

7BHARATHIAR UNIVERSITY, COIMBATORE – 46
M.Sc. BIOINFORMATICS
FOR CANDIDATES ADMITTED DURING THE
ACADEMIC YEAR 2010-2011 AND ONWARDS
(CBCS – University Department)

I Introduction

Bioinformatics is an emerging scientific discipline representing the combined power of biology, mathematics and computers. Bioinformatics is needed to handle the enormous amount of data being generated by researchers identifying the lengthy DNA sequences of humans, plants, animals and microorganisms-life's blueprint and other biological data.

Stored digitally, in computers world wide, are trillions of pieces of information generated by emerging technologies in molecular biology. The amount of public DNA sequence data doubles every 12-14 months and will increase even more dramatically in the coming year. The resulting bottleneck-a wedge between having data and knowing what the data mean-must be overcome to facilitate breakthroughs in medicine, agriculture and environmental sciences.

Fortunately, biology and computer science are converging to unite raw data with powerful software tools and mathematical models. Bioinformatics represents a frontier in biological research and the best path toward finding meaning in a world of complex data.

II Goal

- Improve content and utility of chemical-biological databases
- Develop better tools and databases for comprehensive functional studies
- Develop and improve tools for representing and analyzing sequences similarity and variations
- Create mechanisms to support effective approaches for producing robust, exportable software that can be widely shared

III Bioinformatics and its scope

In last decade, bioinformatics has emerged as a new discipline. Bioinformatics uses advances in the area of computer science, information science, computer and information technology to solve complex problems in life sciences and particularly in biotechnology. Data capture, data ware housing and data mining have become major issues for biotechnologists and biological scientists due to sudden growth in quantitative data in biology such as complete genomes of biological species including human genome, protein sequences, protein 3D structures metabolic pathways databases, cell line and hybridoma information, biodiversity related information. Advancement in information technology, particularly internet, is being used to gather and access ever increasing information in biology and biotechnology. Functional genomics, proteomics, discovery of new drugs and vaccines, molecular diagnostic kits and pharmacogenomics are some of the areas in which bioinformatics has become an integral part of research and development. The knowledge of multimedia databases, tools to carry out data analysis and modeling of molecular and biological systems on computer workstations as well as in a network environment has become essential for any student of bioinformatics.

Bioinformatics, the multidisciplinary area has grown so much that one divides it into molecular bioinformatics, organal bioinformatics and species bioinformatics. Issues related to biodiversity and environment, cloning of higher animals such as Dolly and Polly, tissue culture and cloning of plants brought out that Bioinformatics is not only a support branch of science, but is also a subject that directs future course of research in biotechnology and life sciences. The importance and usefulness of bioinformatics is realized in last few years by many industries. Therefore, large bioinformatics R&D divisions are being established in many pharmaceutical companies, biotechnological companies and even in other conventional industries, dealing with biological. Bioinformatics is thus rated as number one career in the field of Biosciences. The need of trained manpower in this area is on increase but there are very few centers in the world where such training is given at present.

In short, bioinformatics deals with database creation, data analysis and modeling. Data capturing is done not only from printed material but also from network resources. Databases in biology are generally in the multimedia form organized in relational database model. Modeling is done not only on single biological molecule but also on multiple systems thus requiring a use of high performance computing systems.

IV Regulations

a. Eligibility for admission to M.Sc. Course in Bioinformatics

A pass in Bachelors Degree in any one of the following as one of the major subjects: Agriculture, Applied Science, Animal science, Biochemistry, Biology, Biotechnology, Bioinformatics, Botany/Plant Biology, Biochemistry and Plant Biotechnology, Chemistry, Computer Science, Computer Applications (BCA), Information Technology, electronics, Environmental Science, Food Science & Nutrition, Mathematics, Microbiology, Pharmacy, Physics, Statistics, Medical sciences (MBBS/BDS/BVSC) and Zoology .

b. Duration: 2 years with 4 semesters

c. System: Choice based credit system/under semester pattern

d. Other rules and regulations will be formulated by the Bharathiar University then and there

V Fee Structure

A self financing course. The fee structure will be decided by Bharathiar University in the course of time.

VI Question Paper Pattern for 75 Marks

Section A (10*2 =20) Answer all questions

Section B (5*5 =25) Answer any FIVE question out of seven

Section C (2*15 =30) Answer any TWO question out of FOUR

SCHEME OF EXAMINATIONS

Sem	CodeNo.	Subjects	University Examination			
			Internal	External	Total	Credit
I	10BIIA13A	Cell & Molecular Biology	25	75	100	4
	10BIIA13B	Computational Methods for Sequence Analysis	25	75	100	4
	10BIIA13C	Programming for Bioinformatics	25	75	100	4
	10BIIA13D	Pharmacogenomics	25	75	100	4
	10BIIA1EA	Basics of Mathematics & Statistics	25	75	100	4
	10BIIA1GS	Supportive I	12	38	50	2
II	10BIIA23A	Programming in Visual Basics & RDBMS	25	75	100	4
	10BIIA23B	Molecular Interactions	25	75	100	4
	10BIIA23C	Biophysics & Crystallography	25	75	100	4
	10BIIA23D	Biodiversity Informatics	25	75	100	4
	10BIIA2EB	Numerical Methods & Optimization Techniques	25	75	100	4
	10BIIA23P	Practical – I: Wet Lab Protein, Immunology & Pharmacology	40	60	100	4
	10BIIA23Q	Practical II- Computer Programming	40	60	100	4
	10BIIA2GS	Supportive - II	12	38	50	2
III	10BIIA33A	Genomics	25	75	100	4
	10BIIA33B	Proteomics	25	75	100	4
	10BIIA33C	Molecular Modeling & Computer Aided Drug Design	25	75	100	4
	10BIIA33D	Recombinant DNA Technology	25	75	100	4
	10BIIA3EC	Systems Biology	25	75	100	4
	10BIIA3GS	Supportive - III	12	38	50	2
IV	10BIIA43P	Practical III- Biological Sequence Analysis and Computer Aided Drug Design	40	60	100	4
	10BIIA43Q	Practical IV-Molecular techniques	40	60	100	4
	10BIIA47V	Project Work, Viva-Voce			200	8

