

संत गाडगे बाबा अमरावती विद्यापीठ

SANT GADGE BABA AMRAVATI UNIVERSITY

विज्ञान विद्याशाखा
(FACULTY OF SCIENCE)

अभ्यासक्रमिका

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विज्ञान पारंगत सत्र ३ व ४ परिक्षा २०१३-१४

PROSPECTUS

OF

**MASTER OF SCIENCE IN
BIOINFORMATICS**

Semester -I, Winter 2012

Semester-II, Summer-2013

Semester -III, Winter 2013

Semester-IV, Summer-2014



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**Syllabus Prescribed for M.Sc. Semester-I to IV
(Bioinformatics)**

M. Sc. Part-I (Bioinformatics)

Semester-I (Bioinformatics)

- Paper: I - Mathematics and Biostatistics
 Paper: II - Cell and Molecular Biology
 Paper: III - Computer for Biologists
 Paper: IV - Introduction to Bioinformatics

Semester-II (Bioinformatics)

- Paper: V - Biochemistry and Biophysics
 Paper: VI - Genomics
 Paper: VII - Biological Database Management System
 Paper: VIII - Techniques in Bioinformatics

M. Sc. Part-II (Bioinformatics)

Semester-III (Bioinformatics)

- Paper: IX - System Biology
 Paper: X - Proteomics
 Paper: XI - Bio-Programming – I
 Paper: XII - Parasite Informatics

Semester-IV (Bioinformatics)

- Paper: XIII - Molecular Modeling and Drug Design
 Paper: XIV - Chemo-informatics
 Paper: XV - Bio-programming-II
 Paper: XVI - Research Methodology, IPR and Bioethics

**Syllabus Prescribed for M. Sc. Part-I
Semester-I (Bioinformatics)**

Paper I

(Mathematics and Biostatistics)

Unit-I : (Mathematics)

Calculus: Limits, Complete Differentials, Partial differentials of functions with one variable and multiple variables.

Integration: Definite and non-definite integral; Series, Logarithms Mathematical Techniques Ordinary differential equations (first order), Partial differential equations-example from biology. Special functions - Bessel, Legendre

Unit-I : (Mathematics)

2D Coordinate geometry: Equation of a line, circle, ellipse, parabola, hyperbola

3D Geometry: Equation of sphere, cone Trigonometric functions: Sin, Cos, Tan, Co~ Series expansion of these. Functions and other related functions Vector -Addition, subtraction, dot, cross, scalar triple product, divergence, curl of a vector, equation of normal

Matrix algebra: Addition, subtraction, multiplication, transpose inverse, and conjugate of matrix etc.

Logic: Boolean logic Addition, subtraction, multiplication and division using binary, octal and hexadecimal systems Fundamentals of Set theory Fourier transform, Laplace Transform & other standard transforms

Unit-III : (Biostatistics)

Scope of biostatistics, definition, data collection, presentation of data, graphs, charts (scale diagram, histogram, frequency polygon, frequency curve, logarithmic curves). Sampling & selection bias, probability sampling, random sampling, sampling designs, descriptive statistics: Measures of central tendency (arithmetic mean, geometric mean, harmonic mean, median, mode); Partition value, Measures of dispersion (range, quartile deviation, mean deviation and standard deviation), coefficient of variation.

Unit-IV : (Biostatistics)

Correlation and regression analysis (simple and linear) curve fitting (linear, non-linear and exponential), Axioms, models, conditional probability, Bayes rule, Genetic Applications of Probability, Hardy - Weinberg law, Wahlund's Principle, Forensic probability determination, Likelihood of paternity, Estimation of probabilities for multi-locus/multi-allele finger print systems. Discrete probability distributions - Binomial, Poisson, geometric – derivations, Central limit theorem. Continuous probability distribution – normal, exponential, gamma distributions, beta and Weibull distributions, T & F distributions.

Unit-V : (Biostatistics)

Estimation theory and testing of hypothesis, point estimation, interval estimation, sample size determination, simultaneous confidence intervals, parametric tests [t-test, F-test, Chi Squared test for i) goodness of fit, ii) independence of distributes]. Analysis of variance (one-way and two-way classifications). Case studies of statistical designs of biological experiments (CRD, RBD, LSD).

Suggested Reading:

1. Animesh K. Datta (2007) "Basic Biostatistics and its application" First Edition, New Central Book Agency, Ltd, Kolkata.
2. Batschelet E. (1992), "Introduction to Mathematics for Life Sciences", 3rd Edition, Springer- Verlag
3. H. Nell and D. quading. Pure Mathematics (Advance level Mathematics), Vol. 1, 2, 3 Cambridge University Press, 2002.
4. Narayanan, S. and Manicavachaagam Pillai, T.S. (1993) "Calculus, Vol. I and II"; Vishwanathan Printers and Publishers.
5. Nell H. (2002), "Pure Mathematics (Advance level Mathematics)", Vol. 1, 2, 3 Cambridge University Press
6. Parihar and Parihar (2007) "Biostatistics and Biometry" First Edition, Student Edition, Jodhpur
7. Sundar Rao P. S.S., Jesudian G. & Richard J. (1987), "An Introduction to Biostatistics", 2nd edition, Prestographik, Vellore, India.
8. Warren, J; Gregory, E; Grant, R (2004), "Statistical Methods in Bioinformatics", 1st edition, Springer.
9. Zar, J.H. (1984) "Bio Statistical Methods", Prentice Hall, International Edition.

Paper II**(Cell and Molecular Biology)****Unit-I : (Cell Biology)**

Architecture of prokaryotic and eukaryotic cells, Structure of animal and plant cell, cell organelles, structure of cell wall and plasma membrane, Cell cycle, Molecular mechanics of cell cycle in eukaryotes, Cell division – mitosis and meiosis, Types of cells and its functions.

Unit-II : (Cell Biology)

Structure of Cytolplasm, Nucleus, Mitochondria, Ribosome, Golgi bodies, Lysosomes. Endoplasmic Reticulum, Peroxisomes, Chloroplast and Vacuoles, Cell to cell integration, Cell locomotion (Ameoboid, Flagella, Cillar), Components of blood.

Unit-III : (Cell Biology)

Cell process and mechanics, Nucleus- Ultrastructure of nucleolus, Nuclear pore complex (NCP), Import and export mechanism through NCP. Chromosome- Structural organization of chromosome, chromatids, nucleosome model, DNA binding protein interaction.

Unit-IV : (Molecular Biology)

Concept of gene Central dogma, updated central dogma, molecular structure of nucleic acids – structure & forms of DNA & RNA, Replication: structure & function of DNA polymerases, replication in prokaryotes and eukaryotes, replication of chromatin. Transcription - components of transcription machinery, RNA polymerases, processing of RNA. Transcription in prokaryotes & eukaryotes, genetic code, Translation – mechanism, post-translational modification.

Unit-V : (Molecular Biology)

Gene regulation in prokaryotes – Operon concept, Lactose, Histidine and Tryptophan operon, Gene regulation in eukaryotes – Transcriptional level, translational level control.

Suggested Reading:

1. Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K and Walter, P. (2002) "Molecular Cell Biology of the Cell", Fourth Edition, Garland Science, Taylor and Francis Group, USA.
2. De Robertes and De Robertis (2002) "Cell and Molecular Biology", Saunders College, Philadelphia, USA
3. Karp, G. (2005) "Cell and Molecular Biology: Concepts and Experiments"; Fourth Edition, Wiley Publishing Co. USA
4. Krieger, M. (2003) "Molecular Cell Biology"; Fifth Edition, W.H. Freeman and Co., New York.
5. Lewin, B. (2004) "Genes VIII"; Eighth edition, Pearson Education International.
6. Lodish, H., Scott, M.P., Matsudaira, P., Darnell, J., Zipursky, L., Kaiser, C.A., Berk, A. (2003) "Molecular Biology of the Cell" Fifth Edition, W. H. Freeman and Company, England.

