

**PROGRAM ARCHITECTURE, DURATION, SCHEME OF EXAMINATION,  
WORKLOAD/WEEK AND CREDITS**

**For Ph.D. course work**

**(Only for subjects where there is no M.Phil. programs are available)**

**Duration :** One Semester (Six months)

**Total Credit requirement:** 14 credits

**Program Structure:** Ph.D. in Bioinformatics

<b>SEMESTER 1</b>						
<b>Course Code</b>	<b>Nomenclature of Course</b>	<b>Theory marks (end semester examination)</b>	<b>Internal Assessment marks</b>	<b>Maximum marks</b>	<b>Hours /Week</b>	<b>Credits</b>
20BINPH11C1 (Compulsory for all Ph.D. Course work)	Research Methodology	80	20	100	4	4
<b>20MPCC1</b> (Compulsory for all Ph.D. Course work)	Research and Publication Ethics	40	10	50	2	2
20BINPH11C3	Computational and Systems Biology	80	20	100	4	4
20BINPH11C4	Structural Bioinformatics	80	20	100	4	4
<b>Total marks/Credits</b>				<b>350</b>		<b>14</b>

**Note:** The compulsory course on 'Research and Publication Ethics' shall be offered by Ch. Ranbir Singh Institute of Social and Economic Change for all UTDs/Centres/Institutes passed vide Resolution No. 27 of the 271<sup>st</sup> meeting of EC held on 29.7.2020.

\*Internal evaluation will comprise of 2 written assignments and 2 presentations of 05% marks each.

**Program Specific Outcomes:** The students upon completion of Ph.D. coursework in Bioinformatics will be able to:

- PSO1** Produce a well-developed research proposal.
- PSO2** Select an appropriate methodology with which to conduct the research and defend the methodology of their selection.
- PSO3** Understand the various techniques required to carry out the research.
- PSO4** Explore the resources needed to perform the research process and perform proper documentation of their findings.
- PSO5** Present and report their research in acceptable manner for the Life Sciences research community.

**MAHARSHI DAYANAND UNIVERSITY**

**CENTRE FOR BIOINFORMATICS**

<b>Name of the Program</b>	Ph.D. Course work in Bioinformatics	<b>Program Code</b>	BINPH
<b>Name of the Course</b>	Research Methodology	<b>Course Code</b>	20BINPH11C1
<b>Hours/Week</b>	4	<b>Credits</b>	4
<b>Max. Marks.</b>	80	<b>Time</b>	3 Hours
<p><b>Note:</b>The examiner has to set a total of nine questions (two from each unit and one compulsory question consisting of short answer from all units. The candidate has to attempt one question each from each unit along the compulsory question (5 x 16 = 80 marks)</p>			
<p><b>Course Objectives:</b> This course aims to introduce:</p> <ol style="list-style-type: none"> <li>1. Basic properties and structure of biopolymers.</li> <li>2. Different methods of Electrophoresis.</li> <li>3. Theory of centrifugation and application to biological systems.</li> <li>4. Principles and Applications of Spectroscopic methods and NMR</li> <li>5. Theory of lyophilization and its applications to biological systems</li> </ol>			
<p><b>Course Outcomes:</b> Students who complete this course will be able to:</p> <ol style="list-style-type: none"> <li>1. Discuss the basic properties and structure of biopolymers.</li> <li>2. Apply the knowledge gained about electrophoresis while performing practicals.</li> <li>3. Apply various types of Centrifugation and Chromatography techniques.</li> <li>4. Discuss the concept of spectroscopy and its application in life sciences.</li> <li>5. Apply the theory of lyophilisation while performing practicals.</li> </ol>			
<b>Unit - I</b>			
Colloidal solutions of biopolymers and their electrochemical properties, Hydrodynamic properties; Viscosity, diffusion etc of biopolymers; Molecular weight determination, osmotic pressure, reverse osmosis and Donnan effect, Structure of biomembranes and their electrochemical properties, membrane potential, action potential and propagation of impulses; PPI			
<b>Unit - II</b>			
Electrophoresis; different methods of electrophoresis for protein, nucleic acids, small molecular weight compounds and immune precipitates (Immuno electrophoresis). Peptide mapping and combination of electrofocussing and SDS-PAGE. Blotting techniques (Northern, Southern and western blotting); RT-PCR			
<b>Unit - III</b>			
Theory of centrifugation and application to biological systems. Rotors angle/vertical/zonal/continuous flow centrifuge, differential centrifugation density gradient centrifugation. Ultra centrifugation principle and application. Chromatography – adsorption, affinity, partition, Ion-exchange, gel permeation, GLC, TLC, RPC, HPLC etc.			
<b>Unit - IV</b>			
Introduction to principles and applications of (a)Spectroscopic methods (UV, Vis, IR, Fluorescence, ORD, CD, & PAS) (b)NMR, ESR & Mass spectrometry, Use of			