Total Marks: 2250

Credit: 90

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SEM I

CELL AND MOLECULAR BIOLOGY

Objective: To understand the basics of organization, biology and functions of cell, the basic unit of life.

Unit I :

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

Unit II:

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 and regulation – Mitosis, Meiosis.

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-Monosacharides and their derivatives, Disacharides, Polysacharides.

Proteins –Structure of aminoacids, Different levels of organization-Primary, secondary tertiary and Quarternary 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.

Metabolism of glucose: glycolysis, TCA cycle, glycogenesis, glycogenolysis and gluconeogenesis, pentophosphate shunt, ETC. Digestion of protein and protein metabolism, nitrogen balance: transamination, oxidative deamination and urea cycle. Lipid metabolism: beta oxidation. Interconnection of pathways, metabolic regulations.

REFERENCES:

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

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SEM I

COMPUTATIONAL METHODS FOR SEQUENCE ANALYSIS

Objectives: To understand various computational techniques employed to analyze biological data with the use of sequence information.

UNIT-I

Introduction to bioinformatics, Classification of biological databases, Biological data formats, Introduction to single letter code of amino acids, symbols used in nucleotides, data retrieval- Entrez and SRS.

UNIT-II

Introduction to Sequence alignment. Substitution matrices, Scoring matrices – PAM and BLOSUM. Local and Global alignment concepts, Dot plot. Dynamic programming methodology: Needleman and Wunsch algorithm. Smith–Waterman algorithm. Statistics of alignment score. Multiple sequence alignment. Progressive alignment. Database search for similar sequences using FASTA and BLAST Programs.

UNIT-III

Evolutionary analysis: distances, Cladistic and Phenetic methods. Clustering Methods. Rooted and unrooted tree representation. Bootstrapping strategies, Use of Clustal and PHYLIP.

UNIT-IV

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

UNIT-V

Concepts of secondary structure prediction of RNA and Protein. Probabilistic models: Markov chain, Hidden Markov Models-other applications.

REFERENCES

1. S.C. Rastogi, Namita Mendiratta, Parag Rastogi. **Bioinformatics – Concepts, Skills, Applications”**.
2. Andréa’s D. Baxevanis, B.F. Francis Ouellette. **Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins**.

3. Richard Durbin et al. **Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids.**
4. Doolittle R.F **Computer Methods for Macromolecular Sequence Analysis..** (Ed.) (Methods in Enzymology, Vol. 266).
5. Shanmughavel, P. 2005. **Principles of Bioinformatics**, Pointer Publishers, Jaipur, India.
6. Bishop M.J. Rawlings C.J. (Eds.) **DNA and Protein Sequence Analysis. A Practical approach.**
7. Teresa. K. Atwood and David J. Parry-Smith **Introduction to Bioinformatics.**

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SEM I

PROGRAMMING FOR BIOINFORMATICS

Objective: To develop programming skills for Bioinformatics applications.

UNIT-I:

Programming in C

Introduction, Data types, Operators, Expressions, Control Flow, Structures, Input and Output, Functions, Pointers and References, String Processing, File Handling

UNIT-II

Programming in C++

Basic concepts of OOPS-Introduction to C++, C vs C++-data types, variables, constants, operators and statements in c++- Functions in c++- function prototype-definition-inline functions-overloaded functions.

UNIT- III

Programming in PERL

Introduction, Basic Operators and Control Structures, Scalars, Lists, Hashes, File Manipulation, Pattern Matching and Regular Expressions, Subroutines, Text and String Processing

UNIT-IV

BioPERL Programming

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-V

Python Programming

Overview, Data structures, Control Flow, Modules, Basic I/O, Exception Handling, Regular Expressions, File Manipulation, Classes, Standard library

REFERENCES:

1. B.W.Kernighan and D.M. Ritchie **The C Programming Language**, II Edition. Prentice Hall of India.

2. Larry Wall, Tom Christiansen & John Orwant **Programming Perl** –3 ed 2000- O’ Reilly
3. Mark Lutz, **Programming Python**, II Edition., O’ Reilly
4. E. Balagurusamy , **Programming in C++** - Tata Mc. Graw Hill Edition
5. Byron Gottfried.1998. **Programming with C** (Schaum's Outline Series) - Tata McGrawHill Publishing Company .
6. Robert Laffore , **Object oriented programming with c++** -Waite series.
7. Larry. Wall, **Programming Perl** - Tom Christiansen, Orielly Publications

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SEM I

PHARMACOGENOMICS

Subject Description:

It deals with Basic concepts of Drug metabolism and influence of genetic variation on drug response in individuals.