Paper III
(Computer for Biologists)

- Unit-I : (Introduction to Computer)**
Block Structure of a computer, characteristics of computers, classification of computers, Storage devices, Types of memory, Input and Output devices, Operating system – windows, linux etc, System drivers and software, Application software, Window – Introduction, features, desktop: Background screensaver, Customizing desktop, creating, moving, deleting icon.
- Unit-II : (Introduction to MS-Office)**
MS-Word: Introduction to word, features, page setup, views, text formatting, Auto correct, spell check, grammar, table, tabs, indentation, mail merge, print preview, printing of document, hyperlink. **MS-PowerPoint:** Introduction to power point, features, Creation of new presentation, adding slides and text, Editing slide text, saving presentation, text effect, animation, modifying objects and adding images, preparing to deliver a presentation. **MS-Excel:** Introduction to Excel, features, creating and formatting worksheet, Inserting data, entering mathematical formulas and functions, auto fill
- Unit-III : (Introduction to Internet and Networking)**
Introduction to Internet, Type of Internet connection: Direct, dial-up, protocol: TCP/IP, FTP, HTTP, Domain name, electronic mail address, WWW, Search engine, Browser: Internet explorer, Mozilla, Netscape Navigator. **Networking:** Needs and objectives, LAN- Introduction, classification, topology. Topology – Bus, Tree, Ring, Star, Hybrid, WAN, MAN.
- Unit-IV : (Introduction to C programming)**
Algorithms, flow-charts, programming languages, compilation, linking and loading, testing and debugging, documentation, Introduction to C programming, C variable, constant, and operators, data types, arithmetic operators, logical operators.
- Unit-V : (Introduction to C programming)**
Condition: if, if else, while, do while, switch, Nested condition, Looping: for, while, do while, nested loop. Introduction to Array, Array initialization, bound checking, passing array element to a function, initializing a 2-

dimensional array, sorting; Introduction to File Handling : Opening a file, Closing a file, Reading and Writing into a file, Appending to a file.

Suggested Reading:

1. Allen K. R. (2003) "Window 2000 complete" BPB publication, India
2. Balaguruswamy S. (2006) "Programming in ANSI C" Tata Mcgraw Hill
3. Kanetkar Y. (2008) "Let us C" BPB publication, India
4. Rajaraman V. (2006) "Fundamental of Computers"
5. Sharma S (2006) "Fundamental of Computer" BPB publication, India

Paper IV

(Introduction to Bioinformatics)

- Unit-I : (Introduction to Bioinformatics)**
Introduction to Computational Biology and Bioinformatics; Different definitions of Bioinformatics, Bioinformatics – A multidisciplinary Approach, History of Bioinformatics, Emergence of bioinformatics as a separate discipline; Application of Bioinformatics, Scope of Bioinformatics, some of the biological problems that require computational methods for their solution; Role of internet and www in bioinformatics.
- Unit-II : (Biological Data Acquisition)**
The form of biological information; DNA sequencing methods – basic DNA sequencing, automated DNA sequencing, DNA sequencing by capillary array and electrophoresis; Types of DNA sequences – genomic DNA, cDNA, recombinant DNA, Expressed sequence tags (ESTs), Genomic survey sequences (GSSs); RNA sequencing methods; Protein structure determination methods; gene expression data.
- Unit-III : (Databases: Format and Annotation)**
Conventions for databases indexing and specification of search terms; Common sequencing file formats – NBRF/PIR, FASTA, GDE; Files for multiple sequence alignment – multiple sequence format (MSF), ALN format; Files for structural data – PDB format and NMR files; Annotated sequence databases – primary sequence databases (GenBank-NCBI, the nucleotide sequence database-EMBL, DNA sequence databank of Japan-DDBJ; Subsidiary data

storage (ESTs, dbESTs, GSSs), unfinished genomic sequence data, organisms specific databases (EcoGene, SGD, MatDB, TAIR, FlyBase, OMIM, etc.); Protein sequence and structure databases (PDB, SWISS-PROT and TrEMBL); List of Gateways (NCBI, GOLD, MIPS, TIGR, UniGene).

Unit-IV : (Data: Access, Retrieval and Submission)

Data access – standard search engines, Data retrieval tools – Entrez, DBGET and SRS (sequence retrieval systems); Software for data building; Submission of new and revised data.

Unit-V : (Sequence Similarity Searches)

Sequence homology as product of molecular evolution; Sequence similarity searches; Significance of sequence alignment; Sequence alignment – global, local and free-space; Alignment scores and gap penalties; Measurement of sequence similarity; Similarity and homology.

Suggested Reading:

1. Baxevanis, A.D. and Francis Ouellette, B.F. (1998) “Bioinformatics– a practical guide”
2. Mount, D. (2004) “Bioinformatics: Sequence and Genome Analysis”; Cold Spring Harbor Laboratory Press, New York. (ISBN 0-87969-712-1)
3. Sharma, V. Munjal, A. and Shankar, A. (2008) “A text book of Bioinformatics” first edition, Rastogi Publication, Meerut – India.

Practical – I: Practical based on Paper I and II

Mathematics and Biostatistics

1. Calculation of measures of central tendency- Arithmetic mean, median and mode.
2. Computation of partition values - Quartiles, Deciles and percentiles.
3. Geometric mean and harmonic mean.
4. Measure of dispersion- Range, Quartile deviation and mean deviation.
5. Standard deviation and coefficient of variation.
6. Calculation of coefficient of correlation.
7. Computation of rank correlation coefficient.
8. Fitting of straight line.
9. Line of regression and regression coefficient.
10. Fitting of Binomial distribution.

11. Fitting of Normal distribution.
12. Fitting of Poisson distribution.

Cell and Molecular Biology

13. To study morphology of Bacteria by Gram staining
14. To study morphology of Fungi and Yeast
15. Preparation of pure culture by stick plate method
16. Estimation of protein and carbohydrates
17. Restriction digestion of plant genomics DNA
18. Isolation & Purification of genomic DNA from plants
19. Isolation of DNA fragment from Agarose gel
20. Agarose gel electrophoresis of chromosomal & plasmid DNA
21. Estimation of DNA
22. Estimation of RNA
23. Paper Chromatography
24. PCR Analysis (RAPD, Gene Specific Amplifications)
25. Data Analysis by using Nei and Li Similarity Coefficient.

Semester-I

**Distribution of Practical Marks for Practical-I- (Mathematics, Biostatistics, Cell and Molecular Biology)
(Based on Paper-I & II)**

Time: 6Hrs.

Max. Marks:100

- | | |
|---|----------|
| 1) Setting and working on any one exercise based on Biostatistics | 20 Marks |
| 2) Setting and working on any one exercise based on exercise based on Mathematics | 20 Marks |
| 3) Setting and working on any one exercise based on exercise based on Cell Biology | 20 Marks |
| 4) Setting and working on any one exercise based on exercise based on Molecular Biology | 20 Marks |
| 5) Viva-voce | 10 Marks |
| 6) Practical Record | 10 Marks |

Total

100 Marks

Practical – II: Practical based on Paper III and IV.

Computer for Biologists

1. DOS Commands - Internal Commands: Viewing a directory, Changing Directory, Renaming a Directory - File operations: Creating files, removing a file, renaming files, viewing a file – External commands: Copying a disk, Comparing disks
2. Overview of different versions of Windows –Working with Windows- Desktop Basic Layout, Icons, Opening Windows, Window Characteristics, Window Controls, Resize Windows, Arrange Windows, Taskbar.
3. Working with Programs: Basic Program Layout, WordPad Program, Scrolling in Documents, Moving Insertion Point, Delete & Insert Key, Selecting Text, Cut, Copy & Paste, Working with Multiple Programs.
4. Files & Folders: Organization, View Folder Structure, Working with Folders, Search for Files, Organizing Workspace - Personal Desktop, Shortcuts, Start Menu, Start Properties, Display as Menu, Taskbar, Quick Launch.
5. Windows Properties - Navigating Control Panel, Changing Theme, Desktop Settings, Screen Saver Settings, Appearance Settings, Display Settings, Mouse Settings
6. Working with documents: Creating a document, Manage files and folders for documents, working with icons, editing documents - Text formatting and alignment, Indentation.
7. Paragraph formatting - Margins, tabs and page numbering.
8. Working with tables and borders - Printing - Working with Images and Text - Find and replace text - Mail merge.
9. Creating and formatting a presentation –Creation of a new Presentation, Adding Slides and Text to a Presentation, Editing Slide Text, Saving a Presentation, and Running a Slide Show- Adding Tables and charting data – Modifying objects and adding Images, Preparing to deliver a presentation.
10. Creating and modifying a worksheet- Formatting Worksheets – Working with multiple worksheets – Performing Calculations
11. Surfing information using Search Engines, Saving web pages to a disk, Composing E-mail, Sending E-mail.
12. **C Programming:** Flowcharts, Algorithm, Keywords, Identifiers, variables, Constants, Scope of Life of variables- Local and Global variables. Data types, Expressions, Operators – Arithmetic operators, Logical operators, Relational, conditional, Bitwise operators - Input / Output Library functions. Declaration statement

13. Conditional statement: If statement, If... Else statement, Nesting of If...Else statement, Switch statement – Iteration statements

