive - I Database &Sequence Analysis	2	12	38	50	2
II	CORE –V	23A	Perl and Python programming for Bioinformatics	4	25	75	100	4
	CORE –VI	23B	Molecular Interactions	4	25	75	100	4
	CORE –VII	23C	Biophysics and Crystallography	4	25	75	100	4
	CORE -VIII	23D	Pharmacogenomics and Drug Design	4	25	75	100	4
	ELECTIVE – II	2EA	Biodiversity Informatics (or)	4	25	75	100	4
		2EB	Basics of Cheminformatics					
	CORE PRACTICAL– II	23P	Practical – II. Computer Programming	6	40	60	100	4
	SUPPORTIVE –II	GS98	Supportive-II Principles of Drug Design and Discovery	2	12	38	50	2
III	CORE –IX	33A	Genomics and NGS	4	25	75	100	4
	CORE –X	33B	Proteomics	4	25	75	100	4
	CORE –XI	33C	Visual Basic with RDBMS and Multimedia	4	25	75	100	4
	CORE -XII	33D	Molecular Modeling	4	25	75	100	4
	ELECTIVE – I	3EA	Systems Biology (or)	4	25	75	100	4
		3EB	Big Data Analytics					
	SUPPORTIVE – III	GS02	Supportive - III Database &Sequence Analysis	2	12	38	50	2
	CORE PRACTICAL– III	33P	Practical – III Molecular Techniques	6	40	60	100	4
CORE PRACTICAL– IV	33Q	Practical – IV Biological Sequence Analysis and Computer Aided Drug Design	6	40	60	100	4	
IV	PROJECT AND VIVA	47V	Project Work and Viva-Voce				200	8
			SWAYAM –MOOCs– Online 4weeks Course*		-	-	50	2
Total							2300	92

SWAYAM –MOOCs – Online 4weeks course is mandatory and it should be completed within third semester*

PRACTICAL COMPONENTS:

The M.Sc., Bioinformatics Core Practical Examination have the following Marks:

INTERNAL MARKS: 40

S.No.	Category	Marks
1.	Record and Observation note book	20
2.	Model Exams	20
	Total	40

EXTERNAL MARKS: 60

S.No.	Category	Marks
1.	Major Practical	20
2.	Minor Practical	10
3.	Spotters (A, B, C, D and E) 5x3=	15
4.	Record	05
5.	Viva	10
	Total	60

THEORY COMPONENTS:

The M.Sc., Bioinformatics Core and Elective theory Examination have the following Marks.

CORE AND ELECTIVE PAPERS: MAXIMUM MARKS– 100

INTERNAL MARKS: 25

S.No.	Category	Marks
1.	Test	15
2.	Assignment	05
3.	Seminar	05
	Total	25

EXTERNAL MARKS: 75

SECTION– A: 10x2=20 Marks (Question No. 1 to 10)

Answer All questions. All questions carry equal marks.

SECTION– B: 5x5=25 Marks (Question No. 11 to 17)

Answer any FIVE questions. All question carry equal marks.

SECTION– C: 2x15=30 Marks (Question No. 19 to 21)

Answer any TWO questions. All Question carry equal marks.

SUPPORTIVE PAPERS: MAXIMUM MARKS– 50

INTERNAL MARKS: 12

S.No.	Category	Marks
1.	Test	06
2.	Assignment	03
3.	Seminar	03
	Total	12

EXTERNAL MARKS: 38

SECTION– A: 8x1=8 Marks (Question No. 1 to 8)

Answer All questions. All questions carry equal marks.

SECTION– B: 5x2=10 Marks (Question No. 9 to 13)

Answer All questions. All Question carry equal marks.

SECTION– C: 5x4=20 Marks (Question No. 14 to 21)

Answer any FIVE questions out of Eight. All Question carry equal marks.

As Bioinformatics is inter disciplinary subject where students from biology, chemical, physical and computer sciences are admitted. Hence the syllabus is framed to benefit all the students.

Program Objectives:

- To introduce the biology part to the students by explaining cell structure, function of organelles and macromolecules.
- To make the students understand the drug's action, they are informed about the macromolecular structure and interactions.
- To provide the basic knowledge of mathematics and statistics required for bioinformatics.
- To enable the students to write the algorithm by teaching them with computer languages.
- To make the students understand different aspects of molecular modeling and drug design.
- To provide detailed information on Proteomics, Applied genomics and System biology so that the students will understand the drug designing and targeting clearly.
- To make the students to have hands on experience on dry lab as well as wet lab experiments.

Title of the Subject:

CELL AND MOLECULAR BIOLOGY

No. of Credits: 4

Code No:19BIIA13A

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basic concept of cell.
- To know the central dogma of life plays a pivotal role in cell biology.
- To analyze the different structural form of DNA and protein.
- To understand the cell cycle and molecules of life in various aspects.
- To understand the theory of Michaelis – Menten kinetics.

Syllabus

Unit-I: Biology of cell

Cells as a unit of life, structure of prokaryotic and eukaryotic cells. An overview of organelles (Mitochondria, chloroplasts, ER, Golgi, ribosomes, lysosomes and peroxisomes, nucleus and nucleolus). Differences and similarities in plant and animal cells. Cellular membrane: structure, transport, channels, carriers, receptors, endocytosis, membrane potentials.

Unit-II: Central Dogma of Life

DNA replication, Transcription and Translation. Cell-cell interactions and signal transductions: Intercellular junctions, signaling by hormones and neurotransmitters; receptors, G-proteins, protein kinases and second messengers. Protein traffic in cells.

Unit-III: Cell Cycle

Mitosis, Meiosis, Regulation. Mutation – Types of mutations, types of mutagenic agents and their molecular mechanism; DNA repair; Chromosomal types and structure; Mechanism by which genome undergoes changes, recombination, mutation, inversion, duplication, and transposition.

Unit-IV: Molecules of Life

Introduction to carbohydrates–Monosaccharides and their derivatives, Disaccharides, Polysaccharides. Proteins –Structure of aminoacids, Different levels of organization–Primary, secondary, tertiary and quaternary structures. Nucleic acids – Purines, pyrimidines, Nucleosides and Nucleotides, Different structural form of DNA, denaturation and renaturation of DNA. Lipids-Structure and function of Fatty acids, Triacylglycerols, sphingolipids, steroids and glycerophospholipids. Water, small molecules–Alkaloids, glycosides, phenols, oligopeptides, Flavonoids, and terpenoids.

Unit-V: Enzymes

Units of Activity, coenzymes and metal cofactors, temperature and pH effects, Michaelis – Menten kinetics, inhibitors and activators, active site and mechanism of enzyme action, Isoenzymes, allosteric enzymes.

Reference Books:

- Lehninger, A. L. 1984. Principles of Biochemistry. CBS publishers and distributors, New Delhi, India.
- Horton, Moran, Ochs, Rawn, Scrimgeour Principles of Biochemistry Prentice Hall Publishers.
- David. E. Sadava Cell Biology: Organelle Structure and Function Jones & Bartlett publishers.
- Shanmughavel, P. 2005. Principles of Bioinformatics, Pointer Publishers, Jaipur, India.

Course Outcomes:

On successful completion of the course, the students will be able to

- CO 1- Describe the Prokaryotic and Eukaryotic cell and interpret the different stages of cell division
- CO 2- Evaluate the changes in the transcription and translation.
- CO 3- Identify the isoenzymes and coenzymes based on their function
- CO 4- Describe the different structures of carbohydrate, lipids, nucleotides, DNA and Protein

Course Prepared by: Dr.P.Shanmughavel

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

COMPUTATIONAL METHODS FOR SEQUENCE ANALYSIS

No. of Credits: 4

Code No: 19BIIA13B

No. of Teaching Hours: 4/week

Course Objectives:

- To understand the various computational techniques.
- To analyze biological data with the use of sequence information.
- To understand the steps involved in Evolutionary analysis.
- This topic helps to ensure the sequence analysis work successfully without any error.

Syllabus

Unit-I: Outline of Bioinformatics

Introduction and Applications of Bioinformatics. Classification of biological databases, Biological data formats. Introduction to single letter code of amino acids, Symbols used in nucleotides. Data retrieval from Entrez and SRS.

Unit-II: Wide-ranging of Sequence Alignment

Outline and Uses of sequence alignment. Similar sequence search using FASTA and BLAST programs in the database. Pairwise sequence alignment and Multiple sequence alignment. Local and Global alignment with dynamic methodology of Smith-Waterman algorithm and Needleman-Wunsch algorithm. Substitution matrices, Scoring matrices - PAM, BLOSUM and Dot plot. Statistics of alignment score and evaluation.

Unit-III: Evolutionary/Phylogenetic analysis

Overview of the Tree analysis. Cladistics, Phenetics and Distances. Different types of trees for prediction. Overview of Bootstrapping. Tools - Clustal, PHYLIP and Mega. Problems and errors in phylogenetic reconstruction.

Unit-IV: Genome Exploration

Gene finding methods. Gene prediction: Analysis and prediction of regulatory regions. Fragment assembly. Genome sequence assembly, Restriction Mapping and Repeat Sequence finder.

Unit-V: Protein Assessment

Primary sequence information. Secondary structure prediction of RNA and Protein. Probabilistic models: Markov chain and Hidden Markov Models. Tools - ProtParam, GOR, HNN and Sopma.

Reference Books:

- S.C. Rastogi et al. Bioinformatics: Methods and Applications: (Genomics, Proteomics and Drug Discovery) Kindle Edition.

- Andreas D. Baxevanis and B.F. Francis Ouellette. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. ISBN: 978-0-471-47878-2.

