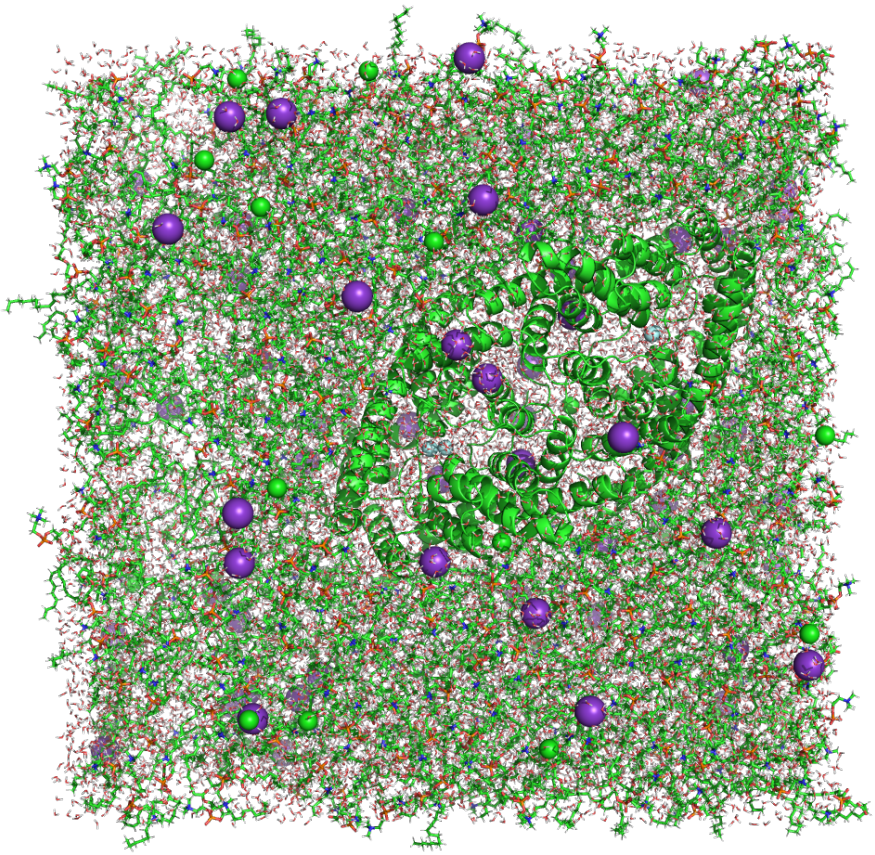
University of Colorado Denver
Department of Chemistry

QM/MM Input Preparation – PyMOL Tutorial



Developers: Abigail Chiu[1], Woonghee Lee[1]*
[1] Department of Chemistry, University of Colorado Denver, Denver, CO 80204, USA

Tutorial Contributors
Abigail Chiu[1], Jennifer Nguyen[1]
[1] Department of Chemistry, University of Colorado Denver, Denver, CO 80204, USA

Contents

Introduction

The Poky Suite is a software suite that for multidimensional NMR analysis, 3D structures calculations and more. It integrates multiple different software packages to provide automated and visualized platforms for resonance assignments, structure calculation, dynamic studies, computer-aided drug design, etc.

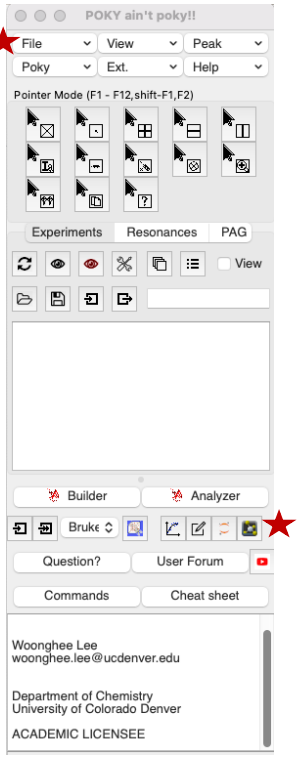
- Read QMMM input file and display the QM atoms on the screen.
- After user select/modify the list of QM atoms by clicking on the screen, write the serial numbers of QM atoms to a file that can later be incorporated into the QMMM input file.

