



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science & Commerce
(Autonomous)**
Matunga,
Mumbai – 400 019,
Maharashtra

Program: Master of Science

Course: Bioinformatics

Syllabus for M.Sc. Semester I & II

**(As per Choice Based Semester and Grading System with effect
from Academic Year 2023-2024)**

Introduction:

Last two decades have witnessed the emergence of Bioinformatics as a major thrust area in the global scientific scenario. It is the interface between the two most rapidly advancing fields of biological and computational sciences. Bioinformatics is a scientific discipline and asset of skills that has now become one of the most important information gathering, data mining, and knowledge building tools in recent research and clinical applications.

In the current pandemic bioinformatics has played a major role in studying the genomics of COVID-19. It helped in studying the impact of Hydroxychloroquine on COVID. Bioinformatics came out as one of the essential tools to analyze viral data as it provides vital information about the genetic makeup of the virus and assists directly in the development of drugs or vaccines against the deadly disease.

This course is of two years imparting technical skills for producing industry ready candidates. Post Graduate Bioinformatics course content includes Biological sciences (Cell biology, Biochemistry, Molecular biology, Proteomics, Immunology), Biostatistics, Machine learning, Chemical sciences (Drug designing, Analytical techniques like HPLC, GC, HPTLC, IR, Mass Spectroscopy), Computational sciences (Java, Linux, Perl, Mongodb, Python), Clinical Research and Clinical Data Management, Bioinformatics in Genomics and Proteomics, Sequence Analysis , Structural Biology, Drug Designing, Molecular Modeling and Simulations, Cheminformatics, Immunoinformatic, QSAR, Research Methodology and Scientific Writing.

In the second-year students are introduced to Research Methodology and Scientific Writing. Research culture is inculcated by pursuing a compulsory 3 months dissertation project. They are trained to present their research work in scientific conferences and research meet. They also publish their research work in eminent journals. This adds a feather to cap while they apply for PhD programs in India and abroad.

The course is specially designed to cater to the requirements of the pharmaceutical and biotech industries as well as emerging sectors like biopharmaceuticals, clinical research, data science, and information technology. Opportunities are arising in areas like big data, data analytics, drug designing, bio-analytics, hospitals, research & development labs, data Science companies, biotechnology & healthcare companies, sequence assembly, genomic sequence analysis, functional genomics, genotyping, pharmacogenomics, database administration, etc.

We are blessed with a team of renowned scientists and faculty members across industry and academics who are prompt and enthusiastic and have helped students build lucrative careers in the said fields.

The proposed program for Masters in Bioinformatics is a two-year program which has been successful in developing young minds into bright researchers and industry professionals.

Objectives of The Course:

- Develop trained manpower in the field of Bioinformatics with specific emphasis for fulfilling expectations of Indian Pharma and Biotech industry.
- To develop skills needed to collect, understand, analyze and manage data generated through high throughput technology.
- Explain how the boundaries of knowledge in this professional discipline are advanced through research and enable students to conduct research through targeted research projects.
- To give exposure to the students in national and international work.

Eligibility:

Bachelor degree from a recognized university in any of the following disciplines:

- Science (Biochemistry, Biology, Bioanalytical Science five years integrated, Biophysics, Botany, Biotechnology, Chemistry, Environmental Science, Life Sciences, Physics, Mathematics, Microbiology, Statistics or Zoology)
- Agriculture
- Medicine
- Pharmacy
- Veterinary Science
- Computer Science

Staffing Pattern for The Course:

- Instrument technician - 01
- Technical assistance - 02
- Lecturer - 03 (Full Time)
- Lecturer - 01 (Part Time)
- Remaining workload will be shared with visiting faculty.

Faculty:

Post graduate or PhD degree in the subject of Bioinformatics, Bioanalytical Science, Biochemistry, Biotechnology, Chemistry, Computers Science, Information technology, Microbiology, Life Science, Molecular Biology, Botany, Zoology, and Statistics, Mathematics with B+ grade and NET / SET.

SYLLABUS IN BRIEF

Distribution of Credits

Semester I

Paper code	Paper	Paper Name	Credit
GNKPSBI1501	Mandatory Paper - I	Fundamental of Biology & Bioinformatics	4
GNKPSBI2501	Mandatory Paper- II	Introduction to Programming Languages and Databases	4
GNKPSBI3501	Elective Paper	Bioinformatics and Sequence Analysis	3
GNKPSBI4501	Research Methodology	Research Methodology	2+2 = 4
GNKPSBI1P501	Mandatory Paper I – Practical	Fundamental of Biology & Bioinformatics	2
GNKPSBI2P501	Mandatory Paper II – Practical	Introduction to Programming Languages and Databases	2
GNKPSBI3P501	Elective Paper - Practical	Bioinformatics and Sequence Analysis	1

Semester II

Paper code	Paper	Paper Name	Credit
GNKPSBI1502	Mandatory Paper-I	Advance Biology & Structural Bioinformatics	4
GNKPSBI2502	Mandatory Paper-II	Java Programming, Introduction to Linux and Machine Learning	4
GNKPSBI3502	Elective Paper	Genomics & Proteomics in Bioinformatics, NGS	3
GNKPSBI4502	ON JOB TRAINING	ON JOB TRAINING	4
GNKPSBI1P502	Mandatory Paper I – Practical	Advance Biology & Structural Bioinformatics	2
GNKPSBI2P502	Mandatory Paper II – Practical	Java Programming, Introduction to Linux and Machine Learning	2
GNKPSBI3P502	Elective Paper - Practical	Genomics & Proteomics in Bioinformatics, NGS	1



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)**
Matunga, Mumbai – 400 019, Maharashtra

Syllabus for M.Sc. Semester I

Program: Master of Science

Course: Bioinformatics

Mandatory Paper: I

**(As per Choice Based Semester and Grading System with effect
from Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023-

2024) Mandatory Paper I

Course Title: Fundamental of Biology & Bioinformatics

Paper Code: GNKPSBI1501

Credits: 04

No. of Lectures:

60 Marks: 100

Learning Objectives:

- To learn about the bioinformatics databases, databanks, data format and data retrieval from the online sources.
- To make students understand the essential features of the interdisciplinary field of science for better understanding biological data.
- To provide the student with a strong foundation for performing further research in bioinformatics.
- To understand and explore the sequence comparison tools for nucleotide and protein sequences.
- To interpret the results of sequence alignments (Pairwise - local and global alignments as well as multiple sequence alignments).
- To study basis of cell biology.
- This course will enable students to understand structure of Biomolecules and their Metabolism.
- To lay a foundation of Enzyme Kinetics.

Learning Outcome:

- Gain an overview of cells - their origin and evolution. Students will understand the structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles. They will apply their knowledge of cell biology to selected examples of changes or losses in cell function.
- Students will be able explain/describe the synthesis of proteins, lipids, nucleic acids, and carbohydrates and their role in metabolic pathways along with their regulation. Students will be able to use current biochemical techniques to plan and carry out experiments.
- Introduce what bioinformatics is and why it is important.
- Provide an overview of the application areas of bioinformatics, with a focus on the topics that will be taught.
- Locate and use the main databases at the NCBI and EBI resources.
- Know the difference between databases, tools, repositories and be able to use each one to extract specific information.

Semester I

Unit		Title	No. of lectures
Unit 1		Cell Biology	15
	1.1	Structure and Function of cells and intracellular organelles (of both prokaryotes and eukaryotes)	
	1.2	Cell Membranes- fluid mosaic model and its functions. Membrane transport, Na-K Pump	
	1.3	Structure, various models, its function. Cellular transport - simple diffusion, facilitated diffusion, active transport, nuclear transport, osmosis exocytosis and endocytosis	
	1.4	Structure and Function of cells and intracellular organelles (of both prokaryotes and eukaryotes)	
	1.5	Cytoskeleton- Introduction to microfilaments, microtubules, and intermediate filaments, Nucleation	
	1.6	Mechanism of cell division including (mitosis and meiosis) and concept of motors. Programmed cell death	
	1.7	Characteristics of cancerous cells; Agents promoting carcinogenesis; molecular basis of cancer therapy, Tumor markers - AFP, CEA, hCG; Telomere replication; Telomerase and its role in cancer and aging.	
	1.8	Neurotransmitters	
Unit 2		Structure of Biomolecules and their Metabolism	15
	2.1	Nucleic Acids: RNA and DNA	
	2.2	Different Structural Forms of DNA; Different Types of RNA.	
	2.3	Carbohydrates: Structure and Classification, Glycosaminoglycans, Proteoglycans and Glycoproteins	
	2.4	Lipids: Structure and Classification, Acylglycerols; Phospholipids, Sphingolipids, Cholesterol and Membranes; Isoprenoids, Icosanoids and their biological importance	
	2.5	Carbohydrates: Structure and Classification, Glycosaminoglycans, Proteoglycans and Glycoproteins	
	2.6	Glycolysis, Feeder, pyruvate oxidation, the Krebs cycle, and oxidative phosphorylation.	
Unit 3		Enzyme Kinetics	15
	3.1	Introduction to Enzymes	
	3.2	Units of activity, coenzymes and metal cofactors.	
	3.3	Temperature and PH effects	
	3.4	Michaelis – Menten Kinetics	
	3.5	Feedback inhibition and activation	
	3.6	Ribozyme and abzymes	

Unit 4	Introduction to Bioinformatics & Sequence Analysis	
4.1	Introduction to the Bioinformatics and its application	15
4.2	Importance, goals / scope, opportunities & Limitations of Bioinformatics	
4.3	Various file formats for bio- molecular sequences	
4.4	Basic Concepts of sequences similarity, Identity, homology, orthologues, Paralogues	
4.5	Concepts of sequence alignments, Dot Matrix, Dynamic Programming, Heuristic Programming,	
4.6	Algorithms: Needleman & Wunch, Smith & Waterman	
4.7	Scoring matrices: Basic concepts of scoring matrix, PAM and BLOSUM series and principles based on which these matrices are derived	

Semester I Evaluation Pattern

Internal: 25

External: 75

M.Sc. Bioinformatics (2023-2024)

Mandatory Paper I - Practical

Course Title: Fundamental of Biology & Bioinformatics

Paper Code: GNKPSBI1P501

Credits: 02

Marks: 50

1. Biochemical estimation of DNA.
2. Biochemical estimation of RNA.
3. Estimation of vitamin C using UV- Vis spectrophotometer.
4. 2D separation of amino acids, plant pigments using paper chromatography.
5. Thin layer chromatography analysis of modern drug.
6. Pair-wise global alignments of protein/ DNA sequences using Needleman-Wunsch algorithm
7. Pair-wise local alignments of protein and DNA sequences using Smith-Waterman algorithm
8. Identification of similar and divergent sequences:
 - a. BLAST
 - b. FASTA
 - c. PSI BLAST
 - d. PHI BLAST

References:

- Bioinformatics: Sequence and Genome Analysis by Mount D., Cold Spring Harbor Laboratory Press, New York. 2004
 - Bioinformatics- a Practical Guide to the Analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellette, B.F., Wiley India Pvt Ltd. 2009
 - Introduction to Bioinformatics by Teresa K. Attwood, David J. Parry-Smith. Pearson Education. 1999
 - Introduction to Bioinformatics Algorithms, Neil C. Jones, Pavel Pevzner
 - Introduction to Bioinformatics - S. Sundararajan and Balaji
 - Instant notes – Bioinformatics – Westhead, Howard parish and Twyman. Viva books Pvt. Limited. Chennai
 - Bioinformatics basic methods and applications – S.C. Rastogi
 - Essential Bioinformatics by Jin Xiong, 2006
 - ORENGO, C., JONES, D. & THORNTON, J.: Bioinformatics: genes, proteins and computers. 2003. Bios Scientific Publishers, Ltd. Oxford
 - Ingvar Eidhammer, Inge Jonassen, William R. Taylor: Protein Bioinformatics. 2003 John Wiley And Sons Ltd (UK) 2. HIGGINS, D. & TAYLOR, W.: Bioinformatics: sequence, structure, and databank. 2000. Oxford University Press, Oxford, UK
 - M. Lesk. (2002) Introduction to Bioinformatics Oxford University Press 68. G.B Fogel D.W Corne (2002) Evolutionary Computation in Bioinformatics
 - Voet, Donald, Voet Judith, Pratt, Charlotte W. Fundamentals of Biochemistry: Life at the molecular Level 2nd Edition. Publisher: Asia, John Wiley & Sons. 2006.
 - Nelson David L., Cox Michale. Lehninger Principles of Biochemistry 5th Edition. Publisher: New York. W. H. Freeman. 2008.
 - R C Rastogi, Biochemistry 2nd edition, 2003.
 - Kleinsmith and Harden, The World of the cell, Becker, Academic Internet Publishers; 5th edition (2006)
 - Geoffrey M. Cooper and Robert E. Hausman. The Cell: A Molecular Approach, Fourth Edition
 - Harvey Lodish. Molecular cell Biology. W. H. Freeman; Sol edition (2007)
-



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)**
Matunga, Mumbai – 400 019, Maharashtra

Syllabus for M.Sc. Semester I

Program: Master of Science

Course: Bioinformatics

Mandatory Paper: II

**(As per Choice Based Semester and Grading System with effect from
Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023- 2024)

Mandatory Paper II

Course Title: Introduction to Programming Languages and Databases

Paper Code: GNKPSBI2501

Credits: 04

No. of Lectures:60

Marks: 100

Learning Objectives:

- Explore various programming paradigms as well as principles of building object-oriented software
- Solidify your understanding of Computer Science in theory and practice related to biological data.
- Learn the essential elements of computing theory including logic, proof techniques, combinatorics, algorithm analysis, discrete data models (sets, relations, trees), and finite automata.

Learning Outcomes:

- Understand dynamic memory management techniques using pointers, constructors, destructors, etc.
- Classify inheritance with the understanding of early and late binding, usage of exception handling, generic programming.
- Understand generic programming, templates, file handling.

