START

System Preparation

GET YOUR PDB
(RCSB, literature, etc.)

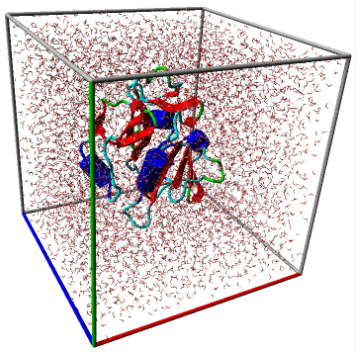
pippo.pdb

PREPARE FILE FOR GMX
(pdb2gmx)

conf.gro
topol.top
posre.itp

GENERATE BOX
(editconf)

box.gro



ADD WATER
(solvate)

solv.gro

ADD IONS
(grompp + genion)

ions.gro

Simulation

ENERGY MINIMIZATION
(grompp + mdrun)

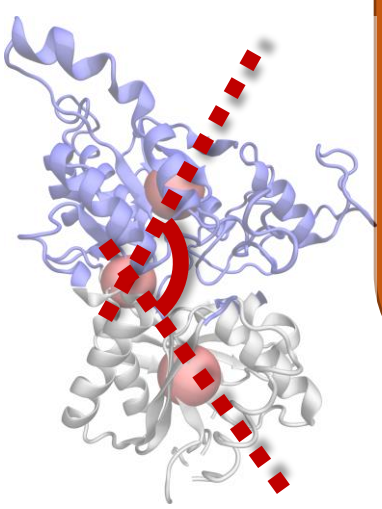
1em.gro
1em.xtc
1em.trr
1em.edr
1em.cpt
1em.log

POSITION RESTRAINTS
EQUILIBRATION
(grompp + mdrun)

2nvt.gro
2nvt.xtc
2nvt.trr
2nvt.edr
2nvt.cpt
2nvt.log

PRODUCTION
(grompp + mdrun)

3md.gro
3md.xtc
3md.trr
3md.edr
3md.cpt
3md.log



ANALYSIS
(rms, cluster, rmsf, gyrate,
distance, mindist, ..)

END