Installation instructions

Conda environments

To avoid clashing, it is advisable to have independent environments for different projects. If `conda` is being used as the package manager, create:

```
conda create --name data_visualization
conda create --name fair_data
```

Data Visualization

1. Activate the environment of choice via `conda activate data_visualization`
2. Run:

```
conda install -c conda-forge --file requirements_dataviz.txt
```

3. Open a jupyter session `jupyter notebook` and open the notebook `DataViz.ipynb`

FAIR Data

This module employs a library called `py-iochem` which must be installed beforehand.

1. Activate the environment of choice via `conda activate fair_data`
2. Run:

```
conda install -c conda-forge --file requirements_fairdata.txt
```

3. Enter the `py_iochem` directory (`cd py_iochem`)
4. Run `python -m pip install .` (do not forget the period at the end!) - to install the library from the local directory.
5. Go back to the previous directory (`cd ..`) and open a jupyter session `jupyter notebook` to open the notebook `FAIRData.ipynb`