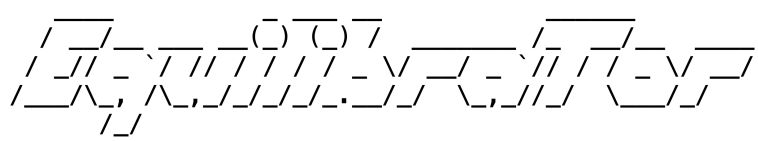


PROTEIN PDB

GENERATE TOPOLOGY FOR PROTEIN

[protein PDB input]

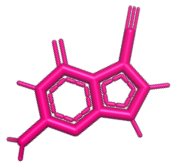
↓

[gmx pdb2gmx -f ...]

↓

[protein.gro] [topol.top]

LIGAND PDB



CONVERT LIGAND PDB TO MOL2

[ligand PDB input]

↓

[obabel -ipdb -omol2 ... -h]

↓

[ligand.mol2]

MERGE TOPOLOGIES

[protein.gro] [ligand.gro]

↓

[merge_topologies()]

↓

[merged.gro]

GENERATE TOPOLOGY FOR LIGAND

[ligand.mol2]

↓

[acpype -i ... -l -o gmx -b ...]

↓

[ligand outputs (e.g., *.gro)]

CREATE THE SIMULATION BOX

[protein.gro or merged.gro]

↓

[gmx editconf -c -d 1.2 -bt cubic]

↓

[box.gro (centered, boxed)]

SOLVATE THE SYSTEM

[box.gro] [spc216.gro]

↓

[gmx solvate -cp ... -cs ... -o ... -p ...]

↓

[solvated.gro] [topol.top (updated)]

NEUTRALIZE THE SYSTEM

[ions.mdp] [solvated.gro] [topol.top]

↓

[gmx grompp → ions.tpr]

↓

[echo SOL | gmx genion -s ions.tpr ...]

↓

[sol_ions_gro] [topol.top (updated)]

RUN ENERGY MINIMIZATION

[minim.mdp] [sol_ions_gro] [topol.top]

↓

[gmx grompp → em.tpr]

↓

[gmx mdrun -deffnm em]

RUN NVT EQUILIBRATION

[equilibration.mdp] [em.gro] [topol.top]

↓

[gmx grompp → eq.tpr]

↓

[gmx mdrun -deffnm eq]

RUN NPT EQUILIBRATION

[equilibration_2.mdp] [eq.gro] [topol.top]

↓

[gmx grompp → npt.tpr]

↓

[gmx mdrun -deffnm npt]

MULTIPLE FIGURES

1. Potential energy vs time (ps)
2. Pressure vs time (ps)
3. Temperature vs time (ps)
4. RMSD vs time (ps)
5. RMSF vs residue
6. Radius of gyration vs time (ps)

FRAME PDB FILES