

**Central University of Punjab,  
Bathinda**



**MSc Life Science (Bioinformatics)**

**Session: 2019-21**

**Department of Computational Sciences**

### **Eligibility Criterion for MSc Life Science (Bioinformatics) to be approved by BOS**

Bachelor's degree in any branch of Life Sciences/ Pharmaceutical Sciences / Mathematical Sciences/ Computer Sciences (or applications)/ Physical Sciences/ Chemical Sciences/ Veterinary Sciences/ Agricultural Sciences / Medical Sciences or B.Tech in CSE/IT/BioTech with 55% marks from a recognized Indian or foreign university.

### **Certificate**

The BOS of Department of Computational Sciences certifies that the syllabus of MSc Life Science (Bioinformatics) has been designed to ensure maximal overlap with the CSIR-NET and BINC syllabus.

### **Program Objectives or Expected Skill Development among Students of MSc Life Science (Bioinformatics)**

In line with the syllabus of MSc Life Science (Bioinformatics) it is expected that a student graduating after successful completion of the course shall be

1. Proficient in various aspects of Bioinformatics.
2. Competent to carry out understanding complex information from the concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out the unsupervised research.
3. Shall have scientific temperament.

Multiple courses shall be opted by students from other (allied) departments, however, concerned teacher shall have to use examples from relevant discipline so as to gravitate the students more towards Bioinformatics.

Therefore graduated students of MSc Life Science (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 course. A special effort has been made to enable the student clear national level tests, especially, CSIR-NET and BINC.

### SEMESTER I

Course Code	Course Title	Course Type	Credits		
			L	T	P
LBI.506	Chemical Biology	CFC	2	-	-
LBI.515	Programming - I	CFC	2	-	-
LBI.516	Practicals in Programming - I	CFC	-	-	3
LBI.508	Basics of Biochemistry	CC	2	-	-
LBI.509	Concepts of Genetics	CC	2	-	-
LBI.510	Mathematics for Biologists	CC	4	-	-
LBI.512	Biological Databases and management Systems	CC	4	-	-
LBI.517	Practicals in Biological Databases and management Systems	CC	-	-	3
LBI.518	Perl Programming for life sciences	IDE	2	-	-
<b>Credits</b>			<b>18</b>	<b>-</b>	<b>6</b>
<b>Total Credits</b>			<b>24</b>		

### SEMESTER II

Course Code	Course Title	Course Type	Credits		
			L	T	P
LBI.521	Essentials of Immunology	CC	2	-	-
LBI.511	Sequence Analysis	CC	3	-	-
LBI.530	Programming II	CC	3	-	-
LBI.531	Practicals in Programming II	CC	-	-	3
LBI.522	Statistical Mechanics	DE – I	4	-	-
LBI.532	Maths for Machine Learning	DE – II	2	-	-
LBI.527	Biomolecular Structure Modelling	DE – III	2	-	-
LBI.533	Practicals in Biomolecular Structure Modeling	DE – IV	-	-	2
LBI.534	Python Programming for life sciences	IDE	2	-	-
LBI.542	Credit Seminar – I	SBC	-	-	1
<b>Credits</b>			<b>18</b>	<b>-</b>	<b>6</b>
<b>Total Credits</b>			<b>24</b>		

### SEMESTER III

Course Code	Course Title	Course Type	Credits		
			L	T	P
LBI.557	Datamining and Machine learning	CF	4	-	-
LBI.558	Practicals in Datamining and Machine learning	CF	-	-	3
LBI.553	Complex Algorithms	CC	2	-	-
LBI.555	Molecular Dynamics	CC	4	-	-
LBI.556	Molecular Dynamics (P)	CC	-	-	3
LBI.576	Computational Genomics and Proteomics	CC	2	-	-
Any one of the two below					
LBI.599	M.Sc. Project – I	SBC	-	-	6
LBI.600	M.Sc. Dissertation – I	SBC	-	-	6
<b>Credits</b>			<b>12</b>	<b>-</b>	<b>12</b>
<b>Total Credits</b>			<b>24</b>		

### SEMESTER IV

Course Code	Course Title	Course Type	Credits		
			L	T	P
LBI.571	Systems Biology	CC	4	-	-
LBI.524	Molecular Evolution	CC	4	-	-
LBI.573	Chemiinformatics	DEC	4	-	-
LBI.544	Credit Seminar II	SBC	-	-	1
Any one of the two below (same as previous semester)					
LBI.599	M.Sc. Project – II	SBC	-	-	6
LBI.600	M.Sc. Dissertation – II	SBC	-	-	6
	Two courses need to be chosen from the list of EF/VB courses given by the University	EF/VAC	1+1	-	-
<b>Credits</b>			<b>14</b>	<b>-</b>	<b>17</b>
<b>Total Credits</b>			<b>24</b>		

## Semester-I

**Course Title: Chemical Biology**

**Paper Code: LBI.506**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

### Course Objectives

The purpose of this course is to develop a holistic approach to chemical biology and further leading to a harmonious intellect with sound fundamentals of chemistry. The course will discuss Atomic structure, Chemical equilibrium, kinetics, and solid state within the larger framework of a chemical biology. The course shall promote inquiry, collaboration and chemistry; and giving students the opportunity to develop values through intellectual exercises.

### Learning Outcomes

On completion of the course, the learner will be able to:

1. understand the importance of various atomic models.
2. identify the nature of values in of hybridization.
3. understand the chemical kinetics
4. critically analyse the nuances of solid state.

### Unit I

**8 Hours**

Atomic structure and chemical bonding: Bohr model, spectrum of hydrogen atom, quantum numbers; Wave-particle duality, de Broglie hypothesis; Uncertainty principle; shapes of s, p and d orbitals; Electronic configurations of elements (up to atomic number 30); Aufbau principle; Pauli's exclusion principle and Hund's rule; Orbital overlap and covalent bond; Hybridisation involving s and p orbitals only.

### Unit II

**8 Hours**

Concept of atoms and molecules; Mole concept; Chemical formulae; Concentration in terms of mole fraction, molarity, molality and normality. Chemical equilibrium: Law of mass action; Equilibrium constant, Le Chatelier's principle (effect of concentration, temperature and pressure); Significance of  $\Delta G$  and  $\Delta G_0$  in chemical equilibrium

### Unit III

**6 Hours**

Chemical kinetics: Rates of chemical reactions; Order of reactions; Rate constant; First order reactions; Temperature dependence of rate constant (Arrhenius equation).

### Unit IV

**6 Hours**

Solid state: Classification of solids, crystalline state, seven crystal systems (cell parameters a, b, c,  $\alpha$ ,  $\beta$ ,  $\gamma$ ), close packed structure of solids (cubic), packing in fcc, bcc and hcp lattices;

### Transactional Modes:

Lecture; Tutorial; Problem solving; Self-learning.

**Suggested readings:**

1. Physical Chemistry by A. J. Mee, James Clare Speakman, Heinemann Educational Publishers (1993)
2. Physical Chemistry by P.W. Atkins, Oxford University Press; (2014)

**Course Title: Programming I****Paper Code: LBI.515****Total Hours: 30**

L	T	P	Cr
2	0	0	2

**Course Objective**

By the end of the course, students will have gained a fundamental understanding of programming in Python by creating a variety of scripts and applications for the Web and for systems development. Python is a versatile programming language, suitable for projects ranging from small scripts to large systems. This course emphasizes best practices such as version control, unit testing and recommended styles and idioms. Students will explore the large standard library of Python 3, which supports many common programming tasks.

**Learning Outcomes:**

Upon successfully completing this course, students will be able to “do something useful with Python”.

