2. Prepare ligand

2. Prepare protein

3. Perform Drug-likeness test on SwissADME

1. Obtain ligand from PubChem

1. Download protein crystal as .pdb file

3. Receptor grid generation

Docking

Molecular dynamics simulation

* Visualize ligand poses
* Rank ligand based on best scores
* Select poses based on set preferences
* Select best simulated complex at 100ns under OPLS-2005 force field in Desmond feature of Schrondinger

Cdk1 MDS Workflow