Unit		Title	No. of lectures
Unit 1		Fundamentals of Computing and introduction to Database systems	15
	1.1	Overview and functions of a Computer System	
	1.2	Memory: Register, buffer, RAM, PROM, EPROM, EEPROM	
	1.3	Overview of various computer threats viz. Trojan horses, viruses etc.	
	1.4	Operating systems concepts (Windows, Unix, Linux)	
	1.5	Software Development Life cycle (SDLC)	
	1.6	Concepts of various types of Databases and Data models	
	1.7	Instances, Schemes and E – R Model	

Unit 2		Introduction to C++	
	2.1	Input and Output	
	2.2	Data types and Functions	
	2.3	Derived data types	
	2.4	Structure in C++ and string manipulations	
	2.5	Basic Input output and File handling	
Unit 3		Advanced C++	
	3.1	Basics of object-oriented programming	
	3.2	Concept of Object, class, Constructor and Destructors	
	3.3	Data encapsulation	
	3.4	Inheritance	
	3.5	Polymorphism	
	3.6	Virtual function and friend function	
Unit 4		SQL	
	4.1	Data definition statement; Data Manipulation Statements	
	4.2	Select statement	
	4.3	Data Control Statement	
	4.4	Other Database Objects (Views, Sequences, Synonyms etc)	
	4.5	Security, Grants, Roles, Privileges	

Semester I Evaluation Pattern

Internal: 25

External: 75

M.Sc. Bioinformatics (2023-2024)

Mandatory Paper II - Practical

Course Title: Introduction to Programming Languages and Databases

Paper Code: GNKPSBI2P501

Credits: 02

Marks: 50

1. Basic I/O Programs
 - a. cin
 - b. cout
 - c. Datatypes and variables
2. Conditional and Loops
 - a. If statement

- b. If-else statement
 - c. Nested If-else statement
- 3. Arrays
 - a. 1-D array
 - b. 2-D array
- 4. Functions and structure
 - a. Create functions with no return and with no parameter
 - b. Create functions with return and with parameter
 - c. Create functions with no return and with parameter
 - d. Create functions with return and with no parameter
- 5. String manipulation
 - a. strlen()
 - b. strcpy()
 - c. strcat()
- 6. Class and objects, Encapsulations
 - a. Create class and objects
 - b. Access specifiers: Private, public and protected
- 7. Inheritance
 - a. Single Inheritance
 - b. Multilevel Inheritance
 - c. Multiple Inheritance
 - d. Hybrid Inheritance
- 8. Polymorphism, Virtual Function, Friend Function
 - a. Runtime Polymorphism
 - b. Compile Polymorphism
- 9. Constructor and Destructor
- 10. SQL
 - a. Create table
 - b. Insert values
 - c. Add new column to table
 - d. Remove the record from table
 - e. Constraints
 - f. Calculate average, sum and max
 - g. group by, where, order by

References:

- 1. C++: The Complete Reference, 4th Edition
 - 2. Advanced C++ by BPB.
 - 3. SQL The Complete Reference, 3rd Edition
-



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Syllabus for M.Sc. Semester I

Program: Master of Science

Course: Bioinformatics

ELECTIVE PAPER

**(As per Choice Based Semester and Grading System with effect from
Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023-2024)

Elective Paper

Course Title: Bioinformatics and Sequence Analysis

Paper Code: GNKPSBI3501

Credits: 03

No. of Lectures: 45

Marks: 100

Learning Objectives:

- To learn about the bioinformatics databases, databanks, data format and data retrieval from the online sources.
- To make students understand the essential features of the interdisciplinary field of science for better understanding biological data.
- To provide the student with a strong foundation for performing further research in bioinformatics.
- To understand and explore the derived databases and their applications to biological systems.
- To explore various computational tools for analysis of biomolecular sequences.

Learning Outcomes:

- Provide an introduction to what bioinformatics is and why it is important.
- Provide an overview of the application areas of bioinformatics, with a focus on the topics that will be taught.
- Explain what type of knowledge will be gained.
- Locate and use the main databases at the NCBI and EBI resources.
- Know the difference between databases, tools, repositories and be able to use each one to extract specific information.
- Define and Identify different life skills required in personal and professional life
- Develop an awareness of the self and apply well-defined techniques to cope with emotions and stress.
- Explain the basic mechanics of effective communication and demonstrate these through presentations.
- Take part in group discussions CO5: Use appropriate thinking and problem solving techniques to solve new problems
- Understand the basics of teamwork and leadership

Unit		Title	No. of lectures
Unit 1		Biomolecular Databases	15
	1.1	What are Database, Types of Databases & Biological Databases	
	1.2	Major Bioinformatics resources NCBI, ENTREZ, EMBL-EBI & ExPasy	
	1.3	Literature database e.g. PUBMED & PMC	
	1.4	Nucleic acid database: GENBANK, EMBL, DDBJ Study of Submission Tools	
	1.5	Protein sequence databases: PIR, UniProt, SWISSPROT, TrEMBL, PROSITE, Pfam, INTERPRO / PRINTS	
	1.6	Protein structure databases: NDB, PDB, CCSD, Reactome, PDBSum, PDBTM, CATH, SCOPe	
	1.7	Genome Databases: NCBI, UCSC, GOLD, Ensemble,	
	1.8	Chemical Databases: PubChem, Drug Bank, ZINC	
	1.9	Specialized & Metabolic databases: MBGD, ICTVdb, KEGG, OMIM	
	1.10	Enzyme Database: BRENDA, EXPASY	
Unit 2		Molecular Phylogenetics	15
	2.1	Introduction to Multiple sequence alignment(MSA) and its various algorithm.	
	2.2	Introduction to Multiple sequence alignment(MSA) and its various algorithm.	
	2.3	Definition and description of Phylogenetic trees, Basics & Nature of data in Taxonomy and Phylogeny.	
	2.4	Concept of evolutionary trees – Dendrogram and Phylogram, its representations & Procedure for Phylogenetic tree construction	
	2.5	Methods for Tree construction:	

		a) Distance based method: Clustering based method (NJ & UPGMA), Optimality based method (FM and ME) b) Character based method: Maximum Parsimony and Maximum likelihood method		
	2.6	Phylogenetic Analysis Programs: PHYLIP, PAUP, MEGA4		
Unit 3	OMICS			
	3.1	Introduction to Genomics, Genome annotation and analysis, DNA sequencing technologies, Comparative genomics, Structural genomics, Functional genomics, Pharmacogenomics, Personalized medicine and genomics		
	3.2	Introduction to Proteomics, Protein separation and purification techniques, Mass spectrometry and proteomic analysis, Protein identification and characterization, Protein-protein interactions, Protein expression profiling	15	
	3.3	Introduction to Epigenomics & Structural Biology		
	3.4	Goals of the Human Genome Project, cloning vectors, concept of maps, physical maps, shotgun libraries, DNA polymorphism, nucleotides, DNA sequences.		
	3.5	Restriction enzymes, resource for restriction enzyme (REBASE)		
	3.6	Bioinformatics & Computational Biology a. Data analysis methods for omics data b. Database resources for genomics, proteomics, and other omics data c. Statistical analysis and data mining (Application / case study) d. Machine learning and predictive modeling (Case study)		

Semester I Evaluation Pattern

Internal: 25

External: 75

M.Sc. Bioinformatics (2023-2024)

Elective Paper - Practical

Course Title: Bioinformatics and Sequence Analysis

Paper Code: GNKPSBI3P501

Credits: 01

Marks: 50

1. Exploring the integrated database system viz. Basic, Advanced and LIMITS w.r.t NCBI, EMBL-EBI, ExPasy
2. Sequence databases:
 - a. EMBL
 - b. DDBJ
 - c. GenBank & Submission Tool
 - d. UniProt
 - e. PIR
 - f. SWISSPROT & TrEMBL
3. Domain database:
 - a. PROSITE
 - b. INTERPRO / PRINT
 - c. Pfam
 - d. BLOCK
4. Structure database:
 - a. PDB
 - b. NDB
 - c. CCSD
 - d. Reactome
 - e. PDBSum
 - f. PDBTM
 - g. CATH
 - h. SCOPe
5. Literature & Specialized database:
 - a. KEGG
 - b. PUBMED
 - c. OMIM
 - d. PMC
6. Retrieving genomic information:
 - a. NCBI
 - b. GOLD & Submission Tool
 - c. Ensemble
 - d. UCSC
 - e. MBGD
 - f. ICTVdb

7. Multiple sequence alignment
 - a. Clustal Omega
 - b. T-Coffee
 - c. MUSCLE
8. Phylogenetic tree generation tool & Visualization:
 - a. Simple Phylogeny (EMBL-EBI)
 - b. Tree construction using PAUP & PHYLIP
 - c. Visualization of phylogenetic trees using Tree View
9. Restriction enzyme database: REBASE
10. Database resources for genomics, proteomics, and other omics data studies

References:

- Bioinformatics: Sequence and Genome Analysis by Mount D., Cold Spring Harbor Laboratory Press, New York. 2004
- Bioinformatics- a Practical Guide to the Analysis of Genes and Proteins by Baxevanis, A.D. and Francis Ouellette, B.F., Wiley India Pvt Ltd. 2009
- Introduction to Bioinformatics by Teresa K. Attwood, David J. Parry-Smith. Pearson Education. 1999
- Introduction to Bioinformatics Algorithms, Neil C. Jones, Pavel Pevzner
- Xinkun Wang, Next-Generation Sequencing Data Analysis, CRC Press, 2016, 1e 2. Publications on NGS data analysis from literature.
- G.P. Quinn and M. J. Keough; Experimental design and data analysis for biologists; Cambridge University Press, 2002.
- S. Knudsen; Guide to analysis of DNA microarray data; Wiley, 2nd edition, 2004.
- E. D. Hoffmann and V. Stroobant; Mass spectrometry: Principles and applications; Wiley, 3rd edition, 2007.
- A. Zhang; Advanced analysis of gene expression microarray data; World Scientific Publishing, 2006.
- N. Rodriguez-Ezpeleta; Bioinformatics for High Throughput Sequencing; Springer; 2012.
- Y. M. Kwon and S. C. Ricke; High-Throughput Next Generation Sequencing: Methods and Applications; Humana Press; 2011.
- J. R. Chapman; Protein and Peptide Analysis by Mass Spectrometry, Springer, 2nd edition, 1996.
- Introduction to Bioinformatics - S. Sundararajan and Balaji
- Instant notes – Bioinformatics – Westhead, Howard parish and Twyman. Viva books Pvt. Limited. Chennai
- Bioinformatics basic methods and applications – S.C. Rastogi
- Essential Bioinformatics by Jin Xiong, 2006
- ORENGO, C., JONES, D. & THORNTON, J.: Bioinformatics: genes, proteins and

computers. 2003. Bios Scientific Publishers, Ltd. Oxford

- Ingvar Eidhammer, Inge Jonassen, William R. Taylor: Protein Bioinformatics. 2003 John Wiley And Sons Ltd (UK) 2. HIGGINS, D. & TAYLOR, W.: Bioinformatics : sequence, structure, and databank. 2000. Oxford University Press, Oxford, UK
 - M. Lesk. (2002) Introduction to Bioinformatics Oxford University Press 68. G.B Fogel D.W Corne (2002) Evolutionary Computation in Bioinformatics
-



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)**
Matunga, Mumbai – 400 019, Maharashtra

Syllabus for M.Sc. Semester I

Program: Master of Science

Course: Bioinformatics

RESEARCH METHODOLOGY

**(As per Choice Based Semester and Grading System with effect from
Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023-2024)

Course Title: Research Methodology

Paper Code: GNKPSBI4501

Credits: 04 (02 + 02)

No. of Lectures: 60

Marks: 100

Learning Objectives:

- To be able to restate an investigative question in terms of a statistical model or algorithm
- Successfully relate theoretical concepts to a real-world problem in a written report.
- Provide reproducible statistical analyses using accepted practices of the research community
- Demonstrate the ability to find appropriate research literature appropriate to the investigative task.
- To understand the scope of personality and its development.
- To develop core skills for development of self.
- To cultivate interpersonal skills for successful life.

Learning Outcome:

- They have the versatility to work effectively in a broad range of analytic, scientific, government, financial, health, technical and other positions.
- They have a broad background in Mathematics and Statistics, an appreciation of how its various sub-disciplines are related, the ability to use techniques from different areas, and an in-depth knowledge about topics chosen from those offered through the department.
- They recognize and appreciate the connections between theory and applications
- Define and Identify different life skills required in personal and professional life
- Develop an awareness of the self and apply well-defined techniques to cope with emotions and stress.
- Explain the basic mechanics of effective communication and demonstrate these through presentations.
- Take part in group discussions CO5: Use appropriate thinking and problem-solving techniques to solve new problems
- Understand the basics of teamwork and leadership

Units	Topic	Lectures	Credits
1.1	Research Fundamentals and Terminology		
	<p>Meaning and Objective of research, features of a good research study, types of Research (qualitative and quantitative research)</p> <p>Study designs and variations: basic, applied, historical, exploratory, experimental, ex-post-facto, case study, diagnostic research, crossover design, case control design, cohort study design, multifactorial design</p>	07	01
1.2	Literature Survey Methods		
	<p>Journal and abbreviation, current titles and review, monographs, textbooks, introduction to abstract, Beilstein, subject and author index</p> <p>Digital: Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, Hindex, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Sciurus, Google Scholar, Wiki-databases, Science Direct, SciFinder, Scopus.</p>	08	
2.1	Research Writing		
	<p>Scientific writing- Reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation.</p> <p>Writing Scientific Papers: Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work.</p> <p>Project Proposal and research funding agencies, Research grants, scholarships and funding (CSIR, DBT, DST, DST- INSPIRE Fellowship, ICMR, INSA, BRNS, MoEFCC, UGC-RFSMS, Fulbright</p> <p>Fellowships for Indian students, Lady Tata Memorial Trust, EPA, Bill and Melinda Gates Foundation, Wellcome Trust, Erasmus Mundus)</p>	10	01

2.2	Publication Ethics & Bibliography	05	
	<p>Publication ethics : definition, introduction</p> <p>Best practices/ Standards settings initiative and guidelines COPE, WAME</p> <p>Conflict of interest</p> <p>Publication Misconduct: definition, concept, problems that lead to unethical behavior</p> <p>Violation of publication ethics, authorship and contributorship</p> <p>Identification of publication misconduct</p> <p>Predatory publisher and journals. Use of reference management software (MS Word / Zotero / Mendeley)</p>		
3.1	Statistical Measures & Statistical Inference		
	<p>Mean, mode, median, Variance, standard deviation, coefficient of variation, Raw and Central Moments upto fourth order, measures of skewness and kurtosis</p> <p>Correlation and regression analysis, curve fitting (linear, non-linear, multilinear).</p> <p>Hypothesis testing: Simple and composite hypotheses, Null and alternative hypotheses critical region Type I and Type II Errors Level of significance p- value, power of a test</p> <p>Test of significance viz. Z test, t test, pair t test, chi2 test of goodness of fit</p> <p>Non-parametric tests: median test, sign test, Kruscal-Wallis test</p>	15	01