Goals:

Pharmacogenomic research could lead to the identification of new targets for treatments and it gives a better understanding of the mechanisms of action for treatments. It could also reduce cost and time in the development of new medications.

Objectives:

Students completing this paper should be able to understand the genetic and genomic principle which leads them to facilitate drug discovery and to improve drug therapy.

UNIT – I

Introduction to pharmacogenomics, pharmacodynamics, pharmacokinetics, toxicokinetics and ADME properties, process of drug development-clinical trials phase I, II and III.Physiological drug distribution of protein binding: physiological factors, drug distribution, clinical pharmacodynamics, clinical pharmacokinetics and toxicokinetics.

UNIT – II

Drug concentration, nature of cell membrane, physiological factors related to drug absorption – drugs across cell membrane, route of drug administration, oral absorption and gastro intestinal tract absorption. Metabolic changes of drugs and related organic compounds: General pathways, sites of drug biotransformation, oxidative biotransformation, reductive reactions, hydrolytic reactions, conjugation reactions, factors affecting drug metabolism.

UNIT – III

Factors affecting variability in drug response, drug metabolism, Ayugenomics (integration of Ayurveda & genomics), genetic analysis of human variation, Microsatellite for studying genetic variation, Ayugenomics for human population. Microarray in herbal drug research, Pharmacodynamics, Pharmacogenomics and Pharmacognosy.

UNIT – IV

Analyzing databases for Metabolic Pathways (WIT, KEGG, PathDB, BIOCARTA, PathCase, PharmGKB). Metabolic and Cellular simulation: Gepasi, XPP, Virtual cell. Reconstruction of metabolic pathways (Biocyc, ASGARD).

UNIT – V

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

References:

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

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SEM I

BASICS OF MATHEMATICS AND STATISTICS

Objectives: To understand the basics of mathematical and statistical techniques.

UNIT I: BASIC MATHEMATICS

Matrix Algebra – Types – Determinants – Transpose – Conjugate – Inverse – Eigen values of matrices – Rank – Solving Simultaneous equations in three variables using matrices, Cayley – Hamilton theorem without proof – Verification and Computation of Inverse of a Matrix – Consistency of linear equations.

Vector – Addition, subtraction – Dot product – Cross product (up to 3 vectors) – Scalar triple product – Gradient – Divergence and Curl.

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: BASIC STATISTICS

Ungrouped data and Frequency distribution: Collection – Classification – Tabulation – graphical and diagrammatic representation of numerical data – Graphs – Histogram, Frequency curve.

Statistical Averages: Mean, Median, Mode, SD, Variance and Coefficient of variation.

Correlation and regression analysis: Types of correlation, Methods of studying correlation – Rank correlation – Simple linear regression – Regression Equations.

UNIT IV: PROBABILITY

Random experiment – Definitions of probability – Theorems of Probability: Addition rule – Multiplication Rule – Properties of probability – Conditional probability - Bayes Theorem – Simple Problems.

Random variables – Discrete and Continuous – Probability mass functions – Probability density functions – Cumulative density function and its properties – Distributions Function.

Theoretical distributions – Binomial, Poisson and Normal distributions – Basic ideas and their applications.

UNIT V: 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.

REFERENCES:

1. T.K.Manickavachagam Pillai et al., **Calculus** - Volume I &II .
2. Raymond A.Barnett and Michael R.Ziegler , **Applied Mathematics** .
3. V.K.Kapoor and S.C.Gupta, **Fundamentals of Mathematical Statistics**.
4. S.P.Gupta, **Statistical Methods**.
5. P. R. Vittal, **Allied Mathematics**, Margham Publishers

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SEM II

PROGRAMMING IN VISUAL BASIC WITH RDBMS

Objectives: To understand the basic concepts of databases and to establish a client- server architecture using Visual Basic programming.

UNIT-I

Introduction: Data abstraction, Data models, Instances & schemes E-R Model: Entity and entity sets, Relations and relationship sets, E-R diagrams, Reducing E-R diagrams to tables. Network Data Model: Basic concepts, Hierarchical Data Model: Basic concepts. Introduction to distributed database processing.

UNIT-II

Data definition languages – Data Manipulation language, Data Control language, Data and String Functions, Union and intersect operator, Sub queries, Normal Form, Introduction to PL/SQL , Data types in SQL, Simple PL/SQL programs.

UNIT-III

Visual Basic: Introduction to Client / Server technology, Introduction to Visual Basic features, Data types, Strings, Variant, Constant, Data Arrays, looping and iterative statements.

UNIT-IV

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, simple connectivity program using data control.

UNIT-V

Menu creation, MDI forms, VB scripting, Introduction to ASP.

REFERENCES

1. Silberschatz, **Database System Concepts**, Tata Mac-Graw Hill Publications.
2. J.M.Martin, **Database system organization**, Princeton-Hall.
3. C.J.Date, **Introduction to Database Systems**.
4. J.M.Martin, **Introduction to Database Systems**, Princeton-Hall.
5. Wilteach et.al, **Parallel and Distributed Databases**.
6. **Using Visual Basic**. Que Series. 2001.
7. Gary Cornell, **Visual Basic 6 From the Ground Up**, Tata Mc-Graw Hill.

