# Syllabus for Pre. Ph.D. (Bioinformatics)

# Computational & Systems biology

Theory Marks:80 Internal assessment:20

Note for Examiner: Examiner should set 2 questions from each unit. Each question shall carry 16 marks. Students will have to attempt at least one question from each unit.

#### Unit-1

# **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

# **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

# Bioinfo tools 2 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

# **Introduction to Systems Biology-I (SB)**

Principles of Networks – Graph Theory and information theory of molecular systems Types of biological networks.

#### Unit-5

# Basics of Systems Biology-II (SB)

Biological Network Databases Genomic networks (Gene regulation)

Protein-protein interaction networks; Biochemical flux networks

Students are advised to consult relevant journal articles and reviews to gather the recent information on the above mentioned topics

**Research Methodology** 

Theory Marks:80

#### Internal assessment:20

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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 heir electrochemical properties, membrane potential, action potential and propagation of impulses; PPI

#### Unit-2

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

# Unit-3

Theory of centrifugation and application to biological systems. Rotors angle/vertical/zonal/continous flow centrifuge, differential centrifugation density gradient centrifugation. Ultra centrifugation principle and application. Chromatography – adsorption, affinity, partition, Ion-exchange, gelpermeation, GLC, TLC, RPC, HPLC etc.

#### Unit -4

Introduction to principles and applications of (a)Spectroscopic methods (UV, Vis, IR, Fluorescence, ORD, CD, & PAS) (b)NMR, ESR & Mass spectrometery, Use of radioactive and stable isotopes and their detection in biological systems.

#### Unit-5

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.

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# **Structural Bioinformatics**

Theory Marks:80 Internal assessment:20

Note for Examiner: Examiner should set 2 questions from each unit. Each question shall carry 16 marks. Students will have to attempt at least one question from each unit.

Unit-1 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-2

# **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-3

# **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-4

# **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.

# Unit-5

# **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.

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