Commands to run MDS of Protein in water

Step-1: Preparation of protein.

```
grep -v HOH sk.pdb > sk_clean.pdb
```

Note: You need to perform this step if your protein structure is downloaded from the protein databank.

Step-2: Creation of topology file.

```
gmx pdb2gmx -f sk_clean.pdb -o sk_pro.gro -water spce
```

Step-3: Solvation

```
gmx editconf -f sk_pro.gro -o sk_newbox.gro -c -d 1.0 -bt cubic
```

once the above command is successfully executed then run the following command in terminal

```
gmx solvate -cp sk_newbox.gro -cs spc216.gro -o sk_solvate -p topol.top
```

Step-4: Ionization

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

once the above command is successfully executed then run the following command in terminal

```
gmx genion -s ions.tpr -o sk_ions.gro -p topol.top -pnane NA -nnane CL -
neutral
```

Step-5: Energy Minimization

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

once the above command is successfully executed then run the following command in terminal

```
gmx mdrun -v -deffnm em
```

Step-6: Equilibration

For temperature equilibration:

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

once the above command is successfully executed then run the following command in terminal

```
gmx mdrun -v -deffnm nvt
```

If you want to plot the energy then run the following command

```
gmx energy -f nvt.edr -o temperature.xvg
```

For pressure equilibration:

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

once the above command is successfully executed then run the following command in terminal

```
gmx mdrun -v -deffnm npt
```

If you want to plot the energy then run the following command

```
gmx energy -f npt.edr -o density.xvg
```

Step-7: MD Run

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

once the above command is successfully executed then run the following command in terminal

```
gmx mdrun -v -deffnm md
```