- Identify/characterize/define a problem
- Design a program to solve the problem
- Create pseudo executable code
- Read most of the basic Python code

**Unit 1****8 Hours**

Introduction, gitHub, Functions, Booleans and Modules, Sequences, Iteration and String Formatting, Dictionaries, Sets, and Files

**Unit 2****8 Hours**

Exceptions, Testing, Comprehensions, Advanced Argument Passing, Lambda -- functions as objects

**Unit 3****6 Hours**

Object Oriented Programming, More OO -- Properties, Special methods

**Unit 4****6 Hours**

Iterators, Iterables, and Generators, Decorators, Context Managers, Regular Expressions, and Wrap Up

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.**Suggested Reading and resources:**

1. **Core Python Programming** (<http://corepython.com/>): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It

starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new language features. In the third edition, "the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends."

2. Dive Into Python 3 (<http://www.diveinto.org/python3/>): This book offers an introduction to Python aimed at the student who has experience programming in another language.
3. Python for You and Me (<http://pymbook.readthedocs.org/en/latest/>): Simple and clear. This is a great book for absolute newcomers, or to keep as a quick reference as you get used to the language. The latest version is Python 3.
4. Think Python (<http://greenteapress.com/thinkpython/>): Methodical and complete. This book offers a very "computer science"-style introduction to Python. It is really an intro to Python in the service of Computer Science, though, so while helpful for the absolute newcomer, it isn't quite as "pythonic" as it might be.
5. Python 101 (<http://www.blog.pythonlibrary.org/2014/06/03/python-101-book-published-today/>) Available as a reasonably priced ebook. This is a new one from a popular Blogger about Python. Lots of practical examples. Also available as a Kindle book: <http://www.amazon.com/Python-101-Michael-Driscoll-ebook/dp/B00KQTFHNK>
6. Problem Solving with Algorithms and Data Structures (<http://interactivepython.org/runestone/static/pythonds/index.html>(Links to an external site.)Links to an external site.)
7. Python Course ([http://www.python-course.eu/python3\\_course.php](http://www.python-course.eu/python3_course.php) (Links to an external site.)Links to an external site.)

### References for getting better, once you know the basics

1. **Python Essential Reference** (<http://www.dabeaz.com/per.html>): The definitive reference for both Python and much of the standard library.
2. **Hitchhikers Guide to Python** (<http://docs.python-guide.org/en/latest>): Under active development, and still somewhat incomplete, but there is good stuff.
3. **Writing Idiomatic Python** (<https://www.jeffknupp.com/writing-idiomatic-python-ebook>): Focused on not just getting the code to work, but how to write it in a really "Pythonic" way.
4. **Fluent Python** (<http://shop.oreilly.com/product/0636920032519.do>): All python3, and focused on getting the advanced details right. Good place to go once you've got the basics down.
5. **Python 3 Object Oriented Programming** (<https://www.packtpub.com/application-development/python-3-object-oriented-programming> (Links to an external site.)Links to an external site.): Nice book specifically about Object Oriented programming structure, and how to do it in Python. From local Author and founder of the Puget Sound Programming Python (PuPPy) meetup group, Dusty Phillips.

**Course Title: Practicals in Programming I**  
**Paper Code: LBI.516**  
**Total Hours: 90**

L	T	P	Cr
0	0	6	3

### **Course Objective**

By the end of the course, students will have gained a fundamental understanding of programming in Python by creating a variety of scripts and applications for the Web and for systems development. The objective of this course is to enable the students to explore the large standard library of Python 3, which supports many common programming tasks.

### **Learning Outcomes:**

Upon successfully completing this course, students will be able to “do something useful with Python”.

- Identify/characterize/define a problem
- Design a program to solve the problem
- Create executable code
- Read most Python code
- Write basic unit tests

**Working with Data.** A detailed tour of how to represent and work with data in Python. Covers tuples, lists, dictionaries, and sets. Students will also learn how to effectively use Python's very powerful list processing primitives such as list comprehensions. Finally, this section covers critical aspects of Python's underlying object model including variables, reference counting, copying, and type checking.

**Program Organization, Functions, and Modules.** More information about how to organize larger programs into functions and modules. A major focus of this section is on how to design functions that are reliable and can be easily reused across files. Also covers exception handling, script writing, and some useful standard library modules.

**Classes and Objects.** An introduction to object-oriented programming in Python. Describes how to create new objects, overload operators, and utilize Python special methods. Also covers basic principles of object oriented programming including inheritance and composition.

**Inside the Python Object System.** A detailed look at how objects are implemented in Python. Major topics include object representation, attribute binding, inheritance, memory management, and special properties of classes including properties, slots, and private attributes.

References for getting started

- **The Python Tutorial** (<https://docs.python.org/3/tutorial/>): This is the official tutorial from the Python website. No more authoritative source is available.
- **Code Academy Python Track** (<http://www.codecademy.com/tracks/python>): Often cited as a great resource, this site offers an entertaining and engaging approach and in-browser work.
- **Learn Python the Hard Way** (<http://www.dustindotson.com>): A classic, well-regarded book for learning Python.



[//learnpythonthehardway.org/book/](http://learnpythonthehardway.org/book/)): Solid and gradual. This course offers a great foundation for folks who have never programmed in any language before. [Python 2]

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

**Course Title: Basics of Biochemistry**

**Paper Code: LBI.508**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

### **Course Objective**

By the end of the course, students will have gained a fundamental understanding of Biochemistry. Biochemistry is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics ranging from sub-cellular to large systems.

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

- The structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles.
- The energy metabolism by cellular components in cells and the process of mitotic cell division.
- 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.

### **Unit 1**

**8 Hours**

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

### **Unit 2**

**6 Hours**

**Composition, structure, function and** metabolism of Carbohydrates, Lipids.

### **Unit 3**

**6 Hours**

**Composition, structure, function and** metabolism of Amino Acids and Nucleotides.

### **Unit 4**

**8 Hours**

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

**Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.**

### **Suggested Readings:**

- Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry*. W.H. Freeman & Company. USA.

2. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction*. Blackwell Publishing Professional. USA.
3. Haynie, D.T. (2007). *Biological thermodynamics*. Cambridge University. UK.
4. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). *Biochemistry*. Oxford University Press Inc. New York.
5. Nelson, D. and Cox, M.M. (2013). *Lehninger Principles of Biochemistry*. BI publications Pvt. Ltd. Chennai, India.
6. Ochiai, E. (2008). *Bioinorganic chemistry: A survey*. Academic Press. Elsevier, India.
7. Randall, D. J., Burggren, W. and French, K. (2001). *Eckert animal physiology*. W.H. Freeman & Company. USA.
8. Raven, P.H., Johnson, G.B. and Mason, K.A. (2007). *Biology*. Mcgraw-Hill. USA.
9. Shukla AN (2009). *Elements of enzymology*. Discovery Publishing. New Delhi, India.
10. Voet, D. and Voet, J.G. (2014). *Principles of biochemistry*. CBS Publishers & Distributors. New Delhi, India.

**Course Title: Concepts of Genetics**

**Paper Code: LBI.509**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

**Course Objective**

By the end of the course, students will have gained a fundamental understanding of concepts of genetics. It is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics ranging from sub-cellular to large systems.

**Learning Outcomes:** The outcomes of the subject is to ensure that a student understands the followings:

- a. The structures and organisation of nucleic acids.
- b. DNA replication.
- c. Inheritance patterns

**Unit 1**

**20 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 2**

**17 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 3****17 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 4****18 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; Tutorial; Problem solving; Self-learning.