Course Outcomes:

On successful completion of the course, the students will be able to

- CO 1- The students can able to do the sequence analysis and phylogenetic prediction with their own knowledge.
- CO 2- Also capable to search the protein/gene sequence and structural information in the databases.
- CO 3- Helps to ensure the sequence analysis work successfully without any error.
- CO 4- To analyze biological data with the use of sequence information.

Course Prepared by: Dr.C.Jayaprakash

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PROGRAMMING IN C AND C++

No. of Credits: 4

Code No: 19BIIA13C

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basic aspects of programming.
- Develop an in-depth understanding of functional, logic, and object-oriented programming paradigms.
- Explain and be able to use fundamental programming constructs such as sequencing, decisions and iteration.
- To enhance problem solving and programming skills in C & C++

Syllabus

Unit-I: Introduction to Programming Languages

Introduction–Programming languages – Problem solving Technique: Algorithm, Flowchart, Compiling, Testing and Debugging, Documentation – Data structures – Array, Stack, Queue, Linked List concepts.

Unit-II: Programming in C

C language Introduction – Tokens – Keywords, Identifier, Variables, Constants, Operators – Expression – Data types –Operator precedence – Statement: Input statement, Output statement,

Conditional and Unconditional Control Statement – Looping Statement: while, do–while, for – nested loop – Arrays.

Unit-III: Procedural Concepts in C

C – Procedural Concepts: Structured Programming – Built-in library function – User defined functions – Pointer introduction – Passing pointer in a function – Structure – Union – File handle: Read and Write character from a file.

Unit-IV: Object Oriented Programming and C++

Basic concepts of OOPS– Data hiding–Encapsulation–Inheritance, Polymorphism – Introduction to C++, C vs C++ – data types, variables, constants, operators and statements in C++ – Conditional and looping statements.

Unit-V: Programming and C++

C++ classes - Classes & Objects – Functions in C++ – function prototype-definition–Different forms of Constructor – Destructor – Copy constructor – Inheritance –Single, Multiple and Multi level inheritance – Function & operator overloading –inline functions – Friend and virtual functions – Overloaded functions.

Reference Books:

- B.W.Kernighan and D.M. Ritchie, “The C Programming Language”, 2nd Edition. Prentice Hall of India.
- Byron Gottfried, - “Programming with C” (Schaum's Outline Series) - Tata McGraw Hill Publishing Company – 1998
- E. Balagurusamy - “Programming in C++ ” - Tata McGraw Hill Edition
- Robert Laffore -“Object oriented programming with C++” -Waite series.

Course Outcomes:

On successful completion of the course, the students will be able to

CO-1- Have a good understanding about the concept of C & C++.

CO-2- Be able to explain and make use of data types, variables, constants, assignment statements, and arithmetic and Boolean expressions in writing programs;

CO-3- Understand object-oriented programming using C++

CO-4- Explain and are able to use arrays and structures;

CO-5- Be able to write and read basic codes in C & C++.

Course Prepared by: Prof.N.Jeyakumar

Course Verified by: Prof.N.Jeyakumar

Title of the subject:

RECOMBINANT DNA TECHNOLOGY

No. of Credits: 4

Subject Code No: 19BIIA13D

No. of Teaching hours: 4/week

Course Objectives:

- To familiarize the students to versatile tools and techniques employed in genetic engineering and recombinant DNA technology.
- To understand the theory behind molecular biology techniques and methodologies in biological research.
- To perform basic molecular biology techniques and know the various components and techniques in designing experiments.
- To learn the importance of designing experiments and interpreting results.
- To provide an understanding on the basic concept in Gene cloning.

Syllabus

Unit-I: Introduction to RDNA

Scope of Recombinant DNA Technology, Milestones in Genetic Engineering, Gene cloning Techniques - Vector, types, properties, enzymes in gene cloning - exonucleases, endonucleases, restriction endonucleases, ligases, reverse transcriptase, polymerase, terminal transferases - Homopolymer tailing, linker sand adaptors.

Unit-II: Cloning Vectors

Plasmids; Bacteriophages; M13mp vectors, pUC19 and Blue script vectors, Phagemids, Lambda vectors- Insertion and Replacement vectors, Cosmids, Artificial chromosomes, Mammalian vectors-SV40, vaccinia and retroviral vectors, Expression vectors- pMal, GST, pET-based vectors, Plant based vectors - Ti and Ri as vectors, Yeast vectors, Shuttle vectors.

Unit-III: Gene Transfer and RDNA selection

Methods of gene transfer: Microinjection, electroporation, gene gun, liposome and viral-mediated delivery, Agrobacterium-mediated delivery. Strategies for selection and screening- marker and reporter genes, positive and negative selection, insertion inactivation, α complementation. Polymerase chain reaction –Primer design tools, Fidelity of thermostable enzymes, Types of PCR – multiplex, nested, reverse transcriptase, real time PCR.

Unit-IV: Sequencing

DNA sequencing - Sanger's method, Maxam and Gilbert method and Automated method, Construction of genomic and cDNA libraries; Chromosome walking and jumping, DNA fingerprinting by RFLP and RAPD, Site- directed mutagenesis.

Unit-V: Applications

Gene silencing techniques – siRNA, Micro RNA, principles and application, Gene knockouts and Gene Therapy, Genome editing by CRISPR/Cas9 system, In-silico analysis, manipulation and annotation of DNA sequences for experimental design and cloning experiments.

Reference Books:

- Principles of genetic manipulation; Ed. Old and Primrose, 6th Edition. Blackwell Science.
- Gene Cloning, an introduction – T. A. Brown, Chapman and Hall, 3rd Edition, 1995.
- An Introduction to Molecular Biotechnology: Molecular Fundamentals, Methods and Applications in Modern Biotechnology - M. Wink. Wiley, ed. 2, 2011.

Course Outcomes:

On successful completion of the course, the students will have

CO1-Technical expertise on versatile techniques in Recombinant DNA technology.

CO2-An understanding on application of genetic engineering techniques in basic and applied experimental biology.

CO3-Proficiency in designing and conducting experiments involving genetic manipulation.

Course Prepared by: Dr.V.Hemamalini

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

MATHEMATICAL & STATISTICAL APPLICATIONS IN BIOINFORMATICS

No. of Credits: 4

Code No: 19BIIA1EA

No. of Teaching Hours: 4/week

Course Objectives:

- This course will enable the students to achieve skills in mathematics that are essential for application in bioinformatics.
- Mathematical and statistical frameworks are being increasingly employed to understand and investigate biological processes.
- These frameworks helps in analyzing vast amount of datasets generated from genome and related projects.
- It is thus essential to introduce basic concepts of mathematics, probability and statistics early within the Bioinformatics curriculum.
- This course will enable students to understand and appreciate computational problems in proper perspective.
- In addition, this course will provide a foundation for pursuing higher level courses in Computational Biology.

Unit-I: Matrices

Different types of matrices - Matrix Operations - transpose, inverse, and conjugate systems - symmetric and skew symmetric matrices - Diagonalization of Matrices and Characteristic roots - Equality of Matrices - Adjoint of a matrix - Singular and non-singular matrices - Eigen values and Eigen vector – Rank – **Determinants** - evaluation – Properties - Minors and Cofactors, Multiplication of Determinants, Adjoint, Reciprocal, Symmetric Determinants - Solving Simultaneous equations in three variables using matrices - Solution of a system of linear equations by Cramer's rule and by matrix inversion method - Cayley – Hamilton theorem without proof - Consistency of linear equations. **Vectors** - The concept of a Vector, Vector addition and subtraction, Products of two vectors-Dot product and Cross product, Products of three vectors- scalar triple product and vector triple product, Gradient, Divergence and Curl, equation.

Unit-II: Calculus – Differentiation

Standard results – Derivatives of simple functions – Product Rule – Quotient Rule - Partial Differentiation – Partial derivative of simple functions (3 variables case only) - Euler's Theorem. **Integration** – Standard results – Integrals of simple functions – Definite Integrals – Indefinite Integrals – Integration by parts – Integration by substitution – Integration by partial fractions.

Unit-III: Introduction to Statistics

Classification and tabulation of Data - Diagrammatic and graphic Presentation - frequency curve and its characteristics - Introduction to Central Tendency - Frequency Distributions and **Statistical Measures** (Arithmetic Mean, Median, Mode) - Measures of Dispersion - Methods of Studying Variation, Range, Mean Deviation, Standard Deviation, Variance, coefficient of Variation - **Correlation and regression** – Introduction - Types of correlation, methods of studying correlation - Coefficient of correlation – Probable error – Regression – Simple linear regression - Principles of least squares, - Relation between regression and correlation - Regression Equations.

Unit-IV: Probability

Concept and definitions of Probability - Terms used in probability - Probability of events - axioms of probability - Theorem of probability - Properties of probability - Conditional probability - Baye's theorem, Problem based on Baye's theorem - Random variables: Discrete and continuous random variables, cumulative density function, Probability density and mass functions - Probability distribution- Introduction, binomial distribution, Poisson distribution, Normal distribution - **Test of Hypothesis Sampling** - Population – Sample – Parameter – Statistic – Standard error - Hypothesis-Null Hypothesis – Alternative Hypothesis – Critical Region – Level of Significance – Errors in Sampling – One tailed and two test statistic-test of significance and its test procedure. Test of significance for small samples: Tests based on normal distribution for Single mean, difference of two means - Tests based on t-distribution for single mean, difference of two means, paired test and observed correlation coefficient – F Test – Parametric and Non parametric tests - Chi-square (χ^2) test for goodness of fit. Analysis of variance: One way and two way classifications - PCA, Factor analysis.

