

QSAR (SPCI) and CReM tutorial

Install anaconda or miniconda for your operating system:

<https://www.anaconda.com/products/distribution>

<https://docs.conda.io/en/latest/miniconda.html>

Start conda command prompt and run the following commands which install all necessary packages and register a new kernel for jupyter notebook. A new environment named `add6` will be created. It should be activated after each run of a conda command prompt.

```
conda create -c conda-forge -n add6 rdkit python=3.9 ipykernel scikit-learn  
openbabel dask distributed
```

```
conda activate add6
```

```
python -m ipykernel install --user --name add6 --display-name "Python3  
(add6) "
```

```
pip install CReM
```