**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. Atherly, A.G., Girton, J.R., McDonald, J.F. (1999). *The science of Genetics*. Saundern College publication.
3. Snusted, D.P., Simmons, M. J. (2010). *Principles of Genetics*. John Wiley & Sons, New York.
4. Gupta, P.K. (2009). *Genetics*. Rastogi publications, Meerut, India.
5. Gupta, P.K (2008). *Cytology, Genetics and Evolution*. Rastogi publications, Meerut, India.
6. Jocelyn, E.K., Elliott, S.G., Stephen, T.K. (2009). *Lewin's Genes X*. Jones & Bartlett Publishers, USA.
7. Schaum, W.D. (2000). *Theory & problems in Genetics by Stansfield, out line series* McGrahill, USA.
8. Tamarin, R.H. (1996). *Principles of Genetics, International edtn*. McGrawhill, USA.

**Course Title: Mathematics for Biologists****Paper Code: LBI.510****Total Hours: 60**

L	T	P	Cr
4	0	0	4

**Course Objective**

By the end of the course, students will have gained a fundamental grasp of Cartesian Geometry, vectors Matrices and fundamental calculus. It is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics.

**Learning Outcomes:**

Upon successfully completing this course, students will be able to apply mathematics to create novel solution in bioinformatics.

- Identify/characterize/define a problem
- Design a program to solve the problem
- Create geometric solutions
- Interpret real world problems with calculus

**Unit 1** **15 Hours**  
**Cartesian Geometry**

Vectors, lines in two dimensions, circles, conics, transformation of coordinates, polar coordinates, parametric equations, and the solid analytic geometry of vectors, lines, planes, cylinders, spherical and cylindrical coordinate

**Unit 2** **15 Hours**  
**Differential Calculus**

Functions, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, exact and inexact differentials, partial differentiation.

**Unit 3** **15 Hours**  
**Matrix Algebra**

Addition and multiplication; inverse, adjoint and transpose of matrices, matrix equation, Introduction to vector spaces, matrix eigen values and eigen vectors, diagonalization, determinants (examples from Huckel theory).

**Unit 4** **15 Hours**  
**Integral Calculus**

Basic rules for integration, integration by parts, partial fraction and substitution, definite integrals, evaluation of definite and some standard integrals related to chemistry

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Suggested Readings:**

1. Steiner, E. The Chemistry Mathematics, 2<sup>nd</sup> edition, 2008, Oxford University Press.
2. Doggett, G. and Sucliffe, B.T. Mathematics for Chemistry, 1<sup>st</sup> edition, 1995, Longman.
3. Daniels, F. Mathematical Preparation for Physical Chemistry, 2003, McGraw Hill.
4. Hirst, D.M. Chemical Mathematics, Longman.
5. Barrante, J. R. Applied Mathematics for Physical Chemistry, 3<sup>rd</sup> edition, 2008, Prentice Hall.
6. Tebbutt P. Basic Mathematics for Chemists, 1<sup>st</sup> edition, 1998, John Wiley

**Course Title: Biological Database and Management Systems**

**Paper Code: LBI.512**

**Total Hours: 60**

L	T	P	Cr
4	0	0	4

**Course Objective**

By the end of the course, students will have gained a fundamental grasp of Biological databases and their management systems. It is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics.

**Learning Outcomes:**

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

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

**Unit1****15 Hours**

Biological Databases: Nucleotide Sequence Databases, GenBank, DDBJ, EMBL, Sequence Flatfile and submission process, Protein sequence databases, UniProt, Mapping databases, Genomic databases, PDBsum, PDB, SCOP, CATH, Pathway and molecular interaction databases.

**Unit 2****15 Hours**

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

**Unit 3****15 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 4****15 Hours**

**Internals of RDBMS** Physical data structures, query optimization. Join algorithm statistica and cost base optimization. Transaction processing.concurrency control and recovery management. Transaction model properties, state serizability, lock base protocols, two phase locking.

**Optional Tutorial Part should cover:**

1. Introduction to NCBI Taxonomic Browser
2. DDL & DML: Creating and working with databases, creating tables, dropping tables, primary and secondary keys,
  1. data validation, simple queries using MySQL, cursors, stored procedures.
  2. DTD and XML schema- simple DTD and creation of data in XML.
  3. Design of database architecture - Design, planning, databases, UML Schema, Data models to physical tables.
  4. Accessing molecular biology databases: Entrez, SRS, PIR
  5. Databases: Retrieving, parsing and analysing sequences, structures etc

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Suggested Readings:**

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

2. Elmasri Ramez and Novathe Shamkant, "Fundamentals of Database systems" (2007) Benjamin cummings Publishing Company. ISBN-10: 0321369572.
3. P. Ramakrishnan Rao: Database Management system, (2003) 3EdMcGraw Hill Publications. 9780071230575
4. Jim Gray and A.Reuter " Transaction processing : Concepts and Techniques" Morgan Kaufmann Press.(1997) ISBN- 10: 1558601902
5. V.K .Jain. Database Management system (2002) Dreamtech Press ISBN 8177222279
6. Date C.J. " Introduction to database management" (2009) Vol1, Vol2, Vol3 addison Wesley.
7. Ullman, JD " Principles of Database systems" (1992) Galgottia publication
8. James Martin Principles of Database Management systems" (1985) PHI.

**Paper Code: LBI.517**

**Course Title: Practicals in Biological Database and Management System**

**Total Hours: 90**

L	T	P	Cr
0	0	6	3

### **Course Objective**

By the end of the course, students will have gained a fundamental grasp of Biological databases and their management systems. It is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics.

### **Learning Outcomes:**

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

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

### **Syllabus**

1. Data Definition, Table Creation, Constraints,
2. Insert, Select Commands, Update & Delete Commands.
3. Nested Queries & Join Queries
4. Views
5. High level programming language extensions (Control structures, Procedures and Functions).
6. Front end tools
7. Forms
8. Triggers
9. Menu Design
10. Reports.

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

**Suggested Readings:**

1. Abraham Silberschatz, Henry F.Korth and S.Sudhashan (2005) Database system concepts. 5 Ed McGraw Hill Publications.
2. Elmasri Ramez and Novathe Shamkant, “ Fundamentals of Database systems” (2007) Benjamin cummings Publishing Company. ISBN-10: 0321369572.
3. P. Ramakrishnan Rao: Database Management system, (2003) 3EdMcGraw Hill Publications. 9780071230575
4. Jim Gray and A.Reuter “ Transaction processing : Concepts and Techniques” Morgan Kaufmann Press.(1997) ISBN- 10: 1558601902
5. V.K .Jain. Database Management system (2002) Dreamtech Press ISBN 8177222279
6. Date C.J. “ Introduction to database management” (2009) Vol1, Vol2, Vol3 addison Wesley.
7. Ullman, JD “ Principles of Database systems” (1992) Galgottia publication
8. James Martin Principles of Database Management systems” (1985) PHI.

**Course Title: Perl Programming for Life Sciences (for other departments)**

**Paper Code: LBI.518**

**Total Hours: 30**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
2	0	0	2

**Course Objective**

By the end of the course, students will have gained a fundamental grasp of Perl Programming. It is a additional capability increasing subject, for life scientists.

**Learning Outcomes:**

Upon successfully completing this course, students will be able to apply perl coding to create novel solution in Life Sciences.

- Identify/characterize/define and solve a coding problem
- Design an approach to create a perl code
- Create algorithmic solutions to the automatable problems

**Unit: 1****7 Hours**

PERL as a scripting language, Installation on various OS, Integrated Development Environment, The Comprehensive PERL Archive Network, BioPerl, Getting started in PERL coding, Running PERL programs.

**Unit: 2****7 Hours**

PERL Basics: Scalar variables, Syntax and semantics, Processing scalar variables, Iteration with while construct, Variable containers, Loops, Conditional statements, Introducing Patterns, Reading and writing files, Case study: Making Motif Search tool.

