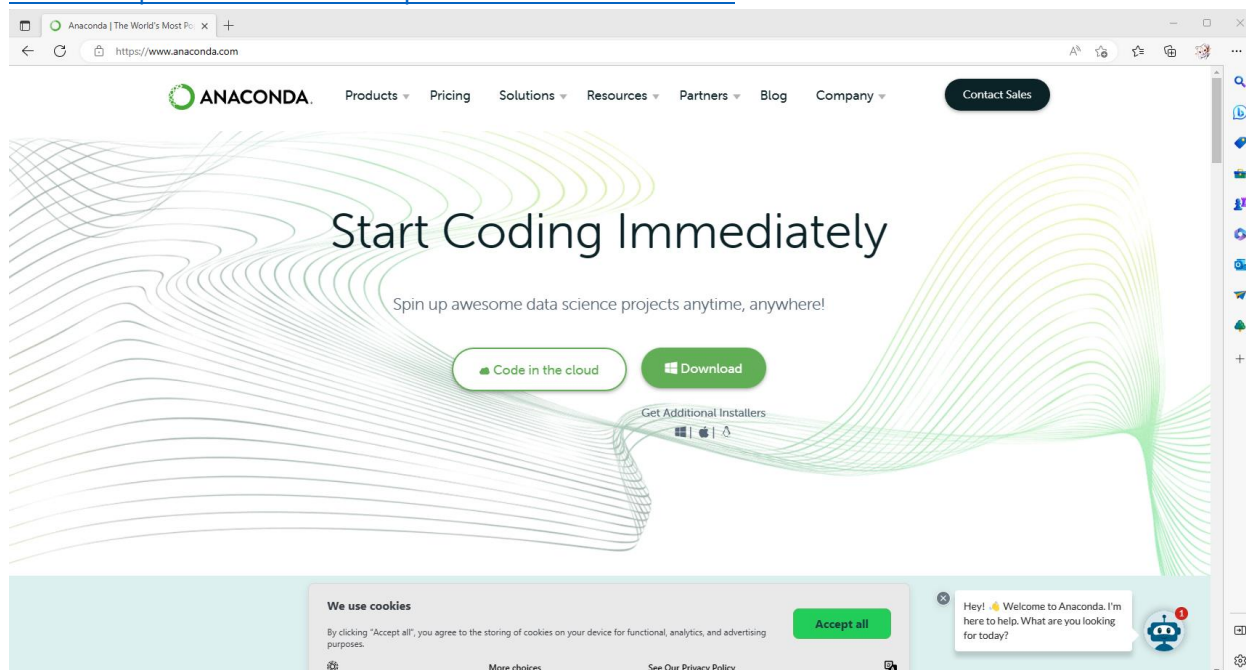


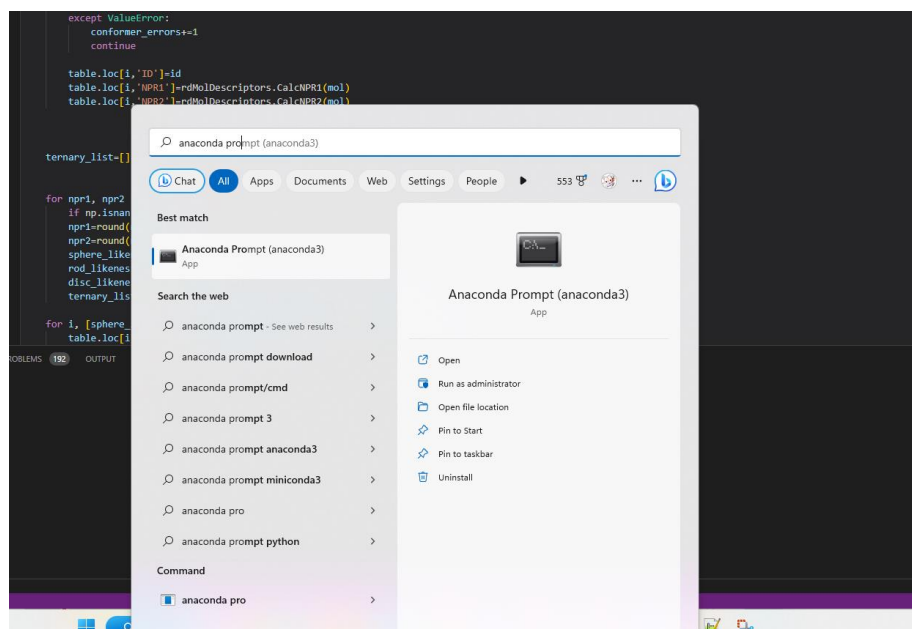
Step 1) Install Anaconda

[Anaconda | The World's Most Popular Data Science Platform](https://www.anaconda.com)



Step 2) Install RDKit

2a) Open an Anaconda prompt window. You may do this from the Anaconda Navigator or simply search for “anaconda prompt”



2b) In the command window, run these two commands to install RDKit

