MD ANALYSIS UGM 2024

Freie Universität Berlin

molecular design.lab

OpenMMDL

A Workflow for Molecular Dynamics Simulations of Protein-Ligand Complexes

Setup Simulation Analysis

Valerij Talagayev,

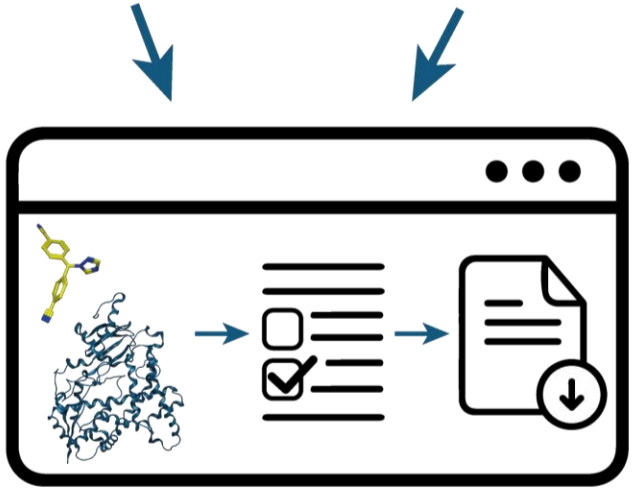
PhD Student, Wolber Lab

Freie Universität Berlin

Setup Simulation Analysis

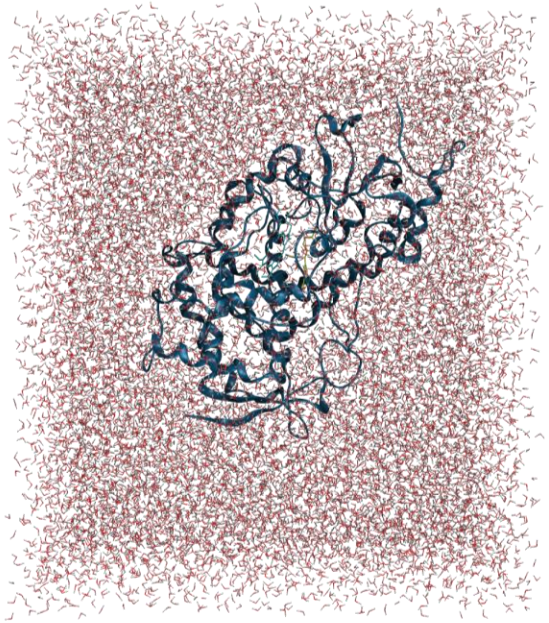
Setup

AmberTools PDBFixer



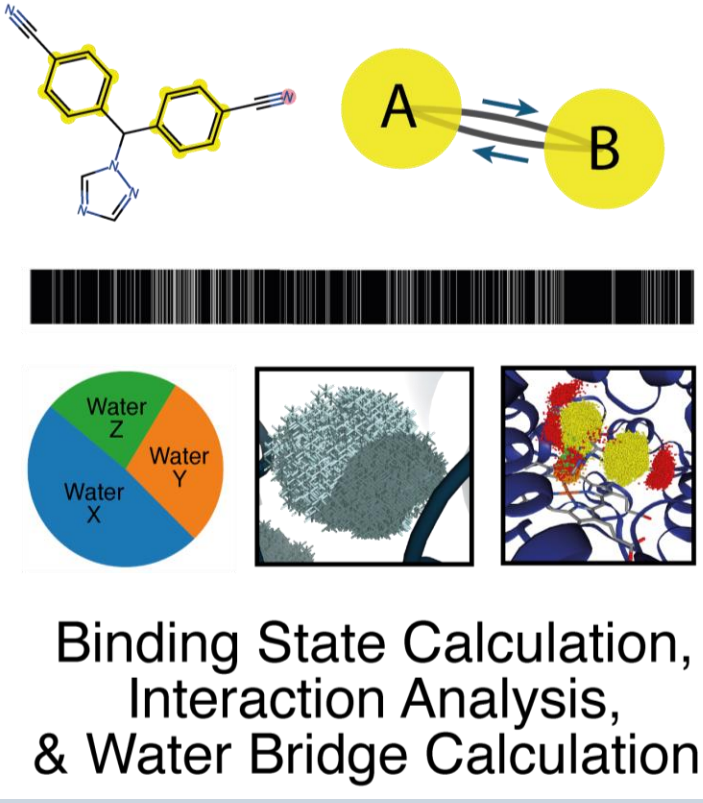
Structure-, System-
& simulation-configuration