Introduction to Bioinformatics

14. Arrays: Concept of Single and Multidimensional arrays, Array declaration, and initialization of arrays.
15. Functions: User defined and library functions
16. File Handling: Opening a file, Closing a file, Reading and Writing into a file, Appending to a file
17. SRS of Biological Databases
 - a. National Center for Biotechnology Information (NCBI)
 - b. Nucleotide/ Genome Databases
 - c. Protein Sequence Database
 - d. Structure databases
 - e. Protein Pattern Databases
18. Different file formats
 - a. Genbank
 - b. Genpept
 - c. FASTA
 - d. EMBL
 - e. NBRF/PIR, GDE
19. Entrez and Literature Searches.
 - a. PubMed
 - b. PubMed central
 - c. OMIM / OMIA
 - d. Citation matcher
20. File format conversion
 - a. FmtSeq
 - b. ReadSeq
 - c. Sequence Manipulation Suite
21. Protein Structure Database – MMDB, Swiss-Prot, PDB, PDB file format
22. Sequence Alignment – BLAST, FASTA
23. Sequence Analysis
 - a. Dot Plot
 - b. Pairwise alignment
 - c. Multiple Sequence Alignment
24. Phylogenetic analysis using PHYLIP, Phylodraw, PAUP, Treeview, JalView
25. Softwares
 - a. BioEdit.

- b. GeneDoc
 - c. ClustalW / X, MEGA, MEME
26. Visualization Tool
- a. RasMol
 - b. Cn3D
 - c. MolMol
27. Submission Tools for new and revised data

Semester-I

Distribution of Practical Marks for Practical-II:- (Computer for Biologists and Introduction to Bioinformatics) (Based on Paper-III & IV)

Time: 6Hrs.

	Max. Marks:100
1) Setting and working on any one exercise based on Computer	20 Marks
2) Setting and working on any one exercise based on Computer programming	20 Marks
3) Setting and working on any one exercise based on Databases	20 Marks
4) Setting and working on any one exercise based on Data Processing & Analysis	20 Marks
5) Viva-voce	10 Marks
6) Practical Record	10 Marks
Total	100 Marks

Syllabi for Semester-II (Bioinformatics)

Paper V

(Biochemistry and Biophysics)

Unit-I : (Biochemistry)

Water- Water as the universal biological solvent, concept of osmolarity, water relationship

Carbohydrates- Monosaccharides, oligosaccharides, polysaccharides, peptidoglycans, proteoglycans and glycoproteins, biological importance of carbohydrates

Lipids- Fatty acids, acylglycerols, phospholipids, sphingolipids, sterols, membrane Icoprenoids, Icosanoids and their biological significance.

Unit-II : (Biochemistry)

Levels of protein structure – primary, secondary, tertiary and quaternary with examples; alpha helix, beta sheet and beta turn; domains and structural motifs; Ramchandran plot, Rossmann fold, Immunoglobulin fold; Double helical structure of DNA – DNA polymorphism; types of RNA and its secondary and tertiary structure.

Unit-III : (Biochemistry)

Transcription- Prokaryotic and eukaryotic Transcription-RNA polymerases- general and specific transcription factors- regulatory elements- mechanism of transcription regulation- Transcription termination; Post transcriptional modification Translation- Genetic code- Prokaryotic and eukaryotic, **Translation** - translational machinery-Mechanism of initiation- elongation and termination-Regulation of translation.

Unit-IV : (Biophysics)

Diffusion and Osmosis, Osmotic pressure, osmolarity of fluids and electrolyte balance. Donnan membrane equilibrium, dialysis. Viscosity, Measurement and applications, Surface tension, Measurements and viscosity of blood, Electrochemical Techniques - principles of redox reactions, Centrifugation principles, basic principles and laws of sedimentation. Preparative and analytical ultracentrifuges, Sedimentation equilibrium methods, Types of separation methods in preparative centrifuges, Differential and density gradient centrifugation.

Unit-V : (Biophysics)

Absorption Spectroscopy basic principles, analysis of biopolymers, effects of absorption, basic laws of light absorption, optical rotatory dispersion, circular dichroism, Rayleigh Scattering, Size and shape of Macro molecules, Method of Direct visualization, Macro molecules as Hydro dynamic particles, Macro molecular Diffusion, Ultra centrifugation, Viscometry, X-ray crystallography (Determination of 3D structure By X-ray Diffraction) single crystal diffraction, Fibre diffraction, NMR spectroscopy

(3D structure determination), of biological systems, Electron Microscopy, Neutron Scattering, Light Scattering, Luminescence, optical activity, Magnetic optical activity, IR, laser- Raman and ESR/EPR Mass Spectroscopy.

Suggested Reading:

1. Banwell, C.N. (1983) "Fundamentals of Molecular Spectroscopy"; Tata McGraw Hill Publishing Company, New Delhi, India.
2. Cantor, C.R. and Schimmel, P. (1985) "Biophysical Chemistry Vol. 1 and 2"; W.H. Freeman and Company, New York, US.
3. Freifelder, D. (1982) "Physical Biochemistry"; W.H. Freeman and Company, New York, USA.
4. Horton, R, Moran, L, Scrimgeour, G, Perry, M, Ravon, D (2005) "Principles of Biochemistry", 4th edition, Prentice-Hall of India, Kolkata.
5. Leach, A.R. (1992) "Molecular Dynamics Simulation", John Wiley and Sons, New York, USA
6. Narayanan, P (1999) "Introductory Biophysics"; New Age Publishing House, Mumbai, India.
7. Palmer, T (2004) "Enzyme: Biochemistry, Biotechnology, Clinical Chemistry" Affiliated-East-West Press, India.
8. Resnick, R., Halliday, D. and Walker (2001) "Fundamentals of Physics", Sixth edition, John Wiley and Sons, USA.
9. Roy R. N. (2007) "A text book of Biophysics" First Edition, New Central Book Agency, Ltd, Kolkata.
10. Satyanarayana, U (2005) "Biochemistry", Books Allied (P) Ltd, Kolkata.
11. Talwar, GP, Srivastava LM, (Editor) (2003) "Textbook of Biochemistry and Human Biology", 3rd edition, Prentice-Hall of India Pvt Ltd, New Delhi.
12. Tipler, P.A. (1999) "Physics for Engineers and Scientists"; Fourth edition, W.H. Freeman and Company, USA.
13. Vasantha Pattabhi and N. Gautham. (2001) "Biophysics"; Narosa Publishing Company, New Delhi, India.
14. Voet, D (2004), "Biochemistry", 3rd edition, Wiley, USA.

**Paper VI
(Genomics)**

Unit-I : (Introduction to Genomics)

Introduction to genomics- scope and application, Computational genomics, Organization of the prokaryotic and eukaryotic genomes, Genome maps and types, current sequencing technologies, partial sequencing, gene identification, gene prediction rules and software, Genome databases; Annotation of genome, Genome diversity: taxonomy and significance of genomes – bacteria, yeast, *Caenorhabditis*, *Homo sapiens*, *Arabidopsis*, etc.

Unit-II : (Functional Genomics)

Microarray - Gene Expression, methods for gene expression analysis; DNA array for global expression profile; Types of DNA array, Array databases; Applications of DNA microarray – analysis of gene expression, differential gene expression under different conditions and during development of organisms, Human Genome Project - Construction of physical maps; Basics of radiation hybrid maps; Sequencing of the entire human genome, annotation and analysis of genome sequences: sequence repeats, transposable elements, gene structure, Pseudogenes

Unit-III : (Computational Genome Analysis)

Introduction to genome analysis, Gene analysis; gene order; chromosome rearrangement; compositional analysis; clustering of genes; composite genes; Basics of Single Nucleotide Polymorphisms, detection and its implications; dbSNP and other SNP related database, Gene Prediction method, Prediction of ORFs, Prediction of signal sequence (Promoter, Primers, Splice site, UTR etc); BLAST, PSI BLAST, PHI BLAST; Epitope prediction; Gene expression analysis; Genome annotation

Unit-IV : (Comparative Genomics)

Relevance of comparative genomics; orthologs and paralogs; Comparative genomics of prokaryotes; Minimal genome; Vertical and horizontal gene transfer, Comparative genomics of organelles; Comparative genomics of eukaryotes, Differences and similarities in genomes of organisms; Evolution of protein families; Applications of comparative genomics in reconstruction of metabolic pathways

Unit-V : (Phylogenetic analysis)

Phylogenetics, cladistics and ontology; Phylogenetic representations – graphs, trees and cladograms; Classification and ontologies; Steps in phylogenetic analysis; Methods of phylogenetic analysis – similarity and distance tables, distance matrix method; Method of calculation of distance matrix (UPGMA, WPGMA); The Neighbour Joining Method; The Fitch/Margoliash method; Character-based Methods – maximum parsimony, maximum likelihood; Reliability of Phylogenetic trees; Steps in constructing alignments and phylogenies; Limitations of phylogenetic algorithms; Phylogenetic softwares – PAUP, PHYLIP, MacClade.

