FACULTY OF LIFE SCIENCES

SYLLABUS

FOR

M.Sc. (BIO-INFORMATICS)
(For Colleges)
(Semester: I - IV)

Examinations: 2019-20

GURU NANAK DEV UNIVERSITY
AMRITSAR

M.Sc. Bioinformatics (Semester System) (For Colleges)

SCHEME OF COURSE

SEMESTER-I

Code		Title of Course	Course Hours	Max. Marks
BI	511	BASIC CONCEPTS IN BIOLOGY	3	75
BI	512	DATABASE MANAGEMENT AND DATA MINING	3	75
BI	513	BASIC BIOSTATISTICS	3	75
BI	514	COMPUTER FUNDAMENTALS, NETWORKING 'WEB TECHNOLOGY AND BASICS OF C PROGRAMMING LANGUAGE	3	75
BI	515	INTRODUCTION TO BIOINFORMATICS & BIOLOGICAL DATABASES	3	75
BI	516	PRACTICALS BASED ON BI-512 & BI-514	9	75
BI	517	PRACTICALS BASED ON BI-515	9	75
		TOTAL	**33**	**525**

M.Sc. Bioinformatics (Semester System) (For Colleges)

SCHEME OF COURSES

SEMESTER-II

Code	Title of Course	Course Hours	Max. Marks
BI 521	CONCEPTS IN MOLECULAR BIOLOGY & R-DNA TECHNOLOGY	3	75
BI 522	PROGRAMMING IN PERL FOR BIOINFORMATICS	3	75
BI 523	BASIC MATHEMATICS	3	75
BI 524	COMPUTATIONAL METHODS FOR SEQUENCE ANALYSIS	3	75
BI 525	STRUCTURAL BIOLOGY AND BIOINFORMATICS	3	75
BI 526	PRACTICALS BASED ON BI-522	9	75
BI 527	PRACTICALS BASED ON BI-524 & BI-525	9	75
	TOTAL	33	55

M.Sc. Bioinformatics (Semester System) (For Colleges)

SCHEME OF COURSES

SEMESTER-III

Code		Title of Course	Course Hours	Max. Marks
BI	631	Genomics and Proteomics	3	75
BI	632	Advanced Algorithms for Computational Biology	3	75
BI	633	System Biology and Metabolic Pathway Engg.	3	75
BI	634	Molecular Modeling and Computer Aided Drug Design	3	75
BI	635	Introduction to Data Analysis using R Programming	3	75
BI	636	Practicals based on BI-633, BI-634	9	75
BI	637	Practicals based on BI-631 & 635.	9	75
BI	638	Seminar on Emerging Trends in Bioinformatics	2	25
*BI	639	Industrial / Institutional Visit	**Satisfactory/ Not Satisfactory**	
		TOTAL	35	550

*Note:- Report of BI 639 Industrial/ Institutional Visit to be evaluated by panel of 3 Internal Examiners as Satisfactory/ Not Satisfactory.

M.Sc. Bioinformatics (Semester System) (For Colleges)

SCHEME OF COURSES

SEMESTER-IV

Code	Title of Course		Course Hours	Max. Marks
BI 640	MAJOR PROJECT		20	200
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		TOTAL	20	200
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Grand Total (Contact Hours)   :   121
Maximum Marks   :   **1800**

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No. BI 511: BASIC CONCEPTS IN BIOLOGY

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:

Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Diversity of cell size, shape, structure of pro and eukaryotic cells – isolation and growth of cells, cell motility, cilia, flagella of eukaryotes and prokaryotes, Cell theory. Sub cellular fractionation and criteria of functional integrity. Cellular organelles with special emphasis on plasma membrane, cell wall and their structural organization, Cellular energy transactions – role of mitochondria and chloroplast. Stem cell biology and introduction to cloning and its applications

SECTION-B

Carbohydrates – Mono, Oligo, Polysaccharides. Proteins – Primary, Secondary (Including types of secondary structures such as helices, strands, loops etc.), Super Secondary Structures, Tertiary and Quaternary Structure. Lipids – Fatty Acids, Structural and Storage Lipids and their Biological Importance. Nucleic Acids – Basic Structure of DNA & RNA.

Overview of metabolic pathways such as glycolysis, citric acid cycle, oxidative phosphorylation, pentose phosphate pathway and gluconeogenesis and their regulation.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

SECTION-C

Enzyme nomenclature and classification, substrate specificity, active site, factors affecting enzyme activity: proximity and orientation, covalent catalysis, and acid-base catalysis. Kinetics of single substrate enzyme reaction: Michaelis-Menten equation, effect of temperature and pH on enzyme activity, types of enzyme inhibition (reversible and irreversible). **Enzyme regulation: Allosteric and covalent modifications of enzymes**. Practical demonstration of enzyme reaction.

SECTION-D

Immunology: Innate and adaptive immunity, cells and organs of immune system, structure and functions of immunoglobulins, Genetics of antibody diversity, antigens characteristics, antigen-antibody interactions, MHC I & II polymorphism, MHC-Peptide interactions, antigen processing and presentation.
T-cell and B-cell maturation, activation, and differentiation. humoral and cell mediated immunity, Principles of diagnostic kits, precipitation and agglutination techniques, ELISA, immunoelectrophoresis and immunofluorescence. Practical demonstration of lymphocytes isolation and ELISA.

Text / Reference Books:
1. Lehninger, A.L. Nleson, DL and Cox, MM (2005). Principles of Biochemistry, 4th Ed., *Worth Publishers, New York*
2. Benjamin. E (2004). Immunology, *Willey and Liss, New York.*
3. Kubey, J and Goldby, R.A. (2003). Immunology Freeman and Cp., *New York.*
4. Palmer T. (2001). Enzymes: Biochemistry, Biotechnology and Clinical Chemistry. *Horwood Publishing, Chivhester.*
5. Master, IRW (2000). Animal Tissue Culture, *Oxford University Press, New York.*
6. Buchnan B.B., Grissem W. and Jones, R.L. (2000). Biochemistry and Molecular Biology of Plants. *American Society for Plant Physiologists, Maryland.*
7. Nicholas C.Price (1999). Fundamental of Enzymology, 3rd Edition, *Oxford University Press*.
8. Damal, J, Lodish, H. and Baltimore, D. (1990). Molecular Cell Biology, 2nd Edition, *Scientific American Books, New York.*
9. De Roberties, E.D and De Roberties , E.M (1987). Cell and Molecular Biology, 8th Ed, *Lippincott   Williams and Wilkins Publication.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

COURSE NO. BI- 512: DATABASE MANAGEMENT AND DATA MINING

Time: 3hrs **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Introduction, Characteristics of Data base approach, Database users, Intended uses of databases, Implication of database approach. Database System Concepts and Architecture, Data Models, Schemas and Instances, DBMS Architecture and data independence, database languages, Classification of DBMS.

