BHARATHIDASAN UNIVERSITY, TIRUCHIRAPPALLI – 620 024.
M.Sc. Bioinformatics - Course Structure under CBCS
(For the candidates admitted from the academic year 2008-2009 onwards)

Semester	Course	Course Title	Ins. Hrs / Week	Credit	Exam Hrs	Marks		Total
						Int.	Extn.	
I	Core Course – I (CC)	Cell Biology and Biodiversity	6	4	3	25	75	100
	Core Course – II (CC)	Bioinformatics Resources and Applications	6	4	3	25	75	100
	Core Course – III (CC)	Computer Programming	6	4	3	25	75	100
	Core Course – IV (CC)	Molecular Biology and Genetic Engineering	6	4	3	25	75	100
	Core Course – V (CC)	Practical – I : Computer Programming	6	5	3	40	60	100
		Total	**30**	**21**				**500**
II	Core Course – VI (CC)	Computational Biology	6	4	3	25	75	100
	Core Course – VII (CC)	Mathematics for Bioinformatics	6	4	3	25	75	100
	Core Course – VIII (CC)	Experimental Techniques for Biomolecules	6	4	3	25	75	100
	Core Course – IX (CC)	Practical – II : Computational Biology and Statistical Package	6	5	3	40	60	100
	Elective – I	Structural Bioinformatics	6	4	3	25	75	100
		Total	**30**	**21**				**500**
III	Core Course –X (CC)	Database Management Systems	6	5	3	25	75	100
	Core Course – XI (CC)	Genomics and Proteomics	6	5	3	25	75	100
	Core Course – XII (CC)	Practical – III : Genomics, Proteomics and Database Management Systems	6	4	3	40	60	100
	Elective – II	Any one as given in the list	6	4	3	25	75	100
	Elective – III	Any one as given in the list	6	4	3	25	75	100
		Total	**30**	**22**				**500**
IV	Core Course – XIII (CC)	Advanced Computer Programming	6	5	3	25	75	100
	Core Course – XIV (CC)	Practical – IV : Molecular Modelling, and Advanced Computer Programming	6	4	3	40	60	100
	Elective – IV	Any one as given in the list	6	5	3	25	75	100
	Elective – V	Any one as given in the list	6	5	3	25	75	100
	Project Work Dissertation 80 Marks Viva 20 Marks	Dissertation=80 Marks [2 reviews –20+20=40 marks Report Valuation = 40 marks] Viva = 20 Marks	6	7	-	-	-	100
		Total	**30**	**26**				**500**
		Grand Total	**120**	**90**				

Elective II

EC-II.1 Molecular Modelling and Drug Designing
EC-II.2 Drug and Pharmaceutical Technology
EC-II.3 Cancer Biology

Elective III

EC-III.1 Chemoinformatics
EC-III.2 Medicinal Chemistry
EC-III.3 Bioinformatics Algorithms

Elective IV

EC-IV.1 Applied Bioinformatics
EC-IV.2 Stem Cell in Health Care
EC-IV.3 Medical Informatics

Elective V

EC-V.1 Information Management
EC-V.2 Networks and Distributed Computing
EC-V.3 Machine Learning in Bioinformatics

Note:

Core Courses include Theory, Practicals & Project

No. of Courses	14 - 17
Credit per Course	4 - 5
Total Credits	70

Elective Courses

(Major based / Non Major / Internship)

No. of Courses	4 – 5
Credit per Course	4 – 6
Total Credits	20

	Internal	External
Theory	25	75
Practicals	40	60

Project

Dissertation	80 Marks	[2 reviews – 20+20	=	40 marks
		Report Valuation	=	40 marks]
Viva	20 Marks			20 marks

Passing Minimum in a Subject

CIA	40%	Aggregate 50%
UE	40%	

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SEMESTER – I

CC - I CELL BIOLOGY AND BIODIVERSITY

UNIT – I

Biology of Cells: Prokaryotic and Eukaryotic cells – Cell organelles and its functions - Differences and similarities in plant and animal cells — Cell surface and Cellular interactions - Cell membrane and Permeability: Membrane organization – Membrane proteins - Transport across the plasma membrane - Mechanisms of transport in animals and in vascular plants - Cell Cycle and Cell division (mitosis & meiosis).

UNIT – II

Biological Thermodynamics – Active sites and structure of an Enzyme – Mechanism of an enzyme action - 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, and nucleic acids – chemical bonds in biomolecules.

UNIT – III

Overview of protein and nucleic acid structure – Levels of protein structure - α-helix, β-sheet and β-turns –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

Evolution: Concepts and theories of Organic evolution – Mechanisms producing genetic diversity – Origin of species – Hardy-Weinberg equilibrium – Adaptive radiation – Patterns of evolution.
Biodiversity: Genetic, Species and Ecosystem diversity – Values and Uses of Biodiversity – Conservation of Biodiversity – Databases on Biodiversity – Biodiversity and Biotechnology.

UNIT – V

Biology of Environment: Basic ecological principles – Dynamics of an ecosystem –Energy flow in an ecosystem - Community ecology – Human impact on resources and ecosystems - Environmental pollution - Population ecology –Co evolution - Importance of biodiversity in homeostasis of an ecosystem.

Reference Books:

1. E.D.P. De Robertis and E.M.F. De Robertis, Jr., Cell and Molecular Biology, Eighth Edition, B.I. Waverly Pvt Ltd, New Delhi, 1996.
2. Robert H.Tamarin, Principle of Genetics, The McGraw Hill companies, Inc., 1999.
3. Mukherji, S. and Ghosh, A.K., Plant Physiology, Tata McGraw Hill Publishing Company Limited, New Delhi, 1996.
4. Donald T. Haynie, Biological Thermodynamics, Cambridge University Press, 2001.
5. J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, 5th edition, W. H. Freeman & Co. New York (2002).
6. J.L. Jain, Fundamentals of Biochemistry, S. Chand & Company LTD, 1999.
7. Krishnamurthy K.V., An Advanced Textbook on Biodiversity – Principles and Practice, Oxford & IBH Publishing Co. Pvt. Ltd., New Delhi, 2003.
8. Jha, A.P. Genes and Evolution, Macmillan India Ltd, 1993.
9. Sharma, P.D., Elements of Ecology, Rastogi Publications, Meerut, 1989.
10. Odum, E.P., Fundamentals of Ecology. W.B.Saunders Company, Philadelphia, 1971.
11. J.L. Chapmann & M.J.Reiss, Ecology- Principles and Applications, Cambridge University Press, 1999.

