THIRUVALLUVAR UNIVERSITY

MASTER OF SCIENCE

M.Sc. BIO INFORMATICS

DEGREE COURSE
UNDER CBCS
(with effect from 2012-2013)

The Course of Study and the Scheme of Examinations

S.NO	Part	Study Components	Course Title	Ins. hrs /week	Credit	Title of the Paper	Maximum Marks		
SEMESTER I							**CIA**	**Uni. Exam**	**Total**
1		Main	Paper -1	4	4	Introduction to Bioinformatics	25	75	100
2		Main	Paper -2	4	4	Biochemistry and Bio-Physics	25	75	100
3		Main	Paper -3	4	4	Computer Programming using C	25	75	100
4		Main Practical	Practical-1	5	0	Statistical Bioinformatics	0	0	0
5		Main Practical	Practical-2	5	0	Biochemistry and Molecular Biology	0	0	0
6		Main Practical	Practical-3	5	0	Computational Biology	0	0	0
7		Elective	Paper -1	3	3	A) Cytogenetics (or) B) Cell Biology (or) C) BioInstrumentation	25	75	100
				30	**15**		**100**	**300**	**400**
SEMESTER II							**CIA**	**Uni. Exam**	**Total**
6		Main	Paper -4	5	5	Genomics and Proteomics	25	75	100
7		Main	Paper-5	5	5	Statistical Bioinformatics	25	75	100
8		Main Practical	Practical-1	5	5	Statistical Bioinformatics	40	60	100
9		Main Practical	Practical -2	5	5	Biochemistry and Molecular Biology	40	60	100

10		Main Practical	Practical -3	5	5	Computational Biology	40	60	100
11		Elective	Paper -2	3	3	A) Molecular Biology and Biotechnology (or) B) Genetic Engineering (or) C) Relational Database Management Systems	25	75	100
12		Compulsory Paper		2	2	Human Rights	25	75	100
				30	**30**		**220**	**480**	**700**
SEMESTER III							**CIA**	**Uni. Exam**	**Total**
13		Main	Paper-6	4	4	Molecular Modeling and Drug Designing	25	75	100
14		Main	Paper-7	4	4	Advanced Programming in Bio-informatics	25	75	100
15		Main	Paper-8	4	4	Chemoinformatics	25	75	100
16		Main	Practical -4	5	0	Molecular Modeling and Programming	0	0	0
17		Main	Practical-5	5	0	Genomics and Proteomics	0	0	0
18		Main	Practical -6	5	0	DBMS and Biocomputing	0	0	0
19		Elective	Paper-3	3	3	A) Genetic Algorithm (or) B)Drug Discovery (or) C)Computational Chemistry	25	75	100
				30	**15**		**100**	**300**	**400**
SEMESTER IV							**CIA**	**Uni. Exam**	**Total**
20		Main	Paper -9	6	6	Systems Biology	25	75	100
21		Main	Paper-10	6	6	Project Work/Dissertation and *viva voce*	25	75	100
22		Main	Practical -4	5	5	Molecular Modeling and Programming	40	60	100
23		Main	Practical -5	5	5	Genomics and Proteomics	40	60	100
24		Main	Practical -6	5	5	DBMS and Biocomputing	40	60	100
25		Elective	Paper -4	3	3	A)Bio-diversity Informatics (or) B)IPR and Biosafety (or) C) Protein Engineering	25	75	100
				30	**30**		**195**	**405**	**600**

Subject	**Papers**	**Credit**	**Total Credits**	**Marks**	**Total marks**
MAIN	10	4-5	46	100	1000
MAIN PRACTICAL	6	4-5	30	400	600
ELECTIVE	4	3	12	100	400
COMPULSORY PAPER	1	2	2	100	100
Total	**21**		**90**		**2100**

THIRUVALLUVAR UNIVERSITY

M.Sc. BIOINFORMATICS

SYLLABUS
UNDER CBCS
(with effect from 2012-2013)

SEMESTER I

PAPER – 1

INTRODUCTION TO BIOINFORMATICS

Objective:

To introduce classic bioinformatics theory to students by focusing on how computer techniques can be used for the storage, analysis, prediction and simulation of biological sequences (DNA, RNA and Proteins).

UNIT-I

Bioinformatics - Definition - Biological & Specialized Databases - Nucleic acid sequence databases: GenBank, EMBL, DDBJ - Protein sequence databases: SWISS-PROT, TrEMBL, PIR_PSD - Genome Databases at NCBI, EBI, TIGR, SANGER - Virtual Library.

UNIT-II

Bioinformatics servers - NCBI - EBI - GENOMENET - Bibliographic resources and literature databases - PUBMED, MEDLINE, AGRICOLA - Database Searching techniques - ENTREZ - Data Mining - techniques & tools - Data Warehousing - Top Down & Bottom up approaches.

UNIT-III

Sequence patterns & representation - consensus, regular expression, contigs, motifs and blocks - Sequence Analysis - FASTA - BLAST - Scoring matrices - PAM and BLOSUM - Pairwise alignments - Multiple sequence alignments - CLUSTALW and Pileup - dendrograms and its interpretation.

UNIT-IV

Phylogenetic analysis - taxonomy and phylogeny - molecular evolution - Data used in Taxonomy and Phylogeny - Phylogenic trees - Definition and description - types of trees - tree construction - tree analysis - homologous - orthologous - paralogous - Phylip and phylogenetic analysis.

UNIT-V

Application of Bioinformatics - Drug designing - Drug discovery cycle - Role of Bioinformatics in drug design - Target identification - lead discovery - Structure-based drug design - Modeling of target- small molecule interactions.

Text Books:

Attwood, T.K. and Parrysmith, D.J. 2001. Introduction to Bioinformatics. Pearson Education (Singapore) Pvt. Ltd., New Delhi.

Mani, K. and Vijayaraj, N. 2004. Bioinformatics - A practical approach. Aparna Publications, New Delhi.

Harshawardhan Bal - Bioinformatics - Primciples and Applications, 1st Edition 2005, TMH, New Delhi.

Reference Books:

Bryan Bergersen, M.D. 2003. Bioinformatics computing. Pearson Education (Singapore) Pvt. Ltd., New Delhi.

Rastogi, S.C., Menderatta, M. and Rastogi, P. 2004. Bioinformatics - concepts, skills and applications. CBS Publishers & Distributors, New Delhi.

Westhead, D. R., Parish, J. H. and Twyman, R.M. 2003. Bioinformatics. Viva Books Pvt. Ltd., New Delhi.

Sahai, S., 1999. Genomics and Proteomics: Functional and computational aspects. Viva Books Pvt. Ltd., New Delhi.

Mount, David W. 2001. Bioinformatics sequence and genome analysis. Cold Spring Harbor Laboratory Press, New Delhi.

Pennigton, S.R., and Dunn, M.J. 2002. Proteomics. Viva Books Pvt. Ltd., New Delhi.

Baxevanis, En Andreas D. and Francis Ouellette, B.F. 2003. Bioinformatics: A practical guide to the analysis of genes and proteins. John Wiley & Sons, New Delhi.

PAPER – 2

BIOCHEMISTRY AND BIOPHYSICS

Objective:

To impart knowledge to the candidates on structural, functional and dynamic aspects of biological components

UNIT-I

Classification, Structure, Properties and Biological role of Carbohydrates. Carbohydrate Biosynthesis, Metabolism - Glycolysis, TCA cycle and ATP bioenergetics.

UNIT-II

Structure, classification. Properties and Biological role of Lipids. Storage of fatty acids. Lipid, Biosynthesis, Metabolism. Utilization of fatty acids for energy production - β Oxidation.

UNIT-III

Introduction to protein structure - Composition and dynamic structural properties, primary and higher level protein organization. Structural components of Nucleic acids. DNA structure, function and sequence. Properties, structure and types of RNA. Nucleic acid Metabolism - Conformational properties of proteins - Ramachandran, Chandrasekaran and Sasisekaran plots, secondary, super secondary, tertiary and quaternary structure of protein.

UNIT-IV

Biophysics - Introduction - Thermodynamics - Laws of thermodynamics - Energy states - Ground and Excited states - Electromagnetic spectrum - Absorption of light by atoms & molecules - Paulis exclusion principle - Coupling of chemical reactions - Endergonic and exergonic coupling - Redox reactions - Hydrogen half cell.

UNIT-V

ATP synthesis - ETC in chloroplast and mitochondria - Oxygen electrode - Classification, Characteristics of enzymes - Biological role - Enzyme Kinetics, Regulation of enzyme activity and Factors affecting enzyme kinetics - Formulation and significance of Michaelis - Menton Equation.

Text Books:

Berg, J.M., Tymoczko, J. L. and Stryer, L. 2002. Biochemistry. 5th Edn. W.H Freeman and Company, New York.