Suggested Reading:

1. Bergman N. H. (2007), "Comparative genomics" Volume 2, Humana Press
2. Cantor C.R., Smith C.L., (1993) "Genomics: the science and technology behind the Human Genome Project" John Wiley and Sons
3. Choudhuri S., Carlson D. B. (2008), "Genomics: fundamentals and applications" Informa Healthcare
4. Clark M (2000), "Comparative genomics" Springer
5. Griffiths A. J. F., Miller J.H., Suzuki D.T., (2000) "An Introduction to Genetic Analysis" W.H. Freeman and Co., Publishers.
6. Pevsner J (2009), "Bioinformatics and functional genomics", Edition 2, John Wiley and Sons
7. Primrose S. B., Twyman R. M. (2004), "Genomics: applications in human biology" Wiley-Blackwell
8. Primrose S. B., Twyman R. M. (2006), "Principles of gene manipulation and genomics" Wiley-Blackwell
9. Saccone C., Pesole G., (2003), "Handbook of comparative genomics: principle and methodology" John Wiley and Sons
10. Suhai S (2000), "Genomics and proteomics: functional and computational aspects" Springer

Paper VII**(Biological Database Management System)****Unit I : (Introduction to BDBMS)**

Database & Database users, Characteristics of Database, Database System applications, Database System Versus File Systems, Concepts and Architecture, Data Models, Schemas & Instances, DBMS architecture and Data

Independence, Database languages & Interfaces, View of Data, Data Models, Database Languages, Database, Users and Administrators, Database System Structure

Unit II : (Introduction Data models)

ER Model: Keys, Constraints, Design Issues, Extended ER features, Reductions of ER Schema to Tables. Relational Model: Structure, Relational Algebra; Hierarchical Model, Network Model, Object Oriented Model

Unit-III : (Structured Query Language)

Basic Structure, Set Operations, Aggregate Functions, Null Values, Nested Sub queries, Views, Integrity: Domain constraints, Joined Relations, Data-Definition Language, Embedded SQL, Dynamic SQL; Locking techniques, Granularity of Data Items – Database System Architecture and information retrieval: Centralized and Client-Server Architecture, Distributed DBMS, Data Mining, Data Integration, Data Warehousing

Unit IV : (Relational Database and Storage)

Pitfalls in Relational Design Database, Functional dependencies, Decomposition Normal Forms – 1NF, 2NF, 3NF & Boyce-Codd NF, Overall Database Design Process, Multi-valued Dependencies, Data Storage – Ordered indices, Static Hashing, Dynamic Hashing - Transaction Management – Security and Authorization.

Unit V : (Introduction to MySQL)

Introduction to MySQL, basics installation, server technology architecture, Basic MySQL datatype, Database languages, Transaction Management, Storage Management, Database Administrator, Database Users, Overall System Structure, MySQL connectivity

Suggesting Reading:

1. Date, C.J. (2000) "An introduction to Database systems"; Seventh Edition, Addison Wesley Publishers.
2. Elmasri and Navathe (2004) "Fundamentals of Database systems" Fourth Edition, Addison Wesley Publishers.
3. Silberschatz, A., Korth, H.F. and Sudarshan, S. (2002) "Database system Concepts"; Fourth Edition, McGraw Hill Publishers.
4. Ullman, J. D. (2001) "Principles of Database systems"; Second Edition, Galgotia Publications

Paper VIII**(Techniques in Bioinformatics)****Unit-I : (Biological Databases)**

Primary Sequence & Structure Databases: Genbank, SwissProt/Uniprot, EMBL, PIR, PDB, MMDB, NDB, CSD, KEGG etc. Derived (Secondary) Databases of Sequences and Structure: Prosite, PRODOM, PRINTS, Pfam, BLOCK, INTERPRO etc. SSOP, CATH, DSSP, FSSP, RNAbase, Genome Databases (at NCBI, EBI, TIGR, SANGER), High-throughput genomics sequences (EST, STS, GSS), ENSEMBL.

Unit-II : (Advanced techniques)

Algorithms for derivation of and searching sequence patterns: MeMe, PHI-BLAST, SCanProsite and PRATT, Algorithms for generation of sequence profiles: Profile Analysis method of Gribskov, HMMer, PSI-BLAST; Basic concepts on identification of disease genes, role of bioinformatics-OMIM database, reference genome sequence, integrated genomic maps, gene expression profiling; identification of SNPs, SNP database (DbSNP). Role of SNP in Pharmacogenomics, SNP arrays.

Unit-III : (Singles in DNA)

Introduction, DNA linguistics, Convey equation, Consensus, CG-islands, HMM, Gibbs sampling, Gene Prediction – introduction, statistical approaches, Spliced alignment, Reverse gene finding, some other problems.

Unit-VI : (Genome Rearrangement)

Introduction, Break point graphs, Signed Permutation, Transformation of permutation, Searching for the safe reversals, Algorithms for sorting by reversals, Capping chromosomes, Caps and tails, Genome duplication.

Unit-V : (DNA microarray)

DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), ArrayExpress, SAGE databases DNA microarray: understanding of microarray data, normalizing microarray data, detecting differential gene expression, correlation of gene expression data to biological process and computational analysis tools (especially clustering approaches)

Suggested Reading:

1. Baxevanis, A.D. and Francis Ouellette, B.F. (1998) "Bioinformatics—a practical guide to the analysis of genes and proteins" John Wiley and Sons
2. Des Higgins, Willie R. Taylor, Willie Taylor (2000) "Bioinformatics: sequence, structure, and databanks : a practical approach" Oxford University Press
3. Mount, D. (2004) "Bioinformatics: Sequence and Genome Analysis"; Cold Spring Harbor Laboratory Press, New York. (ISBN 0-87969-712-1)
4. Sharma, V. Munjal, A. and Shankar, A. (2008) "A text book of Bioinformatics" first edition, Rastogi Publication, Meerut – India.
5. Stanley Letovsky (1999) "Bioinformatics: databases and systems" Springer

Practical – III: Practical based on Paper V and VI**Biochemistry and Biophysics**

1. Experiment based on Osmosis by using Potato Osmoscope
2. SDS-PAGE Analysis of Protein
3. Calculation of Viscosity Index
4. Measurement of Surface Tension
5. Working and Principle of Biological Instruments (Ultra centrifuge, NMR Spectroscopy, Mass Spectroscopy, Electron Microscopy and Scanning Electron Microscopy)
6. Trypsin inhibitor activity.
7. To demonstrate kinetic behavior of enzymes by using spectrophotometer.
8. Separation of lipids by thin layer chromatography.
9. To study the characteristics of UV absorption spectra of Proteins.
10. To prepare the buffers & measurement of pH.
11. To determine the titration curve of amino acids & calculate the pKa values.
12. To determine the Tm of DNA.
13. Denaturation & Renaturation of DNA.
14. To determine the osmotic fragility of RBC.
15. Qualitative tests for-carbohydrates, proteins, amino acids and lipids.
16. Preparation of standard buffers and determination of pH.
17. Verification of Beer-Lambert's Law.
18. Estimation of carbohydrate by anthrone method.
19. Estimation of blood glucose by Folin-Wu method.
20. Estimation of amino acids by ninhydrin method.

21. Separation of amino acids and sugars using paper and thin layer chromatography.
22. Determination of saponification value and iodine number of fats.
23. Estimation of ascorbic acid.
24. Titration curve for amino acids and determination of pK value.
25. Sorenson-formol titration for amino acid estimation

Genomics

26. Sequence Analysis
27. Gene Analysis and identification
28. Genome databases
29. Annotation of genome
30. Perditiion of ORFs
31. dbSNP and other SNP related database
32. Prediction of signal sequence
33. Promoter
34. Primers
35. Splice site
36. UTR
37. Software
38. BioEdit
39. GENSCAN
40. GeneMark
41. HMMgene
42. Staden
43. Sequin
44. Glimmer
45. Mummer
46. Phylogenetic analysis using PHYLIP, Phylodraw, PAUP, Treeview, JalView.

Semester-II

Distribution of Practical Marks for Practical-III:- (Biochemistry and Biophysics and Genomics) (Based on Paper-V & VI)

Time: 6Hrs.