CC – II - BIOINFORMATICS RESOURCES AND APPLICATIONS

UNIT - I

Overview of Bioinformatics – Literature databases – NCBI – PubMed – Sequence and Structure databases – Genomics and Proteomics – Biodiversity - Systems Biology

UNIT – II

Protein and Nucleic Acid Sequence Databases – PIR, Swiss-prot, GenBank – pattern and motif searches – PROSITE, BLOCKS, PRINTS, PFAM – structure databases – PDB – structural classification – SCOP, CATH - Protein structure visualization tools – RasMol, Swiss PDB Viewer

UNIT - III

Sequence alignment: Scoring matrices - Substitution matrices (PAM and BLOSUM) - Local and Global alignment concepts – Dotplot - Dynamic programming methods - Statistics of alignment score - Databases searching - FASTA and BLAST searches - Multiple sequence alignment – CLUSTALW -

TCOFFEE- Structure based sequence alignments - Profile methods – Gribskov profile – PSI-BLAST - HMMER

UNIT - IV

Genome Mapping, Sequencing, Assembly and Annotation – Genome projects – Genomic variations – Genome expression – Computational approaches in comparative Genomics – MUMMER -Genomic identification – Biomedical Genome Research – Proteomics – Computer gel analysis and protein identification software - Informatics solutions for proteomics – Interactomics- Systems biology (basic concepts)

UNIT - V

Evolutionary analysis - sequence level - distances - clustering methods - construction of dendrograms - rooted and un-rooted tree representation - 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. G. Gibson & S.V.Muse, A Primer of Genome Science, Sinauer Associates, Inc. Publishers, 2002.
5. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ, 2005.
6. A. M.Campbell & L. J. Heyer, Discovering Genomics, Proteomics & Bioinformatics, CSHL Press, 2003.
7. C.S. Tsai, An Introduction to Computational Biochemistry, Wiley-Liss, New York, 2002.
8. T.E. Creighton, Protein Function A Practical Approach, Oxford university press, 2004.
9. S.R. Pennington & M.J. Dunn, Proteomics – from protein sequence to function, BIOS Scientific Publishers, 2002.

CC – III COMPUTER PROGRAMMING

UNIT – I

Introduction to C - Identifiers and Keywords - Constants, Variables and Data types - Operators and expressions - Data Input and Output –

UNIT II

Control Structures - *if* and *switch* statements - *while*, *do-while* and *for* statements – *goto* statement - Arrays - Character strings - Simple programs.

UNIT - III

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 - IV

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.

UNIT - V

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.

Reference Books

1. Byron S. Gottfried, Schaum's outline of Theory and Problems of Programming with C, Tata McGraw-Hill, New Delhi, 1991.
2. Brain W. Kernighan and Dennis. M. Ritchie, The C Programming Language, Second Edition, Printice-Hall of India, 1988.
3. S.Parthasarathy, Essentials of Computer Programming in C for Life Sciences, Ane Books, New Delhi, 2008.
4. Sumitabha Das, UNIX Concepts and Applications, 3rd Edition, Tata McGraw-Hill, New Delhi, 2003.
5. Thomas A. Powell, HTML & XHTML, The Complete Reference, 4th Edition, Tata McGraw-Hill, New Delhi, 2007.

CC - IV MOLECULAR BIOLOGY AND GENETIC ENGINEERING

UNIT – I

Sequence organization of prokaryotic and eukaryotic DNA – Mitochondria and chloroplast DNA – 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 in prokaryotes and eukaryotes – operon concept – lac, trp – promotor, attenuator – terminator and operator – transcription factors – allosteric enzymes and feed back inhibition – repression – Gene transfer mechanisms - transformation, conjugation, transduction – Genetic linkage and crossing over and genetic mapping of chromosomes

UNIT – III

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

UNIT – IV

DNA sequencing – DNA sequencing by base specific cleavage and by primed enzymatic synthesis – insertions and deletions – 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 – siRNA

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 Weinhein, Germany, 1987.
5. Prokop, Ales, Bajpai, Rakesh K., and Ho, Chester S., Recombinant DNA Technology and Applications, McGraw-Hill, New York, 1991.
6. Nicholl D.S.T., An Introduction to Genetic Engineering, 2nd Edn., Cambridge University Press, UK, 2002.
7. Griffiths A.J.F., Gelbart W.M., Lewontin, R.C., Miller J. H. Modern Genetic Analysis (Integrating Genes and Genomes), 2nd Edn., W.H. Freeman, New York, 2002.
8. T. A. Brown, Genomes, 2nd Edition, BIOS Scientific Publishers, Ltd.,Oxford, UK, 2002.

