Schedule of Seven days

Online Skill Development Program

on

"Molecular Dynamics Simulations and In-Silico Drug Designing"

09 – 15 December 2021

Day	Time	Experiment
Day 1	06:00 pm – 08:30 pm	Introductory lecture on Molecular Dynamics Simulations and In-Silico Drug Designing.
		Protein retrieval and Active site prediction (RCSB – PDB, Discovery studio, CASTp)
Day 2	06:00 pm – 08:30 pm	Selection of ligand and Dataset preparation (PubChem, ChemSpider, Open Babel)
		Drug likeliness of compound and Screening of ligands on basis of Lipinski rule of 5
Day 3	06:00 pm – 08:30 pm	Ligand property prediction and screening (DriLiTo, ADMET-SAR, Swiss-ADME)
		Homology modelling for structure of unknown proteins
Day 4	06:00 pm – 08:30 pm	Protein and Ligand Preparation on ADT
		Docking in Autodock Vina
Day 5	06:00 pm – 08:30 pm	Docking in PyRx
		ProteInteraction of Protein-ligand residues in the active site using LigPlot
Day 6	06:00 pm – 08:30 pm	Poses analysis using PyMol
		Molecular Dynamics Simulation using GROMACS (Part 1)
Day 7	06:00 pm – 08:30 pm	Molecular Dynamics Simulation using GROMACS (Part 2)
		Analysis of the plots of simulation
		Final discussion/Conclusion, Certificate distribution & Feedback