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SEM II

MOLECULAR INTERACTIONS

Objective: to understand the basic concepts of interaction, how biological molecules interact with each other and the experimental techniques to study these molecules.

UNIT-I

Fundamentals of atomic and molecular orbitals:

Theory of atomic and molecular orbitals; Linear combination of atomic orbitals; Quantitative treatment of valency bond theory and molecular orbital theory; Resonance structures; σ -bonds and π -bonds.

UNIT-II

Fundamentals of chemical bonding and non-bonding interactions:

Electrovalent bond, stability of electrovalent bond. Co-valent bond – partial ionic character of co-valent bonds. Shape of orbitals and hybridization. Co-ordination bond, Vander Waals forces; Metallic bond. Molecular geometry- VSEPR Theory.

UNIT-III

Folding pathways: Principles of protein folding, role of chaperons, hydrophobic interactions, electrostatic interactions, non-bonded interactions. Beta turns, gamma turns, types of helices, disulphide bridge.

UNIT –IV

Molecular interactions: protein-protein, protein-DNA, DNA-Drug, Protein-Lipid, Protein-Ligand, Protein-Carbohydrate interaction, Metalloprotein. π ... π interactions, C-H... π interactions.

UNIT-V

Spectroscopy: Principles, Theory, Instrumentation and Application of UV, IR, NMR and Circular dichroism (CD) to macro molecules. Stereochemistry of proteins and nucleic acids.

REFERENCES:

1. Albert cotton, F. 1971. **Chemical Application of Group Theory**. John Wiley and Sons, Inc. New York. 386 pp.
2. Spice, J. E. 1964. **Chemical Bonding and Structure**. Pergamon Press Ltd., Headington Hill Hall, Oxford. 395 pp.
3. Winter, m. j. 1996. **Chemical Bonding**. Oxford University Press, Inc., New York. 91 pp.
4. Ernest Eliel, 1996. **Stereochemistry of carbon compounds**, Prentice Hall
5. Shanmughavel, P. 2005. **Principles of Bioinformatics**, Pointer Publishers, Jaipur, India.

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SEM II

BIOPHYSICS AND CRYSTALLOGRAPHY

Objective: To get an insight into the biophysical techniques to analyze protein molecules

UNIT – I.

Introduction to protein structure: Physical and chemical properties of aminoacids and polypeptides. Theoretical and experimental methods for determination of size of proteins. Physical nature of non covalent interactions. Conformational properties of proteins, Ramachandarn Plot, Secondary, Super Secondary, tertiary and quaternary structure of proteins.

UNIT – II.

Protein structure modeling: Homology modeling, Threading, Fold recognition, Vector based method, neural network. Model refinement and validation. **Functional classification of proteins:** Cell surface receptors, GPCR's, Kinases, Channel proteins, Ubiquitin

UNIT - III.

Biophysical Techniques: Principles, Process and Applications of Thin layer chromatography, Column chromatography (ion exchange and affinity only) , HPLC, Uni Directional and 2 D Electrophoresis, UV Visible spectroscopy, NMR and MALDI - TOF

UNIT – IV.

X-ray crystallography of small molecules; x-ray generation ; its application; unit cell and x-ray anomalous scattering; lattices, Bragg's Law; atomic scattering factor and structure factor; phase problem; intensity data collection and reduction; direct method of solving a small molecule; refinement of crystal structure, hydrogen bonding

UNIT – V.

X-ray crystallography of macromolecules. Isolation and purification of protein (chromatography, electrophoresis), crystallization (sitting and hanging drop method). Protein structure determination-molecular replacement technique; multiple isomorphous replacement method, synchrotron radiation and its uses; multi wavelength anomalous diffraction method. Calculation of electron density map, interpretation of electron density map. Refinement of the structure. Structure validation methods.

REFERENCES:

1. Thomas. E. Creighton **Proteins Structures and Molecular Properties** Freeman and Company
2. Cantor and Schimmel **Biophysical Chemistry Part II Techniques for the study of biological structure and function** Freeman and Company
3. Thomas M Devlin **Textbook of Biochemistry** Wiley LISS Fifth edition
3. Stephen Neidle **Nucleic Acid Structure and Recognition**
4. Leonard Banaszak **Foundations of Structural Biology**
5. Philip E. Bourne **Structural Bioinformatics** John Wiley & sons
6. Shanmughavel, P. 2005. **Principles of Bioinformatics**, Pointer Publishers, Jaipur, India.

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SEM II

BIODIVERSITY INFORMATICS

Objective

To aware of digitized biodiversity data resource available nationally and internationally and to utilize the same effectively to conserve biodiversity.

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

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

UNIT-IV

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.

References

1. Global Biodiversity: Status of the Earth's Living Resources. Water Conservation Monitoring Centre (1992), Chapman & Hall, London.
2. Systematics and Conservation Evaluation- Forey, P.L., C.J. Humphries and R.I Vane-Wright (eds) (1994), Clarendon press, Oxford.
3. Biodiversity: Measurement & Estimation –Hawksworth, D.I. (Ed.) (1995), Chapman & Hall, London.
4. Alice, 1990. A Biodiversity database system. Alice software partnership. Cnhos, D.A.L. Canhos, V.P and Kirsop, B.E (eds) 1994. Linking Mechanisms for biodiversity information, Tropical foundation, Tropical Foundation, Campinas, Brazil.