Unit-V: Introduction to R

How R works - Data sets included in R - Objects –Operators - The data editor – Useful R functions - Graphics with R – Data frames and lists - File operations - Mathematical operations, Basic matrix computation - Basic graphics (high-level plotting, low-level plotting, interacting with graphics) - Statistical analyses with R - Hypothesis testing and data handling: Parametric and nonparametric tests, Chi-square test, t-tests, ANOVA, Correlation and regression, Principal component Analysis – Packages in R - Bioconductor - Loops and vectorization - Expression Set Class, Data annotation, biomaRt, Network analysis - Writing a program in R - Writing own functions -**Matlab**- key features, basic functionalities - tool box, data types, variables, operators, vectors, matrix operations, Control structures The Matlab interface - Writing in script files - Importing data – Plotting - Using in-built functions - Creating your own functions - Basic programming in Matlab (including for loops) – Case study with biological examples.

Reference Books:

- Basic mathematics by Serge A. Lang, 1988, Springer publisher
- Narayanan Manicavachagom Pillay, Calculus Vol I, S. Viswanathan Publications.
- S.C.Gupta and V.K. Kapoor, Fundamentals of Mathematical Statistics.
- Gentle, James E.; Härdle, Wolfgang K. Mori, Yuichi (Eds.). Handbook of Computational Statistics
- Ewens, W.J. and Grant, 2001. Statistical Methods in Bioinformatics: An Introduction, Springer-Verlag
- Mathur Sunil K. Statistical bioinformatics with R. Publisher: Academic Press, 2010 ISBN: 9780123751041.
- Michael R. King, Nipa A. Mody, “Numerical and Statistical Methods for Bioengineering: Applications in MATLAB”, Cambridge University Press, 2011.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Workout basic mathematical problems in bioinformatics.

CO 2- Analyse the statistical significance of any biological data.

CO 3- Write R codes and Matlab programs for biological problems.

CO 4- Apply the mathematical and statistical knowledge in programming.

CO 5- Develop new coding functionalities.

Course Prepared by: Dr.S.Usha

Course Verified by: Prof.N.Jeyakumar

Title of the subject:

BIOSTATISTICS

No of Credits: 4

Code No: 19BIIA1EB

No of teaching hours: 4/week

Course Objectives:

- This course will enable the students to achieve skills in statistics that are essential for application in bioinformatics.
- Statistical frameworks are being increasingly employed to understand and investigate biological processes.
- These frameworks helps in analyzing vast amount of datasets generated from genome and related projects.
- It is thus essential to introduce basic concepts of probability and statistics early within the Bioinformatics curriculum.
- This course will enable students to understand and appreciate computational problems in proper perspective.
- In addition, this course will provide a foundation for pursuing higher level courses in Computational Biology.

Syllabus

UNIT-I: Introduction to statistics and Data collection

Statistics – Definition – Statistical methods – Basic principles – Variables – Measurements, functions– Collection of Data – Primary and Secondary – Types and methods of data collection – Procedure – Merits and Demerits – Classification and tabulation of data – Diagrams and graphs.

UNIT-II: Central tendency and dispersion

Measures of Central tendency – Mean, Median, Mode, Geometric Mean – Merits and Demerits – Dispersion and measure of dispersion – Range, Standard deviation, quartile deviation – Merits and Demerits – Co-efficient of variations.

UNIT-III: Correlation and Regression

Skewness and Kurtosis – Correlation – Types and method of correlation – Regression – Simple regression equation fitting – Prediction, similarities and dissimilarities of correlation and regression.

UNIT-IV: Distribution and Hypothesis tests

Distribution – Binomial, Poisson, Normal – Statistical inference – Sampling methods – Simple hypothesis testing – Students “t”- test – Chi square test.

UNIT-V: Non Parametric Test

Sign test, Wilcoxon signed rank test, one sample Run Test, Median test, Kruskal Wallis H test, Kolmogorov Smirnov test, Mann Whitney U test

Reference Books:

- Schaum's Outline Statistics by Murray.R, Spiegel, Larry.J.Stephens, 4th edition, McGraw Hill Companies.
- Zar, J. - Bio-statistical Analysis, Prentice Hall of India.
- An introduction to Bio-Statistics by N.Gurumani.2009 – MJP Publications.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Understand the basics of Biostatistics and data collection & classification methods

CO 2- Know the types of central tendency and dispersion for different data analysis

CO 3- Understand the concept and methods of Correlation and Regression.

CO 4- Understand the types of Distribution, Hypothesis test and Non parametric test.

Course Prepared by: Dr.S.Usha

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PRACTICAL – I

WET LAB – MICROBIAL AND PHYTOCHEMICAL TECHNIQUES

No. of Credits: 4

Code No: 19BIIA13P

No. of Teaching Hours: 6/week

Course Objectives:

- To understand the isolation of three different microorganisms in a single aspect.
- To know the collection of microbes, plants and blood samples.
- To make students understand preliminary phytochemical analysis from plant extracts.

MICROBIOLOGY LAB

1. Isolation of bacteria from soil - serial dilution technique
2. Isolation of fungi from soil - serial dilution technique
3. Isolation of actinomycetes from soil - serial dilution technique
4. Screening microbes for antibiotic production
5. Extraction of proteins from microbes, plant and blood
6. Separation of protein and molecular weight determination using SDS-PAGE
7. Staining the gel - CBB and Silver staining

PHYTOCHEMISTRY LAB

8. Extraction of secondary metabolites from medicinal plants - Cold percolation method
9. Extraction of secondary metabolites from medicinal plants - Soxhlet method
10. Preliminary Phytochemical analysis of plant extracts
11. Antibiotic bioassay-inhibitory activity (Disc Diffusion)
12. Tissue culture - callus induction
13. Tissue culture - cell suspension culture

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- A step by step procedure describes the isolation methods.

CO 2- Skillful in comparison and interpretation of the result with the standard reports.

CO 3- Able to identify the expected compound present or absent in the taken sample.

CO 4- Capable to prepare the Gel and do the staining processes individually.

Course Prepared by: Dr.M.Jeyam & Dr.C.Jayaprakash

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PERL AND PYTHON PROGRAMMING FOR BIOINFORMATICS

No. of Credits: 4

Code No: 19BIIA23A

No. of Teaching Hours: 4/week

Course Objectives:

The objectives of this course include the following:

1. Utilise the UNIX/LINUX environment effectively to perform a range of system-level tasks.
2. Analyse, write and apply shell and Perl scripts of medium complexity to solve system-level problems and form an appropriate skill set.
3. Give students a thorough understanding of the Python and provide an exposure of effective Python programming
4. Construct and apply regular expressions in shell and to process text, search files and validate formats
5. Experience learning a programming language "on our own"
6. Understand the syntax and semantics of the Perl and Python languages and to develop and implement various types of programs in them
7. Understand various forms of data representation and structures supported by the Programming language and to understand their appropriate applications

Syllabus:

Unit - I

UNIX/LINUX Operating System - UNIX - File system - Overview - Text processing - Commands and Operation - UNIX filenames and file protections - working with directories - loops and IF statements - Different File Editors - Mastering the special features of the UNIX system - Advanced Unix commands - Configuring services in Unix

- - Networking Utilities Introduction to Linux - System Processes - User Management - Types of users, Creating users- Granting Rights - File Quota, File-System Management and Layout - Login Process- Linux shells (bash and tcsh) - Shell Programming Networking on Linux - Printing and print sharing- ftp service, http service.

Unit - II

PERL Basics - Data types – Operators – variables –Variable Interpolation- Cont–Scalars, Lists, Hashes - Arrays – Array functions – Push and Pop , Shift and unshift – Hash Functions, Using Hashes for the Genetic Code, Gene Expression Data Using Hashes - **PERL Subroutines, Modules & Objects** - Subroutines - for calculation, Reference to subroutine - Arguments, Passing Data to Subroutines - Passing arrays and hashes to subroutines. Modules - Perl standard modules-Library - **Object oriented Perl** – Working with objects - Perl and Databases – Perl and DBM

Unit - III

PERL Regular Expression and File handling – Pattern-matching - Substitutions, Transliteration, Split and join functions - Quantifiers - File handling concepts - Writing to Files - Opening and Closing a File handle - Directory Manipulation - Common Gateway Interface - CGI.pm Module - Simple CGI programs, Passing Parameters via CGI, Perl and the Web - Perl control statements - **PERL programs** for Sequences and Strings – Representing Sequence data, store a DNA sequence, concatenating DNA fragments, Transcription. Motifs – Finding motifs, counting nucleotides. Genbank – Files and libraries. Protein Data Bank – files and folders, PDB files. Blast – String matching and homology, blast output files - **BioPERL:** General Bioperl classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local Database).

UNIT- IV

Introduction to Python - Installing Python - Environment Setup - Python interpreter - Identifiers, Keywords and Indentation - Comments - Python Data Types - Python variables - Operators - Lists in Python - operations, methods, parameters – Iterators - Generators, Comprehensions and Expressions - Tuples - Python Dictionaries and Sets - operations and methods

UNIT- V

Files - reading and writing files, command line arguments - Exception handling - Modules and Packages - Functions - Control Statements and Regular Expression - string functions and methods - Web Programming with Python - Using Databases in Python - Introduction to Biopython - Sequence objects - Database search using Biopython, Advanced modules in Biopython - Python For Data Analysis - Array Function, Processing, Input and Output

References:

1. Thomas, R. A., & Yates, J. (1987). Advanced Programmer's Guide to Unix System. V. McGraw-Hill Book Company.
2. Cozens, S., & Wainwright, P. (2000). Beginning Perl. Wrox Press.
3. Tisdall, J. (2001). Beginning Perl for Bioinformatics. O'Reilly Media, Inc.
4. Sedgewick, R., Wayne, K., & Dondero, R. (2015). Introduction to programming in Python: An interdisciplinary approach. Addison-Wesley Professional.
5. Chang, J., Chapman, B., Friedberg, I., Hamelryck, T., De Hoon, M., Cock, P., Antao, T., & Talevich, E. (2010). Biopython Tutorial and Cookbook. *Update*, 15-19.
6. Martelli, A. (2006). Python in a Nutshell. O'Reilly Media, Inc."

