Course Title: In Silico Innovation: Computer-Aided Drug Design and Network Pharmacology

Course Description:

This course introduces computational approaches for drug discovery, integrating bioinformatics, structure-based and ligand-based drug design, and network pharmacology. Students will gain hands-on experience in sequence analysis, molecular modeling, docking, ADMET prediction, and systems-level network analysis of drug–target interactions.

Module I: Introduction to Bioinformatics and Biological Databases

Overview:
This module introduces the fundamentals of bioinformatics and the use of biological databases for molecular data analysis, functional annotation, and drug discovery applications.

Topics Covered:

- Introduction to bioinformatics: scope and applications in drug discovery
- Biological data types: DNA, RNA, and protein sequences
- Functional annotation of sequences
- Sequence data retrieval and database overview
- Key bioinformatics tools and workflows for molecular analysis

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Module II: Sequence Analysis and Molecular Biology Tools

Overview:
This module focuses on computational methods for sequence comparison, functional prediction, evolutionary studies, and support for molecular biology experiments.

Topics Covered:

- Sequence similarity searching using BLAST
- Conserved domain analysis with CDD BLAST
- Open Reading Frame (ORF) detection and gene prediction
- Multiple Sequence Alignment (MSA) and evolutionary analysis
- Phylogenetic tree construction and interpretation
- In silico PCR and primer design strategies
- Primer validation and optimization

Module III: Computer-Aided Drug Design (CADD)

Overview:
This module provides comprehensive knowledge of computational approaches in drug discovery, from target identification to molecular interaction analysis and simulation.

Topics Covered:

- Drug discovery pipeline and target identification
- Structure-based and ligand-based drug design principles
- Protein structure analysis and chemical representation
- Ligand preparation and chemical structure drawing
- Drug-likeness evaluation and physicochemical profiling
- ADME and toxicity prediction
- Protein structure modeling, AlphaFold prediction, and model validation
- Pharmacophore modeling for lead identification
- Molecular docking and protein–ligand interaction analysis
- Interpretation of docking results
- Molecular dynamics and flexibility analysis of protein–ligand complexes

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Module IV: Network Pharmacology

Overview:
This module focuses on systems-level drug discovery, integrating pharmacology with network biology to understand multi-target drug actions and biological pathways.

Topics Covered:

- Concepts of network and systems pharmacology
- Multitarget drug discovery strategies
- Identification of bioactive compounds from natural sources
- Prediction of compound–target interactions and disease-associated targets
- Protein–protein interaction (PPI) network construction and analysis
- Hub target identification using network topology
- Functional enrichment (Gene Ontology) and pathway (KEGG) analysis
- Construction of drug–target, target–pathway, and integrated drug–target–pathway networks
- Docking validation of key targets

Course Learning Outcomes (CLOs):

After completing this course, students will be able to:

1. Retrieve and analyze biological sequence data using bioinformatics tools.
2. Perform sequence alignment, phylogenetic analysis, and primer design.
3. Apply CADD approaches, including docking, pharmacophore modeling, and molecular dynamics.
4. Evaluate drug-likeness, ADME, and toxicity profiles of lead compounds.
5. Construct and analyze network pharmacology models for multi-target drug discovery.
6. Integrate computational tools for systems-level drug discovery insights.

Assessment:

- **Class Attendance:** 20%
- **Practical / Assignments:** 40%
- **Case Study / Project:** 40%