5. Uhlir, P.F, 1980. The public international law of Civilian remote sensing: an overview. In: Mink, P.D. (ed), American Enterprise, the law, and the commercial use of space, Vol II. National Legal Center for the public interest, Washington, Dc.
6. Heywood, V.H., Watson, R.T.1995. Global Biodiversity Assessment. Published for the United Nations Environment programme, Cambridge University press, Cambridge.
7. P.Shanmughavel (2010) Bioinformatics Applications in Forestry, VDM Verlag, Germany.

Web Resource

www.Biodiv.org
www.wri.org/wri/biodiv/
www.wcmc.org.uk

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SEM II

NUMERICAL METHODS & OPTIMIZATION TECHNIQUES

Objective: To understand the basic concepts of numerical methods and optimization techniques

UNIT-I: ERRORS IN MODELLING

Errors involved in the construction of a mathematical model of the real physical process - Errors in Numerical Calculations – Errors in the numerical approximation of the mathematical model (truncation errors) – Errors in a series approximation – Errors in the actual computation using a computer (round off errors).

UNIT-II: MINIMIZATION OR MAXIMIZATION OF FUNCTION

Problems with Minimum number of iterations

One Dimensional Optimization: Golden section Method, parabolic interpolation and Brent's method in one dimension, one-dimensional search with first derivatives. Second-order Derivative: Newton-Raphson method,

Multidimensional Optimization: Univariate Method – Pattern Directions – Powell's Method – Conjugate directions – Algorithm – Quadratic Convergence - Downhill simplex method in multi dimensions, Indirect Search Methods – Gradient - Steepest decent(Cauchy) method – Conjugate gradient(Fletcher-Reeves) method - Procedure.

UNIT-III: RANDOMIZED MINIMIZATION TECHNIQUES

Monte-Carlo minimization.

Genetic algorithms – Representation of Design Variables – Representation of Objective function and Constraints – Genetic Operators.

Simulated annealing – Procedure – Features.

UNIT-IV: FOURIER TRANSFORM

Fourier Transform of Discretely Sampled Data – Discrete convolution – Periodic sequence and Circular convolution –Linear Convolution through circular convolution –Fast Fourier

Transform(FFT) – Discrete in Time(DIT) – Discrete in Frequency(DIF) – Algorithm – Computation of inverse DFT - Simple problems.

UNIT-V: NUMERICAL SOLUTIONS OF ODEs

Solution by Taylor's series Method - Euler's Method – Modified Euler Method – Midpoint Method, Runge-Kutta Method, Predictor–Corrector Methods - Adam's-Moulton Method - Milne's Method – Simultaneous and Higher Order Equations, Methods to solve stiff equations (Implicit Euler Method and Explicit Euler Method).

REFERENCES:

1. **Sastry,S.S. (1993).** Introductory methods of numerical analysis. **Prentice hall of India pvt Ltd., New Delhi.**
2. **Chapra,S.C. / Raman and Canale, P.** Numerical methods for Engineers with personal computer applications.
3. **Venkatraman, M.K. (1999), International student Edition,** Numerical methods in science and engineering. **National publishing company, Chennai.**
4. T. Veerarajan, **Engineering Mathematics,** Tata Mc. Graw-hill Publishing Company.
5. Singiresu S. Rao, **Optimization Techniques** New Age International (P)Limited.

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SEM I & II

PRACTICAL – I. WET LAB – PROTEIN, IMMUNOLOGY AND PHARMACOLOGY

Protein Lab

1. Isolation of Microbes (*fungi, bacteria and Actinomycetes*) from soil – serial dilution techniques
2. Screening of microbes for enzymes (amylase) production - plate and enzyme assay method
3. Isolation/Extraction of intracellular and extra cellular enzymes
4. Construction of purification table for any one enzyme
5. Molecular weight determination (SDS – PAGE)

Immunology Lab

6. Methods for bleeding
7. Counting of blood cells- Haemocytometre count
8. Preparation of serum from blood
9. Blood grouping – Haemoagglutination
10. ELISA

Pharmacology Lab

11. Screening of microbes for antibiotic production
12. Antibiotic bioassay-inhibitory activity
13. Extraction of medicinal plants using Cold percolation and Soxhlet methods
14. Preliminary Phytochemical analysis of plant extracts
15. Tissue culture technique for secondary metabolite production

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SEM I & II

PRACTICAL - II. COMPUTER PROGRAMMING

MS-Office and HTML.

1. Working with MS-Office Packages –One Exercise each in Word, Excel, Power Point and Access.
2. Working with HTML Tags and HTML Forms. Creating HTML Pages (At least five different pages to be created using all tags learnt).

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
- 18) 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 Programming

1. Program to store a DNA sequence
2. Program to concatenate DNA fragments
3. Program to convert DNA to RNA

4. Program to calculate reverse compliment of DNA sequence
5. Program to read protein sequence data from a file
6. Program to print the elements of a array
7. Program to take an element off the end of an array
8. Program to take an element off the beginning of an array
9. Program to put an element at the beginning of an array
10. Program to put an element at the end of an array
11. Program to reverse an array
12. Program to get the length of an array
13. Program to insert an element at a random position in an array
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
18. 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

Mini project using Visual Basic and RDBMS

VISUAL BASIC AND RDBMS

1. Create Tables, queries, and Simple PL/SQL Programs.
2. Construct user interface with manipulation and validation
3. Provide Database Connectivity and hence produce Reports.

