PROSPECTUS
OF
MASTER OF SCIENCE IN
BIOINFORMATICS
Semester-I, Winter 2012
Semester-II, Summer 2013
Semester-III, Winter 2013
Semester-IV, Summer 2014

Price Rs.12/-
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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

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)

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

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)

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:
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-

Suggested Reading:

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 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:

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.

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

Time: 6Hrs.

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<td>1) Setting and working on any one exercise based on Biostatistics</td>
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<td>2) Setting and working on any one exercise based on Mathematics</td>
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<td>3) Setting and working on any one exercise based on Cell Biology</td>
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<td>4) Setting and working on any one exercise based on Molecular Biology</td>
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<td>5) Viva-voce</td>
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<td>6) Practical Record</td>
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Total 100 Marks

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

Computer for Biologists


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.


5. Windows Properties - Navigating Control Panel, Changing Theme, Desktop Settings, Screen Saver Settings, Appearance Settings, Display Settings, Mouse Settings


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


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


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

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: 6 Hrs.  
Max. Marks: 100

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<td>Setting and working on any one exercise based on Databases</td>
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<td>Setting and working on any one exercise based on Data Processing &amp; Analysis</td>
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|   |   | 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

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; Ramachandran 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.
Suggested Reading:


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, Peridiction 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:

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)

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:
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-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:

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
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.
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. Perdition 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

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
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

Semester-II

Distribution of Practical Marks for Practical-IV:- (Biological Database Management System and Techniques in Bioinformatics)

(Based on Paper-VII & VIII)

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<th>Time: 6Hrs.</th>
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<tbody>
<tr>
<td>1) Setting and working on any one exercise based on RDBMS</td>
<td>20 Marks</td>
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<tr>
<td>2) Setting and working on any one exercise based on Primary Sequence &amp; Structured Databases</td>
<td>20 Marks</td>
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<tr>
<td>3) Setting and working on any one exercise based on Blast Analysis</td>
<td>20 Marks</td>
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<tr>
<td>4) Setting and working on any one exercise based on Microarray Analysis</td>
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<td>Viva-voce 10 Marks</td>
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<td>6) Practical Record</td>
<td>10 Marks</td>
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<tr>
<td><strong>Total</strong></td>
<td><strong>100 Marks</strong></td>
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</tbody>
</table>
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:
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:
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:

Practical based on Paper IX and X

System Biology
1. Microbial Database
2. MLVA
3. HBMMMD
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

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
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 Bioperl / 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:**


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**Paper XIV (Chemo-informatics)**

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


**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)**

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:
3. Gasteiger J. Engel T. “A textbook of Chemoinformatics” Wiley-VCH GmbH & Co. KGaA
5. Lavine B. (2005), “Chemometrics and chemoinformatics” American Chemical Society

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:

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),

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)

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:

**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

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<td>1</td>
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<td><strong>Total</strong></td>
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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
- Pharmac-o-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)

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<td>(1) Hypothesis</td>
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<td>(2) Viva based on the project.</td>
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<td>(3) Depth of Work</td>
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<td>(4) Conduct of project work</td>
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<tr>
<td>(5) Project Record</td>
<td>20 Marks</td>
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<tr>
<td><strong>Total</strong></td>
<td><strong>100 Marks</strong></td>
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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.
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 Newton’s 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.

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