**Unit: 3****8 Hours**

Advance data structure and programming in PERL: Arrays, Hashes, Sub-routines, Getting organized: Visibility and Scope of big programs, Modules

**Unit: 4****8 Hours**

Regular expression and Text mining: The Match Operator, Match Operator Modifiers, The Substitution Operator, Substitution Operator Modifiers, Translation, Translation Operator Modifiers, More complex regular expressions, Case study: UniProt database parsing.

**Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.**

**Suggested Readings:**

1. Moorhouse M, Barry P (2005): Bioinformatics Biocomputing and Perl: An Introduction to Bioinformatics Computing Skills and Practice, Book, John Wiley & Sons
2. Dwyer R. A. (2003): Genomic Perl: From Bioinformatics Basics to Working Code, Volume 1, Book, Cambridge University Press
3. Tisdall J (2003): Mastering Perl for Bioinformatics, Book, O'Reilly
4. Hietaniemi J, John Macdonald J, Orwant J (1999): Mastering Algorithms with Perl, Book, O'Reilly
5. Bradnam K & Korf I (2012): Unix and Perl Primer for Biologists, Web tutorial at [http://korflab.ucdavis.edu/Unix\\_and\\_Perl/current.html](http://korflab.ucdavis.edu/Unix_and_Perl/current.html)
6. Robert's PERL tutorial  
<http://www.physics.rutgers.edu/~kotliar/perl tut.html>
7. Collection of PERL tutorials at <http://perl-tutorial.org/>

**SEMESTER II****Course Title: Essentials of Immunology****Paper Code: LBI.521****Total Hours: 45**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
2	0	0	2

**Course Objective**

By the end of the course, students will have gained a fundamental understanding of immune system and to understand the concept of immune-based diseases as either a deficiency of components or excess activity as hypersensitivity. It is a fundamental subject, necessary for gaining insights into the application possibilities of immuno-informatics ranging from sub-cellular to large systems.

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

- a. Antigenicity
- b. Mechanisms of Antibody diversity
- c. MHC and HLA systems
- d. Inflammation and autoimmunity



**Unit: 1****12 Hours**

**Immune system:** The cells and organs of immune system. Recognition of self and nonself, Humoral immunity-immunoglobulins, basic structure, classes and subclasses, structural and functional relationships, nature of antigen, antigen-antibody reaction

**Unit: 2****13 Hours**

Molecular mechanisms of antibody diversity and Cellular immunity: Organization of genes coding for constant and variable regions of heavy chains and light chains. Mechanisms of antibody diversity, class switching. Complement system, their structure, functions and mechanisms of activation by classical, alternative

**Unit: 3****10 Hours**

Structure and functions of Major Histocompatibility Complex (MHC) and Human Leukocyte Antigen (HLA) system, polymorphism, distribution, variation and their functions. Organization and rearrangement of T-cell receptor genes (TCR).

**Unit: 4****10 Hours**

**Immune System in Health and Diseases:** Inflammation, hypersensitivity and autoimmunity, Immunity to microbes, immunity to tumors, AIDS and immunodeficiencies, hybridoma technology and vaccine development associated challenges for chronic and infectious diseases.

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Suggested Readings:**

1. Kindt, T.J., Osborne, B.A. and Goldsby, R.A. (2007). *Kuby Immunology*. 7<sup>th</sup> Edition. W.H. Freeman, USA.
2. Abbas. (2008). *Cellular and Molecular Immunology*. CBS Publishers & Distributors, India.
3. Charles, A. and Janeway, J.R. (1994). *Immunobiology: The immune system in health and disease*. Blackwell Publishing, USA.
4. Delves, P.J., Roitt, I.M. and Seamus, J.M. (2006). *Roitt's essential immunology (Series-Essentials)*. Blackwell Publishers, USA.
5. Elgert, K.D. (2009). *Immunology: Understanding the immune system*. Wiley-Blackwell, USA.
6. Paul, W.E. (1993). *Fundamental immunology*. Raven Press, SD, USA.
7. Sawhney, S.K. and Randhir, S. (2005). *Introductory practical biochemistry*. Alpha Science International Ltd. New Delhi, India.
8. Tizard. (2008). *Immunology: An Introduction*. Cengage Learning, Thompson, USA.

**Course Title: Sequence Analysis**

**Paper Code: LBI.511**

**Total Hours: 30**

L	T	P	Cr
3	0	0	3

### **Course Objective**

By the end of the course, students will have gained a fundamental understanding of sequence analysis. It is a fundamental subject, necessary for gaining insights into the application possibilities of sequence based bioinformatics ranging from sub-cellular to large systems.

**Learning Outcomes:** The outcomes of the subject is to ensure that a student can apply the knowledge of the following

- a. Data storage formats
- b. Pairwise alignments
- c. Sequence patterns and profiling
- d. Multiple sequence alignment

### **Unit 1**

**9 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 2**

**7 Hours**

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

### **Unit 3**

**8 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 4**

**6 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; Tutorial; Problem solving; Self-learning.

### **Suggested Readings:**

1. A.D. Baxevanis *et. al.*, Current Protocols in Bioinformatics, (2005) Wiley Publishers
2. David W.Mount Bioinformatics (2001) Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
3. Computational Molecular Biology by P. A. Pevzner, Prentice Hall of India Ltd, (2004) ISBN81-203-2550-8
2. D.E.Krane and M.L.Raymer Fundamental concepts of Bioinformatics (2003) Pearson Education ISBN 81-297-0044-1

3. N.Gautham Bioinformatics Narosa publications. (2006) ISBN-13: 9781842653005

**Course Title: Programming II**

**Paper Code: LBI.530**

**Total Hours: 45**

L	T	P	Cr
3	0	0	3

**Course Objective**

By the end of the course, students will have gained a advanced conceptual knowledge of programming in Python by creating a variety of codes with a unit of linear algebra. Python is a versatile programming language, suitable for projects ranging from small scripts to large systems. This course emphasizes best practices such as version control, unit testing and recommended styles and idioms. Students will explore the large standard library of Python 3, which supports many common programming tasks.

**Learning Outcomes:**

Upon successfully completing this course, students will be able to “do something useful with Python”.

- Identify/characterize/define a numerical problem
- Design a program to solve the data parsing problem
- Create Time code
- Read most of the basic Python code

**UNIT 1**

**10 Hours**

Intro to OOP- Define Classes- Create Objects- Understand methods and attributes- Work with `self`

**UNIT 2**

**10 Hours**

Advanced OOP concepts - Work with class and static methods- Inheritance and polymorphism

**UNIT 3**

**10 Hours**

File handling- Work with JSON, CSV or XML files- Python pickle- Functional programming- List comprehensions- Iterators and Generators

**UNIT 4**

**15 Hours**

Solving  $Ax = b$  for square systems by elimination (pivots, multipliers, back substitution, invertibility of A, factorization into  $A = LU$ ), Complete solution to  $Ax = b$  (column space containing b, rank of A, nullspace of A and special solutions to  $Ax = 0$  from row reduced R); Basis and dimension (bases for the four fundamental subspaces); Least squares solutions (closest line by understanding projections); Orthogonalization by Gram-Schmidt (factorization into  $A = QR$ )

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

### **Suggested Reading and resources:**

1. **Core Python Programming** (<http://corepython.com/>): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new language features. In the third edition, "the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends."
2. **Dive Into Python 3** (<http://www.diveinto.org/python3/>): This book offers an introduction to Python aimed at the student who has experience programming in another language.
3. **Python for You and Me** (<http://pymbook.readthedocs.org/en/latest/>): Simple and clear. This is a great book for absolute newcomers, or to keep as a quick reference as you get used to the language. The latest version is Python 3.
4. **Think Python** (<http://greenteapress.com/thinkpython/>): Methodical and complete. This book offers a very "computer science"-style introduction to Python. It is really an intro to Python in the service of Computer Science, though, so while helpful for the absolute newcomer, it isn't quite as "pythonic" as it might be.
5. **Python 101** (<http://www.blog.pythonlibrary.org/2014/06/03/python-101-book-published-today/>) Available as a reasonably priced ebook. This is a new one from a popular Blogger about Python. Lots of practical examples. Also available as a Kindle book: <http://www.amazon.com/Python-101-Michael-Driscoll-ebook/dp/B00KQTFHNK>
6. **Problem Solving with Algorithms and Data Structures** (<http://interactivepython.org/runestone/static/pythonds/index.html>) (Links to an external site.)
7. **Python Course** ([http://www.python-course.eu/python3\\_course.php](http://www.python-course.eu/python3_course.php)) (Links to an external site.)

