Central University of Punjab

M.Sc. Bioinformatics

Session: 2021-2023

Department of Computational Sciences

School of Basic Sciences

Graduate Attributes

In line with the syllabus of M.Sc. Bioinformatics it is expected that a student graduating after successful completion of the course shall be able to understand in various areas of Bioinformatics, basic knowledge in Mathematics, and knowledge in applied fields like Computer Science. Further, they apply the knowledge, general competence, and analytical skills on an advanced level, needed in industry, consultancy, education, research, or public administration. Therefore graduated students of M.Sc. Bioinformatics would be a valuable asset for nation by virtue of his/her scientific abilities. The student can expect gainful employment in academic/research/industry by undertaking this programme.

Course Structure of the Programme

SEMESTER I							
S. No.	**Course Code**	**Course Title**	**Course Type**				
				L	**T**	**P**	**Cr**
1	LBI.507	Molecular Biology and Methods in Biology	CC	3	0	0	3
2	LBI.511	Sequence Analysis	CC	3	0	0	3
3	LBI.510	Mathematics for Biologists	CC	3	0	0	3
4	PCP.519	Python Programming	CC	3	0	0	3
5	LBI.508	Basics of Biochemistry	CF	3	0	0	3
6	PCP.520	Entrepreneurship	CF	1	0	0	1
Choose any one of these courses/MOOC							
7	LBI.509	Concepts of Genetics	DE	3	0	0	3
8	BOT.554	Evolutionary Biology	DE	3	0	0	3
9	BCH.512	Animal Cell Culture Technology	DE	3	0	0	3
10	ZOL.525	Nanobiology	DE	2	1	0	3
Interdisciplinary course offered from other departments							
12	XXX.XXX	Interdisciplinary Course	IDC	2	0	0	2
Total				**21**	**0**	**0**	**21**

SEMESTER II							
S. No.	**Course Code**	**Course Title**	**Course Type**				
				L	**T**	**P**	**Cr**
1	CCC.554	Fundamentals of Molecular Simulations	CC	3	0	0	3
2	LBI.557	Data Mining and Machine learning	CC	3	0	0	3
3	LBI.576	Computational Genomics and Proteomics	CC	3	0	0	3
4	CCC.525	Computational Methods	CC	3	0	0	3
6	LBI.571	System Biology	CF	3	0	0	3
6	XXX.XXX	Value Added Course	VAC	2	0	0	2
Choose any two of these courses/MOOC							
7	LBI.524	Molecular Evolution	DE	3	0	0	3
8	LBI.526	Biomolecular Structure Modelling and Drug Designing	DE	3	0	0	3
9	ZOL.552	Cancer Biology	DE	3	0	0	3
10	LMM.525	Stem Cell and Regenerative Medicine	DE	3	0	0	3
11	BCH.527	Developmental Biology	DE	3	0	0	3
Total				**23**	**0**	**0**	**23**

SEMESTER III							
S. No.	**Course Code**	**Course Title**	**Course Type**				
				L	**T**	**P**	**Cr**
1	CCC.551	Research Methodology	CC	3	0	0	3
2	LBI.512	Biological Databases and Management Systems	CC	3	0	0	3
3	LBI. 517	Biological Databases and Management Systems Lab (Practical)	SB	0	0	4	2
4	LBI.558	Data Mining and Machine learning Lab (Practical)	SB	0	0	4	2
5	CCC.555	Molecular Simulations Lab (Practical)	SB	0	0	4	2
6	LBI.569	Computational Genomics and Proteomics Lab (Practical)	SB	0	0	4	2
7	LBI.572	Enriching Bioinformatics	DEC	2	0	0	2
8	CCC.528	Computational Methods Lab (Practical)	SB	0	0	4	2
9	LBI.600	Research Proposal	SBE	0	0	8	4
Total				**8**	**0**	**28**	**22**

SEMESTER IV							
S. No.	**Course Code**	**Course Title**	**Course Type**				
1	LBI.600	Dissertation	SBE	0	0	40	20
Total				**0**	**0**	**40**	**20**
Grand Total				**86 Credits**			

L: Lectures; T: Tutorial; P: Practical

MOOCs may be taken upto 40% of the total credits (excluding dissertation credits). MOOC may be taken in lieu of any course but content of that course should match a minimum 70%. Mapping will be done by the department and students will be informed accordingly.

Mode of Transaction: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Evaluation Criteria for Theory Courses

A. Continuous Assessment (Course wise): [25 Marks]
Two or more of the given methods (Surprise Tests, in-depth interview, unstructured interview, Jigsaw method, Think-Pair Share, Students Teams Achievement Division (STAD), Rubrics, portfolios, case based evaluation, video based evaluation, Kahoot, Padlet, Directed paraphrasing, Approximate analogies, one sentence summary, Pro and con grid, student generated questions, case analysis, simulated problem solving, media assisted evaluation, Application cards, Minute paper, open book techniques, classroom assignments, homework assignments, term paper).

B. Mid Semester Test: Based on Subjective Type Test [25 Marks]

C. End Semester Test: Based on Subjective (70%) and Objective (30%) Type Test [50 Marks]

The objective type will include one word answers, fill-in the blank, sentence completion, true/false, MCQs', and matching, analogies. The subjective type will include a very short answer (1-2 lines), short answer (one paragraph), essay type with restricted response, and essay type with extended response.

Core, Discipline Elective, Compulsory Foundation, Value Added and Interdisciplinary Courses			Discipline Enrichment Course		Entrepreneurship Course	
	Marks	Evaluation	Marks	Evaluation	Marks	Evaluation
Internal Assessment	25	Various	-	-	-	-
Mid-semester test (MST)	25	Subjective	50	Objective	25	Objective
End-semester test (EST)	50	Subjective (70%) Objective (30%)	50	Objective	25	Subjective

Evaluation Criteria for Practical Courses:

Evaluation	Marks
Maintaining the lab records/notebooks	10
Continuous assessment	20
Attendance	10
Final practical examination	50
Viva-voce	10

CF: Compulsory Foundation, CC: Core Course, DE: Discipline Elective, DEC: Discipline Enrichment Course, IDE: Inter-Disciplinary Elective, SBC: Skill-based Core, SBE: Skill-based Elective, VAC: Value Added Courses
L: Lecture, T: Tutorial, P: Practical

* Every student has to take 1 IDE (Inter-Disciplinary Elective) course of 2 credits from other disciplines in 1st semester of the program.

