

You can open all xvg file with xmgrace

Task1: `gmx energy -f step6.0_minimization.edr -o potencial.xvg`
Select potential (13), press enter two time.

Task2:

Temperature:

`gmx energy -f step6.1_equilibration.edr -o step6.1-temp.xvg`
select Temperature (17), press enter two time.

repeat it for all equilibration states:

`gmx energy -f step6.2_equilibration.edr -o step6.2-temp.xvg`
`gmx energy -f step6.3_equilibration.edr -o step6.3-temp.xvg`
`gmx energy -f step6.4_equilibration.edr -o step6.4-temp.xvg`
`gmx energy -f step6.5_equilibration.edr -o step6.5-temp.xvg`
`gmx energy -f step6.6_equilibration.edr -o step6.6-temp.xvg`

Pressure:

`gmx energy -f step6.1_equilibration.edr -o step6.1-pressure.xvg`
select Temperature (18), press enter two time.
repeat for all steps till step6.6_equilibration.

Task3: First we need to make index files:

```
gmx make_ndx -f prot.pdb -o prot.ndx (then write keep 1)
```

We have index file now, we can calculate rmsd:

```
gmx rms -f traj.xtc -n prot.ndx -s prot.pdb -o rmsd-protein.xvg
```

Task4:

```
gmx rmsf -f traj.xtc -n ga.ndx -s prot.pdb -o rmsf-prot.xvg -res yes -fit yes
```

Task5:

First we need to make ndx for for our ligand (p0g)

```
gmx make_ndx -f prot.pdb -o p0g.ndx
```

Keep 13

```
gmx sasa -f traj.xtc -n p0g.ndx -s prot.pdb -o sasa-p0g.xvg
```

Select group 0 and hit enter