Swami Ramanand Teerth Marathwada University, Nanded

Syllabus M.Sc. Bioinformatics (Revised)

Choice Base Credit System (CBCS) Pattern- (June – 2014 pattern) (W. e. f. 2015-16)

M. Sc. Bioinformatics Second Year (Third Semester)

Paper No.	Paper Title	External (ESE)	Internal (CA)	Total
BI –XI	Statistics for Bioinformatics	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI –XII	Chemo Informatics and Drug Designing	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI – XIII	Systems Biology	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
*BI -XIV (Elective)	Object Oriented Programming	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI -XV	Seminar	25 Marks		Credit : 1
			Total for Sem: III	**Credit :17**

M. Sc. Bioinformatics Second Year (Fourth Semester)

Paper No.	Subject Title	External (ESE)	Internal (CA)	Total
BI –XVI	Biological Database Management	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI –XVII	Programming using Perl and Python	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI –XVIII	Genomics and Proteomics	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
*BI -XIX (Elective)	Structural Bioinformatics	75 Marks	25 Marks (2 Test:15 Marks + Assignments:10 Marks)	Credit :4 (100 Marks)
BI – XX	Seminar	25 Marks		Credit : 1

Lab Course Work (Annual Practical)	Lab Course Work -V	75 Marks	25 Marks	Credit :4 (100 Marks)
	Lab Course Work -VI	75 Marks	25 Marks	Credit :4 (100 Marks)
	Lab Course Work -VII	75 Marks	25 Marks	Credit :4 (100 Marks)
	Lab Course Project Work -VIII (Dissertation/ Elective Lab Course Work)	75 Marks	25 Marks	Credit :4 (100 Marks)
			Total for Lab Course Work (Annual)	**Credit :16**
			Total for M.Sc. I Year: Sem. I + Sem. II + Lab Course Work (Annual)	**Credit: 50**
			Total for M.Sc. (I Year + II Year)	**Credit:100**
			Total for Sem: IV	**Credit :17**

Note: *Paper –IV (Elective): Transfer of Credit as per Students Choice
**The Evaluation of Seminar Should be from panel of Experts.

CA- Continuous Assessment
ESE- End of Semester Examination

M.Sc. Bioinformatics (Semester Pattern) III Semester

BI : XI Statistics for Bioinformatics **Marks: 100** **Hours: 45**

Unit I Introduction

Definition of statistics, population Concept of Data – Discrete and continuous data, Representation of data – Tabulation, Graph, Chart Diagrams, What Are Events? Complements.
Entropy and Related Concepts: Information theory, Entropy Relative Entropy Scores and Support Inference

Unit II Probability theory

Probability, sample space mutually exclusive and exhaustive events. Probabilities of Events Conditional Probabilities Independence of Events, axiomatic definition of probability, addition theorem of probability, multiplication theorem of probability, conditional probability, byes theorem

Unit III Measure of central tendency, dispersion

Definition, formula, and computation for ungrouped and grouped data of Arithmetic Mean – Combine mean, weighted mean, GM, HM. Median, Mode .
Quartiles – Definition, formula, and computation for ungrouped and grouped data.
Range – Definition for ungrouped and grouped data. SD, MD, Mean deviation about (mean mode median), variance: real life examples. Correlation and regression.

Unit IV Continuous and discrete distribution

Probability Distributions – Discrete and Continuous
Discrete Probability Distributions – One Bernoulli trial, The Binomial, Distribution, The Hyper geometric Distribution, The Uniform Distribution, The Geometric Distribution, The Poisson distribution, Approximations
Continuous Distributions – The Uniform Distribution, the Normal, Distribution, the Exponential Distribution, The Gamma Distribution, The Beta Distribution. Tests of statistics: z test, t test, f test, chi square test.

Unit V Random variables:

Continuous random, variables, discrete random variables, pdf, pmf, mgf, problem.
Design of experiment (ANOVA- One way, Two way)
Introduction to Matrices: addition, multiplication.

