Executed In Parallel
Toil: Management System

Intermidate MD

Post-Processing

Compute BFE

Complex Parameterization

End-State MD (REMD)

Restraint Files

Split Complex Into Guest and Host System

Run Complex Intermidate States

Post Analysis Complex MD Runs

Run Recetor Intermidate States

Post Analysis Receptor MD Runs

Run Ligand Intermidate States

Post Analysis Ligand MD Runs

Compute BFE With MBAR