ZOL: Department of Zoology
LHG: Department of Human Genetics and Molecular Medicine
BOT: Dept of Botany
SCH: Dept. of Biochemistry

Semester I

Course Title: Molecular Biology and Methods in Biology

L	T	P	Cr
3	0	0	3

Course Code: LBI.507
Total Hours: 45

Learning outcome is to:

- Demonstrate the mechanism of biomolecules to act in a cell or an organism
- Describe the structure and regulation of genes
- Apply and effectively communicate scientific reasoning related to concepts of selecting drug targets
- Demonstrate correlation between genome and transcriptome
- Understand the purpose of the cell's performing transcription and translation.

Course Content

Unit I **11 Hours**

DNA structure, classic experiments, semi-conservative model of DNA replication: Unit of replication, enzymes involved, replication origin and replication fork, leading and lagging strand, fidelity of replication.

Unit II **12 Hours**

RNA synthesis and processing: transcription factors and machinery, formation of initiation complex, transcription activator and repressor, RNA polymerases, capping, elongation, and termination. RNAprocessing, RNAediting, splicing, and polyadenylation

Unit III **12 Hours**

Molecular cloning of DNA or RNA fragments in bacterial and eukaryotic systems. PCR: principal and working concept, in-silico designing of specific and non-specific primers, validation of primers design, troubleshooting with primers.

Unit IV **10 Hours**

The world of Non-Coding RNAs: various types and their respective roles, Antisense transcription and non-coding RNAs.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Jocelyn E Krebs, Elliott S Goldstein, Stephen T Kilpatrick (2012). Lewin's Essential Genes. ISBN: 9781449644796 Edition: 3, Jones & Bartlett

2. EJ Gardner, MJ Simmons and DP Snustad.(1991). Principles of Genetics. ISBN: 9780471504870 Edition: 8, John Wiley & Sons

3. Venki Ramakrishnan, Jennifer A Doudna (2019). Gene Machine:The Race to Decipher the Secrets of the Ribosome. ISBN: 9781786076717. Oneworld Publications

4. Mercadante, A. A., Dimri, M., & Mohiuddin, S. S. (2020). Biochemistry, Replication and Transcription. In *StatPearls*. StatPearls Publishing.

5. Hoerter, J. E., & Ellis, S. R. (2020). Biochemistry, Protein Synthesis. In *StatPearls*. StatPearls Publishing.

Web-resources:

- https://ocw.mit.edu/courses/biology/7-01sc-fundamentals-of-biology-fall-2011/molecular-biology/dna-replication/
- Replication: Mechanism of Replication (Basic), 3-D Animation Library
- Replication: Mechanism of Replication (Advanced), 3-D Animation Library
- Transcription Animation (Basic)

Course Title: Sequence Analysis

L	T	P	Cr
3	0	0	3

Course Code: LBI.511
Total Hours: 45

Learning Outcomes: The outcomes of the subject is to ensure that a student can understand and apply the main algorithms and methods used in

pairwise and multiple alignment
searching of sequence databases
hidden Markov models of biological sequences
finding and discovery of motifs in biological sequences

understand the biological contexts in which to apply biological sequence analysis

Course Content

Unit I **13 Hours**

Basic concepts of sequence similarity, identity and homology, homologues, orthologues, paralogues and xenologues Pairwise sequence alignments: basic concepts of sequence alignment, Needleman and Wunsch, Smith and Waterman algorithms for pairwise alignments, gap penalties

Unit II **10 Hours**

Scoring matrices: basic concept of a scoring matrix, PAM and BLOSUM series, Comparison of PAM and BLOSUM, Tools such as BLAST (various versions of it) and FASTA.

Unit III **12 Hours**

Multiple sequence alignments (MSA): basic concepts of various approaches for MSA (e.g. progressive, hierarchical etc.). Algorithm of CLUSTALW (including interpretation of results), concept of dendrogram and its interpretation.

Unit IV **10 Hours**

Sequence patterns and profiles: Basic concept and definition of sequence patterns, motifs and profiles, profile-based database searches using PSI- BLAST, analysis and interpretation of profile-based searches.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. David W.Mount (2001) Bioinformatics. Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
2. P. A. Pevzner (2004) Computational Molecular Biology. Prentice Hall of India Ltd, ISBN81-203-2550-8
3. D.E.Krane and M.L.Raymer (2003) Fundamental concepts of Bioinformatics. Pearson Education ISBN 81-297-0044-1
4. N.Gautham (2006) Bioinformatics. Narosa publications ISBN-13: 9781842653005
5. Andreas D. Baxevanis, Gary D. Bader, David S. Wishart (2020) Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins 4th Edition.Wiley Publishers, ISBN-10 : 1119335582
6. Yoon, Byung-Jun, Qian, Xiaoning (2021) Recent Advances in Biological Network Analysis. Springer International Publishing, ISBN 978-3-030-57172-6.

Web Resources

1. https://iop.vast.ac.vn/theor/conferences/smp/1st/kaminuma/SWISSPROT/index.html
2. http://ggdc.dsmz.de/

Course Title: Mathematics for Biologists

L	T	P	Cr
3	0	0	3

Course Code: LBI.510
Total Hours: 45

Learning Outcomes: At the end of the course, the students will be able to:

- Identify and describe the basic mathematical techniques that are commonly used by chemists.
- Develop skills in vectors, matrices, differential calculus, integral calculus and probability.
- Apply the principles to a number of simple problems that have analytical solutions.
- Design different methods to problems related to chemistry.

Course Content

Unit I **10 Hours**
Vectors in 2D, 3D and in general, circles, transformation of coordinates, polar coordinates, parametric equations.

Unit II **12 Hours**
Functions, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, partial differentiation.

Unit III **12 Hours**
Addition and multiplication; inverse, adjoint and transpose of matrices, matrix equation, Introduction to vector spaces, matrix eigen values and eigen vectors, diagonalization, determinants.

Unit IV **10 Hours**
Basic rules for integration, integration by parts, partial fraction and substitution, definite integrals, evaluation of definite

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested readings

1. E. Kreyszig (2011) Advanced Engineering Mathematics (Wiley India Pvt.

Ltd., New Delhi, India).
2. L. A. Pipes (1985) Applied Mathematics for Engineers and Physicist (McGraw-Hill, Noida, India).
3. D. G. Zill (2012) Advanced Engineering Mathematics (Jones & Barlett Learning, Massachusetts, USA).
4. P. K. Chattopadhyay (2000) Mathematical Physics (New Age International (P) Ltd., New Delhi).
5. E.Steiner (2008) The chemistry Mathematics Book,, Oxford University Press.
6. F. Daniels (1959) Mathematical for Physical Chemistry : Mc. Graw Hill.
7. D.M. Hirst, Longman (1979) Chemical Mathematics .
8. Tebbutt (1994) Basic Mathematics for Chemists, Wiley.
9. G. Arfken, H. Weber and F. Harris (2012) Mathematical Methods for Physicists (Elsevier Academic Press, Massachusetts, USA).