SECTION-B

Database Design: Informal Design guidelines for relation Schemas, Functional Dependencies, Normalization and its forms like 1NF, 2NF, 3NF, BCNF, 4NF and 5NF. Data modeling using ER diagram, ER Model Concepts, Notation for ER Diagrams.

SECTION-C

The relational Model, Relational Model Concepts, Relational Model Constraints, Introduction to Relational Algebra.

SQL: Introduction, Data Definition in SQL, Quries in SQL, Update statement in SQL, Views SQL, Simple programs in PL/SQL. Procedures, Functions, Cursors, Triggers in PL/SQL.

SECTION-D

Data Mining, Definition, Data Mining and KDD, Data Mining on relational databases, Data Warehouses, Transactional Databases etc. Data Mining Functionalities, Pattern Minning.Association Analysis, Classification and Prediction, Cluster Analysis, Evolution Analysis, Data Mining on Biological data.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Text/Reference Books:

1. Kurth and Sudarshan. Database System Concepts. 4th Edition. *Tata McGraw Hill. New Delhi. (2002)*

2. Elmasari and Navathe, Fundamentals of Database Systems, *Prentice Hall (India), 2001.*

3. Jiawei Han, Micheline Kamber, Data Mining Concepts and Techniques- *Morgan Kaufmann Publisher, 2001.*

4. Date C.J. Database System 7th edition. *Pearson Education (2001).*

5. Schaum Series. Relational Database Systems. *Tata McGraw Hill. New Delhi (2001).*

6. Iwindell, S.R., Miller R R, Myers G S A (Eds) Internet for Molecular Biologists. *Horizon Scientific Press. Norfolk. (1996).*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No. BI 513: Basic Biostatistics

Time: 3 Hrs.   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Elementary statistics: Representation of data- discrete data, continuous data, histogram, polygons, frequency curves. Mean, Median, Quartiles, Percentile, Skewness, Standard deviation, Variance, Box and whisker diagrams (box plots), Scatter diagrams, Introduction to statistical sampling from a population, Random Sampling.

SECTION-B

Probability:

Experimental Probability, Probability when outcomes are equally likely, Subjective Probabilities, Probability laws Probability rules for Combined events, Conditional Probability and Independent Events, Probability trees, Bayes theorem.

SECTION-C

Random Variables and Probability

Discrete random variables, their Probability Mass function, Probability Density Function Mean and variance. Binomial and Poisson Distributions

Continuous Random variables, their Probability Mass function, Probability Density Function Mean and variance, Normal Distribution

Cumulative distribution function

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

SECTION-D

Multivariate Analysis

Regression and correlation:, Linear Correlation, Scatter Diagrams, Least Square Regression lines, Standard error of estimate, explained and unexplained variation, correlation coefficient, Regression function, Linear correlation coefficient and regression lines.

Hypothesis Testing: Fischer test, Chi Square test, Student t-test, One way ANOVA

Text / Reference Books:

1 Brian S., Ripley D. and Venables W. N. (2002). Modern Applied Statistics. *Springer Verlag.*

2 J. Crawshaw and J Chamber (2002), Advanced Level Statistics, 4th Edition, *Melson Thornes.*

3 Kapoor V.K. and Gupta S.C. (2000) Fundamentals of Mathematical Statistics. *Sultan Chand and Company, New Delhi*

4 Gupta S.P. (2000). Statistical Methods. *Sultan Chand and Company, New Delhi.*

5 Mendenhall W. and Sincich T. (1995). Statistics for Engineering and Sciences (IVth edition). *Prentice Hall.*

6 Elhance D.N. (1984). Fundamentals of Statistics. *Kitab Mahal, Allahabad.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No. BI 514   Computer Fundamentals, Networking, Web Technology and Basics of C Programming Language

Time: 3 Hrs.   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A
Fundamentals of Computing: Introduction to computer, Operation of processor; Number Systems and Digital Circuits; ALU; Memory Chips (ROM, RAM, DRAM), Storage Devices, Memory Hierarchy; I/O Devices; Moore's Law, Classification of computers (Notebook, Personal Computers, Workstation, Mainframes, Minicomputers, Microcomputers, Supercomputers). Introduction to Computer Viruses.

Computer Networking: OSI reference model, Network Topologies, Router, Switch, Data Communication (ISDN, Cable Modem), Concept of Wireless networking, LAN, WAN, MAN. **Introduction to Internet**: World Wide Web, Advantages of Web, Web Terminology, Telnet, FTP.

SECTION-B
HTML: Introduction, common tags, creating hyper links, incorporation of images; Tables; Frames; Formatting of text with fonts; Dynamic HTML; cascading style sheets; Creation of Background images, HTML object models; dynamic positioning; direct animation path control.

SECTION-C
Introduction to programming and C Language: The basic model of computing, algorithm and flow charts, programming languages, compilation, linking, testing, debugging and Documentation. Concept of Structured programming and Introduction to C Language**,** Character set, variables and identifiers, Built in data types,

SECTION-D
Operators: Arithmetic operators and expressions, constants and literals, Relational operators and logical connectivity, Basic input/output statement, Conditional statement and loops
Arrays: Definition and its types. **Functions:** modular programming and functions, standard library of C function. Function prototype and function definition, calling a function, Structure, Union, pointers

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Text / Reference Books: -

1. Gurvinder Singh, Rachhpal Singh (2005). A Textbook on Windows Based Computer Courses, *Kalyani Publishers*, *Jalandhar*

2. Rachhpal Singh, Mamta Verma, Sonia Mahindru (2005). A Textbook of Scripting Language and Web

3. Designing, *Kalyani Publishers*, *Jalandhar*

4. Kapila H. (2003). PC Computing Window Based Computer System. *Dinesh Publishers, Jalandhar.*

5. Bayross I. (2002). Programming in Visual Basic 6.0. *BPB Publication, New Delhi.*

6. Norton's P. (2001). Introduction to Computing Fundamental. *McGraw Hill Education, New Delhi.*

7. Sinha P.K. (2001). Fundamental of Computers. *BPB Publication, New Delhi.*

8. Denis Ritchie, Programming in C, *TMT, Fourth Edition. 2000.*

9. Herbert Schildt, Programming in C, *TMH, Fifth Edition. 2002.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No. BI 515 Introduction to Bioinformatics & Biological Databases

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A
Introduction to Genes and Proteins, The central dogma, Promoter and other regulatory sequences, Genetic Code, ORFs, Introns and Exons, Splicing, Splice variants,

Introduction to Bioinformatics: History of Bioinformatics and milestones,
objectives and applications of Bioinformatics. Introduction to Data Generating Techniques**:** Restriction Enzymes, Gel Electrophoresis, Blotting and Hybridization, Cloning, PCR, DNA Sequencing, Next Generation sequencing.

