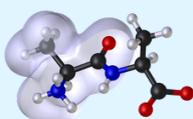


One Day Workshop on

# Bioinformatics and Healthcare: Concepts, Tools and Applications

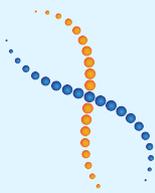
**Session 1**



## 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

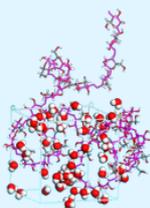
**Session 3**



## 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



27th February 2026

10:00 AM - 5:00 PM



Room No: H25, Second Floor, Academics complex, IIITDM Kancheepuram



Registration Fees: 300/- for students and 400/- for faculties

Registration link: <https://onlinesbi.sbi.bank.in/sbicollect/>

Instructions for registration: [Click Here](#)



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