**CABANA Workshop: Chemoinformatics in Drug Discovery**

**Quick guide to Install requirements**

**Install Conda** (This step allow python installation, and conda will help to install RDKit in next step)

1.-Download the installer for Python 3.7 version (<https://www.anaconda.com/distribution/>)

2.-Open a terminal, and move to the folder that contains Anaconda installation file.

Run the command:

bash Anaconda-latest-Linux-x86\_64.sh



Anaconda installer file name

Follow the prompts on the installer screens.

3.- Test your installation

Run the command:

conda list

A list of installed packages must be displayed.

Additional information:

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| --- | --- |
| **Anaconda documentation** | <https://docs.conda.io/projects/conda/en/latest/user-guide/install/linux.html> |
| **Digital Ocean tutorial** | <https://www.digitalocean.com/community/tutorials/how-to-install-anaconda-on-ubuntu-18-04-quickstart> |

**Install RDKit.**  (In our experience, an easy way is installing is with conda)

1.-Create a conda environment with the RDKit

Run the command:

conda create -c rdkit -n my-rdkit-env rdkit

2.- Activate environment:

In the same shell, run the command:

conda activate my-rdkit-env rdkit

Note: to deactivate the environment, run the command conda deactivate, but please do not deactivate the environment until finish next step.

Additional information:

|  |  |
| --- | --- |
| **RDKit documentation** | <http://rdkit.org/docs/Install.html> |

**Install libraries** (Python packages)

Run the command:

pip install jupyter notebook

Visit this github repository <https://github.com/BarbaraDiazE/CABANA_CHEMOINFORMATICS>

and download the file **requirements.txt** (or copy the content and save in a .txt file)

move to the folder that contains the file and run:

pip install -r requirements.txt

Now you can deactivate virtual environment by run:

conda deactivate

**Any Questions or support**, send us a message:

[debi\_1223@hotmail.com](mailto:debi_1223@hotmail.com)

Edgar.Lopez.593@hotmail.com