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CC – V PRACTICAL - I : Computer Programming

1. Find the pH of a solution given the concentration of H^+ (or) OH^- ions
2. Compute the area and the circumference of the circle
3. Compute the volume of a cylinder and cone
4. Convert the given Fahrenheit value to centigrade scale (or vice versa)
5. Compute the relative centrifugal force using r_max (in cm) and rpm value
6. Compute the rpm value using r_max (in cm) and RCF value
7. Find the biggest of three given numbers using if-else statement
8. Compute all possible roots of quadratic equation using if-else statement
9. Find the molecular weight of a DNA with n base pairs in length
10. Find the molecular weight of a given dephosphorylated oligonucleotide sequence
11. Find the molecular weight of a given DNA sequence, after checking for phosphorylation
12. Find the sum of n natural numbers
13. Compute the sum of n odd numbers
14. Find the factorial of a given integer number
15. Compute the nature of the solution based on the pH value using switch case statement.
16. Compute all possible roots of quadratic equation using switch - case
17. Reverse the given integer number and store it in a variable
18. Compute the sum of individual digits up to a single digit of a given number
19. Calculate sedimentation time (in hrs. & mins.) using clearing factor and sedimentation coefficient
20. Compute the average of n given values
21. Arrange the n given numbers in ascending order
22. Reverse a given string (without using the built in string function)
23. Checking for palindrome of a given string (without using the built in string function)
24. Arrange the given names in alphabetical order

25. Compute the mean, median, mode, variance, standard deviation for a set of given values
26. Compute the matrix addition, subtraction and multiplication (use different functions for each operation)
27. Generate n fibonacci numbers using ‘static’ storage class (define a function)
28. Swap two given numbers using pointers (use a separate function to swap)
29. Swap two given numbers without using additional variable (write separate swap function)
30. 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

CC-VI - COMPUTATIONAL BIOLOGY

UNIT - I
Sequence alignment algorithms: pairwise alignment - Local and Global alignment concepts - dynamic programming methodology-Needleman and Wunsch algorithm, Smith-Waterman algorithm -– Databases searches for homologous sequences - FASTA and BLAST - Statistics of alignment score – p-value – E-value

UNIT - II
Multiple sequence alignment – methods of multiple sequence alignment Progressive alignment – Clustal W, T-Coffee – Application of multiple sequence alignment - PRINTS, BLOCKS, PRINTS, PRODOM, PFAM – principles and methods – methods for phylogenetic tree construction – NJ, ML and MP – evolutionary models

UNIT – III
Protein 3-D structure comparison and alignment – structure superposition – RMSD – structure alignment methods – DALI, SSAP, CE – multiple structure alignment

UNIT - IV

Protein Secondary structure prediction – Chou-Fasman, Garnier-Osguthorpe-Robson (GOR) methods – Neural network concepts and secondary structure prediction – amphipathic helix prediction – transmembrane structure prediction

UNIT - V

Fragment assembly - Genome sequence assembly - Gene finding methods: content and signal methods – Analysis and prediction of regulatory regions - - Probabilistic models: Markov chain – random walk - Hidden Markov models – Gene identification and other applications.

Reference Books

1. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press, New Delhi (2003).
2. David W. Mount, Bioinformatics – Sequence and Genome analysis, Cold Spring Harbor Laboratory Press, New York, 2001.

3. D. Higgins and W. Taylor (Eds), Bioinformatics- Sequence, structure and databanks, Oxford University Press, New Delhi (2000).

4. R. Durbin, S.R. Eddy, A. Krogh and G. Mitchison, Biological Sequence Analysis, Cambridge Univ. Press, Cambridge, UK (1998).

5. A. Baxevanis and B.F. Ouellette. Bioinformatics: A practical Guide to the Analysis of Genes and Proteins, Wiley- Interscience, Hoboken, NJ (1998).

6. Michael S. Waterman, Introduction to computational Biology, Chapman & Hall, (1995).

7. P.E. Bourne and H. Weissig (Eds.) Structural Bioinformatics, John-Wiley and Sons, 2003

8. C. Gibas and P. Jambeck, Developing Bioinformatics Computer Skill, 1st Edition, O'Reilly, 2001O'Reilly, 2001.

CC – VII - MATHEMATICS FOR BIOINFORMATICS

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 and Poisson distributions – Z-score, P-value and E-value – Hidden Markov models –

Neural networks – applications in bioinformatics - Needleman and Wunsch algorithm, Smith-Waterman algorithm

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

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, 3rd Edn, Oxford University Press, New Delhi, 2002.
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 – VIII EXPERIMENTAL TECHNIQUES FOR BIOMOLECULES

UNIT – I

Isolation and purification of proteins - Crystallization 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 – High throughput techniques in Crystallography

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. Van Holde, 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 PRACTICAL–II: COMPUTATIONAL BIOLOGY AND STATISTICAL PACKAGES

1. Search on NCBI – PubMed bibliographic search – different options – author name, keyword in title, abstract, title and/or abstract, related articles – different display options
2. Search on EMBL for nucleic acid sequences
3. Study of sequence formats by ReadSeq and TranSeq
4. Perform a similarity search of PIR database for the given protein sequence
5. Perform a similarity search of SwissProt database for the given protein sequence
6. Computation of protein sequence features using PROTPARAM tool
7. Retrieving genomic information using GOLD database
8. Perform pairwise sequence alignment for a set of two analogous proteins
9. Motif searching in derived databases PRINTS and BLOCKS databases
10. Structure exploration using PDB
11. To list SCOP lineages and CATH architecture description for a set of proteins
12. Structure visualization using RASMOL software
13. Structure visualization using PYMOL software
14. Pairwise sequence alignment by LALIGN tool
15. Sequence similarity search using NCBI-BLAST tool
16. To retrieve amino acid sequences (in FASTA format) of Bowman-Birk inhibitors from different species (monocots and dicots) and perform multiple alignment with ClustalW to evaluate their homology. To compare and comment on the conservation disulfide bridge pattern between monocots and dicots.
17. Searching metabolic pathway information in KEGG database and MetaCyc
18. PHYLIP –
    i) To perform phylogenetic analysis by neighbor joining method using the Kimura two-parameter model for a set of nucleotide sequences.
    ii) To perform phylogenetic analysis by neighbor joining method using the Dayhoff PAM matrix for a set of amino acid sequences (ribonucleases)
19. Calculation of mean, median, mode, variance and standard deviation.