4.1	Communication Skills & Public Speaking		
	<p>Introduction to Personality Development The concept of personality, SWOT analysis, Attitude & Motivation Attitude - Concept - Significance - Factors affecting attitudes - Positive attitude – Advantages –Negative attitude- Disadvantages, Concept of motivation</p> <p>Self-esteem Term self-esteem - Symptoms - Advantages - Do's and Don'ts to develop positive self-esteem – Low self esteem - Symptoms - Personality having low self esteem - Positive and negative self esteem. Interpersonal Relationships – Defining the difference between aggressive, submissive and assertive behaviors - Lateral thinking</p> <p>Aspects of Personality Development Body language - Problem-solving - Conflict and Stress Management - Decision-making skills - Leadership and qualities of a successful leader – Character building -Team-work – Time management - Work ethics –Good manners and etiquette.</p> <p>The art of participating in Group Discussion – Facing the Personal (HR & Technical) Interview -Frequently Asked Questions - Psychometric Analysis - Mock Interview Sessions.</p>	15	01

Internal Evaluation: 50 Marks

External Evaluation: 50 Mark

References:

- BIOSTATISTICS by P.N. Arora & P.K. Malhan
 - Biostatistics, B ANNADURAI
 - Intuitive Biostatistics: A Nonmathematical Guide
 - The Art of Public Speaking, STEPHEN LUCAS
 - TED Talks: The Official TED Guide to Public Speaking, CHRIS ANDERSON
-



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)**
**Matunga, Mumbai – 400 019,
Maharashtra**

Syllabus for M.Sc. Semester II

Program: Master of Science

Course: Bioinformatics

Mandatory Paper I

**(As per Choice Based Semester and Grading System with effect
from Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023-2024)

Mandatory Paper I

Course Title: Advance Biology & Structural Bioinformatics

Paper Code: GNKPSBI1502

Credits: 04

No. of Lectures: 60

Marks: 100

Learning Objectives:

- To teach concept of Central Dogma. Describe the general principles of gene organization and expression in both prokaryotic and eukaryotic organisms.
- To give a grounding in the Recombinant DNA technology and recent advancement in field of Molecular Biology.
- To study introduction of structural bioinformatics, conformational analysis of proteins and nucleic acids.
- To understand the protein structure prediction, and molecular interactions.
- This course will enable the students to: understand the levels of structural organization. of macromolecules and experimental methods of structure determination.
- Helps to understand the approaches for structure analysis and acquire knowledge of various algorithms & methods of structure prediction.
- Understand the genomic information.
- Describe the genome annotation pipeline, including manual and automated annotation

Learning Outcomes:

- Students will analyze structural-functional relationships of genes and proteins from bacteria to eukaryotes using genomic methods based on evolutionary relationships.
- Students will be able to explain the synthesis of proteins and nucleic acids with their regulation at the epigenetic, transcriptional, translational, and post-translational levels
- Acquire skills to use different approaches for prediction of protein structure.
- To understand the structural organization, structural properties and various techniques employed in the structure determination of Biological macromolecules – DNA, Protein.
- Advances understanding about primary and secondary structures of proteins
- Expansions understanding about tertiary and quaternary structures of proteins
- Designate about protein folding and its significance and helps to gain knowledge for the same.
- Use the UCSC genome browser to explore the available annotation tracks for a gene of interest.
- Helps in interpretation of the structure for a protein sequence based on an identified template.

Semester I

Unit		Title	No. of lectures
Unit 1		Concept of Central Dogma	15
	1.1	Concept of Central Dogma & Recombinant DNA Technology	
	1.2	DNA Replication, various enzymes involved, DNA topology, super coiling of DNA, origin of replication	
	1.3	Transcription – enzymes involved, sigma factor, DNA binding sites, initiation, elongation and termination	
	1.4	Translation or protein synthesis – enzymes or factors involved polyribosome	
	1.5	Operon model in prokaryotes and eukaryotes, lac operon, trp operon	
	1.6	Gene splicing, post translation modifications	
Unit 2		Recombinant DNA Technology	15
	2.1	History of rDNA Technology, enzymes involved – restriction endonucleases, ligases etc.	
	2.2	Cloning vectors – plasmids, bacteriophage vectors for eukaryotes- YAC.	
	2.3	DNA manipulation–cutting and joining DNA using nucleases and ligases, linkers and adapters	
	2.4	Cloning strategies, construction of libraries	
	2.5	Transformation of DNA into host cells, Screening for recombinants, blue white screening	
	2.6	DNA fingerprinting techniques	
	2.7	Application of recombinant DNA technology	
Unit 3		Molecular Biology Techniques	15
	3.1	Protein/DNA/RNA probes, southern and western blotting, In situ hybridization	
	3.2	DNA Sequencing	
	3.3	Microarray	
	3.4	Flow cytometry	
	3.5	Capillary Electrophoresis	
	3.6	PCR and Real time PCR	
Unit 4		Introduction to Protein Structures & Prediction Methods	
	4.1	Overview of structural bioinformatics – understanding structural basis for biological phenomena– challenges in structural bioinformatics	

	4.2	Macromolecular Structure: Protein - Primary, Secondary, Super secondary, Tertiary and Quaternary structure, Potential energy maps, Ramachandran map, Co-ordinate systems	
	4.3	Macromolecular interactions: Protein – Protein (Proteomic analysis of Post-translational Modification- Phosphorylation, ubiquitination, and glycosylation) , Protein – Nucleic acids , Protein – carbohydrates, etc. Yeast two Hybrid Technique, Tools to study protein interaction: STRING, MIPS (other equivalent methods)	
	4.4	Principles of protein folding and methods to study protein folding, Anfinsen Experiment	
	4.5	Prediction of protein structure: secondary structure prediction methods: First, second and third generation methods.	
	4.6	Prediction of protein Tertiary structure prediction: Homology modeling, fold recognition and ab initio methods	
	4.7	Validation of protein tertiary structure using Ramachandran Plot/RAMPAGE/SAVES (or other equivalent methods)	

15

Semester II Evaluation Pattern

Internal:25

External: 75

M.Sc. Bioinformatics (2023-2024)

Mandatory Paper I - Practical

Course Title: Advance Biology & Bioinformatics

Paper Code: GNKPSBI1P502

Credits: 02

Marks: 50

1. Isolation of plasmid DNA and chromosomal DNA
2. Restriction digestion of DNA
3. Ligation
4. PAGE separation of human serum proteins
5. To perform Polymerase Chain Reaction of gene of interest
6. Demonstration of DNA Sequencer
7. Demonstration of Flow cytometer
8. Demonstration of Real time PCR
9. Secondary structure prediction using various available tools
10. Tertiary structure and function prediction using homology modeling, Fold recognition and ab initio method
 - a. Modeller
 - b. I TASSAR

c. ROBETTA / ROSETTA

11. Validation of predicted structure by SAVES server or verify 3d (other equivalent methods)
12. Visualization of 3D protein structure using
 - a. Rasmol
 - b. PyMol
 - c. Chimera
13. Binding pocket prediction – Castp; Glycosylation, phosphorylation sites prediction (other equivalent methods)
14. Structural Blast – VAST & DALI

References:

- Primrose, S.B. and Twyman, R.M. (2006) Principles of Genetic Manipulation and Genomics. Seventh Edition. Blackwell Publishing, USA.
- Winnacker, E-L.(1987) From Genes to Clones. VCH Publishers, USA.
- SambrookJ.and Russell D.2001.Molecular Cloning: A Laboratory Manual, 3rd edition. Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York.
- B. M. Turner, Chromatin and Gene Regulation: Molecular Mechanisms in Epigenetics
- Russell Peter J. iGenetics: A Molecular Approach 3rd edt.: Pearson International Edition. Publisher: New York, Pearson ISBN: 9780321610225.
- Cesareni Giovanni, Gimona Mario, Sudol Marius, Yaffe Michael (Editors). Modular Protein Domains. Publisher: Weinheim Wiley-VCH. 2005. ISBN: 352730813X.
- Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890.
- Webster David (Editor). Protein Structure Prediction: Methods and Protocols (Methods in Molecular Biology) Volume 143. Publisher: New Jersey Humana Press. 2000. ISBN: 0896036375.
- Sternberg Michael J. E. Protein Structure Prediction: A Practical Approach. Publisher: USA, Oxford University Press. 1997. ISBN: 0199634953.
- R.M. Twyman, “Principles of Proteomics (Advanced Text Series)”, Bios Scientific, 2004. 2
- Daniel C. Liebler ,” Introduction to Proteomics: Tools for the New Biology”, Humana Press Inc., 2002
- Ian M. Rosenberg , “Protein Analysis and Purification: Benchtop Techniques “- , Springer, 2005 2. Philip L.R. Bonner, “Protein Purification”, Taylor & Francis, 2007
- David W Mount, “Bioinformatics- Sequence and genome analysis”, Cold Spring Harbor Laboratory Press, second edition, 2004
- S. R. Pennington, M. J. Dunn, “Proteomics: from Protein Sequence to Function”, Springer publications, first edition, 2001.
- Timothy Palzkill,“Proteomics”,Springer, 2002.
- Igor Jurisica, Dennis Wigle. Knowledge Discovery in Proteomics. 2006. Chapman & Hall / CRC Pennington SR (Ed), Dunn M. J. (Ed) Proteomics: from protein sequence to function. 2002 Viva Books Pvt. Ltd.
- Srivastava Sudhir (Ed). Informatics in Proteomics 2005 Taylor & Francis Group / CRC



Shiromani Gurdwara Parbandhak Committee's

**Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Syllabus for M.Sc. Semester II

Program: Master of Science

Course: Bioinformatics

Mandatory Paper: II

**(As per Choice Based Semester and Grading System with effect from
Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023-2024)**Mandatory Paper II****Course Title: Java Programming, Introduction to Linux and Machine Learning****Paper Code: GNKPSBI2502****Credits: 04****No. of Lectures:****Marks: 100****Learning Objectives:**

- Gain knowledge about basic Java language syntax and semantics to write Java programs and use concepts such as variables, conditional and iterative execution methods etc.
- Understand the fundamentals of object-oriented programming in Java, including defining classes, objects, invoking methods etc. and exception handling mechanisms.
- Understand the principles of inheritance, packages and interfaces.
- Machine Learning is broad and fast growing sub-field of Artificial Intelligence.
- This course introduces students to the basic concepts and techniques of Machine Learning.
- The objective of this course is to develop the skills required for Machine Learning Technologies with use of Python to analyze data, create beautiful visualizations, and problem solving using powerful machine learning algorithms.

Learning Outcomes:

- Identify classes, objects, members of a class and relationships among them needed for a specific problem.
- Have a good understanding of the fundamental issues and challenges of machine learning: data, model selection, model complexity, etc.
- Appreciate the underlying mathematical relationships within and across Machine Learning algorithms and the paradigms of supervised and un-supervised learning.
- Be able to design and implement various machine learning algorithms in a range of real-world applications.
- Application of Biological data using ML.
- Implementation & Evaluation of various machine learning algorithms

Unit		Title	No. of lectures
Unit 1		Core Java and Advanced Java	
	1.1	An introduction to Object-Oriented Programming	
	1.2	Object-oriented programming and Java	
	1.3	Introduction to Java basics	
	1.4	Objects, Arrays, Conditionals and Loops	
	1.5	Creating Classes and Applications in Java, methods	
	1.6	Managing Simple Events and Interactivity	15

	1.7	Creating User Interfaces with AWT	
	1.8	Packages and Interfaces	
	1.9	Exception	
Unit 2	JDBC		
	2.1	Introduction to JDBC	
	2.2	Client Server Application	
	2.3	Java Drivers: Type 1 Drivers, Type 2 Drivers, Type 3 Drivers, Type 4 Drivers	
	2.4	Difference Between Java Drivers	
	2.5	Executing SQL Statements	
	2.6	Programs on Open a JDBC connection to connect database, create a table using JDBC	
	2.7	Insert values using JDBC, retrieve data using JDBC, Close a JDBC connection	
Unit 3	Introduction to Linux and Basic Linux commands		
	3.1	History and design	
	3.2	Principles of Linux	
	3.3	Functions of Linux OS	
	3.4	Basic shell commands	
	3.5	Understanding Linux file permissions	
	3.6	Basic script building and File creation in Linux	
Unit 4	Introduction to Machine Learning in Bioinformatics		
	4.1	Introduction	
	4.2	Importance of machine learning	
	4.3	Types of machine learning	
	4.4	Supervised Learning	
	4.5	Unsupervised learning	
	4.6	Semi supervised learning	

Semester II Evaluation Pattern

Internal: 25

External: 75

M.Sc. Bioinformatics (2023-2024)

Mandatory Paper II - Practical

Course Title: Java Programming, Introduction to Linux and Machine Learning

Paper Code: GNKPSBI2P502

Credits: 02

Marks: 50

1. Programs on Classes and Constructors, Destructor
 - a. Create a class and functions
 - b. Create a class and constructor to allocate memory
 - c. Create destructor to deallocate the memory
2. Programs on Inheritance and Polymorphism:
 - a. Implement Single Inheritance
 - b. Implement Multiple Inheritance
 - c. Implement Multilevel Inheritance
 - d. Implement Hierarchical Inheritance
 - e. Create Runtime Polymorphism
 - f. Create Compile Time Polymorphism
3. Arrays and Loops and Conditional Statement
 - a. Create and access 1-D array
 - b. Create and access 2-D array
 - c. Implement while loop
 - d. Implement do-while loop
 - e. Implement for loop
 - f. Implement if conditional statement
 - g. Implement if-else conditional statement
 - h. Implement Nested if-else conditional statement
4. Create AWT components on:
 - a. Frame
 - b. Button
 - c. Text Field
 - d. Checkbox
 - e. Radio Button

5. Create SWING components on:
 - a. jFrame
 - b. JButton
 - c. JTextField
 - d. JCheckbox
 - e. JRadio Button
 - f. JOptionPane
6. Create programs on packages
7. JDBC
 - a. Open a JDBC connection
 - b. Create a table using JDBC
 - c. Insert values using JDBC
 - d. Retrieve data using JDBC
 - e. Close a JDBC connection
8. LINUX Commands
 - a. Demonstration of Linux installment
 - b. Understand the working of UNIX, UNIX file system
 - c. Basic UNIX commands
 - File System Commands
 - ls and ls with options
 - d. Study of Commands:
 - tr, head, tail, wc, sort
 - find, file, ,split
 - e. Comparing files: od, cmp, comm, diff, uniq
 - f. Filter Commands: Grep, egrep, fgrep

References:

1. Java: The Complete Reference (English, Schildt Herbert).
 2. Core and Advanced Java, Black Book, Recommended by CDAC, Revised and Upgraded Kindle Edition
 3. Fundamentals of Linux: Explore the essentials of the Linux command line Kindle Edition
 4. Practical Guide to Linux Commands Editor, by Mark G. Sobell.
 5. Breiman, Leo, Friedman, J. H., Olshen, R. A. and Stone, C. J. (1984).
 6. Classification and regression trees. Monterey, CA: Wadsworth and Brooks/Cole Advanced Books and Software.
-



Shiromani Gurdwara Parbandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce
(Autonomous)
Matunga, Mumbai – 400 019, Maharashtra

Syllabus for M.Sc. Semester II

Program: Master of Science

Course: Bioinformatics

ELECTIVE PAPER

**(As per Choice Based Semester and Grading System with effect from
Academic Year 2023-2024)**

M.Sc. Bioinformatics (2023- 2024)

Elective Paper

Course Title: Genomics & Proteomics in Bioinformatics, NGS

Paper Code: GNKPSBI3502

Credits: 03

No. of Lectures: 45

Marks: 100

Learning Objectives:

- To study prokaryotic and eukaryotic genomes, general methods of genome sequencing techniques, genome analysis and annotations, genome mapping techniques and applications of genomics.
- To understand the proteins enclosed by the genes with respect to structure, function, protein – protein interactions, techniques for separation and analysis, database and applications.
- Thorough knowledge of basic concepts underpinning Bioinformatics & NGS Data
- Define whole genome sequencing.
- Knowledge and skill in NGS Data Analytics
- Appreciate and explore the comparative genomics databases.
- Recognize various algorithms used for comparisons of full genome and gene order.
- Know the concepts of SNPs and their significance.
- Realize and appreciate the proteomics concepts and technology.

