Using PyMol in the Caricato Group

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What is PyMol?

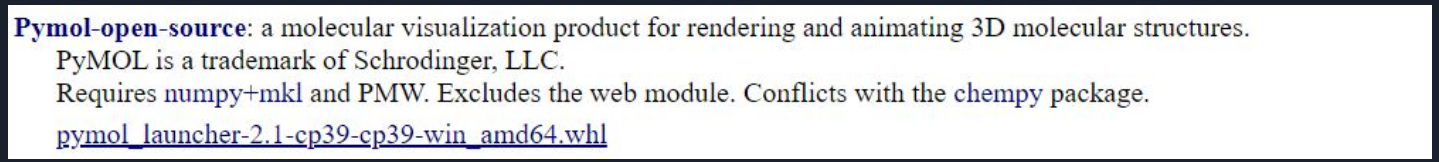
- PyMol is a molecular visualization program with similar functionality to VMD
- It’s written in Python, which makes it easy to write scripts and automate processes

Before Installing PyMol

- Installing the open-source version of PyMol can be a little tricky
- I recommend installing the latest version of Python (currently 3.9) before continuing
  - Pip is automatically installed when installing Python which saves a few steps
- Numpy is also required before installing PyMol
  - This can be done by simply typing ‘pip install numpy’ in the console
- You should also install pyqt5 by doing ‘pip install pyqt5’
  - This is necessary to display the GUI for PyMol

Installing PyMol

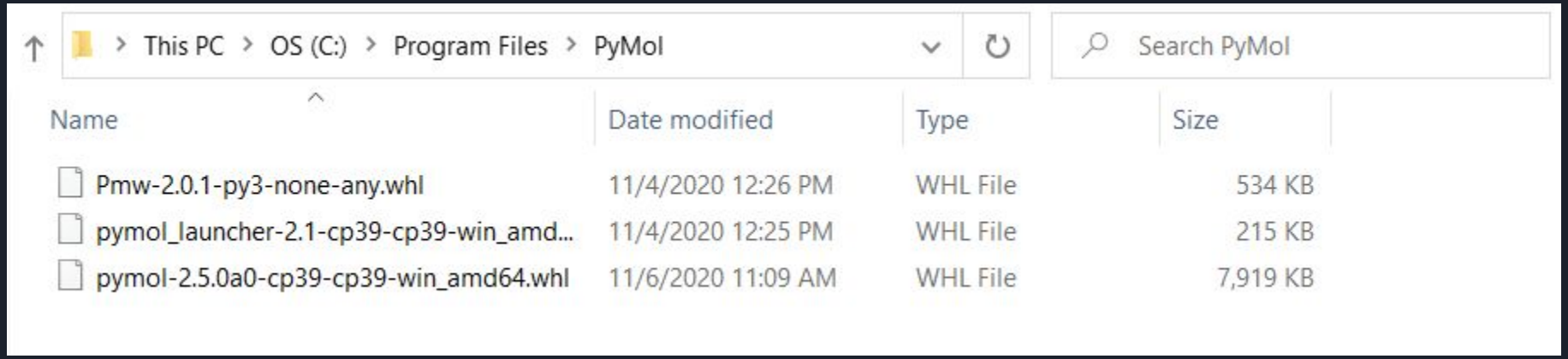
- Navigate here and find the appropriate version of PyMol for your Python version - you can click pymol-open-source from the large list at the top of the page to automatically scroll to the right spot
- Download the ‘pymol_launcher-2.1-cp39-cp39-win_amd64.whl’ file and ‘pymol-2.5.0a0-cp39-cp39-win_amd64.whl’
- The ‘cp39’ portion of the file corresponds to Python version 3.9
  - There are other versions available if you already have a different version of Python installed