20. Regression analysis and plotting of graphs, bar diagrams, pi charts.
21. Student's 't' test
22. Chi-square test

EC – I STRUCTURAL BIOINFORMATICS

UNIT – I

Overview of structural bioinformatics – understanding structural basis for biological phenomena – challenges in structural bioinformatics – integration of structural data with other data – Structure Databases – PDB, NDB, CCD - Structural Classification – SCOP, CATH, FSSP - Structural genomics

UNIT – II

Conformational Analysis of proteins– Forces that determine protein structure – polypeptide chain geometries – Ramachandran Map – potential energy calculations – observed values for rotation angles – structure comparison and alignment

UNIT – III

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

UNIT – IV

Structure Prediction Methods – Homology Modeling – Fold Recognition Methods – a*b initio* methods –Rosetta – CASP – prediction of secondary structure – Chou-Fasman, Garnier-Osguthorpe-Robson (GOR) methods – transmembrane structure prediction – solvent accessibility calculations and prediction.

UNIT – V

Interactomes – macromolecular interactions - protein-protein interactions – protein-DNA interactions – protein-ligand interactions – interactions databases – BIND, ProNIT - Docking – principles and methods

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., 1999.
3. P.E. Bourne and H. Weissig (Eds.) Structural Bioinformatics, John-Wiley and Sons, 2003.

SEMESTER - III

CC – X - DATABASE MANAGEMENT SYSTEMS

UNIT - I

Introduction – History of database systems - Database system applications – Database systems vs File systems – View of data: Data abstraction – Instances and Schemas – Database users and administrators - Transaction management – Database system structure – Advantages and disadvantages

UNIT - II

Database Models: Basic concepts and structure of Entity relationship data model, Relational data model, Object-oriented data model, Object-relational data model, Network data model and Hierarchical data model . Integrity and security – Normalization – Constraints - Indexing and Hashing

UNIT - III

SQL basics – SQL languages: DDL, DML, TCL, DCL and non procedural languages - MySQL data types, operators and functions – Working with databases and tables – working with data – Joins – Sub queries – Transactions. Introduction to PL/SQL - simple PL/SQL programs

UNIT - IV

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

UNIT - V

SRS: An integration platform for databanks and analysis tools in bioinformatics - The Kleisli query system as a backbone for bioinformatics data integration and analysis - Integration challenges in gene expression data management – Discovery link

Reference Books:

1. Abraham Silberchatz, Henry F. Korth, S. Sudharshan, Database System Concepts (5th Edition), McGraw Hill, 2002(Text book for units I & II).
2. James Martin, Computer database organization, Prentice Hall of India, 1977.
3. James Martin, Principles of Database management, Prentice Hall of India, 1976.
4. Bipin C. Desai, An introduction to database systems, Galgotia publications pvt. Ltd., New Delhi, 2003(Text book for units I & II).
5. Peter Rob Carlos Coronel, Database systems, design, implementation & management, Course technology, 2000.
6. Database systems – A practical approach to design, implementation and management, Thomas cannolly and Carolyn begg, Pearson Education, 2002.
7. Vikram Vaswani, The Complete Reference MySQL, Tata McGraw-Hill, New Delhi, 2002 (Text book for unit III).
8. Zoe Lacroix and Ternce Critchlow, Bioinformatics - Managing Scientific Data, Morgan Kaufmann publishers, 2003 (Text book for units IV & V).

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CC – XI - 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. Comparative genomic databases – PEDANT, Cluster of Orthologous Groups (COG), Kyoto Encyclopedia of Genes and Genomes (KEGG) – Metabolic reconstruction – Network Databases –Statistical data on available genome sequenced species - Pathway Databases.

UNIT – III

Human genome (HGMP) 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 in medicine.

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.

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CC – XII PRACTICAL - III: GENOMICS, PROTEOMICS AND DATABASE MANAGEMENT SYSTEMS

(FIFTEEN practical from Section A and FIVE practical from Section B)

Section A: Genomics and Proteomics

1. Comparative genomic analysis by Integrated Microbial Genomes and Microbiomes tools and HGT-DB tools
2. Comparative genome annotation by VISTA tools
3. Bacterial operon prediction by OperonDB tools
4. Gene prediction by WebGene, ORF finder and COG database
5. Promoter and regulan prediction by Virtual FootPrint
6. Prediction of secondary structure of rRNA by rRNA project and mFOLD server
7. Sequence assembly and finishing by GAP4/TIGR assembler/phRed/phRAP software and dbEST and dbSTS databases
8. Cloning vector construction by FastPCR, pDRAW software, WebCutter server and Plasmid Genome Database
9. Identification of coding region by CRITICA and CodanDB tools
10. Identification of mutations in genes by GeneSNP-VISTA software
11. Recombination frequency analysis by MEGA, RAS and RAT software
12. Metabolic pathway prediction by UB-BBD and Pathway Hunter Tool
13. Metabolic reaction and pathway construction by KASS and e-ZYME software
14. Protein network prediction by Sting and KEGG Net servers
15. Protein bulk properties prediction by WinGene/WinPep software
16. Protein modification site prediction by GlyMod, PhosMod, AceMod tools and WinPep software
17. 2D gel data analysis by SWISS-2D GEL DB and NCI Flicker web server/software
18. Microarray data analysis by NCBI-OMNIBUS, TIGR Archive Viewer and TH4/BioConductor/BASE software
19. Mass spectroscopy data analysis by MSDB and Mascot/PeptIdent/GFS server
20. Microbial strain improvement by CellDesigner and Systems Biology Workbench (Demo).

Section B: Database Management

21. Create a database and demonstrate MySQL – Data types
22. Create a database and demonstrate MySQL – Functions
23. Create a database and demonstrate MySQL – Operators
24. Create a protein sequence database using DML & DDL
25. Create a biology literature database using DML & DDL
26. Create a disease database to explain the concept of Joins and Sub-queries.

27. Create a genome information database to explain the RDBMS concepts.

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ELECTIVE - II

EC – II.1 MOLECULAR MODELLING AND DRUG DESIGN

UNIT - I

Basic concepts of molecular structure (bond length, bond angle, torsion angle and non-covalent interactions – Molecular structure and internal energy - Energy minimization of small molecules – Empirical representation of molecular energies – Use of force fields and the molecular mechanics method –Discussion of global energy minimum – Molecular representation in graphics.