Learning Outcomes:

- Appreciate the importance of full genome comparisons and helps in further research studies.
- Genome mapping solves the complicated puzzle of genes with pieces of information coming from laboratories all over the world and helps to detect the functions of the genes.
- Helps of proteomics studies may lead to better treatments in future.
- Understand the different platforms for first and second-generation sequencing
- Understand the advantage and disadvantage of different types of first and second generation sequencing
- Understand the different platforms for third generation sequencing.
- Understand the different types of high throughput sequencing.
- Understand the library preparation methods for different types of high throughput sequencing.
- Understand the types of sequencing methods used in different platforms
- Understand the different file formats used in NGS data analysis
- Understand the different sources of publicly available NGS datasets and how to retrieve them
-

Unit		Title	No. of lectures
Unit 1		Genomics & Proteomics	15
	1.1	Introduction to Genomics & Proteomics, Need, scope and challenges, Applications	
	1.2	Prediction of Introns, Exons and its identification tools, Open Reading Frame (ORFs)	
	1.3	Predictions of genes, promoters, splice sites, regulatory regions: basic principles, application of methods to prokaryotic and eukaryotic genomes and interpretation of results. (Synteny and gene order) Mutations and diseases	
	1.4	Identification of disease genes using OMIM database (Case study), Microarray studies, reference genome sequence, integrated genomic maps, gene expression profiling	
	1.5	Orphan GPCRs, Identification of Orphan GPCRs, Reverse Pharmacology, Reverse Pharmacology for Orphan GPCRs, Deorphanisation	
	1.6	Protein Identification with antibodies, protein sequence determination by chemical degradation/ Edman's degradation, Short-gun proteomics for proteome profile	
	1.7	Computational tools- advanced tools for data analysis at ExPasy, INTERPRO and other equilavant tools	
Unit 2		History & evolution of sequencing	15
	2.1	GENE prediction & Genome Alignments: BLAST2GO, MUMmer, Pip Maker, VISTA, Comparison of Gene Order Comparative Genomics Databases: COG, VirGen, CORG, Single Nucleotide Polymorphism, dbSNP and other SNP-related databases	
	2.2	History & evolution of sequencing: First-generation technologies – Sanger dideoxy sequencing, Maxam-Gilbert sequencing. Technologies used in Human Genome Project. Shotgun sequencing. Advantages and disadvantages of first generation sequencing. Next (second)-generation sequencing – difference between first and next generation sequencing, NGS platforms – Roche 454, ABI SOLiD, Ion torrent, Illumina. Advantages and disadvantages of second generation sequencing.	

	2.3	Third-generation sequencing: PacBio, Oxford nanopore. Advantages and disadvantages of third generation sequencing. Comparison of output, accuracy and types of errors of first, second and third generation sequencing technologies. Introduction to NGS technologies: DNA-seq, RNA-seq, ChIP-seq, Hi-C, Metagenomics, Single cell sequencing.
Unit 3		Data Analysis in Genomics and Transcriptomics
	3.1	Preparation for sequencing: Different sample preparation methods for different type of NGS (DNASEq, RNASeq, ChIPSeq, Metagenomics, Single cell), Adaptors, Index, Barcode. Library preparation methods - Bridge amplification, Emulsion PCR. Sequencing methods – sequencing by synthesis, ion semiconductor, SMRT, nanopore.
	3.2	Data formats & Pre-processing: Data formats overview – FASTQ, subreads, nanopore data, single cell data. Single-end, Paired-end, Mate-pair. NGS Data sources – NCBI , SRA, EBI-ENA, DDBJ-SRA, GEO; Retrieving data from data sources - SRA toolkit; Aspera connect. Sequence quality measures – Phred quality score. Quality check – tool – FASTQC, Pre-processing: Trimmomatic, Fastx-toolkit.
	3.3	Introduction to NGS Data Analysis: Assembly (overview) -principles, output file formats – contigs, scaffolds, assembly quality assessment – N50, total length, no. of contigs/scaffolds; Mapping (overview) – Principles, tools – BWA, Bowtie, SAMtools, output file formats – BAM, SAM, mapping alignment assessment – no. of reads mapped, concordant reads; Visualizations tools – IGV.

15

Semester II Evaluation Pattern

Internal: 25

External: 75

M.Sc. Bioinformatics (2023-2024)

Elective Paper Practical

Course Title: Genomics & Proteomics in Bioinformatics, NGS

Paper Code: GNKPSBI3P502

Credits: 01

Marks: 50

1. Detection of general signals, regulatory regions and promoter prediction (Minimum 5)
2. Microarray Studies: GEO database
3. GPCR Database
4. EST Database
5. Functional annotation and analysis of genome-scale sequence: BLAST2GO
6. SNP Database: DbSNP & identification of mutational genes
7. Whole Genome Sequencing:
 - a. MUMmer
 - b. Pipmaker
 - c. VISTA
8. Identification of repetitive elements: Repeat Masker Tool
9. NGS:
 - a. Working with NGS databases and file formats
 - b. Variant calling and filtering using BCF tools
 - c. SAMtools
 - d. FASTQC
 - e. Cutadapt & Trimmomatic
 - f. Reference genome mapping and alignment using BWA /bowtie
 - g. De Novo assembly using velvet/spades
 - h. Determining quality of the assembly using Quast tool
 - i. Metagenomics
 - j. Prokka
 - k. Visualize Insertions/deletion

References:

1. Sándor Suhai, Genomics and Proteomics: Functional and Computational Aspects, Kluwer Academic Publishers, 2002
2. Azuaje F & Dopazo J. 2005. Data Analysis and Visualization in Genomics and Proteomics. John Wiley & Sons.
3. Akay M. (Ed) Genomics and Proteomics Engineering in Medicine and Biology 2007 WileyInterscience John Wiley & sons, Inc. Publication, USA
4. "Microbial Genomics And Proteomics" by Niyaz Ahmed
5. Christendat D, et al. Structural proteomics of an archeon. Nat. Struct. Biol. 2000;7(10):903–909. [PubMed]
6. Discovering Genomics, Proteomics and Bioinformatics 2nd edition - by A. Malcolm Campbell and Laurie J. Heyer. by Cold Spring Harbor Laboratory Press 2006.
7. Principles of Genome Analysis and Genomics (3rd Ed.) by Primrose, S.B. and Twyman, R.M., Blackwell Publishing Company, Oxford, UK. 2003
8. Introduction to Proteomics – Tools for the new biology (1st Ed.) by Liebler, D.C., Humana Press Inc., New Jersey, USA. 2002
9. Bioinformatics and Functional Genomics by Pevsner, J., John Wiley and Sons, New Jersey, USA. 2003
10. Bioinformatics: Sequence and Genome Analysis by Mount, D., Cold Spring Harbor Laboratory Press, New York. 2004

Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
MATUNGA, MUMBAI-400019

MOTTO

Essence of Wisdom is Service to Humanity

VISION

To emerge as a Centre of Excellence in Higher Education.

MISSION

To create strong analytical minds with scientific temper, fostering global competencies through the spirit of humanism thereby bringing about holistic development of the students

by remaining in sync with the teachings of Guru Nanak Dev Ji.

QUALITY POLICY

To attain excellence in all our endeavours namely teaching, research and continuing education; adopt self-evaluation as a measure for continuous improvement and ensure accountability.

Based on the provided motto, vision, mission, and quality policy, program outcomes for a Science program of our college are:

Postgraduate Science Program Outcomes:

PO1	Advanced Understanding: Attain an advanced understanding of specialized scientific areas and theories, building upon undergraduate knowledge.
PO2	Advanced Analytical Skills: Develop advanced analytical and problem-solving skills for complex scientific issues.
PO3	Research Proficiency: Acquire proficiency in scientific research, contributing significantly to the advancement of knowledge.
PO4	Leadership Skills: Develop leadership skills to lead scientific initiatives and contribute to the scientific community.
PO5	Interdisciplinary Collaboration: Collaborate effectively with interdisciplinary teams for comprehensive scientific solutions.
PO6	Innovation and Creativity: Foster innovation and creativity in scientific research and practice.
PO7	Professionalism: Demonstrate professionalism and excellence in all scientific endeavours.
PO8	Quality Improvement: Embrace self-evaluation and continuous improvement for achieving excellence in scientific pursuits.

Programme Specific Outcomes (PSOs) for MSc in Bioinformatics

Sr. No.	A student completing M.Sc. in Bioinformatics will be able to:
PSO 1	Impart a thorough understanding of all the essential ideas, apply the knowledge, skills, and resources in biology, information technology, bioinformatics, and soft skill development.
PSO 2	Gain knowledge and demonstrate the working of various instruments used in the pharma, biopharmaceuticals and bioinformatics industry for research activities and on job training.
PSO 3	Ideate and apply entrepreneurial and IPR skills for innovations in pharma and biopharma industries.
PSO 4	Develop strong communication and interpersonal skills, with the ability to work effectively in a team.
PSO 5	Acquire research and development positions in the various fields of bioinformatics and competent employment positions in allied fields. Also, be equipped for competitive exams in the field.
PSO 6	Exhibit proficiency in NGS technologies, Drug Discovery, QSAR, Immunoinformatic, Machine Learning, Clinical Trials, IT and Biostatistics as a stepping stone in comprehending industry demands and hype surrounding big data analysis.

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester III and IV

(Major paper- I/II/Elective)

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Program Structure
Semester-III

Course Code	Course Name	Teaching Hours		Credits Assigned		
		Theory	Practical	Theory	Practical	Total
GNKPSBIMJ1503	Biophysical techniques, IPR, Cheminformatics & Combinatorial chemistry (Major Paper-I)	60	60	4	2	6
GNKPSBIMJ2503	PYTHON Programming language and Machine learning in bioinformatics (Major Paper-II)	60	60	4	2	6
GNKPSBIEL1503	Immunoinformatic & Drug Designing (Elective Paper)	45	30	3	1	4
GNKPSBIRP503	Research project (RP)	--	--	--	--	4
Total		165	150	11	05	20

Semester-IV

Course Code	Course Name	Teaching Hours		Credits Assigned		
		Theor y	Practica l	Theory	Practica l	Total
GNKPSBIMJ1504	Drug Discovery, Clinical trial & Mass Spectrometry (Major Paper-I)	60	60	4	2	6
GNKPSBIMJ2504	PERL and R programming language for bioinformatics (Major Paper-II)	60	60	4	2	6
GNKPSBIEL1504	Molecular Docking, Simulation & QSAR (Elective Paper)	45	30	3	1	4
GNKPSBIRP504	Research project (RP)	--	--	--	--	4
Total		165	150	11	05	20

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester III

(Major paper- I)

**Name of the paper: Biophysical techniques, IPR, Cheminformatics &
Combinatorial chemistry
(GNKPSBIMJ1503)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Bioinformatics

Course: MSc-II Bioinformatics

Semester-III Major Paper- I

Course Title: Biophysical techniques, IPR, Cheminformatics & Combinatorial Chemistry

Course Code: GNKPSBIMJ1503

Credits: 4

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	To recognize the importance of IPR and to educate the pupils on basic concepts of Intellectual Property Rights.
2	To learn the procedure of obtaining Patents, Copyrights, Trade Marks & Industrial Design
3	To understand the principles of physical sciences that form the basis of the techniques and instrumentation used in the research field.
4	The main objective of this course is to give the students a thorough understanding of biophysical techniques used in industry.
5	Emphasize the significance of chemical libraries.
6	Understanding the principles of cheminformatics, including the use of computational methods to analyze and interpret chemical data.
7	Learning how to use software tools and databases for chemical structure representation, searching, and analysis.
8	Exploring the applications of cheminformatics in drug discovery, materials science, and other fields.
9	Understanding the principles of combinatorial chemistry, including the synthesis of large libraries of diverse chemical compounds.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Analyze and interpret the statutory provisions of different forms of IPRs in simple forms	1, 2, 6, 7	3	U, Ap. R, E, C
CO 2	Apply Filing of patent, Copyrights, Trademarks and Industrial Design	1, 2, 6, 7	3	U, Ap. R, E, C
CO 3	Understand various analytical methods and the workings of various microscopy techniques	1, 2, 3, 4	1, 2	U, Ap. An, R, E
CO 4	Explain the basic principles of separation methods such as chromatography, electrophoresis and centrifugation; identify core areas of application of these techniques in experiments and projects and analyse and troubleshoot the results obtained.	1, 2, 3, 4	1, 2	U, Ap. An, R, E
CO 5	Analyze and interpret chemical data using computational methods and software tools.	2, 9	1, 5, 6	U, R, E, C
CO 6	Capability to create effective visual representations of models and datasets.	2, 9	1, 5, 6	U, R, E, C
CO 7	Apply high-throughput screening techniques to evaluate the biological activity of combinatorial libraries	2, 9	1, 5, 6	U, R, E, C
CO 8	Utilize molecular modeling techniques such as molecular docking and QSAR analysis to predict chemical properties and biological activities.	2, 9	1, 5, 6	U, R, E, C