SECTION-B
Introduction to Databases, Introduction to Biological Databases, Types of Databases,
Literature Databases: PUBMED,PMC, EuropePMC, Biomed Central , Public Library of Sciences
Nucleic acid and protein databases: GenBank, EMBL, DDBJ, Uniprot-KB, SWISSPROT
Database Retrieval and Deposition Systems: SRS, Entrez, Bankit, Seqin.

SECTION-C
Biotechnological Databases: EST, STS, GSS, SNP, GEO,
Gene Ontology
Pattern Databases: InterPro, Prosite, Pfam, ProDom,
Databases for species identification and classification: GBIF, taxonomy browser at NCBI, BOLD.
Various human, plants and animal databases: NCBI Genome Ensembl Genome project, Flybase, Maize GDB, Human GDB, TAIR, EcoGene.

SECTION-D

Structural Databases: PDB, NDB, Pubchem etc.
RNA and Carbohydrate databases: Rfam, miRBase, NONCODE, UniCarbKB
File formats: GenBank, FASTA, MSF, PDB, SMILES, CML, SDF etc.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Text / Reference Books:

1. Mount D. W. (2004). Bioinformatics & Genome Analysis. *Cold Spring Harbor Laboratory Press.*

2. Baxevais B.F. and Quellette F. (2004). Bioinformatics A Practical Guide to the Analysis of Genes and Proteins. *Wiley-Interscience*.

3. Eidhammer I., Jonassen I. and Taylor W. R. (2004). Protein Bioinformatics: An Algorithmic Approach to Sequence and Structure Analysis. *Mathematics.*

4. Orengo C.A., Jones D.T. and Thornton J.M. (2003). Bioinformatics: Genes Proteins and Computers. *Bios Scientific Pub.*

5. Bourhe P. E. and Weissig H. (2003). Structural Bioinformatics (Methods of Structural Analysis). *Wiley-Liss.*

6. C. Braden and C. Tooze (1991). Introduction to Protein Structure" *Garland Publishing Inc., New York.*

7. Brown. T.A. (2002). Genomes (Second Edtion). *Oxford: Wiley-Liss.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No. BI-516: Practical based on BI-512 & BI-514

Time: 9 periods (Each Period of 1 hour) per week   **Max. Marks: 75**

Part- A

Marks: 60

DBMS

Exercises to understand RDBMS: Oracle/PosGre SQL etc.; Usage of important commands/instructions.

Operating Systems & Networking

1 Introduction to operating systems (DOS, Windows, Linux etc) and their installation.
2 Basic DOS commands
3 Basic Linux commands
4. Working with Telnet and FTP

HTML

1 Exercises on HTML.

Basics of C Language

Write at least 25 programs including the following. The programs should cover the corressponding topics studied in the theory part.

   To show the use of standard input (scanf) and standard output (printf)functions

   To show the use of variables and keywords.

   To show the use of arithmetic operators, relational operators, logical operators,unary operators, assignment operator, arithmetic assignment operators andconditional operator.

   To show use of library functions like sqrt, POW, tan, log etc.

   To show the precedence of operators.

   To show the use of getchar, putchar, gets, puts, getch, getche.

   To Expertise branching statements like if, if-then, if-then-else.

   To Expertise Looping Statement like while, do-while, for loops.

   To show the utility of union and structures.

   To create functions and to show different calls: Call by reference, Call by value.

   To show the utility of pointers and various type of pointers like Pointer to a variable, Pointer to a function, Pointer to union and structures.

   Write a program for addition and multiplication of two matrices.

PART-B

Marks: 15

Practical Assignment

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–I)

Course No.BI-517: Practical based on BI-515

Time: 9 periods (Each Period of 1 hour) per week

Max. Marks: 75

PART-A

Marks: 60

To Study & analyse various biological databases

 NCBI, EBI, Expasy

To Study and analyse various other databases like

 EST, Gene Ontology, GEO

Study of Protein Databases RCSB, SWISSPROT, PubChem etc.

Study of Nucleic acid databases like Gene Bank, EMBL, miRBase etc.

 To retrieve sequences from NCBI/EBI/ExPasy and submit in BLAST/FASTA/CLUSTAL W

Study of Biodiversity Informatics using various tools GBIF (Global Biodiversity Information Facility). BOLD, Taxonomic Browser at NCBI etc.

Study Carbohydrates and lipid databases: UniCarbKB

 EMBOSS installation and perform the above operations using EMBOSS. Each student should install it on a PC.

Search for other freeware and install.

PART-B
Practical Assignment

Marks: 15

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI – 521: Concepts in Molecular Biology & rDNA Technology

Time: 3 Hrs **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Properties of DNA: renaturation and denaturation of DNA, Cot curves, DNA banding patterns.
DNA replication-an overview, Enzymes of replication, prokaryotic replication mechanisms, eukaryotic DNA replication, repair of DNA.

SECTION-B

Molecular basis of transcription: types of RNA and RNA polymerases in prokaryotes and eukaryotes, control of transcription in prokaryotes and eukaryotes, post transcriptional processing of mRNA
Molecular basis of translational: genetic code, translational process, control of translation and initiation, post-translational modifications and transport, protein trafficking and sorting.

SECTION-C

Regulation of gene expression in prokaryotes: Operon concept, lytic cascade and lysogenic repression in phase, regulation of gene expression in eukaryotes.

SECTION-D

Introduction to recombinant DNA technology- Historical perspectives, Enzymes involved in manipulation of genetic material: (Restriction endonucleases, DNA ligases, DNA polymerases. Lambda and Plasmid vectors.

