COMMANDS TO RUN MDS OF PROTEIN-LIGAND COMPLEX

Step-1: Preparation of protein and ligand.

- Use Discovery studio software.

Step-2: Preparation of protein topology file

gmx pdb2gmx -f receptor.pdb -o receptor.gro

Step-3: Preparation of ligand topology file.

- Use the Swiss Param online server.

Use the below command to generate the ligand.gro file

gmx editconf -f LIG.pdb -o lig.gro

Step-4:

1. Merging of the receptor.gro and ligand.gro file to create the complex.gro file.
2. Modification of topol.top file.

Step-5: Solvation

gmx editconf -f complex.gro -o newbox.gro -bt dodecahedron -d 1.0

Once the above command is executed, run the following command

gmx solvate -cp newbox.gro -cs spc216.gro -p topol.top -o solv.gro

Step-6: Ionization

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

Once the above command is executed, run the following command

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

Step-7: Energy Minimization

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

Once the above command is executed, run the following command

gmx mdrun -v -deffnm em

Step-8: Ligand Restrain

gmx make_ndx -f lig.gro -o index_lig.ndx

Once the above command is executed, run the following command

gmx genrestr -f lig.gro -n index_lig.ndx -o posre_lig.itp -fc 1000 1000 1000

Step-9: Modification of topol.top file.

Step-10: Generation of Thermostat.

gmx make_ndx -f em.gro -o index.ndx

Step-11: Equilibration

Temperature equilibration:

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

Once the above command is executed, run the following command

gmx mdrun -v -deffnm nvt

Pressure equilibration:

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

Once the above command is executed, run the following command

gmx mdrun -v -deffnm npt

Step-12: MD run

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

Once the above command is executed, run the following command

gmx mdrun -v -deffnm md