

Installation Instructions

- All the scripts described here can be found in the “scripts” folder
- All the installation steps are only required for a first-time user.
- Creation of the conda environment with all the necessary tools installed requires around 400 MB of disk space.

| Installation | |
|--------------|--|
| 1. | <p>Install Miniconda (or anaconda). Follow the instructions on their website. <i>(If you are new to conda and not planning to use the powerful python tools in it, I recommend using Miniconda since it requires less disk space. The full anaconda installation comes with many useful tools but it will take at least a few GB.)</i></p> <ol style="list-style-type: none"> Miniconda https://docs.conda.io/en/latest/miniconda.html (Alternative: Anaconda https://www.anaconda.com/) |
| 2. | Download the “scripts” folder I shared for later use. <i>(or you may just download the scripts you want)</i> |
| 3. | <p>Install software packages in the conda environment:</p> <div style="border: 1px solid black; padding: 5px;"> <p>WINDOWS USER ONLY:</p> <ol style="list-style-type: none"> Do EITHER (ai) or (aii): <i>(requires internet connection)</i> Start the “Anaconda Prompt (Miniconda3)” from your start menu or search it with the system search tool. <i>(if you have installed Anaconda instead, it would be “Anaconda Prompt (Anaconda3)”)</i> <ol style="list-style-type: none"> Type the following command: <div style="border: 1px solid black; padding: 2px; display: inline-block;">conda create -y -n chemtools-win10 -c conda-forge -c msys2 smina pymol-open-source m2-base openbabel</div> For Miniconda, this command install the conda environment with selected software in “%USERPROFILE%\miniconda\envs\chemtools-win10”. <ol style="list-style-type: none"> If you want to install it elsewhere or change the name of environment, replace “-n chemtools-win10” with “-p \FULL\PATH\to\your\target\location\envname” e.g. if you want to install the tools in “D:\” and rename it to “newname”, replace “-n chemtools-win10” in the command with “-p D:\newname”. <i>(Openbabel automatically installs with smina but explicitly stating it just to be safe)</i> Check the path to your environment and modify corresponding variables in the files provided in the “scripts” directory <p>UNIX USERS ONLY: (Should work for major distribution of Linux, haven’t tested on Mac)</p> <ol style="list-style-type: none"> Open a terminal If your conda is not in your path and/or initialized e.g. via the option to add related commands to the .bashrc/.zshrc during the anaconda installation process or with `conda init <shell name>`, you will need to execute the following command, <div style="border: 1px solid black; padding: 2px; display: inline-block;">eval "\$(XXX/conda shell.<shell name> hook)"</div> <p>where:</p> <ol style="list-style-type: none"> “XXX” is the full path to your conda executable <shell name> is the name of your shell <ol style="list-style-type: none"> Usually bash for Linux. For Mac it may be bash or zsh, depends on OS version <ol style="list-style-type: none"> Note that I wrote the scripts in bash, for now it should still be installed on Mac although the default shell has changed to zsh for newer Mac versions. I haven’t tested whether they can be run directly by zsh yet. If you don’t want to change the default shell on Mac, just call bash explicitly as you run the shell scripts I provide. Do EITHER (di) or (dii): (requires internet connection) <ol style="list-style-type: none"> Execute the following command: <div style="border: 1px solid black; padding: 2px; display: inline-block;">conda create -y -n chemtools -c conda-forge smina pymol-open-source openbabel</div> For Linux users, default installation path would be “~/conda/envs/chemtools”. If you want to install it elsewhere or change the name of environment, replace “-n chemtools” with “-p /FULL/PATH/to/your/target/location/envname” e.g. if you want to install the tools in “~/Desktop” and rename it to “newname”, replace “-n chemtools-win10” in the command with “-p ~/Desktop/newname”. <i>(Openbabel automatically installs with smina but explicitly stating it just to be safe)</i> Check the path to your environment and modify corresponding variables in the files provided in the “script” directory. </div> |

4. Start PyMOL:

WINDOWS USER ONLY: ASSUMING you installed anaconda3/miniconda3 with “Just Me” option:

- a. If you installed “Miniconda3” start PyMOL by double-clicking “miniconda-local-pymol.bat”.
- b. If you installed “Anaconda3”, start PyMOL by double-clicking “anaconda-local-pymol.bat”.

