

BHARATHIDASAN UNIVERSITY, TIRUCHIRAPPALLI – 620 024.

M. Sc. Bioinformatics - Course Structure under CBCS

(For the candidates admitted from the year 2005-2006 onwards)

Seme ster	Course	Course Title	Ins. Hrs / Week	Credit	Exam Hrs	Marks		Total
						Int.	Ext.	
I	Core Course – I (CC)	Biological Systems	6	4	3	25	75	100
	Core Course – II (CC)	Molecular Biology and Genetic Engineering	6	4	3	25	75	100
	Core Course – III (CC)	Computer Programming	6	4	3	25	75	100
	Core Course – IV (CC)	Practicals –I: Computer Programming	6	4	3	25	75	100
	Elective Course – I (EC)	---	6	4	3	25	75	100
II	Core Course – V (CC)	Bioinformatics-I: Computational Biology	6	4	3	25	75	100
	Core Course – VI (CC)	Mathematical and Statistical Techniques	6	4	3	25	75	100
	Core Course – VII (CC)	Practicals - II: Bioinformatics and Computational Biology	6	4	3	25	75	100
	Elective Course – II (EC)	---	6	4	3	25	75	100
	Extra Disciplinary Course – I (EDC)	---	3	2	3	25	75	100
	Extra Disciplinary Course – II (EDC)	---	3	2	3	25	75	100
III	Core Course – VIII (CC)	Bioinformatics -II: Experimental Techniques for Biomolecules	6	4	3	25	75	100
	Core Course – IX (CC)	Genomics and Proteomics	6	4	3	25	75	100
	Core Course – X (CC)	Biophysics and Stereochemistry	6	4	3	25	75	100
	Core Course – XI (CC)	Practicals - III : Advanced Bioinformatics Lab	6	4	3	25	75	100
	Elective Course – III (EC)	---	6	4	3	25	75	100
IV	Core Course – XII (CC)	Database Management System	6	4	3	25	75	100
	Project Work Viva voce 25 marks Dissertation 75 marks	----	24	8	-	-	-	100
			120	72				

The Department of Bioinformatics will offer the following Elective Courses :

1. Information Management
2. Molecular Modelling and Drug Design
3. Applied Bioinformatics

The Department of Bioinformatics will offer the following Extra Disciplinary Courses :

1. Basic Bioinformatics
2. Bioinformatics Algorithms

SEMESTER – I

CC - I BIOLOGICAL SYSTEMS

UNIT – I

Biology of Cells : Prokaryotic and Eukaryotic cells – E. coli & Yeast – Cell organelles - Differences and similarities in plant and animal cells – Principles of Membrane organization – Membrane proteins – Types of Cell function – Cell division, mitosis & meiosis

Cell Transport, across plasma membrane, mechanisms of transport, transport in animals, transport in vascular plants.

UNIT – II

Cell Energetics and respiration : Energy, life's driving force, energy capture – photosynthesis, role of ATP in energy cycle - Fats and protein as alternate energy sources.

Key Biomolecules – lipids, polysaccharides, proteins, nucleic acids – chemical bonds in biomolecules – hydrogen bond - peptide bond – phosphate bond

UNIT – III

Overview of protein and nucleic acid structure – Levels of protein structure - α -helix, β -sheet and β -turns – Ramachandran Map - Super secondary structures – Domains - quaternary structure.

DNA and RNA structure - helical structures of DNA - Watson and Crick model – Different forms of DNA - A, B and Z forms - RNA secondary structure - DNA as genetic material, genes in action, gene regulation.

UNIT – IV

Life Diversity and Evolution : Prokaryotes and viruses, fungi, molds and lichens - origin of species - macro evolution.

Plant diversity and animal diversity – Management of Plant Biodiversity – Principles and Practice – Biodiversity Information – Management and Communication – Databases on Biodiversity

UNIT – V

Biology of Environment : Basic ecological principles, population ecology, community ecology – Principle of animal behaviour, social behaviour, food chain & food-web in ecosystem, human impact on world ecosystems, importance of biodiversity in homeostasis of an ecosystem.

Emerging areas in Biology : Transgenic and knock out mice technology, in vitro fertilization.

Reference Books

Lehninger A.L., Principles of Biochemistry, CBS Publishers and Distributors, New Delhi, 1984.