Course Code: PCP.519

L	T	P	Cr
3	0	0	3

Course Title: Python Programming
Total Hours: 45

Learning Outcomes: At the end of the course students will be able to explain and learn Python Programming to build applications in their core domain. Python is becoming popular in artificial intelligence and machine learning. MicroPythonis subset of Python Programming useful to port in hardware for embedded and IoT applications.

Course Content

Unit I **12 hours**

Introduction, Data Types and Operators: Installation and working with Python, Variables and data types in python, Perform computations and create logical statements using Python's operators: Arithmetic, Assignment, Comparison, Logical, Membership, Identity, Bitwise operators, list, tuple and string operations

Unit II **11 hours**

Python Decision making and Loops: Write conditional statements using If statement, if ...else statement, elif statement and Boolean expressions, While loop, For loop, Nested Loop, Infinite loop, Break statement, Continue statement, Pass statement, Use for and while loops along with useful built-in functions to iterate

over and manipulate lists, sets, and dictionaries. Plotting data, Programs using decision making and loops

Unit III **11 hours**

Python Functions and Modules: Defining custom functions, Organising Python codes using functions, Create and reference variables using the appropriate scope, Basic skills for working with lists, tuples, work with dates and times, get started with dictionaries, Importing own module as well as external modules, Programming using functions, modules and external packages

Unit IV **11 hours**

Python File Operations: An introduction to file I/O, use text files, use CSV files, use binary files, Handle a single exception, handle multiple exceptions, Illustrative programs.

Transaction Mode: Lecture, tutorial, problem solving

Suggested Readings

1. Gowrishankar S, Veena A, (2018). **"**Introduction to Python Programming", 1st Edition, CRC Press/Taylor & Francis.
2. Jake VanderPlas, (2016). **"**Python Data Science Handbook: Essential Tools for Working with Data", 1st Edition, O'Reilly Media.
3. Aurelien Geron, (2019). "Hands-On Machine Learning with Scikit-Learn and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems", 2nd Edition, O'Reilly Media.
4. Wesley J Chun, (2015). "Core Python Applications Programming", 3rd Edition, Pearson Education India.

Course Title: Basics of Biochemistry

L	T	P	Cr
3	0	0	3

Course Code: LBI.508
Total Hours: 45

Learning Outcomes: The outcomes of the subject is to ensure that a student comprehends the following:

a) The structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles.

b) The energy metabolism by cellular components in cells and the process of mitotic cell division.

c) Influences of changes or losses in cell function; including the responses to environmental or physiological changes, or alterations of cell function brought about by mutation.

Course Content

Unit I **12 Hours**

Principles of biophysical chemistry Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.

Unit II **12 Hours**

Carbohydrates and Glycobiology: Monosaccharides: types, characteristics and properties; disaccharides, oligosaccharides, polysaccharides. Cabohydrate metabolism: Central pathways of carbohydrate metabolism – regulatory mechanisms, bioenergetics and significance.Gluconeogenesis from TCA intermediates / amino acids / acetyl-CoA. Lipids: Classification, structure, properties; biological significance. Lipid metabolism: Catabolism: Oxidation of fatty acids. Anabolism: Biosynthesis of fatty acids, Biosynthesis of triglycerides, phospholipids, sterols

Unit III **11 Hours**

Composition, structure, function and metabolism of Amino Acids and Nucleotides. Nucleotides and Nucleic Acids: Purine and pyrimidine nucleotides: biosynthesis and its regulation. Deoxyribonucleotides: biosynthesis and regulation. Biosynthesis of nucleotide coenzymes. Catabolism of purine and pyrimidine nucleotides. Amino Acids: Biosynthethic pathways and their regulation. Catabolism of amino acids.

Unit IV **10 Hours**

Enzymology: Classification, Principles of catalysis, Mechanism of enzyme catalysis, Enzyme kinetics, Enzyme regulation, Isozymes.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2019). Biochemistry 9th edition. W.H. Freeman & Company. USA, ISBN: 9781319248062

2. Nelson, D. and Cox, M.M. (2021). Lehninger Principles of Biochemistry. W H Freeman & Co; 8th edition, ISBN-10: 1319228003

3. Ochiai, E. (2010). Bioinorganic chemistry: A survey. Academic Press. Elsevier, India, ISBN: 978-0120887569

4. Shukla AN (2009). Elements of enzymology. Discovery Publishing. New Delhi, India, ISBN-10 : 8183564038

5. Voet, D. and Voet, J.G. (2014). Principles of biochemistry. CBS Publishers & Distributors. New Delhi, India, ISBN-10: 0470570954

Web Resources

1. https://higheredbcs.wiley.com/legacy/college/boyer/0471661791/animations/animations.htm?newwindow=true
2. http://lifescienceinteractive.com/tag/biochemistry-2

Course Code: PCP.520

L	T	P	Cr
1	0	0	1

Course Title: Entrepreneurship

Total Hours: 15

Learning Outcomes: On the completion of this course, students will be able

a. To absorb an entrepreneurial mind-set.

b. To learn what is entrepreneurship and its impact

c. To develop understanding about problems and prospects in entrepreneurship.

d. To gain insights about entrepreneurial behaviour and skills.

e. To develop understanding about writing business plan/project proposals & managing start-up issues.

UNIT I **4 Hours**

Introduction:

- The concept of entrepreneurship, the history of entrepreneurship
- Entrepreneurial Structure; Nature, Characteristics, functions and its role in economic development
- Entrepreneurship- problems and prospects in India

UNIT II **4 Hours**

The Entrepreneur

- Entrepreneurial Behaviour and Skills
- The entrepreneurial decision process
- The skill gap analysis, role models
- The entrepreneurial success stories

Unit III **3 Hours**

E-Cell

- The concept of E-cells
- The significance, and activities conducted by E-cell

- Benefits of Joining E-Cells

Unit IV **4 Hours**

- Role of industries/entrepreneur's associations and self-help groups
- Funding opportunities for start-ups. Basic start-up problems
- Contents of business plan/ project proposal
- Barriers and gateways to communication, the ability of personal selling and negotiation.

Transactional Modes: Videos and quizzes through the on-line LMS; Classroom learning (Videos, In-class Activities); Assignments and Projects; and Practical Experiences including challenges.

Suggested Readings

1. G. K. Varshney, (2012). *Fundamentals of Entrepreneurship*, Sahitya Bhawan Publications, .
2. R. Roy, (2011). *Entrepreneurship*, 2nd Edition, Oxford, .
3. B. K. Mehta, (2018). *Entrepreneurship and Small Business*, SBPD Publishing House.