Labeling techniques, nick translation, end labeling, primer extension, random priming methods, cDNA library: reverse transcription, DNA primers, linkers, adaptors, library construction and screening.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Text / Reference Books:
1. Glick B.R. (2003*). Molecular Biotechnology ASM Press Washington DC, U.S.A.*

2. Old R. W. and Primrose S.B. (2002). Principles of Gene Manipulation. *Blackwell Publishing.*

3. Lewin, B. (2000). Gene VII, 7th Ed., *Oxford University Press.*

4. Sambrook, J., Fritsch, E.F. and Maniatis, T. (2000). Molecular Cloning: A Laboratory Manual,. *Cold Spring Harbor Laboratory Press, New York.*

5. Henry, R. J. (1997). Practical Applications of Plant Molecular Biology, *Chapman and Hall.*

6. Glover, D. M. and Hames, B. D. (1995). DNA Cloning: A Practical Approach, *IRL Press, Oxford.*

7. Primrose, S. B. (1994). Molecular Biotechnology, 2nd Edition, *Blackwell Scientific Publishers. Oxford.*

8. Damal, J, Lodish, H. and Baltimore, D. (1990). Molecular Cell Biology, 2nd Edition*, Scientific American Books, New York.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI- 522: Programming in PERL for Bioinformatics

Time: 3 Hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four
Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are
required to attempt five questions, selecting at least one question from each Section. The fifth
question may be attempted from any Section.

SECTION-A

Getting started with PERL, Perl's Benefits, Versions of Perl, Downloading & installing perl in
Linux/Windows environment, How to run perl Programs in linux/windows environment, Error
Messages, Debugging, Perl interpreters, Perl scripts. CPAN (Comprehensive Perl Archive
Network)

Scalar Values and scalar variables, Assignment, Statements, Blocks, Arrays, Hashes, Operators,
Operator precedence, Conditional and logical operators, Binding operators, loops, I/O: Input
from STDIN, Built in File handlers, Input from file, Input from file named on command line,
Output to file,

SECTION-B
Regular expression, Pattern matching, Meta symbols, Pattern modifiers, Subroutines and
modules, built-in functions.

Applications of Perl in Bioinformatics: Representing strings and sequenced data
in Perl,   Program to store a DNA sequence, Concatenating DNA fragments,
DNA to RNA transcription, Reading proteins   from   files,   Finding   motifs,
Counting nucleotides, Exploding strings into arrays, Operating on strings.

SECTION-C
Generating random numbers, A program to simulate DNA mutation, Generating random
DNA, Analyzing DNA, Translating DNA into proteins, Reading DNA from Files in
FASTA format, Separating Sequence and Annotation from GenBank, files. Parsing PDB
files, parsing BLAST output.

SECTION-D

Introduction to Bioperl:- Bioperl objects: Sequence objects, Location objects, Interface objects
etc. Using Bioperl:- Accessing sequence data from local and remote databases(Bio:: DB::
GenBank etc.). Indexing and accessing local databases (Bio:: Index::*.bp_index.pl,bp_fetch.pl,
Bio::DB::*). Transforming formats of database, sequence files(SeqIO) and alignment
files(AlignIO); introduction to manipulation of sequences using Bioperl

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Text/Reference Books: -

1   James D.Tisdall, *(2001).* "Beginning Perl for Bioinformatics,*"O"Rilley and Associates,*

2   Cynthia Gibas & Per Jamesbeck, *(2000).* " Developing Bioinformatics Computer Skills, "*O"*

     Rilley & Associates.

3   Rex A.Dawyer, "Genomic Perl", *Cambridge University Press.*

4   Randal L.Schawrtz and Tom Phoneix, *(2000).* Learning Perl, 3rd Edition: *"O" Rilley*

5   D. Curtis Jamison. *Perl Programming for Biologists.* Hoboken, N.J.: Wiley-Liss, 2003.

6.   James D.Tisdall, *(2003).* "Mastering Perl for Bioinformatics, "*O"Rilley and Associates.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI- 523: Basic Mathematics

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

Note: Question should be based on very simple and basic examples as the students are from both non-medical and medical background.

SECTION-A

Fundamentals of Set Theory: Concept of Set, Product Set, Relations, Functions, Graphical representation of some well known functions (periodic function, polynomial function, absolute value function, greatest integer function, signum function).

Real and Complex Numbers: Concept of different kinds of numbers, integers, Rationals Irrationals, reals and complex numbers, Operations with complex numbers.

SECTION-B

Matrices and Vectors: Concept of Matrix, Matrix Algebra: Addition, Subtraction, Multiplication, Transpose inverse and conjugate of a Matrix, Determinants, Vectors in space, Addition, Subtraction, Dot, Cross, Scalar triple product.

SECTION-C

Differentiation: Intuitive idea of Complete Differentials, Derivatives as rates of change.

Applications to maxima and minima, increasing and decreasing functions, Partial Differentiation.

SECTION-D

Limits: Concept of Limit of a function.
Integration: Finding function from its derivative, Indefinite & Definite Integral, calculating areas (simple cases only).
Coordinate Geometry: Equation of a line, circle, Parabola and Sphere.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Recommended Books:

1   H. Nell and D. Qualing (2002), Pure Mathematics (Advanced Level Mathematics) Vol. 1,

    2, 3, *Cambridge University Press*.

2   Brown R. (1994). Theory and Problems of Differential Equations. *Tata Mcgraw Hill*

    Company Ltd., New Delhi.

3   Edward Batschelet (1992) "Introduction to Mathematics for Life Sciences", 3rd Edition,

    Springer-Verlag.

4   Spiegel M.R. (1974). Theory and Problems of Advanced Calculus. *Tata Mcgraw Hill*

    Company Ltd., New Delhi.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI- 524: Computational Methods for Sequence Analysis

Time: 3hrs **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Sequence alignment: scoring matrices, PAM, BLOSUM, Local and global alignment concepts;

Dot matrix sequence comparison; Dynamic programming; Needleman-Wunch algorithm, Smith-Waterman algorithm; Statistics of alignment score.

Multiple sequence alignment: progressive alignment, scoring MSA, CLUSTALW, PILEUP, iterative methods of MSA, database searches for homologous sequences, FASTA and BLAST, PSSM searching, PSI-BLAST and PHI-BLAST.

SECTION-B

Evolutionary analysis: Relationship of phylogenetic analysis to sequence alignment, Genome complexity, concept of evolutionary trees, Methods-maximum parsimony method, distance methods, the maximum likelihood approach. Sequence alignment based on evolutionary model, reliability of phylogenetic predictions, complications from phylogenetic analysis.