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SEM III

GENOMICS

Objectives: To understand the genome architecture and to extract information like gene function, gene regulation, protein evolution and targets for drug designing.

UNIT – I

Introduction to Genomics: Definition of Genome, Genome sequencing, Genome map: Types of Genome maps and their uses, High and low-resolution map, Map elements, Polymorphic markers, Types of maps: Cytogenetic, Linkage map, Transcript map, Physical map, Comparative map, Integrated map, STS content maps, Map repositories: NCBI – Entrez Human genome map viewer, OMIM – Online Mendelian Inheritance in Man, Linkage map resources: CEPH reference pedigree, CHLC – Cooperative human linkage center, Radiation hybrid map resources. Practical uses of genome maps: Locating genomic regions, Target identification, Arrangement of genes, SNP diagnosis, Positional specific cloning,

UNIT – II

Genome Anatomy: The anatomy of the Eukaryotic Genome –The special features of metaphase chromosomes, where are the genes in the genome? Families of genes, pseudogenes – Eukaryotic organelle genomes, Repetitive DNA content of the human genome.

Transcriptomes and Proteomes

Genome Expression in outline; The RNA content of the Cell– the Transcriptome – yeast and human; The Protein content of the cell - the link between the Transcriptome and the Proteome.

UNIT – III

Annotation of the Genome: Structural annotation (Locating coding regions and other structural elements of the gene). Various approaches in gene prediction: ORF prediction, Gene prediction in prokaryotes and eukaryotes, Hidden Markov Model, Pattern discrimination, Evaluation of gene prediction methods, Prediction of promoter sequences, Functional annotation: (Prediction of gene function), Employing the similarity in the sequence, gene family and metabolic pathway. Employing the conserved domain, Profile and motif comparison, EST Comparison. Analysis of Human Genome.

UNIT – IV

Comparative Genomics:

Purpose and Methods of comparison, Tools for genomic comparison: Applications of Comparative Genomics, Reconstruction of metabolic pathway, Predicting regulatory elements, Identifying targets, examination of domain function, analysis of conserved strings.

Genome projects and Model Organism research -Yeast; Drosophila; C. elegans; and Mouse – a comparative analysis. Comparative genomics as an aid to gene mapping and in the study of human diseases.

UNIT – V

Functional Genomics:

Gene expression analysis by cDNA micro arrays, SAGE, Strategies for generating ESTs and full length inserts; EST clustering and assembly; EST databases (DBEST, UNIGENE); Expression and regulation of entire set of genes, Sporulation Vs Vegetative condition in yeast and *Bacillus*.

REFERENCES

1. **Active Conversation of Non-coding Sequences revealed by three way species comparisons.** Inna Dubchak et al. 2000. Genome Research. 10, 1305–1306.
2. Andreas D. Baxevanis and B.F. Francis Ouellette. A, **Bioinformatics A Practical Guide to the Analysis of Genes and Proteins.** Ed. John Wiley & Sons, Inc., Publications (For mapping and comparative Genomics and COG and other database repositories).
3. David W. Mount, 2001. **Bioinformatics Sequence and Genome Analysis,** Cold Spring Harbor Laboratory Press.
4. Shanmughavel, P. 2005. **Principles of Bioinformatics,** Pointer Publishers, Jaipur, India.
5. Shanmughavel, P. 2006. **Trends in Bioinformatics,** Pointer Publishers, Jaipur, India.
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7. **Encyclopedia or *Escherchia coli* genes and Metabolism.** Peter D. Karp et al. 1996. Eco-Cyc: Nucleic Acids Research. 10: 86-90.
8. **Structural Genomics and its importance for Gene Function Analysis.** Jeffrey et al. 2000. Nature Biotechnology. 18:283 – 287.
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10. **The Comprehensive Microbial Resource.** Jeremy D. Peterson et.al. 2001. Nucleic Acids Research. 29: 123 – 125.
11. **The Molecular Biology Database Collection: Updated Compilations of Biological Database Resources.** Baxevanis A.D. 2001. Nucleic Acids Research. 29 p 1-10.
12. **Genomes.** T.A. Brown, 2001. Taylor and Francis Group.

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SEM III

PROTEOMICS

Objectives : Taxonomy, structure - function relationship and functional aspects of the entire set of cell proteins.

UNIT – I

Protein classification: Structural elements and terminology, Helix, Sheet, Strand, Loop and coil, Active site, Architecture, Blocks, Class and Domains, Fold, Motif, PSSM, Profile. Principles of classification: Based on structural features, Phylogenetic relationship, CATH – Classification by Class, Architecture, Topology, Homology, SCOP - Structural Classification of Protein, FSSP – Fold classification based on structure – structure alignment, MMDB – Molecular Modeling Database, SARF – Spatial arrangement of backbone fragments

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

Analytical protein and peptide separations - 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

Tools 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.