Course Title: Concepts of Genetics

L	T	P	Cr
3	0	0	3

Course Code: LBI.509
Total Hours: 45

Learning Outcomes: At the end of the course, the students will be able to:

a) Comprehensive understanding of the chemical basis of **heredity.**

b) Comprehensive and detailed understanding of genetic methodology and how quantification of heritable traits in families and populations provides insight into cellular and molecular mechanisms.

Course Content

Unit I **12 Hours**

Introduction and scope of genetics, DNA as genetic material: Double helical structure, Structure of DNA and RNA, Different types of DNA molecules, forces stabilizing nucleic acid structure, super coiled DNA, properties of DNA, denaturation and renaturation of DNA and Cot curves. DNA replication: Basic mechanism of DNA replication.

Unit II **13 Hours**

Cell division and Cell cycle: Mitosis, Meiosis Concepts of Linkage analysis and gene mapping: Coupling and repulsion phase linkage, Crossing over and recombination. Population genetics: Application of Mendel's laws to populations, Hardy-Weinberg principle, inbreeding depression and heterosis, inheritance of quantitative traits.

Unit III **10 Hours**

Gene Interaction: Sex determination and Sex linked inheritance, Sex determination in humans, *Drosophila* and other animals, Sex determination in plants, Sex linked genes and dosage compensation.

Unit IV **10 Hours**

Chloroplast and Mitochondrial inheritance, Yeast, *Chlamydomonas/Neurospora* Chromosomal aberrations: Types of changes– deletions, duplications, inversions, translocations,Change in chromosome number: trisomy and polyploidy.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Reading

1. Anthony, J.F., Miller, J.A. ,Suzuki, D.T., Richard, R.C., Gilbert, W.M. (2020). An introduction to Genetic Analysis 12th edition. W.H. Freeman publication, USA, ISBN:9781319401399
2. Atherly, A.G., Girton, J.R., Mcdonald, J.F. (1999). The science of Genetics. Saundern College publication, ISBN-10 : 0756782554
3. Snusted, D.P., Simmons, M. J. (2010). Principles of Genetics. John Wiley & Sons, New York, ISBN-10 : 1118129210
4. Klug, W.S., Cummings, M.R., Spencer, C. A., Palladino M.A. (2019) Concepts of Genetics Eleventh Edition. Pearson Education India, ISBN-10 : 9353940400
5. Gupta, P.K. (2009). Genetics. Rastogi publications, Meerut, India, ISBN: ISBN-10 : 8193775708
6. Gupta, P.K (2008). Cytology, Genetics and Evolution. Rastogi publications, Meerut, India, ISBN-10 : 9350781360
7. Jocelyn, E.K., Elliott, S.G., Stephen, T.K. (2018). Lewin's Genes X. Jones & Bartlett Publishers, USA, ISBN: 9781284104493
8. Schaum, W.D. (2000). Theory & problems in Genetics by Stansfield, outline series McGrahill, USA, ISBN-10 : 0071369155

Web Resources

1. http://www.bio-alive.com/animations/genetics.htm
2. http://highered.mheducation.com/sites/0072835125/student_view0/animations.html

SEMESTER II

Course Title: Fundamentals of Molecular Simulations

L	T	P	Cr
3	0	0	3

Paper Code: CCC.554

Total Lectures: 45

Learning Outcomes: At the end of the course, the students will be able to:

- learn the modelling of small to large molecular environments
- understand various force field for biomolecular simulation in details
- learn different methods for simulating large systems
- gain the knowledge about different molecular simulation techniques
- understand the dynamics of the structural transitions

which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

Course Content

Unit I **11 Hours**

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.

Force Fields and Molecular Representation – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic

Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints, (e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?
Example: Protein, Nucleic Acid, Small Molecule Force Field, Water Models.

Unit II **11 Hours**

Methods for Simulating Large Systems

a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists

b) Boundaries – Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary

c) Long-range Interactions – The Ewald Sum, The Reaction Field Method

Unit III **12 Hours**

Energy Minimization and Related Analysis Techniques

(a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum?
Introduction to Equilibrium Statistical Mechanics
(a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles

Unit IV **11 Hours**

Simulation Methods:

Monte Carlo: The Metropolis method

Molecular Dynamics: (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method (f) Pressure Control: Andersen's Method

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. M.P. Allen and D.J. Tildesley (2017). Computer Simulation of Liquids 2nd Edition, Oxford University Press.
2. D. Frenkel and B. Smit (2001). Understanding Molecular Simulation 2nd Edition, Academic Press.
3. A. R. Leach (2001). Molecular Modelling Principles and Applications 2nd Edition. Pearson.
4. S. Alavi (2020). Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH.

Course Title: Data Mining and Machine Learning

L	T	P	Cr
3	0	0	3

Course Code: LBI.557
Total Hours: 45

Learning Outcomes: On completion of the course the student should be able to:

- learn the data cleaning, cross-validation, and application of regression analysis
- gain knowledge about distance matrices, various methods of clustering as well as dimensionality reduction
- apply several techniques for information retrieval and text mining

Course Content

Unit I **10 Hours**

Introduction: Overview of Machine Learning field, terminology alert: true positive, false positive, Confusion matrix, Bias and variance

Unit II **12 Hours**

Unsupervised Methods: Clustering: Distance Metrics, K-Means, leader, Jarvis-Patrick, hierarchical clustering; Dimensionality Reduction: Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Partial Least Squares – Discriminant Analysis (PLS-DA)

Unit III **12 Hours**

Supervised Methods: Classification: k-nearest neighbors algorithm (K-NN), naïve Bayes, decision trees, boosting and bagging, Bonferroni Correction

Unit IV **11 Hours**

Classification: Ensemble methods, random Forests; Support vector machines Neural networks, Recommendation systems; Outlier detection.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Helder I., N. (Ed.). (2021). Bioinformatics. Exon Publications.
2. Alonso-Betanzos, A., & Bolón-Canedo, V. (2018). Big-Data Analysis, Cluster Analysis, and Machine-Learning Approaches. Advances in experimental medicine and biology, 1065, 607–626. https://doi.org/10.1007/978-3-319-77932-4_37
3. Applied Predictive Modeling by Max Kuhn and Kjell Johnson; 2013.
4. An Introduction to Statistical Learning and Applications in R by James, Witten, Hastie, Tibshirani; 2014.
5. Python for Data Analysis by Wes McKinney; 2013
6. Data Mining: Concepts and Techniques, Third Edition by Han, Kamber, and Pei, 2011

Web Resources

https://www.youtube.com/playlist?list=PLblh5JKOoLUICTaGLRoHQDuF_7q2GfuJF
https://www.youtube.com/playlist?list=PLblh5JKOoLUKxzEP5HA2d-Li7IJkHfXSe

Course Title: Computational Genomics and Proteomics

L	T	P	Cr
3	0	0	3

Course Code: LBI.576
Total Lecture: 45

Learning Outcomes: At the end of the course, the students will be able to:

- learn the importance of DNA-Protein Interactions During Transcription
- gain a deep knowledge about the role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling
- apply probabilistic modeling techniques for the building of transcriptional regulatory networks which will help them to use the techniques of computational proteomics in their further potential careers in academia and industry.