Reference Books:

1. Fundamentals of statistics- S.C. Gupta, V.K. Kapur- Himalaya
2. Statistics: concepts and applications by Frank, Harry & Althoen, S. C., Cambridge University Press,
3. Introduction to probability and statistics by Lipschutz, S. & Schiller, J. J., New York.
4. Statistical methods in bioinformatics: an introduction by Ewens, W. J. & Grant, G.Springer,
5. Handbook of computational statistics: concepts and methods by Gentle, Hardle,-Springer
6. Introduction of Mathematics for Life science- E. Batschelet - Springer
7. Discrete Mathematics- Semyour Lipschutz & Marc Lipson-McGraw Hill
8. Statistical Methods - Gupta-Himalaya
9. Biostatistics – P. Hanamantrao- Himalaya
10. Introduction to Biostatistics Dr. Pranabkumar Banerjee

Practical (Lab Course Work –V)

Experiments based on given syllabus by using data from biological experiments

M.Sc. Bioinformatics (Semester Pattern) III Semester

BI : XII Chemo Informatics and Drug Designing Marks: 100 Hours: 45

Unit I: Introduction

Chemoinformatics definition, scope of chemoinformatics, history of chemoinformatics, why to use informatics methods in chemistry?

Unit II: Representations of chemical compounds

Introduction, Computer Representations of Chemical Structures: Graph Theoretic Representations, Linear Notations, Connection Tables, Canonical Representations of Molecular Structures. 2D structure databases, Reaction Databases, The Representation of Patents and Patent Databases.
Representations of 3D molecular structures: Experimental 3D Databases, 3D Database Searching. Theoretical 3D Databases: Structure-Generation Programs,

Unit III: Molecular Descriptors

Introduction, Descriptors Calculated from the 2D Structure: Simple Counts, Physicochemical Properties, Molar Refractivity.
Structure Searching: Substructure Searching, Screening Methods, Similarity searching, Conformational Search and Analysis: Systematic and Random Conformational Search.

Unit IV: Drug and Drug-Targets

Drug: definition, "Drug-Likeness" and Compound Filters, rule of five. Lead Compound: definition, natural and synthetic resources of lead compounds. Drug targets: Enzymes, receptors, carrier proteins, structural proteins, nucleic acids, etc.

Unit V: Drug designing

Combinatorial Synthesis and Combinatorial Library, QSAR, 3D Pharmacophores. Screening Methods: High-throughput screening, Virtual Screening. Protein–Ligand Docking. The Prediction of ADMET Properties, Toxicity Prediction.

Reference Books:

1. Handbook of Chemoinformatics, volume 1, by John Gastiger, Thomas Engel, WILEY-VCH
2. Guidebook on Molecular Modelling in Drug Designing-Ed. N Claude Cohen-Elsevier
3. An Introduction to Chemoinformatics, by Andrew R. Leach & Valerie j. Gillet, Springer
4. Instant Notes in Medicinal Chemistry, by G. Patrick, BIOS Scientific
5. Discovering Genomics, Proteomics, & bioinformatics- Campbell & Heyer-Pearson

Practical (Lab Course Work –V)

Experiments based on syllabus

M.Sc. Bioinformatics (Semester Pattern) III Semester

BI : XIII Systems Biology **Marks: 100** **Hours: 45**

Unit I Enzymology

Enzyme general characteristics, nomenclature and classification. Methods of isolation, purification and characterization of enzymes. Concept of enzyme assay, enzyme activity, coenzymes and isoenzymes. Enzyme kinetics: Michaelis - Menten Equation - form and derivation, steady state enzyme kinetics. Significance of Vmax and Km.

Unit II Enzymology

Enzyme inhibition - types of inhibitors - competitive, non-competitive and uncompetitive, their mode of action and experimental determination.
Immobilized Enzymes: Relative practical and economic advantage for industrial use,
Various methods of immobilization ionic bonding, adsorption, covalent bonding (based on R groups of amino acids), microencapsulation and gel entrapment.