Max. Marks:100

- | | |
|--|----------|
| 1) Setting and working on any one exercise based on Biochemistry | 20 Marks |
| 2) Setting and working on any one exercise based on Biophysics | 20 Marks |
| 3) Setting and working on any one exercise based on Genome Predictions | 20 Marks |
| 4) Setting and working on any one exercise based on Genome Analysis by Softwares | 20 Marks |
| 5) Viva-voce | 10 Marks |
| 6) Practical Record | 10 Marks |

Total

100 Marks

Practical – IV: Practical based on Paper VII and VIII

Biological Database Management System

1. Structure Query Language
2. Exercise in RDBMS (MYSQL)
 - a. Data Definition Language (DDL) statements: Creating database, Selecting database, Deleting database, Creating table, Modifying Table, Deleting table
 - b. Data Manipulation statements: Inserting, updating and deleting records Retrieving Records Retrieving specific rows and columns
 - c. Use of MySQL operators – Arithmetic operators, Comparison Operators, Logical operators,, Math functions, Aggregate functions
 - d. String operations
 - e. Limiting, Sorting and grouping query results
 - f. Handling null values
 - g. Renaming or aliasing table and column names
 - h. Using subqueries
 - i. Using Joins – joining a table to itself, joining multiple tables
 - j. Use of Indexes

- k. Security Management
- l. Granting and Revoking rights on tables

Techniques in Bioinformatics

3. Primary Sequence & Structure Databases
 - a. Genbank
 - b. SwissProt/Uniprot
 - c. EMBL
 - d. PIR
 - e. PDB
 - f. MMDB
 - g. NDB
 - h. CSD
 - i. KEGG – pathway database
4. PHI-BLAST
5. PSI-BLAST
6. Identification of SNPs
7. SNP database (DbSNP)
8. DNA Microarray Analysis
 - a. GenSprings GX
 - b. R console
 - c. DNA Helix

Semester-II

Distribution of Practical Marks for Practical-IV:- (Biological Database Management System and Techniques in Bioinformatics) (Based on Paper-VII & VIII)

Time: 6Hrs.	Max. Marks:100
1) Setting and working on any one exercise based on RDBMS	20 Marks
2) Setting and working on any one exercise based on Primary Sequence & Structured Databases	20 Marks
3) Setting and working on any one exercise based on Blast Analysis	20 Marks
4) Setting and working on any one exercise based on Microarray Analysis	20 Marks)
Viva-voce	10 Marks
6) Practical Record	10 Marks
Total	100 Marks

Syllabus for Semester-III (Bioinformatics)

Paper IX : (System Biology)

Unit-I : (Introduction to System Biology)

System Biology – Introduction, Need for system analysis in Biology, System Biology approaches, Dynamic Analysis, Organization of living cells, Components vs. Systems, Links and functional states, Links to Networks.

Unit-II : (Introduction to System Biology)

Biochemical Reaction Kinetics – Rate equation approach, Biochemical Reaction Modeling, Basics principles and assumptions, elementary reactions, complex reaction, Michaelis-Menten equation for EK, Stochastic Modelling and Simulation, Modelling of Cell communication networks.

Unit-III : (Reconstruction of Biochemical Networks)

Basic features, Reconstruction methods, Organism specific source of information, Strategies relating to In silico Modeling of biological processes, Metabolic Networks, Regulation of metabolic networks, Signaling Networks.

Unit IV : (Introduction to Synthetic Biology)

Synthetic Biology - Introduction, Relevant aspects of Biological system, Emergence of Synthetic biology, Technological enablers, Tools in Synthetic biology, Gene Expression Patterns. E-cell and V-cell Simulations and Applications.

Unit V : (Introduction to R programming)

R programming – Introduction and preliminaries, Simple manipulation, Objects and Modules, Orders, Arrays, Lists, Reading data from files, Loops and conditions, Functions creation, Packages.

Suggested Reading:

1. B. O. Palsson “System Biology – Properties of Reconstructed Networks” Cambridge University Press
2. Olaf Wolkenhauer. (2010) “System Biology – Dynamic Pathway Modeling”
3. Andres Kriete, Roland Eils (2006) “Computational systems biology” Academic Press
4. Andrzej K. Konopka (2007) “Systems biology: principles, methods, and concepts” CRC Press/Taylor & Francis

5. Lilia Alberghina (2008) "Systems biology: definitions and perspectives" 2 Edition, Springer
6. Uri Alon (2007) "An introduction to systems biology: design principles of biological circuits" Chapman & Hall/CRC
7. W. N. Venables, D. M. Smith; "An Introduction to R (Version 2.8.1.)", R developer Core team.

Paper X
(Proteomics)

Unit-I : (Introduction to Proteomics)

Introduction to Proteomics: Scope and Application, Complexity of the problem: Post translational modification, Phosphorylation, Methods of studying proteins, establishing protein-protein interactions, Practical application of proteomics and current research technology, Protein databases

Unit-II : (The Proteome and Proteome technology)

Introduction; Expression proteomics (express profile); Cell map proteomics; Protein separation technology - 2D-Gel Electrophoresis, liquid chromatography, affinity chromatography (for cell map proteomics); X-ray diffraction, NMR, mass spectroscopy and its uses in protein identification; Forward and Reverse Proteomics

Unit-III : (Computational Protein Structure Prediction)

Secondary structure: Basic principles on which the prediction methods of first, second and third generation are based; algorithms of Chou Fasman, GOR methods; Predicting the secondary structures using these methods and analysis; concepts in measuring the accuracy of predictions (Q3, Segment overlap, Mathew's correlation coefficient etc.) **Tertiary Structure:** Theoretical basis of the methods for structure prediction and choice of appropriate prediction approach; basic principles and protocol of Homology Modeling; Databases of models; Basic principles for fold recognition, 1D profiles and threading approaches, basic principles of ab-initio structure prediction and the broad approaches, Structure Validation methods

Unit-IV : (Comparative Proteomics)

Protein structure comparison and classification: classes, folds; the concepts in 3D structure comparison, purpose of structure comparison, algorithms such as FSSP, VAST and DALI. Visualization of structures using Rasmol or SPDBViewer or CHIME, Basic concepts in molecular modeling, different types of computer representations of molecules, Concepts of force fields: representations of atoms and atomic interactions, potential energy representation, Genomics and Proteomics

Unit-V : (Advance Proteomics)

Molecular force field model, molecular dynamics, hydrogen bonds, Computation and minimization of RMSD over rotation, Solution to the problems of minimization of RMSD over rotation and translation, Solvent accessible surface of a protein.

Suggested Reading:

1. Azuaje F., Dopazo J., (2005) "Data analysis and visualization in genomics and proteomics" John Wiley and Sons
2. Dubitzky W. Granzow M. Berrar D (2007) "Fundamentals of data mining in genomics and proteomics"
3. Gu Jenny, Bourne P. (2009) "Structural bioinformatics" Wiley-Blackwell
4. Kraj A, Silberring J, (2008) "Proteomics: introduction to methods and applications" John Wiley & Sons
5. Liebler D.C, (2002), "Introduction to proteomics: tools for the new biology" Humana Press
6. Mishra N.C., (2010), "Introduction to Proteomics: Principles and Applications" John Wiley and Sons
7. Pennington S.R., Dunn M. J. (2001), "Proteomics: from protein sequence to function" BIOS
8. Reinders J, Sickmann A., (2009) "Proteomics: methods and protocols" Humana Press
9. Suhai S. (2000) "Genomics and proteomics: functional and computational aspects" Springer
10. Veetstra T.D., Yates J.R. (2006) "Proteomics for biological discovery" John Wiley and Sons
11. Polanski A., Kimmel M. (2007) "Bioinformatics" Springer Verlag Berlin Heibel berg

Paper XI**(Bio-Programming – I)****Unit-I : (Introduction to PERL)**

Introduction to PERL, History and uses, PERL Basics, Data types, Basic Operators, Control Statements: if, if else, if elsif else, Loops: do, while, until, for, foreach, labels, lists, Arrays and associative arrays

Unit-II : (Introduction to PERL)

Pattern matching: Regular expressions, Matching and substitution, Atoms and assertions, Subroutines and functions: structure and invocations, parameter matching, scope Files and I\O: file handles, opening, closing, reading and writing, formats, manipulating files, Modules: Extending PERL functionality, obtaining and installing, Object oriented PERL

Unit-III : (Introduction to ODBC)

DBM Databases and DBM Hashes, Design of DBI, DBI Methods, DBI Environment Variables, DBD Interface Modules, Fixed Length Random-Access Databases, Variable-Length Databases, Win32 Database Interface, Perl Graphics, Using the GD.pm graphics lib