Downloading Poky

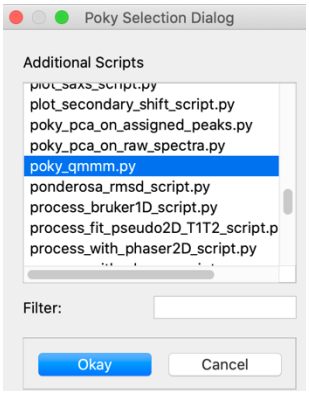
- Before starting the tutorial, you need to download the current version of Poky which can be found at https://poky.clas.ucdenver.edu.
    - You can follow the tutorial on the Installation Page to download Poky for your specific computer system.

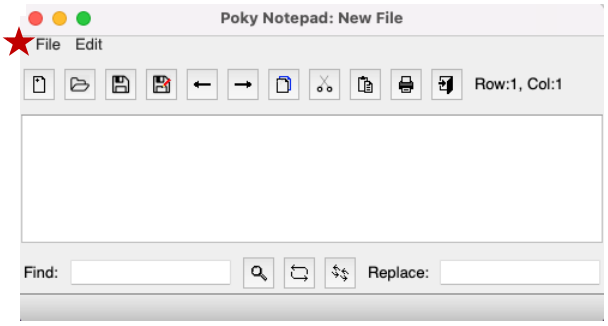
You will be using PyMOL through the POKY program.
[All directions are on the Poky website: https://poky.clas.ucdenver.edu.]

Opening Structure in PyMOL through Poky



1) Open POKY
2) Open POKY notepad (you can open it through **file → "Poky Notepad"** or by clicking the icon under the Analyzer button)
   - If you hover over the icons, it will appear the name
3) Go to **File → Poky Scripts → Find Additional Modules from Poky GitHub Repository → poky_qmmm.py** to load the QMMM script

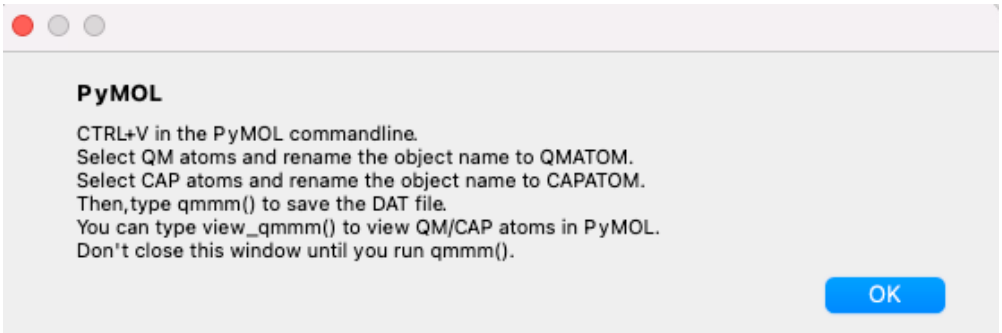




4) Click **File → Run Python Module**
   - This will result in a python shell to open up
5) It will ask you for your PDB file → Open PDB file
   - You have the option to create a new DAT file, or you can use an existing file

Creating a new DAT file

6) You will hit **cancel** if you want to make a completely new DAT file
   - A screen will pop up for you to name your new file → Click Save
   - There will be a window that pops up with directions → do not close this window until you run qmmm()



7) It will automatically open PyMOL

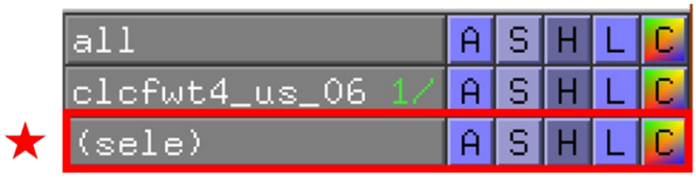
- You will follow the steps in the pop-up box

8) CTRL+V to paste the link into the PyMOL command line → press enter

- Now you have your structure loaded

Selecting CAP atom(s)

9) Select your CAP atom(s) by clicking on them; if they are selected, you will see a red dot in the center of them.
   - If you selected the wrong atom(s), just select it again so that it unselects
10) Once you select your CAP atoms(s), a new box will show up on the right-hand side



