Value Added Certificate Course, 2024-25

On

"Computer-Aided Drug Design: Hands-On Skill Development"

Department of Bioinformatics, B.J.B Autonomous College

Objective of the course:

- To introduce students to the principle and applications of computer-aided drug design (CADD).
- To provide hands-on experience in molecular docking using AutoDock Vina and PyMOL.
- To explore the concepts and application of Quantitative Structure-Activity Relationship (QSAR) in drug design.
- To enable student to apply CADD techniques in real-world drug discovery projects.

Expected Outcomes:

Upon completion of the course, students will be able to:

- Understand the basics of CADD, including molecular docking and QSAR.
- Perform molecular docking simulation using AutoDock Vina.
- Visualize and analyze molecular interaction using PyMOL.
- Apply QSAR methods to predict the biological activity of chemical compound.
- Develop and implement small-scale drug design project using CADD tools.

Course Structure:

- Duration: 30 hours (10 days, 3 hours/day)
- Target Audience: UG/PG students interested in Life science, Chemistry, bioinformatics, and related fields.
- Time Schedule: In all working days from 2pm to 5pm.
- Class Size: 31 students
- Mode of learning: Blended (online/offline)
- Assessment: Practical exam and project work.

Examination and Certification:

- Assessment:
    - Practical Exam: Hands-on task to solve drug design problem using CADD tools.
    - Project work: Competition and presentation of a mini-project in drug design.
- Certification: Provided by the Department of Bioinformatics

Resource Person:

- Mr. Sabyasachi Mohanty, Head of Department, Department of Bioinformatics

Syllabus

Unit – 1: Introduction to Computer-Aided Drug Design

I. Overview of Drug Discovery Process
II. Introduction to CADD: Principle and Techniques
III. Introduction to Molecular Docking: Concepts and Applications
IV. Hands-on Session: Setting Up the Environment (AutoDock Vina and PyMOL)

Unit – 2: Molecular Docking with AutoDock Vina

I. Basics of Molecular Docking: Binding Affinity and Scoring Functions
II. Preparing Ligands and Receptor for Docking
III. Running Docking simulations with AutoDock Vina
IV. Hands-on Session: Performing Docking Studies on the Sample Targets

Unit – 3: Visualization and Analysis with PyMOL

I. Introduction to PyMOL: Interface and Features
II. Visualization Docking Results: Ligand-Receptor Interactions
III. Hands-on Session: Analyzing Docking Poses and Interaction Maps
IV. Case Studies: Successful Drug Design Using Molecular Docking

Unit – 4: Introduction to QSAR and its Applications

I. Concepts of QSAR: Historical Background and Importance
II. QSAR Modeling: Descriptor Calculation and Model Building
III. Hands-on Session: Creating QSAR Models using Software Tools
IV. Validating QSAR Models: Statistical Analysis and Predictive Power

Unit – 5: Advanced Topics and Project work

I. Combining Docking and QSAR for Drug Design
II. Introduction to Other CADD Techniques: Pharmacophore Modeling, ADMET Prediction
III. Hands-on Session: Implementing a Mini-Project in CADD
IV. Project Presentation: Students present their findings and projects

Books and Resources:

- *Molecular Modeling: Principle and Application* by Andrew R. Leach
- *The Art of Molecular Dynamics Simulation* by D. C. Rapaport
- *Principle of Computer-Aided Drug Design* by Thomas J. Perun and C. L. Propst
- *Molecular Docking: Basics, Advance and State-of-Art* by Belal F. M. Zaki
- *Introduction to Quantitative Structure-Activity Relationship (QSAR) Methodology* by Kunal Roy
- *Molecular Docking for Chemist* by Suleyman Temel
- *PyMOL User's Guide* by Warren L. DeLano