Unit-IV : (Introduction to HTML and CGI)

Basics structure of HTML, Basics HTML TAGS, URL Encoding, CGI Environment Variables, Handling forms, Accessing form Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action

Unit-V : (Introduction to Bio-PERL)

Overview, basic installation, Sequence Objects, Location objects, Accessing sequence Installing Bioperl, General Bioperl Classes, Sequences (Bio::Seq Class, Sequence Manipulation), Features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan), Databases (Database Classes, Accessing a local database), Implementing REBASE, Introduction to BioPERL modules

Suggested Reading:

1. Arun Jagota (2004) “Perl for Bioinformatics” Arun Jagota
2. D. Curtis Jamison (2003) “Perl programming for biologists” Wiley-IEEE

3. D. Curtis Jamison (2008) “Perl Programming For Bioinformatics & Biologists” Wiley-India
4. James D. Tisdall (2003) “Mastering Perl for bioinformatics” O’Reilly Media, Inc
5. Jules J Berman (2008) “Perl: The Programming Language” Jones & Bartlett Learning
6. Randal L. Schwartz, Tom Phoenix, Brian D. Foy (2008) “Learning Perl” O’Reilly Media, Inc
7. Vittal R. Srinivas (2005) “Bioinformatics: A Modern Approach” PHI Learning Pvt. Ltd

Paper XII**(Parasite Bioinformatics)****Unit-I : (Introduction to Parasitic Diseases)**

Biology of Parasites - Life Cycle, Infectivity, Demographic distribution of strains (Malaria, Leishmaniasis, Trypanosoma, Filariasis), Role of bioinformatics in Diseases monitoring.

Unit-II : (Introduction to Parasitic Diseases)

Parasite Genome and Proteome Databases (AnoBase, ENSEMBL, Notre Dame, PlasmoDB), Vectors of parasites – Biology of vectors, Application of Bioinformatics Data Mining tools for Identification of: Parasite-specific genes/ gene products (e.g. house-keeping genes, genes essential for survival), Resistant Genes.

Unit-III : (Techniques to study Parasitic Diseases)

Full Genome Comparison, Gene Prediction, Signal sequence prediction, Protein sequence comparison and analysis, Protein structure comparison and analysis, Micro Array and Proteomics Data Analysis, Structural genomics of parasites.

Unit-IV : (Introduction to Host-parasite interaction)

Host-parasite interaction: Recognition and entry processes of different pathogens like bacteria and viruses into animal and plant host cells; alteration of host cell behavior by pathogens, virus-induced cell transformation, pathogen-induced diseases in animals and plants; cell-cell fusion in both normal and abnormal cells.

Unit-V : (Introduction to Host-parasite interaction)

Host-Parasite and Host-Vector-Parasite Interactions, Pathway databases (KEGG, BioCyc, Pathguide, REACTOME), Multi-Drug Resistance - Mechanism of MDR: genomic, molecular, cellular, Identification of genes responsible for MDR, Approaches to novel drug discovery for parasite, Challenges and opportunities in vaccine development, Plant Parasites and diseases - Disease resistance genes of plants, Plant-pathogen interactions.

Suggested Reading:

1. Bush, A. O., Fernandez, J. C., Esch, G.W. & Seed, R. J., "Parasitism", Cambridge University Press, 2001.
2. Melville, S.E., "Parasite genomics protocols", New Jersey. Humana Press, 2004.
3. Lately, A.N, Pune, "A modern textbook of Parasitology", Narendra prakashan, 1991.
4. Wyler, D.J. "Modern parasite biology: cellular immunological and molecular aspects", Ed., 1990

Practical based on Paper IX and X**System Biology**

1. Microbial Database
2. MLVA
3. HBMMD
4. DSMZ
5. RIDOM
6. GPMS

Proteomics

7. Protein Sequence Databases
8. Protein Structure Databases
9. Protein Sequence Analysis by BioEdit
10. Advanced Visualization Software and 3D representations
11. Coordinate generations and inter-conversions
12. Secondary Structure Prediction
 - a. GORIV
 - b. Online Secondary structure prediction tools
13. Fold Recognition, *ab initio* (Rosetta Server)
14. Homology based comparative protein modeling
15. Energy minimizations
16. Validation of models

- a. WHATIF
 - b. PROSA
 - c. PROCHECK
 - d. VERIFY 3D
 - e. RAMPAGE
17. Protein Structure Alignment
 18. Protein Structure Comparison
 19. Modeller9v7
 20. Geno-3D
 21. Discovery Studio Server

Semester-III**Distribution of Practical Marks for Practical-V:- (System Biology and Proteomics)****(Based on Paper-IX & X)****Time: 6Hrs.****Max. Marks:100**

- | | |
|---|----------|
| 1) Setting and working on any one exercise based on Databases | 20 Marks |
| 2) Setting and working on any one exercise based on Structural Prediction | 20 Marks |
| 3) Setting and working on any one exercise based on Validation of Models | 20 Marks |
| 4) Setting and working on any one exercise based on Structural Alignment | 20 Marks |
| 5) Viva-voce | 10 Marks |
| 6) Practical Record | 10 Marks |

Total**100 Marks****Practical based on Paper XI and XII****Bio-Programming – I and Parasite Informatics**

1. Exercise in Structured Programming
Basic Operators and Control Flow, Basic Perl Data Types, References, Matrices, Complex/Nested Data Structures, Scope (my, local, our), Function/Subroutines, System and User Function, The

local Operator, Variable-length Parameter Lists, Notes on Lexical Variable, File handle and File Tests, stat and stat Functions, Formats, Directory Access & Manipulation, Process Management, Formatting Data, System Information

2. Exercise in Regular Expressions
Uses of Regular Expressions, Patterns, Single-Character Patterns, Grouping Patterns (Sequence, Multipliers, Parentheses as memory, Alternation) Anchoring Patterns, Precedence, Matching Operators, Ignoring Case, Different Delimiter, Variable Interpolation, Special Read-Only Variables, Substitutions, Split and Join Functions, Dynamic Programming, Approximate String Matching
3. Exercise in CGI
URL Encoding, CGI Environment Variables, Handling forms, Accessing form Input, Extra Path Information, CGI.pm Module, Passing Parameters via CGI, Less Typing, Sever Side Includes, Debugging CGI programs, Stepping through programs, Breakpoints, Line Action
4. Exercise in CPAN Database Modules
DBM Databases and DBM Hashes, Design of DBI, DBI Methods, DBI Environment Variables, DBD Interface Modules, Fixed Length Random-Access Databases, Variable-Length Databases, Win32 Database Interface, Perl Graphics, Using the GD.pm graphics library
5. Exercise in Bioperl
Installing Bioperl, General Bioperl Classes, Sequences (Bio::SeqClass, Sequence Manipulation), features and Location Classes (Extracting CDS), Alignments (AlignIO), Analysis (Blast, Genscan),
Databases (Database Classes, Accessing a local database), Implementing REBASE
6. Exercise in HTML
Basics structure of HTML, Formatting text with HTML, Adding local and remote links, Adding graphics, creating lists in HTML, Creating tables in HTML, Frames, and Forms.
7. Parasite Bioinformatics
 i% ICTV database
 i% Parasite Genome and Proteome Databases.
8. Genome Comparison
9. Gene Prediction (Parasite)
10. Signal sequence prediction (Parasite)
11. Protein sequence comparison and analysis
12. Protein structure comparison and analysis (from parasite genome)

Semester-III

Distribution of Practical Marks for Practical-VI:- (Bio-Programming – I and Parasite Informatics)

(Based on Paper-XI & XII)

Time: 6Hrs.	Max. Marks:100
1) Setting and working on any one exercise based on Programming/Regular Expressions	20 Marks
2) Setting and working on any one exercise based on CGI / CPAN Database Modules	20 Marks
3) Setting and working on any one exercise based on Biopperl / HTML	20 Marks
4) Setting and working on any one exercise ' based on parasite informatics	20 Marks
5) Viva-voce	10 Marks
6) Practical Record	10 Marks
Total	100 Marks

Syllabus Semester-IV (Bioinformatics)

Paper XIII

(Molecular Modeling and Drug Design)

Unit-I : (Concepts in Molecular Modeling)

Introduction; Coordinate System; potential energy surfaces molecular graphics; Computer hardware and software; Mathematical concepts – introduction of molecular mechanics & quantum mechanics

Unit-II : (Molecular Mechanics)

Features of molecular mechanics, force fields; Bond structure and bending angles – electrostatic, Vander Waals and non-bonded interactions, hydrogen bonding in molecular mechanics; Derivatives of molecular mechanics energy function; Calculating thermodynamic properties using force field; Transferability of force field parameters, treatment of delocalized *pi* system; Force field for metals and inorganic systems – Application of energy minimization

Unit-III : (Molecular Dynamics Simulation Methods)

Molecular Dynamics using simple models; Molecular Dynamics with continuous potentials and at constant temperature and pressure; Time-dependent properties; Solvent effects in Molecular Dynamics; Conformational changes from Molecular Dynamics simulation. Introduction, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzman velocity, time steps, duration of the MD run. Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions.