radioactive and stable isotopes and their detection in biological systems.

Automatic analyzer for amino acids, protein sequencer, peptide synthesizer & nucleic acid synthesizer. Cell sorters and their applications. Theory of lyophilization and its applications to biological systems. Introduction to principles and working of light and electron microscope.

**References:**

1. Biochemical calculations (1976) by Irwin H. Seghal (John Wiley and Sons Inc.).
2. Physical biochemistry (1982) by D. Freifilder (W.H. Freeman and Company).
3. A biologist's guide to principles and techniques in practical biochemistry (1986) by Keith Wilson, Kenneth H. Goulding (ELBS).
4. An introduction to practical biochemistry (2004) by Plummer D.T. (Tata McGraw Hill Publishers Co. Ltd., New Delhi).
5. Upadhyay, A. (2009). Biophysical chemistry. Himalaya Publishing House.

<b>Name of the Program</b>	Ph.D. Course work in Bioinformatics	<b>Program Code</b>	BINPH
<b>Name of the Course</b>	Computational and Systems Biology	<b>Course Code</b>	20BINPH11C3
<b>Hours/Week</b>	4	<b>Credits</b>	4
<b>Max. Marks.</b>	80	<b>Time</b>	3 Hours
<p><b>Note:</b> The examiner has to set a total of nine questions (two from each unit and one compulsory question consisting of short answer from all units. The candidate has to attempt one question each from each unit along the compulsory question (5 x 16 = 80 marks)</p>			
<p><b>Course Objectives:</b> This course aims to introduce:</p> <ol style="list-style-type: none"> <li>1. Different type of Biological Databases.</li> <li>2. Tools for DNA Sequence Analysis.</li> <li>3. Tools for Protein Sequence Analysis.</li> <li>4. Types of Biological Networks.</li> <li>5. Protein Protein Interaction Networks.</li> </ol>			
<p><b>Course Outcomes:</b> Students who complete this course will be able to:</p> <ol style="list-style-type: none"> <li>1. Discuss and explore the various Biological Databases.</li> <li>2. Analyze the DNA sequences with the available computational tools.</li> <li>3. Analyze the Protein sequences with the available computational tools.</li> <li>4. Explain working knowledge of the modeling that underpins much of systems biology.</li> <li>5. Exhibit strong skills in critical analysis and synthesis of scientific information using different computational tools.</li> </ol>			
<b>Unit - I</b>			
<p><b>Biological data</b> 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.</p>			
<b>Unit - II</b>			
<p><b>DNA sequence analysis</b> Sequence annotation and sequence analysis-Phylogeny of gene (blast, fasta, HMMer) and residue conservation. Primer design and T<sub>m</sub> Calculation, DNA Restriction pattern analysis. Condon bias and its effect on the protein expression with reference to various expression system.</p>			
<b>Unit - III</b>			
<p><b>Bioinfo tools 2 Protein sequence and structure insights (PSSI)</b> 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.</p>			
<b>Unit - IV</b>			
<p><b>Introduction to Systems Biology-I (SB)</b> Principles of Networks – Graph Theory and information theory of molecular systems; Types of</p>			

biological networks.