Devlin, T. M. 2002. Text book of Biochemistry - with clinical correlations. 5th Edn. John Wiley & Sons Inc., New York, USA.

Freifelder, D. and Malcinski, G.M. 1993. Essentials of Molecular Biology, 2nd Edn. Jones & Bartletl Publishers Inc., London.

Nelson, D.L. and Cox, M.M. 2005. Lehninger's Principles of Biochemistry, 4th Edn. Replika Press Pvt. Ltd., New Delhi.

Voet, D. and Voet, J.G. 1990. Biochemistry. John Wiley and Sons Inc., New York.

Reference Books:

Atherly, A.G., Girton, J.R. and McDonald, J.F. 1999. The science of Genetics – Saunders College Publishers, New Delhi.

Bickerstaff, G.F.1997. Immobilization of Enzymes and Cells. Humana Press, New Jersey, USA.

Bray, A., Raff, L. and Watson, R. 1994. Molecular biology of the Cell. 3rd Edn. Garland Publishing Company, New York.

Click, B.R. and Pastumak, J.J. 1998. Molecular Biotechnology - Principles and application of recombinant DNA. American Society of Microbiologists Press, Washington.

Cooper, G.M. and Hausman, R. E. 2004. The Cell: A Molecular Approach, 3rd Edn. American Society of Microbiologists Press, Washington.

Karp, G. 1996. Cell and Molecular Biology: Concepts and Experiments. John Wiley & Sons, New York.

Micklos, D.A., Freyerr, G. A. and Crotty, D. A. 2003. DNA Science, 2nd Edn. Cold Spring Harbor Laboratory Press, New York.

Primrose, S. B. 1994. Molecular Biotechnology, 2nd Edn. Blackwell Scientific Publishers, Oxford.

PAPER – 3

COMPUTER PROGRAMMING USING C

Objectives:

To equip students in programming using C and its application in bioinformatics exercises.

UNIT-I

Introduction to Computer - History of Computing - Computer characteristics - Components of Computer - Modes of operation - Types of Programming Languages - Parallel computing - Single user and Multi user system - Linux Clusters - Distributed Computing - Future of Computing - Role of computer in Biology (Biocomputing)

UNIT-II

Introduction to Operating Systems - MS windows commands, UNIX basic commands - General purpose, file handling, vi editor & environment - Linux - basic commands - Internet browsers - HTML, DHTML, XML - web page design tools - cgi-bin scripts - Linking - Text Formatting - Adding Images - Tables - Frames to web pages

UNIT-III

Introduction to C - History of C - Identifiers and Keywords - Data Types -Constants, Variables and arrays - Operators and expressions - Data Input and Output - Preparing and Running a complete C program - Control Structures - if and switch statements - while, do-while and for statements - goto statement - Arrays - Character strings - Simple programs.

UNIT-IV

User defined Functions in C - Defining and accessing functions - Passing arguments - Function prototypes - Recursion - Storage classes - Pointer Declarations - Passing pointers to functions - Pointers and arrays - Operations on pointers - Arrays of pointers - Dynamic memory allocation.

UNIT-V

Structures: User defined data types in C - Structures - Declaring structures and Accessing members - Array of structures - Structure within structure - Unions - File operations - open, close, reading and writing - Random access files - Linked list - Preprocessor directives - Macros - Command line arguments.

Text Books:

Byron S. Gottfried, Schaum's outline of Theory and Problems of Programming with C, Tata McGraw-Hill, New Delhi, 1991.

Brain W. Kernighan and Dennis. M. Ritchie, The C Programming Language, Second Edition, Prentice-Hall of India, 1988.

Sumitabha Das, UNIX Concepts and Applications, 3rd Edition, Tata McGraw-Hill, New Delhi, 2003.

H.M.Deitel, P.J. Deitel and A.B. Goldberg, Internet and WWW - How to program, 3rd Edition, Prentice - Hall of India pvt ltd, New Delhi, 2005.

Ethan Cerami, XML for Bioinformatics, Springer International edition, 2005.

ELECTIVE

PAPER – 1

A. CYTOGENETICS

Objectives:

To know the terminology and literature of cytogenetics; chromosome structure, and function; cytogenetic techniques that can be employed in plant genetics and improvement.

UNIT-I

Prokaryotic and eukaryotic cells -. Structure and function of cell organelles (chloroplasts, mitochondria, ER, ribosomes, endosomes, lysosomes, peroxisomes, hydrogenosome). - Nucleus, nucleolus, nuclear pore complex. Chromatin and nucleosome - Cell 10ignaling and cell receptors. Signal transduction (G-1 proteins, etc.) - Mitosis and meiosis.

UNIT-II

Prokaryotic and Eukaryotic genome organizations - Molecular basis of life - DNA as the Genetic Material - Definitions of the Gene - Chemistry of the Gene - Gene as the unit of mutation and recombination - Mechanism of replication and transcription - Gene as the unit of expression Regulation of gene expression in Bacteria, yeast, Mitochondria & chloroplast.

UNIT-III

Structure and function of chromosomes. - chemical composition - types of chromosomes; lampbrush chromosomes, polytene chromosomes, B chromosomes - variations in chromosome structure: duplications, deletions, inversions, and translocations, isochromosomes, ring chromosomes, centric fusions and fissions.

UNIT-IV

Changes in chromosome number - aneuploidy and euploidy in both plants and animals, their origins, cytogenetic effects, use in crop breeding, and adaptive significance - Variant chromosomal systems. - asexual reproduction, modified sexual reproduction (various forms of parthenogenesis), chromosome diminution and elimination.

UNIT-V

Cell aging and cell senescence, programmed cell death- molecular aspects, regulation of cell death, PCD in leaf senescence, in response to stress – Apoptosis – Role of different genes, cell organelles during apoptosis – genetic control of apoptosis.

Text Books:

Alberts. B., Bray, D., Lewis, J., Raff, M., Roberts, K. and Watson, J. D. 1989. Molecular biology of the Cell (2nd edition). Garland Pub. Inc., New York.

De Robertis, E.D.P. and De Robertis, E.M.F. 1995. Cell and Molecular Biology. 8th end., B.I. Waverly Pvt. Ltd., New Delhi.

Hartl, D. L. and Jones, E. W. 2001. Genetics: Principle and Analysis (4th edition). Jones & Bartlett Pub., USA.

Snustad. D. P.and Simmons M. J. 2000. Principles of Genetics (2nd edition). John Wiley and Sons, Inc., USA.

Reference Books:

Atherly, A. G., Girton, J. R. and McDonald, J. F. 1999. The Science of Genetics. Saunders College Pub. Fort Worth, USA.

Bumham, C. R. 1962. Discussions in Cytogenetics. Burgess Pub. Co., Minnesota.

Busch, H. and Rothblum, L. 1982. Volume X. The Cell Nucleus Rdna Part A, Academic Press.

Khush, G. S. 1973. Cytogenetics of Aneuploids. Academic Press New York, London.

Karp, G. 1999. Cell and Molecular Biology – Concepts and experiments. 2nd edn. Harris, D (ed.), John Wiley & sons, New york.

Kleinsmith, L.J. & Kish, V.M. 1995. Principles of Cell and Molecular Biology. 2nd edn., McLaughlin, S., Trost, K., Mac Elree, E. (eds)., Harper Collins Publishers, Newyork.

Lewin, B. 2000. GENE VII. Oxford University Press, New York, USA.

Lewis, R. 1997. Human Genetics: Concepts & Applications (2nd edition). WCB McGraw Hill, USA.

Malacinski, G. M. And Freifelder, D. 1998. Essentials of Molecular Biology (3rd edition) Jones & Bartlet Publishers, Inc. London.

Russel, P. J. 1998. Genetics (5th edition). The Benjamin/Cummings Pub. Co., Inc. USA.

PAPER – 1

B. CELL BIOLOGY

Objectives:

To know the terminology and literature of cytogenetics; chromosome structure, and function; cytogenetic techniques that can be employed in genetics and improvement of life systems.

UNIT-I

Prokaryotic and eukaryotic cells -. Structure and function of extracellular matrix or ECM (cell wall) and membranes - Structure and function of cell organelles (chloroplasts, mitochondria, ER, ribosomes, endosomes, lysosomes, peroxisomes, hydrogenosome). - Nucleus, nucleolus, nuclear pore complex. Chromatin and nucleosome - Cell signalling and cell receptors - Signal transduction.

UNIT-II

Mitosis and meiosis; molecular basis of cell cycle - Phases of Cell Cycle, functional importance of each phase - Numerical and structural variations in chromosomes and their significance. Study of polytene, lampbrush and B-chromosomes - structure, behaviour and significance.

