Getting Started with RDKit and Jupyter Notebooks

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The actual tutorial will be in the Jupyter notebook

However, there are a few steps that need to be done before you can get started, if you have never used a Jupyter notebook before, or in particular RDKit

Please follow these steps before the Jupyter tutorial in case things go wrong, so that we can have a smooth session :)

How to use the Jupyter Notebook

Download and install Anaconda https://www.anaconda.com/products/individual

Two ways to create the environment:

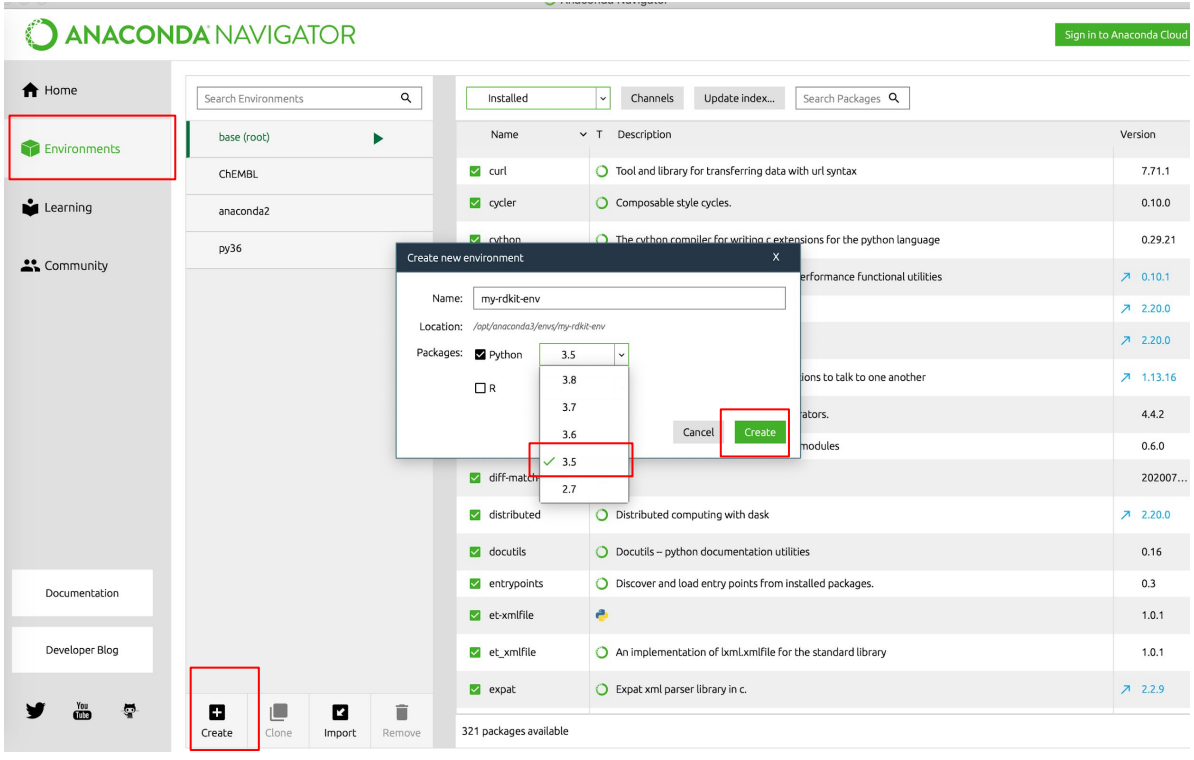
1. Command line

```
$ conda create -c conda-forge -n my-rdkit-env rdkit
$ conda activate my-rdkit-env
$ conda install -c conda-forge notebook
$ jupyter notebook
```