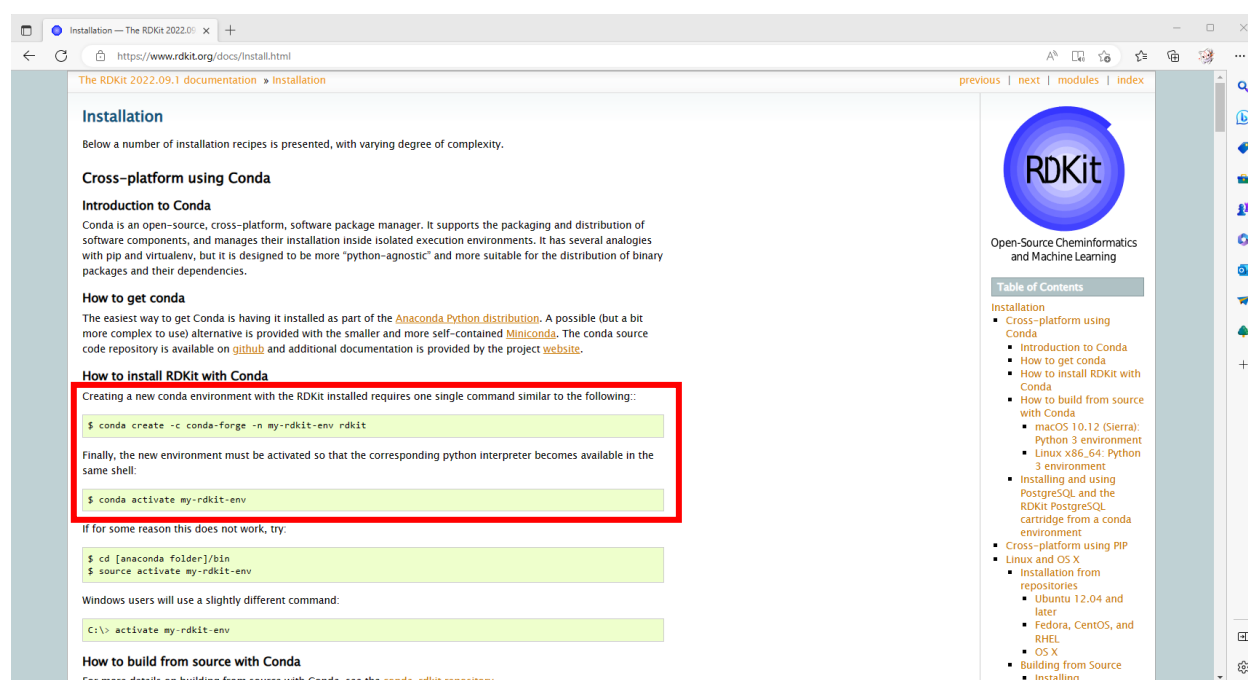
```
conda create -c conda-forge -n my-rdkit-env rdkit

conda activate my-rdkit-env
```

Note: RDKit requires the use of its own virtual environment. The first command both creates the virtual environment and installs RDKit within it. Any additional python libraries you intend to use alongside RDKit must also be installed within this venv (this will be covered in step 4).

