Quick Start Guide: MD Simulation of a Protein in Water (GROMACS)

Input Files:

protein.pdb (without water and any ligands)

ions.mdp

minim.mdp

nvt.mdp

npt.mdp

md.mdp

Step 1: Prepare the Topology

gmx pdb2gmx -f protein.pdb -o protein_processed.gro

When prompted, select the desired force field and water model

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Step 2: Defining the Unit Cell & Adding Solvent

Defining the Unit Cell

gmx editconf -f protein_processed.gro -o protein_newbox.gro -c -d 1.0 -bt cubic

Adding Solvent

gmx solvate -cp protein_newbox.gro -cs spc216.gro -o protein_solv.gro -p topol.top

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Step 3: Adding Ions

Prepare the system for ion addition

gmx grompp -f ions.mdp -c protein_solv.gro -p topol.top -o ions.tpr

Add ions to neutralize the system and reach physiological salt concentration

gmx genion -s ions.tpr -o protein_solv_ions.gro -p topol.top -pname NA -nname CL -neutral -conc 0.15

When prompted, select the SOL group.

Step 4: Energy Minimization

Prepare the system for Energy Minimization

gmx grompp -f minim.mdp -c protein_solv_ions.gro -p topol.top -o em.tpr

Run Energy Minimization

gmx mdrun -v -deffnm em

Step 5: NVT Equilibration

Prepare the system for NVT Equilibration

gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr

Run NVT Equilibration

gmx mdrun -v -deffnm nvt

Step 6: NPT Equilibration

Prepare the system for NPT Equilibration

gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

Run NPT Equilibration

gmx mdrun -v -deffnm npt

Step 7: Production MD

Prepare the system for Production MD

gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md.tpr

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Run Production MD

gmx mdrun -v -deffnm md