Advanced Computer-Aided Drug Design and Drug Discovery

Course Outline

Instructors:

Ruhul Kuddus Shiddiky
Founder & CEO, Omics-Lab BD
Research Assistant at Bioinformatics Lab, IUB.
Research Assistant at Bioinformatics Lab (Dry), University of Rajshahi.
M.Pharm Thesis Student at Phytopharmacology Lab (Wet & Dry), Department of Pharmacy

Sajib Ghosh
Co-founder & Lead Trainer, Omics-Lab BD
Research Assistant at Bioinformatics Lab, IUB.
Research Assistant at Bioinformatics Lab (Dry), University of Rajshahi.
M.Pharm Thesis Student at HEAT Project (Wet & Dry), Department of Pharmacy

Course Contents	
Session-1	**Introduction** • Introduction and Definition of Bioinformatics • Brief History of Bioinformatics • Major Research Fields of Bioinformatics • Applications of Bioinformatics • Bioinformatics in Modern Drug Discovery
Session-2	**CADD Workflow** • Software Installation • Publication-Ready Advanced CADD Pipeline • Target Identification & PDB ID Selection • Ligand Collection and Library Construction • Insilco Pass Prediction • Structure Conversion and Optimization • Protein Preparation & Energy Minimization
Session-3	**Homology Modelling** • Homology Modelling of Target Protein • Quality Assessment • Ramachandran Plot Evaluation • Fundamentals of Molecular Docking
Session-4	**Molecular Docking Analysis** • Software Installation • Active Site Prediction and Grid Box Generation • Blind Molecular Docking

	• Site Specific Molecular Docking • Redocking For Protocol Validation
Session-5	**Post Docking Analysis** • Software Installation • Complex generation • Publication Quality Visualization • 2D & 3D Interaction Figure Generation • Publication Ready Docking Table
Session-6	**Drug Likeness & ADMET Analysis** • Lipinski Rule of 5 • Drug Likeness Evaluation • Oral Bioavailability Evaluation • Absorption, Distribution, Metabolism & Excretion Analysis • Toxicity Analysis • Publication-Ready Table Generation
Session-7	**Molecular Dynamics Simulation** • Basic Fundamentals of MD Simulation • Overview of the MD Trajectories • RMSD • RMSF • SASA • Radius of Gyration • Hydrogen Bonding • PCA • MM-PBSA & MM-GABSA
Assignment	