Unit III . Metabolic Pathways

Photosynthesis - Light harvesting complexes; mechanisms of electron transport; photoprotective mechanisms; CO2 fixation-C3, C4 and CAM pathways.
Respiration– Glycolysis, Citric acid cycle; mitochondrial electron transport and ATP synthesis; alternate oxidase; photorespiratory pathway.
Nitrogen metabolism **-** Nitrate and ammonium assimilation; amino acid biosynthesis, Nucleotide biosynthesis- de novo and salvage.

Unit IV. More on Metabolic Pathways

Databases: KEGG, PathDB, EcoCyc and MetaCyc, EMP, Malaria Parasite Metabolic Pathways Boehringer Mannheim - Biochemical Pathways.
LIGAND - Biochemical Compounds and Reactions. ENZYME – Enzymes; BRENDA - Comprehensive Enzyme Information System. Full Genome Annotation through knowledge of Metabolic Pathways Organism Specific Metabolic Pathways. Comparison of Metabolic Pathways

Unit V. Metabolic Pathway Engineering

Mathematical modeling of metabolic pathways. Engineering of Metabolic Pathways
Representation of Metabolic Pathways. Generation and Dynamic Representation of Metabolic Pathways
Deriving Common Principles from the Metabolic Pathways Knowledge - E.g. deriving sets of enzymes specific for various reactions (e.g. oxidation), Alternative paths for synthesis of metabolites etc.

Reference Books:

1. Enzymes- Palmer & Bonner - Woodhead Publishing
2. Cohn and stumpt- Outline of Biochemistry- Wiley India
3. Gene Regulation and Metabolism-Ed. Collado Vides and Hofestad-
4. Fundamentals of Enzymology- Price and Stevens-Oxford
5. Fundamentals of Biochemistry- D., Voet, Voet, J.G. & Pratt, C. W. John Wiley & Sons.
6. Lehninger Principles of Biochemistry - D. L. Nelson & M. M. Cox, W. H. Freeman & Co.
7. The Enzyme Reference- D. L. Purich & R. D. Allison- Academic Press.
8. Metabolic Engineering -G.N. Stephanopoulos, A. A. Aristidou & J. Nielsen Academic Press.
9. Gene regulation and metabolism: postgenomic computational approaches. Collado-Vides, J. & Hofestadt, R. Cambridge, The MIT Press.

Practical (Lab Course Work –VI)

Experiments based on syllabus

M.Sc. Bioinformatics (Semester Pattern) III Semester

BI : XIV Object Oriented Programming Marks: 100 Hours: 45

Unit I: An Introduction and overview of Java

A Short History of Java, Features of Java, Comparison of Java and C++, Java Tools And Editors (Appletviewer,Jar,Jdb). Java Environment. Types of Comments, Built In Data Types, Variables and Constants(Final Keyword Related to variables), Operators, Memory Allocation Using new Operator., Output using println() method, Control Statements, Arrays, Simple Java Program.

Unit II: Objects and Classes

Defining Your Own Classes, methods and objects, using this keyword, constructors, types of constructors, constructor overloading, static variables and methods, access specifiers (private, protected and public), packages-creating, accessing and using packages, Garbage collection, finalize() method.

Unit III: Inheritance and Interfaces

Inheritance Basics and Types of Inheritance, use extends keyword, Super class, Subclass and use of Super Keyword, Method Overriding, Use of final keyword related to method and class, Use of Abstract class, Defining and Implementing Interfaces, interface variables and interface methods.

Unit IV: Exception Handling, Strings, Streams and Files:

Dealing Errors, types of exception, exceptions handling using try and catch, using throws keyword, uses finally block. String class and String Buffer Class, Stream classes, Byte Stream classes, Character Stream Classes, Using the File class, Creation of files, Reading/Writing characters and bytes, Handling primitive data types.

Unit V: Applet Programming with Graphical User Interface

Applet Life Cycle, Applet HTML Tags, Passing parameters to Applet, Repaint() method, User Interface Components with AWT in applet, Buttons and Labels, Checkboxes and Radio Buttons, Lists and Combo Boxes, Dialogs (Message, confirmation, input (like file selection).