UNIT-III

Prokaryotic and Eukaryotic genome organizations - Molecular basis of life - DNA as the Genetic Material - Definitions of the Gene - Chemistry of the Gene - Gene as the unit of mutation and recombination - Mechanism of replication and transcription - Gene as the unit of expression Regulation of gene expression in Bacteria, yeast, Mitochondria & chloroplast.

UNIT-IV

Cell differentiation - Physiological aspects of cellular differentiation - Totipotency of plant cells, Organogenesis, Embryogenesis, and Cytodifferentiation - Differentiation of sieve tube elements and tracheids/ vessels, specialized cell types like laticifers, transfer cells, secretory cells, and aleurone layer.

UNIT-V

Cell aging and cell senescence, programmed cell death- molecular aspects, regulation of cell death, PCD in leaf senescence, in response to stress - Apoptosis- Role of different genes, cell organelles during apoptosis - genetic control of apoptosis.

Text Books:

De Robertis, E.D.P. and De Robertis, E.M.F. 1995. Cell and Molecular Biology. 8th end., B.I. Waverly Pvt. Ltd., New Delhi.

Kleinsmith, L.J. & Kish, V.M. 1995. Principles of Cell and Molecular Biology. 2nd edn., McLaughlin, S., Trost, K., Mac Elree, E. (eds)., Harper Collins Publishers, Newyork.

Reference Books:

Alberts. B., Bray, D., Lewis, J., Raff, M., Roberts, K. and Watson, J. D. 1989. Molecular biology of the Cell (2nd edition). Garland Pub. Inc., New York.

Hartl, D. L. and Jones, E. W. 2001. Genetics: Principle and Analysis (4th edition). Jones & Bartlett Pub., USA.

Snustad. D. P.and Simmons M. J. 2000. Principles of Genetics (2nd edition). John Wiley and Sons, Inc., USA.

PAPER – 1

C. BIOINSTRUMENTATION

Objective:

To impart training in analytical techniques to use and utilize the modern instruments and its technology for application-oriented one

UNIT-I

Centrifugation: Low speed, high speed, and Ultra and Refrigerated centrifuges. Principles and Operation methods of Weighing devices, pH, salinity and conductivity meters. Preparation of Buffers and stock solutions of media/reagents. Preparation of normality, ppm, molar and percentage solutions. Calibration of stage and ocular meter for micrometry and Haemocytometer.

UNIT-II

Spectrometry: UV, IR, NMR and A.A.Spectroscopy. Mass spectroscopy and fluorescence spectroscopy-Protein crystallography and X-ray diffraction

UNIT-III

Electrophoresis:Gel electrophoresis, Polyacrylamide gel electrophoresis (PAGE & SDS PAGE) and Agarose gel electrophoresis, comet assay. Two dimensional electrophoresis, Vertical electrophoresis. Horizontal electrophoresis, Paper electrophoresis- Southern Blot, Northern Blot, Western Blot, DNA finger printing-.

UNIT-IV

Extraction methods: Crude extracts. Distillation, Separation procedures. Chromatography: Principles, working procedure, functions and application of CC, TLC, PC, GC, GLC, HPLC, HPTLC, Fourier Transform IR and MS.

UNIT-V

Principles of Bioinformatics: Collection and storing of sequences, alignment of pairs of sequences, multiples sequences alignment, database searching for sequences.

Text Books:

Becker, J.M., Caldwell, G.A. and Zachgo, E.A. 1996. Biotechnology: A Laboratory Course, 2nd Edn. Academic Press, Inc., San Diego, California.

Brown, T.A 1991. Molecular Biology Labfax. Bios Scientific Publishers Limited, Oxford.

Harborne, J.B. 1998. Phytochemical Methods, 3rd Edn. Chapman & Hall, London.

Mount, D.W. 2003. Bioinformatics: Sequence and Genome Analysis. CBS Puiblishers and Distributors, New Delhi.

Punia, M.S. 1999. Plant Biotechnology and Molecular Biology - A Laboratory Manual. Scientific Publishers, Jodhpur, India.

Willard, H.H., Merritt, L., Dean, J.A., Settle, F.A. Instrumental Methods of Analysis, 1st Edn. CBS Publishers and Distributors, New Delhi.

Wilson, K. and Walker, J. 1997. Practical Biochemistry: Principles and Techniques. Cambridge University Press, Cambridge.

Reference Books:

Bishop, M.J. and Rawlings, C.J. 1987. Nulceic acid and Protein sequence analysis: A Practical Approach. IRL Press, Oxford.

Cannel, J.P. 1998. Natural Products Isolation. Humana Press, New Jersey, USA.

Chirikjian, J.G.1995. Biotechnology: Theory and Techniques Vol.II.Genetic Engineering, Mutagenensis, Separation Technology. Jones and Bartlett Publishers, London, England.

Darbre, P. D. 1988. Introduction to Practical Molecular Biology. John Wiley & Sons Ltd., New York.

Krawelz, S.A. and Womble, D.D. 2003. Introduction to Bioinformatics: a theoretical and Practical approach. Humana Press Inc., New Jersey, USA.

Sharma, B.K 1996. Instrumental Methods of Chemical Analysis, 15th Edn. Goel Publishing House, Meerut.

CORE PRACTICAL – I

STATISTICAL BIOINFORMATICS

Compilation and analysis of data

Standard déviation, MEAN, MODE

ANOVA

T-Test

Chi-square analysis

HMM

Neural network analysis

Bootstrapping

Jack-knife method

CORE PRACTICAL – II

BIOCHEMISTRY AND MOLECULAR BIOLOGY

Preparation of buffers and use of pH meter

Estimation of carbohydrates

Determination of sugars, reducing and non-reducing sugars

Estimation of proteins

Isolation, purification and separation of proteins- Western Blotting.

Estimation and separation of lipids

Separation of lipids by TLC and paper chromatograms.

Quantification and separation of chlorophyll pigments

Determination of acid value of oil.

Estimation of free fatty acids

Isolation and separation of Enzymes

Absorption spectrum for chlorophyll

Measurement of redox potential

CORE PRACTICAL – III

COMPUTATIONAL BIOLOGY

Biological databases (sequence, structure and specialized databases)

Data retrieval using ENTREZ

Database file formats

Gene finding (Genscan)

Protein prediction

Sequence search

Sequence alignment

Phylogenetic tree construction

Find the pH of a solution given the concentration of H^+ (or) OH^- ions

Compute the relative centrifugal force using r_max (in cm) and rpm value

Compute the rpm value using r_max (in cm) and RCF value

Find the molecular weight of a DNA with n base pairs in length

Find the molecular weight of a given dephosphorylated oligonucleotide sequence

Find the molecular weight of a given DNA sequence, after checking for phosphorylation

Computing amino acid composition of a given protein sequence. Read the sequence from a data file.

Computing base composition of a given nucleotide sequence. Read the sequence from a data file.

Note: Test all your programs on different platforms (windows, linux/unix)

SEMESTER II

PAPER – 4

GENOMICS and PROTEOMICS

Unit-I

Human genome-physical structure and genetic content-Genome structure and anatomy of prokaryotic and eukaryotic genome-nuclear genomes-organelle genomes-Plasmid genome-Repetitive DNA-sequence repeats-transposable elements-pseudo genes-Comparative genome analysis-genome databases-organisms-specific databases-Genome analysis and annotation-gene ontology and community annotation--experimental verification-limitations

Unit-II

Genome mapping-genetic linkage-markers-genetic mapping techniques–physical mapping techniques—Genome sequencing methods - Maxam-Gilbert sequencing-Chain termination method- Genome mapping resources-map elements-genetic markers-types of maps-genomic mapping resources-integrated mapping resources-comparative maps-Gene prediction methods-fine structure of gene-prediction programmes-Prediction of promoters-characterization strategies and consideration

Unit-III

Genomes of model organisms-*E.coli- Archaeoglobus fulgidus-Saccharomyces cerevisiae-Arabidopsis thaliana-Caenorhabditis elegans- Drosophilla melanogaster*– Human genome project- SNP-Genetic diversity in anthropology-Evolution of genomes-Metabolomics and its application - metabolic pathways database system and integration of file formats-pathway reconstruction methods- flux balance analysis tools-metabolic pathway lay-out tools

Unit-IV

Proteomics introduction-Protein sequencing methods-2D gel electrophoresis and Mass spectra-Tools for proteome technology-Protein identification from 2D gel, mass spectra and sequence data-Protein property prediction-bulk, active sites, modification sites, interactive sites, location, localization, stability, shape, domains properties, secondary and tertiary structures–comprehensive commercial packages-Expasy proteomics tools-Protein identification programs-Muscot- PeptIdent- Protein prospector-GFS

Unit-V

Proteome databases and resources-Comparative proteomics methods-2D gel databases-Protein interaction data bases and resources – Metabolomics databases- and tools - Systems biology resources and its applications-Application of genomics and proteomics to medicine, toxicology and pharmaceuticals

Reference Books:

Baxevanis D and Ouellette BFF, "*Bioinformatics: A practical guide to the analysis of genes and proteins ",*(3rd Ed), John Wiley & Sons, Inc., 2005.