Simulation



Preparation, Simulation
& Postprocessing

Analysis



Binding State Calculation,
Interaction Analysis,
& Water Bridge Calculation

Setup

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- Flask based Web application
  - Based upon OpenMM Setup
  - Contains two preparation options
  - Adjustment of Simulation Settings

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OpenMMDL Setup

Start Over | Quit

This PDB file contains 12 chains. Select which ones to include.

Chain	# Residues	Content	Include?
A	750	Protein	☑
B	745	Protein	☑
C	4	MAN, BMA, NAG	☐
D	2	NAG	☐
E	5	MAN, BMA, NAG	☐
F	4	MAN, BMA, NAG	☐
G	2	NAG	☐
H	4	MAN, BMA, NAG	☐
A	4	7VF, NAG	☐
B	2	7VF, NAG	☐
A	116	HOH	☐
B	81	HOH	☐

Select All | Select None

A heterogen is any residue other than a standard amino acid or nucleotide. Do you want to delete heterogens?

Keep all heterogens

Continue

Setup

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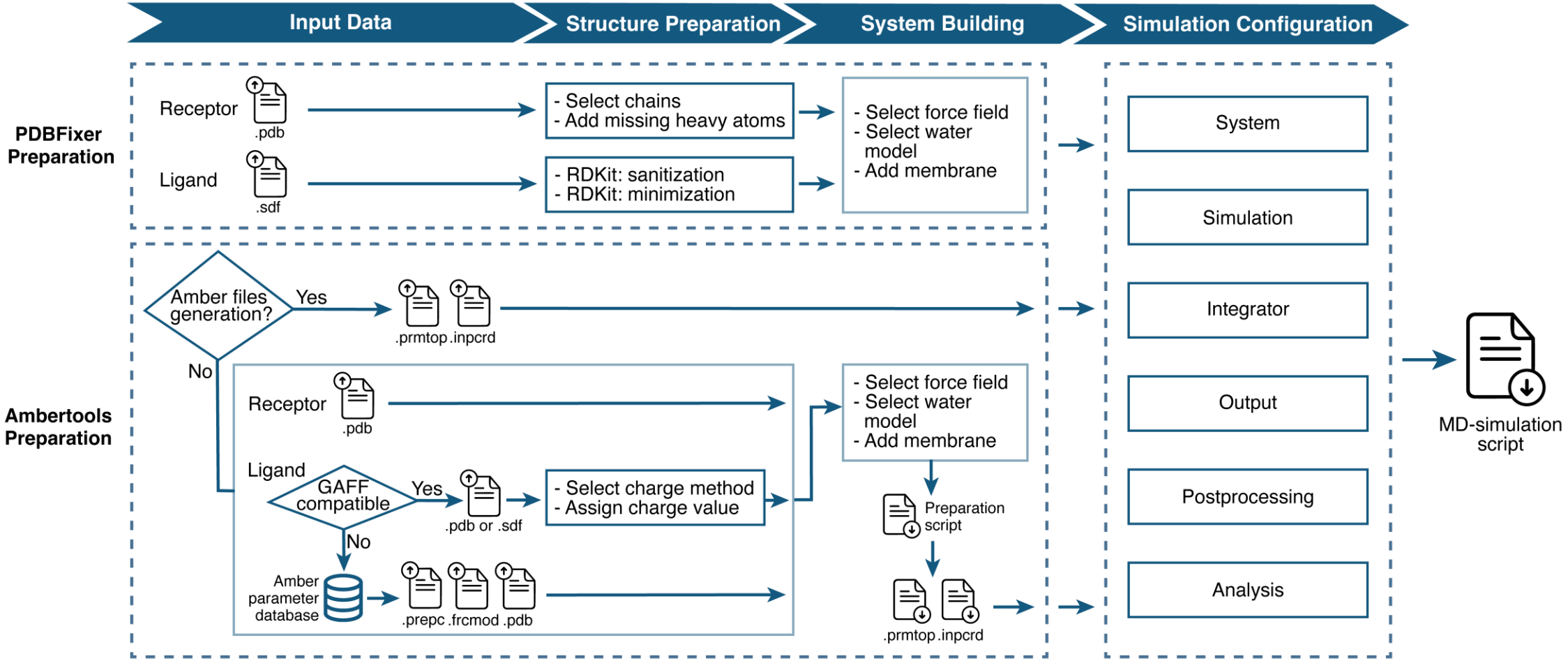

