

Course structure for Direct Ph.D. in Bioinformatics

Why direct Ph.D.

This is a mid-stream option where students can move into the direct Ph.D programme after successful completion of one semester course work, provided they meet the requirements specified by the university.

No. of seats: 3

Eligibility:

1. Candidate should have a consistently good academic record and a minimum of 55 percent of aggregate marks, or a minimum final grade point average (FGPA) of 6.0 in a 10 point scale awarded by a recognized university in India or abroad, are eligible for admission.
2. A candidate should have a Master's degree in sciences or related Science discipline
3. A student with completed M.Phil. in Science stream or an allied field may also apply for direct Ph.D.
4. A candidate may be either a fresh M.Phil graduate or someone with professional experience
5. Candidate with NET/JRF qualifications will be given preference

The intended focus of the proposed course shall be Computational Interactomics

During the past two decades Bioinformatics has emerged as major field of research in life sciences. As a consequence the importance of a course in bioinformatics cannot be overstated. This is an emerging field which has huge implication for the identification of novel drug targets (among protein-protein, protein-membrane interaction interface and development of new drug molecules. In the last few years of its establishment in Western world bioinformatics has resulted in a number of novel therapeutic molecules. A number of bioinformatics courses have been introduced by various State / Central Universities to cater the increasing demands of skilled manpower in pharmaceutical and biotechnology industries. The Central University of Punjab has identified Bioinformatics as core area for research and has undertaken to strive for the generation of state-of-the-art infrastructure for Bioinformatics research in order to develop high skilled scientific man-power. As a step forward in this direction, a Centre for Bioinformatics has been established.

We propose to initiate PhD programme to train skilled manpower in bioinformatics. The objective of the course is to generate solutions for the regional problems of cancer and other pollution-related diseases. The rationale behind computational interactomics is rooted in the success of rational drug discovery. The availability of the high resolution structural information coupled with a techniques like high-throughput fragment-based drug design have had a number of success stories. However, these latest developments have blurred the conventional demarcations of the molecules involved. A new array of putative targets for drug development have been identified, for instance, the targeting of small molecules interacting with the superficial grooves on protein surface (Such shallow pockets are involved in the protein-protein interaction). The process of protein-protein interaction (PPI) inhibitor design is based on the combined principles of protein-ligand interaction and protein-protein interaction. This implies that successes from the approaches based on protein-ligand-interactions-only will plateau soon. There are a number of “non-conventional” drug-target interactions which are generally overlooked in the conventional drug-discovery protocols, but have been successful. The study of the interaction interfaces, especially the protein-protein, protein-membrane, protein-carbohydrates and protein-nucleic acids, require development of novel “interaction orientation determining” algorithms and scoring functions for the interaction affinity calculation. Such techniques fall under the ambit of “Computational Interactomics” and the PhD synopsis would be designed with the same focus. The students would be working in the following fields:

- a. Development of novel tools for the *in silico* interaction mapping.
- b. Understanding the phasic evolution of molecular interaction through techniques like Molecular Dynamics.
- c. Development of novel and improvement of existing interaction modulators of protein:partner (which could be small molecule/protein/membrane/DNA) etc.
- d. Understanding the structural plasticity of protein (and other biomolecules).
- e. Development of low-resolution forcefields for protein-protein interaction behaviour replication *in silico*.

The Centre for Bioinformatics has one assistant Professor, eligible for guiding students for doctoral research. In running of the course work the following faculty from sister departments can contribute.

Structure for course work for PhD in Bioinformatics

Semester I						
S.No.	Subject Code	Subject Name	Credit Hours			Maximum Marks
			Theory	Practical	Total	
1	BIN.901	Research Methodology	5		5	100
2	BIN.902	Computer Applications	5		5	100
3	BIN.903	Biomathematics	4		4	100
4	BIN.904	Sequence and Structural Bioinformatics	4		4	100
5	BIN.905	Credit Seminar		12	6	200
Total					24	600

**Proposed Syllabi for PhD Course work (Bioinformatics)
Central University of Punjab**

Semester I

Subject Code: BIN. 901
Subject Name: Research Methodology

L	T	P	Credits	Marks
5	0	0	5	100

Course Objective: The objective of this subject is to ensure that a student learns basis of scientific research and statistical methods to arrive at and verify the conclusions drawn.