More information here if you have trouble with this step:

<https://www.rdkit.org/docs/Install.html>



The RDKit 2022.09.1 documentation » Installation

Installation

Below a number of installation recipes is presented, with varying degree of complexity.

Cross-platform using Conda

Introduction to Conda

Conda is an open-source, cross-platform, software package manager. It supports the packaging and distribution of software components, and manages their installation inside isolated execution environments. It has several analogies with pip and virtualenv, but it is designed to be more "python-agnostic" and more suitable for the distribution of binary packages and their dependencies.

How to get conda

The easiest way to get Conda is having it installed as part of the [Anaconda Python distribution](#). A possible (but a bit more complex to use) alternative is provided with the smaller and more self-contained [Miniconda](#). The conda source code repository is available on [github](#) and additional documentation is provided by the project [website](#).

How to install RDKit with Conda

Creating a new conda environment with the RDKit installed requires one single command similar to the following:

```
$ conda create -c conda-forge -n my-rdkit-env rdkit
```

Finally, the new environment must be activated so that the corresponding python interpreter becomes available in the same shell:

```
$ conda activate my-rdkit-env
```

If for some reason this does not work, try:

```
$ cd [anaconda folder]/bin
$ source activate my-rdkit-env
```

Windows users will use a slightly different command:

```
C:\> activate my-rdkit-env
```

How to build from source with Conda

For more details on building from source with Conda, see the [conda-rdkit repository](#).

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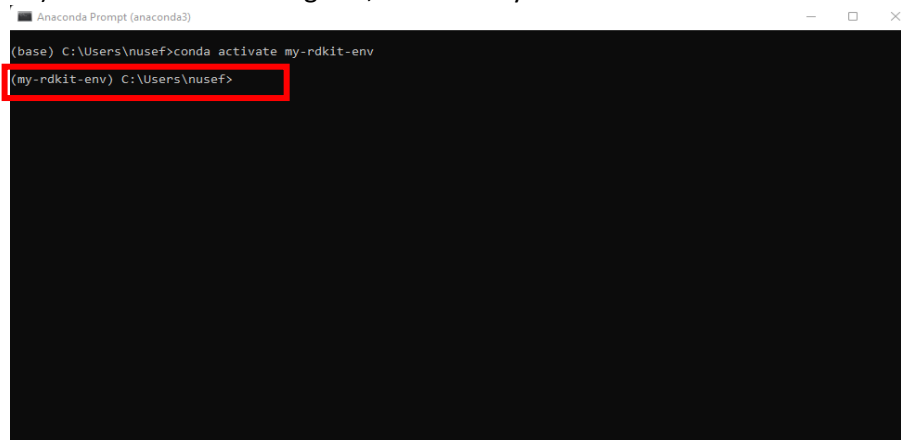
- Installation
 - Cross-platform using Conda
 - Introduction to Conda
 - How to get conda
 - How to install RDKit with Conda
 - How to build from source with Conda
 - macOS 10.12 (Sierra): Python 3 environment
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 - Installing and using PostgreSQL and the RDKit PostgreSQL cartridge from a conda environment
 - Cross-platform using PIP
 - Linux and OS X
 - Installation from repositories
 - Ubuntu 12.04 and later
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 - OS X
 - Building from Source
 - Installing

Step 3) Optional, but highly recommend to install a code editor such as VSCode if you haven't already.

<https://code.visualstudio.com/>

Step 4) Install the necessary python libraries to use the included notebooks.

4a) In the anaconda navigator, make sure your RDkit venv is active.



```
Anaconda Prompt (anaconda3)
(base) C:\Users\nusef>conda activate my-rdkit-env
(my-rdkit-env) C:\Users\nusef>
```

The screenshot shows a terminal window titled "Anaconda Prompt (anaconda3)". The first line shows the command `(base) C:\Users\nusef>conda activate my-rdkit-env` being executed. The second line shows the prompt changing to `(my-rdkit-env) C:\Users\nusef>`, which is highlighted with a red rectangular box, indicating that the environment is now active.

4b) Use pip to install the libraries from the included requirements.txt file.

This can quickly be done with the following command:

```
pip install -r "YourSystemFilePath/requirements.txt"
```