Simulation

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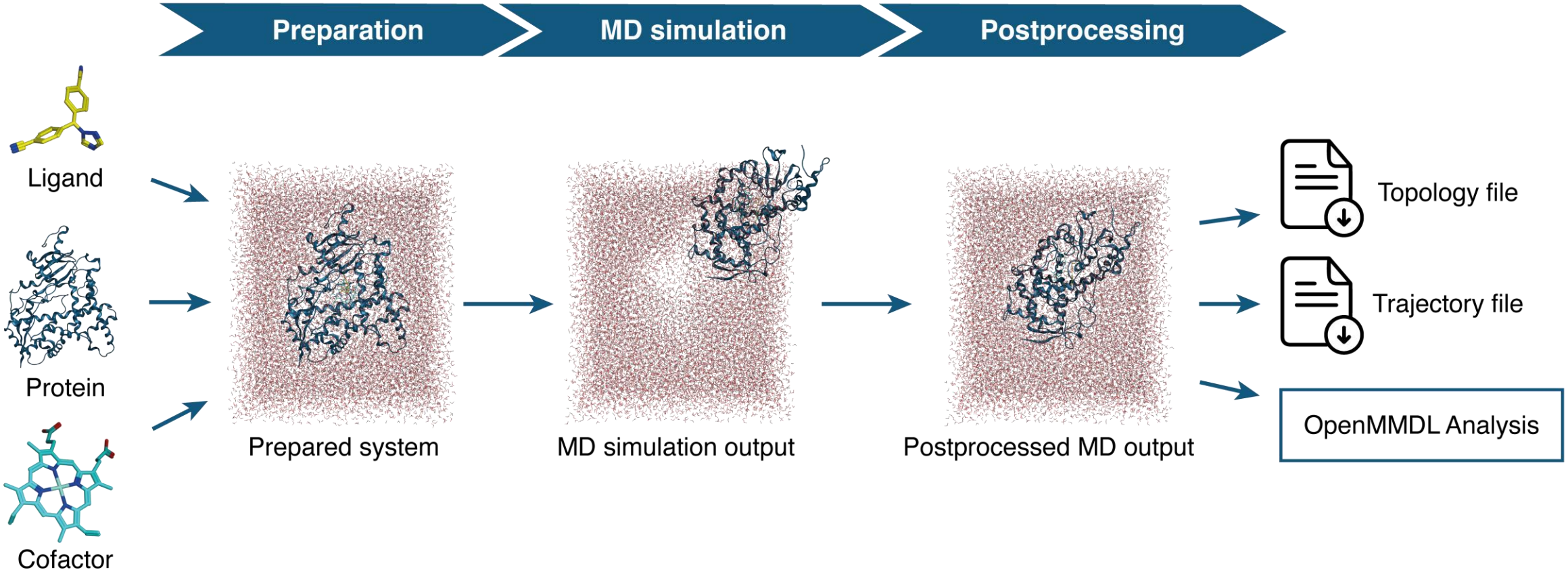
- Simulation with the settings obtained from Setup
  - Complex building
  - Postprocessing
    - MDTraj & MDAnalysis



Analysis

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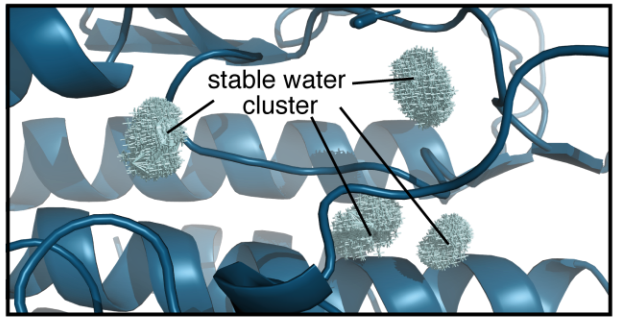
- Analysis of MD simulation trajectory

