IIITD&M Kancheepuram

SIDI

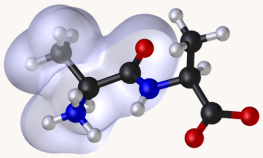
School of Interdisciplinary Design & Innovation

Product Research and Innovation in bioMedical Engineering (PRIME) Lab

One Day Workshop on

Molecular Modeling and Bioinformatics for Healthcare

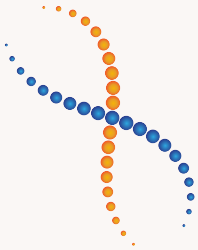
Session 1



Introduction to Molecular Modeling and Bioinformatics

- Overview of molecular modeling in healthcare applications
- Role of bioinformatics in drug discovery and precision medicine
- Tools and databases used in molecular modeling.

Session 2



Protein Structure Prediction and Analysis

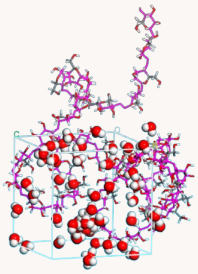
- Homology modeling and molecular dynamics simulations
- Protein-ligand docking basics (AutoDock, ClusPro, etc.)
- Energy minimization and stability assessment

Session 3

Computational Drug Design

- Virtual screening and drug repurposing
- QSAR modeling and molecular docking case study
- ADME-Tox prediction tools (SwissADME, pkCSM)

Session 4



Molecular Dynamics Simulations

- Preparing the System: Protein, Ligand, and Solvent Setup
- Running MD Simulations Using GROMACS/NAMD/AMBER
- Analyzing Trajectories: RMSD, RMSF, Hydrogen Bonds, and SASA
- Free Energy Calculations (MM-PBSA/MM-GBSA) and Case Studies

25th February 2025

10:00 AM - 5:00 PM

Room No 413, 4th Floor, Laboratory complex, IIITDM Kancheepuram

Registration Fees: 200/- for students and 400/- for faculties

Registration link: https://www.onlinesbi.sbi/sbicollect/icollecthome.htm?corpID=634626

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