**Basics of Systems Biology-II (SB)**

Biological Network Databases Genomic networks (Gene regulation) Protein-protein interaction networks; Biochemical flux networks

**References:**

1. Waterman, M. S. (1995). *Introduction to computational biology: maps, sequences and genomes*. CRC Press.
2. TL, W. J. (Ed.). (2003). *Computational biology and genome informatics*. World Scientific.
3. Aluru, S. (Ed.). (2005). *Handbook of computational molecular biology*. CRC Press.
4. Haubold, B., & Wiehe, T. (2006). *Introduction to computational biology: an evolutionary approach*. Springer Science & Business Media.
5. Kitano, H. (2001). *Foundations of systems biology*. The MIT Press Cambridge, Massachusetts London, England.
6. Klipp, E., Herwig, R., Kowald, A., Wierling, C., & Lehrach, H. (2005). *Systems biology in practice: concepts, implementation and application*. John Wiley & Sons.

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CENTRE FOR BIOINFORMATICS

<b>Name of the Program</b>	Ph.D. Course work in Bioinformatics	<b>Program Code</b>	BINPH
<b>Name of the Course</b>	Structural Bioinformatics	<b>Course Code</b>	20BINPH11C4
<b>Hours/Week</b>	4	<b>Credits</b>	4
<b>Max. Marks.</b>	80	<b>Time</b>	3 Hours

**Note:** The examiner has to set a total of nine questions (two from each unit and one compulsory question consisting of short answer from all units. The candidate has to attempt one question each from each unit along the compulsory question (5 x 16 = 80 marks)

**Course Objectives:**

This course aims to introduce:

1. Protein Structure Prediction Techniques.
2. Molecular Modeling and Dynamics studies.
3. Drug Discovery and Development Strategy.
4. Structural Bioinformatics Tools.
5. QSAR Methodology.

**Course Outcomes:**

Students who complete this course will be able to:

1. Account for the structure of proteins, DNA and RNA
2. Model the novel protein structures and simulate the structures using molecular dynamics applications.
3. Explain basic principles of experimental methods used for the determination of the structure of macromolecules.
4. Use computer programs to visualize three-dimensional structures and analyze the relationship between structure and function.
5. Perform Docking studies and access various online tools and databases for the purpose of *in silico* drug designing.

**Unit - I**

**Protein Structure Prediction** Introduction, Protein Stability and Folding, Application of Hydrophobicity, Superposition of Structures, DALI methods, Evolution of Protein Structures, CASP, Secondary Structure Prediction, Homology Modelling, Fold Recognition, ROSETTA, LINUS.

**Unit - II**

**Molecular Modeling and Dynamics** Introduction, Molecular Dynamics using simple molecules, Signification of Times steps & Temperature Conformational energy calculations and molecular dynamics, Docking by Energy minimization, Ramachandran Plot.

**Unit - III**

**Drug Discovery and Development** Drug Discovery Cycle, The Lead compound, Pharmacophore, Bioinformatics in drug discovery and development, chemical databases, ADME and Toxicity, Virtual Screening, Molecular Docking, Structure and Ligand Based Drug Designing, Case studies.

**Unit - IV**

**Structural Bioinformatics tools** Tools for Molecular Visualization and Analysis: RASMOL, PYMOL, VMD, SWISS-PDB Viewer. Molecular Modeling and Docking: Swiss-Model, Arguslab, Hex, DOCK and Autodock. Online Tools: Biology Workbench, Marvin Sketch, Chemskech, Pubchem.

**Quantitative tools** Introduction to QSAR methodologies, Types of QSAR methods – 2D, 3D, 4D, 5D and 6D-QSAR methodologies, Descriptors classification, Application of QSAR in molecular design.

**References:**

1. Leach, A. R., & Gillet, V. J. (2007). An introduction to chemoinformatics. Springer.
2. Mannhold, R., Kubinyi, H., & Folkers, G. (2005). Chemoinformatics in drug discovery (Vol. 23). T. I. Oprea (Ed.). Weinheim:: Wiley-VCH.
3. Mannhold, R., Kubinyi, H., & Folkers, G. (2006). Chemoinformatics in drug discovery (Vol. 23). John Wiley & Sons.
4. Gu, J., & Bourne, P. E. (Eds.). (2009). Structural bioinformatics (Vol. 44). John Wiley & Sons.
5. Brown, J. B. (Ed.). (2018). Computational Chemogenomics. Humana Press.
6. Wei, D., Xu, Q., Zhao, T., & Dai, H. (Eds.). (2015). Advance in structural bioinformatics. Springer.