Reference Books:

1. Complete reference Java by Herbert Schildt(5th edition)
2. Java 2 programming black books, Steven Horlzner
3. Programming with Java , A primer ,Forth edition , By E. Balagurusamy
4. Java servlet Programming by Jason Hunter, O'Reilly
5. Core Java Volume-I-Fundamentals, Eighth Edition, Cay S. Horstmann, Gary Cornell,

Practical: (Lab Course Work –VI)

Programs based on the syllabus

M.Sc. Bioinformatics (Semester Pattern) IV Semester

BI : XVI Biological Database Management Marks: 100 Hours: 45

Unit I: Introduction

Database designing, data capturing; Data Abstraction, Data Models, Instances & Schemes; Textual Databases; Introduction to Distributed Database Processing. Basic concepts and applications of Network Data Model, Hierarchical Data Model, Multimedia Databases E-R Model – E-R diagrams; Entity and entity sets; Relations and relationship sets; Reducing E-R Diagrams to tables. Basic concepts of – Indexing and Hashing; ISAM; B+ Tree indexed files; Static Hash functions; Dynamic Hash functions.

Unit II ORACLE, SQL

Oracle Architecture, Oracle objects - Tables, Views, Indexes, Sequences, Synonyms, Snapshots, Clusters. Database ,Tablespace, Data files, Data Blocks, Extents, Segments, Rollback Segments; Oracle Background Processes, control file, Redo log file, Archive log file; Security, Users, Grants, Roles. Backup & Recovery (Archiving); Physical Storage & Logical Storage.
User Defined Columns; PL/SQL Interface/ Triggers; Packaged Procedure; Calling Report from a Form. Menu - Default Menus; PL/SQL in Menu Modules, Menu Security. Select Statements, Data Definition Statements, Data Manipulation Statements, Data Control Statements.

Unit III. More on SQL

SQL commands used to create table, modify table structure, drop table, rename table. SQL commands used to change the data within the database – inserting of records in the tables, updation of all or specific set of records in tables, viewing the attributes of table's column. Querying data – Selecting the data from table using Arithmetic and logical Operators, Range searching and pattern matching, Function, group function, scalar function. Defining Constraints – Types: I/O constraints like Primary Key, Foreign key, Null and Unique constraints. Business constraints like check constraints. Levels: Table level constraints, column level constraints, creating and deletion of constraints using the Alter Table clause. Joining multiple tables, joining a table to itself. Security Management using SQL – Granting rights on user objects such as Tables, Views, and Sequences; Revoking rights on user objects such as Tables, Views, and Sequences.

Unit IV. PL/SQL

PL/SQL blocks; exception handling, triggers handling with cursors in PL/SQL blocks; Types of cursors: Implicit and Explicit cursors.

Unit V. Introduction to Front-end application development

Introduction to Front-end application development, working with code and forms, variables, procedures and controlling program executor, standard controls, data access. Establishing connection to various databases. Need of metadata standards & ontology.

Reference Books:

1. SQL, PL/SQL: the programming language of oracle by I. Bayross, BPB Publications.
2. DBMS by Bipin Desai-
3. Oracle SQL & PL/SQL Handbook: a guide for data administrators, developers, and business analysis by J. Palinski, Delhi, Pearson Education, 2003.
4. Database System Concepts by Hanery Korth and Abraham Silberschatz, TMH
5. An Introduction to Database Systems by C.J. Date, Addison-Wesley.
6. ORACLE: Power Objects Handbook by Bruce Kolste, David Peterson.

Practical ((Lab Course Work –VII)

Experiments based on syllabus

M.Sc. Bioinformatics (Semester Pattern) IV Semester

BI : XVII Programming using Perl and Python Marks: 100 Hours: 45

Unit I: Introduction and art of Programming

Introduction , computer program & programming language, Perl's benefits, portability, speed & program maintenance, Installing perl on your computer, how to run perl Program, text editor, finding help.
Individual approaches to programming, bio programming strategies, the programming process.