Installing PyMol

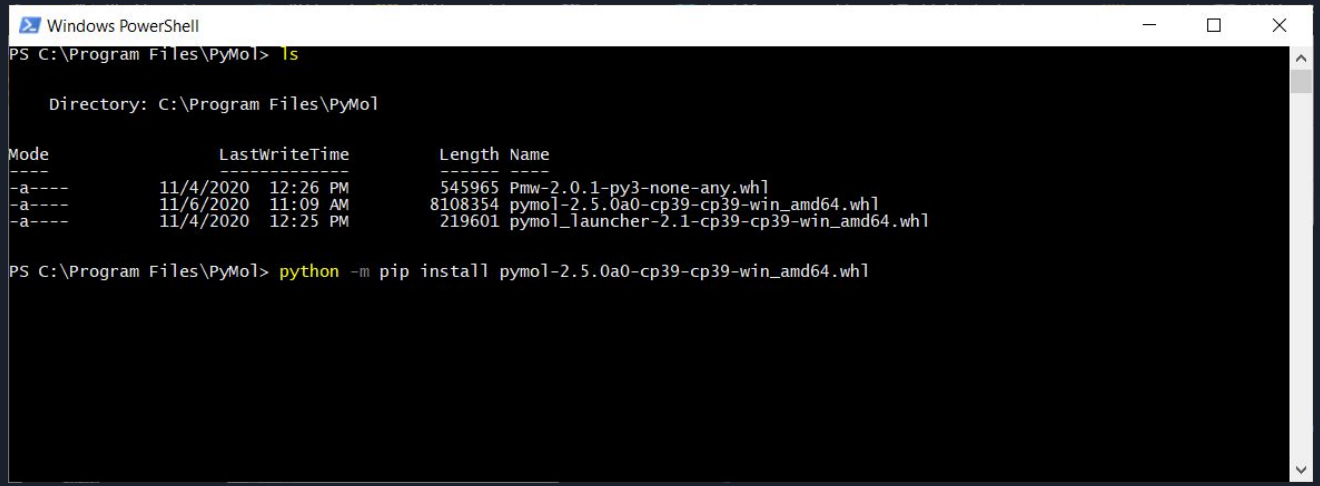
Pmw-2.0.1-py3-none-any.whl
Pmw-2.0.1-py2-none-any.whl

- Next, download ‘Pmw-2.0.1-py3-none-any.whl’
- If you already installed pip and Numpy as described previously, you shouldn’t have to download any more .whl files from here
- You should now have a directory that looks something like this - the location and naming of the directory is up to you



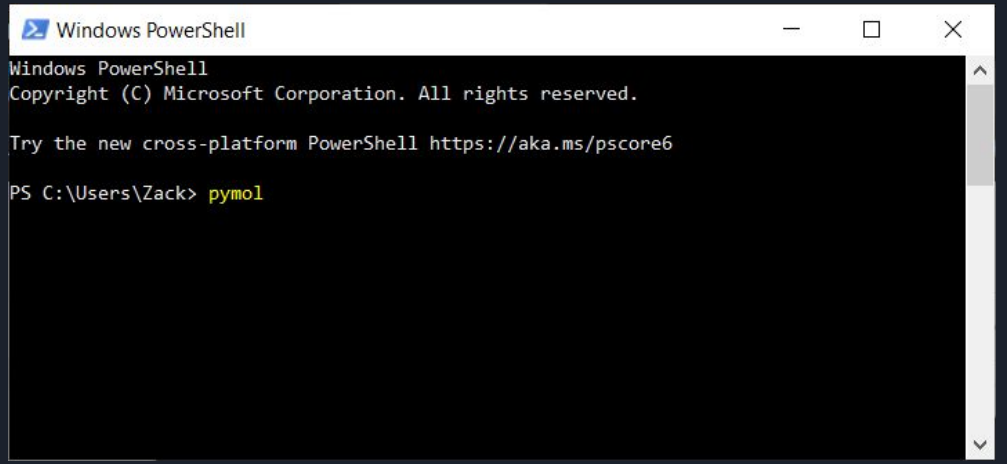
Installing PyMol

- Now open a console in that directory
  - On windows you can Shift+Right Click -> Open Powershell window here
  - You can also open a command prompt and ‘cd’ to the directory manually
- Enter ‘python -m pip install pymol-2.5.0a0-cp39-cp39-win_amd64.whl’ and run the command