Course Content

Unit I **12 Hours**

DNA- Protein interaction: Process of DNA-Protein Interactions During Transcription, Network identification and processing. Protein- Protein Interactions: Processing of the Proteome, Prediction of Post-translational modifications, Protein Degradation.

Unit II **10 Hours**

Role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling; identification of SNPs, Vector Screening

Unit III **12 Hours**

DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), understanding of microarray data, normalizing microarray data, Raw read quality assessment, Mapping data visualization, detecting differential gene expression.

Unit IV **11 Hours**

Building predictive models of transcriptional regulatory networks using probabilistic modeling techniques. Viral Informatics: Virome, Comparative metagenomic analysis using VIROME. Metagenomics

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Sándor Suhai (2002). Genomics and Proteomics. Springer US
2. CAMPBELL (2007). Discovering Genomics, Proteomics and Bioinformatics. Pearson Education
3. Richard P. Grant (2004). Computational Genomics: Theory and Application. Horizon Bioscience
4. Gracia KC, Husi H. (2019) Computational Approaches in Proteomics. Brisbane (AU): Codon Publications, PMID: 31815395.

Web Resources

1. http://virome.dbi.udel.edu

Course Title: Computational Methods

L	T	P	Cr
3	0	0	3

Paper Code: CCC.525

Total Hours: 45

Learning Outcomes: At the end of the course, the students will be able to solve:

- the large scale systems of linear, non-linear and simultaneous equations
- the matrix and determinants, interpolations, polynomial and spline interpolation
- the numerical differentiation and integration
- complex curve fitting methods, explicit schemes to solve differential equations
- the simple optimisation, vectorisation.

After, completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

Course Content

Unit I **11 Hours**

Introduction: Errors, Siccessive Approximation, Taylor's Series, Polynomial Evaluation

Matrix and Determinants: Pivotal Condensation Method, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit II **11 Hours**

System of Linear Algebraic Equations: System of Linear Equations, Guass Elimination Method, Importance of Diagonal Dominance, Gauss Seidel Iteration Method, Matrix Inversion Method: Gauss-Jordan's Matrix-Inversion Method

Unit III **13 Hours**

Interpolations: Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms

Numerical differentiation and integration: Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor's series, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration.

Curve Fit: least square, straight line and polynomial fits.

Unit IV **10 Hours**

Numerical Solution of Differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. V. Rajaraman (1993) Computer Oriented Numerical Methods, PHI.
2. E. Balaguruswamy (2017) Numerical Methods, Tata McGraw Hill.
3. F.Acton (1997) Numerical Methods that Work, Harper and Row, 1997.
4. S. D. Conte and C.D.Boor (2005) Elementary Numerical Analysis, McGraw Hill.
5. S. S. Shastri (2012) Introductory Methods of Numerical Analysis, PHI.

Course Title: Systems Biology

L	T	P	Cr
3	0	0	3

Course Code: LBI.571
Total Hours: 45

Learning Outcomes: At the end of the course, the students will be able to:

- relate the various biological pathways with consensus network motifs and therefore decipher the functioning
- figure out the optimal structure for analyzing deep sequencing data
- understand the main features of biological networks.
- apply mathematical modelling to discuss relevant issues in Biology
- present a research paper in Systems Biology

Course Content

Unit I **11 Hours**

Introduction to system biology, networks, path, degree, cluster coefficient, scale-

free networks and relevance, power law. Transcription networks, basic concepts, elements of Transcription networks, logic input functions,

Unit II **12 Hours**

Lac operon, Auto-regulation, a network motif: patterns, randomized networks and network motif, the feed forward loop (FFL) network motif, Dynamics of CI-FFL, II-FFL with logical gates, Convergent evolution of FFLs.

Unit III **12 Hours**

Temporal programs and the global structure of transcription networks: SIM, Bi-Fans, DORs, Interlocked FFL in B. subtilis sporulation network, Network motifs in developmental, signal-transduction and neuronal networks

Unit IV **10 Hours**

Kinetic proofreading and conformational proofreading, Demand rule for gene regulation, optimal gene circuit design: cost of LacZ protein, fitness function and optimal expression level.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Leonie Ringrose (2017). Epigenetics and Systems Biology.ISBN:9780128030769, Elsevier Science
2. Markus W. Covert (2017).Fundamentals of Systems Biology:From Synthetic Circuits to Whole-cell Models. ISBN:9781498728478, CRC Press
3. Bor-Sen Chen, Cheng-Wei Li (2016). Big Mechanisms in Systems Biology:Big Data Mining, Network Modeling, and Genome-Wide Data Identification. ISBN:9780128097076, Elsevier Science
4. Edda Klipp, Wolfram Liebermeister, Christoph Wierling, Axel Kowald (2016). Systems Biology, A Textbook. ISBN:9783527675661, Wiley
5. Uri Alon (2020). An Introduction to Systems Biology: Design Principles of Biological Circuits. Chapman & Hall, Second Edition, ISBN: 13: 978-1-4398-3717-7
6. Hake, S. and Wilt, F. (2003). Principles of Developmental Biology. W.W. Norton and Company, New York, USA.

Web resources:

lac operon

- The lac operon
  https://www.youtube.com/playlist?list=PLLbr-

B8cNbo6v4kc68JowzUeAYdh6gdQH
https://www.youtube.com/watch?v=9Y55Y_c_KLk

Course Title: Molecular Evolution

L	T	P	Cr
3	0	0	3

Course Code: LBI.524
Total Hours: 45

Learning Outcomes: After completing the course the student should be able to

- describe evolutionary processes that give rise to variation in sequences and genomes and how these influence the architecture of the genome, contents and variation in base composition
- explain and justify different models for sequence and genome evolution
- choose, apply and evaluate bioinformatics methods for studying genetic variation in and between species.

