Commands to Analyze the MD Simulation of protein-ligand complex output Data

**Step-1: Bringing Protein to the center of the box**

gmx trjconv -s md.tpr -f md.xtc -o md\_center.xtc -pbc mol -center

Step-2: Calculation of RMSD

gmx rms -s md.tpr -f md\_center.xtc -o rmsd.xvg -tu ns

Step-3: Calculation of RMSF

gmx rmsf -s md.tpr -f md\_center.xtc -o rmsf.xvg -res

Step-4: Calculation of Radius of Gyration

gmx gyrate -s md.tpr -f md\_center.xtc -o gyrate.xvg

Step-5: Calculation of Total Number of Hydrogen bonds

gmx hbond -s md.tpr -f md\_center.xtc -num hydrogen.xvg -tu ns

Step-6: Calculation of Total Solvent Accessible Surface Area

gmx sasa -s md.tpr -f md\_center.xtc -o area.xvg -tu ns

Step-7: Calculation of Binding Energy

gmx grompp -f ie.mdp -c npt.gro -t npt.cpt -p topol.top -n index.ndx -o ie.tpr

gmx mdrun -deffnm ie -rerun md.xtc

gmx energy -f ie.edr -o interaction\_energy.xvg