### **References for getting better, once you know the basics**

1. **Python Essential Reference** (<http://www.dabeaz.com/per.html>): The definitive reference for both Python and much of the standard library.
2. **Hitchhikers Guide to Python** (<http://docs.python-guide.org/en/latest>): Under active development, and still somewhat incomplete, but there is good stuff.
3. **Writing Idiomatic Python** (<https://www.jeffknupp.com/writing-idiomatic-python-ebook>): Focused on not just getting the code to work, but how to write it in a really "Pythonic" way.
4. **Fluent Python** (<http://shop.oreilly.com/product/0636920032519.do>): All python3, and focused on getting the advanced details right. Good place to go once you've got the basics down.

## 5. Python 3 Object Oriented Programming

(<https://www.packtpub.com/application-development/python-3-object-oriented-programming> (Links to an external site.)Links to an external site.): Nice book specifically about Object Oriented programming structure, and how to do it in Python. From local Author and founder of the Puget Sound Programming Python (PuPPy) meetup group, Dusty Phillips.

### Course Title: Practicals in Programming II

Paper Code: LBI.531

Total Hours: 90

L	T	P	Cr
0	0	6	3

### Course Objective

By the end of the course, students will have gained a practical advanced conceptual knowledge of programming in Python by creating a variety of codes. Python is a versatile programming language, suitable for projects ranging from small scripts to large systems. This course emphasizes best practices such as version control, unit testing and recommended styles and idioms. Students will explore the large standard library of Python 3, which supports many common programming tasks.

### Learning Outcomes:

Upon successfully completing this course, students will be able to “do something useful with Python”.

- Identify/characterize/define a numerical problem
- Design a program to solve the data parsing problem
- Create Time series code
- Read most of the advanced Python code
- Introduction to Numpy and Pandas
- Visualizations with Matplotlib and Seaborn
- Statistical analysis to understand our data
- Data cleaning and normalization.
- Advanced Pandas models
- Hierarchical indexing
- Data Wrangling and transformations
- Advanced visualizations
- Introduction to Machine Learning
- Intro to Regressions- Linear and logistic regression using Scikit Learn
- Intro to Classification- Classification with K nearest Neighbours- Decision Trees and Random Forest

### Suggested Readings and resources:

1. **Core Python Programming** (<http://corepython.com/>): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new

language features. In the third edition, "the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends."

2. Dive Into Python 3 (<http://www.diveinto.org/python3/>): This book offers an introduction to Python aimed at the student who has experience programming in another language.
3. Python for You and Me (<http://pymbook.readthedocs.org/en/latest/>): Simple and clear. This is a great book for absolute newcomers, or to keep as a quick reference as you get used to the language. The latest version is Python 3.
4. Think Python (<http://greenteapress.com/thinkpython/>): Methodical and complete. This book offers a very "computer science"-style introduction to Python. It is really an intro to Python in the service of Computer Science, though, so while helpful for the absolute newcomer, it isn't quite as "pythonic" as it might be.
5. Python 101 (<http://www.blog.pythonlibrary.org/2014/06/03/python-101-book-published-today/>) Available as a reasonably priced ebook. This is a new one from a popular Blogger about Python. Lots of practical examples. Also available as a Kindle book: <http://www.amazon.com/Python-101-Michael-Driscoll-ebook/dp/B00KQTFHNK>
6. Problem Solving with Algorithms and Data Structures (<http://interactivepython.org/runestone/static/pythonds/index.html>) (Links to an external site.)Links to an external site.)
7. Python Course ([http://www.python-course.eu/python3\\_course.php](http://www.python-course.eu/python3_course.php)) (Links to an external site.)Links to an external site.)

### References for getting better, once you know the basics

1. **Python Essential Reference** (<http://www.dabeaz.com/per.html>): The definitive reference for both Python and much of the standard library.
2. **Hitchhikers Guide to Python** (<http://docs.python-guide.org/en/latest/>): Under active development, and still somewhat incomplete, but there is good stuff.
3. **Writing Idiomatic Python** (<https://www.jeffknupp.com/writing-idiomatic-python-ebook>): Focused on not just getting the code to work, but how to write it in a really "Pythonic" way.
4. **Fluent Python** (<http://shop.oreilly.com/product/0636920032519.do>): All python3, and focused on getting the advanced details right. Good place to go once you've got the basics down.
5. **Python 3 Object Oriented Programming** (<https://www.packtpub.com/application-development/python-3-object-oriented-programming>) (Links to an external site.)Links to an external site.): Nice book specifically about Object Oriented programming structure, and how to do it in Python. From local Author and founder of the Puget Sound Programming Python (PuPPy) meetup group, Dusty Phillips.

**Course Title: Statistical Mechanics I****Paper Code: LBI.522****Total Hours: 60**

L	T	P	Cr
4	0	0	4

**Course Objective**

By the end of the course, students will have gained a practical advanced conceptual knowledge of statistical mechanics. It is a versatile subject, which is critical for some projects ranging from small to large systems. This course shall emphasize the ability of a student to

**Learning Outcomes:**

Upon successfully completing this course, students will be able to “do something useful with Python”.

- Identify/characterize/define a Statistical mechanics problem
- Create partition function
- Apply the concepts of thermodynamics
- Read and understand publications with applied stat mech

**Unit I:****18 Hours****Mathematical Review of Classical Mechanics:**

Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations

Classical approach to Ensembles:

Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and its ensembles

Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

**Unit II****18 Hours****Elementary Probability Theory**

Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem

Distributions & Fluctuations:

Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable

**Unit III****18 Hours**

**Basic Thermodynamics:** Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

**Unit IV****18 Hours**

**Bose-Einstein distribution:** Einstein condensation. Thermodynamic properties of ideal BE gas.

**Fermi-Dirac distribution:** Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

### **Suggested Readings**

1. Statistical Mechanics, by Donald A McQuarrie
2. Introduction to Modern Statistical Mechanics, by David Chandler
3. Statistical Mechanics, by Kerson Haung
4. Statistical Mechanics, by Patria

### **Course Title: Mathematics for Machine Learning**

**Paper Code: LBI.532**

**Total Hours: 30**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
2	0	0	2

### **Course Objective**

Broadly speaking, Machine Learning refers to the automated identification of patterns in data. As such it has been a fertile ground for new statistical and algorithmic developments. The purpose of this course is to provide a mathematically rigorous introduction to these developments with emphasis on methods and their analysis with one unit of linear algebra for mathematical connectivity.

### **Learning Outcomes:**

Upon successfully completing this course, students will be able to apply mathematics to create novel solution in datamining and machine learning.