Baxevanis D and Ouellette BFF, 2002. *Bioinformatics: A practical guide to the analysis of genes and proteins* (2rd Ed), John Wiley & Sons, Inc.

Brown TA, "*Genomes",* (2nd Ed), BIOS Scientific Publishers, Oxford, UK., 2002.

Sensen CW, "*Essentials of Genomics and Bioinformatics"*, Wiley-VCH, 2002.

Sensen CW, "*Hand book of Genome Research"*, Wiley-VCH Verlag GmBh & Co, Weinheim,2005.

Pennigton SR and Dunn MJ, „ *Proteomics"*, Viva Books Pvt. Ltd, New Delhi,2002.

PAPER – 5

STATISTICAL BIOINFORMATICS

Objective:

To introduce the students in mathematical and statistical tools and techniques.

UNIT-I

Role of statistics in Biology and Bioinformatics - Collection and Representation of Experimental data - Measures of Central Tendency and Location: Arithmetic Mean, Median, Mode, Position of averages, Geometric Mean, Harmonic mean and percentile - Measures of Dispersion: Range, Interquartile range, mean deviation, variance and standard deviation.

UNIT-II

Correlation and Regression: Correlation coefficient - Types of correlation - Regression equation - Principles of least squares - Linear regression - Biological significance of correlation and regression - Tests of significance: Basis of statistical inference - Student's 't' test for mean, difference of means and test for correlation and regression coefficients – Chi - square test - Analysis of Variance

UNIT-III

Basic concepts of Probability - Sample space and Events - The use of counting methods in probability - Addition law - Conditional probability - Simple problems involving the estimation of probabilities - Normal Distribution and Binomial and Poisson distributions - Z-score, P-value and E-value - Hidden Markov Models - Neural Networks - Applications of probability concepts in Bioinformatics

UNIT-IV

Matrices: Matrix algebra - Types of matrices - determinant - inverse, rank of matrix - solution of simultaneous equations - rotation matrices and co-ordinate transformation
Vectors: Vector algebra - addition and subtraction of vectors - product of vectors, dot & cross products - scalar triple product - vector calculus - gradient, divergence, curl of a vector & identities - applications.

UNIT-V

Basic differentiation of algebraic and trigonometric functions - Maxima and Minima - Integration of simple functions - Definite and non-definite integrals - Table of integrals - Numerical methods for differentiation and integration - applications to systems biology

Text Books:

Gupta, S.C. and Kapoor, V.K. 2002.Fundamentals of Mathematical Statistics, 11th Edition, Sultan Chand & Sons, New Delhi.

Jordan, D.W. and Smith, P. 2002. Mathematical Techniques, 3rd Edn, Oxford University Press, New Delhi.

Forthofer, L. 1995. Introduction to Biostatistics, Academic Press, New York.

Sokal, Robert R. and Rohlf, F.J. 1987. Introduction to Biostatistics (Biology-Statistics Series), W.H. Freeman & Company, New York..

Batschelet, E. 1991. Introduction to Mathematics for Life Scientists, 2nd Edn., Springer International Student Edn., Narosa Publishing House, New Delhi.

ELECTIVE

PAPER – 2

A. MOLECULAR BIOLOGY AND BIOTECHNOLOGY

Objectives:

To advance the students to acquire knowledge in molecular biology and biotechnology theories and skills.

UNIT-I

Cell structure - Prokaryotic and eukaryotic. Ultra structure of a plant cell, structure and function of cell wall and plasma membrane. Membrane properties, dynamic nature and movement of substances across cell membranes. Cell cycle - major molecular events.

UNIT-II

DNA as the genetic material - Griffith's experiment. DNA replication: semi -conservative mode, mechanics of DNA replication, enzymes and accessory proteins involved. Transcription - RNA polymerase, transcription factors, regulatory elements, transcriptional and post transcriptional modifications of mRNA. Gene regulation in Prokaryotes and Eukaryotes.

UNIT-III

Translation: Mechanism of initiation, elongation and termination of polypeptide, synthesis. Regulation of translation, post translational modifications of proteins. Protein targeting to different organelles (Chloroplasts, Mitochondria and Nucleus). Antisense RNA and ribozyme technology.

UNIT-IV

Gene and gene mapping. - rDNA technology - Molecular markers in genome analysis: RFLP, RAPD and AFLP. Application of molecular markers in germplasm accession, biodiversity and taxonomic studies, Marker-aided Breeding. Micro satellites, SCAR (sequence characterized amplified regions), SSCP (single strand conformational polymorphism), AFLP, QTL, map base cloning, molecular marker-assisted selection.

UNIT-V

Concept of genomics and its applications. Organelle genomes, Genomic Libraries (YAC, BAC) - recovery of clones. Analytical techniques. DNA sequencing, PCR, analysis of cloned genes. Microarray technology. Applications. Proteomics concept and applications. Comparative genomics.

Text Book:

Celis, J. E. 1998. Cell Biology: A Laboratory Handbook, 2nd Edn. Vols. 1 to 4. Academic Press, San Diego.

Devlin, T. M. 2002. Text book of Biochemistry - with clinical correlations. 5th Edn. John Wiley & Sons Inc., New York, USA.

Punia, M.S. 1999. Plant Biotechnology and Molecular Biology - A Laboratory Manual. Scientific Publishers, Jodhpur, India.

Snustad, P., Michael, D. and Simmons, J. 2000. Principles of Genetics, 2nd Edn. John Wiley & Sons, Inc., New York.

Watson, J.D., Hopkins, N. H., Roberts, J. W. Steitz, J.A. and Weiner, A. M. 1987. Molecular Biology of the Gene, 5th Edn. Benjamin/Cummings Publication, California.

Reference Books:

Becker, J.M., Caldwell, G.A. and Zachgo, E.A. 1996. Biotechnology: A Laboratory Course, 2nd Edn. Academic Press, Inc., San Diego, California.

Berger, S.L. and Kimmel, A.R. 1998. Methods in Enzymology Vol 152, Guide to Molecular Cloning Techniques. Academic Press, lnc., San Diego.

Campbell, W. Robinson, J. and Howell, A. 1985. Comprehensive Biotechnology, Vol.4, 1st Edn. Pergaman-Press, England.

Chirikjian, J.G.1995. Biotechnology: Theory and Techniques Vol.II.Genetic Engineering, Mutagenensis, Separation Technology. Jones and Bartlett Publishers, London, England.

Freifelder, D. and Malcinski, G.M. 1993. Essentials of Molecular Biology, 2nd Edn. Jones & Bartletl Publishers Inc., London.

Glover, D. M. and Hames, B. D. 1995. DNA Cloning: a Practical Approach. Glover, IRL Press, Oxford.

Goeddel, D.V. 1990. Methods in Enzymology Vol 185, Gene Expression Technology. Academic Press, lnc., San Diego.

Harvey, L.P., Berk, A.S., Lawrence, Z. Matsudaria, P., Baltimore, D. and Damell, J.E. 2000. Molecular Cell Biology, 4th Edn. Media Connected. W.H Freeman and Company, New York.

Meyers, R.A. 1995. Molecular Biology & Biotechnology - A comprehensive desk reference. VCH Publishers, New York.

Micklos, D.A., Freyerr, G. A. and Crotty, D. A. 2003. DNA Science, 2nd Edn. Cold Spring Harbor Laboratory Press, New York.

Sambrook, J. and Russel, D.W. 2001. Molecular Cloning: A Laboratory Manual, 3rd Edn. Cold Spring Harbor Press, Cold Spring Harbor, New York.

PAPER – 2

B. GENETIC ENGINEERING

Objective:

To train the candidates in genetics up to the level of genes and molecules

UNIT-I

Scope and principles of Genetic Engineering, Molecular Tools and Their Applications. rDNA technology - Nucleic acid Isolation, purification. Yield Analysis. Restriction enzymes - properties, types, functions and modification enzymes.

UNIT-II

Gene Cloning Vectors: Plasmid, bacteriophages, phagemids, cosmids, Artificial chromosomes, cDNA Synthesis and Cloning - mRNA enrichment, reverse transcription, DNA primers, linkers, adapters and their chemical synthesis, library construction and screening. T - DNA - binary vectors, co integrate vectors. PCR principles and its applications.