Stable Water Clustering

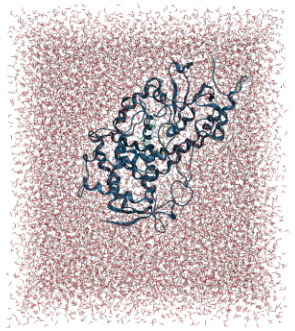
A



representative waters.pdb

interacting residues.csv

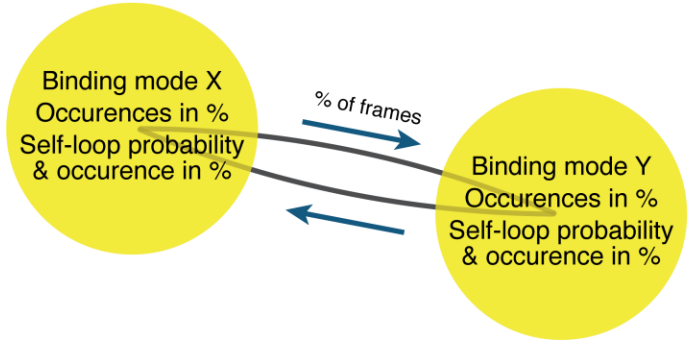
3D visualization of stable water clusters



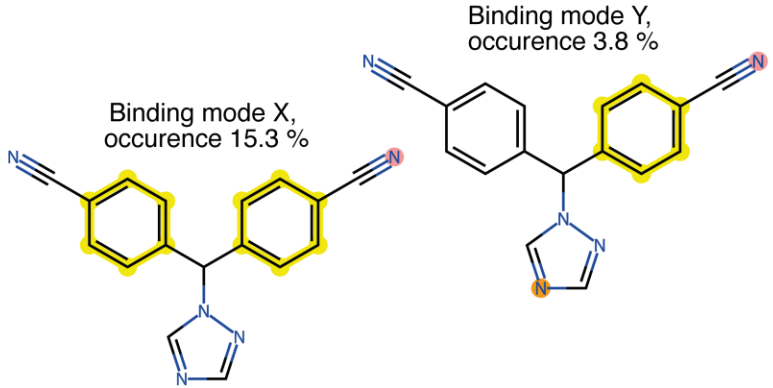
Simulation Output

Binding Mode Generation

B



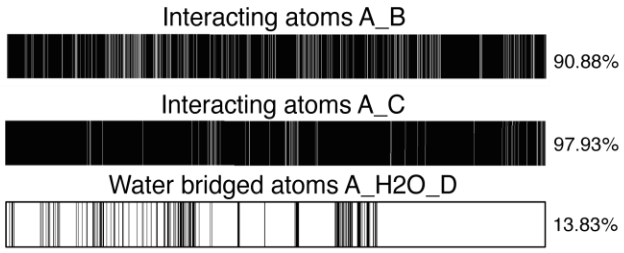
Markov state transition graphs



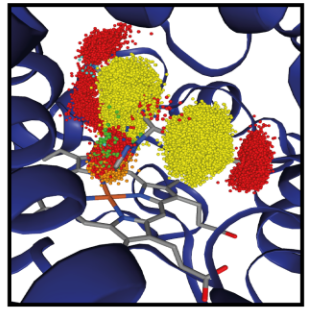
2D depiction of top binding modes

Interaction analysis

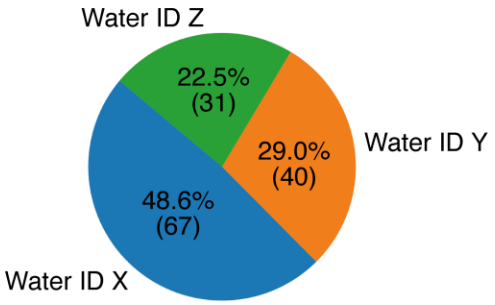
C



Interaction bar plots



Interaction visualization



Water bridge pie charts

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