SECTION-C

Gene prediction in prokaryotic genomes, gene prediction in eukaryotes, evaluation of gene prediction methods, promoter prediction in *E.coli* and promoter prediction in eukaryotes.

SECTION-D

Prediction of protein secondary structure from the amino acid sequence- Use of sequence patterns for protein structure prediction, Identifying Structural features of proteins from sequence elements (motifs, domains etc.). Prediction and Identification of B Cell Epitopes using protein sequences.

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Text/Reference Books:

1. S.C. Rastogi, N. Mendiratla and P.Rastogi (*2004)*, Bioinformatics Mthods and Aplications-Genomics, Proteomics and Drug Discovery, *Prentice Hall (India).,*

2. I.Korf, M.Yandell & Joseph Bedell (*2003). BLAST, *O'Reilly.*

3. A.D.Baxevanis and B.F.F.Ouellette, (*2002).* Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, *John Wiley and Sons (ASIA) Pvt. Ltd.,*

4. D.W.Mount, (*2001).* Bioinformatics: Sequence and Genome Analysis, *Cold Spring Harbour Laboratory Press, New York,*

5. R.Durbin, S.Eddy, A.Krogh, G.Mitchison, (*1988).* Biological Sequence Analysis – Probability Models of Proteins and Nucleic acids, *Cambridge University Press.*

6. Bishop M. J., Rawings C.J. (1997) DNA and Protein Sequence Analysis. A Practical Approach, *IRL Press, Oxford.*

7. *Schwede T. and Peitsch M (2009).* Computational Structural Biology. Methods and Applications. *World Scientific.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI- 525: Structural Biology and Bioinformatics

Time: 3hrs **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A
Protein structure determination methods (principles of X-Ray diffraction, NMR and CD Spectroscopy), Mass Spectroscopy (Principles of Mass Spectroscopy, Use of Mass Spectroscopy in Peptide mapping, Post translational modification analysis and Protein sequencing). Conformational properties of proteins: Dihedral angles (Phi, Psi and Omega), Rotameric structures, Ramachandran plots- hard sphere approach, soft potentials, Sequence and structure Motifs and Domains.

SECTION-B
Nucleic acid Conformational flexibility: Sugar puckering, Backbone torsional flexibility, Glycosyl Rotation, Basic Helical Descriptors and their values in A, B, Z DNA, Methods for prediction of RNA structures. Principles of protein folding, Classification of three dimensional structure of protein in protein data banks (SCOP, CATH, PFAM).

SECTION-C
Secondary structure Prediction methods: First, second, third and fourth generation methods based on *ab initio*, Neural network models, Nearest neighbor methods, Hidden markov model including CHOU-FASMAN, GOR, PHD, PSIPRED, SOPM. Concepts, algorithms and their limitations. Benchmarking, CASP, CAFASP

SECTION-D
Methods for Prediction Tertiary structures of Proteins (Knowledge-based Structure prediction, Fold recognition, Ab initio methods for structure prediction). Assessement of Protein Structure predictions, Protein Structure Comparison and alignment: Introduction to Graph Theory, Distance Matrices, Structural alignment algorithms (CE, VAST, ALIGN, DALI, SSAP).

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Text/Reference Books:-

1 Creightons T.E. (2005). Proteins: Structures and Molecular Properties. *WH Freeman Publishers.*

2 Mount D. W. (2004). Bioinformatics & Genome Analysis. *Cold Spring Harbor Laboratory Press.*

3 Baxevais B.F. and Quellette F. (2004). Bioinformatics a Practical Guide to the Analysis of Genes and Proteins. *Wiley-Interscience*.

4 Friefelder D. M. (2004). Physical Biochemistry: Applications to Biochemistry and Molecular biology. *Blackwell Publishing.*

5 Eidhammer I., Jonassen I. and Taylor W. R. (2004). Protein Bioinformatics: An algorithmic approach to sequence and structure analysis. *Mathematics.*

6 Bourhe P. E. and Weissig H. (2003). Structural Bioinformatics (Methods of structural Analysis). *Wiley-Liss.*

7 Orengo C.A., Jones D.T. and Thornton J.M. (2003). Bioinformatics: Genes Proteins and Computers. *Bios Scientific Pub.*

8 Sheehan D. (2000). Physical Biochemistry. *WH Freeman Publishers*.

9 C. Braden and C. Tooze (1991) Introduction to Protein Structure" *Garland Publishing Inc., New York.*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI- 526: Practical based on BI-522

Time: 9 Periods (Each Period of 1 Hour) Per Week   **Max Marks: 75**

PART-A

PERL & Bioperl

Write programs from each unit including the following:
1. Write a Program to show the concept of standard input/output.
2. Write a Program to declare and use variables.
3. Write a Program to use the operators.
4. Write a Program for the type conversion.
5. Write a Program to implement the conditional statements.
6. Write a Program to show the use of loops, nested loops
7. Write a Program which uses NEXT, LAST, REDO statement.
8. Write the programs that show the all-possible operations on arrays, lists.
9. Write a Program to implement the stack.
10. Write a Program to use hashes.
11. Write a Program to show the concept of subroutine.
12. Write programs to CREATE, RENAME, STATUS of a file and READ/WRITE
    operation on file.
13. Write a Program to search of a file in a directory.
14. Programs related with Regular Expression
    • Searching for a regular expression in a file.
    • Searching and Replacing a regular expression an a file
15. Program to access local database
16. Program to access remote database
17. Program to transform sequence and alignment files
18. Program to obtain basic sequence statistics

PART-B

Marks: 15

Practical Assignment

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–II)

Course No. BI -527: Practical based on BI-524 & BI-525
Time: 9 Periods (Each Period of 1 Hour) Per Week

Max. Marks: 75

PART-A

Marks: 60

To analyze protein sequence using Secondary Structure prediction Methods: GOR, CHOU-FASMAN, PSIPRED, PHD, SOPM etc.

Secondary structure of RNA using M fold.

To predict tertiary structure of protein by Modeller, swill model, PHYRE^2 etc.

To retrieve various structures of Proteins from RCSB, their classification systems using CATH/SCOP etc.

To down-load structures of proteins in software like RASMOL, SPDBV and analysis of structures in these software

To study the atomic co-ordinate files of various structures

Similarity searches using various tools like

BLAST/ FASTA

BLAST N

BLAST P

BLAST X

To align, superimpose and compare three dimensional structures of the proteins using 3D- alignment software

To predict gene/ORF for genomic/DNA sequences of prokaryotic and eukaryotic origin.