Unit-IV : (Molecular Modeling in Drug Discovery)

Deriving and using 3D pharmacophore; Molecular Docking; Structure based methods to identify lead compounds; *de novo* ligand design; Applications of 3D Database Searching and Docking, Finding new drug targets to treat diseases – Pharmacophore identification - Structure based drug design -Molecular Simulations

Unit-V : (Structure Activity Relationship)

QSARs and QSPRs, QSAR Methodology, Various Descriptors used in QSARs: Electronic; Topology; Quantum Chemical based Descriptors. Use of Genetic Algorithms, Neural Networks and Principle Components Analysis in the QSAR equations

Suggested Reading:

1. Andrew R. Leach (2001) "Molecular Modeling – Principles and Applications"; Second Edition, Prentice Hall, USA
2. Fenniri, H. (2000) "Combinatorial Chemistry – A practical approach", Oxford University Press, UK.
3. Gordon, E.M. and Kerwin, J.F. (1998) "Combinatorial chemistry and molecular diversity in drug discovery"; Wiley-Liss Publishers
4. Lednicer, D. (1998) "Strategies for Organic Drug Discovery Synthesis and Design"; Wiley International Publishers
5. Swatz, M.E. (2000) "Analytical techniques in Combinatorial Chemistry"; Marcel Dekker Publishers

Paper XIV**(Chemo-informatics)****Unit-I : (Introduction to Chemo-informatics)**

Chemo-informatics: Introduction, scope and application, Basics of Chemo-informatics, Current Chemo-informatics resources for synthetic polymers, pigments. Primary, secondary and tertiary sources of chemical information, Databases: Chemical Structure Databases (PubChem, Binding database, Drugbank), Database search methods: chemical indexing, proximity searching, 2D and 3D structure and substructure searching. Drawing the Chemical Structure: 2D & 3D drawing tools (ACD ChemsSketch) Structure optimization.

Unit-II : (Introduction to Chemo-informatics)

Introduction to quantum methods, combinatorial chemistry (library design, synthesis and deconvolution), spectroscopic methods and analytical techniques, Representation of Molecules and Chemical Reactions: Different types of Notations, SMILES Coding, Structure of Mol files and Sd files (Molecular converter, SMILES Translator). Similarity search of the molecule (Zinc Database).

Unit-III : (Introduction to Chemo-informatics)

Analysis and use of chemical reaction information, chemical property information, spectroscopic information, analytical chemistry information, chemical safety information, Drug Designing: Prediction of Properties of Compounds, QSAR-Data Analysis, Structure-Activity Relationships, Electronic properties, Lead Identification, Molecular Descriptor Analysis.

Unit-IV : (Introduction to Chemo-informatics)

Target Identification: Molecular Modeling and Structure Elucidation: Homology Modelling (Modeller 9v7, PROCHECK), Visualization and validation of the Molecule (Rasmol, Pymol Discovery studio), Applications of Chemo-informatics in Drug Research - Chemical Libraries, Virtual Screening, Prediction of Pharmacological Properties.

Unit-V : (Introduction to Chemo-informatics)

Drug Discovery: Structure based drug designing, Docking Studies (Target Selection, Active site analysis, Ligand preparation and conformational analysis, Rigid and flexible docking, Structure based design of lead compounds, Library docking), Pharmacophore - Based Drug Design, Pharmacophore Modeling (Identification of pharmacophore features, Building 2D/3D pharmacophore hypothesis), Toxicity Analysis-Pharmacological Properties (Absorption, Distribution and Toxicity), Global Properties (Oral Bioavailability and Drug-Likeness) (ADME, OSIRIS, and MOLINSPIRATION)

Suggested Reading:

1. Bajorath J (2004), "Chemoinformatics: Concepts, Methods and Tools for Drug Discovery" Humana Press
2. Leach A, Gillet V, "An Introduction to Chemoinformatics" Revised edition, Springer
3. Gasteiger J. Engel T. "A textbook of Chemoinformatics" Wiley-VCH GmbH & Co. KGaA
4. Bunin B. Siesel B. Guillermo M. "Chemoinformatics: Theory, practice & products", Springer
5. Lavine B. (2005), "Chemometrics and chemoinformatics" American Chemical Society
6. Casteiger J. and Engel T (2003) "Chemoinformatics" Wiley-VCH
7. Bunin Barry A. Siesel Brian, Morales Guillermo, Bajorath Jürgen. Chemoinformatics: Theory, Practice, & Products Publisher: New York, Springer. 2006. ISBN: 1402050003.
8. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: WileyVCH; 1st edition. 2003. ISBN: 3527306811.
9. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic, 2003. ISBN: 1402013477.
10. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4 Volumes), 2003. Publisher: Wiley-VCH. ISBN: 3527306803.

**Paper XV
(Bio-Programming – II)****Unit I : (Introduction to Java)**

Why JAVA is important to the internet, the continuing revolution, an overview of JAVA, Object Oriented Programming, Data types- Variables and Arrays, the simple types, floating point types, Operators, Control statements, Class fundamentals, Declaring objects, Assigning object reference variables, Introducing methods, Constructors, The this keyword; Garbage collection, using objects as parameters, Argument passing, Retaining objects, Recursion, Introducing Access control, Understanding static; Nested and inner classes, exploring the string class, Using command line arguments.

Unit II : (Introduction to Java)

Inheritance: Basics, Member access and inheritance. Using super: to call super class constructors, Creating a multilevel hierarchy, Method overriding, Dynamic method dispatch, Using abstract classes, Using final with inheritance, Using final to prevent overriding, Using final to prevent inheritance, The object class

Packages and Interfaces: Packages, Defining a package, Understanding class path, Access protection: Importing packages, Defining an interface, Implementing interfaces, Applying interfaces, Variables in interfaces, Exception Handling: Fundamentals, Exception types, Uncaught exceptions, Using try and catch, Displaying a description of an exception. Multiple catch clauses, Nested statements, throw, throws; Java's built in exceptions, Creating own exception subclasses, Using exceptions

Unit III : (Introduction to Java)

Multithreaded programming: The Java thread model. Thread priorities, Synchronization, Messaging, The thread class and the run able interface. The main thread: creating a thread, Implementing run able, extended thread, Choosing an approach, creating multiple threads, Using is alive () and join(), Thread priorities; Synchronization :Using synchronized methods, the synchronized statement, Inter-thread communication, Deadlock, Suspending resuming and stopping threads, Using multithreading.

Unit IV : (Introduction to Java)

I/O Applets: I/O basics - Streams, Byte streams and character streams. The predefined streams; Reading console Input: reading characters, reading strings, Writing files, Applets, Fundamentals, The transient and volatile modifiers, using instance of, Native methods, Problems with native methods

Unit V : (Introduction to Bio-Java)

Installing Bio-Java, Symbols, Basic Sequence Manipulation (DNA to RNA, Reverse Complement, motif as regular expression), Translation (DNA to Protein, Codon to amino acid, Six frame translation), Proteomics (Calculate the mass and pI of a peptide), Sequence I/O (File Formats conversions), Locations and Features (Point Location, Range Location, Feature modifications), BLAST and FASTA (Blast and FastA Parser, extract information from parsed results), Counts and Distributions, Weight Matrices and Dynamic Programming, User Interfaces.