UNIT - II

Basic principles of molecular dynamics and Monte Carlo Simulation for conformational analysis - ab initio – Density-Functional Theory and semiemperical methods**.**

UNIT - III

Macromolecular modeling – Identification and mapping of active sites - 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 –pharmocophore identification and novel drug design.

UNIT – IV

Cancer and related diseases – mechanism and action of available anti-cancer drugs - New targets for anti-cancer drugs - Drugs that rescue mutant p53's and tubulin.

UNIT – V

Enzyme background – Theories of enzyme inhibition - Enzyme inhibition as a tool for drug development – Structured-based drug design – structural bioinformatics in drug discovery - 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. Smith, 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

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EC – II.2 DRUG AND PHARMACEUTICAL TECHNOLOGY

UNIT - I

Development of Drug and Pharmaceutical Industry: Therapeutic agents, their use and economics- Regulatory aspects.

UNIT - II

Drug metabolism: physico chemical principles, radio activity-pharma kinetic action of drugs on human bodies.

UNIT - III

Bulk drug manufacturers- Type of reactions in bulk drug manufacture and processes- Special requirement for bulk drug manufacture.

UNIT - IV

Compressed table- wet granulation-dry granulation or slugging-direct compression-tablet presses- coating of tablets, capsules-sustained action dosage forms-parental solution-oral liquids-injections-ointment-topical applications- Preservation, analytical methods and test for various drug and pharmaceuticals-packing: packing techniques, quality management, GMP.

UNIT - V

Therapeutic categories such as vitamins-laxatives- analgesics- nonsteroidal contraceptives-Antibiotics, biologicals- hormones.

Reference Books

1. Leon Lachman et al, *Theory and Practice of Industrial Pharmacy*, 3 Edition, Lea and Febiger, 1986.
2. Remington's, *Pharmaceutical Science*, Mark Publishing and Co.

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EC – II.3 CANCER BIOLOGY

UNIT - I

Regulation of Cell cycle- Mutations that cause changes in signal molecules- effects on receptor-signal switches- tumour suppressor genes- Modulation of cell cycle-in cancer- Different forms of cancers- Diet and cancer.

UNIT - II

Chemical Carcinogenesis- Metabolism of Carcinogenesis- Natural History of Carcinogenesis- Targets of Chemical Carcinogenesis- Principles of Physical Carcinogenesis- X-Ray radiation – Mechanism of radiation Carcinogenesis.

UNIT - III

Oncogenes- Identification of Oncogenes- Retroviruses and Oncogenes- detection of Oncogenes- Growth factor and Growth factor receptors that are Oncogenes- Oncogenes / Proto Oncogenes activity- Growth factors related to transformations.

UNIT - IV

Clinical significances of invasion- heterogeneity of metastatic phenotype- Metastatic cascade- Basement membrane disruption- Three step theory of invasion- Proteinases and tumour cell invasion.

UNIT - V

Different forms of therapy- Chemotherapy- Radiation Therapy- Detection of Cancers- Prediction of aggressiveness of Cancer- Advances in Cancer detection.

Reference Books

1. King R.J.B., *Cancer Biology*, Addision Wesley Longmann Ltd, U.K., 1996.
2. Ruddon.R.W., *Cancer Biology*, Oxford University Press, Oxford, 1995.
3. Maly B.W.J., *Virology a practical approach*, IRL press, Oxford, 1987.
4. Dunmock.N.J and Primrose S.B., *Introduction to modern Virology*, Blackwell Scientific Publications, Oxford, 1988.

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ELECTIVE - III

EC – III.1 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

1. Chemometrics and chemoinformatics. Washington, DC: American Chemical Society, 2005.
2. Bunin, Barry A. Chemoinformatics: Theory, Practice, and Products. Dordrecht: Springer, 2007.
3. Bajorath, Juergen, ed. Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery. Totowa, N.J.: Humana Press, 2004.
4. Gasteiger, Johann; Engle, Thomas, eds. Chemoinformatics: A Textbook. Weinheim, Germany: Wiley-VCH, 2003.
5. Gasteiger, Johann, ed. Handbook of Chemoinformatics: From Data to Knowledge. Volume 4. Weinheim, Germany: Wiley-VCH, 2003.
6. Leach, Andrew R.; Gillet, Valerie J. An Introduction to Chemoinformatics. Dordrecht: Kluwer, 2003.
7. Oprea, Tudor I. Chemoinformatics in Drug Discovery. Weinheim: Wiley-VCH, 2005.
8. Pirrung, Michael C. Molecular Diversity and Combinatorial Chemistry: Principles and Applications. Amsterdam: Elsevier, 2004.
9. Ekins, Sean, ed. Computer Applications in Pharmaceutical Research and Development. Hoboken, N.J.: Wiley, 2006.
10. Ferenc Darvas, András Guttman, György Dormán. Chemical Genomics. Marcel Dekker Inc, New York, 2005.
11. John B. Taylor, Comprehensive Medicinal Chemistry (Volume I-VI). Pergamum Press, England, 2005.

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EC – III.2 MEDICINAL CHEMISTRY

UNIT - I

Introduction to Medicinal Chemistry-Folk and Herbal Medicine -Introduction to Important Functional Groups in Medicinal Chemistry-Physico-chemical Aspects and Principals of Drug Action-Functional Groups and Isosteres (peptidomimetics)

UNIT - II

Introduction to Computational Molecular Modeling- Quantitative Structure Activity Relationships (QSAR) Metabolism and Prodrugs - Drug-Receptors Interactions and Receptor-Effector Theories- Enzymes: catalysis, representative mechanisms of action and inhibition/inactivation-Receptors and transporters -DNA-interactive drugs.

