

## Introduction for the test case of pyGRETA, pyPRIMA and pyCLARA



### Step 1a:

1. Go to Directory of pyGRETA and there to the subdirectory env.
  2. Start a console and create a conda environment for pyGRETA.  
`conda env create -f pyGRETA.yml`
  3. When the creation is done, activate the environment.  
`conda activate pyGRETA`
  4. In the console, go to the pyGRETA subdirectory code.  
`cd ../code`
  5. Make sure in the file `config.py` the path to the database is correct (lines 68 and 70) and make further changes if necessary or wanted.
  6. Run the python script `runme_step1A.py`  
`python runme_step1A.py`
- If an Error “No such file or directory” occurs, check if all the data from the instructions is correctly placed in the database folder. Otherwise, wait until it is finished.



### Step 1b:

1. Still in the console, go to Directory of pyPRIMA and there to the subdirectory env.  
`cd ../../pyPRIMA/env`
2. Again, create a conda environment, this time for pyPRIMA.  
`conda env create -f pyPRIMA.yml`
3. When the creation is done, activate the environment.  
`conda activate pyPRIMA`
4. In the console, go to the pyPRIMA subdirectory code.  
`cd ../code`
5. Make sure in the file `config.py` the path to the database is correct (lines 68 and 70) and make further changes if necessary or wanted.
6. Run the python script `runme_step1B.py` and wait until it is finished.  
`python runme_step1B.py`



### Step 2:

1. After that, go to Directory of pyCLARA and there to the subdirectory env.  
`cd ../../pyCLARA/env`
2. As before, create the conda environment for pyCLARA.  
`conda env create -f pyCLARA.yml`
3. When the creation is done, activate the environment.  
`conda activate pyCLARA`
4. In the console, go to the pyCLARA subdirectory code.  
`cd ../code`
5. Make sure in the file *config.py* the path to the database is correct (lines 68 and 70) and make further changes if necessary or wanted.
6. Run the python script *runme\_step2.py* and wait until it's finished.  
`python runme_step2.py`



### Step 3A:

7. Go back to Directory of pyGRETA and directly to the subdirectory code.  
`cd ../../pyGRETA/code`
8. Activate the environment again.  
`conda activate pyGRETA`
9. Run the python script *runme\_step3A.py* and wait until it is finished.  
`python runme_step3A.py`



### Step 3B:

1. Finally, go to the subdirectory code of the pyPRIMA directory.  
`cd ../../pyPRIMA /code`
2. Activate the environment again.  
`conda activate pyPRIMA`
3. Run the python script *runme\_step3B.py* and wait until it is finished.  
`python runme_step3B.py`