Krishnamurthy K.V., An Advanced Textbook on Biodiversity – Principles and Practice, Oxford & IBH Publishing Co. Pvt. Ltd., New Delhi, 2003.

J. M. Berg, J.L. Tymoczko and L. Stryer, Biochemistry, 5th Edition W.H. Freeman, 2002.

Mukherji, S. and Ghosh, A.K., Plant Physiology : Tata McGraw Hill Publishing Company Limited, New Delhi, 1996.

Rastogi, S.C., Biochemistry, Tata McGraw Hill Publishing Company Limited, New Delhi, 1993.

Sharma, P.D., Elements of Ecology, Rastogi Publications, Meerut, 1989.

CC - II MOLECULAR BIOLOGY AND GENETIC ENGINEERING

UNIT – I

DNA replication – transcription and translation – codon and anticodon concepts – inhibitors of transcription and translation

Gene as the unit of expression – spontaneous mutation, induced mutation – reversed and suppression mutation – DNA repair mechanism

UNIT – II

Gene regulation – operon concept – lac, trp – promotor, attenuator – terminator and operator – transcription factors – allosteric enzymes and feed back inhibition – repression.

Mendelian laws – Sex chromosome and sex-linked inheritance – linkage and crossing over and genetic mapping of chromosomes – transformation, conjugation, transduction.

UNIT – III

Basics of recombinant DNA technology – Introduction to cloning, cloning vectors – expression of the clones, gene selection, maximizing gene expression, restriction enzymes and mapping of DNA, plasmid & phage vectors

UNIT – IV

DNA sequencing – DNA sequencing by base specific cleavage and by primed enzymatic synthesis – insertions and deletions – chromosomal structure function in prokaryotes and eukaryotes – chromosome walking, selection, immunological identification of clones – PCR & RFLP, RAPD techniques, bio-chips and DNA finger printing

UNIT – V

Applications of recombinant DNA technology – commercial aspects of recombinant proteins - cloning in plants – direct transfer of DNA into plant cells – transgenic plants – transgenic animals – gene transfer by nuclear injection – gene therapy – pharmaceuticals – anti-sense RNA technique.

Reference Books

1. Benjamin Lewin, Genes VIII, Pearson - Prentice Hall International Edition, New Delhi, 2004.
2. Freifelder D. Molecular Biology, Jones and Bartlett Publishers Inc. 1987.
3. Watson, J.D., et al., Recombinant DNA, 2nd ed. Scientific American Books, New York, 1992.
4. Winnacker E. L. From Genes to Clones, VCH Weinheim, Germany, 1987.
5. Prokop, Ales, Bajpai, Rakesh K., and Ho, Chester S., Recombinant DNA Technology and Applications, McGraw-Hill, New York, 1991.

CC – III COMPUTER PROGRAMMING

UNIT – I

Identifiers and Keywords - Constants, Variables and Data types - Operators and expressions - Data Input and Output - Control Structures - *if* and *switch* statements - *while*, *do-while* and *for* statements - *goto* statement - Arrays - Character strings - Simple programs

UNIT - II

User defined Functions - 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 - III

User defined data types - 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

UNIT - IV

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

UNIT – V

PERL – string comparison – searching databases – string manipulation programs – BioPERL – fundamentals – applications of BioPERL.

Reference Books

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

2. Brian W. Kernighan and Dennis. M. Ritchie, The C Programming Language, Second Edition, Printice-Hall of India, 1988.
3. Sumitabha Das, UNIX Concepts and Applications, 3rd Edition, Tata McGraw-Hill, New Delhi, 2003.
4. L.Wall, T.Christiansen and J.Orwant, Programming Perl, 3rd Edition, O'Reilly, 2000.
5. J. Tisdall, Mastering Perl for Bioinformatics, O'Reilly, 2003.
6. <http://bio.perl.org/>

CC – IV PRACTICALS – I : COMPUTER PROGRAMMING

1. Sum of the digits of a given number.
2. Fibonacci number generations.
3. Factorial of a given number
4. Sorting numbers
5. Sorting names in alphabetical order
6. Reversing a given string
7. Checking for palindrome
8. Mean, median, mode and standard deviation calculations.
9. Storing and retrieving amino acid sequences using structure data types
10. Swapping two values using pointers
11. Computing amino acid composition of a given protein sequence (using pointers and structure data types)
12. Finding sequence patterns using PERL.
13. String Comparison using PERL/Bio PERL
14. Creating a web page to get protein sequence data and compute and display amino acid composition
15. Creating a web page to get nucleic acid sequence data and compute and display base composition

