

Ionic Density Map generator

Author: Eddy BARRAUD

Contact: eddy.barraud@outlook.fr

Public access: <https://github.com/Eddy-Barraud/IDM>

Requirements : numpy pandas matplotlib seaborn mdtraj

This app is converting pairdist XVG files to Ionic Density Maps (IDM). The python script behind the app is using [Seaborn](#) and [MDTraj](#) libraries.

IDM represents the normalized probability to find an ion at a given distance of each protein residue along the simulation time.

1. Generate with GROMACS a pairdist XVG file using a command like the one below :

```
gmx pairdist -f 12.npt_9.xtc -s 12.npt_9.tpr -n index.ndx -refgrouping res -selgrouping all -o 12.npt_9.pairdist.xvg
```

When asked, enter the protein group number, then a group with ions (Na, NaW, Na-Cl, etc...)

2. Then, generate a topology file of that system, named **sys.gro** (IMPORTANT), using a command like below :

```
gmx editconf -f 12.npt_9.gro -n index.ndx -o sys.gro
```

When asked, enter a group that contains the protein AND the ions, i.e., a group containing the two groups entered at step 1.

3. Copy the 12.npt_9.pairdist.xvg and the sys.gro files to the same folder as the app IDM.Gen.exe
4. Run the script.

```
python IonicDensityMap.py
```

It will convert each XVG file to a map named filename.density.png, only if the map file is not already present.

Another file, named filename.mindist.png, is created, it corresponds to a heatmap of the minimum distance between each residue and any of the ions across time.