Title of the subject:

MOLECULAR INTERACTIONS

No. of Credits: 4

Subject Code No: 19BIIA23B

No. of Teaching hours: 4/week

Course Objectives:

- To acquire a thorough and comprehensive understanding of various types of chemical bonding.
- To impart advanced knowledge on protein Structure, its characteristics property and significance in biological systems.
- To introduce the concepts on structure of chemical compounds that is considered important in understanding the interaction of biomolecules.
- To understand the structural and dynamic properties of biomolecules with special emphasis on stereochemistry and conformational analysis.
- To gain knowledge on principles of spectroscopy for structural elucidation.
- To understanding the structural properties and energy minimization in protein folding process.

Syllabus

Unit-I: Chemical Bonding

Introduction and characteristics: ionic bond, covalent bond, coordination bond and hydrogen bond. Factors affecting covalent bond strength. Non-bonded interactions - electrostatic interactions and Van der Waals interactions. Hydrophobic interactions and Hydrophilic interactions. Bond stretching interactions and Metallic bond.

Unit-II: Theories of Chemical Bonding

Valence bond Theory - Sigma bond, Pi bond and Hybridization. Types of interaction between atoms - Bond distance, Bond angle, Torsion Angle, Bond energy and Dipole-Dipole interactions. VSEPR theory - Shape of orbitals and orbital hybridization. Molecular orbital theory and its applications.

Unit-III: Protein Folding

Principles of protein folding. Role of chaperones, folding pathways. Methods to study protein folding - phi, psi & omega angles with distance. Zwitterion, Disulfide Bridge and Ramachandran Plot. Types of Helices, Beta turns, Gamma turns. FSSP, VAST and DALI.

Unit-IV: Macromolecular interactions

Protein-Protein, Protein-Nucleic acids, Protein-carbohydrates, Protein-drug or small molecule interactions. Metalloprotein, Sequence and structure based methods to predict protein-protein interaction. Stereochemistry of proteins and nucleic acids.

Unit-V: Fundamentals of Spectroscopy

Quantum mechanics - Wave properties - Absorption Spectra - Ultraviolet Spectra of Proteins and Nucleic Acids - NMR Spectroscopy - Chemical Shifts - Spin-Spin Splitting - Magnetic Resonance Imaging - Electron Spin Resonance - Circular Dichroism of Proteins and Nucleic acids - Optical Rotatory Dispersion - Infrared Spectroscopy - Raman Spectroscopy - Structure Determination with Vibrational Spectroscopy - Applications.

Reference Books:

- Tewari K.S. Vishnoi N.K. (1998) “A Text book of organic chemistry”, Vikhyas publishing house.
- Gordon G. Hammes. (2005) “Spectroscopy for the Biological Sciences”, John Wiley & Sons.
- Creighton T.E. (1993) “Proteins-structures and molecular properties”, Freeman WH.
- Carl Branden & John Tooze. (1999) “Introduction to Protein Structure” Garland Publishing, New York & London.
- David Micha. (2009) “Molecular Interactions” John Wiley & Sons.

Course Outcomes:

On successful completion of the course, the students will have

CO 1- Predict and justify that changes in the subcomponents of a biological polymer affect the functionality of the molecule.

CO 2- Define models that illustrate the interactions between biomolecules.

CO 3- Analyze data to identify how molecular interactions affect structure and function.

Course Prepared by: Dr.C.Jayaprakash

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

BIOPHYSICS AND CRYSTALLOGRAPHY

No. of Credits: 4

Code No: 19BIIA23C

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basic aspects and applications of crystallography.
- To know the computational software's to visualize and compare the protein structure and sequences.
- To analyze the conformational properties of protein using Ramachandran plot.
- To understand the steps various chromatography techniques.
- To utilize the different databases for further analysis of study.

Syllabus

Unit-I: Introduction to protein structure

Physical and chemical properties of aminoacids and polypeptides. Secondary, Super Secondary, tertiary and quaternary structure of proteins. Theoretical and experimental methods for determination of size of proteins. Physical nature of non-covalent interactions. Conformational properties of proteins, Ramachandran Plot.

Unit-II: Structural Bioinformatics

Homology modeling, Threading, Fold recognition, Model refinement and validation. Vector based method, neural network. Structural databases- PDB, CATH (Classification by Class, Architecture, Topology), SCOP - Structural Classification of Protein, FSSP – Fold classification based on structure – structure alignment, MMDB – Molecular Modeling Database, SARF – Spatial arrangement of backbone fragments. mmCIF formats used for archiving structures. Comparison of structures by tools – PyMOL, Chimera.

Unit-III: Functional Bioinformatics

Cell surface receptors, GPCR's, Kinases, Channel proteins, Ubiquitin. Biophysical Techniques: Principles, Process and Applications of Thin layer chromatography, Column chromatography (ion exchange and affinity only), HPLC; Low Resolution Techniques: CD spectroscopy and DLS. 1Directional and 2D Electrophoresis, UV Visible spectroscopy. High Resolution Techniques: NMR, X-ray crystallography

Unit-IV: X-ray crystallography Introduction

X-ray generation; its application; unit cell lattices, Bragg's Law; synchrotron radiation and its uses; Symmetry, Atomic scattering factor and structure factor; phase problem; intensity data collection and reduction; hydrogen bonding.

Unit-V: X-ray crystallography of macromolecules

Isolation and purification of protein, crystallization (sitting and hanging drop method). Protein structure determination-molecular replacement technique; multiple isomorphs replacement method, multi wavelength anomalous diffraction method and x-ray anomalous scattering; Calculation of electron density map, interpretation of electron density map. Refinement of structure. Structure validation methods.

Reference Books:

- Thomas. E. Creighton Proteins Structures and Molecular Properties Freeman and Company
- Cantor and Schimmel Biophysical Chemistry Part II Techniques for the study of biological structure and function Freeman and Company
- Thomas M Devlin Textbook of Biochemistry Wiley LISS Fifth edition
- Stephen Neidle Nucleic Acid Structure and Recognition
- Leonard Banaszak Foundations of Structural Biology
- Philip E. Bourne Structural Bioinformatics John Wiley & sons
- Shanmughavel, P. 2005. Principles of Bioinformatics, Pointer Publishers, Jaipur, India.
- J. Drenth: Principles of protein x-ray crystallography. Springer, New York (1994)
- C. Brandén & J. Tooze: Introduction to Protein Structure. Second Edition, Garland, New York (1998).

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the Physical and chemical properties of amino acids and model 2D and 3D structure of a target from the sequence.

CO 2- Interpret the model refinement and validation of Protein structure.

CO 3- Evaluate the atomic scattering factor and structure factor of macromolecules.

CO 4- Visualize and compare the protein structures using bioinformatics tools.

Course Prepared by: Dr.N.Sundara Baalaji

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PHARMACOGENOMICS AND DRUG DESIGN

No. of Credits: 4

Code No: 19BIIA23D

No. of Teaching Hours: 4/week

Course Objectives:

- To give strong foundations of pharmacogenomics, Pharmacodynamics, and toxicogenomics and stages in drug development.
- To make the students understand drug interaction and metabolism of the drug in the host
- To realize the importance of ayugenomics and to utilize the microsatellite and microarray techniques gene analysis.
- To make the students understand the importance of pharmacogenomics in disease treatment.
- To utilize the available sequences to model the target and to use computational tools and software to design a drug.

UNIT-I: Introduction to Pharmacogenomics

Introduction to pharmacogenomics, pharmacodynamics, pharmacokinetics, toxicogenomics and ADME properties. Process of drug development-clinical trials phase I, II, III and IV. Route of drug administration. Nature of cell membrane, physiological factors related to drug absorption and drug distribution.

UNIT-II: Drug Metabolism and Ayugenomics

Biotransformation (Metabolism) of drugs and related organic compounds - General pathways, sites of drug biotransformation. Oxidative reactions, reductive reactions, hydrolytic reactions, conjugation reactions, factors affecting drug metabolism and variability in drug response. Ayugenomics (integration of Ayurveda & genomics). Microsatellite in studying genetic variation. Microarray in herbal drug research, Pharmacodynamics, Pharmacogenomics and Pharmacognosy.

UNIT-III: Pharmacogenomics in the disease treatment

Pharmacogenomics in the treatment of cancer, neurodegenerative diseases, cardiovascular diseases. Pharmacogenomics in pharmaceutical industry, Ethical issues related to Pharmacogenomics, Pharmacogenomics and ethnopharmacology, Benefits of Pharmacogenomics.

UNIT-IV: Ligand designing

2-D and 3-D database searching, Structure-based and Ligand based drug design for all classes of targets, SPROUT, LUDI. Structure Activity Relationship studies. QSAR studies, 3D QSAR, CoMFA, Verlot Algorithm, Craig Plot, Topliss scheme. Pharmacophore identification and novel drug design. ADME prediction - SwissADME, PreADMET.

UNIT-V: Modeling and Docking

Druggable Targets, Macromolecular modeling- *Ab initio* modeling; Phyre 2 server. Homology Modeling; Modeller. Threading; RAPTOR. Validation of the Model – Ramachandran Plot. PROCHECK. Binding site; Q-Site finder, Catalytic site atlas. Molecular docking; ArgusLab, AutoDock, GLIDE. Drug-receptor interaction. Pymol, Rasmol viewer.