Unit		Title	No. of lectures	CO Mapping
Unit 1		Patinformatics	15	
	1.1	Introduction to IPR & its type		CO 1
	1.2	Patent & Types of Patent Application		CO 1
	1.3	Patent prosecution		CO 1
	1.4	IPR: Patents and reading the patent		CO 1
	1.5	Copyrights		CO 2
	1.6	Trademarks		CO 2
	1.7	TRIPS Agreement		CO 2
	1.8	Patinformatics		CO 2
	1.9	Patent Mapping		CO 2
	1.10	Patent Landscape Analysis & Reporting		CO 2
	1.11	Patent databases		CO 2
Unit 2		Biophysical techniques - I	15	
	2.1	Properties of electromagnetic radiation		CO 3 & CO 4
	2.2	Wavelength and Energy		CO 3 & CO 4
	2.3	The Interaction of Light with Matter		CO 3 & CO 4
	2.4	The Beer-Lambert Law		CO 3 & CO 4
	2.5	Types of Spectroscopy		CO 3 & CO 4
	2.6	UV-vis Spectrophotometer		CO 3 & CO 4
	2.7	Turbidimetry and Nephelometry		CO 3 & CO 4
	2.8	X-ray spectroscopy		CO 3 & CO 4
	2.9	Infrared and Raman Spectroscopy		CO 3 & CO 4
	2.10	Nuclear Magnetic Resonance Spectroscopy		CO 3 & CO 4
	2.11	Microscopic techniques		CO 3 & CO 4
Unit 3		Biophysical techniques - 2	15	
	3.1	Liquid chromatography		CO 3 & CO 4
	3.2	Thin layer chromatography and HPTLC		CO 3 & CO 4
	3.3	High Performance Liquid Chromatography		CO 3 & CO 4
	3.4	Adsorption chromatography		CO 3 & CO 4
	3.5	Partition chromatography		CO 3 & CO 4
	3.6	Affinity chromatography		CO 3 & CO 4
	3.7	Ion-exchange chromatography		CO 3 & CO 4
	3.8	Gas chromatography		CO 3 & CO 4
	3.9	Centrifugation techniques: Principal, type of centrifuge and application.		CO 3 & CO 4
	3.10	Electrophoresis: AGE and PAGE		CO 3 & CO 4
	3.11	2-D electrophoresis		CO 3 & CO 4
	3.12	Isoelectric focusing		CO 3 & CO 4
Unit 4		Introduction to Cheminformatics & Combinatorial Chemistry	15	
	4.1	Representation and manipulation of Molecular		CO 5 & Co 6

		structures (2D and 3D)		
	4.2	Substructure searching		CO 5 &Co 6
	4.3	Conformational Search and analysis		CO 6 & CO 7
	4.4	3D Pharmacophore generation		CO 6 & CO 7
	4.5	Diverse and focused libraries		CO 7 & CO 8
	4.6	Library enumeration		CO 7 & CO 8
	4.7	Library design strategies		CO 6 & CO 8
	4.8	Product-based library design		CO 6 & CO 8

References:

1. Bunin Barry A. Siegel Brian, Morales Guillermo, Bajorath Jürgen. Chemoinformatics Theory, Practice, & Products Publisher: New York, Springer. 2006. ISBN: 1402050003.
2. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: WileyVCH; 1st edition. 2003. ISBN: 3527306811.
3. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic , 2003. ISBN: 1402013477.
4. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge(4 Volumes), 2003. Publisher: Wiley-VCH. ISBN:3527306803.
5. Bunin BA. 2006. Chemoinformatics: Theory, Practice and Products. Springer Gasteiger J & Engel T. 2003. Chemoinformatics: A Textbook. Wiley-VCH. HinchliffeA. 2003.

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics

Semester-III Major I Practical

Course Title: Biophysical techniques, IPR, Cheminformatics & Combinatorial chemistry (Major Practical Paper- I)

Course Code: GNKPSBIMJ1P503

Credits: 02

No of Practical (Hours): 60

Marks: 75 M

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	To study working principle and application of various analytical instruments.
2	To separate phytochemicals using HPTLC, HPLC and GC.
3	Teach students how to analyze structure-activity relationships in chemical datasets to identify key structural features influencing biological activity.
4	Students will understand various software/ tools and databases commonly used in chemoinformatics, such as ChemDraw, RDKit, Open Babel, PubChem, and ChEMBL.
5	Familiarize students with different methods of representing chemical structures including SMILES notation, molecular graphs, and 3D coordinates.
6	Students will understand how to visualize chemical data effectively using techniques such as 2D and 3D molecular rendering, scatter plots, histograms, and heatmaps.
7	Present case studies illustrating the practical applications of chemoinformatics in drug discovery, materials science, and other fields. Encourage students to critically evaluate the strengths and limitations of different chemoinformatics approaches.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Use the technique of HPTLC, HPLC and GC to identify phytochemicals.	1,2,3	1,2	U, R, An, E, C
CO 2	Use the technique of infrared spectroscopy to establish which functional groups are present in an unknown organic molecule.	1,2,3	1,2	U, R, An, E, C
CO 3	Students should demonstrate proficiency in using software tools and databases commonly employed in chemoinformatics, including but not limited to ChemDraw, RDKit, Open Babel, PubChem, and ChEMBL.	1,2,3,8	1,5,6	U, R, E, C

CO 4	Students should be able to effectively retrieve chemical data from public databases, store it in appropriate formats, and manage large datasets efficiently.	1,2,3,8	1,5,6	U, R, E, C
CO 5	Students should be able to represent chemical structures using various methods, including SMILES notation, molecular graphs, and 3D coordinates, and understand the significance of each representation.	1,2,3,8	1,5,6	U, R, E, C
CO 6	Students should be able to calculate molecular descriptors and fingerprints accurately and understand their importance in chemical similarity searching and QSAR modeling.	1,2,3,8	1,5,6	U, R, E, C
CO 7	Students should be able to apply methods for measuring chemical similarity and diversity, such as Tanimoto coefficient, Euclidean distance, and PCA, to analyze and interpret compound datasets	1,2,3,8	1,5,6	U, R, E, C
CO 8	Students should demonstrate the ability to critically evaluate chemoinformatics approaches, assess their strengths and limitations, and apply appropriate methods to solve real-world chemical problems.	1,2,3,8	1,5,6	U, R, E, C

List of Experiments:

1. HPTLC separation of modern drug from its formulation (e.g. Diclofenac sodium)
2. HPLC separation of modern drug from its formulation (e.g. Diclofenac sodium)
3. Gas Chromatographic separation of volatile sample.
4. IR analysis of a modern drug (e.g. Diclofenac Sodium)
5. Importance of 3D structures and method of generation from 1D & 2D representations.
6. Drawing, edit and manipulating 2D and 3D structures and understanding various file formats to represent molecular structures (To be restricted to small molecules) along with Substructure/Exact/similar structure-based searching & filters based on physicochemical property
7. Chemical structure representation and storage in special file formats (Any 4)
8. Generating and analyzing conformations using different methods.
9. Generation and validation of 3D Pharmacophore and selective best Pharmacophore map.

References:

1. Bunin Barry A. Siegel Brian, Morales Guillermo, Bajorath Jürgen. **Chemoinformatics: Theory, Practice, & Products**. Publisher: New York, Springer. 2006. ISBN: 1402050003.

2. Gasteiger Johann, Engel Thomas. Chemoinformatics: A Textbook. Publisher: WileyVCH; 1st edition. 2003. ISBN: 3527306811.
 3. Leach Andrew R., Valerie J. Gillet. An introduction to chemoinformatics. Publisher: Kluwer academic , 2003. ISBN: 1402013477.
 4. Gasteiger Johann, Handbook of Chemoinformatics: From Data to Knowledge (4 Volumes), 2003. Publisher: Wiley-VCH. ISBN:3527306803.
 5. Bunin BA. 2006. Chemoinformatics: Theory, Practice and Products. Springer Gasteiger J & Engel T. 2003. Chemoinformatics: A Textbook. Wiley-VCH. HinchliffeA. 2003.
 6. Molecular Modelling for Beginners. John Wiley & Sons. Leach AR. 1996. Molecular Modelling: Principles and Applications. Longman.
 7. F.K. Brown (1998). "Chapter 35. Chemoinformatics: What is it and How does it Impact Drug Discovery". Annual Reports in Med. Chem. 33: 375.doi:10.1016/S0065- 7743(08)61100-8.
 8. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer, Anamaya Publishers, 2008.
-

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester III

(Major paper- II)

**Name of the paper: PYTHON Programming language and Machine
learning in bioinformatics
(GNKPSBIMJ2503)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Bioinformatics

Course: M.Sc. II Bioinformatics

Semester-III Major II Paper- II

Course Title: PYTHON PROGRAMMING LANGUAGE AND MACHINE LEARNING IN BIOINFORMATICS

Course Code: GNKPSBIMJ2503

Credits: 4

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Become familiar with Python's fundamentals, including ways to develop simple applications
2	Understand the underlying concepts employed in currently used Machine Learning and Biopython applications.
3	Acquire the skill of Python programming.
4	Acquire the basic skills of machine learning.
5	Discover generalized patterns that cover a large proportion of how Python code is used in bioinformatics
6	Learn how to use Python modules for pattern matching, structured text processing, online data retrieval, and database access
7	Learn how to apply the principles and techniques of object-oriented programming

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Analyze the syntax and semantics of diverse coding elements of a Python program	2, 9	1,6	U, R, E, C
CO 2	Select an appropriate problem-solving algorithm for a given bioinformatic problem	2, 9	1,6	U, R, E, C
CO 3	Select an appropriate data structure to store and efficiently manipulate Biological data	2, 9	1,6	U, R, E, C

CO 4	Construct regex patterns for Biological data	2, 9	1,6	U, R, E, C
CO 5	Extract patterns and replace strings with regex Evaluate the rationale behind these problem-solving algorithms	2, 9	1,6	U, R, E, C
CO 6	Implement problem-solving algorithms efficiently using regex	2, 9	1,6	U, R, E, C
CO 7	Select an appropriate problem-solving algorithm using Biopython	2, 9	1,6	U, R, E, C
CO 8	Evaluate published research that employs algorithmic problem-solving strategies using Biopython	2, 9	1,6	U, R, E, C
CO 9	Use and analyse an appropriate problem-solving algorithm using Biopython	2, 9	1,6	U, R, E, C
CO 10	Characterize the machine learning algorithms as supervised learning and unsupervised learning and apply the various algorithms of supervised and unsupervised learning	2, 9	1,6	U, R, E, C
CO 11	Analyze the concept of neural networks for learning linear and non-linear activation functions	2, 9	1,6	U, R, E, C
CO 12	Implement and apply Numpy package	2, 9	1,6	U, R, E, C

Unit		Title	No. of lectures	CO Mapping
Unit 1		Introduction to Python and OOPs Concept	15	
	1.1	Basic of python commands		CO 1
	1.2	Numbers and other data types, Expressions and Operators		CO 1
	1.3	Decisions and Loops, List, Tuples and Dictionary		CO 2
	1.4	String Functions		CO 2
	1.5	Functions		CO 3
	1.6	Object-Oriented Programming		CO 3
Unit 2		Regular Expression and Pattern Matching	15	
	2.1	Introduction to Regular expressions		CO 4
	2.2	RegEx Module, RegEx Functions		CO 5
	2.3	Metacharacters		CO 5
	2.4	Special Sequences		CO 6
	2.5	Split and Join function		CO 6
Unit 3		Biopython	15	
	3.1	Introduction		CO 7
	3.2	Working with sequences		CO 7
	3.3	Sequence objects		CO 8
	3.4	Sequence annotation objects		CO 8
	3.5	Sequence Input/ Output		CO 9
	3.6	BLAST and other sequence search tools		CO 9
	3.7	Entrez Database,PDB Module, Motif Objects		CO 9
	3.8	Genome Analysis, ,Plotting		CO 9
	3.9	How Biopython helps in ML		CO 9
Unit 4		Machine Learning using Numpy	15	
	4.1	Installing and Importing NumPy		CO 10
	4.2	What is NumPy, What is Array, Types of Array What is Dimension, Exploring-Row Before Column Why?		CO 11
	4.3	Creating an Array from a Tuple, creating a Zero-Dimensional Array, Avoiding Errors of "Multiple Arguments", Creating a 1-D Array, creating a 2-D Array, creating a 3-D Array, Understanding NumPy Data Type, Forcing a Data Type of an Array		CO 12
	4.4	Important Statistics Functions in NumPy		CO 12
	4.5	Machine learning applications in number theory and Time Series Analysis		CO 12
	4.6	Use of Other Libraries like Pandas, Tensorflow, Scikit-Learn, Scipy etc.		CO 12

References:

1. Mark Lutz, David Ascher (2003) Learning Python. O'Reilly & Associates
2. Alan Gauld (2000) Learn To program Using Python Addison –Wesley
3. AlexMartelli (2003) Python in a Nutshell, O'Reilly
4. Python - The Complete Reference (English, Brown Martin C.)
5. Python Cookbook, Third edition
6. Python Programming: A modular approach by Pearson
7. Python Data Science Handbook
8. NumPy for Beginners: first Step to learn Data Science

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics

Semester-III Major II Practical

**Course Title: PYTHON Programming language and Machine learning in bioinformatics
(Major Practical Paper- II)**

Course Code: GNKPSBIMJ2P503

Credits: 02

No of Practical (Hours): 60

Marks: 75

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Become familiar with Python's fundamentals, including ways to develop simple applications
2	Understand the underlying concepts employed in currently used Machine Learning and Biopython applications.
3	Acquire the skill of Python programming.
4	Acquire the basic skills of machine learning.