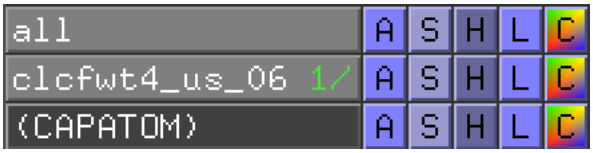
ASHLC = **A**ction, **S**how, **H**ide, **L**abel, **C**olor

- Pick your atoms and rename it by clicking **"A" → "rename selection"**

- Delete the old name (sele) and change it. Because Python is capitalization sensitive, you have to make sure it is capitalized → Rename it to CAPATOM → Press Enter

Selecting QM atom(s)

11) In order to select the QM atom(s), make sure you hide the CAPATOM
    - You click on the CAPATOM box, and it will be unselected (it will become unhighlighted) → now you can select your QM atom(s)



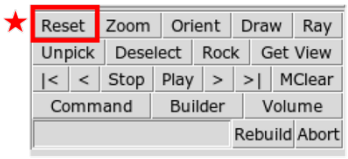
- Rename it by clicking **"A" → "rename selection"** → Delete old name (sele) → Rename to **QMATOM** → Press Enter

Saving DAT file

12) Type **qmmm()** in the PyMOL command line to save the DAT file → Press Enter
    - Now it should be saved, and you can check to make sure that the file is in your folder/directory

Viewing CAP and QM Atom(s)

13) In the PyMOL command line, type **view_qmmm()** → Press Enter
    - This will zoom in on the atom(s) and change the color to red
        - Use your mouse to zoom back out or hit "Reset" at the PyMOL graphics system for the view to go back to normal
    - You can change the color manually if you don't like the red color



To Change the color → click **"C"**

If you want to see what is in the DAT file…
- Open it up, and when you make a new DAT file, it will only have your QM and CAP atom

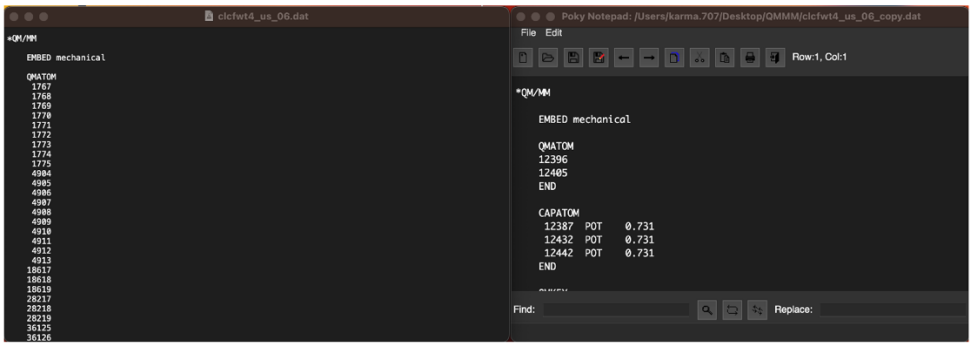
Once you are done with everything, you can close the pop-up window (or press okay). When you close the pop-up, it will show what is inside your DAT file.

```
QMATOM
12387
12432
12442
END

CAPATOM
 12396  POT    0.731
 12405  POT    0.731
END
```

Use an existing DAT file

1) Open POKY notepad
2) Go to **File → Poky Scripts → Find Additional Modules from Poky GitHub Repository → poky_qmmm.py** to load the QMMM script
3) Click **File → Run Python Module**
4) It will ask you for your PDB file → Open PDB file
5) Select your DAT file → Select Open
6) Follow the same procedure for loading structure, selecting your QM and CAP Atom(s), saving, and viewing.



Original DAT file

New CAP and QM Atoms added to existing DAT file

Woonghee Lee*, Mehdi Rahimi, Yeongjoon Lee, Abigail Chiu.
POKY: a software suite for multidimensional NMR and 3D structure calculation of biomolecules.
Bioinformatics. Sep 15, 2021. 37(18):3041-3042. https://doi.org/10.1093/bioinformatics/btab180