Reference Books:

- J.H. Block and J.M. Beale Jr. 2004. Organic medicinal and Pharmaceutical chemistry. Lippincott Williams and Wilkins, New York.
- B.Patwaradhan.2007. Drug discovery and development. New India publishing agency, New Delhi.
- L.Shargel and A.B.C.Yu.1999. Applied Biopharmaceutics and Pharmacology. McGraw-Hill, New York.
- D.M. Brown.2004. Drug delivery systems in Cancer therapy. Humana press, Totowa, New Jersey.
- Rothstein, Pharmacogenomics: Social, ethical and clinical dimensions, Wiley Less.
- Jin Xiong. Essential Bioinformatics. Cambridge University Press.
- Andrew R. Leach Molecular Modeling: Principles and Applications.

Course Outcomes:

On successful completion of the course, the students will be able to

CO1-Understand pharmacogenomics and describe the metabolism of the drug right from administration to excretion and biotransformation.

CO2- Relate the traditional medicinal system to the modern scientific results through Ayugenomics; apply modern research tools in the area of Pharmacogenomics.

CO 3- Understand the genes affecting the efficacy of the drugs in the treatment of some important diseases.

CO 4- Model and validate the target structures and to *in silico* identification of lead molecules through docking.

Course Prepared by: Dr.M.Jeyam

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

BIODIVERSITY INFORMATICS

No. of Credits: 4

Code No: 19BIIA2EA

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basic Biological diversity of life.
- To know the distributed databases and web- accessible resources
- To analyze the software for identification of Assessing existing biodiversity databases
- To understand the probabilistic and deterministic method for analyzing biodiversity data.

Syllabus

Unit-I: Biological diversity of life

Methods for species identification & classification- Information needs in biodiversity assessments and inventorying programmes- Role of information technology in distributing biodiversity information.

Unit-II: Introduction to biodiversity informatics

Assessing, analyzing and documenting biodiversity- Morphological and molecular characterization of biodiversity- Introduction to biodiversity database: endangered animals, endemism and Red data books- Biodiversity registers.

Unit-III: Network and Databases

Designing information systems to support biodiversity conservation- Networks for distributing information- Distributed Databases and Web- Accessible Resources.

Unit-IV: Software for biodiversity informatics

Software for identification of Assessing existing biodiversity databases on the world- wide web- Probabilistic and deterministic identification, Delta, MicroIS, AVIS, ICTV.

Unit-V: Global biodiversity information system

Overview of the UNEP/GEF biodiversity data management project (BDM) – CBD and bioethics– General agreement on trade and traffics.

Reference Books:

- Global Biodiversity: Status of the Earth's Living Resources. Water Conservation Monitoring Centre (1992), Chapman & Hall, London.
- Systematics and Conservation Evaluation- Forey, P.L., C.J. Humphries and R.I Vane-Wright (eds) (1994), Clarendon press, Oxford.

- Biodiversity: Measurement & Estimation -Hawkswoth, D.I. (Ed.) (1995), Chapman & Hall, London.
- Alice, 1990. A Biodiversity database system. Alice software partnership. Canhos, D.A.L. Canhos, V.P and Kirsop, B.E (eds) 1994. Linking Mechanisms for biodiversity information, Tropical foundation, Tropical Foundation, Campinas, Brazil.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the role of information technology in distributing biodiversity information.

CO 2- Involve the biodiversity assessments and inventorying programmes.

CO 3- Interpret the morphological and molecular characterization of biodiversity.

CO 4- Evaluate the Red data books and Biodiversity registers.

Course Prepared by: Dr.P.Shanmughavel

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

BASICS OF CHEMINFORMATICS

No. of Credits: 4

Code No: 19BIIA2EB

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basics of cheminformatics and their application.
- To aware the various chemical information sources.
- To analyze the pharmacokinetic properties of small molecules using ADMET calculation.
- To understand the steps in pro drug design.
- To utilize the bioinformatics tools and software in different aspects.

Syllabus

Unit-I: Basic Mathematics and Statistics

Graph theory and molecular numerology; Logic, sets and functions; Algorithms, integers and matrices; Mathematical reasoning, induction and recursion; Counting; graphs, trees and sets, basic probability and statistics; Markov processes.

Unit-II: Foundations of Chemistry and Biology

Basic Stereochemistry, Group Theory, Amino acids and Proteins and Properties; pKa, pH and ionization of acids and bases; Protein structure - Primary structure, Secondary structure - helix & sheet; Tertiary structure; Quaternary structure; covalent and non-covalent forces that maintain structures. Physical properties of proteins - charge, size, hydrophobic, protein binding – structural aspects; antibodies; transport; nucleotide binding; catalytic enzymes; basic concepts of combinatorial chemistry. Introduction to drug action, pro drug design and applications.

Unit-III: Chemical information sources

History of scientific information communication-chemical literature-chemical information-chemical information search-chemical information sources-chemical name and formula searching-analytical chemistry-chemical history-biography-directories and industry sources.

Unit-IV: Bioinformatics

Introduction; Experimental sources of biological data; Publicly available databases; Gene expression monitoring; Genomics and Proteomics; Metabolomics; Visualisation of sequence data; Visualization of structures using Rasmol or SPDB Viewer or CHIME; Genetic basis of disease; Personalised medicine and gene-based diagnostics; Legal, ethical and commercial ramifications of bioinformatics.

Unit-V: Pharmaceutical applications of molecular modeling

Introduction to drugs, structure-based drug design. QSAR and 3D-QSAR Methods. Pharmacophore Design, Ligand-Based Design and De Novo Drug Design Virtual screening/docking of ligands. Protein structure. Drug action enzymes. Drug action receptors. Drug design target interaction. Prediction of Binding Modes, Protein–ligand binding free energies, Fragment-Based Drug Design; Absorption, Distribution, Metabolism, Excretion & Toxicology (ADMET) prediction; Calculation of Physico-Chemical Properties, Biological and Physico-Chemical Predictive Model Building.

References:

- "Mathematical Methods for Physicists" Arfken, Academic Press 1985
- Schaum's Outline of Probability and Statistics, Murray R Spiegel, John J. Schiller, R. Alu Srinivasan
- Stereochemistry, by David G. Morris, Eddie Abel
- Introduction to Protein Structure: Second Edition, Carl Branden, John Tooze
- Combinatorial Chemistry and Molecular Diversity in Drug Discovery, Eric M. Gordon, James F. Kerwin
- Computer-Aided Drug Design: Methods and Applications, T.J. Perun C.L. Propst
- Chemical Information Sources (Mcgraw-Hill Series in Advanced Chemistry), Gary Wiggins
- Introduction to Bioinformatics, Teresa K. Attwood, David Parry-Smith
- Molecular Modeling: Basic Principles and Applications, 3rd Edition, Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the chemical formula and structure of compounds.

CO 2- Interpret the mathematical reasoning, induction and recursion using statistical approach.

CO 3- Evaluate the drug action and target interaction using bioinformatics tools

CO 4- Identify the experimental sources of biological data and analyse the personalized medicine and gene-based diagnostics.

Course Prepared by: Dr.P.Shanmughavel

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PRACTICAL II - COMPUTER PROGRAMMING

No. of Credits: 4

Code No: 19BIIA23P

No. of Teaching Hours: 6/week

Course Objectives:

- To make the students understand the basic aspects of programming.
- Practice the use of conditional and looping statements.
- Gain skills to handle strings and files.
- Explain and be able to use fundamental programming constructs such as sequencing, decisions and iteration.
- To program with advanced features of the C, C++ and PERL.

Programming in C

I. Character array manipulations

- 1) Read and Display a character array
- 2) Reverse print the array (String Reverse)
- 3) Length of the array
- 4) Copying the contents of one array to another (String Copy)
- 5) Copy the Uppercase character of one array as Lowercase character to another array
- 6) Checking whether a string is a palindrome or not
- 7) Copy the left 'n' characters of one array to another
- 8) Copy the last 'n' characters of one array to another
- 9) Copy the middle 'n' characters of one array to another
- 10) Concatenate two character arrays (String Concatenate)
- 11) Counting the numbers of Words, Lines and characters in an array
- 12) Counting the numbers of Uppercase and Lowercase Alphabets, Digits and special characters in an array
- 13) Check the number of occurrences of a pattern
- 14) Check the occurrences of a pattern and skip the same.
- 15) Check the occurrences of a pattern and replace it with a different pattern

II. Pointers and Character Array

- 16) Pattern Counting
- 17) Pattern Skipping
- 19) Pattern Replacing

III. Files and Command Line Arguments

- 19) Read data from the keyboard and write it in the file (char by char)
- 20) Read data from the file and display it on the screen (char by char)
- 21) Display the content of all the files (Cat all the files)

- 22) Copy data from one file to another
- 23) Pattern Count
- 24) Line in which the pattern occurs with line number
- 25) Grep all files (Pattern match all the files)

Programming in PERL

I PERL Basics

1. Program to print the elements of a array
2. Program to take an element off the end of an array
3. Program to take an element off the beginning of an array
4. Program to put an element at the beginning of an array
5. Program to put an element at the end of an array
6. Program to reverse an array
7. Program to get the length of an array
8. Program to insert an element at a random position in an array

II PERL Bioinformatics Programming

9. Program to store a DNA sequence
10. Program to concatenate DNA fragments
11. Program to convert DNA to RNA.
12. Program to calculate reverse compliment of DNA sequence
13. Program to read protein sequence data from a file
14. Program to find motifs in a protein sequence
15. Program to count nucleotides in a sequence
- 16 Program to find the percentage of hydrophobic amino acids in a sequence
- 17 Program to find the percentage of G and C in a DNA sequence
19. Program to append ATGC to a DNA sequence using subroutines
19. Program to concatenate two strings using subroutines
20. Program to count the number of given motifs
21. Program to convert DNA to RNA using subroutines
22. Program to find if a DNA is stable or not

Course Outcomes:

On successful completion of the course, the students will be able to

CO-1- Have a good understanding about the concepts of C & PERL.