- Identify/characterize/define a machine learning problem
- Design a program to calssify, find regression and cluster entities
- Create automated machine dependent solutions
- optimize real world problems

### **Unit 1**

Symmetric matrices and positive definite matrices (real eigenvalues and orthogonal eigenvectors, tests for  $x'Ax > 0$ , applications); Linear transformations and change of basis (connected to the Singular Value Decomposition - orthonormal bases that diagonalize A);

### **Unit 2**

The Statistical Theory of Machine Learning: Classification, Regression, Aggregation;

### **Unit 3**

Empirical Risk Minimization, Regularization; Suprema of Empirical Processes Algorithms and Convexity: Boosting;

### **Unit 4**

Kernel Methods Convex Optimization Online Learning: Online Convex Optimization; Partial Information Bandit Problems; Blackwell's Approachability

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.



### Suggested Readings

1. Steiner, E. The Chemistry Mathematics, 2<sup>nd</sup> edition, 2008, Oxford University Press.
2. Doggett, G. and Sucliffe, B.T. Mathematics for Chemistry, 1<sup>st</sup> edition, 1995, Longman.
3. Daniels, F. Mathematical Preparation for Physical Chemistry, 2003, McGraw Hill.
4. Hirst, D.M. Chemical Mathematics, Longman.
5. Barrante, J. R. Applied Mathematics for Physical Chemistry, 3<sup>rd</sup> edition, 2008, Prentice Hall.
6. Tebbutt P. Basic Mathematics for Chemists, 1<sup>st</sup> edition, 1998, John Wiley

### Course Title: Biomolecular Structure Modelling

Paper Code: LBI.527

Total Hours: 60

L	T	P	Cr
2	0	0	2

### Course Objective

The course covers advanced methods and strategies used in medicinal chemistry research with a focus on computer-aided drug design. The course includes protein–ligand interactions, docking, chemo-informatics, molecular dynamics simulations, free energy calculations..

### Learning Outcomes:

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

- describe different types of protein–ligand interactions and characterise binding pockets
- use different search methods to find compounds with specific properties in large compound databases
- set up, perform and evaluate different virtual screening methods using large datasets
- account for and set up molecular dynamics simulations and free energy calculations

### Unit 1

**15 Hours**

Introduction to drug designing, drug design to discovery and development, drug metabolism, toxicity and pharmacokinetics, toxicology considerations, problems and drawbacks on drug discovery and development.

### Unit 2

**15 Hours**

Identification and validation strategies Drug Target classification, identification and validation strategies, Design and development of combinatorial libraries for new lead generation

### Unit 3

**15 Hours**

Structure-based design–‘de novo’ design methodologies 3D-database searching techniques, docking. QSAR:

**Unit 4****15 Hours**

Statistical techniques behind QSAR, classical QSAR, molecular descriptors 3D QSAR and COMFA; Basic principles of molecular modeling, molecular dynamics simulation techniques.

**Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.**

**Suggested Readings:**

1. *Grant, Guy H.; Richards, W. Graham* **Computational chemistry** Oxford: Oxford Univ. Press, 1995
2. *Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo* **Molecular design : concepts and applications** Weinheim: Wiley-VCH, c2008

**Course Title: Practicals in Biomolecular Structure Modelling**

**Total Hours: 60**

**Paper Code: LBI.533**

L	T	P	Cr
0	0	2	1

**Course Objective**

The course covers advanced methods and strategies used in medicinal chemistry research with a focus on practical aspects of computer-aided drug design. The course includes protein-ligand interactions, docking, cheminformatics, molecular dynamics simulations, free energy calculations. Application of these techniques in virtual screening, structure-based design, and ligand-based design will be addressed and used in computer exercises.

**Learning Outcomes:**

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

- Identify different types of protein-ligand interactions and characterise binding pockets
- Apply different search methods to find compounds with specific properties in large compound databases
- Evaluate different virtual screening methods using large datasets
- Devise and set up molecular dynamics simulations and free energy calculations

The following experiments should be conducted by the students:

**A. Molecular Recognition**

1. Prediction of Protein-ligand interaction sites
2. Prediction of Protein-protein interaction sites
3. Prediction of Protein-membrane interaction sites
4. Prediction of Protein-nucleic acid interaction sites

**B. Docking**

1. Protein Ligand Docking using
  - 1) Autodock
  - 2) Vina
  - 3) Dock

2. Protein-protein docking by HADDOCK or other similar methods

C. Modelling macromolecular structure

1. Homology modeling
2. *ab-initio* structure modelling

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

**Suggested Readings:**

1. *Grant, Guy H.; Richards, W. Graham* Computational chemistry Oxford: Oxford Univ. Press, 1995
2. *Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo* Molecular design : concepts and applications Weinheim: Wiley-VCH, c2008

**Course Title: Python Programming for Life Sciences**

**Paper Code: LBI.534**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

**Course Objective:**

The main goal of this course is to teach life science students how to write computer programs to analyze biological data. The students will learn how to use Python, an object-oriented computer language that is an ideal combination of power and simplicity. Our philosophy in this class is to learn Python in a hands-on way, through tutorials and weekly homeworks that challenge the student to break down problems into manageable units. In the second half of the course, students will apply their Python skills to address a bioinformatics problems.

**Learning Outcomes**

- How to manipulate large datasets using read, write, and comparative functions.
- How to create customized statistical tests using simulations. Real biological data often violate critical assumptions of standard statistical tests. The more sophisticated biologist knows how to account for complexities of the data through permutation and randomization.
- How to construct a pipeline of different programs that automates genomic analysis.
- Most importantly, this class will provide students the means to break down a scientific hypothesis into its fundamental elements, a necessary prerequisite to coding for the answers.

**Unit 1**

**10 Hours**

Installing Python; Basic usage. Basic Elements & Syntax  
Strings, Lists and Tuples

**Unit 2** **7 Hours**  
Dictionaries  
Loops, comparisons

**Unit 3** **7 Hours**  
Definitions & functions  
Classes

**Unit 4** **6 Hours**  
Midterm, Randomization & permutation assignments  
Graphing & stats (R and matplotlib)

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

**Suggested Readings and resources:**

1. **Core Python Programming** (<http://corepython.com/>): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new language features. In the third edition, "the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends."
2. Dive into Python 3 (<http://www.diveinto.org/python3/>): This book offers an introduction to Python aimed at the student who has experience programming in another language.

**Course Title: Credit Seminar -I**  
**Paper Code: LBI.542**

L	T	P	Cr
0	0	2	1

**Objective:** The objective of Credit Seminar would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:  
Maximum Marks: 50

S.No.	Criteria	Marks
1	Content	20
2	Presentation Skills	20
3	Handling of queries	10

**Course Title: Datamining and Machine learning**

**Paper Code: LBI.557**

**Total Hours: 60**

**Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.**

L	T	P	Cr
4	0	0	4

**Unit 1**

**8 Hours**

Introduction: Overview of Machine Learning field with intro to statistics Data Cleaning, imputation, cross-validation, and interpreting results Probability and Statistics Regression

**Unit 2**

**14 Hours**

Unsupervised Methods: Clustering: Distance Metrics, K-Means, leader, Jarvis-Patrick, hierarchical clustering; (The students should note that the correlation of gene expression data to biological process and computational analysis tools involves many clustering techniques) Clustering: Self-organized maps, EM-algorithm; Dimensionality Reduction: PCA, LDA, Sammon's

**Unit 3**

**20 Hours**

Supervised Methods: Classification: K-NN, naïve Bayes, decision trees, boosting and bagging; Classification: Ensemble methods, random Forests; Support vector machines Neural networks; Introduction to Deep learning

**Unit 4**

**18 Hours**

Application Areas: Information retrieval and text mining, and n-grams; Recommendation systems; Outlier detection  
Active learning; Frequent Pattern mining and APRIORI; Reinforcement learning

**Suggested Readings:**

1. Data Mining: Concepts and Techniques, Third Edition by Han, Kamber, and Pei, 2011.
2. Pattern Recognition and Machine Learning by Christopher Bishop; 2007.
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.