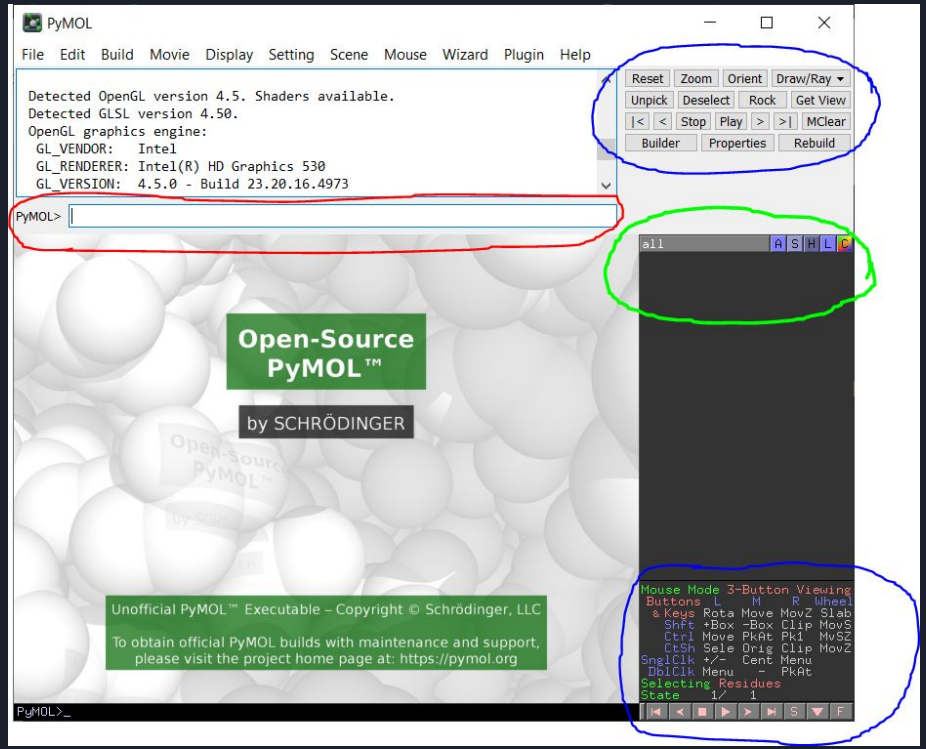
Finishing installation

- If all went well, PyMol should now be ready for use
- You can launch PyMol by simply typing ‘pymol’ in the console window
- The full Windows installation guide can be found here
    - You’ll see that we didn’t necessarily follow the same instructions listed here
- You should be able to launch PyMol from any directory, but this may depend on your Python installation and if Python is in your system’s PATH environment variable



PyMol is installed

- After opening PyMol, you should see a window that looks like this
- The command bar is circled in red - this is where you can input various commands and run functions
- The area circled in green is where all of the objects, such as molecules or shapes you load will be listed
- The areas in blue generally will not be used, but the ‘Reset’ button at the top can be handy if the zoom or orientation gets messed up

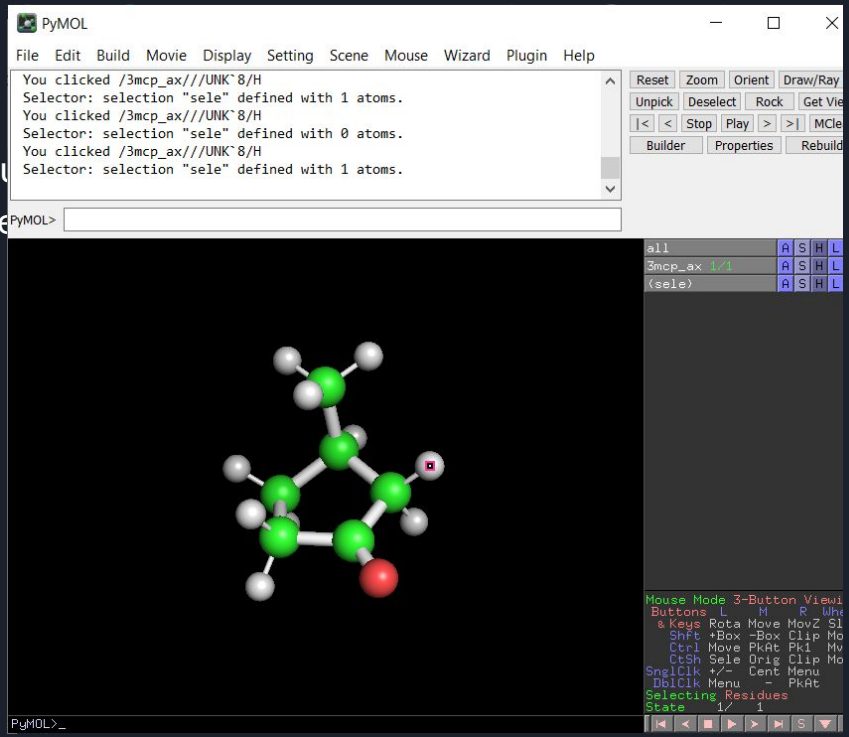


Using the toolbar and basic functionality

- Files can be loaded in by selecting ‘File ->Open’ then navigating to your molecular structure file.
- Ctrl+Z and Ctrl+Y can be used for undo/redo as in other programs
- ‘Build’ and ‘Movie’ will not be used and can be ignored for now
- ‘Display’ and ‘Setting’ can be used to change various components of the scene like background color, the type of molecular representation, and colors for different elements
- The rest of the toolbar will generally not be used