PART-B

Marks: 15

Practical Assignment

Course No. BI- 631: Genomics & Proteomics

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four).Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Overview of Genome Anatomy- Anatomy of prokaryotic and eukaryotic genome. Characteristics of Human Genome - sequence repeats, transposable elements, gene structure and pseudogenes. Analyzing gene expression – DNA microarray- design, analysis, visualization of data and Stanford microarray database.
Genomic Mapping – Different types of Genome maps and their uses, Genetic and Physical mapping techniques. Practical uses of genome maps

SECTION-B

Comparative Genomics:- (Viruses, Microbes, Pathogens, Eukaryotes). Comparative Genomics Databases: - (UCSC Genome Browser, COG, VirGen,, PLANTGDB , Gramene)
Genome Alignment Tools:- (BLAST2, MUMmer, VISTA).
Genetic Markers -RFLP, Mini- and Micro satellite, STS, SSCP, RAPD

SECTION-C

Overview of proteomics: Introduction to proteomics technology; Experimental Techniques, Current Applications of proteomics in varied biological system; Bioinformatics in proteomics; Protein folding.
Comparative proteomics- Differential 2D gel, plant proteomics research and pharmacogenomics

SECTION-D
Protein-Protein Interaction Networks, databases and software:- (DIP (Database of Interacting Proteins), PPI Server, MINT – a Molecular Interactions Database, GRID - The General Repository for Interaction Datasets, InterPreTS - protein interaction prediction through tertiary structure

Text/Reference Books:-

1. Richard P. Simpson (2004) Proteins and Proteomics. A Laboratory Manual. *Cold Spring Harbor Laboratory Press, New York.*
2. T.B.Kitano (*2003),* Handbook of Comparative Genomics: Principles and Methodology, *Graziano Pesole.*
3. Primrose and Twyman (2003) Principles of Genome Analysis. *Blackwell Publishing, Oxford.*
4. Gibson and Muse, (2003) A Primer of Genome Science. Sinauer Associates Inc. *Publishers, Sunderlands, New York.*
5. Philip E. Bourne, Helge Weissig. (2003) Structural Bioinformatics. *John Wiley & Sons (Asia), Singapore.*
6. Dov Stekal (2003) Microarray Bioinformatics, *Cambridge University Press, Cambridge.*
7. Timothy Palzkill, (*2002)*, Proteomics, *Kluwer Academic Publisher.*
8. Brown TA. (2002) Genomes. *John Wiley & Sons (Asia) Pvt. Ltd. Singapore.*
9. Reiner Westermeier, Tom Naven. (2002) Proteomics in Practice. *Wiley – VCH, Weinheim.*
10. Daniel C. Liebler*, (2001)*, Introduction to Proteomics: Tools for the New Biology, *Humana Press*
11. Hiroaki Kitano*, (2001)*, Foundations of Systems Biology (Ed) *MIT Press.*
12. Pennington S. MJ Dunn. (2001) Proteomics: From Sequence to Function. Bios, *Scientific Pub.Ltd. Oxford.*
13. Liebler (2001) Introduction to Proteomics, Tools for the New Biology. *Humana Press, New Jersey.*
14. Charles R. Cantor, Cassandra L. Smith (1999) Genomics: The Science and Technology behind the Human Genome Project, *John Wiley & Sons (Asia) Pvt. Ltd. Singapore.*
15. P.Clate & R.Backofen (1998), Computational Molecular Biology, *Willy Publication,*

M.Sc. Bioinformatics (Semester System) (For Colleges) (Semester–III)

Course No. BI 632: Advanced Algorithms for Computational Biology

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four).Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A
Algorithms, Complexity, Introduction to the principles and techniques of algorithm design, Use of abstract data types, Standard implementation using appropriate data structures. Complexity theory.

Graphs, Interval Graphs, Measuring Fragments size, Multiple Maps, Double Digest Problem, Classifying multiple solutions, Border block groups, DDPs are NP-Complete, Integer Programming, TSP, Simulated Annealing, Circular Maps, Map Algorithm, Optimization techniques: Basic idea of OT, Golden section.

SECTION-B
Hidden Markov Models, Profile HMMs, Binding Profile HMMs, Motifs Recognitions: Profile Methods and HMM, Physical Mapping of DNA and Genomes, Cloning and Clone Libraries, Libraries of complete digestion, Libraries of partial digestion, Physical genome maps, Mapping by Fingerprinting, Divide and Conquer, Evaluating Finger Printing scheme.

SECTION-C
Introduction to machine learning techniques: - Artificial Neural Network concepts, perceptron, Multilayer Perceptron, Secondary Structure Prediction using ANN, Back propagation Algorithm, Training and testing ANNs. Support vector machines and their applications, Using genetic algorithm and perceptron for feature selection and supervised classification.

SECTION-D

Genetic Algorithms: - Sequence Alignments, Prediction of Protein Structure, Docking Simulations, Ant colony optimization: - Multiple Sequence Alignments, Biomolecular Structure Prediction; Clustering Algorithms: -Hierarchical and non-hierarchical Clustering.

Textbooks and Research Papers:

1. Mount D. W. (2004). Bioinformatics & Genome Analysis. *Cold Spring Harbor Laboratory Press.*
2. Benson G. and Page R. D.M. (2003). Algorithms in Bioinformatics. *Springer.*
3. Pevzner J. (2003). Bioinformatics and Functional Genomics. *Wiley-Liss.*
4. Norvig P. (2003). Artificial Intelligence: A Modern Approach. *Prentice Hall.*
5. Felsenstein J. (2003). Inferring Phylogenies. *Sinauer Associates.*
6. Salemi M., and Vandamme A. (2003). The Phylogenetic Handbook: A Practical Approach to DNA and Protein Phylogeny. *Cambridge University Press.*
7. Fogel G.B. and Corne D.W. (2002). Evolutionary Computation in Bioinformatics. *Humana Press* (*Science).*
8. Krane D.E., Raymer M.L and Marieb E.N. (2002). Fundamental Concepts of Bioinformatics. *Benjamin Cummings.*
9. Ewens W. J. and Grant G. R. (2001). Statistical Methods in Bioinformatics: An Introduction. *Springer Verlag.*
10. Cathy H. Wu and Malarty J. W. (2001). Neural Networks and Genome Informatics. *Elsevier Science.*
11. Nei M. and Kumar S. (2000). Molecular Evolution and Phylogenetics. *Oxford University Press.*
12. Michael Waterman, Chapwan & Hall/CRC, (2000). Introduction to Computational Biology-Maps, sequences and genomes.
13. Pavel A.Pevzner (2000), Computational Molecular Biology- An Algorithmic Approach, *MIT Press.*
14. IEEE Computer, July (2002), Special Issue on Bioinformatics.
15. Gene Myers, Whole Genome DNA Sequencing, IEEE Computational Biology, *May-June 1999.*
16. R.H.Waterston, E.S.Lauder, J.E.Sulston on the Sequencing of Human Genome, PNAs.
17. Durbin R. and Eddy S. (1998). Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids. *Cambridge University Press.*
18. http://www.phrap.org
19. http://www.cs.vnm.edu/~moret/GRAPPA
20. Chopra, S.C.. Numerical methods for engineers.
21. Singirosu S. Rao. Optimization techniques, New Age International (P) Ltd.