5	Discover generalized patterns that cover a large proportion of how Python code is used in bioinformatics
6	Learn how to use Python modules for pattern matching, structured text processing, online data retrieval, and database access
7	Learn how to apply the principles and techniques of object-oriented programming

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Understand and Apply Basic Python programs to implement the algorithms	2,3,4,5	1,6	U, R, E, C
CO 2	Analyse and write List Python programs to implement the algorithms	2,3,4,5	1,6	U, R, E, C
CO 3	Acquire knowledge on Tuples Array and Loops Python programs to implement the algorithms	2,3,4,5	1,6	U, R, E, C
CO 4	Develop Functions on Python programs	2,3,4,5	1,6	U, R, E, C
CO 5	Apply the various OOPs Python programs to implement the algorithms	2,3,4,5	1,6	U, R, E, C
CO 6	Formulate Regular Expression Python programs	2,3,4,5	1,6	U, R, E, C
CO 7	Implement Biopython Python programs	2,3,4,5	1,6	U, R, E, C
CO 8	Apply NUMPY Python programs to implement the algorithms	2,3,4,5	1,6	U, R, E, C

List of Experiments:

1. Write Basic Python programs to implement the various functions and algorithms
2. Write List Python programs to implement the other methods and algorithms
3. Write Tuples Array and Loops Python programs to implement the algorithms
4. Write Functions Python programs
5. Write OOPs Python programs to implement the algorithms
6. Write Regular Expression Python programs to develop the any methods or algorithms
7. Write Biopython Python programs to implement the algorithms
8. Write NUMPY Python programs to implement the algorithms

References:

1. Mark Lutz, David Ascher (2003) Learning Python. O'Reilly & Associates
2. Alan Gauld (2000) Learn To program Using Python Addison –Wesley
3. AlexMartelli (2003) Python in a Nutshell, O'Reilly
4. Python - The Complete Reference (English, Brown Martin C.)
5. Python Cookbook, Third edition

6. Python Programming: A modular approach by Pearson
 7. Python Data Science Handbook
 8. NumPy for Beginners: first Step to learn Data Science
-

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester III

(Elective Paper)

**Name of the paper: Immunoinformatic & Drug Designing
(GNKPSBIEL1503)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Bioinformatics

Course: M.Sc.II Bioinformatics

Semester-III Elective Paper

Course Title: Immunoinformatics & Drug Designing

Course Code: GNKPSBIEL1503

Credits: 3

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Understanding the fundamentals of immunology and the immune system's response to pathogens and diseases.
2	Learning about bioinformatics tools and techniques used in the analysis of immune system data, including sequence analysis, structural analysis, and modelling.
3	Gaining knowledge of Immunoinformatics databases and resources for accessing and analyzing immunological data.
4	Exploring computational methods for predicting and analyzing immunological epitopes, including T-cell epitopes and B-cell epitopes.
5	Understanding the principles of vaccine design and the use of Immunoinformatics tools in vaccine development.
6	Learning about the role of Immunoinformatics in understanding immune responses to infectious diseases, autoimmune disorders, and cancer.
7	Gaining proficiency in molecular modelling techniques for drug design, including structure-based drug design and ligand-based drug design.
8	Understanding the principles of rational drug design and the use of computational methods to identify potential drug targets and lead compounds.
9	Developing critical thinking and problem-solving skills to apply Immunoinformatics and drug designing principles to address real-world challenges in healthcare and biotechnology.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Analyze immunological data using bioinformatics tools and techniques to identify immunogenic epitopes and understand immune responses to diseases.	1,2,3,8	1,5,6	U, R, E, C
CO 2	Utilize computational methods to predict and analyze T-cell and B-cell epitopes for vaccine design and development.	1,2,3,8	1,5,6	U, R, E, C
CO 3	Apply molecular modeling techniques for rational drug design, including structure-based and ligand-based approaches.	1,2,3,8	1,5,6	U, R, E, C
CO 4	Identify potential drug targets and lead compounds using computational methods and databases.	1,2,3,8	1,5,6	U, R, E, C
CO 5	Demonstrate proficiency in the use of Immunoinformatics and cheminformatics tools for drug discovery and optimization.	1,2,3,8	1,5,6	U, R, E, C
CO 6	Design and evaluate vaccines using Immunoinformatics principles to elicit desired immune responses.	1,2,3,8	1,5,6	U, R, E, C
CO 7	Communicate effectively about Immunoinformatics and drug designing concepts and findings both orally and in writing.	1,2,3,8	1,5,6	U, R, E, C
CO 8	Collaborate with interdisciplinary teams to apply Immunoinformatics and drug designing principles to address healthcare challenges.	1,2,3,8	1,5,6	U, R, E, C
CO 9	Apply problem-solving skills to develop innovative solutions in the fields of immunology, drug discovery, and vaccine development.	1,2,3,8	1,5,6	U, R, E, C

Unit		Title	No. of lectures	CO Mapping
Unit 1		Introduction to Immune systems, Antibodies, Receptors and MHC	15	
	1.1	Innate and adaptive immunity in vertebrates Infectious diseases & Contemporary challenges		CO 1
	1.2	Categories of vaccines & Autoimmune diseases		CO 1
	1.3	Immunoglobulin classes and subclasses		CO 2
	1.4	Antigen processing and presentation		CO 2
	1.5	CDR and LDR regions and sequence numbering		CO 3
	1.6	Humanization of antibodies by design, Immunogenetics & immunogenomics		CO 3

		Hybridoma technology: applications		
	1.7	The B-cell surface receptor for antigen (BCR)		CO 6
	1.8	The T-cell surface receptor for antigen (TCR)		CO 7
	1.9	The major histocompatibility complex (MHC), MHC polymorphism , Causes of MHC polymorphism, MHC supertypes		CO 6
	1.10	Epitopes: Affinity Maturation , Recognition of Antigen by B cells, Neutralizing Antibody		CO 7
Unit 2		Immunoinformatics and Vaccinology	15	
	2.1	Overview of Immunoinformatics		CO 4
	2.2	Reverse vaccinology		CO 5
	2.3	Rational Vaccine design		CO 5
	2.4	Databases & tools: IMGT & IEDB, BciPep, Epitome, CED, Ag-Ab.		CO 6
	2.5	Molecular interactions, Specificity and characterization		CO 6
	2.6	Ag-Ab: Sequential and conformational epitopes,		CO 6
	2.7	MHC- peptide designing tool		CO 7
	2.8	T cell, B cell epitope prediction tool		CO 7
Unit 3		Introduction to Molecular descriptors & molecular similarities	15	
	3.1	2D atomic descriptors		CO 7
	3.2	3D Molecular descriptor		CO 7
	3.3	Similarities based on 2D fingerprints		CO 8
	3.4	Similarities based on 3D structure		CO 8

References:

1. OleLund, "ImmunologicalBioinformatics", MITpress, September 2005. 2. DarrenFlower, "InSilicolmmunology", Springer,2006.
2. Darren R Flower, "Immunoinformatics: Predicting Immunogenicity in Silico", HumanaPress,2007. 2. Rammensee, "Immunoinformatics- Bioinformatics Strategies for Better Understanding of Immune Function", Wiley,2003.
3. Text book of Immunology by Kuby, 2008
4. Text book of Immunology by Riott, 2006
5. Essential of Immunology by Roit
6. Immunology by Nandini Shetty
7. W. E. Paul; Fundamental Immunology, Raven Press
8. Immunoinformatics: A Brief Review by Namrata Tomar and Rajat K. De
9. Indian Patent Act as amended by Act No 15 April 2015
10. Brennan, M. Chem. Eng. News 2000, 78 (27), 4–5
11. Diamond v Chakrabarty, 447 U.S. 303 (1980).

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics**Semester-III Elective Paper****Practical****Course Title: Immunoinformatics & Drug Designing****Course Code: GNKPSBIEL1P503****Credits: 01****No of Practical (Hours): 30****Marks: 50****Course Objectives:**

Sr. No.	Course objectives
The course aims at:	
1	Introduce students to bioinformatics tools and databases for analyzing immunological data, including sequence analysis tools, epitope prediction algorithms, and protein structure prediction software.
2	Teach students how to perform sequence alignment and phylogenetic analysis to study evolutionary relationships among immune-related genes and proteins.
3	Guide students through the analysis of immunological data, including interpretation of experimental results, statistical analysis, and presentation of findings.
4	Teach students how to calculate molecular descriptors using software packages such as RDKit, ChemAxon, and Dragon, and guide them in selecting relevant descriptors for specific chemical compounds.
5	Provide hands-on experience in molecular docking and molecular dynamics simulations to study protein-protein interactions and predict protein structures relevant to immunology.
6	Familiarize students with immunoinformatics databases and resources, such as ImmPort, IEDB, and VDJdb, and teach them how to retrieve and analyze immunological data from these repositories.
7	Train students in visualizing and interpreting immunoinformatics data using software tools such as PyMOL, Chimera, and R, and guide them in generating meaningful insights from complex datasets.
8	Explain the concept of molecular descriptors and their importance in quantitative structure-activity relationship (QSAR) modeling and chemoinformatics.

9	Guide students in analyzing structure-activity relationships in chemical datasets using molecular descriptors, and interpreting the relationship between chemical structure and biological activity.
---	------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Students will gain proficiency in using bioinformatics tools and databases for analyzing immunological data, including sequence analysis tools, epitope prediction algorithms, and protein structure prediction software.	1,2,8	1,5,6	U, R, E, C
CO 2	Students will learn how to design peptide vaccines by predicting antigenic epitopes, selecting appropriate immunogenic regions, and optimizing vaccine constructs.	1,2,8	1,5,6	U, R, E, C
CO 3	Students will gain an understanding of molecular docking techniques and their applications in studying protein-protein interactions relevant to immunology.	1,2,8	1,5,6	U, R, E, C
CO 4	Students will demonstrate proficiency in calculating molecular descriptors using software tools, and understand the significance of different descriptors in describing chemical compounds.	1,2,8	1,5,6	U, R, E, C
CO 5	Students will gain the ability to analyze structure-activity relationships in chemical datasets using molecular descriptors, and interpret the relationship between chemical structure and biological activity.	1,2,8	1,5,6	U, R, E, C
CO 6	Students will learn methods for dimensionality reduction and feature selection in molecular descriptor space, and apply these techniques to select informative descriptors for QSAR modeling.	1,2,8	1,5,6	U, R, E, C

List of Experiments:

1. Browsing and searching sequence & structure databases to retrieve data for Immunoglobulin: sequence and structure
2. Study of Antibody sequence and structure: Antibody numbering: Kabat & Chothia methods
3. Visualization of structure & mapping CDRs on structure
4. Study of variable and constant domains, Drawing topology diagram
5. Study of Ag-Ab interactions epitopes (Any Tool working/Demo)
6. Prediction of conformational epitopes (Any Tool working /Demo)

7. Prediction of cytotoxic and helper T cell epitopes: MHC Class I epitopes and MHC Class II epitopes.
8. Web-based tools for vaccine design (Any Tool working/Demo)
9. Generating and understanding various molecular descriptors and their significance with the chemical properties.

References:

1. OleLund, "Immunological Bioinformatics", MITpress, September 2005.
 2. DarrenFlower, "InSilicoimmunology", Springer, 2006.
 3. Darren R Flower, "Immunoinformatics: Predicting Immunogenicity in Silico",
 3. Ranganathan, S., & Schönbach, C. (Eds.). (2014). Immunoinformatics (Vol. 1184). Springer.
 4. Flower, D. R. (Ed.). (2007). Bioinformatics for immunomics (Vol. 323). Springer.
 5. Schönbach, C., Ranganathan, S., & Brusic, V. (Eds.). (2015). Immunoinformatics: Predicting immunogenicity in silico (2nd ed.). Springer.
 6. Text book of Immunology by Kuby, 2008
 7. Text book of Immunology by Riott, 2006
 8. Essential of Immunology by Roit
 9. Immunology by Nandini Shetty
 10. W. E. Paul; Fundamental Immunology, Raven Press
 11. Immunoinformatics: A Brief Review by Namrata Tomar and Rajat K. De
 12. Todeschini, R., & Consonni, V. (2009). Molecular descriptors for chemoinformatics (Vol. 41). Wiley.
 13. Gasteiger, J., & Engel, T. (2003). Chemoinformatics: A textbook. Wiley-VCH.
 14. Todeschini, R., & Consonni, V. (2000). Handbook of molecular descriptors (Vol. 11). Wiley-VCH
-

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester IV

(Major paper- I)

**Name of the paper: Drug Discovery, Clinical trial & Mass Spectrometry
(GNKPSBIMJ1504)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Chemistry

Course: M.Sc. II Bioinformatics

Semester-IV Major Paper- I

Course Title: Drug Discovery, Clinical trial & Mass Spectrometry

Course Code: GNKPSBIMJ1504

Credits: 4

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Understand the basic concepts and current advances in fields of Mass Spectrometry.
2	Gain Knowledge on Instrumentation Techniques like MS, GC-MS, SFC-MS, ICP-MS, MS-MS and MALDI-TOF
3	Learners will be able to explain key concepts in the design of clinical trials
4	Learners will be able to identify key issues in data management for clinical trials and describe the roles of Regulatory Affairs in clinical trials
5	Gain proficiency in interpreting molecular structures, including small molecules and biological macromolecules such as proteins, nucleic acids, and lipids.
6	Gain an overview of the drug discovery pipeline, including target identification, lead discovery, lead optimization, preclinical development, clinical trials, and regulatory approval.
7	Learn about different types of drug targets, including proteins, nucleic acids, and cell receptors, and understand their role in disease pathology.
8	Understand the principles of rational drug design and learn about different approaches, including structure-based drug design, ligand-based drug design, and phenotypic screening.
9	Gain an overview of the drug discovery pipeline, including target identification, lead discovery, lead optimization, preclinical development, clinical trials, and regulatory approval.
10	Learn about different types of drug targets, including proteins, nucleic acids, and cell receptors, and understand their role in disease pathology.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Acquire mass spectra using several common mass spectrometry platforms and Interpret high resolution mass spectra for chemical formula determination.	1, 2, 3, 4	1, 2	U, Ap. An, R, E
CO 2	Learners will be able to apply Instrumentation Techniques like MS,GC-MS,SFC-MS,ICP-MS, MS-MS and MALDI-TOF on Industrial Aspects.	1, 2, 3, 4	1, 2	U, Ap. An, R, E
CO 3	Learners will be able to apply the principles of clinical trial design, such as using frameworks to create research questions, establish study objectives, effectively communicate trial findings through an understanding of reporting methods, ethical considerations, and regulatory bodies	4, 7, 8, 14	1,2,6	U, Ap. An, R, E
CO 4	Learner will be able to abridge the stages, strategies, ethics and regulations involved in human clinical trials citing appropriate case studies; write and analyze reports related to clinical trial	4, 7, 8, 14	1,2,6	U, Ap. An, R, E
CO 5	Learners can apply molecular docking techniques to predict the binding modes and affinities of small molecules to protein targets, aiding in the identification of potential drug candidates.	1,2,5,8	1,5,6	U, R, E, C
CO 6	Comprehensive Understanding: Demonstrate a thorough understanding of the drug discovery and development process, including the various stages involved, from target identification to regulatory approval.	1,2,5,8	1,5,6	U, R, E, C
CO 7	Critical Thinking and Problem-Solving: Apply critical thinking skills to analyze complex problems and challenges encountered in drug discovery and development, and propose innovative solutions.	1,2,5,8	1,5,6	U, R, E, C
CO 8	Knowledge of Drug Targets: Identify and characterize potential drug targets implicated in various diseases, and evaluate their suitability for drug intervention based on biological and molecular principles.	1,2,5,8	1,5,6	U, R, E, C