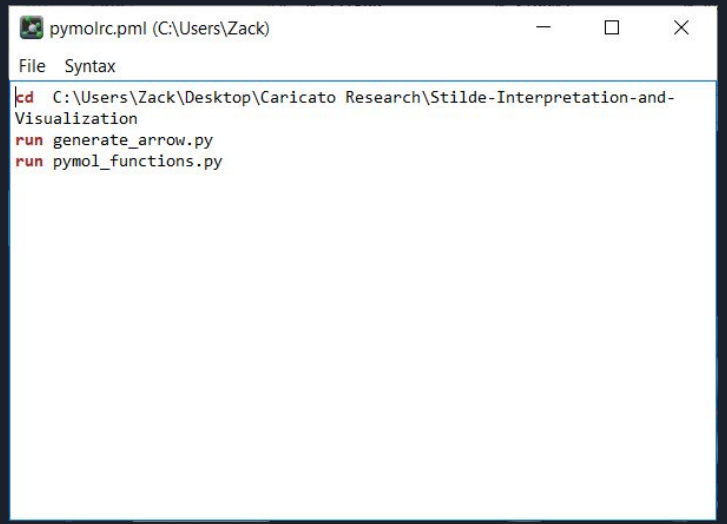
Loading Molecules

- After loading in a file, you can click and drag to rotate the structure
- Using the scroll wheel alone will adjust the ‘slab’ of the molecu
  - essentially moving the camera ‘through’ the molecule (not ve
  useful)
- Ctrl+Shift+Scroll will zoom the molecule in and out normally
- Clicking on an atom will create a variable called ‘sele’ (this is important and will be used later)
  - Clicking the same atom again will deselect it



Pymolrc file

- Pymolrc is a resource file that contains commands that are automatically executed when PyMol is launched
- It can be convenient for automatically changing your working directory, loading necessary scripts, and changing any other settings you frequently use
- Pymol has a built in editor under File -> Edit pymolrc



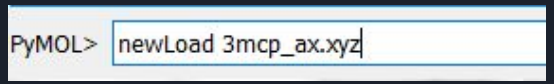
Loading Scripts into PyMol

- Python scripts can be loaded by entering “run scriptname.py”
- Once the script has been loaded in, any functions extended in the script will be accessible in PyMol
    - A Python function must first be passed to the cmd.extend() function defined in the PyMol API before it can be used independently in PyMol

Executing Scripts and functions

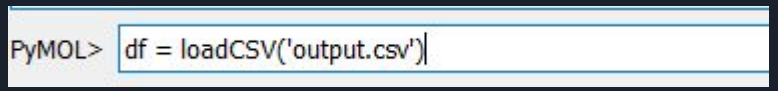
- As mentioned previously, if the function has been “extended” you can simply type the function name followed by its arguments to run it

```
def newLoad(filename):

    cmd.load(filename)
    # Everything ball and stick
    preset.ball_and_stick(selection="all", mode=1)

    # Change carbon color
    cmd.color("gray",selection="elem c")
    return
cmd.extend("newLoad",newLoad)
```

