Course Content

Week	Content/ topic/ activity
1	Overview of Open Access Cheminformatics Toolkits, Software, Workflow Environments, and Databases
2	Identify the Binding Sites, and Basics of Molecular Docking
3	Project 1 – Docking
4	Receptor Flexibility in Structure-Based Drug Discovery
5	Project 2 – Ensemble Docking and Virtual Screening
6	Pharmacophore Modeling and Fragment-Based Drug Design
7	Molecular Dynamics Simulations in Drug Design
8	Free Energy Calculations and Lead Optimization
9	Project 3 – Relative Binding Free Energy Calculation
10	Oral Presentation – Docking or Virtual Screening
11	Oral Presentation – MD Simulations or Free Energy Calculations
12	Oral Presentation – Drug Discovery, Design, or Optimization.
13	MED Seminar (External Speaker)
14	Final Exam