UNIT - III

Combinatorial Chemistry and Rapid Parallel Syntheses - General properties, chemistry, biological action, structure activity relationship and therapeutic applications of Alicyclic compounds-Alkaloids-Vitamins-Hormones

UNIT - IV

Anti-Infective Agents: Anti-viral Agents-Anti-bacterial Agents-Neuroactive Agents: CNS Depressants-CNS Stimulants-Cholinergic Agents-Adrenergic, Dopaminergic and Serotenergic Agents

UNIT - V

Neuroactive Amino Acid Analogs: GABA, Glutamate and Glycine -Cardiovascular Agents (Renin-Angiotensin, etc.)-Antineoplastic Agents (mustards, anti-folates, etc.) -Steroids, Hormones and Cholesterol Lowering Agents

Reference Books

1. Foye's Principles of Medicinal Chemistry, 5th edition; David A. Williams, William O. Foye, Thomas L. Lemke; Lippincott Williams & Wilkins: Philadelphia, 2002.
2. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 11th edition; Delgado & Remers, Eds.; Lippincott Williams & Wilkins: Philadelphia, 2004
3. Delgado, J and Remers, W., "Textbook of Organic Medicinal and Pharmaceutical Chemistry," Lippincott-Raven, Philadelphia, 1998.
4. Perum J. and Propst C.L. Computer-Aided Drug Design Methods and Applications. Marcel Dekker Inc., New York, 1989
5. Richard B. Silver. The Organic Chemistry of Drug Design and Drug Action. Academic Press, Pnen, Inc., USA, 1992

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EC – III.3 - BIOINFORMATICS ALGORITHMS

UNIT - I

Algorithms and Complexity- Biological algorithms versus computer algorithms – The change problem –Correct versus Incorrect Algorithms – Recursive Algorithms – Iterative versus Recursive Algorithms – Big-O Notations – Algorithm Design Techniques.

UNIT - II

Molecular Biology Primer – Exhaustive Search – Mapping Algorithms – Motif-Search Trees – Finding Motifs – Finding a Median String – Greedy Algorithm – Genome Rearrangements – Sorting by Reversals – Approximation Algorithms – A Greedy Approach to Motif Finding.

UNIT - III

DNA Sequence comparison – Manhattan Tourist Problem – Edit Distance and Alignments – Longest Commons Subsequences – Global Sequence Alignment – Scoring Alignment – Local Sequence Alignment – Alignment with Gap Penalties – Multiple Alignment-Gene Predictions – Approaches to Gene Prediction - Spiced Alignment – Divide and Conquer Algorithms.

UNIT - IV

Graphs – Graphs and Genetics – DNA Sequencing – Shortest Superstring Problem – DNA arrays as an alternative sequencing techniques – Sequencing by Hybridization – Path Problems – Fragment assembly in DNA Sequencing – Protein Sequencing and Identification – The Peptide Sequencing Problem – Spectrum Graphs – Spectral Convolution and Alignment – Combinatorial Patter matching.

UNIT - V

Clustering and trees – Gene expression analysis – Hierarchical clustering-k-means clustering – Clustering and corrupted Cliques – Evolutionary Trees – Distance-based tree reconstruction – Reconstruction trees from additive matrices – Evolutionary trees and hierarchical clustering – Character-based tree reconstruction – Small and large Parsimony Problem – Hidden Markov Models- Randomized Algorithms.

Reference Books

1. Neil C. Jones and Pavel A. Pevzner, *An Introduction to Bioinformatics Algorithms*, MIT Press, First Indian Reprint 2005.
2. Gary Benson Roderic page (Eds), *Algorithms in Bioinformatics*, Springer International Edition, First Indian Reprint 2004.
3. Gusfields G, Algorithms *on strings, trees and sequences- Computer Science and Computational Biology*, Cambridge University Press 1997.

SEMESTER - IV

CC – XIII -ADVANCED COMPUTER PROGRAMMING

UNIT I:

Object Oriented Programming (OOP) - Basic concepts and applications - Differences between C and C++ - Functions in C++ - *inline* Functions - Default arguments.

UNIT II :

Function overloading/polymorphism - Classes and objects - Constructors and destructors - Operator overloading and type conversions.

Unit III:

Extending classes - Inheritance and its types - Single level, multilevel, multiple and hybrid inheritance - Pointers to objects and derived classes - Virtual functions - C++ stream classes - Console I/O operations - Simple Data File operations.

Unit IV:

Introduction to PERL – constants and variables – scalar, arrays and hashes - Input and Output Statement - control statements - regular expressions – bioinformatics application programs - string comparison – searching databases

Unit V:

Introduction to BioPERL – Modules - Bio::SeqIO, Bio::PrimarySeq, Bio::Seq, Bio::Search, Bio::DB, (getting files from web, run local blast using modules) – simple bioinformatics application programs

Reference Books

1. E. Balagurusamy, Programming in C++, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 2004.
2. Robert Lafore, Object-Oriented Programming in Turbo C++, Galgotia Publications, New Delhi, 1991.
3. Bjarne Stroustroup, The C++ Programming Language, Second Edition, Addison-Wesley, New Delhi, 1991.
4. W. H. Press, S.A. Teukolsky, W.T.Vetterling and B.P. Flannery, Numerical Recipes in FORTRAN (/ C / C++) , Cambridge Univ. Press, New Delhi, 2000.
5. E. Balagurusamy, Programming with JAVA A Primer, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1999.
6. L.Wall, T.Christiansen and J.Orwant, Programming Perl, 3rd Edition, O'Reilly, 2000.
7. J. Tisdall, Mastering Perl for Bioinformatics, O'Reilly, 2003.
8. Rex A. Dwyer, Genomic PERL, Cambridge Univ. Press, UK, 2003.
9. Harshawardhan P. Bal, PERL programming for Bioinformatics, Tata McGraw-Hill, New Delhi, 2003.
10. htrtp://bioperl.org

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CC – XIV PRACTICAL - IV: MOLECULAR MODELLING AND ADVANCED COMPUTER PROGRAMMING

(TWELVE practical from Section A and EIGHT practical from Section B)