Course Content

Unit I **12 Hours**

Comparison of DNA sequences to calculate gene distance; Convergent and divergent evolution; Mutation Vs. Substitution-Rate of Molecular Evolution. Jukes Cantor Correction and evolutionary distance

Unit II **12 Hours**

Genome evolution, RNA structure and evolution, Compensatory substitutions and the
comparative method, Fitting evolutionary models to sequence data, The influence of thermodynamics on RNA sequence evolution

Unit III **10 Hours**

Molecular clock- Concepts and significance-molecular mechanisms of molecular clock- Neutral theory -gene family organization. Applications of molecular phylogenetics

Unit IV **11 Hours**

Paralogy and Orthology- coordination expression in evolution-genome: content, structure and evolution. Molecular evolution of recently diverged species -

Databases of Molecular evolution.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Darwin, C.R. (1911). On the origin of species by means of natural Selection, or preservation of favoured races in the struggle for life. Hurst Publishers, UK.
2. Dawkins, R. (1996). The Blind Watchmaker, W.W. Norton & Company Jones and Bartlett Publishers.
3. Futuyma, D.J. (2009). Evolution. Sinauer Associates Inc. USA
4. Bromham, L. (2016). An Introduction to Molecular Evolution and phylogenetics. OUP Oxford.
5. Warnow, T.(2019)Bioinformatics and Phylogenetics.Springer International Publishing, ISBN 978-3-030-10836.

Web Resources

1. http://www.bioinf.wits.ac.za/software/fire/evodb/
2. https://www.megasoftware.net/

Course Title: Biomolecular Structure Modelling and Drug Designing

L	T	P	Cr
3	0	0	3

Course Code: LBI.526
Total Hours: 45

Learning Outcomes: On completion of the course the student should be able to:

(a) find relationships between similar kinds of multiple sequences (in msa) and sequence conservation pattern, conserved structural motifs etc.

(b) use different search methods to find compounds with specific properties in large compound databases

(c) explain and make a use of different types of protein–ligand interactions and characterise binding pockets

(d) set up, perform and evaluate different virtual screening methods using large datasets

Course Content

Unit I **10 Hours**

Basics of Biomolecules: Principles of protein and nucleic acid structure: Primary, Secondary, Tertiary structure and Quaternary structure. Protein secondary structure: Introduction, Hydrogen bond, Defining a secondary structure element, Methods for predicting secondary structure

Unit II **12 Hours**

Protein tertiary structure modeling: Basic concepts, Protein folding and Energetics, Comparative modeling, Threading, Ab initio modeling, Modeling protein sidechains, CASP: A blind protein structure prediction competition, CAPRI, Protein Structure Initiative (PSI).

Unit III **12 Hours**

Introduction to drug designing, ADMET, drug metabolism, toxicity and pharmacokinetics. lipinski rule of 5, Identification and validation strategies. Drug Target classification, Concept of Pharmacophore, Functional group considered as pharmacophore, Structure-based drug design, docking, QSAR

Unit IV **11 Hours**

Modelling macromolecular structure: Homology modeling, *ab-initio* structure modeling; Molecular Recognition: Prediction of Protein-ligand interaction sites, Prediction of Protein-protein interaction sites, Prediction of Protein-membrane interaction sites, Prediction of Protein-nucleic acid interaction sites

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Hybrid Biomolecular Modeling. (2019). (n.p.): Frontiers Media SA. ISBN:9782889456994
2. Biomolecular Modelling and Simulations. (2014). United Kingdom: Elsevier Science.ISBN:9780128007891
3. Molecular Modeling of Proteins. (2017). United States: Springer New York. ISBN:9781493954919
4. Biomolecular Simulations in Structure-Based Drug Discovery. (2019). Germany: Wiley. ISBN:9783527342655
5. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo Molecular design : concepts and applications Weinheim: Wiley-VCH, c2008
6. Andrew R.Leach Molecular Modelling Principles and applications. (2001) II ed. Prentice Hall

Web Resources
https://www.uniprot.org/
bioinformatics.org/molvis/phipsi/

Semester III

Course Title: Research Methodology

L	T	P	Cr
3	0	0	3

Course Code: CCC.551

Total Hours: 45

Learning Outcomes: The course Research Methodology has been framed to introduce basic concepts of Research Methods. The course covers preparation of research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, computer laboratory safety issues etc.

Course Content

Unit I **12 hours**

Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion.

Unit II **12 hours**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs). **Entrepreneurship and Business Development:** Importance of entrepreneurship and its relevance in career growth, Types of enterprises and ownership.

Unit III **11 hours**

Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, Technical report writing, Making R and D proposals, Dissertation/Thesis writing, Letter writing and official correspondence, Oral and poster presentation in meetings, Seminars, Group discussions, Use of modern aids; Making technical presentations.

Unit IV **10 hours**

Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies. Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials.

Transaction Mode: Lecture, demonstration, PPT.

Suggested Readings

1. R. Kumar, *Research Methodology*, (2012), SAGE Publications India Pvt. Ltd., New Delhi, India.
2. S. Gupta, *Research Methodology and Statistical techniques*, (2005), Deep and Deep Publications (P) Ltd. New Delhi, India.
C. R. Kothari, *Research Methodology*, (2008) New Age International, New Delhi, India.
4. Standard /Reputed Journal authors' instructions.
5. Web resources: www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
6. Web resources: www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Course Title: Biological Database and Management System

L	T	P	Cr
3	0	0	3

Course Code: LBI.512
Total Lectures: 45

Learning Outcomes: Upon successfully completion of this course, students will be able to

1. apply the concept of RDBMS in understanding the organisation of the biological data in different databases.
2. retrieve the data from different biological databases
3. use principles of DBMS to create novel solutions in bioinformatics.
4. Identify and characterize a data collection, sorting and management problem.
5. Code for an approach to create a Relational DBMS and a non-redundant database.

Course Content

Unit I **8 Hours**

Introduction to Biological Databases: Nucleotide Sequence Databases, GenBank, DDBJ, EMBL, Sequence Flatfile and submission process, Protein sequence

databases, Genomic databases, PDBsum, PDB, SCOP, CATH, Pathway and molecular interaction databases

Unit II **7 Hours**

Database planning and Design concepts General Database Planning and Design – Document or forms – preparation and architexture Entity- Relational ship Model-entities, Attributes, keys, tables design, relationships, roles and dependencies.

Unit III **8 Hours**

Relational DB Introduction to relational DB and transactions. SQL- statements-Data Definition-Manipulation-control-Objects, - Views, sequences and Synonyms. Working with code and forms- Front end development-query sublanguage-modifying relations in SQL.