CO 9	Learners can apply molecular docking techniques to predict the binding modes and affinities of small molecules to protein targets, aiding in the identification of potential drug candidates.	1,2,5,8	1,5,6	U, R, E, C
------	-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	---------	-------	------------

Unit		Title	No. of lectures	CO Mapping
Unit 1		Introduction to Mass spectrometry basic & Hyphenated systems	15	
	1.1	Mass spectrometry		CO 1
	1.2	Components: ion sources, analyzers, detectors, vacuum system		CO 1
	1.3	Application of MS		CO 1
	1.4	Recent advances in field of MS		CO 1
	1.5	Gas chromatography – mass spectrometry (GC_MS)		CO 2
	1.6	High performance liquid chromatography – mass spectrometry		CO 2
	1.7	Supercritical fluid chromatography – mass spectroscopy (SFC-MS)		CO 2
	1.8	Tandem mass spectrometry (MS-MS)		CO 2
	1.9	Inductively coupled plasma – mass spectrometry (ICP-MS)		CO 2
	1.10	MALDI-TOF		CO 2
Unit 2		Introduction to Clinical Research	15	
	2.1	Introduction to Clinical Research		CO 3
	2.2	Terminologies and definition in Clinical Research		CO 3
	2.3	Origin and History of Clinical Research		CO 3
	2.4	Difference between Clinical Research & Clinical Practice		CO 3
	2.5	Types of Clinical Research		CO 3
	2.6	Phases of clinical research		CO 3
	2.7	Clinical Trials in India –The National Perspective		CO 3
	2.8	Post marketing surveillance		CO 3
	2.9	Pharmaceutical Industry – Global and Indian Perspective		CO 3
	2.10	Clinical Trial market		CO 3
	2.11	Career in Clinical Research		CO 3
Unit 3		Regulation in Clinical Research & Data Management	15	
	3.1	Introduction of Clinical Trial Regulation		CO 3

	3.2	European Medicine Agency		CO 3
	3.3	Food and Drug Administration (US FDA)		CO 3
	3.4	Drug and cosmetic act, Schedule Y		CO 3
	3.5	ICMR Guideline		CO 3
	3.6	Project Management, Protocol in Clinical Research, Informed Consent		CO 4
	3.7	Case Report Form : Investigator's Brochure (IB), Selection of an Investigator and Site , Clinical Trial Stakeholders, Contract Research Organization (CRO), Site management organizations (SMO)		CO 4
	3.8	Introduction to CDM: CRF Design , Clinical Data Entry, Electronic Data Capture , Data Validation, Discrepancy Management, Clinical Data Coding, SAE Reconciliation, Quality Assurance & clinical Data Management, Guideline & Regulation in Clinical trial data		CO 4
Unit 4	Drug Discovery and Development		15	
	4.1	Overview of drug discovery, Properties of a drug like molecule, structure based and ligand-based drug design., Introduction to Pharmacology, concept of drugs and various sources of drugs.		CO 5
	4.2	Routes of Drug Administration and Formulations		CO 6
		Introduction to Pharmacokinetics and Pharmacodynamics (ADME) and Toxicity, CYP-450 class of enzymes and drug metabolism.		CO 7
	4.3	Various Pharmacological models for evaluation of drug efficacy and potency (in vitro, in vivo and ex vivo models)		CO 7
	4.4	Evolutionary Classification of the strategies for Drug Discovery		CO 8
	4.5	Basics of Drug Discovery & Development		CO 8
	4.6	Introduction to Drug Discovery and Development: Target identification and validation, Hit identification, Hit-to-lead and lead optimization		CO 9
	4.7	Emerging technologies in Drug Discovery: High throughput and High-content screening		CO 9
	4.8	Regulatory affairs & Hurdles in Drug Development		CO 9

References:

1. W.M.A Niessen, Chromatography – LCMS 2nd and 3rd edition
2. J Mendham, R C Denney, J D Barnes, M J K Thomas, Vogel's Textbook of Quantitative chemical Analysis 6th edition
3. Misra R.P., 1989, Research Methodology: A Handbook, New Delhi, Concept Publishing Company
4. Kumar, R., 2005, Research Methodology - A Step-by-Step Guide for Beginners,(2nd.ed.), Singapore, Pearson Education.
5. Bhattacharya, D.K., 2006, Research Methodology,(2nd.ed.),New Delhi, Excel Books.
6. Panneerselvam R., 2012, Research Methodology, New Delhi, PHI Learning Pvt. Ltd.

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics

Semester-IV Major Paper I Practical

Course Title: Drug Discovery, Clinical trial & Mass Spectrometry (Practical Major Paper- I)

Course Code: GNKPSBIMJ1P504

Credits: 02

No of Practical (Hours): 60

Marks: 75

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	The fundamentals of mass spectrometry, working of in MS instrument and their importance in structural elucidation will be highlighted
2	Learners will be given case studies related to Clinical Data Management
3	Familiarize students with the drug discovery pipeline, including target identification, lead discovery, lead optimization, preclinical testing, and clinical trials.
4	Teach students how to identify and validate potential drug targets using bioinformatics tools, databases, and experimental techniques such as target validation assays.

5	Provide hands-on experience in HTS techniques for screening large compound libraries against drug targets, including assay development, compound screening, hit confirmation, and hit-to-lead optimization
6	Introduce students to molecular modeling techniques, including molecular docking, molecular dynamics simulations, and pharmacophore modeling, and guide them in performing virtual screening to identify potential lead compounds.
7	Provide an overview of FBDD principles and techniques, and guide students in fragment screening, hit identification, and fragment optimization to develop lead compounds with improved binding affinity and selectivity.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Use the techniques of mass spectrometry and elemental analysis to calculate the molecular mass of unknown organic molecules.	1, 2, 3, 8	1,2	U, R, E, C
CO 2	Write and analyze reports related to Clinical Data Management	1, 2, 3, 8	1,6	U, R, E, C
CO 3	Students will demonstrate proficiency in a range of drug discovery techniques, including target identification, high-throughput screening, molecular modeling, lead optimization, and ADME-Tox profiling	1,2,6,8	1,5,6	U, R, E, C
CO 4	Students will gain a comprehensive understanding of the drug discovery process, from target identification and lead discovery to preclinical testing and clinical trials, and appreciate the interdisciplinary nature of drug discovery research	1,2,6,8	1,5,6	U, R, E, C
CO 5	Students will be able to identify and validate potential drug targets using bioinformatics tools, databases, and experimental assays, and assess the therapeutic potential of target candidates.	1,2,6,8	1,2,5,6	U, R, E, C
CO 6	Students will be able to effectively communicate their research findings, collaborate with interdisciplinary teams, and present drug discovery projects in written reports and oral presentations.	1,2,6,8	1,4,5,6	U, R, E, C

List of Experiments:

1. Demonstration and interpretation of LC/MS/MS quantitation of a modern drug (e.g. Diclofenac Sodium).
2. Case study on Clinical Data Management

3. R&D, Quality Assurance in a Pharmaceuticals/Biopharmaceuticals/Biotechnology/food/beverage industry – Field visit and report
4. Target fishing and optimization using computational methods.
5. PK predictions using Swiss ADME
6. Pharmacological models using appropriate software's /tools.
7. Understanding and Optimizing hits and leads.
8. High throughput virtual screening techniques for drug discovery.

References:

1. W.M.A Niessen, Chromatography – LCMS 2nd and 3rd edition
 2. J Mendham, R C Denney, J D Barnes, M J K Thomas, Vogel's Textbook of Quantitative chemical Analysis 6th edition
 3. Misra R.P., 1989, Research Methodology: A Handbook, New Delhi, Concept Publishing Company
 4. Kumar, R., 2005, Research Methodology - A Step-by-Step Guide for Beginners,(2nd.ed.), Singapore, Pearson Education.
 5. Bhattacharya, D.K., 2006, Research Methodology,(2nd.ed.),New Delhi, Excel Books.
 6. Panneerselvam R., 2012, Research Methodology, New Delhi, PHI Learning Pvt. Ltd.
-

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester IV

(Major paper- II)

**Name of the paper: PERL and R programming language for bioinformatics
(GNKPSBIMJ2504)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Bioinformatics

Course: M.Sc. II Bioinformatics

Semester-IV Major Paper- II

Course Title: PERL AND R PROGRAMMING LANGUAGE FOR BIOINFORMATICS

Course Code: GNKPSBIMJ2504

Credits: 4

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Develop efficient algorithms for solving a problem
2	Use the various constructs of a perl programming language viz. conditional, iteration and recursion
3	Implement the algorithms in ‘perl’ language using Biopython
4	Use simple data structures like arrays and dictionary in solving problems
5	Handling File in ‘perl’ and regex.
6	Learn the Fundamentals of R in Bioinformatics
7	Analyse and Implement of Bioconductor, ggplot2.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Analyse the syntax and semantics of diverse coding elements of a Perl program	1,2,3,5,8	1,6	U, R, E, C
CO 2	Select an appropriate data structure to store and efficiently manipulate Biological data	1,2,3,5,8	1,6	U, R, E, C
CO 3	Construct file handling for Biological data	1,2,3,5,8	1,5,6	U, R, E, C
CO 4	Extract patterns and replace strings with regex	1,2,3,5,8	1,6	U, R, E, C
CO 5	Select an appropriate problem-solving algorithm using Bioperl	1,2,3,5,8	1,6	U, R, E, C
CO 6	Use and analyse an appropriate problem-solving algorithm using Bioperl	1,2,3,5,8	1,6	U, R, E, C

CO 7	Analyse the syntax and semantics of diverse coding elements of a R program	1,2,3,5,8	1,6	U, R, E, C
CO 8	Develop skills on R data frames and factors	1,2,3,5,8	1,6	U, R, E, C
CO 9	Construct Bioconductor	1,2,3,5,8	1,6	U, R, E, C
CO 10	Extract data from spreadsheets	1,2,3,5,8	1,5,6	U, R, E, C
CO 11	Implement ggplot, Shiny and dplyr Library	1,2,3,5,8	1,6	U, R, E, C

Unit		Title	No. of lectures	CO Mapping
Unit 1		Introduction to Perl, File handling and Object-oriented Perl	15	
	1.1	Introduction: What is Perl? Why use Perl in Bioinformatics? History of Perl, Availability, Support, Basic Concepts		CO 1
	1.2	Scalar Data: What Is Scalar Data?, Numbers, Strings, Scalar Operators, Scalar Variables, Scalar Operators and Functions		CO 2
	1.3	Arrays and List Data: What Is a List or Array? Literal Representation, Variables, Array Operators and Functions, Scalar and List Context		CO 3
	1.4	Control Structures: Statement Blocks, basic I/O		CO 1
	1.5	Hashes, Hash Variables, Literal Representation of a Hash, using Hashes		CO 2
	1.6	Subroutines, System and User Functions, The local Operator, Object oriented Perl: Introduction to modules, Creating Objects		CO 3
Unit 2		Regular Expression and Database connectivity and Bioperl	15	
	2.1	Concepts of Regular Expressions, Simple Uses of Regular Expressions, metacharacters, quantifiers etc.		CO 4
	2.2	Pattern matching, substitution		CO 5
	2.3	Split and join Functions, Formatting Data, Sorting, Transliteration		CO 6
	2.4	Finding a Substring, Extracting and Replacing a Substring, Variable-length Parameter Lists, Notes on Lexical Variables		CO 4
	2.5	Database Manipulation		CO 5
	2.6	File handles and File Tests, Opening and Closing a File handle, die, Using File handles		CO 6
	2.7	BioPerl: Introduction, Installation procedures, Architecture, Uses of BioPerl		CO 4

Unit 3	Fundamentals of R in Bioinformatics	15	
	3.1 Introducing R and R Studio IDE		CO 7
	3.2 R basics and datatypes		CO 8
	3.3 Factors and Dataframes		CO 9
	3.4 Working with spreadsheets (tabular data), Importing tabular data into R, Summarizing, subsetting, and determining the structure of a data frame.		CO 9
	3.5 Introducing Factors, Plotting and ordering factors, Subsetting data frames		CO 9
	3.6 Advantages of R Programming in bioinformatics		CO 9
	3.7 Tools for R Programming in Bioinformatics		CO 9
Unit 4	Introduction to Bioconductor and ggplot2	15	
	4.1 Installing packages from somewhere else besides CRAN?		CO 10
	4.2 install the BiocManager package and install the vcfR package from Bioconductor using BiocManager		CO 11
	4.3 Introduction to ggplot2, Installing tidyverse, Loading the dataset		CO 12
	4.4 Building your plots iteratively, Faceting, Barplots, Density, ggplot2 themes		CO 12
	4.5 Shiny and dplyr Library and its useful methods		CO 12
	4.6 Applications of R Programming in Bioinformatics		CO 12

References:

1. Beginning Perl for Bioinformatics - O'Reilly Media
2. Perl Cookbook, 2nd Edition by Tom Christiansen, Nathan Torkington
3. Effective Perl Programming by Joseph N. Hall
4. R Programming for Bioinformatics, Robert Gentleman
5. Intro to R and R Studio for Genomics
(URL Link: <https://datacarpentry.org/genomics-r-intro/06-data-visualization.html>)

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics

Semester-IV Practical Major Paper- II

Course Title: PERL AND R PROGRAMMING LANGUAGE FOR BIOINFORMATICS (Practical Major Paper- II)

Course Code: GNKPSBIMJ2P504

Credits: 02

No of Practical (Hours): 60

Marks: 75

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	Become familiar with Perl fundamentals, including ways to develop simple applications
2	Understand the underlying concepts employed in currently used Machine Learning and Biopython applications.
3	Acquire the skill of Perl programming.
4	Acquire the basic skills of machine learning.
5	Discover generalized patterns that cover a large proportion of how Python code is used in bioinformatics
6	Learn how to use Python modules for pattern matching, structured text processing, online data retrieval, and database access
7	Learn how to apply the principles and techniques of object-oriented programming