Section A: Molecular Modeling, Docking

1. To perform the consensus secondary structure prediction for a given protein sequence at NSP@ by selecting six different methods
2. To identify the fold for a given protein sequence using 3-D PSSM fold recognition server
3. To find the structural neighbours of a given protein (2TRX) according to SCOP, CATH, FSSP and CE. To find out if any particular structure is identified by all these classifications.
4. Protein structure prediction and validation
    a. Primary feature computing by PROTPARAM
    b. Secondary structure by SOPMA
    c. 3D structure by PSI-BLAST tool, SWISS-MODEL and SAVS server (MODELER software)
5. Protein structural alignment and classification
    a. Pairwise structural alignment by DALITE server
    b. Multiple structural alignments by DALI/ConSurf server
    c. Structural classification by SCOP and CATH servers
6. Data mining for retrieval chemical information form PUBCHEM and Ligand databases
7. Retrieving pharmacological information from Pharma base and MSDchem database
8. Prediction of binding affinity of ligand by protein-ligand interaction/ReLiBase database tools
9. Ligand design and analysis by ISIS, and VMD software
10. Protein-protein interaction prediction by Hex software
11. Protein-ligand interaction prediction by ArgusLab software
12. Binding site identification of target by Q-site finder server
13. Molecular properties prediction by VEGAZ software
14. Molecular dynamics simulation by GROMOS software
15. Molecular force field analysis by TINKER software
16. Drug activity test by ADMETox tools
17. Analysis of hydrophobic features of target by BioEdit software.

Section B: Advanced Computer Programming

18. Write a C++ program i) to convert temperature given in Farenheit into Celsius and ii) Celsius to Farenheit.
19. Write a C++ program to swap two values using reference variable.
20. Write a C++ program to find all possible roots of a quadratic equation.
21. Write a C++ program to compute the mean and standard deviation of a given n values.
22. Write a C++ program to compute matrix addition, subtraction and multiplication of two matrices using functions
23. Write a C++ program by defining two functions with the same name power() to raise a number m to a power n. One function takes a double value for m and int value for n and the other function having the same name takes a int value for m and int value for n. Write a main function that calls both the functions to demonstrate the function overloading.
24. Write a C++ program using class to find the smallest of two numbers.
25. Write a C++ program with the following specifications :

Define a class to represent a gene sequence data. Include the following members:

Data members:
- Name of the gene
- gene id
- length
- a,t,g,c content

Member functions:
- To read data for a gene
- To compute a,t,g,c content
- To display all the details of a gene

Write a main program to test the program by reading n gene sequences data.

26. Write a C++ program to exchange the private values of two classes using a common friend function.
27. Write a C++ program to find the sum of two complex numbers using overloaded constructors for data input and operator overloading
28. Write a PERL program to compute A, T, G, and C content.
29. Write a PERL program to translate and transcribe a given nucleotide sequence.

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ELECTIVE - IV

EC – IV.1 APPLIED BIOINFORMATICS

UNIT – I

Commercial bioinformatics – Survey of bioinformatics companies in India and abroad – Economics prospects – pharamainformatics – combinatorial chemistry – HT screening – in silico screening - from lead to commercialization

UNIT II

Sequence assembly and Finishing methods - Sequence assemblers – finishing and visualization programmes - Gene expression analysis - Data collection - Image processing - Measures of expression -Finding significant genes - Clustering approaches – SNP – Types - SNP discovery methods - databases and browsers – genotyping - Comparative genomics – algorithms – viewing - genomic alignments – gene prediction and phylogenetic foot printing

UNIT III

Application of genomics to agriculture - gene discovery and gene function - model systems – technologies -methods to introduce novel genes - Pharmaceutical bioinformatics and drug discovery – Introduction - novel gene discovery - methods for identifying novel targets - protein classification and functional assignments – Disease - target gene relationship - Nanotechnology and its applications - Genomics and proteomics in medicine, diagnostics, drug discovery and target findings

UNIT IV

Intellectual Property Rights(IPR): IPR - Importance of IPR, Organization - WIPO & WTO - Agreements and Treaties - GATT-TRIPS - Types of IPR – patents – copyrights - trademarks and trade secrets - Plant Breeder Rights(PBR) - Geographical Indications - Technology Transfer (TT)

- Traditional Knowledge - Importance of patents - Patenting of biological materials - Patenting of biotechnological inventions - Sharing the benefits from biotechnology transfer - IPR in India - IPR impacts on Biotechnology Research in India - significance biotechnological patents in India.

UNIT V

Biosafety & Bioethics: Biosafety - Topics of concern - Hazards of Genetically Engineered Microorganisms – Bioremediation - Framework of biosafety regulations in India (committees, Pressure points for the Biosafety Regulations - Assessment of structural changes.
Ethics – Bioethics - The ethical and social impacts of biotechnology and bioinformatics.

Reference Books

1. T. A. Brown, Genomes, 2nd Edition, BIOS Scientific Publishers, Ltd., Oxford, UK, 2002.
2. Baxevanis D and Ouellette BFF, Bioinformatics: A practical guide to the analysis of genes and proteins (3rd Ed), John Wiley & Sons, Inc., 2005.
3. Sensen CW, 2002. Essentials of Genomics and Bioinformatics, Wiley-VCH.
4. Jenson, O.N., in Proteomics. A Trends Guide (eds Black Stock, Co- and Mann), Elsevier Science, London, 1998.
5. S.R.Pennington and M.J.Dunn, Proteomics, Viva Books Pvt. Ltd., New Delhi, 2002.
4. Relevant papers from Drug Discovery Today - Trends journals
5. N.R.Subbaram, what everyone should know about patents, 2nd Edition, Pharma Book Syndicate, Hyderabad, 2006.
6. Philip W.Grubb, Patents for Chemicals, Pharmaceuticals and Biotechnology-Fundamentals of Global Law practices and strategy, 4th Edition, Oxford University Press, 2006.
7. R.C. Dubey, A Textbook of Biotechnology, S.Chand & Company, 1993.
8. Ben Mepham, Bioethics-an Introduction for the biosciences, Oxford University Press, 2005

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EC – IV.2 STEM CELL IN HEALTH CARE

UNIT - I

Unique properties of stem cells – embryonic stem cells - adult stem cells – umbilical cord stem cells – similarities and differences between embryonic and adult stem cells. Properties of stem cells – pluripotency – totipotency

UNIT - II

Invitro fertilization –culturing of embryos-isolation of human embryonic stem cells – blastocyst – innercell mass – growing ES cells in lab – laboratory tests to identify ES cells – stimulation ES cells for differentiation – properties of ES cells.