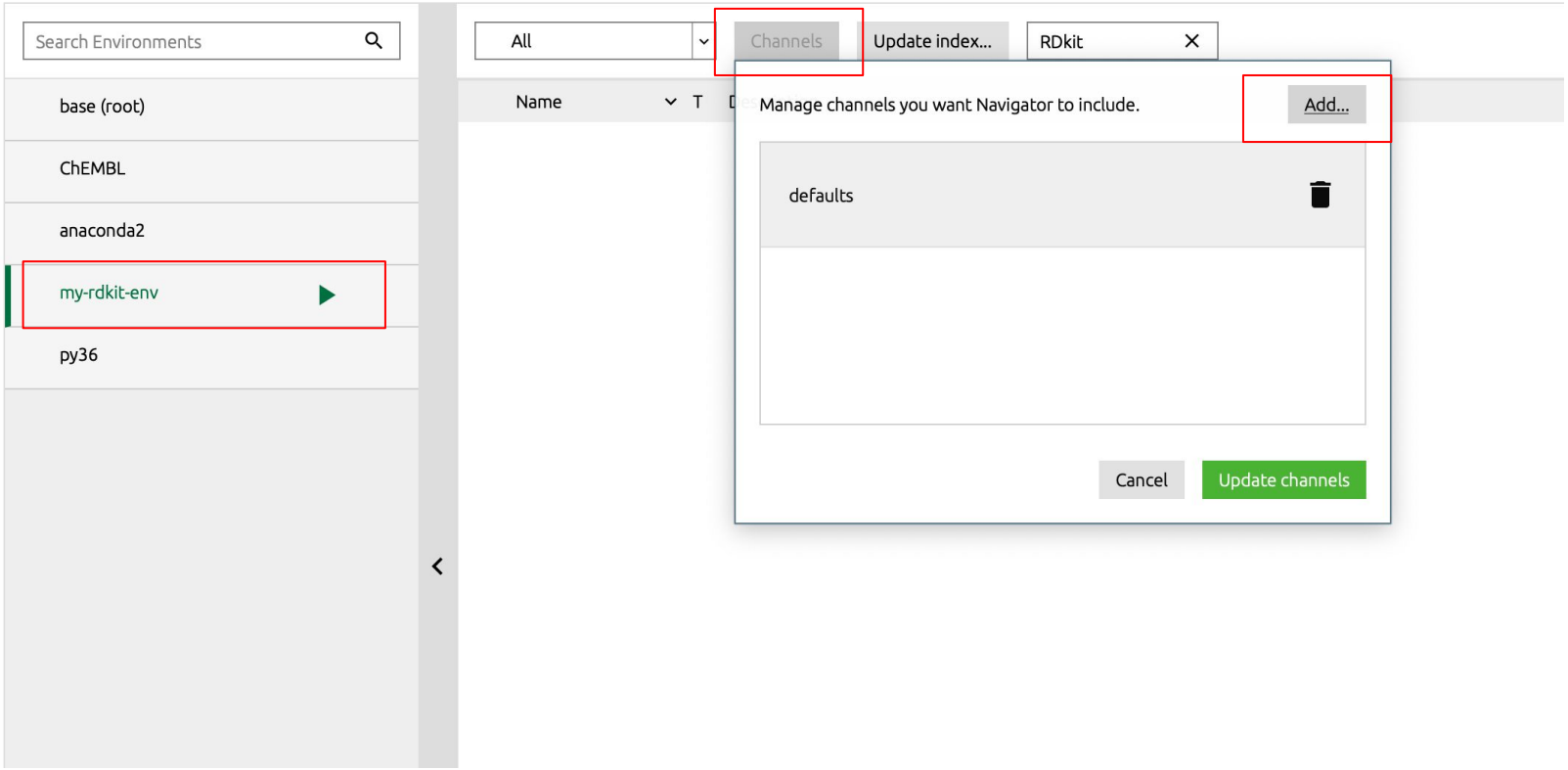
How to use the Jupyter Notebook

YOU MUST SELECT PYTHON 3.5! NOT 3.8!