UNIT-III

Alternative Strategies of Gene Cloning: Cloning interacting genes - Two - and three hybrid systems, cloning differentially expressed genes. Nucleic acid microarrays. Site - directed Mutagenesis and Protein Engineering. Gene Regulation - NA transfection. Primer extension, SI mapping, Rnase protection assay, reporter assays.

UNIT-IV

Expression Strategies for Heterologous Genes: Vector engineering and codon optimization, host engineering, *In vitro* transcription and translatjon, expression in bacteria, expression in Yeasts and plants. Processing of Recombinant Proteins - Purification and refolding, characterization of recombinant proteins, stabilization of proteins. Transposon Tagging. Role of gene tagging in gene analysis, T-DNA and transposon tagging. Identification and isolation of genes through T-DNA or transposon.

UNIT-V

Transgenic and Gene Knockout Technologies: Targeted gene replacement, Chromosome engineering. Chromosome walking, chromosome micro dissection. Gene Therapy - Vector engineering. Strategies of gene delivery, gene replacement/augmentation, gene correction, gene editing, gene regulation and silencing.

Text Books:

Becker, J.M., Caldwell, G.A. and Zachgo, E.A. 1996. Biotechnology: A Laboratory Course, 2nd Edn. Academic Press, Inc., San Diego, California.

Kingsman, S. M. and Kingsman, A. J. 1998. Genetic engineering: Introduction to gene analysis and exploitation in Eukaryotes. Blackwell Scientific Publications, Oxford.

Lewin, B. 2004. Genes VIII. International Edition, Pearson Prentice Hall, Pearson Education, Inc., USA.

Sambrook, J. and Russel, D.W. 2001. Molecular Cloning: A Laboratory Manual, 3rd Edn. Cold Spring Harbor Press, Cold Spring Harbor, New York.

Snustad, P., Michael, D. and Simmons, J. 2000. Principles of Genetics, 2nd Edn. John Wiley & Sons, Inc., New York.

Watson, J.D., Hopkins, N. H., Roberts, J. W. Steitz, J.A. and Weiner, A. M. 1987. Molecular Biology of the Gene, 5th Edn. Benjamin/Cummings Publ., California.

Reference Books:

Atherly, A.G., Girton, J.R. and McDonald, J.F. 1999. The science of Genetics. Saunders College Publishers, New Delhi.

Chirikjian, J.G.1995. Biotechnology: Theory and Techniques Vol.II.Genetic Engineering, Mutagenensis, Separation Technology. Jones and Bartlett Publishers, London, England.

Cooper, G.M. and Hausman, R. E. 2004. The Cell: A Molecular Approach, 3rd Edn. American Society of Microbiologists Press, Washington.

Cseke, L. J., Kaufman, P. B. Podila, G.K. and Tsai., C.J. 2004. Handbook of Molecular and Cellular Methods in Biology and Medicine, 2nd Edn. CRC Press. Florida, USA.

Glick, B.R. and Pastumak, J.J. 1998. Molecular Biotechnology- Principles and application of recombinant DNA, 2nd Edn. ASM Press, Washington.

Glover, D. M. and Hames, B. D. 1995. DNA Cloning: a Practical Approach. Glover, IRL Press, Oxford.

Primrose, S. B. 1994. Molecular Biotechnology, 2nd Edn. Blackwell Scientific Publishers, Oxford.

Scopes, R. K. 1994. Protein Purification: Principles and Practice, 3rd Edn. Springer-Verlag, New York.

Walker, M.R. and Rapley, R. 1997. Route Maps in Gene Technology. Blackwell Science Ltd., Oxford.

PAPER – 2

C. RELATIONAL DATABASE MANAGEMENT SYSTEM

Objective:

The primary goal of this subject is to provide the knowledge on relational database. It imparts the skill on normalization and database design. It inculcates the knowledge on management of databases.

UNIT-I

Introduction - History of database systems - Applications of database systems - Database systems vs. file systems - View of data: Data abstraction - Instances and Schema - Database system structure - Database architecture - Database administrators and users - Transaction - Homogenous and Heterogeneous data - Advantages and disadvantages.

UNIT-II

Types of data models - Relational model - Relational algebra and calculus - Relational databases - Relational languages - Relational-database design - Object-Relational databases and other hybrid databases; Integrity and security - Constraints - Normalization - Indexing and hashing.

UNIT-III

SQL languages: Data Definition Language (DDL) - Data Manipulation Language (DML) - Transaction Control Language (TCL) - Data Control Language (DCL) - Basics of SQL - MySQL datatypes - MySQL operators - MySQL Functions

UNIT-IV

Working with databases using MySQL commands - Working with tables using MySQL commands - Working with datas using MySQL commands - Joins - Subqueries - Transactions.
Basics of PL SQL and simple PL SQL programs.

UNIT-V

Managing scientific data: Introduction - Challenges faced in the integration of biological information - Data management and data integration in Bioinformatics - Issues to address while designing a biological information system - SRS: An integration platform for database and analysis tools in bioinformatics - An integration challenges in gene expression data management - discovery link

Text Books:

Silberschatz, Korth and Sudarshan, Database System concepts, Tata McGraw-Hill, New Delhi, 2006.

Vikram vaswani, The complete reference for MySQL, Tata McGraw-Hill, New Delhi, 2004.

Lacroix Critchlow, Bioinformatics - Managing scientific data, Elsevier, New Delhi, 2003.

CORE PRACTICAL - I

STATISTICAL BIOINFORMATICS

Estimation and Hypothesis Testing

Design of Observational Studies

Design of Randomised Trials

Comparing Groups of Continuous Data

Comparing Groups of Categorical Data

Correlation and Linear Regression

Sample Size Calculations

Measures of Disease and Confounding

Logistic Regression

Analysis of Survival Data

Analysis of Correlated Data

Statistics in Medical Journals

Advanced Issues in Trials

Missing Data

CORE PRACTICAL – II

BIOCHEMISTRY AND MOLECULAR BIOLOGY

Microscopy: Bright field, Phase contrast & Fluorescence microscopy

Instrumental methods for Cell Biology

Sub cellular fractionation and marker enzymes

Histochemical techniques for Plant cells and tissues

Mitosis - Onion root tip squash with heamatoxylin staining.

Meiosis - Tradeschantia anther squash with Acetocarmine staining

Chromosome morphology observation and detection by Mutants.

Model building using space filling/ball and stick models

Isolation of Mitochondria

Isolation of chloroplast

Isolation, purity determination and quantification of DNA from Coconut endosperm by SSC buffer method.

Isolation, purity determination and quantification of RNA

DNA amplification using Thermocycler.

Blotting Techniques - Southern, Northern & Western.

Hybridization - Autoradiography - Demonstration

Gel documentation system - Demonstration.

Calibration of pH meter & preparation of Buffers 4, 7 & 9 pH.

Preparation of Normal (NaOH), PPM (Cr+) and Molar (Sucrose) & % solutions.

Aborption Frequency of any extract using UV Spectrophotometer.

Agarose Gel Electrphoresis - using DNA sample.

PAGE - any protein sample.

Southern Blotting.

Designing of Scientific Experiment.

Column Chromatography.

Thin Layer Chromatography.

Paper Chromatography.

CORE PRACTICAL – III

COMPUTATIONAL BIOLOGY

Sequence comparison

Structure analysis

Pattern recognition

Proteome analysis using tools

Exon finding

Genome homology

Molecular visualization using Rasmol

SEMESTER III

PAPER – 6

MOLECULAR MODELING AND DRUG DESIGNING

Objective:

To familiarize the students in using computer techniques for molecular modeling and drug designing.

Unit-I

Basic concepts of molecular modeling and simulation–Molecular graphics-Interaction forces-Molecular force fields representations-Energy minimization -Molecular mechanics methods-Force field software packages--Molecular dynamics simulation

Unit-II

Computational quantum chemistry principles-*Ab-initio* methods- Semi-empirical methods- Density Functional Theory-Monte Carlo quantum mechanical simulation

Unit III

Principles and methods of Docking –Ligand designing methods- Drug-receptor interactions- Classical SAR/QSAR studies and their implication to the 3D modeler–2D/3D database searching-Pharmacophore identification and novel drug design

Unit-IV

Drug discovery and pharmacoinformatics- Target finding in genomes and proteomes-Genomics on drug discovery-Restoring P53 dependent tumor suppression and cancer therapy

Unit-V

Enzyme background-Theory of enzyme inhibition-Enzyme inhibition as a tool for drug development - Structural based drug design - Structural Bioinformatics in drug discovery-Screening of drug databases

Reference Books:

Bergeron B (2003) *Bioinformatics computing*, Prentice-Hall of India, New Delhi.

Boune PE and Weissig H (2003) *Structural Bioinformatics*, Wiely-Liss,Inc, New York.

