**Gromacs** for Molecular Dynamics Simulations

These are the basic commands to perform simple peptide in water simulation to get a feel of protein folding process via MDS. These commands will work for Gromacs 2018.X versions.

**pdb2gmx module of gromacs ‘gmx’ command** generates a necessary topology file, position restraint file and force field compliant .gro file from input PDB

* gmx pdb2gmx -f ubq.pdb -o ubq\_pro.gro -water spce

**editconf module** generates a box of given dimension and type around the protein

* gmx editconf -f ubq\_pro.gro -o ubq\_box.gro -c -d 1.0 -bt cubic

**solvate** module fills up the box with water molecules

* gmx solvate -cp ubq\_box.gro -cs spc216.gro -o ubq\_solv.gro -p topol.top

**Adding counter ions**

Grompp compiles the files into a .tpr file and genion adds ions

* gmx grompp -f ions.mdp -c ubq\_solv.gro -p topol.top -o ions.tpr
* gmx genion -s ions.tpr -o ubq\_ions.gro -p topol.top -pname NA -nname CL -np 2

**Minimization**

* gmx grompp -f minim.mdp -c ubq\_ions.gro -p topol.top -o em.tpr
* gmx mdrun -v -deffnm em
* gmx energy -f em.edr -o potential.xvg

**Heating (NVT)**

* gmx grompp -f nvt.mdp -c em.gro -p topol.top -o nvt.tpr -r em.gro
* gmx mdrun -deffnm nvt
* gmx energy -f nvt.edr -o temperature.xvg

**Equilibration (NPT)**

* gmx grompp -f npt.mdp -c nvt.gro -t nvt.cpt -p topol.top -o npt.tpr -r nvt.gro
* gmx mdrun -v -deffnm npt
* gmx energy -f npt.edr -o pressure.xvg
* gmx energy -f npt.edr -o density.xvg

**Production MD (NPT)**

* gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md\_01.tpr
* gmx mdrun -v -deffnm md\_01

**Trajectory correction with respect to PBC**

* gmx trjconv -s em.tpr -f em.trr -o em\_mod.trr -pbc mol -ur compact
* gmx trjconv -s nvt.tpr -f nvt.trr -o nvt\_mod.trr -pbc mol -ur compact
* gmx trjconv -s npt.tpr -f npt.trr -o npt\_mod.trr -pbc mol -ur compact
* gmx trjconv -s md\_01.tpr -f md\_01.xtc -o md\_01\_mod.xtc -pbc mol -ur compact

RMSD Graph

* gmx rms -s md\_01.tpr -f md\_01\_mod.xtc -o rmsd.xvg