Unit II : Sequence & Strings, Basic Operators

General introductions to DNA & protein sequence, Standard IUB/IUPAC nucleic acid codes, Standard IUB/IUPAC amino acid codes, A program to store a DNA sequence, Concatenating DNA fragments.
Introduction to genetics code & codon table, translating codons to amino acids (using hashes), translating DNA into proteins, sequence file formats, FASTA format, Transcription:- DNA & RNA.
Scalar variables, Arithmetic operators, comparison operators, logical operators, assignment operators, auto increment & auto decrement operators, Concatenating & repeating string operators.

Unit III: File Handling, Lists & Arrays, Pattern Matching

Opening a file, reading a file, writing a file, closing a file, determining a status of a file. Introduction to lists, storing lists in array variables, more about lists & arrays, Array library function.
How pattern matching works, pattern matching operators, anchoring the patterns, patterns matching function, program to calculate the reverse complement.

Unit IV : Control Flow & Looping Statements, Subroutines & Hashes

If statements, If – else, while, until, single line conditional statement, the 'For' statement the 'for each' statement, the 'do' statement, the last, next, redo, continue statements.
Introduction & advantage of subroutines, writing subroutines, use of local variable & passing parameter to subroutines, returning a value from subroutines, passing data to subroutines, hashes & its creations from an array variables.

Unit V: Introduction to Python and R programming

Introduction to BioPerl. Brief introduction of Python; comparison with Perl
R Programming

Reference Books:-

1.) James Tisdall 2001 "Beginning Perl For Bioinformatics" O'reily & Associates.
2.) R. Schwartz , Foy and Phoenix, "Learning Perl" –O'Reilly
3) Learning Perl- Larry Wall
4) Kernel Methods in Computational Biology-Ed. Scholkopt, Tsuda, Vert-
5) Bioinformatics Technologies- Yi Ping Chen-Springer
6) Mastering Perl for Bioinformatics-James D. Tisdall- Oreally
7) Algorithms in Bioinformatics-Ed. Gary Benson, Roderic Page- Springer
8) Building Bioinformatics Solutions –Cornod Bessant, I Shadforth, Oakley-oxford

Practical ((Lab Course Work –VII)
Experiments based on syllabus

M.Sc. Bioinformatics (Semester Pattern) IV Semester

BI : XVIII Genomics and Proteomics Marks: 100 Hours: 45

Unit I Methods in Genomics

Chemical synthesis and Sequencing of DNA. Polymerase chain reaction and its applications
Introduction sequencing strategies for whole genome analysis, sequence data analysis.
Gene function by sequence comparison Global expression profiling : whole genome analysis of mRNA and protein expression, microarray analysis, types of microarrays and their applications

Unit II Methods in Proteomics

Methods of protein sequencing: Edman degradation, Tryptic and/or Chymotryptic Peptide Mapping.
Chemical and Physical Considerations in Protein and Peptide Stability,
Different methods for protein engineering, Site-directed mutagenesis, gene shuffling, and direct evolution. .
Isolation and purification of proteins, Stability and activity based approaches of protein engineering.

Unit III. Genome Alignments and Comparative Genomics

BLAST2, MUMmer PipMaker VISTA. Comparison of Gene Order- GeneOrder
Viruses, Microbes, Pathogens Eukaryotes.
COG, VirGen, CORG, HOBACGEN, Homophila, XREFdb, Gramene, Single Nucleotide Polymorphism, dbSNP and other SNP-related databases

Unit IV Protein-Protein Interaction Networks, databases and software

DIP (Database of Interacting Proteins), PPI Server, BIND - Biomolecular Interaction Network Database
PIM –Hybrigenics, PathCalling Yeast Interaction Database, MINT - a Molecular Interactions Database\
GRID - The General Repository for Interaction Datasets, InterPreTS - protein interaction prediction through tertiary structure

Unit V Genomics & Proteomics

Mapping of protein interactions: Two hybrid, phage display etc. Experimental Techniques: 2 D PAGE, Mass spectrometry, Bioinformatics Approaches.
Concept of Functional genomics, Toxicogenomics, Pharmacogenomics, Metagenomics

Reference Books:

1. Principles of Genome analysis and Genomics-Primrose and Twyman-Blackwell Publishing
2. Principles of Proteomics-R.M Twyman-BIOS advanced text
3. Functional Genomics-Stephen Hunt, Livesey- Oxford
4. Genetic Programming-W. Banzhaf, Nordin, Keller, Francone- Elsevier
5. Protein Science-Arthur M. Lesk- Oxford
6. Comparative Genomics-Nicholas H Bergman-Humana Press
7. Bioinformatics of Genome Regulations and StructureEd. Nikolay Kolchanov- Ralf Hofestaedt-Springer
8. Bioinformatics: sequence and genome analysis by David Mount, cold springer harbour press.
9. Introduction to proteomics: tools for the new biology by Liebler, D.C. & Yates, J.R.III, Humana Press
10. Proteomics: from protein sequence to function by Pennington, S. R. & Dunn, M. J.: Viva Books

Practical ((Lab Course Work –VII)

Experiments based on syllabus

M.Sc. Bioinformatics (Semester Pattern) IV Semester

BI : XIX Structural Bioinformatics Marks: 100 Hours: 45

Unit I Macromolecular Structure

Protein - Primary, Secondary, Super secondary, Tertiary and Quaternary structure
Nucleic acid – DNA and RNA, Carbohydrates, 3D Viral structures
Principles of protein folding and methods to study protein folding. Structure of Ribosome
Macromolecular interactions –Protein – Protein, Protein – Nucleic acids, Protein - carbohydrates

Unit II. Macromolecular x-ray crystallography

Principles of crystallography, Methods to study 3D structure. Co-ordinate systems
Fitting and refinement; Validation Analysis of 3D structures, Mass spectrometry and computational approaches in structural biology

Unit III Molecular modeling

An Overview. Introduction and challenges
Molecular modelling methods – Conformational searching, Potential energy maps, Ramachandran maps, Ab-initio methods, Semi-empirical methods Empirical methods.

Unit IV. Conformational analysis

Introduction and Methods – Molecular fitting. Conformations: global vs. local
Force fields: expressions for stretch, bond, torsion, etc.
Energy Minimization – Non-derivative and derivative methods. Free energy calculations
Global optimization (simulated annealing, Tabu search, genetic algorithms)
Applications of energy minimization

Unit V. Methods for 3D structure prediction

Knowledge based & Fold recognition Advance techniques in Prediction of 3D Structure –
Hidden Markov Model, Neural networks, Rossetta Stone, Genetic algorithms. Designing of molecules like drug, inhibitors using – Structure based & ligand based docking methods. Different Scoring schemes

Reference Books:

1. Principles of protein X-ray Crystallography by Jan Drenth, Springer-Verlag.
2. Computational Molecular Biology-Pavel A. Pevzner-PHI
3. DNA Protein Interactions-Andrew Travers and Malcolm Buckle- Oxford
4. Handbook of Hidden Markov models in Bioinformatics-Martin Gollery- CRC Press
5. Microarrays for an Integrative Genomics-I.S. Kohane, Kho, Butte-
6. Structural Bioinformatics - Methods of biochemical Analysis Philip E. Bourne (Ed), H. Weissig Wiley-Liss,
7. Introduction to Protein Structure by Branden, Carl & Tooze, John, Garland Publishing.
8. Molecular Modeling: Principles and Applications by Andrew Leach, Prentice Hall.
9. Prediction of protein structure and the principles of protein conformation by Fasman, G.D. Plenum Press
10. Protein Bioinformatics-Eidhammer, Jonassen, Taylor-Wiley

Practical ((Lab Course Work –VII)

Experiments based on syllabus

Lab Course Project Work-VIII
(Dissertation/ Elective Lab Course Work)

Guidelines for Dissertation work

1. The dissertation will be allotted during III semester
2. Students will design experiment of dissertation under guidance of supervisor
3. Selection of topic relevant to priority to areas of biotechnology
4. Collection of literature from various sources
5. Planning of research experiments
6. Performing the experiments with scientific and statistical analysis
7. Writing and compilation of dissertation report
8. Presentation of experimental data in schedule of practical examination
9. Dissertation to be carried out individually by each student