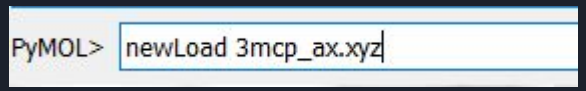


Python syntax vs PyMol syntax

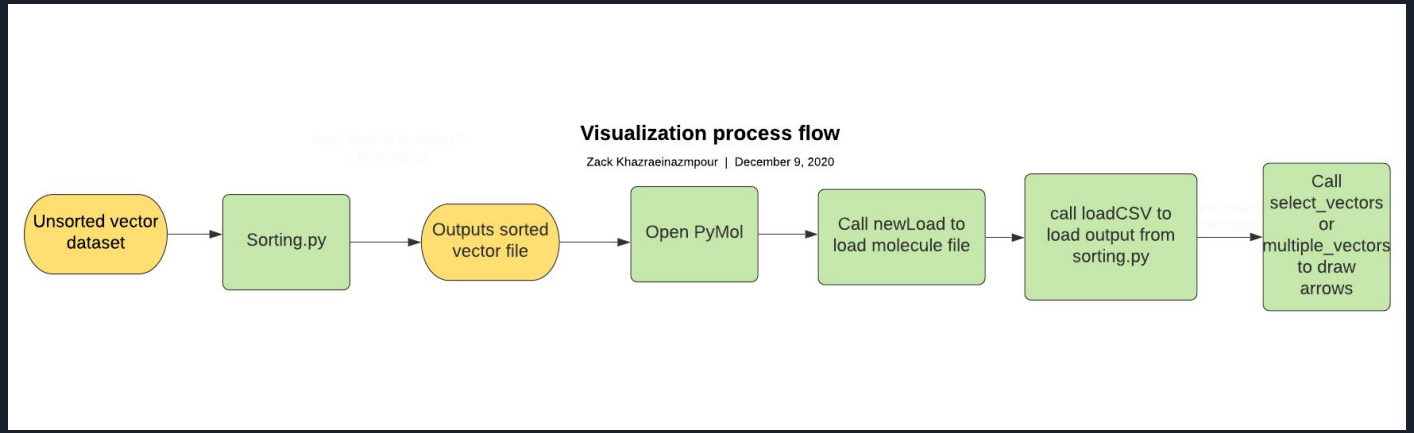
- Some functions can be called without any special syntax like parentheses or quotes
- However, if you want to do something like assign a function's return value to a variable in PyMol, you must use correct python syntax
  - In particular, this is necessary for the loadCSV function because the dataframe must be passed to select_vectors
- In general, any built-in Python function can also be run from the command line in PyMol
  - For example, you can call *print(df)* to print a dataframe at any time



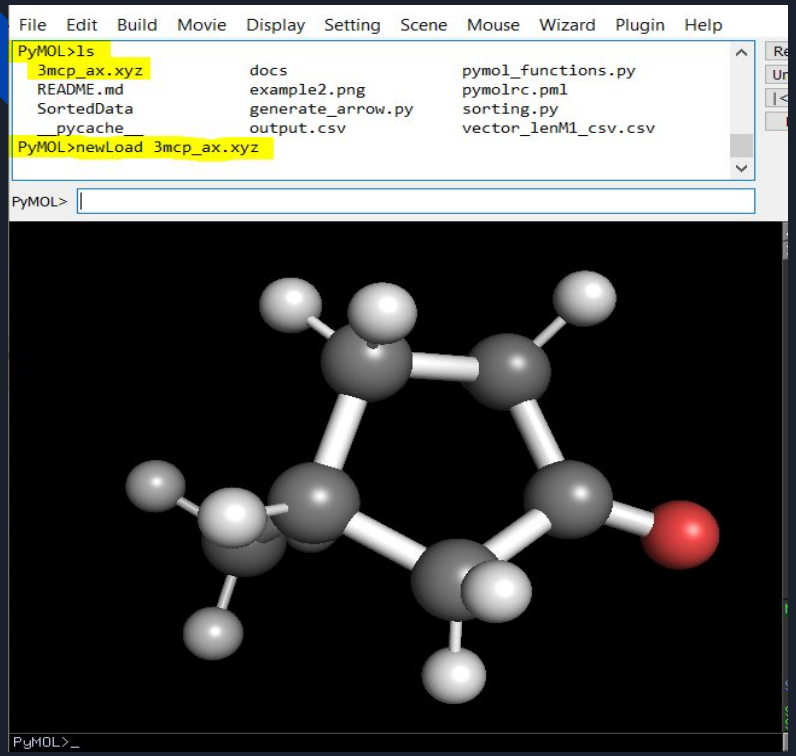
- Correct Python syntax must be used here