Unit IV **7 Hours**

Transaction processing, concurrency control and recovery management. Transaction model properties, state serizability, lock base protocols, two phase locking.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Mukesh Negi (2019). Fundamentals of Database Management System:Learn Essential Concepts of Database Systems. ISBN:9789388176620. BPB PUBN publications
2. Chopra Rajiv (2016). Database Management System (DBMS): A Practical Approach, 5th Edition. ISBN:9789385676345. S CHAND & Company Limited publications.
3. Monelli Ayyavaraiah, Arepalli Gopi (2017). Database Management System.ISBN:9789386369703. Horizon Books (A Division of Ignited Minds Edutech P Ltd) publications
4. Date C.J. (2009). Introduction to database management. Vol1, Vol2, Vol3 addison Wesley.
5. Abraham Silberschatz, Henry F.Korth and S.Sudhashan (2005) Database system concepts. 5 Ed McGraw Hill Publications.
6. Elmasri Ramez and Novathe Shamkant (2007). Fundamentals of Database systems. Benjamin Cummings Publishing Company. ISBN-10: 0321369572.

7. P. Ramakrishnan Rao (2003). Database Management system, 3EdMcGraw Hill Publications. 9780071230575

Web Resources

1. https://www.ncbi.nlm.nih.gov/
2. expasy.org
3. https://www.rcsb.org/

Course Title: Biological Database and Management System Lab (Practical)

L	T	P	Cr
0	0	4	2

Course Code: LBI.517
Total Hours: 60

Learning Outcomes: Upon successfully completing this course, students will be able to apply principles of DBMS to create novel solutions in bioinformatics.

a. Identify/characterize/define and solve a data collection, sorting and management problem
b. Design an approach to create a Relational DBMS
c. Create non-redundant databases

Course Content

1. Data Definition,
2. Table Creation,
3. Constraints,
4. Insert,
5. Select Commands,
6. Update & Delete Commands.
7. Nested Queries & Join Queries
8. Views
9. Functions [skip first/last]
10. Reports.

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Mukesh Negi (2019). Fundamentals of Database Management System:Learn Essential Concepts of Database Systems. ISBN:9789388176620. BPB PUBN publications

2. Chopra Rajiv (2016). Database Management System (DBMS): A Practical Approach, 5th Edition. ISBN:9789385676345. S CHAND & Company Limited publications.

3. Monelli Ayyavaraiah, Arepalli Gopi (2017). Database Management System.ISBN:9789386369703. Horizon Books (A Division of Ignited Minds Edutech P Ltd) publications

4. Abraham Silberschatz, Henry F.Korth and S.Sudhashan (2005) Database system concepts. 5 Ed McGraw Hill Publications.

5. Elmasri Ramez and Novathe Shamkant, " Fundamentals of Database systems" (2007) Benjamin Cummings Publishing Company. ISBN-10: 0321369572.

6. P. Ramakrishnan Rao: Database Management system, (2003) 3EdMcGraw Hill Publications. 9780071230575

Web Resources

https://www.ncbi.nlm.nih.gov/
expasy.org
https://www.rcsb.org/

Course Title: Data Mining and Machine Learning Lab (Practical)

L	T	P	Cr
0	0	4	2

Course Code: LBI.558
Total Lecture: 60

Learning Outcomes: On completion of this module, students should be able to:

- learn the issues involved in dealing with large amount of data
- deal with the principles of a number of machine learning algorithms
- implement and apply different machine learning algorithms on large data sets
- know how to analyse large data sets
- familiar with potential applications of different algorithms
- critically analyse and evaluate a research area

Course Content

1. Basics of Data Mining: dimensionality reduction
2. Principal Component Analysis (PCA)
3. Regression analysis
4. k-Nearest Neighbors algorithm (K-NN)
5. Random forest
6. Support Vector Machine (SVM)
7. Decision trees
8. Heat-Maps
9. Hierarchical clustering

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Leskovec, J & Rajaraman, A. & Ullman, J (2014). *Mining of Massive Datasets*.
2. Doupe, P., Faghmous, J., & Basu, S. (2019). Machine Learning for Health Services Researchers. *Value in health : the journal of the International Society for Pharmacoeconomics and Outcomes Research*, *22*(7), 808–815.
3. Lan, K., Wang, D. T., Fong, S., Liu, L. S., Wong, K., & Dey, N. (2018). A Survey of Data Mining and Deep Learning in Bioinformatics. *Journal of medical systems*, *42*(8), 139.
4. Bishop, C. (2007). *Pattern Recognition and Machine Learning*.

Web Resources

https://www.youtube.com/playlist?list=PLblh5JKOoLUICTaGLRoHQDuF_7q2GfuJF
https://www.youtube.com/playlist?list=PLblh5JKOoLUKxzEP5HA2d-Li7IJkHfXSe

Course Title: Molecular Simulations Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.555

Total Hours: 60

Learning Outcomes: At the end of the course, the students will be able to:

- learn the basics of Linux environment
- use the remote computing as a tool for high performance computation
- use different energy minimization techniques
- create molecular model from scratch, and high definition images using various graphics tools
- gain the practical in-hand experience of various modeling and classical simulation tools
- learn the use of different insilico techniques for biomolecular simulations

which will enhance their employability in their further potential carrers in academia and industry

Course Content

1. Linux basics and remote computing
2. Coordinate generations and inter-conversions of small molecules
3. Energy minimizations and optimization, *ab initio methods*
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Secondary Structure Prediction, Fold Recognition
7. Molecular Dynamics with GROMACS
    a. Water structure and dynamics
    b. Binary Mixtures
    c. HP36 in Water
    d. Serotonin1A in Membrane Bilayers
8. Review of Molecular Dynamics Principles

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group

discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids 2nd Edition, Oxford University Press, 2017.
2. D. Frenkel and B. Smit, Understanding Molecular Simulation 2nd Edition, Academic Press, (2001)
3. A. R. Leach, Molecular Modelling Principles and Applications 2nd Edition. Pearson, 2001.
4. S. Alavi, Molecular Simulations: Fundamentals and Practice 1st Edition, Wiley-VCH, 2020

Course Title: Computational Genomics and Proteomics Lab (Practical)

L	T	P	Cr
0	0	4	2

Course Code: LBI.569
Total Hours: 60

Learning Outcomes: On completion of the course the student should be able to:

- Identify different types of protein–DNA interactions and characterise different biological networks.
- Apply different search methods to find function and putative structure with specific properties in large compound databases
- Evaluate different virtual screening methods using large datasets

Course Content

The following experiments should be conducted by the students:

A. Genomics

1. Retrieve the gene sequences by exploring and querying the nucleic acid databases.
2. Find the chromosomal location of gene sequence and basic experiments in NCBI mapviewer.
3. Practicals on ORFfinder, GenScan
4. Prediction of Protein-nucleic acid interaction sites

B. Proteomics

1. Retrieve the protein sequences by exploring and querying the protein databases.
2. Practicals with MultiDent, AACompIdent, Protparam
3. Databses PDB, SCOP, CATH, Pfam
4. Secondary structure Prediction-GOR, SOPMA
5. Prediction of Protein- protein interaction

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Bioiformatics: A Practical Approach- K.Mani& N. Vijayaraj-Aparna Publishers NewDelhi
2. How to program, Dietel&Dietel , Pearson edn.