Doucet J-P and Weber J (1997) *Computer aided molecular design: Theory and Application*. Academic Press.

Gasteiger J and Engel T (2003) *Chemoinformatics*. Wiely-VCH and Co Ltd.

Leach AR (2001) *Molecular modeling: Principle and application*. Pearson Education Ltd.

Mannhold R, Kubinyi H and Timmerman H (2003) *Bioinformatics-From genomes to drugs*, Wiley-VCH. Basic technologies

Sensen CH (2002) Essentials of Genomics and Bioinformatics, Wiley-VCH.

Silverman RB (2004) *The organic chemistry of drug design and drug action*, Academic press, New York

Veszpremi T and Feher M (1999) *Quantum chemistry: Fundamentals to applications*, Plenum Publishing, New York.

PAPER – 7

ADVANCED PROGRAMMING IN BIOINFORMATICS

Objective:
To enable the students to acquire advanced training in Java, BioJava, Perl, Bioperl, Python

UNIT-I

JAVA - Introduction to object oriented programming - Basic Syntax - Control Structures - Arrays - Strings - Files and Streams - Applets; Introduction to JDBC (Java Database Conectivity) - JDBC Architecture, JDBC Drivers, Connecting to Database and accessing databases - Threads - Java beans.

UNIT-II

BIOJAVA: Introduction - Sequence Manipulation. Translation: DNA to Protein, Codon to amino acid, Six frame translation. Proteomics: mass and pI of a peptide - Sequence File Format conversions, Locations and Features. BLAST and FASTA parsing, Weight Matrices and Dynamic Programming

UNIT-III

PERL: Modules:- defining, storing and using modules; Data and control structures:- Operators and Control Flow, Data Types & structure, Function/Subroutines - File handling; Regular Expressions:- patterns - grouping and anchoring - string matching; Object oriented programming:- Classes, Objects, Methods.
BIOPERL: General Bioperl Classes, Sequences, Sequence Manipulation, Features and Location Classes. Alignments: AlignIO. Analysis: Blast, Genscan; Databases: Database Classes, Accessing a local database.

UNIT-IV

Common Gateway Interface:- HTML form elements, GET, POST & HEAD Method, CGI Environment Variables, Handling forms, Passing Parameters via CGI, Debugging CGI programs.
WEB DESIGNING & XML: HTML Specifications and Syntax, XML Basics, Style Sheets, XML Applications, Java Script.

UNIT-V

PYTHON: Overview, Data structures, Control Flow, Modules, Basic I/O, Regular Expressions, File Manipulation, Classes, Standard library.

Text Books:

Herbertz Schildt, The complete Reference Java J2SE 5 Edition, Mc Graw Hill, Osborne, 2005.

E Balaguruswamy, Programming with Java, Tata Mc Graw Hill, New Delhi, 1999.

Larry Wall, Tom Christiansen & John Orwant, Programming Perl –3rd ed, O'Reilly, 2000.

James D. Tisdall, Beginning Perl for Bioinformatics, O'Reilly, 2001

Mark Lutz , Programming Python - 2nd Ed., O' Reilly, 2003.

Eric Ladd, J.O'Donnell, Using HTML 4, XML and JAVA, Prentice Hall of India QUE, 1999.

Brown, The complete reference - Perl, Tata Mc Graw Hill, New Delhi, 2004.

PAPER – 8

CHEMOINFORMATICS

UNIT-I

Computational chemistry-history-objectives-Computational techniques-software-databases-hardware and network-organization-Computers and chemical structures-chemical nomenclature-use and limitation of models and modeling- Computer graphics for structural analysis of small molecules

UNIT-II

Representation and manipulation of 2D and 3D structures-substructure-3D pharmacophore searching-Molecular descriptors-2D and 3D descriptors-data verification and manipulation-Computational models-deriving QSAR equations-designing a QSAR experiment-Statistical techniques-similarity methods-2D finger prints-similarity co-efficients-2D and 3D descriptors methods

UNIT-III

Selecting diverse set of compounds-cluster analysis-dissimilarity based selection methods-cell based methods-evaluation methods-Analysis of high-throughput screening data-data visualization-data mining methods-Virtual screening-drug likeliness-structural based virtual screening-prediction of ADMET properties-Combinatorial chemistry and ligand design-library enumeration-library design strategies-Lead structure discovery and development

UNIT-IV

Applications of quantum and molecular methods-Molecular mechanics for modeling of drugs-Quantum mechanics for modeling of drug structure-Molecular dynamic simulation in drug development process-QSAR to molecular graphics-Biocatalyst design and application

UNIT-V

Sources of chemical information-online resources-activity searching-synthesis modeling-trends and developments-Chemical genomics-advantages and limitation-chemical genetics-diversity based approach-*In silico* chemical genomics-Process optimization-Resources for chemical genomics (Pharmabase and MSDchem)

Reference Books:

Chemometrics and chemoinformatics. Washington, DC: American Chemical Society, 2005.

Bunin, Barry A. Chemoinformatics: Theory, Practice, and Products. Dordrecht: Springer, 2007.

Bajorath, Juergen, ed. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery. Totowa, N.J.: Humana Press, 2004.

Gasteiger, Johann; Engle, Thomas, eds. Chemoinformatics: A Textbook. Weinheim, Germany: Wiley-VCH, 2003.

Gasteiger, Johann, ed. Handbook of Chemoinformatics: From Data to Knowledge. Volume 4. Weinheim, Germany: Wiley-VCH, 2003.

Leach, Andrew R.; Gillet, Valerie J. An Introduction to Chemoinformatics. Dordrecht: Kluwer, 2003.

Oprea, Tudor I. Chemoinformatics in Drug Discovery. Weinheim: Wiley-VCH, 2005.

Pirrung, Michael C. Molecular Diversity and Combinatorial Chemistry: Principles and Applications. Amsterdam: Elsevier, 2004.

Ekins, Sean, ed. Computer Applications in Pharmaceutical Research and Development. Hoboken, N.J.: Wiley, 2006.

Ferenc Darvas, András Guttman, György Dormán. Chemical Genomics. Marcel Dekker Inc, New York, 2005.

John B. Taylor, Comprehensive Medicinal Chemistry (Volume I-VI). Pergamum Press, England, 2005.

ELECTIVE

PAPER – 3

A. GENETIC ALGORITHM

Objectives:

To know the application of genetic algorithms in science and engineering to solve practical problems and as computational models of natural evolutionary systems.

UNIT-I

Genetic Algorithms: An Overview - A Brief History of Evolutionary Computation - Elements of Genetic Algorithms - A Simple Genetic Algorithm - Genetic Algorithms and Traditional Search Methods.

UNIT-II

Genetic Algorithms in Problem Solving - Evolving Computer Programs - Data Analysis and Prediction - Search/Optimization method - Neural Network method.

UNIT-III

Gnetic algorithms (GA) in machine learning (computer programs, data analysis and prediction, neural networks) - GA in scientific models (interactions among learning, evolution, and culture; sexual selection; ecosystems; evolutionary activity).

UNIT-IV

Applications of Genetic Algorithms - in sequence analysis: Global and Local alignment - Needleman and Wunsch algorithm - Smith and Waterman algorithm - in protein analysis - Folding - Docking - Molecular design - Side chain modeling.

UNIT-V

Neural network - Concepts and secondary structure prediction - probabilistic models - Hidden Markov model - Heuristic approach - Gene identification and other applications.

Text Books

Melanie Mitchell, 1998. An Introduction to Genetic Algorithms.
Terresa K. Attwood and David J. Parry - Smith. Introduction to Bioinformatics.

Reference Books:

Richard Durbin, Sean Eddy, Anders Krogh and Graeme Mitchison, 1997. Biological sequence analysis: Probablistic models of proteins and nucleic acids. Cambridge University.

PAPER – 3

B. DRUG DISCOVERY

Unit-I

Methods and strategies involved in the drug discovery process: Identification potential drug targets-approaches to screening for lead molecules-Sources of lead molecules, including natural products, synthetic libraries, and in silico structure-based molecules-Lead optimization-Promise of personalized medicine.

Unit-II

Experimentation in drug discovery: High-throughput flow cytometry-Metal enhanced fluorescence-NMR-X-ray crystallography-Coupled luminescent methods-Molecular MR imaging

Unit-III

Combinatorial chemistry in drug discovery process-High throughput screening: evolution of technology and methods-QSAR models as tools for drug virtual screening-cell card systems for simulations of multiple cell lines

Unit-IV

Strategies and methods in monitoring and targeting protein-protein interactions-Protein kinase inhibitors in drug discover-GABA and glutamate receptor ligands and their therapeutic potentials-Targets and approaches for cancer drug discovery

Unit-V

Design and pharmaceutical applications of prodrugs- Cancer cell proteomics-strategies in the design of antiviral drugs-application of systems biology in drug discovery-RNA based therapy- Prodrugs and intellectual property rights

Reference Books:

Shayne Cox Gad, Drug discovery today. Wiley-Interscience, 2005.