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

SEMESTER – II

CC – V Bioinformatics - I : Computational Biology

UNIT - I

Analysis of DNA and Protein Sequences - distributions, frequency statistics– Protein and Nucleic Acid Sequence Databases – PIR, Swiss-prot, GenBank – pattern and motif searches - BLOCKS, PRINTS, PFAM – Structure Databases – PDB - Structure – Classification, alignment and analysis – SCOP, CATH, FSSP

UNIT - II

Sequence alignment: Scoring matrices- PAM and BLOSUM- Local and Global alignment concepts - dynamic programming methodology-Needleman and Wunsch algorithm, Smith-Waterman algorithm - Statistics of alignment score - Multiple sequence alignment – Progressive alignment – Databases searches for homologous sequences - FASTA and BLAST

UNIT – III

Protein Secondary structure prediction – Chou-Fasman, Garnier-Osguthorpe-Robson (GOR) methods – Predicting 3D structure – comparative (homology) modeling, threading (fold recognition) and ab initio methods – Rosetta – CASP – Protein structure visualization tools – RasMol, Swiss PDB Viewer

UNIT - IV

Fragment assembly - Genome sequence assembly - Gene finding methods: content and signal methods - Background of transform techniques – Fourier Transform and gene prediction – Analysis and prediction of regulatory regions - Neural network concepts and secondary structure prediction - Probabilistic models: Markov chain – random walk - Hidden Markov models – Gene identification and other applications.

UNIT - V

Evolutionary analysis: distances - clustering methods - rooted and un-rooted tree representation - Bootstrapping strategies – phylogenetic trees – PHYLIP.

Reference Books

1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi (2003).
2. D. Higgins and W. Taylor (Eds), Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi (2000).
3. R. Durbin, S.R. Eddy, A. Krogh and G. Mitchison, Biological Sequence Analysis, Cambridge Univ. Press, Cambridge, UK (1998).
4. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ (1998).
5. Michael S. Waterman, Introduction to computational Biology, Chapman & Hall, (1995).
6. C. Gibas and P. Jambeck, Developing Bioinformatics Computer Skill, 1st Edition, O'Reilly, 2001.

CC – VI MATHEMATICAL AND STATISTICAL TECHNIQUES

UNIT – I

Nature of biological and clinical experiments – collection of experimental data - Measures of central tendency of a set of observations - Purpose of statistical investigations - arithmetic mean - mean of grouped data - median – mode - range, mean deviation, variants and standard deviation.

UNIT – II

Correlation and Regression - Scatter diagram – Karl Pearson's Coefficient of Correlation - Correlation Coefficient for a bivariate frequency distribution - Rank correlation - Linear regression - Principles of least squares – Student's 't' test for mean, difference of means – paired 't' test for difference of means – test for correlation and regression coefficients – Chi-square test for goodness of fit and independence of attributes - Simple problems based on biochemical data.

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 distribution – Z-score, P-value and E-value – Hidden Markov models - applications in biology.

UNIT – IV

Matrices : Matrix algebra – Types of matrices – determinant – inverse, rank of matrix – solution of simultaneous equations.

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 – applications.

Reference Books

1. S.C. Gupta and V.K. Kapoor, Fundamentals of Mathematical Statistics, 11th Edition, Sultan Chand & Sons, New Delhi, 2002.
2. D.W. Jordan and P. Smith, Mathematical Techniques, Oxford University Press, New Delhi, 1997.
3. L. Forthofer, Introduction to Biostatistics, Academic Press, 1995.
4. Robert R. Sokal and F.J. Rohlf, Introduction to Biostatistics (Biology-Statistics Series), W.H. Freeman & Company, New York, 1987.
5. E. Batschelet, Introduction to Mathematics for Life Scientists, 2nd Edn., Springer International Student Edn., Narosa Publishing House, New Delhi, 1991.