CO-2- Be able to write and read basic codes in C & C++.

CO-3- Be able to explain and make use of data types, variables, constants, assignment statements, and arithmetic and Boolean expressions in writing programs.

CO-4- Explain and are able to use arrays and structures.

Course Prepared by: Prof.N.Jeyakumar

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

GENOMICS AND NGS

No. of Credits: 4

Subject Code No: 19BIIA33A

No. of Teaching hours: 4/week

Course Objectives:

- To understand the genome architecture and to extract information like gene function, gene regulation, protein evolution and targets for drug designing.
- To provide students with the skills from acquisition of genomic data to its analysis.
- To provide general and unique aspects of Next Generation Sequencing (NGS) through various tools.
- To understand how genomics applications are used to unravel the biology of life and the basic principles of omics-techniques.

Syllabus

Unit-I: Genome Organisation

Anatomy of the Eukaryotic and Prokaryotic Genome, Repetitive DNA Content of Genomes. How genes work, Gene-protein relations, Genetic fine structure, Mutational sites Complementation, **Genome Mapping** – Mapping Genomes, Genetic and Physical Maps, Sequencing Genomes, Methodology for DNA Sequencing, Assembly of a Contiguous DNA Sequence, understanding a Genome Sequence, Locating the Genes in a Genome Sequence, Determining the Functions of Individual Genes.

Unit-II: Genome Analysis

DNA Sequencing databases, Sequence analysis programs, Pairwise sequence alignment, Multiple sequence alignment, The first complete genome sequence and database, DNA sequencing, Genomic sequencing, Sequencing cDNA Libraries of expressed genes, Accuracy and computers storage of sequence, Sequence formats, Conversions of one sequence format to others.

Unit-III: Gene Prediction and Genome Rearrangement

Introduction, testing the reliability of an ORF Prediction, gene prediction methods and tools, The Biological Problem, Permutations .Analyzing Genomes with Reversals of Oriented Conserved Segments, Applications to Complex Genomes, **Comparative Genomics** – Completed genomes, Sequence assembly and gene identification, functional classification of genes.

Unit-IV: Introduction to Next Generation Sequencing.

What is Next Generation Sequencing? How it is different from traditional sequencing/Microarrays? Various NGS technologies/platforms. Experiment types and

applications. Workflows for various NGS experiments (variant discovery and expression profiling). Algorithms and tools for NGS readalignment, SNP calling. Various file formats - SAM, VCF, BED, WIG, and PILEUP. DNaseq genetic variations. NGS and personal genome sequencing. Whole genome sequencing. Target sequencing. Sequencing Mapp ability. Refined alignment. Base qualityRecalibration. Variants identification. Four different workflows for mutation discovery(CrossBow, Bowtie, BWA, MAQ).

Unit-V: NGS related Theories and Experiments.

RNAseq - Biological theories on RNAseq experiments. Major scientific advance usingRNAseq. Alignment - Gene expression analysis, Differential expression analysis. Alternativesplicing - TopHat and Cufflinks for RNAseq.

ChIPseq - Introduction and biological theories on ChIPseq analysis. DNA fragment evaluation. Peak identification. Two condition comparison. Saturation analysis. Motif findingand related theories.

Reference Books:

- Brown, T.A. 2002 Genome. John Wiley Press, US.
- Campbell, A.M. & Heyer, L.J. 2002 Discovering Genomics, Proteomics and Bioinformatics. Benjamin/Cummings.
- Primrose and Twyman 2003 Principles of Genome Analysis & Genomics. Blackwell.
- Pasternak 2000 An Introduction to Molecular Human Genetics. Fitzgerald.
- Dale and Schartz 2003 From Genes to Genomes. Humana.
- Stuart M. Brown. Next-Generation DNA Sequencing Informatics, Second Edition. New York University School of Medicine (ISBN-13: 978-1621921236).
- Xinkun Wang. Next Generation Sequencing Data Analysis, CRC Press. (ISBN13: 9781482217889).

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Explain genomic technologies and the ways in which genomic data are stored.

CO 2- Have hands-on experience on various bioinformatics tools available for analyzing genes and genomes.

CO 3- To handle biological data generated by the sequencing projects and its analysis.

Course Prepared by: Dr.V.Hemamalini (I,II&III)& Dr.C.Jayaprakash (IV&V)

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PROTEOMICS

No. of Credits: 4

Code No: 19BIIA33B

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the structure of entire cellular proteins.
- To know the phylogenetic relationship via tree construction.
- To analyze the methodology of MALDI-TOF analyzers.
- To predict the secondary structure using different algorithm.
- To understand the functional proteome analysis.

Syllabus

Unit-I: Protein classification

Structural elements and terminology: Helix, Sheet, Strand, Loop and coil, Active site, Architecture, Blocks, Class and Domains, Fold, Motif, PSSM. Principles of classification: Based on structural features, Phylogenetic relationship. Properties of protein in solution and in membranes. Interaction with other molecules like lipids, carbohydrates, metal Ions.

Unit-II: Protein structure prediction

Use of sequence pattern, leucine zipper, coiled coil, transmembrane, signal peptide, cleavage site. Secondary structure prediction: Chou – Fasman / GOR method, Neural network, nearest neighbor method, tertiary structure prediction, threading profile, contact potential, modeling.

Unit-III: Bioanalysis of protein and peptides

Complex protein and peptide mixtures, Extracting proteins from biological samples, Protein separation before digestion: 1D and 2 D Electrophoresis, Immobilized pH gradient, Sample preparation, First dimension criteria, second dimension criteria, Stabilization, Detecting protein on gel: Electro blot, Image analysis, Digital imaging, Spot detection and quantification, Gel matching. Data Analysis – Database for 2D gel.

Unit-IV: Tool of Proteomics

Mass Spectrometry for protein and peptide analysis: MALDI-TOF Analyzers, ESI Tandem MS instrument, Tandem Mass Analyzers, The Triple Quadrupole Mass Analyzer, The Ion Trap Mass Analyzer, Q-TOF & Fourier Transform–Ion Cyclotron Resonance, MS Instrument.

Unit-V: Functional Proteome Analysis

Integrated Proteome Analysis - Phage antibody as tool, Protein expression analysis, High throughput analysis for proteomics. Automation of proteomic analysis. Proteomics in plant breeding: Objectives, principles and methods, Genetic diversity analysis, Distribution of

varieties, lines and cultivars, Mutant characteristics, Variability between organ and developmental stage, Identification of abiotic stress, Genetic mapping of protein markers.

Reference Books:

- Lehninger, A. L. 1984. Principles of Biochemistry. CBS publishers and distributors, New Delhi, India
- Horton, Moran, Ochs, Rawn, Scrimgeour. Principles of Biochemistry. Prentice Hall Publishers.
- David. E. Sadava. Cell Biology: Organelle Structure and Function. Jones & Bartlett publishers.
- Shanmughavel, P. 2005. Principles of Bioinformatics, Pointer Publishers, Jaipur, India.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the different secondary structure of protein.

CO 2- Interpret the properties of protein in solution and in membranes.

CO 3- Evaluate the variability between organ and developmental stage.

CO 4- Identify the immobilized pH gradient and describe the digital imaging, Spot detection and quantification.

Course Prepared by: Dr.N.Sundara Baalaji

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

VISUAL BASIC WITH RDBMS AND MULTIMEDIA

No. of Credits: 4

Code No: 19BIIA33C

No. of Teaching Hours: 4/week

Course Objectives:

- To gain knowledge on relational data and its management.
- To set the data into formats suitable for feeding in traditional RDBMS.
- To design Logical Database Schema and Mapping it to implementation level schema through Database Language Features.
- To provide knowledge of incorporating SQL/ PL/SQL with programming languages.
- To understand the practical problems of Concurrency control and its solutions Gain knowledge about failure and Recovery mechanisms.
- To inculcate knowledge on RDBMS concepts and Programming with Visual Basic.
- This course gives an exposure to Multimedia and its application.

Syllabus

Unit-1:Introduction

Data Abstraction, Schemas and Instances - Data Models: Data modeling using Entity Relationship (ER) Model -entity and entity sets, relations and relationship sets, E-R diagrams - Reductions of ER Schema to Tables - Overview of the QBE Language - Hierarchical and Network Model Relational Model - Object Oriented Model - Introduction to distributed database processing.

Unit-II: Recovery and Security

Database Recovery Techniques - Database Security - Distributed databases and Client-Server Architecture - Concepts for Object Database - Enhanced Data Models for Advanced Application Emerging Database Technologies and Application

Unit-III: Database Languages

Data definition languages – Data Manipulation language, Data Control language, Data and String Functions, Union and intersect operator, Sub queries, Normal Form – 1NF, 2NF, 3NF & Boyce-Codd NF, Introduction to PL/SQL - Basics concepts of SQL and SQL commands - Nested Queries- Aggregate Functions- Null Values - PL/SQL interface - Data types in SQL, Simple PL/SQL programs.

Unit-IV: Visual Basic

Introduction to Visual Basic features, Data types, Strings, Variant, Constant, Data Arrays, looping and iterative statements. Introduction to application development using VB - Codes and forms, variables, procedures and controlling program executor, standard controls -Simple controls, Command buttons, text boxes, labels, list box, drive list box, directory list box, file list box, combo box, check box, timer control, functions in Visual Basic. Introduction to data connectivity, different database connectivity approaches, data access using data control, connecting to oracle database using visual basic, Menu creation, MDI forms, VB scripting, Introduction to ASP.