An introduction to Computational Biochemistry. (C. Stain Tsai, A. John Wiley and Sons, Inc., publications).

Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Vol. 1. Principles and Practice, edited by M. E. Wolff, John Wiley & Sons: New York, 1995.

A Practical Guide to Combinatorial Chemistry, edited by A. W. Czarnik and S. H. DeWitt, American Chemical Society: Washington DC, 1997.

Principles of Medicinal Chemistry, 4th Edition, edited by W.O. Foye, T.L. Lemke, and D. A. Williams, Williams and Wilkins: Philadelphia, 1995.

Medicinal Chemistry: Principles and Practice, edited by F.D. King, Royal Society of Chemistry: Cambridge, 1994.

PAPER – 3

C. COMPUTATIONAL CHEMISTRY

Unit-I

Molecular Mechanics and Force Fields:Force fields, potential energy functions, inter and intramolecular interactions, empirical parameters- Molecular mechanics calculations, energy minimization, conformational analysis, vibrational frequencies, and normal mode analysis-Molecular Simulations: Monte Carlo Simulations-Importance sampling and Metropolis sampling-Basic algorithms and technical details- Moves

Unit-II

Molecular Dynamics Simulations: Equations of motion and force calculations- Diffusion-Integration schemes- Liquid Water-Models-Properties-Ensembles-Canonical and microcanonical Monte Carlo-Isothermal-isobaric Ensemble Monte Carlo-Grand-Canonical Ensemble Monte Carlo-Constant T and P molecular dynamics

Unit-III

Liquids: Solvents (Polar and nonpolar)-Solutions- Acidity and Basicity, and Computation of pKa-Continuum Solvation Models-Structure and Dynamics of Proteins: Protein Structure and PDB-Building Models for Protein Structure and Energy Calcultions-Normal Mode Analysis-Molecular Dynamics of Proteins

Unit-IV

Solvation: Free Energy Simulations.-Free Energy Perturbation-Free energy of solvation-Partition coefficients-Thermodynamic Integration and Umbrella Sampling-Potential of Mean Force for Condensed Phase Reactions-Hydrophobic Effects and Ion-Pair Interactions in Water

Unit-V

Quantum Mechanics: Gaussian and GaussView- Hartree-Fock Theory and Basis Sets-Semiempirical Methods- Electron Correlations-Density Functional Theory-Combined QM/MM Methods.- Why and How to Combine QM and MM-Solvation and Solvent Effects: Polarization-Reaction profiles in soluton-Protein-Ligand Interactions- Modeling Enzymatic Reactions

Reference Books:

A Computational Approach to Chemistry" David M. Hirst, Blackwell Scientific Publications, Oxford 1990

A Handbood of Computational Chemistry: A Practical Guide to Chemical Stucture and Energy Calculations" Tim Clark, Wiley-Interscience 1985.

Computer Simulation of Liquids" Allen and Tildesley, Oxford 1987

Computer Simulation Methods: Applications to Physical Systems" Gould and Tobochnik, Addison-Wesley 1988.

Computer Simulation of Biomolecular Systems: Theoretical and Experimental Applications vol. 1 and 2" van Gunsteren, Weiner, and Wilkinson, ESCOM 1993.

Bajorath, Juergen, ed. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery. Totowa, N.J.: Humana Press, 2004.

CORE PRACTICAL – IV

MOLECULAR MODELING AND PROGRAMMING

Simple genetic algorithm

Genetic algorithm and problem solving

Genetic algorithm in scientific models

Sequence alignment algorithm

Structure prediction - HM Model

Determination of Partition coefficient of established drugs by shake flask method to find out the distribution of drug. (2 to 3 experiments)

QSAR related experiments - calculation of molecular connectivity index values for Ibuprofen, Atropine, Propranalol, Epinephrine and methadone (Minimum of 3 experiments will be given for work out).

Molecular modeling experiments- Molecular Graphics (3D structure) - conformational analysis to correlate physicochemical parameters with biological activity using various molecular modeling software such as AMBER, CAMSEQ, FRODO and SYBL (minimum of 5 experiments will be given).

Study of Pharmacophore models by using software (2 experiments)

Designing a novel molecule and fitting with receptor for invitro activity evaluation - experiments related to this is given (minimum of 3 experiments)

Calculation of F and R substituent constants (2 experiments)

CORE PRACTICAL – V

GENOMICS AND PROTEOMICS

Data mining for retrieving information using NCBI, KEGG, PUBMED and BRENDA databases

Biological sequence analysis

Motif and domain analysis

Phylogenetic analysis

Protein structure prediction and validation

Protein structural alignment and classification

Protein function prediction

Sequence-structure-function prediction

CORE PRACTICAL – VI

DBMS AND BIOCOMPUTING

1. Study of DBMS, RDBMS and ORDBMS.
2. To study Data Definition language Statements.
3. To study Data Manipulation Statements.
4. Study of SELECT command with different clauses.
5. Study of SINGLE ROW functions (character, numeric, Data functions).
6. BioJava programming
7. Bioperl programming
8. RasMol script

SEMESTER IV

PAPER – 9

BIO-COMPUTING

UNIT-I

Cell - Basic unit of life - Cell types, Gene, Protein, Central dogma of Molecular biology, post transcription & translation modifications - Chromosome - Structure and function.

UNIT-II: Computer Basics

Introduction to Computer - History of Computers - Types - Operating System, File handling - Internet browsers - HTML, XML, Scripting language - Introduction to C - Data types, Running & compiling a C programme - I/O statements - Control Statement - Structure - Data files - Life Science application program.

UNIT-III: Introduction to Bio-Computing

Role of Computer in Biology - Future in Bio-Computing, Applications of Bio-Computing, Finding Articles and Journals - Search for technical reports & Conference Papers - Intelligent agent - Use of Intelligent Agent - Characteristics of Intelligent agent.

UNIT-IV: Bio-Informatics and Bio-Computing

Introduction to Bioinformatics - Definition - History - Applications in various field - Software related to bioinformatics - Downloading - Installing - Running - Data Mining - Biological database - Types - Sequence and Structure - Data bases.

UNIT-V: Application of Bio-Computing

Sequence searching - BLAST & FASTA - Multiple sequence alignment - ClustalW, finding evolutionary relationship between organism - Phytogenetic analysis (basic concepts only) - Phylip - Motifs & Domain search - CADD - Molecular Modeling.

Reference Books:

Bio-Computing by P.M.Pardalos, J.C.Principe, A.M.Lesla, Introduction to bioinformatics, 3rd Oxford University press,, New Delhi, 2007.

S.Parthasarathy, Essentials of Programming in C for Life Sciences, Anc Books India Pvt. Ltd., New Delhi, 2008

Bioinformatics Biocomputing and perl and Addison - wesly

Baxevanis: A practical guide of genes and proteins, Wiley - Interscience

Introduction to Bioinformatics, Teresa K.Atwood and David J.Parry-Smith

Andrew R Molecular modeling principles and applications Leach, Harlow

PAPER – 10

SYSTEMS BIOLOGY

Unit-I

E-CELL: Organization-History-Research group-modeling methods-formalism-techniques-numerical simulation algorithm-mathematical analysis methods-software environment-projects models-applications-chemotaxis-molecular clock-circadian rhythms-oxidation stress-multi-enzyme systems

Unit-II

Systems biology projects: Disease oriented models-T1Dbase-HDBase-technology development-software development-cytoscape-SBML-Repeat masker- Human Proteome Folding Project-Applications

Unit-III

CSD-DB: Organization-objectives-databases-general and database structure-statistics and mathematics-methodologies-software development and computer environment-software tools (SCECoR@CSD.DB-ECOCoR@CSD.DB)-service team-Transcriptome DB-mXP-GmD@CSD.DB

Unit-IV

Systems biology software project: About the project-model inter change-code use-bio-models-online services-SBML Layout viewer-SBML validation-simulation translator-model repository-SBW broker-Jurnac-J-designer-BioSpice-BioUMC-CellDesigner –Dizzy-Oscill8

Unit-V

Virtual cell project: Virtual cell NRCAM-Virtual cell software-modeling project-FRAP-Radiobiology software-Functional genomics and systems biology groups-virtual rice project-Yeast systems biology network-EST project of Systems biology-ERATS-Systems biology cancer project

Reference Books:

Hiroaki Kitano (editor). Foundations of Systems Biology. MIT Press: 2001. ISBN 0-262-11266-3

