

SDF, PDB



Docking

3D poses



Mapping

Perturbation network



Simulation setup

Free energy simulation

Bound

Free



MBAR

Perturbation network analysis



$\Delta\Delta G$ of binding

Maestro

Marvin Tools

rDock

Manual

FESetup

Sire/SOMD

Sire/analyse_freenrg

freenrgworkflows

Protocol refinement