CC - VII Practicals II : Bioinformatics and Computational Biology

1. Study of Internet resources in Bioinformatics - E.g. NCBI, ICGB, EMBL-EBI.
2. Searches on NCBI - PubMed bibliographic databases. Concept of boolean operators.
3. Expert Protein Analysis System (ExPASy) – Primary & Secondary structure tools - analysis & prediction
4. Multiple alignment – Domain / Motif databases – BLOCKS, PRINTS, SBASE and PFAM
5. Protein Structure and Classification databases – PDB, SCOP, CATH, FSSP, PDBSUM
6. Evaluation of protein structure by Swiss PDB viewer or by any other suitable programs like Insight-II.
7. Calculation of phi – psi angles and Ramachandran plot for a given protein structure.
8. Comparison of 3D structures of proteins and nucleic acids – RMSD values.
9. Calculation of mean, median, mode, variance and standard deviation.
10. Regression analysis and plotting of graphs, bar diagrams, pi charts.

SEMISTER – III

CC-VIII Bioinformatics – II : Experimental Techniques for Biomolecules

UNIT – I

Isolation and purification of proteins - Crystallisation of protein – Crystal Structure – Bravais Lattice – Symmetry elements and operations – Point groups – Space groups – Bragg's law – X-ray diffraction - Proteins structure determination by X-ray

diffraction - Phase determination - Calculation of electron density map - Interpretation of electron density map - Refinement of the structures - Electron crystallography of proteins.

UNIT – II

Electronic energy levels – electronic transitions – selection rules – types of spectra – IR, UV – visible spectroscopy - Measurement of Infrared (IR) spectrum – Theory of IR spectroscopy – IR spectra of polyatomic molecules – biological examples – Theory of UV - visible spectroscopy – application of UV spectra to proteins – measurement of molecular dynamics by fluorescence spectroscopy

UNIT – III

The principle of Nuclear Spin – Spin flipping – theory of Nuclear Magnetic Resonance – spectral parameters in NMR – intensity, chemical shift, spin-spin coupling, relaxation times, line widths, nuclear Overhauser effect (NOE), chemical exchange, paramagnetic centers – application of NMR in biomolecular structure determination.

UNIT - IV

Principles of electrophoresis – SDS PAGE – Molecular weight determination of proteins - 2D-gel electrophoresis – capillary electrophoresis - principles of chromatography – Gel & ion exchange chromatography – applications

UNIT – V

Micro array techniques and their applications in biology - Mass spectroscopy - ESI and MALDI-TOF - protein finger printing.

References Books

1. W.Kemp, organic spectroscopy, 3rd edition, ELBS, McMillan, London, 1991.
2. C.N.Banwell and E.M.McCash, fundamentals of molecular spectroscopy, 4th edition, Tata McGraw Hill, New Delhi, 1995.
3. I.Howe, D.H.Williams and R.D.Bowen, Mass Spectrometry, principles and applications, 2nd edition, McGraw Hill, London, 1981.

4. Mass Spectroscopy for Biotechnology by Gary Siuzdak, Academic Press, 1995
5. Basic HPLC and CE of Biomolecules by Cunico, Gooding and Wehr, Bay Bioanalytical Lab, 1998.
6. Principles of Physical Biochemistry by Van Holde, Prentice Hall, 2000.
7. Helen C. Causton, John Quackenbush and Alvis Brazma, A Beginner's Guide: Microarray Gene Expression Data Analysis, Blackwell Publishing, USA, First Indian Reprint, 2004.
8. Vasantha Pattabhi and N. Gautham, Biophysics, Narosa Publishing House, New Delhi, 2002.

CC - IX GENOMICS AND PROTEOMICS

UNIT - I

Genome map & types – Polymorphic markers – Genome database (GDB) – NCBI Entrez Human genome map viewer – Online Mendelian Inheritance in Man (OMIM) – Mouse Genome database – Annotation of Genome – structural annotation – gene prediction approaches – Open Reading Frame (ORF) prediction – Hidden Markov Model – Pattern discrimination – Prediction of promoter sequences – Functional annotation – prediction of gene function – sequence similarity – gene family and metabolic pathway – conserved domain, Profile and motif comparison – EST comparison.

UNIT – II

Genome diversity – taxonomy and significance of genomes – Bacterial, Yeast, Coenorabditis, Homo sapiens, Arabidopsis thaliana.
Comparitive genomic databases – PEDANT, Cluster of Orthologous Groups (COG), Kyoto Encyclopedia of Genes and Genomes (KEGG) – Metabolic reconstruction.

UNIT – III

Human genome and genomic analysis – sequence repeats, transposable elements, gene structure, pseudogenes – Gene analysis – gene order – chromosome rearrangement – compositional analysis – clustering of genes – composite genes.