If an error occurs, you may try the following:

a. Correct the path to anaconda/miniconda installation

- i. Find the correct path by doing the following:

- Start the Anaconda Prompt
- Type the following command:

```
conda env list
```

You will see a list of installed conda environment.

```
# conda environments:
#
base * C:\ProgramData\Miniconda3
chemtools-win10 C:\Users\...\.conda\envs\chemtools-win10
```

- Copy the location near “base”, using the above example it would be:

```
C:\ProgramData\Miniconda3
```

- ii. Open the “XXX-pymol.bat” file with a text editor, e.g. RIGHT CLICK on the script then click “edit.”

(Windows 11: the “Edit” option may only appear after you click “show more options”.)
Then, replace “%USERPROFILE%\miniconda3” or “%USERPROFILE%\anaconda3” in line 9 with the copied line,

```
8 rem Define the path to anaconda
9 set CONDAPATH=%USERPROFILE%\miniconda3
```

Save the file after you are done editing.

b. Correct the path to the chemtools-win10

- i. Find the path to the installed environment:

- Start the Anaconda Prompt
- Type the following command:

```
conda env list
```

You will see a list of installed conda environment.

```
# conda environments:
#
base * C:\ProgramData\Miniconda3
chemtools-win10 C:\Users\...\.conda\envs\chemtools-win10
```

- Copy the location near “chemtools-win10”

- ii. Open the “XXX-pymol.bat” file with a text editor (Refer to the instruction in (aii) if necessary)

- Replace “%USERPROFILE%\miniconda3\envs\%ENVNAME%” or “%USERPROFILE%\anaconda3\envs\%ENVNAME%” line 15 with the line you copied.

```
14 rem Define the path to the installed environment
15 set ENVPATH=%USERPROFILE%\miniconda3\envs\%ENVNAME%
```

UNIX USER ONLY: Start PyMOL by the following commands:

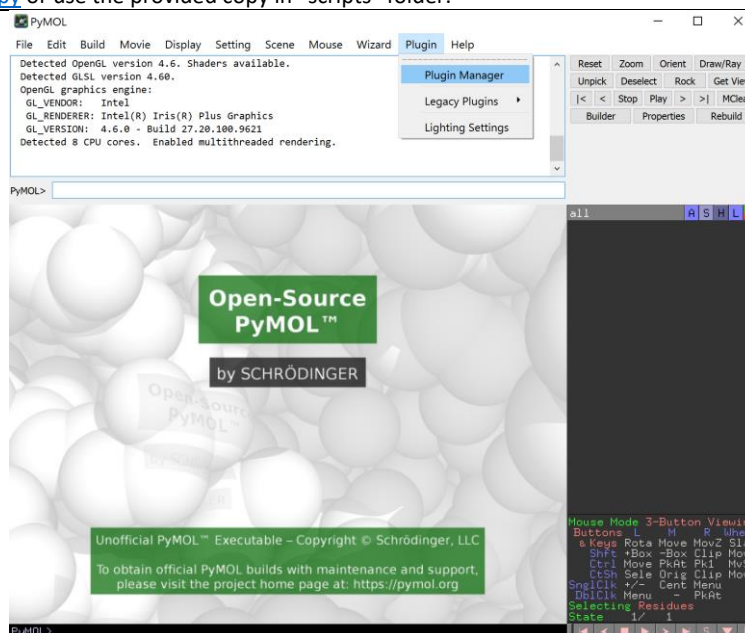
```
conda activate chemtools #or whatever env. name you have set it to
```

```
pymol & # to run it at the background so you don't need to open another terminal to use the command line
```