Unit 1 **5 Lectures**

General principles of research: Meaning and importance of research, critical thinking, formulating hypothesis and development of research plan, review of literature, interpretation of results and discussion.

Unit 2 **10 Lectures**

Technical writing: Scientific writing that includes the way of writing Synopsis, research paper, poster preparation and presentation, and dissertation.

Unit 3 **5 Lectures**

Library: Classification systems, e-Library, web-based literature search engines

Unit 4 **16 Lectures**

Entrepreneurship and business development: Importance of entrepreneurship and its relevance in career growth, characteristics of entrepreneurs, developing entrepreneurial competencies, types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship) employment, self-employment and entrepreneurship, financial management-importance and techniques, financial statements-importance and its interpretation, and Intellectual Property Rights (IPRs).

Suggested Reading

1. Gupta, S. (2008). *Research methodology and statistical techniques*. Deep & Deep Publications (P) Limited, New Delhi.
2. Kothari, C. R. (2014). *Research methodology (s)*. New Age International (p) Limited. New Delhi.
3. Sahay, Vinaya and Pradumna Singh (2009). *Encyclopedia of Research Methodology in life sciences*. Anmol Publications. New delhi
4. Kauda J. (2012). *Research Methodology: A Project Guide for University Students*. Samfunds litteratur Publications.
5. Dharmapalan B. (2012). *Scientific Research Methodology*. Narosa Publishing House ISBN: 978-81-8487-180-7.
6. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials*.3/e (with SPSS). Decker Inc. USA.
7. Rao, P. P., S. Sundar and Richard, J. (2009). *Introduction to Biostatistics and Research Methods*. PHI learning.
- 8.
- 9.
- 10.

11. Christensen, L. (2007). *Experimental Methodology*.
Boston: Allyn & Bacon.

Subject Code: BIN. 902

Subject Name: Computer Applications

L	T	P	Credits	Marks
5	0	0	5	100

Objectives

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

- Convey the essential characteristics of a set of data by representing in tabular and graphical forms and computing relevant measures of average and measures of variation
- Explain or predict values of a dependent variable based on the values of one or more independent variables
- Estimate the characteristics of populations based on their sample data
- Test specific hypotheses about populations based on their sample data
- Use appropriate procedures to analyse qualitative data
- Demonstrate competence in the use of statistical packages for analysis of data

Unit 1

14 Hours

Fundamentals of Computers: Block Diagram of Computer, Hardware Components, Introduction to computer network and World Wide Web, Sharing Data over Network, Internet Terminology, Searching over Internet, Google: advance Search Operations, Email, Checking Plagiarism using Internet

Unit 2

14 Hours

Introduction to Word Processing and Microsoft Office, Creating and Saving Documents, Text Formatting, Tables, Document Review Option, Mail Merge, Inserting Table of Contents, Reference Management.

Introduction to Spreadsheet and Microsoft Excel, Text Formatting, Formulas, Charts, Table formatting, Sorting Records, Filtering the content.

Unit 3

14 Hours

Computer Configuration, Memory Hierarchy, Software Structure, Introduction to Operating System, Operating System types and functions. Introduction to Disk Operating System, DOS Internal and External Commands, Introduction to Windows operating System, Windows Task Manger.

Unit 4

14 Hours

Introduction to MS Paint, Figure Designing components in MS Paint

Introduction to Microsoft PowerPoint, Layout Selection, Designing and Formatting Slides, Slide Design and background formatting, Bullets and Numbering, Transition Style, Custom Animations, Hyperlink to Local files and Web Pages, Movies and Sound, Slide Timings.

Suggested Reading

1. Gookin, D. (2007). MS Word for Dummies. Wiley.
2. Harvey, G. (2007). MS Excel for Dummies. Wiley
3. Sinha, P.K., Computer Fundamentals, BPB Publications.