UNIT – IV

Introduction to Proteome - proteome and technology - information and the proteome – Primary attributes for protein identification - protein species of origin - Protein N- and C-terminal sequence tags - cross species protein identification - Modifications that influence protein change on 2-D PAGE - Detection and analysis of co- and post-translational modification.

UNIT - V

Proteome databases: protein sequence database, SWISS-PROT, TrEMBL, specialized protein sequence databases, PROSITE, BLOCKS, 2-D PAGE databases, PDB, genomic databases, OMIM, Metabolic databases, Some specific metabolic databases - application of proteomics to medicine, proteomics, toxicology and Pharmaceuticals

Reference Books

1. Wilkins M.R., Williams K.L., Appel D.F., Hochstrasser (eds) 1997. Proteome Research: New Frontiers in Functional Genomics Springer- Verlag Berlin Heidelberg, New York.
2. Bentley D.R., in Genomics (eds Dixon G.K., Coppin L.G. and Living Stone D.), Bios Scientifics, London, 1998.
3. Bauw, G. and Monatgu, M.V., in Differenmtially expressed genes in plant: A bench manual (eds Hansen, E and harper G.), Taylor and Francis, London, 1997.
4. T. A. Brown, Genomes, 2nd Edition, BIOS Scientific Publishers, Ltd., Oxford, UK, 2002.
5. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001.
6. Eugene V. Koonin and Michael Y. Galperin, Sequence, Evolution Function, Computaional Approaches in Comparative Genomics, Kluwer Academic Press, Massachuttes, 2003.
7. Jenson, O.N., in Proteomics. A Trends Guide (eds Black Stock, Co- and Mann), Elsevier Science, London, 1998.

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

CC – X BIOPHYSICS AND STEREOCHEMISTRY

UNIT – I

Levels of structures in biological macromolecules – Central questions in biophysics – basic strategies in biophysics

UNIT – II

Conformational Analysis – Forces that determine protein and nucleic acid structure, polypeptide chain geometries – Ramachandran Map – potential energy calculations – observed values for rotation angles – hydrogen bonding – hydrophobic interactions and water structure – ionic interactions – disulphide bonds – prediction of protein structure

UNIT – III

Nucleic acids – general characteristics of nucleic acid structure – geometries, glycosidic bond – rotational isomers and ribose puckering - forces stabilizing ordered forms – base pairing – base stacking – tertiary structure of nucleic acids

UNIT – IV

Stereochemistry : Principles – Chirality, Symmetry in organic compounds, Molecular isomerism : Time scales and energy criteria, conformational principles, conformational space, Types of movements – vibrational, Rotational, torsion angles, Conformational analysis, calculation of surface areas, Volumes and radius of biomolecules.

UNIT – V

Application of stereochemical principles : Conformation of open chain compounds, Chiral compounds, Macromolecular stereochemistry, Determination of relative and absolute configuration.

Reference Books

1. C.R.Cantor & P.R.Schimmel, Biophysical Chemistry Part - I, W.H. Freeman & Co., in San Fransisco, 1980.
2. C. Branden and J. Tooze, Introduction to Protein Structure, Garland Publishing Inc., New York., 1991.
3. R. Glaser, Biophysics, Springer, 2000.
4. Stereochemistry of Organic Compounds by Ernest. L.Eliel etal., John Wiley & Sons, 1994.
5. Stereochemistry – Conformation & Mechanism by P.S.Kalsi, New Age International Ltd., 1990.

CC – XI PRACTICALS - III : ADVANCED BIOINFORMATICS LAB

1. Introduction to sequence data banks - Protein sequence databank, NBRF-PIR, Swiss-PROT, Signal peptide databank, UniPROT.
2. Nucleic acid sequence databanks – GenBank, EMBL nucleotide sequence databank, DDBJ, AIDS virus sequence databank, rRNA data bank, UniGene.
3. Pairwise alignment - Global alignment using Needleman-Wunsch algorithm – source code development & testing
4. Pairwise alignmen t- Local alignment using Smith-Waterman algorithm - source code development & testing
5. BLAST, FASTA algorithms to search and analyze sequence databank.
6. Multiple alignment - CLUSTALW
7. Phylogenetic Trees - PHYLIP
8. Build a structure for a given sequence using Homology modeling
9. Generate a hydropathy profile for a given protein sequence
10. Compute the dot matrix plot to detect internal repeats in a protein/DNA sequence.