UNIT-V: Overview of Multimedia Software Tools

Text, Sound, Images, Animation and Video - Authoring, Editing and Authoring Tools - Graphics and Image Data Representations - File Formats - Digitization of Audio and Video objects - Color Models in Images – Color - Models in Video - Basics of Digital Audio – MIDI - Multimedia Data Compression - Multimedia Communication & Retrieval - Basic Principles of Animation and Drawing Tools.

Reference Books:

- Database System Concepts. Silberschatz, Tata Mac-Graw Hill Publications.
- Database system organization. J.M.Martin, Princeton-Hall.
- Introduction to Database Systems. C.J.Date
- Introduction to Database Systems. J.M.Martin, Princeton-Hall.
- Visual Basic 6 From the Ground Up. Gary Cornell Tata Mc-Graw Hill.
- TayVaughan ,”Multimedia”, 5th Edition, Tata McGraw Hill, 2001.
- Ze-Nian Li, Mark S. Drew ,”Fundamentals of Multimedia”, Prentice Hall of India, 2004.

- James D. Foley, Andries van Dam, Steven K Feiner, John F. Hughes, “Computer Graphics Principles and Practice, 2nd Edition in C, Audison Wesley, ISBN – 981-235-974-5
- William M. Newman, Roberet F. Sproull, “Principles of Interactive Computer Graphics”, Second Edition, Tata McGraw-Hill Edition.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1-To analyse Relational Data Base design methodology.

CO 2- Acquire knowledge in fundamentals of Relational Data Base Management System.

CO 3- Able to handle with different Data Base languages.

CO 4- Beable to effectively develop applications with full functionality and a graphical user interface using the language Visual Basic.

CO 5- Create Presentations and Perform Animation using Multimedia tool.

Course Prepared by : Dr.S.Usha

Course Verified by : Prof.N.Jeyakumar

Title of the Subject:

MOLECULAR MODELING

No. of Credits: 4

Code No: 19BIIA33D

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students better understanding about the structure of the protein molecule and Modeling
- To make the students understand the electron atom types and molecular properties
- To make the students with the strong view on force field and interactions
- To make the students with strong knowledge on energy minimization and its applications
- To make the students with detailed study on molecular dynamics simulation

Syllabus

Unit-I

Introduction to the concept of molecular modeling. Molecular structure and internal energy. Molecular graphics and its applications. Coordinate systems – Cartesian, Polar, spherical and internal coordinate systems.

Unit-II

Introduction to computational quantum mechanics: one electron atom, poly electronic atoms and molecules, Schrodinger equations, Hartree Fock equations, Roothaan hall equations, Born–

Oppenheimer (BO) approximation; calculating molecular properties using semi empirical and *ab initio* methods.

Unit-III

Molecular mechanics: general features of molecular mechanics - force field, bond stretching, angle bending, torsional terms, non-bonded interactions; CHARMM, YETI. Force field parametrisation and transferability.

Unit-IV

Potential energy surfaces, contour map. Local and Global energy minima; energy minimization: derivative and non-derivative methods; GROMACS. Applications of energy minimization.

Unit-V

Molecular dynamics simulation methods: molecular dynamics using simple models, molecular dynamics with continuous potential, setting up and running a molecular dynamic simulation; DESMOND. Monte Carlo simulation of molecules.

References:

- Molecular Modeling: Principles and Applications. Andrew R. Leach
- Basic principles and applications Hans-x
- Yvonne C. Martin. Designing bioactive molecules three-dimensional techniques and applications.
- Exploring QSAR. Leo, Albert, Hockma, D.H.Hansch, Corwin.
- Principles of Bioinformatics, Shanmughavel, P. 2005 , Pointer Publishers, Jaipur, India.
- Shanmughavel, P. 2006. Trends in Bioinformatics, Pointer Publishers, Jaipur, India.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Understand the molecular structure and its functional importance

CO 2- Clear view on computations quantum mechanics and methods for calculating molecular properties

CO 3- Understand the Physical properties of macromolecular structure and broader concept of energy minimization and its applications

CO 4- Protein structural stability, atoms movement in a molecule by Molecular Dynamics

Course Prepared by: Dr.M.Jeyam

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

SYSTEMS BIOLOGY

No. of Credits: 4

Code No: 19BIIA3EA

No. of Teaching Hours: 4/week

Course Objectives:

- To make the students understand the basic aspects and applications of Systems Biology.
- To know the micro array analysis, hierarchical clustering, and self-organizing maps.
- To analyze the virtual erythrocytes and the levels of simulation.
- To understand the steps in yeast two hybrid system and peptide mass fingerprinting.
- To utilize the information from various pathway database for further research.

Syllabus

Unit-I: Introduction to Systems Biology

What is Systems Biology? Integrating Networks. Methods of study: Micro array – definition, types of array, Micro array analysis: Hierarchical clustering, Self-organizing maps. Applications of Micro Array in systems biology.

Unit-II: Metabolomics

Digestion of proteins and protein metabolism, Urea Cycle, Transport metabolism, Carbohydrate metabolism – metabolism of glucose – glycolysis, TCA cycle, glycogenesis, Pentose phosphate shunt, Electron transport. Lipid metabolism: beta oxidation. Interconnection of pathways, metabolic regulations. Interconnection of pathways, metabolic regulation, Phylogeny, RNA secondary Structure, Gene Prediction.

Unit-III: Computational Cell Biology

Principle and levels of simulation – Virtual Erythrocytes, Pathological analysis. Flux Balance Analysis; Graphical Biological Network Editor and Simulator (Cell Designer).

Unit-IV: Location Proteomics

Protein subcellular location- Pattern Recognition. Predicting ligand-binding function, Use of gene cluster, detecting protein – protein interaction. Methods for Protein-Protein Interaction Analysis- Yeast Two Hybrid System (Y2H); Peptide Mass Fingerprinting (PMF).

Unit-V: Creative Bioinformatics

Novel use for database. Use of EST database – Unigene, gene discovery, Primer design, Restriction mapping, Position specific cloning, KEGG, SNP database, Target identification, Epitope identification. Spatial Signaling Dynamics – Methods and Quantification of receptor signaling.

Reference Books:

- Foundation of Systems Biology – Hi Roaki Kitano
- Introduction to Systems Biology – Sangdun Choi
- Shanmughavel, P. 2005. Principles of Bioinformatics, Pointer Publishers, Jaipur, India.
- Shanmughavel, P. 2006. Trends in Bioinformatics, Pointer Publishers, Jaipur, India.
- The underlying pathway structure of biochemical reaction networks. Christopher H. Schilling *et. al.* 1998. PNAS. 95:4193-8
- Towards metabolic phenomics: Analysis of Genomics Data Using Flux Balances. Christopher H. Schilling *et. al.* 1999. *Biotechnology. Prog.* 15: 288-295.
- The Minimal Gene Complement of *Mycoplasma genitalium*. Claire M. Fraser *et. al.* 1995. *Science*, 270: 397- 403.
- Molecular Classification of Cancer: Class Discovery and Class prediction by Gene Expression Monitoring. Golub TR. *et. al.* 1999. . *Science*, 286: 531 – 537.
- The *Escherichia coli* MG. 1655 *in silico* metabolic genotype: its definition, characteristics and capabilities. Jeremy S. Edwards *et. al.* 2000. PNAS. 97:5528-33.
- Whole cell simulation: a grand challenge of the 21st Century. Masaru Tomita, 2001. *Trends in Biotechnology.* 19: 205-210
- Cluster Analysis and Display of Genome – wide expression patterns. Michael B.Eisen *et. al.* 1998, *Proc. Natl. Acad. Sci. USA.* 95: 14863 – 14868.
- A general definition of metabolic pathways useful for systematic organization and analysis of complex metabolic networks. Stephen Schuster *et. al.* 1999. *Nature Biotechnology.* 19: 326-332.
- Of micro array and meandering data points. Steven R. Gullans, 2000. *Nature Genomics.* 26: 4-5.
- A gene expression database for the molecular pharmacology of cancer. Uwe Scherf *et. al.* 2000. *Nature genetics*, 24: 236-244
- The transcriptional program in the response of Human Fibroblast to Serum Viswanth R. Iyer 1999. *Science.* 283: 83-87.
- Mount, David, W., (2001); Bioinformatics: Sequence and Genome

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the microarray technique and analyze the result in various aspects.

CO 2- Interpret the various metabolic pathways.

CO 3- Reorganize the pattern using neural network method.

CO 4- Understand the concept of Quantification of receptor signaling.

CO 5- Know about primer design and epitope identification.

Course Prepared by: Dr.N.Sundara Baalaji

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

BIG DATA ANALYTICS

No. of Credits: 4

Code No: 19BIIA3EB

No. of Teaching Hours: 4/week

Course Objectives:

- Able to select and implement appropriate data structures to solve big data problems and also write Map and Reduce codes for distributed processing of data.
- Interested students will also have an opportunity to learn the basics of functional programming in Scala.
- Capable to perform batch processing operations on Big data on your own computer as well as on an Amazon EC2 instance.

Syllabus

Unit-I: Basics of Big Data

Introduction to Big Data and its Applications. Linear data structures and Non-linear data structures. Algorithm design.

Unit-II: Environment and Databases

Distributed Computing Environment for Big Data. NoSQL databases for Big Data Storage Applications (HBase). Distributed Processing of data using MapReduce & Pig. In-memory distributed processing using Apache Spark. Data Storage on Cloud (Amazon S3 & Dynamo DB).