REFERENCES

1. Daniel C. Leibler, (2002), **Introduction to Proteomics: Tools for New Biology**, Humana Press, Totowa, NJ.
2. Branden, Carl and Tooze John. 1999. **Introduction to Protein Structure** (2nd. Ed.), Garland Publishing, NY, USA.
3. Mount, David, W., (2001); **Bioinformatics: Sequence and Genome Analysis**, Cold Spring Harbor Lab. NY, USA
4. Pennington, S, (Editor), M. J. Dunn (Editor); (2001); **Proteomics: From Proteins Sequence to Function**, Springer Publications
5. Palzkill, Timothy; (2002); **Proteomics**, Kluwer Academic Publishers
6. Suhai, Sandor, (ed), (2000); **Genomics and Proteomics : Functional and Computational Aspects**, Plenum Pub. Corp.
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10BIIA33C

SEM III

**MOLECULAR MODELING & COMPUTER
AIDED DRUG DESIGN**

Objectives: To understand the concepts of molecular modeling and computational approaches for drug design.

Unit I

Introduction to the concept of molecular modeling, molecular structure and internal energy, applications of molecular graphics, coordinate systems, potential energy surfaces, discussion of local and global energy minima

Unit II

Introduction to computational quantum mechanics: one electron atom, poly electronic atoms and molecules, Hartree Fock equations; calculating molecular properties using ab initio and semi empirical methods

Unit III

Molecular mechanics: general features of molecular mechanics force field, bond stretching, angle bending, torsional terms, non-bonded interactions; force field parametrisation and transferability; energy minimization: derivative and non-derivative methods, applications of energy minimization.

Unit IV

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

Unit V

Macromolecular modeling, design of ligands for known macro molecular target sites, Drug-receptor interaction, classical SAR/QSAR studies and their implications to the 3-D modeler, 2-D and 3-D database searching, pharmacophore identification and novel drug design, molecular docking,

Structure-based drug design for all classes of targets.

REFERENCES

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

10BIIA33D

SEM III

Recombinant DNA Technology

Subject Description: This paper provides the student the knowledge in genetic engineering, vectors in gene cloning, transformation in higher organisms and the applications of rDNA technology

Objective: The objective of the paper is to introduce the Bioinformatians to application of rDNA technology.

Goal: This paper will help the student to understand the techniques in recombinant DNA technology.

UNIT –I

Introduction to cloning and rDNA technology, Cloning vectors: Plasmids (pUC 18 and Ti plasmids), Bacteriophages (λ phage), Plasmids, Cosmids (pJB8), SV40, retrovirus and Artificial Chromosomes (BAC, YAC).

UNIT-II

Strategies in gene cloning: restriction, ligase, insertion into vector, cloning, transformation into host cell, Enzymology of Recombinant DNA. Screening for recombinant (Insertional inactivation, Colony/in situ hybridization, radioactive antibody test, Xgal, complementation and physical methods)

UNIT-III

Methods of gene transfer and genome sequencing:CaPO₄ mediated gene transfer, liposomes, electroporation, electro fusion, micro-injection, particle bombardment. DNA sequencing (Sanger and Coulson method; Maxam and Gilbert method and Automated method) - Chromosomal walking, transposons, construction of genomic and cDNA libraries; molecular markers- RAPD, RFLP.

UNIT- IV

Transgenic plants – high yielding, salt, draught, herbicide, disease resistant. Transgenic animals - for improved livestock production.

UNIT-V

rDNA in medicine: Vaccines, enzymes, blood factors, interferon, gene therapy, DNA fingerprinting and its applications in forensic sciences.

REFERENCES:

1. Principles of genetic manipulation; Ed. Old and Primrose, 6th Edition. Blackwell Science publication
2. Gene Cloning, a introduction – T. A. Brown, Chapman and Hall publications, 3rd Edition, 1995

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SEM III

SYSTEMS BIOLOGY

Objectives

To understand the gradual maturation of Genomics and Proteomics into Biology *insilico*.
Convergence of Genomics, Proteomics, Transcriptomics and Metabolomics into Phenomics.

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 Arrays in systems biology.

UNIT – II

Metabolomics & Metabolic Pathways

Digestion of proteins and protein metabolism, Transport metabolism, Carbohydrate metabolism – metabolism of glucose – glycolysis, TCA cycle, glycogenesis, Pentose phosphate shunt, Electron transport, Interconnection of pathways, metabolic regulation. Translating biochemical networks into linear algebra.

UNIT – III

Whole cell simulation: Principle and levels of simulation - Virtual Erythrocytes, Pathological analysis. Flux Balance Analysis

UNIT IV

Relationship analysis: Predicting ligand-binding function, Use of gene cluster, detecting protein – protein interaction.

UNIT – V

Creative Bioinformatics: Novel use for database. Use of EST database – Unigene, gene discovery, Primer design, Restriction mapping, Position specific cloning, SNP database, Target identification, Epitope identification.

REFERENCES

1. Andreas D. Baxevanis and B. F. Francis Ouellette, **Bioinformatics A Practical Guide to the Analysis of Genes and Proteins**. Ed. John Wiley & Sons, Inc., Publications (For Micro array).
2. Challa S. S. R. Kumar, Joseph Hornes, Carola Leuschner, **Nanofabrication towards Biomedical applications**. Ed. Wiley-VCH Verlag GmbH & Co.
3. Shanmughavel, P. 2005. **Principles of Bioinformatics**, Pointer Publishers, Jaipur, India.
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5. **The underlying pathway structure of biochemical reaction networks**. Christopher H. Schilling *et. al.* 1998. PNAS. **95**:4193-8
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7. **The Minimal Gene Complement of *Mycoplasma genitalium***. Claire M. Fraser *et. al.* 1995. *Science*, **270**: 397- 403.