SEMISTER – IV

CC - XII: DATABASE MANAGEMENT SYSTEMS

UNIT - I

Introduction- purpose of database system- data models- database languages- Transaction management – Storage management- DBA- database users- system structure.

UNIT - II

E-R model- Hierarchical model- Network Model.

UNIT - III

Structural Relational databases- Relational Algebra - Tuple Relational Calculus- Domain Relational Calculus, Relational Commercial languages (SQL, QBE, Quel, etc.) - MySQL – database creation – modification - searching – simple programs – - Integrity constraints- Normalization.

UNIT - IV

Indexing and Hashing- Query Processing- Concurrency Control- Security- Sequence analysis, Sequence Data Banks, Structural Data banks - DOS, Windows and UNIX based sequence analysis packages. Analysis Tools for Data Banks - BLAST, FASTA etc.

UNIT - V

Advanced Database Concepts - Emerging Applications in Genomic databases.

Reference Books

1. Abraham Silberchatz, Henry F. Korth, S. Sudharshan, Database System Concepts (5th Edition), McGraw Hill, 2005.
2. Elisa Bertino and Lorenzo Martino, Object-Oriented Database Systems: Concepts and Architectures, 1st edition, Addison-Wesley Longman Publishing Co., Inc. Boston, USA, 1993.

3. Vikram Vaswani, The Complete Reference MySQL, Tata McGraw-Hill, New Delhi, 2002.

CC – XIII PROJECT WORK

Dissertation - 75 Marks

Viva - 25 Marks

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EC - I INFORMATION MANAGEMENT

UNIT – I

Information and related notions - Information content - Information entropy - generalized notion of the amount of entropy.

UNIT – II

The nature of information - Role of images - Image formation by individuals and groups - Image through communication data - Structure of information.

UNIT – III

The information transfer network - Transactions - Configuration and characteristics of transactions - Information system and its overall structure.

UNIT – IV

Software for Informatics: Bibliographic and subject specific - Hardware for Informatics : recognizers, compressions, modular design.

UNIT – V

Programming Style: Structured programming concepts - Modular design -System analysis and design: Software life cycle, waterfall model.

References Books

1. D. Soergel, Organizing Information – Principles of databases and retrieval Systems, Academic press, 2000.
2. Charles T.Meadow, Bert R.Boyce and Donald H.Kraft, Text Information Retrieval Systems, Academic Press, 2000.

EC – II MOLECULAR MODELLING AND DRUG DESIGN

UNIT - I

Introduction to the concepts of molecular modeling – Molecular structure and internal energy - Application of molecular graphics – Energy minimization of small molecules – Empirical representation of molecular energies – Use of force fields and the molecular mechanics method –Discussion of global energy minima.

UNIT - II

The techniques of molecular dynamics and Monte Carlo Simulation for conformational analysis - ab initio – Density-Functional Theory and semiempirical methods.

UNIT - III

Macromolecular modeling. Design of ligands for known macromolocular target sites. Drug-receptor interactions. 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.

UNIT – IV

Finding new drug targets to treat disease - New targets for anti-cancer drugs, - Drugs that rescue mutant p53's.

UNIT – V

Enzyme background – Theories of enzyme inhibition - Enzyme inhibition as a tool for drug development – Structured-based drug design - Examples.

Reference Books

1. Andrew Leach, *Molecular Modelling: Principles and Applications* (2nd Edition), Addison Wesley Longman, Essex, England, 1996.
2. Alan Hinchliffe, *Modelling Molecular Structures*, 2nd Edition, John-Wiley, 2000.
3. Alan Hinchliffe, *Molecular Modelling for Beginners*, John-Wiley, 2003.
4. N. Cohen (Ed.), *Guide Book on Molecular Modeling in Drug Design*, Academic Press, San Diego, 1996.
5. D. Frenkel and B. Smit, *Understanding Molecular Simulations. From Algorithms to Applications*. Academic Press, San Diego, California, 1996.
6. C. Rauter and K. Horn, *X-ray crystallography and drug design*, Elsevier, 1984.
7. M. Kalos and P. A. Whitlock. *Monte Carlo Methods*. John Wiley & Sons, New York, 1986.
8. J.A. McCammon and S.C. Harvey. *Dynamics of Proteins and Nucleic Acids*. Cambridge University Press, Cambridge, 1987.
9. D.C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge University Press, Cambridge, England., 1995.

