

Getting Started with RDKit and Jupyter Notebooks

Layla Hosseini-Gerami
Bender Group High-Dimensional Biology IG
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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:

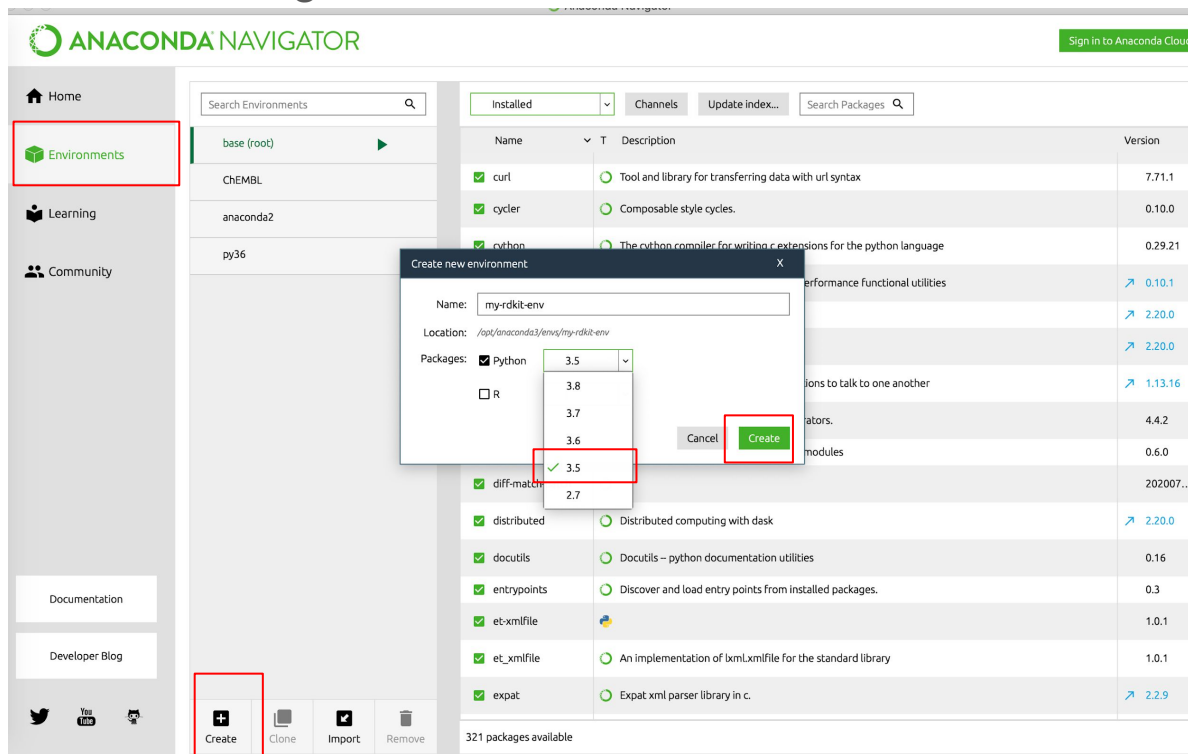
1. Command line

```
$ conda create -c rdkit -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

The screenshot shows the JupyterLab interface with a sidebar on the left displaying a list of environments: `base (root)`, `ChEMBL`, `anaconda2`, `my-rdkit-env` (highlighted with a red box and a green play button), and `py36`. The main panel shows the 'Channels' tab in the top bar, also highlighted with a red box. Below the tabs, a message reads 'Manage channels you want Navigator to include.' and an 'Add...' button is highlighted with a red box. A modal dialog is open, showing a list of channels with 'defaults' at the top. At the bottom of the modal are 'Cancel' and 'Update channels' buttons.

Search Environments

base (root)

ChEMBL

anaconda2

my-rdkit-env

py36

All Channels Update index... RDkit X

Name T Manage channels you want Navigator to include.

Add...

defaults

Cancel Update channels

Make sure you update channels

The screenshot shows the JupyterLab interface. On the left, a sidebar titled "Search Environments" contains a list of environments: "base (root)", "ChEMBL", "anaconda2", "my-rdkit-env" (highlighted with a green bar and a play button), and "py36". The main area displays a table of environments with columns "Name", "Type", and "Channels". The "Channels" column for "my-rdkit-env" shows "RDkit". A dialog box titled "Manage channels you want Navigator to include." is open in the foreground. It has an "Add..." button in the top right. The dialog lists two channels: "defaults" and "rdkit". The "rdkit" channel is highlighted with a red box. At the bottom of the dialog, there are "Cancel" and "Update channels" buttons. The "Update channels" button is highlighted with a red box.

Search Environments

base (root)

ChEMBL

anaconda2

my-rdkit-env

py36

All

Channels

Update index...

RDkit

Name

Type

Channels

Manage channels you want Navigator to include.

Add...

defaults

rdkit

Cancel

Update channels


Now you can search for and install RDKit

Search Environments

base (root)

ChEMBL




anaconda2

my-rdkit-env 

py36

Create Clone Import Remove

All Channels Update index... rdkit

Name	Description	Version
<input checked="" type="checkbox"/> rdkit		2020.0...
<input type="checkbox"/> rdkit-postgresql		2020.0...
<input type="checkbox"/> rdkit-postgresql95		2017.0...

3 packages available matching "rdkit" 1 package selected

Apply Clear

Install Packages



33 packages will be installed

	Name	Unlink	Link	Channel	
1	rdkit	-	2017.09.3.0	rdkit	^
2	*blas	-	1.0	pkgs/main	
3	*boost	-	1.63.0	rdkit	
4	*bzip2	-	1.0.8	pkgs/main	
5	*cairo	-	1.14.12	pkgs/main	
6	*fontconfig	-	2.13.0	pkgs/main	v

* indicates the package is a dependency of a selected package

Apply the installed packages :)

Cancel

Apply



Home



Environments



Learning



Community

[Documentation](#)

[Developer Blog](#)

Applications on

my-rdkit-env

Channels

base (root)

ChEMBL

anaconda2

✓ my-rdkit-env

py36

VS C

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

Applications on my-rdkit-env Channels

 VS Code 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	 Jupyter 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 EnviRnment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features Install

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