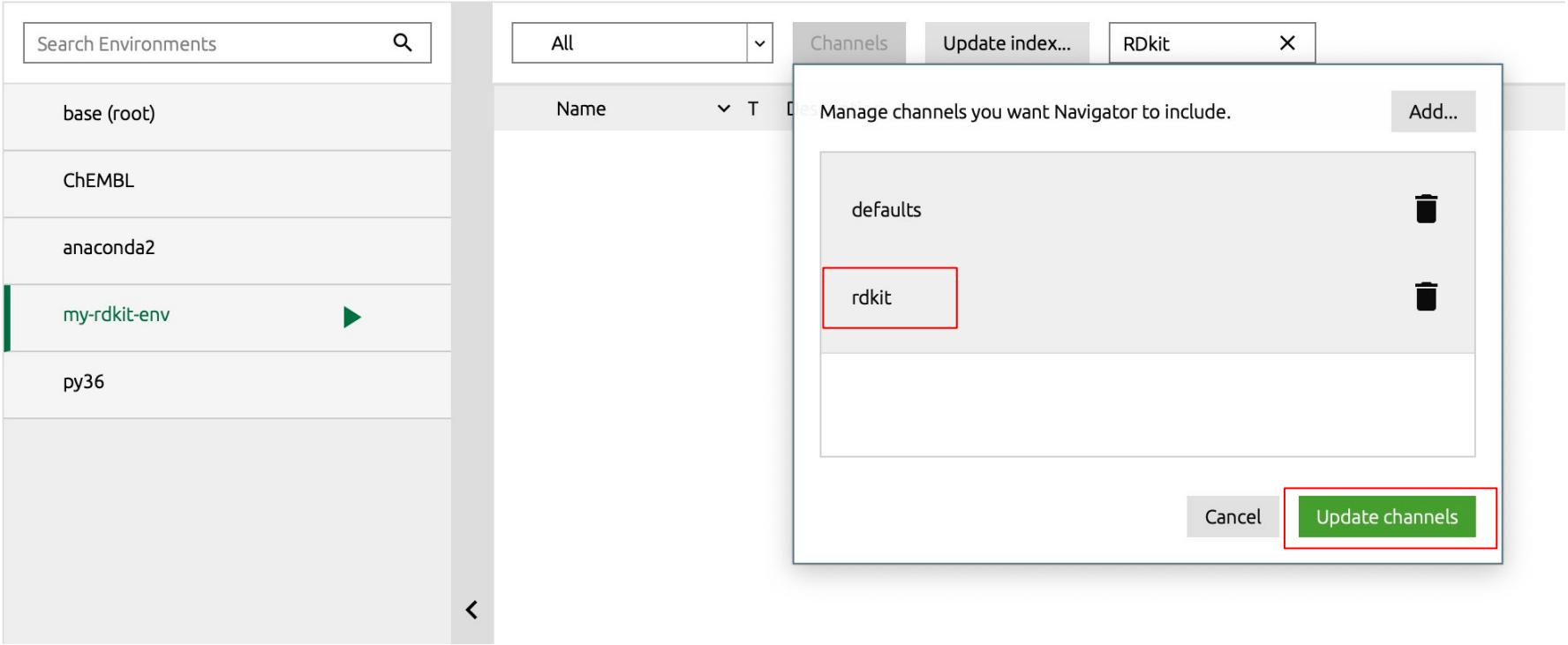
2. Using the Anaconda navigator



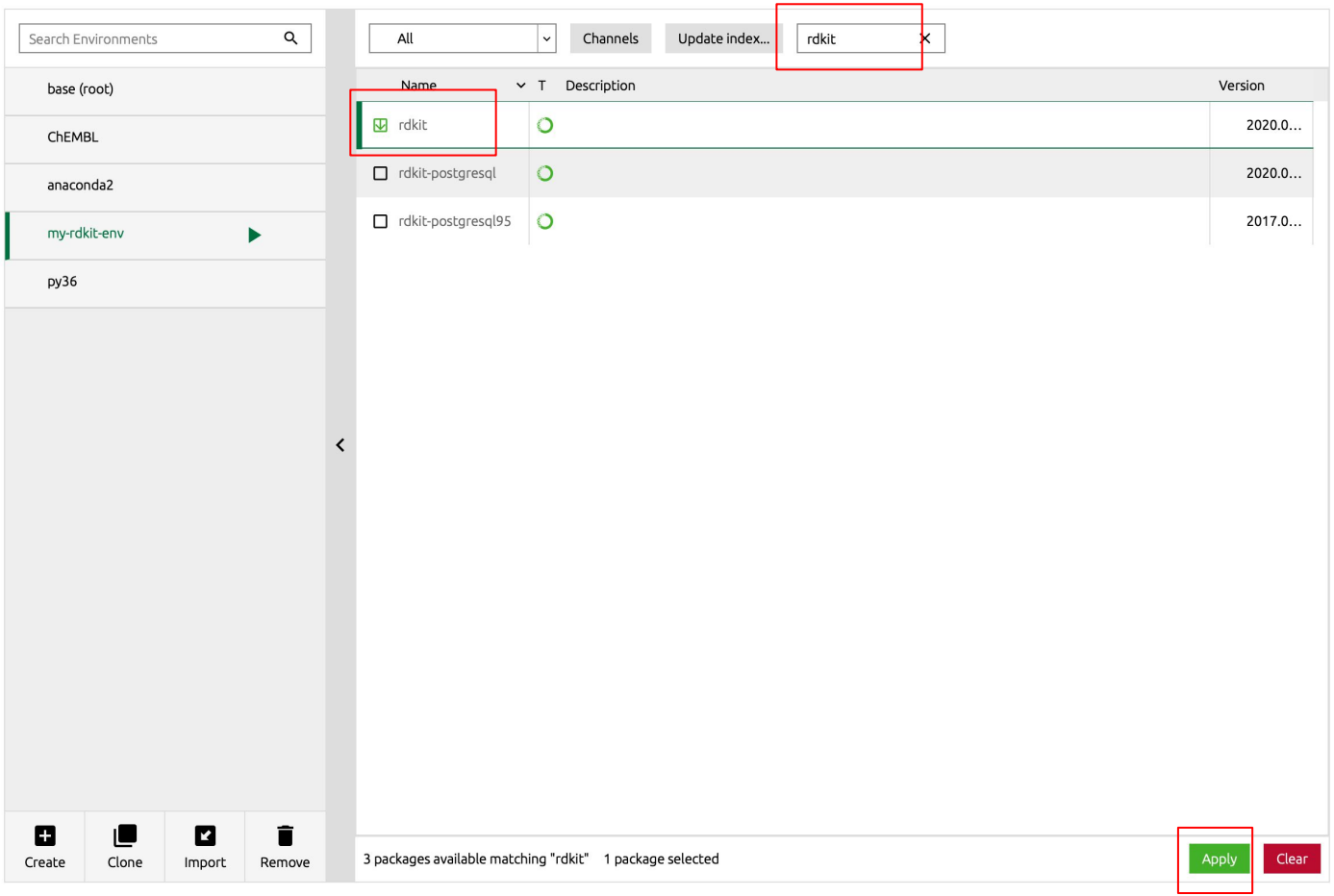
Add rdkit to list of channels

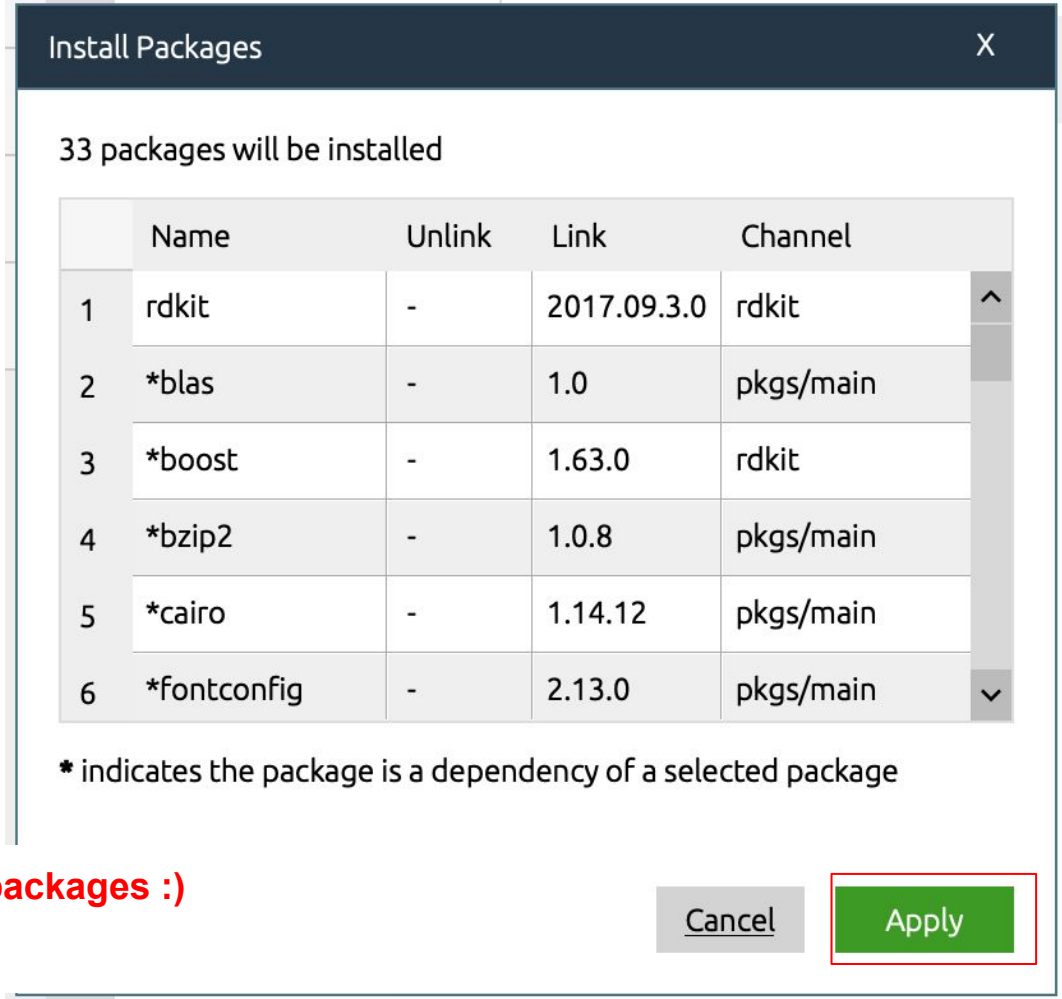


Make sure you update channels

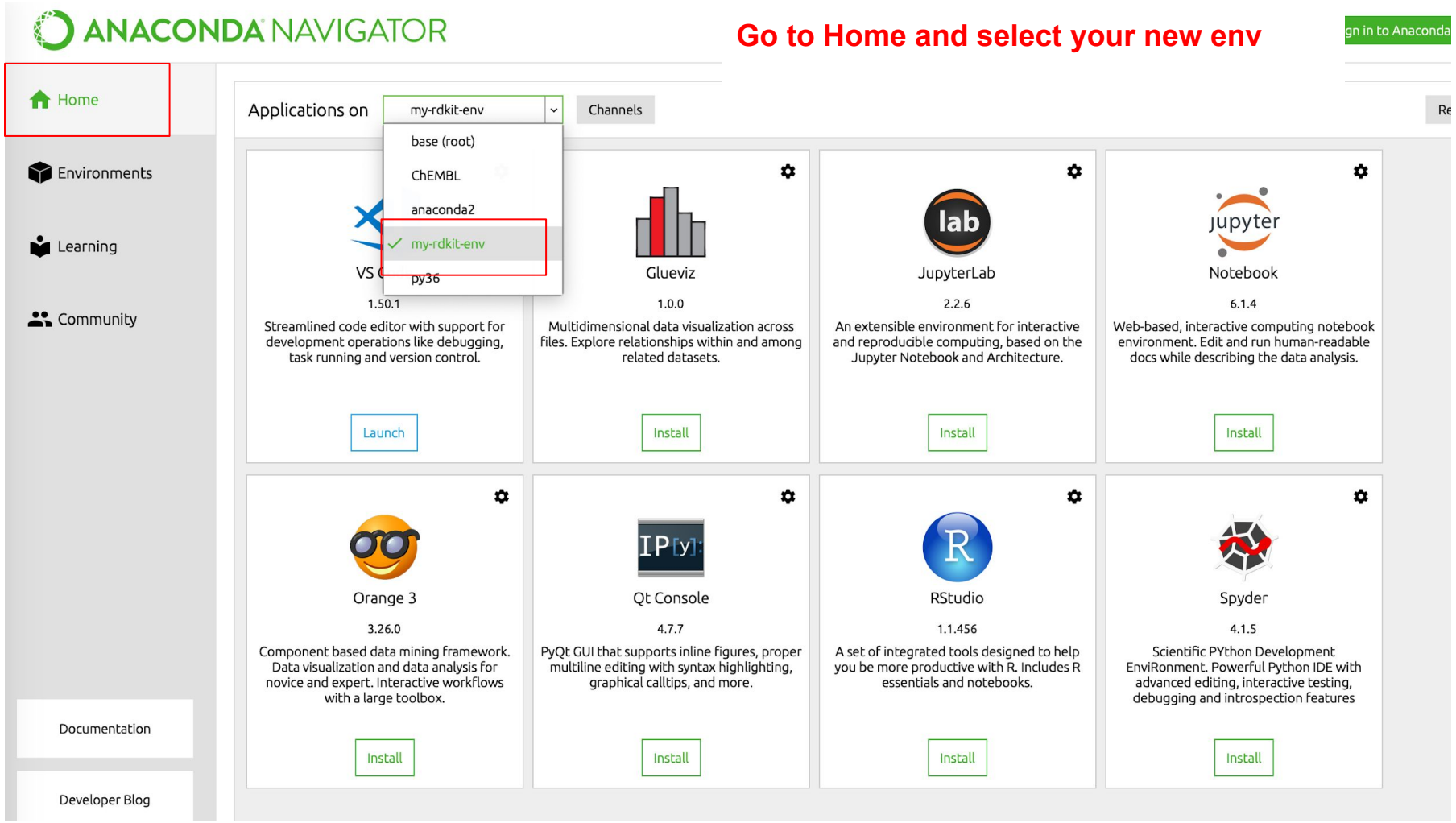


Now you can search for and install RDKit

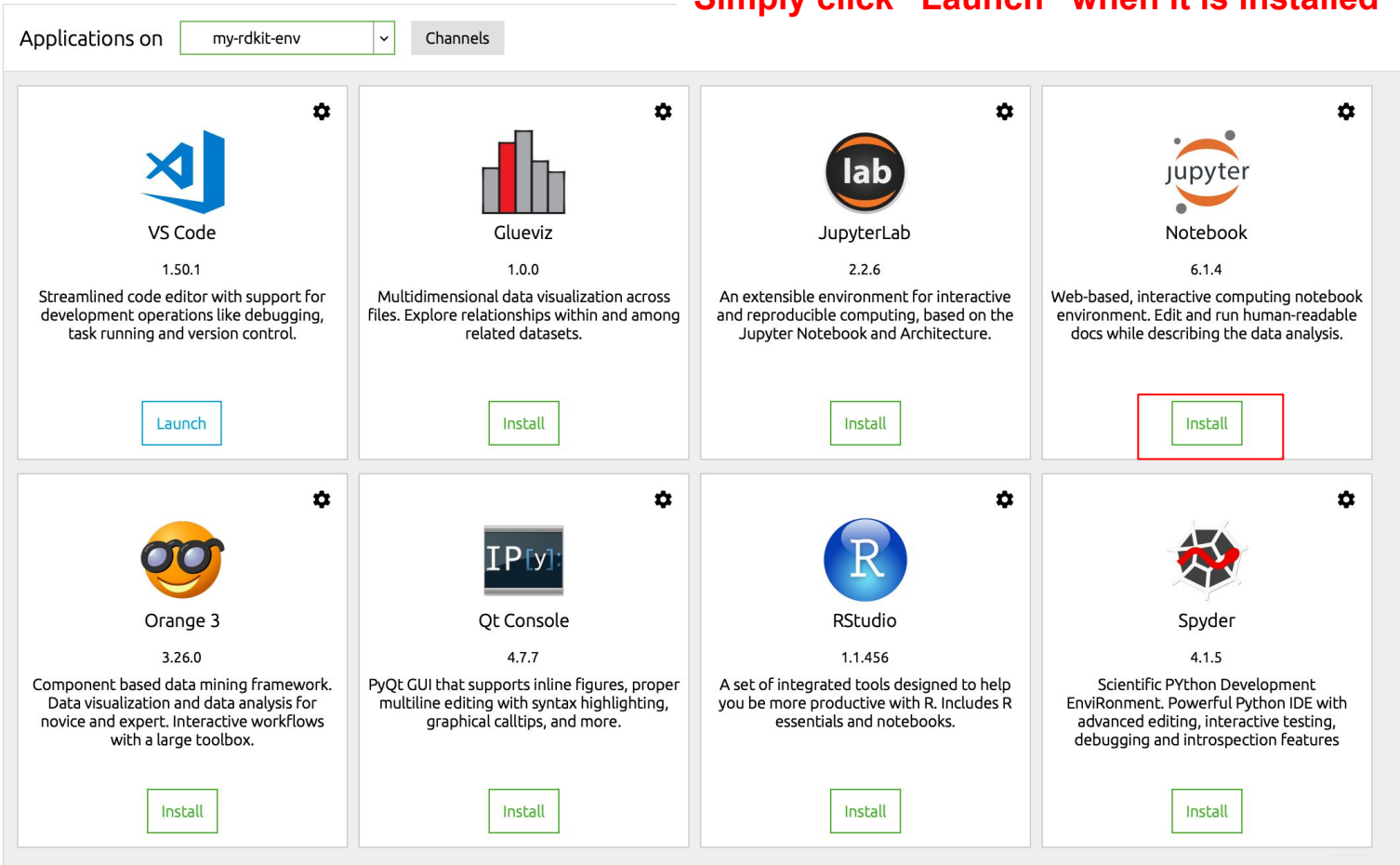




Apply the installed packages :)


ANACONDA NAVIGATOR
Go to Home and select your new env
gn in to Anaconda
Home
Environments
Learning
Community
Documentation
Developer Blog
Applications on
my-rdkit-env
Channels
base (root)
ChEMBL
anaconda2
my-rdkit-env
py36
1.50.1
Streamlined code editor with support for development operations like debugging, task running and version control.
Launch
Glueviz
1.0.0
Multidimensional data visualization across files. Explore relationships within and among related datasets.
Install
JupyterLab
2.2.6
An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Architecture.
Install
Notebook
6.1.4
Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.
Install
Orange 3
3.26.0
Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.
Install
Qt Console
4.7.7
PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.
Install
RStudio
1.1.456
A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.
Install
Spyder
4.1.5
Scientific PYthon Development EnviRonment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features
Install

Install Jupyter Notebook in this env
Simply click “Launch” when it is installed



Now, open the “RDKit_Tutorial.ipynb” and get started!

If you run into issues, try installing the “conda-forge” channel RDKit by adding “conda-forge” to list of channels

Any other issues please email me lh605@cam.ac.uk