EC – III APPLIED BIOINFORMATICS

UNIT – I

Commercial bioinformatics - Definition of bioinformatics company – Bioethics and Biosafety.

UNIT – II

Genome technology - high throughput sequencing and assembly - Micro arrays and genome wide expression analysis - transcriptome, proteome.

UNIT – III

Genomics in medicine - diseases monitoring - profiles for therapeutic molecular targeting - Diagnostics drug discovery and genomics.

UNIT – IV

Pharmacogenomics and its applications - SNPs and their applications - Proteomics in medicine therapeutic target identification.

UNIT – V

Comparative proteomics and its applications - Patenting and the data generation from patent literature for commercial benefits - IPR and bioinformatics - Bioinformatics patents.

Reference Books

1. T. A. Brown, Genomes, 2nd Edition, BIOS Scientific Publishers, Ltd., Oxford, UK, 2002.
2. Jenson, O.N., in Proteomics. A Trends Guide (eds Black Stock, Co- and Mann), Elsevier Science, London, 1998.
3. S.R.Pennington and M.J.Dunn, Proteomics, Viva Books Pvt. Ltd., New Delhi, 2002.
4. Relevant papers from Drug Discovery Today - Trends journals

M.Sc. BIOINFORMATICS

EDC – I BASIC BIOINFORMATICS

UNIT – I

Bioinformatics – An overview, Definition & History; Information Networks – Internet in Bioinformatics – Bioinformatics databases & tools on the Internet.

UNIT – II

Proteins – Amino acids – Peptide bond — Levels of protein structure - α -helix, β -sheet and β -turns – Ramachandran Map - Super secondary structures – Domains - quaternary structure - DNA and RNA structure - Watson and Crick model - A, B and Z forms of DNA - RNA secondary structure.

UNIT – III

Biological Sequence analysis – Pairwise sequence comparison – Sequence queries against biological databases – BLAST and FASTA - Multiple sequence alignments - Phylogenetic alignment.

UNIT - IV

Protein structure visualization tools – RasMol, Swiss PDB Viewer - Structure – Classification, alignment and analysis – SCOP, CATH, FSSP

UNIT - V

Genomics and Proteomics – Sequencing genomes– Genome databases on the web.

Text Books

1. T.K. Attwood and D.J. Parry-Smith, *Introduction to Bioinformatics*, Pearson Education Ltd., New Delhi (2004).
2. D.R. Westhead, J.H. Paris and R.M. Twyman, *Instant Notes: Bioinformatics* – Viva Books Private Ltd, New Delhi (2003).
3. Arthur M. Lesk, *Introduction to Bioinformatics*, Oxford University Press, New Delhi (2003).
4. D. Higgins and W. Taylor (Eds), *Bioinformatics- Sequence, structure and databanks*, Oxford University Press, New Delhi (2000).

EDC – II BIOINFORMATICS ALGORITHMS

UNIT – I

Algorithms – Definition and Example – Biological algorithms versus Computer algorithms – Types of algorithms – iterative, recursive, fast and slow algorithms – Running time of an algorithm – Big O notation

UNIT – II

Algorithm Design techniques – Brute force, branch and bound, greedy algorithms, Dynamic programming, divide and conquer, randomized algorithm – NP complete problems.

UNIT – III

Dynamic Programming Algorithms – Sequence Alignment – Global alignment using Needleman-Wunsch algorithm – Local alignment using Smith-Waterman algorithm – Gap penalties – Fixed and Affine Gap penalties

UNIT – IV

Heuristic Similarity Search algorithms – Approximate Pattern Matching - FASTA algorithm – BLAST algorithm – Comparing a sequence against a database.

UNIT – V

Graph Algorithms – Graphs and Genetics – DNA sequencing – Shortest superstring problem – DNA arrays as an Alternative Sequencing Technique

Text Books

1. N.C. Jones and P.A. Pevzner, An Introduction to Bioinformatics Algorithms, Ane Books, New Delhi, 2005.
2. R. Durbin, S.R. Eddy, A. Krogh and G. Mitchison, Biological Sequence Analysis, Cambridge Univ. Press, Cambridge, UK (1998).