Protein-RNA complex Molecular Dynamics simulation tutorial (Gromacs version 2023)

Input PDB file: Download the protein-RNA complex from RCSB PDB.

Input Gromacs file:

1. ions.mdp,
2. minim.mdp or em.mdp,
3. nvt.mdp
4. npt.mdp,
5. md.mdp

Create a directory example: simulation

$ **mkdir simulation**

Note: Keep all the input Gromacs and pdb file in your working directory created before.

Source the gromacs executable installed on your machine:

$ **source /usr/local/gromacs-2023/bin/GMXRC** (note : use your executable as installed in your machine replacing gmx-2023 accordingly)

example – if your executable is gmx then replace gmx-2023 with gmx in following commands.

1. gmx-2023 pdb2gmx -f 8ID2_sim.pdb -o 8ID2_processed.gro -water tip3p
   - select group 6: (AMBER99SB-ILDN)

2. gmx-2023 editconf -f 8ID2_processed.gro -o 8ID2_cubicbox.gro -c -d 1.0 -bt cubic

3. gmx-2023 solvate -cp 8ID2_cubicbox.gro -cs spc216.gro -o 8ID2_solvated.gro -p topol.top

4. gmx-2023 trjconv -s 8ID2_solvated.gro -f 8ID2_solvated.gro -o 8ID2_solvated_compact.gro -pbc atom -ur compact
   - select group 0: (System)

5. gmx-2023 trjconv -s 8ID2_solvated.gro -f 8ID2_solvated.gro -o 8ID2_solvated_compact.pdb -pbc atom -ur compact

6. gmx-2023 grompp -f ions.mdp -8ID2_solvated_compact.gro -p topol.top -o 8ID2_ions.tpr -maxwarn 1

7. gmx-2023 genion -s 8ID2_ions.tpr -o 8ID2_solv_ions.gro -p topol.top -pname NA -nname CL -neutral
   - select group 14: (SOL)

8. gmx-2023 grompp -f minim.mdp -c 8ID2_solv_ions.gro -p topol.top -o 8ID2_em.tpr

9. gmx-2023 mdrun -v -deffnm 8ID2_em

10. gmx-2023 energy -f 8ID2_em.edr -o potential.xvg
    - select group 10: Potential

11. gmx-2023 make_ndx -f 8ID2_em.gro -o index.ndx
    INPUT: 1|12 (Protein_RNA)

12. gmx-2023 grompp -f nvt.mdp -c 8ID2_em.gro -r 8ID2_em.gro -p topol.top -o 8ID2_nvt.tpr -n index.ndx -maxwarn 1

13. gmx-2023 mdrun -v -deffnm 8ID2_nvt

14. gmx-2023 energy -f 8ID2_nvt.edr -o 8ID2_nvt_temperature.xvg
    - select group 16: Temperature

15. gmx-2023 grompp -f npt.mdp -c 8ID2_nvt.gro -r 8ID2_nvt.gro -t 8ID2_nvt.cpt -p topol.top -o 8ID2_npt.tpr -n index.ndx -maxwarn 1

16. gmx-2023 mdrun -v -deffnm 8ID2_npt

17. gmx-2023 energy -f 8ID2_npt.edr -o 8ID2_npt_pressure.xvg
    - select group 18: Pressure

18. gmx-2023 energy -f 8ID2_npt.edr -o 8ID2_npt_density.xvg
    - select group 24: Density

19. gmx-2023 grompp -f md.mdp -c 8ID2_npt.gro -t 8ID2_npt.cpt -p topol.top -o 8ID2_md.tpr

20. gmx-2023 mdrun -v -deffnm 8ID2_md