**Course Title: Practicals in Datamining and Machine learning**

**Paper Code: LBI.558**

**Total Hours: 90**

L	T	P	Cr
0	0	6	3

**Course Objectives:**

This module aims to introduce students to basic principles and methods of machine learning algorithms that are typically used for mining large data

sets. In particular, we will look into algorithms typically used for analysing networks, fundamental principles of techniques such as decision trees and support vector machines, and finally, neural network architectures. The students will gain practical understanding through a coding exercise where they will implement and apply one machine learning algorithm on a particular large data set.

### **Learning Outcomes:**

On completion of this module, students should:

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

**Basics of Data Mining:** dimensionality reduction

**Support Vector Machines:** common kernel functions; implementation of kernels; non-parametric SVM-based clustering; regression; multiclass SVM

**Decision Trees and Decision Support Systems:** classification tree algorithms (e.g., survival trees, clustering trees, linear splits, class prior, binary splits);

**Neural Networks:** basic principles of self-organisation and supervised learning; representation aspects of neural networks, neural circuits, neurons; learning and neural coding

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

### **Suggested Readings:**

1. Leskovec, J & Rajaraman, A. & Ullman, J (2014). *Mining of Massive Datasets*.
2. Bishop, C. (2007). *Pattern Recognition and Machine Learning*.

**Course Title: Complex Algorithms in Bioinformatics**

**Paper Code: LBI.553**

**Total Hours: 30**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
2	0	0	2

### **Course Objectives:**

This module aims to introduce students to basic principles and methods of optimization algorithms. In particular, we will look into algorithms such as genetic algorithms, swarm intelligence: BCO and ACO.

The students will gain practical understanding through a coding exercise where they will implement and apply one machine learning algorithm on a particular large data set.

### **Learning Outcomes:**

On completion of this module, students should:

- understand the issues involved in dealing with large amount of data
- understand the principles of a number of optimization algorithms
- know how to apply HMM

**Unit 1**

**10 Hours**

TSP; Weight matrices: Sequence weighting, pseudo count correction for low counts, Gibbs sampling, and Psi-Blast

**Unit 2**

**12 Hours**

Hidden Markov Models: Model construction, Viterbi decoding, and posterior decoding, and Baum Welsh HMM learning

**Unit 3**

**8 Hours**

Genetic Algorithm: Real world problems of optimization; BCO; ACO;

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Suggested Readings:**

1. Mastering Algorithms with Perl; Oreilly
2. Algorithms by Robert Sedgewick
3. Art of Computer Programming, Volume 1: Fundamental Algorithms by Donald Ervin Knuth

---

**Course Title: Molecular Dynamics**

**Paper Code: LBI.555**

**Total Hours: 60**

L	T	P	Cr
4	0	0	4

**Course Objective and Learning Outcomes:** The objective of this subject is to ensure that a student learns modelling of biomolecular structures and understanding the dynamics of the structural transitions.

**Unit 1**

**15 Hours**

Biomolecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials in protein and nucleic acid structure. Techniques for Conformational Sampling- Monte Carlo, global optimization, etc.

**Unit 2**

**15 Hours**

Molecular Mechanics: general features, bond stretching, angle bending, improper torsions, out of plane bending, cross terms, non-bonded interactions, Ramachandran diagram point charges, calculation of atomic charges, polarization, van der waals interactions, hydrogen bond interactions, Water models, Force field, all atoms force field and united atom force field.

**Unit 3**

**15 Hours**

**Energy minimization:** Steepest descent, conjugate gradient – Derivatives, First order steepest decent and conjugate gradients. Second order derivatives Newton-Raphson, Minima, maxima saddle points and

convergence criteria.-non derivatives minimization methods, the simplex, sequential univariate, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, Solvent access, Equilibration, cut-offs.

#### **Unit 4**

**15 Hours**

**Simulation methods :** algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

#### **Suggested Readings:**

1. Andrew R. Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach", (2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

**Course Title: Practicals in Molecular Dynamics**

**Paper Code: LBI.556**

**Total Hours: 90**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
0	0	6	3

**Course Objective and Learning Outcomes:** The objective of this subject is to ensure that a student learns practical aspects of biomolecular structures and the understanding of the dynamics of the structural transitions.

1. Advanced Visualization Software and 3D representations with VMD and Rasmol.
2. Coordinate generations and inter-conversions.
3. Secondary Structure Prediction.
4. Fold Recognition, *ab initio method*.
5. Homology based comparative protein modeling.
6. Energy minimizations and optimization.
7. Validation of models.
  - a. WHATIF
  - b. PROSA
  - c. PROCHECK
  - d. VERIFY 3D
8. Protein Structure Alignment.



9. Modeller
10. Structure based Drug Design
  - a. Molecular Docking
  - b. De Novo Ligand Design
  - c. Virtual Screening
11. Ligand based Drug Design
  - a. Pharmacophore Identification
  - b. QSAR
12. Molecular Dynamics with Gromacs
13. Binding Site Identification

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

### Suggested Readings

1. Andrew R. Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach", (2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

### Course Title: Computational Genomics and Proteomics

**Paper Code: LBI.576**

**Total Hours: 30**

L	T	P	Cr
2	0	0	2

#### Unit 1

**7 Hours**

The Importance of DNA-Protein Interactions During Transcription. Initiation-Regulation of Transcription, Synthesis and Processing of the Proteome, The Role of tRNA in Protein Synthesis, The Role of the Ribosome in Protein Synthesis, Post-translational Processing of Proteins, Protein Degradation.

#### Unit 2

**8 Hours**

Role of bioinformatics-OMIM database, integrated genomic maps, gene expression profiling; identification of SNPs, SNP database (DbSNP)

#### Unit 3

**16 Hours**

DNA microarray: database and basic tools, Gene Expression Omnibus (GEO), ArrayExpress, SAGE databases  
understanding of microarray data, normalizing microarray data, detecting differential gene expression,

#### Unit 4

**6 Hours**

Only for yeasts: building predictive models of transcriptional regulatory networks using probabilistic modeling techniques.

**Extra Reading Topics (Not in evaluatory syllabus)**

Genomes, Transcriptomes and Proteomes, The Human Genome and its Importance, Structure of the Eukaryotic and Prokaryotic Genome, the Repetitive DNA Content of Genomes. Mechanism of Genetic Action, Gene-protein relations, Genetic fine structure, Mutational sites Complementation

How Genomes Function, Accessing the Genome, Inside the Nucleus, Chromatin Modifications and Genome Expression, Assembly of the Transcription Initiation Complex, Metagenomics

**Transactional Modes:** Lecture; Tutorial; Problem solving; Self-learning.

**Course Title: M.Sc. Project I**

**Paper Code: LBI.599**

**Total Hours: 180**

L	T	P	Cr
0	0	12	6

**Course Objective and Learning Outcomes:** The objective of dissertation part II 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.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
1.	Report Writing	S/US
2.	Presentation of research work	S/US
3.	Continuous evaluation of student by Guide	S/US
	Total	S/US

S/US = Satisfactory / Unsatisfactory

The final presentation shall be evaluated by a three membered committee consisting of

- COC / OIC of the department
- Another teacher from allied department
- Supervisor (and Co-supervisor if applicable)

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

**Course Title: M.Sc. Dissertation I**

**Paper Code: LBI.600**

**Total Hours: 180**

L	T	P	Cr
0	0	12	6

**Course Objective and Learning Outcomes:** The objective of dissertation part II 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.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
1.	Report Writing	S/US
2.	Presentation of research work	S/US
3.	Continuous evaluation of student by Guide	S/US
4.	Novelty of work	S/US
	Total	S/US

S/US = Satisfactory / Unsatisfactory

The final presentation shall be evaluated by a three membered committee consisting of

- COC / OIC of the department
- Another teacher from allied department
- Supervisor (and Co-supervisor if applicable)

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

**Course Title: Systems Biology**

**Paper Code: LBI.571**

**Total Hours: 60**

L	T	P	Cr
4	0	0	4

### **Course Objective**

This course provides an introduction to cellular and population-level systems biology with an emphasis on synthetic biology, modeling of genetic networks, cell-cell interactions, and evolutionary dynamics. Cellular systems include genetic switches and oscillators, network motifs, genetic network evolution, and cellular decision-making. Population-level systems include models of pattern formation, cell-cell communication, and evolutionary systems biology.