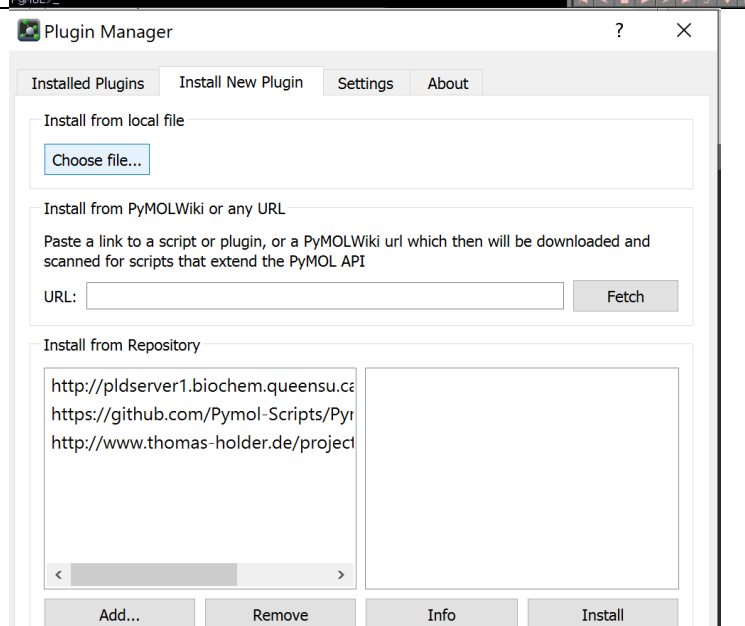
5. Download the optimize plugin from <https://raw.githubusercontent.com/Pymol-Scripts/Pymol-script-repo/master/plugins/optimize.py> or use the provided copy in “scripts” folder.

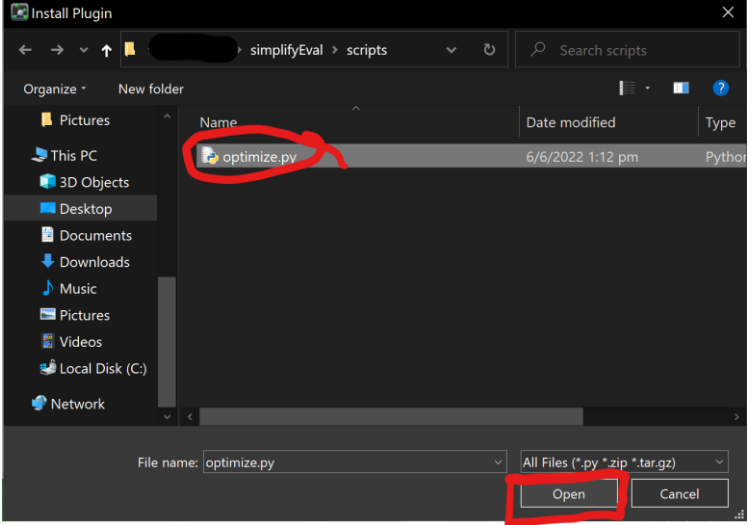
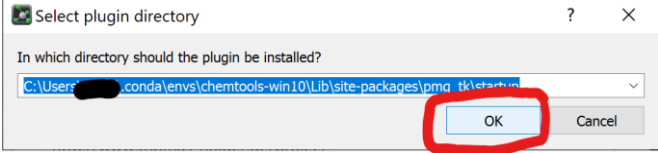
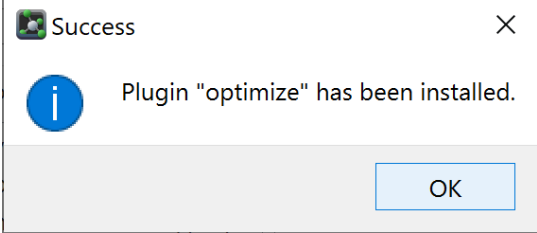
6. Install the Optimize plugin with the PyMOL Plugin Manager.

- a. Opens the plugin manager



- b. Under the “Install New Plugin” Tab, click “Choose file”.



| | |
|---|---|
| <p>c. Choose "optimize.py" and click "open".</p> |  |
| <p>d. Click "OK" as it prompt for the installation directory.</p> |  |
| <p>e. Click "OK" as the installation is completed.</p> |  |
| <p>7. Now you can close PyMOL, or directly proceed to the first exercise.</p> | |