CP Fall, E Marland, J Wagner and JJ Tyson (Editors). "Computational Cell Biology." Springer Verlag: 2002 ISBN 0-387-95369-8

G Bock and JA Goode (eds).In Silico" Simulation of Biological Processes, Novartis Foundation Symposium 247. John Wiley & Sons: 2002. ISBN 0-470-84480-9

E Klipp, R Herwig, A Kowald, C Wierling, and H Lehrach. Systems Biology in Practice. Wiley-VCH: 2005. ISBN 3-527-31078-9

L. Alberghina and H. Westerhoff (Editors) – Systems Biology: Definitions and Perspectives, Topics in Current Genetics 13, Springer Verlag (2005), ISBN 13: 978-3540229681

A Kriete, R Eils. Computational Systems Biology., Elsevier - Academic Press: 2005. ISBN 0-12-088786-X

K. Sneppen and G. Zocchi, (2005) Physics in Molecular Biology, Cambridge University Press, ISBN 0-521-84419-3

D. Noble, The Music of life. Biology beyond the genome Oxford University Press 2006. ISBN-10: 0199295735, ISBN-13: 978-0199295739

Z. Szallasi, J. Stelling, and V.Periwal (eds.) System Modeling in Cellular Biology: From Concepts to Nuts and Bolts (Hardcover), MIT Press: 2006, ISBN 0-262-19548-8

B Palsson, Systems Biology - Properties of Reconstructed Networks. Cambridge University Press: 2006. ISBN 978-0-521-85903-5

K Kaneko. Life: An Introduction to Complex Systems Biology. Springer: 2006. ISBN 3540326669

ELECTIVE

PAPER – 4

A. 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 - Species 2000 and Tree of life.

UNIT-IV

Software for identification of Accessing 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 tariffs.

Text Books:

Kevin J. Gaston and John I. Spicer. Biodiversity - An introduction

Agarwal., K.C., Biodiversity

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.

Biodivesity: Measurement & Estimation - Hawkswoth, D.I. (Ed.) (1995), Chapman & Hall, London.

Alice , 1990. A Bio-Diversity 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, Campinas, Brazil.

Uhlir, P.F,. 1980. The Public international law of Civilian remote sensing: an overview. In: Mink, P.D. (ed), American Enter Prise, The law, and the commercial use of spece, Vol II. National Legal Center for the Public Interest, Washington, Dc.

Heywood, V.H., Watson, R.T. 1995. Global Biodiversity Assessment. Published for the United Nations Environment Programme, Cambridge University Press, Cambridge.

Web Resource

www. Biodiv.org

www.wri.org/wri/biodiv/

www.wcmc.org.uk/

PAPER – 4

B. IPR AND BIOSAFETY

Unit-I

Introduction to Intellectual Property-Types of IP: Patents, Trademarks, Copyright & Related Rights, Industrial Design, Traditional Knowledge, Geographical Indications, Protection of New GMOs; International framework for the protection of IP IP as a factor in R&D; IPs of relevance to Biotechnology and few Case Studies; Introduction to History of GATT, WTO, WIPO and TRIPS

Unit-II

Concept of 'prior art' Invention in context of "prior art"; Patent databases; Searching International Databases; Country-wise patent searches (USPTO, EPO, India etc.); Analysis and report formation

Unit-III

Basics of Patents-Types of patents; Indian Patent Act 1970; Recent Amendments; Filing of a patent application; Precautions before patenting-disclosure/non-disclosure; WIPO Treaties; Budapest Treaty; PCT and Implications; Role of a Country Patent Office; Procedure for filing a PCT application

Unit-IV

Patent filing and Infringement-Patent application- forms and guidelines, fee structure, time frames; Types of patent applications: provisional and complete specifications; PCT and convention patent applications; International patenting-requirement, procedures and costs; Financial assistance for patenting-introduction to existing schemes; Publication of patents-gazette of India, status in Europe and US Patenting by research students, lecturers and scientists-University/organizational rules in India and abroad, credit sharing by workers, financial incentives-Patent infringement- meaning, scope, litigation, case studies and examples

Unit-V

Biosafety Introduction; Historical Background; Introduction to Biological Safety Cabinets; Primary Containment for Biohazards; Biosafety Levels; Biosafety Levels of Specific Microorganisms; Recommended Biosafety Levels
for Infectious Agents and Infected Animals; Biosafety guidelines - Government of India; Definition of GMOs & LMOs; Roles of Institutional Biosafety Committee, RCGM, GEAC etc. for GMO applications in food and agriculture; Environmental release of GMOs; Risk

Analysis; Risk Assessment; Risk management and communication; Overview of National Regulations and relevant International Agreements including Cartagena Protocol.

Important Links

http://www.w3.org/IPR/

http://www.wipo.int/portal/index.html.en

http://www.ipr.co.uk/IP_conventions/patent_cooperation_treaty.html

www.patentoffice.nic.in

www.iprlawindia.org/ - 31k - Cached - Similar page

http://www.cbd.int/biosafety/background.shtml

http://www.cdc.gov/OD/ohs/symp5/jyrtext.htm

http://web.princeton.edu/sites/ehs/biosafety/biosafetypage/section3.html

PAPER – 4

C. PROTEIN ENGINEERING

Unit-I

Fundamentals of protein structures and classes – Protein structure determination – Protein folding pathways and mechanism – Molecular evolution of protein family and diversity

Unit-II

A survey of protein structure and function-Evolution of globins – NAD binding domains-visual pigments – Principles of enzyme catalysis – Enzyme mechanisms: Substrate binding, transition state stabilization and catalysis- Polypeptide folding, protein stability and subunit interaction

Unit-III

Basic outline of protein engineering – Site directed mutagenesis and its application – Directed evolution strategies: Screening and selection methods-mutant library construction-SeSaM method-Identifying target sites for mutagenesis-Diels-Alder reaction-Engineering enzymes for biocatalysts

Unit-IV

Protein engineering and mutant databases – Protein and engineering and designing algorithms-Online protein engineering tools – Software packages for protein engineering

Unit-V

Bacterial and phage display technologies- Catalytic antibodies –Epitope mapping and vaccine development – Protein engineering in drug designing – Artificial and Synthetic enzymes

Reference Books:

Alberghina L (2003) *Protein Engineering in Industrial Biotechnology*, Harwood Academic Publishers.
Boune PE and Weissig H (2003) *Structural Bioinformatics*, Wiely-Liss,Inc, New York.
Cleland JL and Craik CS (1996) *Protein Engineering: Principles and Practice*, Wiley-Liss.
Fersht A (1999) *Structure and Mechanism in Protein Science*, W.H. Freeman and Company, New York.
Lesk AM (2004) *Introduction to Protein Science*, First edition, Oxford University Press.
Primrose SB (1992) *Molecular Biotechnology*, 2nd Edition, Wiely and Sons Ltd.

CORE PRACTICAL – IV

MOLECULAR MODELING AND PROGRAMMING

1. Data mining for retrieval of ligand information
2. Data mining for retrieval of protein-ligand complex information
3. Data mining for retrieval of drug-related information
4. Molecular modeling of macromolecules
5. Prediction of binding packets of receptor
6. Ligand designing and conformational analysis
7 .Molecular docking and analysis
8. Molecular energy computation and minimization
9. Molecular dynamic simulation
10. QSAR tools in drug discovery (QSAR WORLD)
11. Bioactivity analysis

CORE PRACTICAL – V

GENOMICS AND PROTEOMICS

Comparative genomic analysis
Comparative genome annotation
Genome annotation
Bacterial operon prediction
Gene prediction
Promoter and regulan prediction
Phylogenetic foot printing analysis
Prophage prediction
Transposan prediction
DNA repeats prediction
Identification of disease locus
Identification of gene marker locus
Prediction of secondary structure of rRNA
Sequence assembly and finishing
Cloning vector construction
Gene order prediction
Identification of coding region
Identification of mutations in genes
Identification of recombination points in microbial populations
Recombination frequency analysis
Prediction phenotypes of a genome
Comparative metabolomics analysis
Metabolic pathway prediction
Metabolic reaction and pathway construction
Protein network prediction
Protein bulk properties prediction
Protein modification site prediction
2D gel data analysis
Microarray data analysis
Mass spectroscopy data analysis
Microbial strain improvement by Systems Biology Workbench

CORE PRACTICAL – VI

DBMS AND BIOCOMPUTING

Study of GROUP functions (avg, count, max, min, Sum).

Study of various type of SET OPERATORS

(Union, Intersect, Minus).

Study of various type of Integrity Constraints.

Study of Various type of JOINS.

To study Views and Indices.

SBML script

Enzyme script

Gepasi script

Metabolic flux analysis

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