Unit-III: Concepts and Platforms

Performing operations. Concepts for Big Data. Big Data Platforms. Workflow management. Batch Processing.

Unit-IV: Applications and Source

Applications of Streaming Data in Industry. Sourcing Streaming data using Apache Flume. Building real-time data pipeline using Apache Storm. Streaming on Apache Spark.

Unit-V: Advances in Big Data

Regression, Clustering & Classification using Spark MLlib. Building visualizations using Big Data. Case Studies on applications of Big Data Analytics.

Reference Books:

- Parag Kulkarni, Big Data Analytics (Kindle Edition).
- Viktor Mayer-Schonberger and Kenneth Cukier. Big Data: A Revolution That Will Transform How We Live, Work and Think. 2013.

Learning Outcomes:

On successful completion of the course, the students will be able to

CO 1- Competent to retrieve and store data in HDFS & Hbase using MapReduce & Apache Pig.

CO 2- Learn to choose and use tools to ingest structured and unstructured data into big data processing systems and use Hive to perform data transformations. You will also be able to process Big Data on Cloud using Amazon EMR and use OOOIE for managing your workflow.

CO 3- Gifted to build real time data processing systems using Apache Storm and Apache Spark.

CO 4- Talented to perform analytics on the big data using Spark MLlib and get knowledge of tools to visualize results.

Course Prepared by: Dr.C.Jayaprakash

Course Verified by: Prof.N.Jeyakumar

Title of the subject:

PRACTICAL – III: MOLECULAR TECHNIQUES

No. of Credits: 4

Subject Code No: 19BIIA33P

No. of Teaching hours: 6/week

Course Objectives:

- To provide hands on training in the basic techniques that is essential for genetic engineering and recombinant DNA technology.
- To develop their skills in the preparation, identification and quantification of microorganisms.
- To gain insights into the designing of cloning experiments.
- To have experience in the handling of macromolecules (DNA and RNA).

Syllabus

1. Sterilization techniques and Media preparation
2. Preparation and Maintenance of Microbial Culture
3. Plasmid and Chromosomal DNA Preparation from E. coli
4. Pure microbial culture techniques
5. pH measurements and preparation of buffers
6. Spectrophotometric Analysis of DNA
7. Agarose Gel Electrophoretic Analysis of DNA
8. Restriction digestion of bacterial genomic DNA and plasmid DNA
9. Ligation of DNA fragment with plasmid DNA
10. Animal Genomic DNA isolation

11. Plant Genomic DNA isolation
12. Amplification of DNA by PCR
13. Maintenance of Cell lines
14. Cell Viability assay

Reference Books:

- Laboratory Manual Sambrook and Russell, “Molecular Cloning – A Laboratory Manual”, CSHL Press, 2002
- Life Science Laboratory Manual, DST, 2017
- Bansal. MP, Molecular biology and biotechnology: basic experimental protocols, The Energy and Resources Institute (TERI), 2012

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Have technical expertise on versatile techniques in Recombinant DNA technology.

CO 2- Perform various types of practical laboratory work (chemical, biochemical and molecular methods) in a safe way

CO 3- Analyse, interpret and present the results with theoretical background

CO 4- Have hands-on experience on various basic biotechnological techniques for analyzing biomolecules.

Course Prepared by: Dr.V.Hemamalini

Course Verified by: Prof.N.Jeyakumar

Title of the Subject:

PRACTICAL – IV

BIOLOGICAL SEQUENCE ANALYSIS AND COMPUTER AIDED DRUG DESIGN

No. of Credits: 4

Code No: 19BIIA33Q

No. of Teaching Hours: 6/week

Course Objectives:

- To make the students understand the basic aspects and applications of Bioinformatics.
- To know the computational methods for Sequence Alignment.
- To analyze relatedness of the proteins of an organism with that of other organisms.
- To understand the steps in Evolutionary analysis.
- To utilize the information in the sequences for further research.

Syllabus

1. Biological Databanks Sequence Databases, Structure Databases, Specialized Databases
2. Data retrieval tools and methods
3. Database file formats
4. Molecular visualization
5. Gene structure and function prediction (using GenScan, GeneMark)
6. Sequence similarity searching (NCBI BLAST)
7. Protein sequence analysis (ExpASy proteomics tools)
8. Multiple sequence alignment (Clustal)
9. Molecular phylogeny (PHYLP)
10. Analysis of protein and nucleic acids sequences,
11. Sequence analysis using EMBOSS or GCG Wisconsin Package
12. Small molecule building, using ISIS DRAW and CHEM SKETCH
13. Homology Modeling using SPDBV
14. Model structure refinement using SPDBV
15. Model validation using What Check and Pro Check
16. Docking using DOCK or AUTODOCK or AMBER

Reference Books:

- K. Mani and N. Vijayaraj, Bioinformatics a Practical Approach, Aparna Publications, Coimbatore.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describes the database file formats and validates the modeled structure.

CO 2- Interprets the protein structure using molecular visualization tool.

CO 3- Evaluates the evolutionary relationship between different organisms via clustalW.

CO 4- Model 2D and 3D structure of a target from the sequence and Dock the protein and ligand using Auto dock.

Course Prepared by: Dr.P.Shanmughavel

Course Verified by: Prof.N.Jeyakumar

SUPPORTIVE PAPER I

Title of the subject:

DATABASE AND SEQUENCE ANALYSIS

No of Credits: 2

Code no: 19BIIAGS02

No of Teaching hours: 2 hours/week

SEM- I & III

Course Objectives:

- To make the students understand the basic aspects and applications of Bioinformatics.
- To know the computational methods for Sequence Alignment and the Algorithm and Scoring involved in that.
- To analyze relatedness of the proteins of an organism with that of other organisms.
- To understand the steps in Evolutionary analysis.
- To utilize the information in the sequences for further research.

Syllabus

Unit-I: Introduction to Bioinformatics and Biological Databases

Introduction to Bioinformatics, Biological Databases and Data formats, Nomenclature of nucleotides and amino acids, Application of Bioinformatics.

Unit-II: Sequence Alignment

Introduction to sequence alignment, PAM - BLOSUM, Local and Global alignment, Needleman-wunsch algorithm, Smith-waterman algorithm, Multiple sequence alignment, FASTA, BLAST.

Unit-III: Computational Evolutionary Analysis

Evolutionary analysis, Cladistic, and Phenetic methods, Clustering methods, Rooted and Unrooted tree representation.

Unit-IV: Gene Prediction and Analysis

Gene Prediction - GENSCAN, GRAIL, FGENES; Repeat sequence finder- RADAR, REPRO, TRUST; Protein Domain search - Pfam, MOTIF search, SMART.

Unit-V: Macromolecular structure prediction

Structure prediction methods: Chou-Fasman, GOR method, Neural Network, Threading and Fold recognition, Modeling.

References:

- David. W. Mount (2001): Bioinformatics Sequence and Genome Analysis, Cold spring Harbor Lab. NY.USA
- Comparative Genomics Ann Gibbons, 1998, Science.
- Genomes T.A Brown,2001, Taylor and Francis Group.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Describe the file formats, nomenclature of macromolecules and have an idea of Databases.

CO 2- Interpret the algorithms, scoring functions involved in the sequence alignment.

CO 3- Evaluate the phylogenetic relationship of an organism and identify genes, repeats, domains from sequences using bioinformatics tools.

CO 4- Model 2D and 3D structure of a target from the sequence.

Course Prepared by: Dr.M.Jeyam

Course Verified by: Prof.N.Jeyakumar

SUPPORTIVE PAPER-II

Title of the Subject:

PRINCIPLES OF DRUG DESIGN AND DISCOVERY

Code No: 19BIIAGS98

No. of Credits: 2

No. of Teaching Hours: 2/week
SEM- II

Course Objectives:

- To utilize the available sequences to model the target and use computational tools and software to design a drug.
- To acquire knowledge on the computational software to visualize and compare the protein structure and sequences.
- To analyze the conformational properties of protein using Ramachandran plot.

SYLLABUS

Unit-I: Introduction to drug discovery

History of drug design, Drug properties, likeness; Principles of Protein structure - Helix, Sheet, Strand, Loop and Coil, Torsion angles, Active site, Domains, Fold, Motif, PSSM; Structural databases- PDB, CATH, SCOP; Chemical Databases – ZINC, Pubchem, ChEMBL.

Unit-II: Macromolecular modeling

Ab initio modeling; Homology Modeling; Threading; Fold Recognition. Model refinement and validation – Ramachandran Plot, PROCHECK. Prediction of Binding site; ADME prediction; Rasmol viewer.

Unit-III: Quantitative Structure Activity Relationship (QSAR)

SAR, QSAR, Types of physicochemical parameters, experimental and theoretical approaches for the determination of physicochemical parameters. 3D-QSAR software COMFA.

Unit-IV: Molecular docking and Virtual screening

Structure-based drug design and Ligand based drug design; Virtual Screening, Pharmacophore design and identification. Molecular docking- AutoDock, Drug-receptor interaction.

Unit-V: Molecular mechanics and dynamics

General features of molecular mechanics; Energy Minimization - local and global energy minima, applications. Molecular dynamics simulation.

REFERENCE BOOKS:

- Molecular Modeling: Basic Principles and Applications, 3rd Edition, Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers
- Andrew R. Leach Molecular Modeling: Principles and Applications.

Course Outcomes:

On successful completion of the course, the students will be able to

CO 1- Identify and Select the ligands for docking.

CO 2 -Model and validate the target structures and identification of lead molecules through docking.

CO 3- Evaluate the ligand binding and interaction with the target using bioinformatics tools.