UNIT - III

Somatic stem cells – test for identification of adult stem cells – adult stem cell differentiation – trans differentiation – plasticity – different types of adult stem cells.

UNIT - IV

Target identification – Manipulating differentiation pathways – stem cell therapy Vs cell protection - stem cell in cellular assays for screening – stem cell based drug discovery, drug screening and toxicology.

UNIT - V

Gene therapy – genetically engineered stem cells – stem cells and Animal cloning – transgenic animals and stem cells – Therapeutic applications – Parkinson disease - Neurological disorder – limb amputation – heart disease - spinal cord injuries – diabetes –burns - HLA typing-Alzheimer's disease –tissue engineering application – production of complete organ - kidney – eyes - heart – brain.

Reference Books

1. Kursad and Turksen, *Embryonic Stem cells*, Humana Press, 2002.
2. Committee on the Biological and Biomedical applications of Stem cell Research, *Stem cell and future of regenerative medicine*, National Academic press, 2002.

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EC – IV.3 MEDICAL INFORMATICS

UNIT - I

Introduction- Hospital management and information system: functional area- pre-requisites-integrated hospital information systems- health information system- and disaster management plan

UNIT - II

Artificial intelligence- expert systems- materials and methods- computer based patient Records-computer assisted medical education

UNIT - III

Hospital Management and Information systems- structure and functions- computer assisted patient education- computer assisted patient surgery

UNIT - IV

Three-dimensional imaging: limitations of endoscopy and imaging- benefits of virtual endoscopy- materials and methods- limitations- applications- merits and demerits- surgical simulation- virtual environment

UNIT - V

Tele-medicine- needs- materials and methods- Internet tele-medicine- controversial issues-reliability- cost-analysis- applications- tele-surgery- the Internet

Reference Books

1. Mohan Bansal, *Medical Informatics- a primer*, Tata McGraw-Hill, 2003.

2. Charles P. Friedman, Jeremy C. (EDT) Wyatt, Evaluation Methods in Medical Informatics- Springer Verlag, 1997.
3. Hsinnchun Chen, *Medical Informatics: Knowledge Management And Data Mining in Biomedicine*, Springer, 2005.
4. F. T. De Dombal, *Medical Informatics: The Essentials*, Butterworth-Heinemann, 1996.

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ELECTIVE - V

EC – V.1 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.

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EC – V.2 NETWORKS AND DISTRIBUTED COMPUTING

UNIT - I

Reference Model, Network Topologies and Protocols, Types of Networks: Local Area Network (LAN), Wide Area Network (WAN), Metropolitan Area Network (MAN), Network Security (Firewall, Packet Filtering, VPN), Uses of Computer Networks

UNIT - II

OSI & Internet Architecture, IEEE 802 standards, Physical Layer - Transmission Media, Switching. Data Link Layer - Design Issues, Example Data Link Protocols, Data Link layer in the Internet, Media Access Sub layer

UNIT - III

Network Layer - Design Issues, Routing Algorithms, Congestion control algorithm, Router Operation, Router Configuration, Internetworking, IP Addressing, IP Subnet Mask, IPv6 (an overview) Transport Layer – Transport Service, TCP/IP Protocols (TCP, UDP)

UNIT - IV

Design Issues, Conventional Encryption, Classical and Modern Techniques, Encryption and Decryption Algorithms (RSA), Confidentiality, DNS, SNMP, RMON, WWW, E-mail, Digital Signatures

UNIT - V

Introduction to Distributed Computing, Examples, Key Characteristics, Historical background, Basic design issues, User requirements - Introduction to IPC, Building Blocks, Client Server Communication, Group Communication, Remote Procedure Call (RPC).

References Books

1. Tananbaum A.S.,(1999) "Computer Networks", 3rd Ed, PHI
2. Black U.,(1996) "Computer Networks-Protocols, Standards and Interfaces", PHI, 1996
3. George Coulouris, Jean Dollimore, Tim Kindsberg,(2000) "Distributed Systems : Concepts & Design" 3rd Ed, Addison Wesley

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EC – V.3 MACHINE LEARNING IN BIOINFORMATICS

UNIT - I

Introduction-Bayesian modeling-Cox Jaynes axioms- Bayesian inference and induction- models structures- examples.

UNIT - II

Dynamic programming- EM/ GEM algorithms-Markov chain Monte carlo methods-simulated annealing- genetic algorithm-Neural networks.

UNIT - III

Sequence coding- correlations- Prediction: secondary structure, signal peptides and cleavage sites-applications for DNA & RNA nucleotide sequences- Performance evaluation.

UNIT - IV

Introduction- likelihood & Basic algorithms- Learning algorithms- Applications: general aspects, proteins, DNA and RNA

UNIT - V

Models for phylogeny-substitution probabilities-Data likelihood-optimal trees- modeling for array data

References Books

1. Søren Brunak, Pierre F Baldi, *Bioinformatics: The Machine Learning approach,* MIT Press, 2001.
2. Steffen Schulze-Kremer, Molecular Bioinformatics: Algorithms and Applications, Walter de Gruyter, 1996.
3. Balas Kausik Natarajan, *Machine Learning: A Theoretical Approach,* Morgan Kaufmann, 1991.
4. Yi-Ping Phoebe. Chen*, Bioinformatics Technologies*, Springer, 2005.

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