Subject Code: BIN. 903
Subject Name: Biomathematics

L	T	P	Credits	Marks
4	0	0	4	100

The course aims at enabling learners to :

- become precise, exact and logical.
- acquire knowledge of mathematical terms, symbols, facts and formulae.
- develop an understanding of mathematical concepts.
- develop problem solving ability.
- acquire skills in applying the learning to situation including reading charts, tables, graphs etc

Unit 1

14 Hours

Vectors Scalars and vectors Vectors as directed line segments Magnitude and direction of a vector; Null vector and Unit vector Equality of vectors Position vector of a point Algebra of vectors Addition and subtraction of vectors and their properties Multiplication of a vector by a scalar and their properties

Resolution of a vector Resolution of a vector in two dimensions; Resolution of a vector in three dimensions; Section formula

Unit 2

14 Hours

Discrete and Continuous Distributions Binomial, Gaussian, Chi-Square test, Student's t-Test, F-test, Z-test

Unit 3

14 Hours

2D Coordinate geometry: line, circle, ellipse, parabola, hyperbola, **3D Geometry: equations of** Sphere and cone

Unit 4

14 Hours

Probability Theory Sample Space and Events, Axioms of Probability, Conditional Probability, Independent Events, Baye's Formula.

Unit 45

14 Hours

Matrix algebra, addition, subtraction, multiplication, inverse and transpose and determinants

Suggested readings

1. Wayne W. Daniel, Biostatistics, 9e Wiley (2004) ISBN: 978-0-471-45654-4
2. Bernard Rosner, Fundamentals of Biostatistics 6e (2006) Thomson Brooks/Cole ISBN: 0-534-41820-1

L	T	P	Credits	Marks
4	0	0	4	100

Subject Code: BIN. 904

Subject Name: Sequence and Structural Bioinformatics

Unit-1

14 Hours

Biological data Types of biological data (various omics)

Biological Databases Nucleic acid and protein sequence and protein structure databases Overview of available Bioinformatics resources on the web

Unit-2

14 Hours

DNA sequence analysis

Sequence annotation and sequence analysis - Phylogeny of gene (blast, fasta, HMMer) and residue conservation. Primer design and Tm Calculation, DNA Restriction pattern analysis. Condon bias and its effect on the protein expression with reference to various expression system.

Unit-3

14 Hours

Bioinfo tools

Protein sequence and structure insights (PSSI) X-ray, NMR, Comparative modeling, ab initio, threading methods. Structure refining techniques Energy minimization approaches (Steepest descent, Conjugate gradient etc), Basis of Molecular dynamics simulations and its application.

Unit-4

14 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.

Suggested Readings

1. Andrew R. Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. A.D. Baxevanis *et. al.*, Current Protocols in Bioinformatics, (2005) Wiley Publishers
3. David W. Mount Bioinformatics (2001) Cold Spring Harbor Laboratory Press, ISBN 0-87969-608-7
4. Computational Molecular Biology by P. A. Pevzner, Prentice Hall of India Ltd, (2004) ISBN 81-203-2550-8
5. D.E. Krane and M.L. Raymer Fundamental concepts of Bioinformatics (2003) Pearson Education ISBN 81-297-0044-1
6. N. Gautham Bioinformatics Narosa publications. (2006) ISBN-13: 9781842653005
7. Fenniri, H. "Combinatorial Chemistry – A practical approach", (2000) Oxford University Press, UK.
8. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
9. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Subject Code: BIN. 905
Subject Name: Credit Seminar

L	T	P	Credits	Marks
0	0	12	6	200

Objective: The objective of dissertation part I would be to ensure that the student learns the aspects of the Review writing and seminar presentation. Herein the student shall have to write a 5000 words review of existing scientific literature with simultaneous identification of knowledge gaps that can be addressed through future work.

The evaluation criteria for “Review Writing and Presentaion” shall be as follows:

Maximum Marks: 200

S.No.	Criteria	Marks
1.	Review of literature	50
2.	Identification of gaps in knowledge	30
3.	References	20
4.	Content of presentation	30
5.	Presentation Skills	40
6.	Handling of queries	30
Total		200

The synopsis shall be evaluated by a three membered committee consisting of

- a. COC of the department
- b. One external Expert
- c. Supervisor or Co-supervisor
- d. One faculty of allied department