Suggested Reading:

1. Benjamin, Cummings and Booch, G. (1994) "Object Oriented Design and Applications"; Second edition, Addison Wesley Publishers.
2. Horstmann, C.S. (2000) "Computing Concepts with Java 2 Essentials"; Second Edition, John Wiley Publishers
3. Naughton, P. and Schildt, H. (1999) "Java-2: The complete Reference"; Third Edition, McGraw Hill Publishers.
4. Bal H, Hujol J, (2007) "Java for bioinformatics and biomedical application" Springer Japan
5. Lindsey C. S., Tolliver J.S., Lindblad T, (2005) "JavaTech: an introduction to scientific and technical computing with JAVA" Cambridge University Press
6. Srinivas V.R. (2005) "Bioinformatics: A modern Approach" PHI learning Pvt. Ltd

Paper XVI**(Research Methodology, IPR and Bioethics)****Unit I : (Research Methodology)**

Research and Technical Writing: What is research? The process of research – various types of research – research methodology – Hypothesis – research writing – basic principles; publication process – peer review - Journal impact factors – popular journals in Computational Biology & Bioinformatics (brief overview of their scope),

Professional Societies in the field – their role in research and knowledge dissemination, Open Access Publications, Concept of ethics – its application in Scientific Research and Academics, Solving ethical conflicts, moral reasoning & ethical theories, responsibilities and rights

Unit II : (Intellectual Property Rights)

General principles of Intellectual property rights (IPR); Patents and methods; application of patents; Legal implications; International treaties for protection of IP – Bern, Paris, TRIPS, WIPO treaties, Biodiversity convention, etc

Unit III : (Intellectual Property Rights)

Nature of Intellectual Property: Patents, Designs, Trademarks and Copyright. Process of Patenting and Development: technological research, innovation, patenting, development; International cooperation on Intellectual Property, Procedure for grants of patents, Patenting under PCT; Scope of Patent Rights; Licensing and transfer of technology. Patent information and databases, Geographical Indications

Unit IV : (Bioethics)

The legal and socioeconomic impacts of biotechnology; public education of the process of the processes of biotechnology involved in generating new forms of life for informed decision making; Biosafety regulation and national and international guidelines; rDNA guidelines; Experimental protocol approval; levels of containment

Unit V : (Bioethics)

Environmental aspects of biotechnology applications; Use of genetically modified organisms and their release in environment; Special procedures for rDNA-based product production ; Biodiversity and farmers rights; Beneficial applications and development of research focus to the need of the poor; Identification of directions for yield effect in agriculture, aquaculture, etc; Bioremediation

Suggested Reading:

1. Sasson, A. (1988) "Biotechnologies and Development", UNESCO Publications
2. Sasson, A. (1993) "Biotechnologies in developing countries present and future"; UNESCO Publishers

3. Singh, K. "Intellectual Property Rights on Biotechnology"; BCIL, New Delhi
4. Halbert, (2007) "Resisting Intellectual Property" Taylor & Francis Ltd
5. Ramappa T., "Intellectual Property Rights Under WTO", S. Chand

Practical Based on Paper XIII, XIV, XV and XVI

Molecular Modeling, Drug Design, Chemo-informatics , Bio-Programming –II and Research Methodology, IPR and Bioethics

1. Binding site identification
2. Pharmacophore identification
3. Rigid body docking using Autodock and ADT
4. Molecular dynamics simulations using Gromacs
5. Visual Molecular Dynamics (VMD)
6. Docking with LigandFit (Discovery Studio)
7. Receptor and Ligand Optimization
8. Conformational Analysis
9. Concepts of Flowcharting, Algorithm Development
10. Chemo-informatics Software
 - a. AMBER
 - b. ArgusLab 3.0
 - c. BABEL
 - d. ACD/Labs
 - e. Chemos
 - f. VEGA
 - g. HaptiChem
 - h. ChemJun
11. PubChem
12. ChemSketch
13. Chemo-informatics databases
14. Chemical structure representation
15. Smiles - Simplified Molecular Input Line Entry System
16. Molecular Dimension Limited (MDL) file format for chemical connectivity
17. Chemical Structure similarity
18. Fingerprints and search for substructure similarity
19. Generation of 3D structures from 2D representations

20. 3D structure similarity
21. Elements of molecular descriptors
22. Writing Pseudo Codes
23. Working with Objects, Arrays, Conditionals and Loops
24. Creating Classes and Applications in Java
25. Java Applets Basics, Graphics, Fonts and Color
26. Simple Animation and Threads, Advanced Animation, Images and Sound
27. Managing Simple Events and Interactivity
28. Creating User Interfaces with AWT, Modifiers
29. Packages and Interfaces, Exception, Multithreading
30. Streams and I/O, Using Native Methods and Libraries
31. Java Programming Tools, Working with Data Structures
32. Sequence Analysis Packages – EMBOSS, NCBI Tool Kit
33. Dynamic programming
34. Analysis of Biological Sequences
 - a. Basic Blast
 - b. Specialized Blast
35. FASTA

Semester-IV

Distribution of Practical Marks for Practical-VII:- (Molecular Modeling, Drug Design, Chemo-informatics , Bio-Programming –II and Research Methodology, IPR and Bioethics)

(Based on Paper-XIII, XIV, XV & XVI)

Time: 6Hrs.

Max. Marks:100

- | | |
|--|----------|
| 1) Setting and working on any one exercise based on molecular modeling | 20 Marks |
| 2) Setting and working on any one exercise based on molecular dynamics | 20 Marks |
| 3) Setting and working on any one exercise based on programming | 20 Marks |
| 4) Setting and working on any one exercise based on chemo-informatics | 20 Marks |
| 5) Viva-voce | 10 Marks |
| 6) Practical Record | 10 Marks |

Total

100 Marks

Seminars: Two theory classes/ week. Student have to submit script of the seminar.

Projects: Project to the students will be distributed at the beginning of third semester with the consent of HOD and shall be examined during the period of practical examination in IV semester. The student will develop the skill for designing the programs related to Bioinformatics. For this, variety of small research projects designed by the teachers based on the interest of the student and capabilities should be worked out.

The projects should be based on following topics

- Biological database designing
- Biological software designing
- Biological tool designing
- Chemo-informatics
- Comparative genomics and proteomics
- Drug designing
- Molecular modeling
- Parasite bioinformatics
- Pharmaco-informatics
- Plant bioinformatics
- Structural biology
- System biology
- Vaccine designing
- Any recent biological research topics

Semester-IV

Distribution of Practical Marks for Practical-VIII:- (Project Work)

Distribution of Marks for Project :-

Total Marks - 100 (Time : 3 Hrs per Week)

(1) Hypothesis	10 Marks
(2) Viva based on the project.	20 Marks
(3) Depth of Work	30 Marks
(4) Conduct of project work	20 Marks
(5) Project Record	20 Marks

Total

100 Marks

Internal Assessment: It should be based on-

1. Study tour : Educational / Institutional / Industrial tour is compulsory for M. Sc. Bioinformatics
 - Semester I/II: Visit to local research laboratory
 - Semester III/IV: Educational tour to visit the industry / CSIR research laboratory, ICAR laboratory.
2. Seminars.
3. Unit test, Open Book Test and Semester end terminal examination.

List of Equipments:

1. Microscopes
2. Laminar Airflow
3. High speed centrifuge
4. Horizontal gel electrophoresis apparatus
5. Vertical gel electrophoresis apparatus
6. Submarine gel electrophoresis apparatus
7. UV spectrophotometer
8. Sonicator
9. Chromatography Chamber
10. Calculator.
11. Computer systems.
12. LAN
13. Server
14. High speed internet connection
15. Telescope
16. Monochromator
17. Spectrophotometer
18. Babinet's compensator
19. Conductors.
20. Conductivity meter.
21. Printers.
22. CCD Camera.
23. Projector.
24. Online lecture hall.
25. Rosetta Server
26. Discovery Studio Server
27. MySQL Operator
28. Deep Frezer
29. PCR Machine
30. Lyofilizer

31. Spectrometer
32. Plane Transmission Grating (England Make – 15000 LPI)
33. Thermal Conductivity of Solid Kit
34. Wavelength of light by Newtons Ring Method – Complete Setup including travelling microscope, sodium lamp, and lenses.
35. Clement & de Serme's apparatus for specific Heat of gases.
36. Sodium lamp with leak transmitter (35 Watt, 65 Watt)
37. Variable slit
38. Apparatus for conductivity of a semiconductor by Four Probe method
39. Polaroids with circular scale.
40. Double dense flint glass prism.
41. Polarize Microscope
42. LASER light source.
43. **List of Software** : Visualization software, Verify 3D, Whatif, Prosa, Modeller, PAUP, PHYLIP, MacClade, MEME/MAST, eMotif, interproScan, ProSite, ProDom, Pfam., VMD. BABL, MOPAC, Phylodraw, ClusterX, ClusterL.
44. **Databases** : PubMed, PubMed central, OMIM / OMIA, Citation matcher, Nucleotide/ Genome Databases, Protein Sequence Database, Structure databases, Protein Pattern Databases, FmtSeq, ReadSeq, Sequence manipulation Suite, Dot Plot, Pairwise alignment, Multiple Sequence Alignment, BioEdit, GeneDoc, ClustalW / X, MEGA, MEME, RasMol, Cn3D, MolMol, NCBI.