Course No. BI -633: System Biology & Metabolic Pathway Engineering

Time: 3Hrs.   **Max. Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four).Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A
System Biology: Towards System level Understanding of Biological Systems, Properties of models-Robustness, Redundancy, Control, Modular Design, Structure Stabilty. Impacts of System Biology. Rapid Pole-to-pole Oscillations in E. coli, Models for Eukaryotic Gradient Sensing.

SECTION-B
Systems Microbiology - The Cell as a Well-stirred Bioreactor: Michaelis-Menten Kinetics, A Genetic Switch in Lamba Phage, Synthetic genetic switches, Stability analysis, Modeling Escherichia coli chemotaxis, Genetic Oscillators

SECTION-C
Developmental Systems Biology: Whole cell simulation, Computer Simulation of the Cell: Human erythrocyte model & its applications Quorum Sensing, Minimal gene set concept. Emerging Areas in System Biology: such as From Neurons to Brains, Complex Diseases, Organisms and their interactions with environment.

SECTION-D
Regulation of Metabolic Pathways at Enzyme Level: Regulation of enzyme activity, overview of enzyme kinetics, allosteric enzymes, feedback inhibition. Metabolic Pathway databases:-KEGG, EMP, EcoCyc and BioCyc.

Enzymes, Compounds and Reactions databases; LIGAND - Biochemical Compounds and Reactions, ENZYME – Enzymes, BRENDA - Comprehensive Enzyme Information System;, Engineering of Metabolic Pathways.

References:

1. Foundation of System Biology by Hiroaki Kitano.

2. A First Course in System Biology by Eberhard O. Voit.

3. Alberts Bruce *et al,* (2002), Molecular Biology of the Cell. *Garland Science, New York.*

4. Masaru Tomita, (2001). Whole cell simulation: a grand challenge of the 21st century.

5. Trends in Biotechnology, 19: 205-210.

6. Postma, Marten, and Peter J. M. Van Haastert. (2001) Diffusion–Translocation Model for Gradient Sensing by Chemotactic Cells." *Biophysical Journal 81, 3:1314-23.*

7. Narang, Atul, K. K. Subramanian, and D. A. Lauffenburger. (2001) "A Mathematical Model for Chemoattractant Gradient Sensing based on Receptor-regulated Membrane Phospholipid Signaling Dynamics." *Annals of Biomedical Engineering* 29, *8: 677-91.*

8. Hasty, Jeff, Joel Pradines, Milos Dolnik, and J. J. Collins. (2000) "Noise-based Switches and Amplifiers for Gene Expression." *Proc. Natl. Acad. Sci. USA 97: 2075-80.*

9. Elowitz, Michael B., and Stanislas Leibler, (2000). "A Synthetic Oscillatory Network of Transcriptional Regulators." *Nature 403*: *335-8.*

10. Gardner, Timothy S., Charles R. Cantor, and James J. Collins. (2000) "Construction of a Genetic Toggle Switch in Escherichia coli." *Nature 403: 339-42.*

11. Chistoper H. Schilling *et al.*, (1999). Towards metabolic phenomics: Analysis of Genomicsdata using flux balances. *Biotechnol. Prog*. *15: 288-295.*

12. Michael B. Eisen *et al*. (1998). Cluster analysis and display of genome-wide expression patterns. *Proc. Natl. Acad. Sci.* USA 95*: 14863-14868.*

13. Spiro, Peter A., John S. Parkinson, and Hans G. Othmer, (1997) "A Model of Excitation andAdaptation in Bacterial Chemotaxis." Proc. Natl. Acad. Sci. *USA 94: 7263– 68.*

Course No. BI- 634: Molecular Modeling and Computer aided Drug Design

Time: 3Hrs.   **Max. Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four).Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Introduction to the concepts of molecular modeling. Molecular structure and internal energy. Force Field Models: Molecular Mechanics, Energy Minimization and related methods for exploring the energy surface.

Techniques of molecular dynamics, Molecular Dynamics Simulation Methods, Monte Carlo Simulation Methods, Conformational analysis, Use of molecular modeling to discover and design new molecules.

SECTION-B

Concepts in Quantitative structure activity relationships (QSAR): - Objective of QSAR, Development of Hansh QSAR equation, QSAR descriptors, Concept of Pharmacophore, Pharmacophore mapping, Regression Analysis, component Analysis for QSAR: Discriminant analysis, Principle components Regression and Partial least squares.

SECTION-C

Receptors- Structure, function and Pharmacology, Ion channels- Structure, function and Pharmacology, Enzymes and enzyme inhibitors. Classical Antiviral Agents, Design of New Antiviral Agents. DNA as Target for Anticancer Drugs, Mitotic Apparatus as Target for Drugs.

SECTION-D

The drug development process, Rational Drug Design, Role of molecular recognition in drug design, Structure Based Drug Design, Principles and methods of docking, Ligand Based Drug Design, 3D database search approaches, use of 3D pharmacophore models, Druglikeness, Lipinski's rule of Five and Prediction of ADMET properties. The uses and limitations of Computer assisted drug discovery process.