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Perform scripting on Basic Perl programs	1,2,3,5,8	1,5,6	U, R, E, C
CO 2	Acquire the script on Arrays perl programs	1,2,3,5,8	1,5,6	U, R, E, C
CO 3	Apply the knowledge to script on Hashes and Loops perl programs	1,2,3,5,8	1,5,6	U, R, E, C
CO 4	Implement Functions perl programs to implement the algorithms	1,2,3,5,8	1,5,6	U, R, E, C
CO 5	Solve and work with a OOPs perl programs	1,2,3,5,8	1,5,6	U, R, E, C
CO 6	Analyze Regular Expression perl programs to implement the algorithms	1,2,3,5,8	1,5,6	U, R, E, C
CO 7	To write the Bioperl programs to implement the algorithms	1,2,3,5,8	1,5,6	U, R, E, C
CO 8	Apply Basic R programs to implement the algorithms	1,2,3,5,8	1,5,6	U, R, E, C
CO 9	Implement R programs to Bioconductor and ggplot2	1,2,3,5,8	1,5,6	U, R, E, C

List of Experiments:

1. Write script on Basic Perl programs to implement the algorithms
2. Write script on Arrays Python programs to implement the algorithms
3. Write script on Hashes and Loops Python programs to implement the algorithms
4. Write Functions Python programs to implement the algorithms
5. Write OOPs perl programs to implement the algorithms
6. Write Regular Expression perl programs to implement the algorithms
7. Write Bioperl programs to implement the algorithms
8. Write Basic R programs to implement the algorithms
9. Write R programs to Bioconductor and ggplot2

References:

1. Beginning Perl for Bioinformatics - O'Reilly Media
 2. Perl Cookbook, 2nd Edition by Tom Christiansen, Nathan Torkington
 3. Effective Perl Programming by Joseph N. Hall
 4. R Programming for Bioinformatics, Robert Gentleman
 5. Intro to R and RStudio for Genomics
(URL Link: <https://datacarpentry.org/genomics-r-intro/06-data-visualization.html>)
-

**Shiromani Gurudwara Prabandhak Committee's
Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Matunga, Mumbai – 400 019, Maharashtra**

Program: Master of Science

Syllabus

Course: M.Sc. II Bioinformatics

Semester IV

(Elective paper)

**Name of the paper: Molecular Docking, Simulation & QSAR
(GNKPSBIEL1504)**

(As per NEP guidelines-DSC model)

With effect from Academic Year 2024 - 2025)



Guru Nanak Khalsa College of Arts, Science and Commerce (Autonomous)
Department of Bioinformatics

Course: M.Sc. II Bioinformatics

Semester-IV ELECTIVE PAPER

Course Title: Molecular Docking, Simulation & QSAR

Course Code: GNKPSBIEL1504

Credits: 3

No of lectures (Hours): 60

Marks: 100 (75:25)

Course Objectives:

Sr. No.	Course objectives
The course aims at:	
1	To provide an understanding about the various mechanisms taking place in a biological environment with special emphasis to macromolecules, their structural and thermodynamical properties, a necessity for drug designing.
2	To understand molecular dynamics concepts of temperature, ensemble, and periodic boundaries.
3	Learn to use popular molecular modelling software packages for tasks such as molecular visualization, energy minimization, and molecular dynamics simulations.
4	Understand the principles and applications of molecular docking techniques for predicting the binding modes and affinities of small molecules to protein targets.
5	Understand the principles of molecular dynamics simulations and their applications in studying the dynamic behaviour of biomolecular systems, such as protein-ligand interactions and protein folding.
6	Learn about virtual screening methods for prioritizing compound libraries based on their predicted binding affinities and other properties.
7	Thoughtful the structural properties and energy minimization in folding process
8	To set up free energy calculations.
9	Gain proficiency in interpreting QSAR models, including identifying important molecular features associated with biological activity and assessing the predictive performance of the models.
10	Explore the applications of QSAR in drug discovery and development, including virtual screening, lead optimization, and toxicity prediction.
11	Understand how QSAR techniques can be integrated with molecular modeling approaches, such as molecular docking and molecular dynamics simulations, to enhance the understanding of structure-activity relationships.

12	Appreciate the working and parameters for the software.
13	To understand the modelling of molecules including hard potentials, soft potentials, torsion and bend potential.
14	To provide biophysics knowledge to the students this will pave a way for further excellent application of the concepts.

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	To understand the basic concepts which determine the design and discovery of drugs.	1,2,3,5,8	1,5,6	U, R, E, C
CO 2	To absorb the Bioorganic, medicinal and physico-chemical principles behind the rational designing and mechanism of drugs.	1,2,3,5,8	1,5,6	U, R, E, C
CO 3	Helps to determine the drug stereochemistry in drug design and molecular modeling.	1,2,3,5,8	1,5,6	U, R, E, C
CO 4	Understand how quantum mechanical models can be used to describe chemical reactions and properties.	1,2,3,5,8	1,5,6	U, R, E, C
CO 5	Evaluate the accuracy of performed calculations	1,2,3,5,8	1,5,6	U, R, E, C
CO 6	Explain how quantum mechanics can contribute to the understanding of reaction mechanisms in organic chemistry and catalysis.	1,2,3,5,8	1,5,6	U, R, E, C
CO 7	Understand the theory, concepts and terminology of computational chemistry with an emphasis on electronic structure calculations using the molecular-orbital model.	1,2,3,5,8	1,5,6	U, R, E, C
CO 8	Students can analyze and visualize molecular modeling data, including simulation trajectories and binding free energy calculations, to extract meaningful insights and generate informative figures.	1,2,3,5,8	1,5,6	U, R, E, C
CO 9	Learners understand how molecular modeling and simulation techniques can complement experimental approaches in drug discovery, aiding in the interpretation of experimental data and guiding further experimental studies.	1,2,3,5,8	1,5,6	U, R, E, C

Unit		Title	No. of lectures	CO Mapping
Unit 1		Structure-based drug Design, Molecular Modelling & Simulation	15	CO 1
	1.1	Introduction to Molecular docking, validation and Scoring functions		CO 1
	1.2	Overview of molecular modelling, Molecular modelling:- Introduction, force field, quantum chemistry, Schrödinger equation, potential energy functions. energy minimization, local and global minima, saddle point, grid search		CO 1
	1.3	Overview of Molecular Mechanics, Molecular mechanics:- Definition, balls and springs, force fields, bond-stretching, bond-bending, dihedral motions, out of plane angle potential, non-bonded interaction, coulomb interactions, conformational search, united atoms and cut-offs. Derivative methods: - First-order methods; Steepest descent, conjugate gradient, Second order methods; Newton-Raphson method		CO 2
	1.4	Overview of Molecular Dynamics, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, duration of the MD run		CO 3
	1.5	Various methods for conformation generations for docking.		CO 4
	1.6	Software: GROMACS, PYRX, DS/ Chimera		CO 5
Unit 2		Introductions to QSAR and Machine Learning	15	
	2.1	QSAR- Historical aspects, Hansch analysis and Free-Wilson analysis		CO 5
	2.2	SAR versus QSAR, Designing of QSAR experiment		CO 5
	2.3	QSAR methodology, Deriving QSAR equations (Simple and Multiple linear regressions, Principle component regression, Partial Least squares, and Genetic algorithms)		CO 5
	2.4	Selection of diverse sets (Clustering analysis, dissimilarity-based methods, etc)		
	2.5	Introduction to Machine learning (Neural networks, random forest methods, Support vector machines and other deep learning methods such as PyTorch platform)		CO 6
	2.6	Various aspects of validating results from QSAR and machine learning methods. Special emphasis on applicability domains		CO 7
Unit 3		Types of QSAR	15	
	3.1	Introductions to various types of QSAR		CO 7
	3.2	QSARs and QSPRs		CO 7
	3.3	2D QSAR : Linear free energy relationships descriptors for QSAR - experimental and theoretical, statistical parameters and their significance, correlation coefficient, cross-validated		CO 7

		correlation coefficient, standard error, F-value, boot-strap analysis, randomization		
	3.4	3D-QSAR model- Introduction , History, Methodology		CO 8
	3.5	Comparative Molecular Field Analysis (CoMFA), Comparative Molecular Similarity Index Analysis (CoMSIA), Comparative residue-interaction analysis (CoRIA), COMBINE 3D QSAR, AFMoC, etc		CO 8
	3.6	Brief overview of Higher order QSAR methods (4D to 6D)		CO 7 & Co 8

References:

1. Bunin BA. 2006. Chemoinformatics: Theory, Practice and Products. Springer Gasteiger J & Engel T. 2003. Chemoinformatics: A Textbook. Wiley-VCH. HinchliffeA. 2003.
2. Molecular Modelling for Beginners. John Wiley & Sons. Leach AR. 1996. Molecular Modelling: Principles and Applications. Longman.
3. Bioinformatics : Databases, Tools & Algorithms – Orpita Bosu and Simminder Kaur Thukral (Oxford Higher Education)
4. A Text Book of Bio-informatics - Singhal and Singhal (Pragati Prakashan) Molecular Modelling and drug Design (Leech) Textbook of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor Francis Publication.
5. Molecular Modeling for Beginners: Alan Hincliffe
6. Text Book of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor and Francis Publication.
7. Bioinformatics basic methods and applications – S.C. Rastogi
8. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe, John Wiley & Sons Ltd. 2008 2.
9. Molecular Modeling and Simulation – An interdisciplinary Guide by Tamar Schlick, SpringerVerlag. 2000
10. Textbook of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor Francis Publication.
11. Text Book of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor and Francis Publication
12. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890
13. Computational Chemistry and Molecular Modeling-Principles and Applications by Ramachandran
14. Molecular Modeling and Simulation – An interdisciplinary Guide by Tamar Schlick, SpringerVerlag. 2000

Examination:

- **Internal Examination (25 Marks):** 20 Marks exam (Presentation). And 5 Marks for Class Participation etc.
- **End Semester theory examination (75 Marks):** Weightage of each unit will be proportional to the number of lecture hours as mentioned in the syllabus. Duration of exam: 2hours 30mins
- **Combined passing of 40% with minimum 20% in Internal Component.**

Course: M.Sc. II Bioinformatics**Semester-IV Elective Practical Paper****Course Title: Molecular Docking, Simulation & QSAR (Practical Elective Paper)****Course Code: GNKPSBIEL1P504****Credits: 01****No of Practical (Hours): 30****Marks: 50****Course Objectives:**

Sr. No.	Course objectives
The course aims at:	
1	Understand the principles and algorithms behind molecular docking and familiarize students with different types of docking methods (e.g., rigid docking, flexible docking, induced-fit docking).
2	Gain proficiency in using popular docking software such as AutoDock, AutoDock Vina, PyRx and DOCK. Learn how to prepare protein and ligand structures for docking simulations.
3	Understand the principles of molecular dynamics simulations and their applications in biomolecular systems and learn about force fields, integration algorithms, and simulation protocols used in MD simulations
4	Gain proficiency in using MD simulation software such as GROMACS, AMBER, and NAMD and learn how to set up and run MD simulations for biomolecular systems.
5	Understand the principles of QSAR and its applications in drug design and chemical biology and learn about the concept of molecular descriptors and their role in QSAR modeling.
6	Learn how to build QSAR models using regression techniques, machine learning algorithms, and statistical methods and understand the importance of model validation, cross-validation, and external validation in assessing QSAR model performance.

7	Interpret QSAR models to understand the relationship between chemical structure and biological activity and identify key structural features influencing biological activity and make informed decisions in drug design.
---	--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

Course Outcomes (COs):

Sr. No.	On completing the course, the student will be able to:	POs addressed	PSOs addressed	Cognitive Levels addressed
CO 1	Students will demonstrate proficiency in setting up and running molecular docking simulations using popular software tools and choose appropriate docking methods and parameters for specific ligand-protein systems.	1,2,3,7,8	1,5,6	U, R, E, C
CO 2	Students will be able to interpret docking results, including binding poses, binding energies, and ligand-protein interactions and learn how to identify potential lead compounds based on docking scores and binding affinities.	1,2,3,7,8	1,5,6	U, R, E, C
CO 3	Students will demonstrate proficiency in setting up and running molecular dynamics simulations for biomolecular systems.	1,2,3,7,8	1,5,6	U, R, E, C
CO 4	Students will be able to analyze MD trajectories to extract structural and dynamic information and studies related to protein dynamics, conformational changes, and ligand binding/unbinding events.	1,2,3,7,8	1,5,6	U, R, E, C
CO 5	Students will be able to interpret QSAR models to understand the relationship between chemical structure and biological activity and will gain insights into structure-activity relationships (SAR) and identify key structural features influencing biological activity.	1,2,3,7,8	1,5,6	U, R, E, C
CO 6	Students will develop the ability to critically evaluate QSAR models, assess model reliability, and identify potential limitations and biases.	1,2,3,7,8	1,5,6	U, R, E, C

List of Experiments:

1. Performing Molecular simulation studies in solvent methods using GROMACS.
2. Virtual screening and docking studies using Pubchem (Any Virtual Screening database) PyRx / Autodock Vina
3. Visualization using Discovery studio Visualizer / Chimera
4. Performing QSAR AUTODOCK studies on at least 3 sets (different molecular targets with

at least 50 molecules) and validation of these models (at least 8-10 parameters).

References:

1. Bunin BA. 2006. Chemoinformatics: Theory, Practice and Products. Springer
 - Gasteiger J & Engel T. 2003. Chemoinformatics: A Textbook. Wiley-VCH.
 - HinchliffeA. 2003.
 2. Molecular Modelling for Beginners. John Wiley & Sons. Leach AR. 1996
 3. Molecular Modelling: Principles and Applications. Longman.
 4. Bioinformatics : Databases, Tools & Algorithms – Orpita Bosu and Simminder Kaur Thukral (Oxford Higher Education)
 5. A Text Book of Bio-informatics - Singhal and Singhal (Pragati Prakashan)
Molecular Modelling and drug Design (Leech) Textbook of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor Francis Publication.
 6. Molecular Modeling for Beginners: Alan Hincliffe
 7. Text Book of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor and Francis Publication.
 8. Bioinformatics basic methods and applications – S.C. Rastogi
 9. Molecular Modelling for Beginners, (2nd Edition) by Alan Hinchliffe, John Wiley & Sons Ltd. 2008
 10. Molecular Modeling and Simulation – An interdisciplinary Guide by Tamar Schlick, SpringerVerlag. 2000
 11. Textbook of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor Francis Publication.
 12. Text Book of Drug Design and Discovery (Edited by Povl Krogsgaard – Larsen, Tommy Liljefors and Ulf Madsen) Taylor and Francis Publication
 13. Höltje Hans-Dieter, Sippl Wolfgang, Rognan Didier, Folkers Gerd. Molecular Modeling: Basic Principles and Applications. Publisher: New York, Wiley-VCH. 2003. ISBN: 3527305890
 14. Computational Chemistry and Molecular Modeling-Principles and Applications by Ramachandran
 15. Molecular Modeling and Simulation – An interdisciplinary Guide by Tamar Schlick, SpringerVerlag. 2000
-