### **Learning Outcomes:**

At the end of the course, the student is expected to be able to:

- identify the optimal structure for analyzing deep sequencing data
- discuss the main features of biological networks.
- use mathematical modelling to discuss relevant issues in Systems Biology
- understand the main results published on a research paper
- prepare a presentation based on a research paper in Systems Biology

### **Unit 1**

**15 Hours**

Transcription networks, basic concepts, Auto-regulation, a network motif, the feed forward loop network motif

### **Unit 2**

**15 Hours**

Temporal programs and the global structure of transcription networks, Network motifs in developmental, signal-transduction and neuronal networks

### **Unit 3**

**15 Hours**

Robustness of protein circuits, the example of bacterial chemotaxis, Robust patterning in development

### **Unit 4**

**15 Hours**

Kinetic proofreading, optimal gene circuit design; Rules for gene regulation based on error minimization, Simplicity in biology

**Transactional Modes:** Lectures; Tutorials; Problem solving; Self-learning.

### **Suggested Readings**

1. An Introduction to Systems Biology: Design Principles of Biological Circuits by Uri Alon, Chapman & Hall, ISBN 1-58488-642-0.
2. Hake, S. and Wilt, F. (2003). Principles of Developmental Biology. W.W. Norton and Company, New York, USA.
3. Hall, B.K. and Hallgrimsson, B. (2007). Strickberger's Evolution. Jones and Bartlett Publishers, India.
4. Lewin, R. (2004). Human Evolution - An Illustrated Introduction. Wiley-Blackwell, USA.

**Course Title: Molecular Evolution**

**Paper Code: LBI.524**

**Total Hours: 60**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
4	0	0	4

### **Course Objective**

The course will cover the mutational processes; the evolutionary forces affecting mutations; the evolution of DNA sequences; the molecular clock; selection and drift at the molecular level; how variation in nucleotide composition gives rise to polymorphisms and SNPs. It will also cover the basic mechanisms that generate variation in genomes and how these affect

the genome, including recombination, duplication, horizontal gene transfer, and mutational biases. We will also address models for sequence and genome evolution, including the statistical methods for analyzing evolutionary processes, for example selection based on sequence data.

### **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.

### **Unit 1**

**15 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 2**

**15 Hours**

Hardy-weinberg equilibrium – Heterozygosity, gene frequency and heterozygosity; Loss of heterozygosity-mutant alleles-theta as the measure

### **Unit 3**

**15 Hours**

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

### **Unit 4**

**15 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:** Lectures; Tutorials; Problem solving; Self-learning.

### **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

**Course Title: Chemoinformatics****Paper Code: LBI.573****Total Hours: 60**

L	T	P	Cr
4	0	0	4

**Course Objectives:**

Cheminformatics is an emerging field at the intersection of chemistry, physics, biology, mathematics and computer science. It typically deals with (i) storage, analysis and search of chemical information (databases), (ii) development of predictive models linking structure of molecules and their physico-chemical or biological properties, and, (iii) in silico design of new compounds or materials possessing desirable properties. Chemoinformatics approaches are widely used in pharmaceutical industry in order to perform a virtual screening, lead optimization and early ADME/Tox predictions.

**Learning outcomes:**

On successful completion of this module, students should be able to: the students will obtain some knowledge and will get training in

1. Data organization and search in chemical databases;
2. QSAR and pharmacophores modelling;
3. Chemical data visualization and analysis
4. Virtual screening tools and efficiency assessments

**Unit I:****15 Hours**

Chemoinformatics as a theoretical chemistry discipline: definition, main concepts and areas of application. Representing chemical structures on computer. Molecular graphs. Connectivity tables. Adjacency and distance matrices. Linear representations SMILES and SMIRKS. Hashed fingerprints. Exchange formats for chemical structures (MOL, SDF,...) and reactions (RXN et RDF). Chemical Databases. Different types of searching structures in the databases: exact match, sub-structural, super-structural and by similarity.

**Unit 2****15 Hours**

- Molecular descriptors. Definition and main requirements. Different types of descriptors: constitutional, topological indices, geometry-based, surface-based, substructural fragments, lipophilicity, etc.
- Development and validation of QSAR/QSPR models. Data preparation. Statistical parameters assessing models performance. Cross-validation. Models applicability domain. Ensemble modeling.

**Unit 3****15 Hours**

- Molecular Interaction Fields. 3D QSAR. Molecular fields' similarity
- Pharmacophore approach Pharmacophore features. Ligand- and structure-based pharmacophores. Merged and shared pharmacophores. Pharmacophore-based virtual screening

**Unit 4****15 Hours**

- Chemical Space concept. Graph-based chemical space: scaffolds, frameworks and R-groups. Scaffold tree approach. Descriptor-based

chemical space: distance and similarity metrics. Data visualization: Generative Topographic Mapping. Network-like similarity graphs. Activity landscapes. Bioisosteres. Activity cliffs.

- Virtual screening workflow. Drug-likeness filters and structural alerts. Parameters of screening efficiency.

**Transactional Modes:** Lectures; Tutorials; Problem solving; Self-learning.

**Suggested Readings:**

- A. Leach, V. Gillet “An Introduction to Chemoinformatics”, Springer, 2007
- “Tutorials in Chemoinformatics”, A. Varnek, Ed. , WILEY, 2017

**Course Title: Credit Seminar -II**  
**Paper Code: LBI.544**

L	T	P	Cr
0	0	12	6

**Objective:** The objective of Credit Seminar would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:  
Maximum Marks: 50

S.No.	Criteria	Marks
1	Content	20
2	Presentation Skills	20
3	Handling of queries	10
Total		50

**Course Title: M.Sc. Project II**  
**Paper Code: LBI.599**  
**Total Hours: 180**

L	T	P	Cr
0	0	12	6

**Course Objective and Learning Outcomes:** The objective of dissertation part II 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.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
1.	Report Writing	S/US
2.	Presentation of research work	S/US
3.	Continuous evaluation of student by Guide	S/US

Total

S/US

S/US = Satisfactory / Unsatisfactory

The final presentation shall be evaluated by a three membered committee consisting of

- a. COC / OIC of the department
- b. Another teacher from allied department
- c. Supervisor (and Co-supervisor if applicable)

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

**Course Title: M.Sc. Dissertation II**

**Paper Code: LBI.600**

**Total Hours: 180**

L	T	P	Cr
0	0	12	6

**Course Objective and Learning Outcomes:** The objective of dissertation part II 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.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
1.	Report Writing	S/US
2.	Presentation of research work	S/US
3.	Continuous evaluation of student by Guide	S/US
4.	Novelty of work	S/US
	Total	S/US

S/US = Satisfactory / Unsatisfactory

The final presentation shall be evaluated by a three membered committee consisting of

- a. COC / OIC of the department
- b. Another teacher from allied department
- c. Supervisor (and Co-supervisor if applicable)

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