Web Resources

https://www.uniprot.org/

Course Title: Enriching Bioinformatics

L	T	P	Cr
2	0	0	2

Course Code: LBI.572

Total Hours: 30

Learning outcomes: On completion of the course the student should be able to:

- Apply different skills to perform in competitive exams.
- To speed up the problem solving task in specific time period which is necessary to secure well in exams
- revisit and revise the courses offered
- Solve exercises, mock tests and practice tests for competitive examinations

Course Content

Unit I **8 Hours**

Overview of replication, DNA damage and repair mechanisms, homologous and site-specific recombination

Unit II **7 Hours**

Cell Signalling: Signalling through G-protein coupled receptors, signal transduction pathways

Unit III **8 Hours**

Zygote formation, cleavage, blastula formation, embryonic fields, gastrulation and formation of germ layers in animals

Unit IV **7 Hours**

Codominance, incomplete dominance, pleiotropy, sex linkage, sex limited and sex influenced characters

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Suggested Readings

1. Anthony, J.F., Miller, J.A. ,Suzuki, D.T., Richard, R.C., Gilbert, W.M. (1998). An introduction to Genetic Analysis. W.H. Freeman publication, USA.

2. Scott, F. and Gilbert, S.F. (2010). Developmental Biology. Sinauer Associates, Inc. USA.

3. Slack, J.M.W. (2005). Essential Developmental Biology, Wiley-Blackwell, USA.

4. Alberts, B., Bray, D., Lews, J., Raff, M., Roberts, K. and Watson, J.D. (2010). Molecular Biology of the cell. Garland publishers, Oxford.

5. Celis, J.E. (2006). Cell biology: A laboratory handbook, Vol 1, 2, 3. Academic Press, UK.

6. Gupta, P.K. (2008). Cytology, Genetics and Evolution. Rastogi publications

Web Resources

1. https://www.embibe.com/exams/csir-net-question-paper/amp/
2. https://www.examrace.com/CSIR/CSIR-Sample-Old-Papers/Life-Sciences/

Course Title: Computational Methods Lab (Practical)

L	T	P	Cr
0	0	4	2

Paper Code: CCC.528

Total Hours: 60

Learning Outcomes: At the end of the course, the students will be able to:

- learn computer code for the large scale systems of transcendental and polynomial equations
- understand numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
- learn the computer code for numerical differentiation and integration, differential equations, complex curve fitting, and simple optimisation

After completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

Course Content

To write and execute computer programs in Fortran/Python language for the following problems:

1. Solution of transcendental or polynomial equations by the Newton Raphson method.
2. Matrix summation, subtraction and multiplication.
3. Matrix inversion using Gauss-Jordan's Matrix-Inversion Method.
4. Solution of Simultaneous Linear Equations: Gaussian Elimination, Gauss Seidel Iteration Method.
5. Finding Eigen values and Eigenvectors.
6. Newton/Lagrange interpolation based on given input data.
7. Numerical first order differentiation of a given function.
8. Numerical integration using Trapezoidal, Simpson's 1/3, Gaussian Quadrature methods.
9. Solution of first order differential equations using the Rung-Kutta method,
10. Monte Carlo integration.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings

1. Y.Kirani Singh and B.B.Chaudhuri, MATLAB Programming, Prentice-Hall India, 2007

2. Rudra Pratap, Getting Started with Matlab 7, Oxford, Indian University Edition, 2006
3. E. Balaguruswamy, Numerical Methods, Tata McGraw Hill (2017).
4. V. Rajaraman, Computer oriented numerical methods, PHI Learning Pvt. Ltd., (2018).

Course Title: Research Proposal

L	T	P	Cr
0	0	8	4

Course Code: LBI.600
Total Hours: 120

Course Objective and Learning Outcomes: The objective of this course would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

What Students would do:
Students will prepare a research proposal based on literature review and extensive student-mentor interactions involving regular discussions, meetings and presentations. Each student will submit a research/dissertation proposal of the research work planned for the M.Sc. dissertation with origin of the research problem, literature review, hypothesis, objectives, methodology to carry out the planned research work, expected outcomes and bibliography.

Students will have an option to carry out dissertation work in industry, national institutes or Universities in the top 100 NIRF ranking. Group dissertation may be opted, with a group consisting of a maximum of four students. These students may work using a single approach or multidisciplinary approach. Research projects can be taken up in collaboration with industry or in a group from within the discipline or across the discipline.

Evaluation Criteria:
The evaluation of the dissertation proposal will carry 50% weightage by supervisor and 50% by HoD and senior-most faculty of the department.

Dissertation Proposal (Third Semester)

	Marks	Evaluation
Supervisor	50	Dissertation proposal and presentation
HoD and senior-most faculty of the department	50	Dissertation proposal and presentation

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.

Semester IV

Course Title: Dissertation

L	T	P	Cr
0	0	40	20

Course Code: LBI.600

Total Hours: 600

Course Objective and Learning Outcomes: The objective of dissertation would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

Students will carry out their research work under the supervision of a faculty member. Students will interact with the supervisors through meetings and presentations on a regular basis. After completion of the research work, students will complete the dissertation under the guidance of the supervisor. The dissertation will include literature review, hypothesis, objectives, methodology, results, discussion, and bibliography.

Evaluation Criteria:

The evaluation of dissertation in the fourth semester will be as follows: 50% weightage for continuous evaluation by the supervisor which includes regularity in work, mid-term evaluation, report of dissertation, presentation, and final viva-voce; 50% weightage based on average assessment scores by an external expert, HoD and senior-most faculty of the department. Distribution of marks will be based on report of dissertation (30%), presentation (10%), and final viva-voce (10%). The final viva-voce will be through offline or online mode.

Dissertation (Fourth Semester)		
	Marks	Evaluation
Supervisor	50	Continuous assessment (regularity in work, mid-term evaluation) dissertation report, presentation, final viva-voce
External expert, HoD and senior-most faculty of the department	50	Dissertation report (30), presentation (10), final viva-voce (10)

Transactional Modes: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning, Online tools.