Reference Books:-

1. Richard B Silverman (2004). The Organic Chemistry of Drug Design and Drug Action, *Elsevier Publishers, Ireland.*

2. Povl Krogsgaard-Larsen *et.al.* (2002). Textbook of Drug Design and Discovery, *Taylor & Francis Publishers, New York.*

3. Andrew R.Leach. (2001). Molecular Modelling; Principles and Applications, *Prentice Hall Publications, New Delhi.*

4. Arup K Ghose (2001). Combinatorial Library Design and Evaluation, *Marcel Dekker Publishers, New York.*

5. Alan L. Harvey (1998). Advances in Drug Discovery Techniques, *John Wiley & Sons, New York.*

6. Penelope W Codding (1998). Structure-Based Drug Design, *Springer Publishers, Berlin.*

7. Nicholas Cohen (1996). Guidebook on Molecular Modeling in Drug Design, *Academic Press, New York.*

Course No. BI- 635: Introduction to Data Analysis using R Programming

Time: 3hrs   **Max Marks: 75**

Instructions for the Paper Setters:
Eight questions of equal marks (Specified in the syllabus) are to be set, two in each of the four Sections (A-D). Questions may be subdivided into parts (not exceeding four).Candidates are required to attempt five questions, selecting at least one question from each Section. The fifth question may be attempted from any Section.

SECTION-A

Itroduction to R, Getting and Installing R on Windows and Linux systems, Installation of R-Packages, Basic operations and commands for starting, closing, navigating directories, listing objects etc., The R Interpreter

Overview of R Language: Expressions, Objects, Symbols, Functions, Special Values, Constants, Operators, Expressions, Control Structures (Conditional Statements and Loops)

R Objects: Primitive Object Types, Vectors, List, Matrices, Arrays, Factors, Data Frames, Formulas, Time Series, Shingles, Dates and Times, Connections, Attributes and Class, Symbols and Environments.

SECTION-B

Functions: The function keyword, Arguments, Return Values, Functions as Arguments.

Object Oriented Programming in R: Defining Classes, New objects, Accessing Slots, Working with Objects.

Working with Data: Entering data within R, Saving and Loading R-Objects, Importing data from External Files, Exporting Data, Importing Data from Data bases, Database Connection R-Packages. Combining Data Sets, Transformations, Binning Data.

SECTION-C

Data Visualization and Graphics: An. Overview of R Graphics, Scatter Plots, Bar Charts, Pie Charts, Plotting Distributions, Box Plots. Lattice Graphics, ggplot2
Basic Statistics with R: Mean, Range, Quartile, Correlation, Covariance, Simple Linear Regression models.
Basic Cluster Analysis: Hierarchical Clustering, K-means- Clustering**,** Principle Component Analysis

SECTION-D

Introduction to Sequence Analysis using R Base and Bioconductor, Key Bioconductor Packages. Use of R in Analysis of Expression Data, Analysis of NGS Data (RNA-Seq, ChIP-Seq, VAR-Seq)

Text / Reference Books: -

1. Joseph Adler, R in a Nutsell, A Desktop Quick Reference. *O'reily 2012.*

2. Vince Buffalo, Bioinformatics Data Skills *O'reily 2015*

3. Algorithms Jones N and Pevzner P (2004) An Introduction to Bioinformatics Algorithms. MIT Press, Massachusetts, 435 pages.

4. Sequence Analysis Durbin, R, Eddy, S, Krogh, A, Mitchison, G. (1998) Biological Sequence Analysis: Probabilistic Models of Proteins and Nucleic Acids. Cambridge University Press, UK, 356 pages.

5. Parida L (2008) Pattern Discovery in Bioinformatics: Theory & Algorithms. CRC Press, London, 526 pages.

6. Profiling Bioinformatics Gentleman, R, Carey, V, Dudoit, S, Irizarry, R, Huber, W (2005) Bioinformatics and Computational Biology Solutions Using R and Bioconductor. Springer, New York, 473 pages.

Course No. BI- 636: Practicals based on BI-633 & BI-634

Time: 9 Periods (Each Period of 1 Hour) Per Week

Max. Marks: 75

Time: 3 Hrs

PART-A

Course No. BI -636   **Marks: 60**

Practical: - Based on BI- 633

Insilico Biotechnology
Primer designing software: Primer3, Primer-BLAST
NEBcutter: A program to cleave DNA with restriction enzymes
PSORTb v.2.0 for **bacterial sequences**
WoLF PSORT: Advanced computational tool for protein subcellular localization prediction of **eukaryotic sequences**
iPSORT for **classification of eukaryotic N-terminal sorting signals.**
CELLO v.2.5 : subCELlular localization prediction
KEGG: Kyoto Encyclopedia of Genes and Genomes
CellDesigner: Modelling tool for Biochemical Network
Reactome: A curated pathway database
Cytoscape :   A platform for visualizing complex networks

Practical: - Based on BI- 634
   1**.** Drawing chemical structures using Marvin Beans/Chemsketch etc. and studying their properties
   2. To carry out energy minimization on a protein/Nucleic acid/carbohydrate.
   3. To carry out molecular dynamics on a protein.
   4. To carry out rigid body docking between two given molecules e.g. protein-protein, protein nucleic acid, protein-ligand etc.
   5. To carry out flexible Protein-Ligand docking using Autodock and elaborate it for virtual screening of a small ligand database.
   6. Experiment to design a pharmacophore model from a set of ligands.
   7. Practical to demonstrate active site finding using LigBuild, CaspP etc.
   8. Scaffold Hopping using ReCore.

PART-B

Marks: 15

Practical Assignment

Course No. BI- 637: Practicals based on BI-631 & 635

Time: 9 Periods (Each Period of 1 Hour) Per Week

Max. Marks: 75

PART-A

Marks: 60

Practical: - Based on BI-631

- Comparative Genomics Tools and Databases: - (UCSC Genome Browser, VISTA Genome Browser, CoGe, VirGen, PLANTGDB, Gramene)
- IntAct: Molecular Interaction Database,
- BioGRID: Database of Protein, Chemical, and Genetic Interactions,
- InterPreTS - protein interaction prediction through tertiary structure.
- MAGICTOOL: For microarray data analysis

Practical: - Based on BI-635
R- Programming
1. Downloading and Installing R on Windows and Linux
2. Basic operations on Functions, Variables, Objects and Classes, Models and Formulas
3. Finding and Installing Packages inside R and from other repositories
4. Importing data from Text files and other software
5. Data visualization using scatter Plots, Line Graphs, Bar Charts, Box Plots
6. Practicals on Clustering
7. Practicals on Expression and NGS data analysis using Bioconductor
.

Marks: 15

PART-B

Practical Assignment

Course No. BI -638
Seminar on emerging trends in Bioinformatics

Max. Marks: 25

BI-640: MAJOR PROJECT

Max. Marks: 200