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9. **The *Escherichia coli* MG. 1655 *in silico* metabolic genotype: its definition, characteristics and capabilities.** Jeremy S. Edwards *et. al.* 2000. PNAS. **97**:5528-33.
10. **Whole cell simulation: a grand challenge of the 21st Century.** Masaru Tomita, 2001. *Trends in Biotechnology*. **19**: 205-210
11. **Cluster Analysis and Display of Genome – wide expression patterns.** Michael B.Eisen *et. al.* 1998, *Proc. Natl. Acad. Sci. USA*. **95**: 14863 – 14868.
12. **A general definition of metabolic pathways useful for systematic organization and analysis of complex metabolic networks.** Stephen Schuster *et. al.* 1999. *Nature Biotechnology*. **18**: 326-332.
13. **Of micro array and meandering data points.** Steven R. Gullans, 2000. . *Nature Genomics*. **26**: 4-5.
14. **A gene expression database for the molecular pharmacology of cancer.** Uwe Scherf *et. al.* 2000. *Nature genetics*, **24**: 236-244
15. **The transcriptional program in the response of Human Fibroblast to Serum** Viswanth R. Iyer 1999. *Science*. **283**: 83-87.

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SEM III

**PRACTICAL – III - BIOLOGICAL
SEQUENCE ANALYSIS & COMPUTER AIDED DRUG DESIGN**

- Biological Databanks Sequence Databases, Structure Databases, Specialized Databases
- Data retrieval tools and methods
- Database file formats
- Molecular visualization
- Gene structure and function prediction (using GenScan, GeneMark)
- Sequence similarity searching (NCBI BLAST)
- Protein sequence analysis (ExpASy proteomics tools)
- Multiple sequence alignment (Clustal)
- Molecular phylogeny (PHYLP)
- Analysis of protein and nucleic acids sequences,
- Sequence analysis using EMBOSS or GCG Wisconsin Package
- Small molecule building, using ISIS DRAW and CHEM SKETCH
- Homology Modeling using SPDBV
- Model structure refinement using SPDBV
- Model validation using What Check and Pro Check
- Docking using DOCK or AUTODOCK or AMBER

REFERENCE:

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

PRACTICAL – IV - MOLECULAR TECHNIQUES
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SEM III

Isolation and Molecular techniques

1. Pure culture techniques
2. Preparing competent culture
3. Microbial genomic DNA isolation
4. Microbial plasmid isolation
5. Plant genomic DNA isolation
6. Animal genomic DNA isolation

rDNA Technology

7. Restriction mapping with Lambda DNA
8. Ligation
9. PCR(Polymerase Chain Reaction)
10. Blotting techniques
11. PAPD
12. RFLP

SUPPORTIVE PAPER I (I SEMESTER)

10BIIA1GS

SEM I

BASICS OF OMICS CONCEPTS

Unit I

Definition of Genome, NCBI, OMIM, Practical uses of genome maps, Locating genomic regions, Target identification , Arrangement of genes, SNP Diagnosis.

Unit II

Annotation of Genome- structural annotation by Genscan and Genmark and functional annotation by pattern searching, TMPred.

Unit III

Comparative Genomics- Profile Comparison, Motive Comparison, EST Comparison, human genome Project.

Unit IV

Protein Classification – Helix, Sheet, Strand, Loop and Coil, Active site, Class and Domains, Fold, Motif, PSSM, Profile.

Unit V

CATH- Classification by Class, Architecture, Topology, Homology, SCOP- Structure Classification of Proteins.FSSP- Fold Classification based on Structure- Structure alignment, MMDB – Molecular Modeling Database,SARF-Special arrangement.

References:

1. Mount David W. (2001); Bioinformatics: Sequence and Genome Analysis, Cold spring Harbor Lab. NY.USA.
2. Introduction to Protein Structure (2nd Ed) Brander, Carl and Tooze John. 1999.
3. Bioinformatics : A Practical Guide to analysis of Gene and Proteins. Ed. Andreas D.Barevanii and B.F. Francis Ouellette.

SUPPORTIVE PAPER II (II SEMESTER)

10BIIA2GS

SEM II

FUNDAMENTALS OF INSILICO MODELING FOR DRUG DESIGNING

Unit I

Concept of Molecular Modeling, Molecular Structure and Internal energy, Molecular graphics and its applications, Local and Global energy minima.

Unit II

Introduction to Computational Quantum mechanics, One Electron atom, Polyelectronic atoms and molecules, Hartree- Fock equations.

Unit III

Molecular Mechanics, Bond Stretching, Angle bending, Torsional terms, Non-Bonded Interactions , Energy minimization and its application.

Unit IV

Macromolecular Modeling, Design of ligands for known macromolecular target sites, Drug-Receptor interaction.

Unit V

SAR/QSAR Studies and their implications to the 3 D molecular, 2D and 3D database Searching, Molecular Docking.

References:

1. Molecular Modeling principles and Applications Andrew R Leach.
2. Designing bioactive Molecules Three – Dimensional Techniques and Applications, Yvonne C.Martin.

SUPPORTIVE PAPER III (III SEMESTER)

10BIIA3GS

SEM III

DATABASES AND SEQUENCE ANALYSIS

Unit I

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

Unit II

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

Unit III

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

Unit IV

Gene finding methods, Gene prediction methods, Repeat sequence finder.

Unit V

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

References:

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