- Correct Python syntax is not necessary here



- A diagram illustrating the general flow for drawing arrows in PyMol. The next couple slides show what the expected output should be for the functions in PyMol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PyMOL>ls
3mcp_ax.xyz docs pymol_functions.py
README.md example2.png pymolrc.pml
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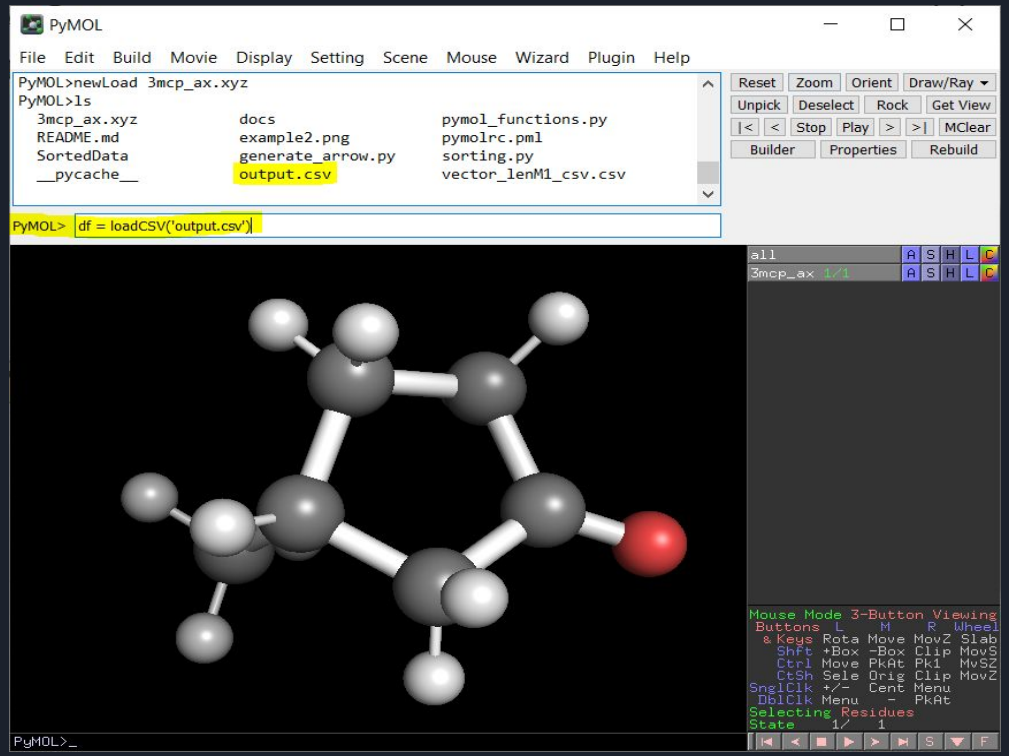
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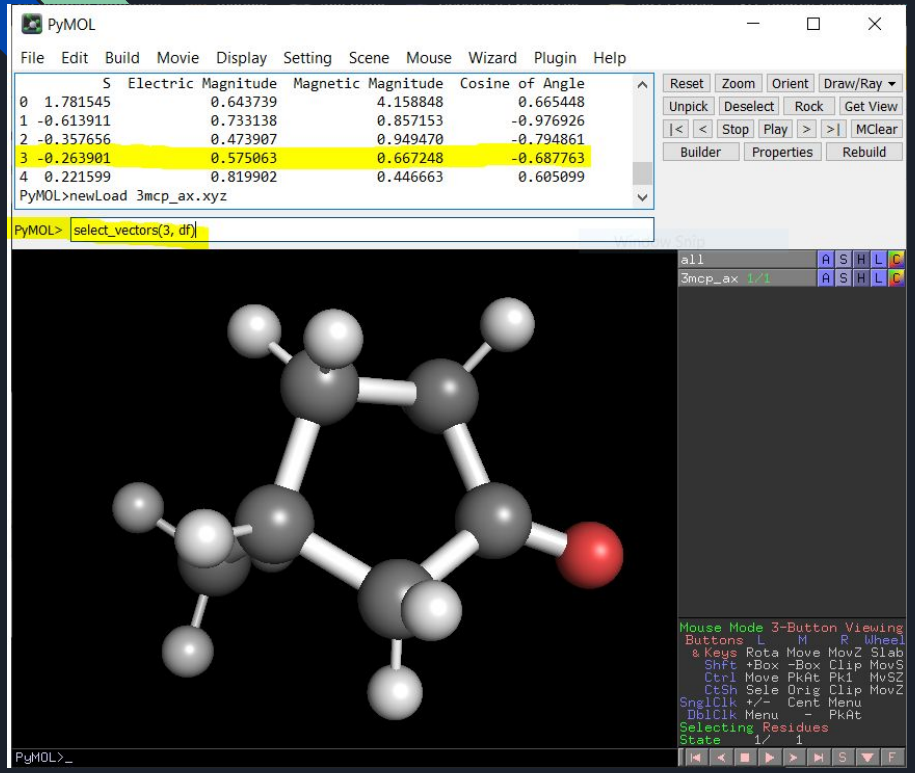
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3 -0.263901 0.575063 0.667248 -0.687763
4 0.221599 0.819902 0.446663 0.605099
PyMOL>newLoad 3mcp_ax.xyz
PyMOL> select_vectors(3, df)
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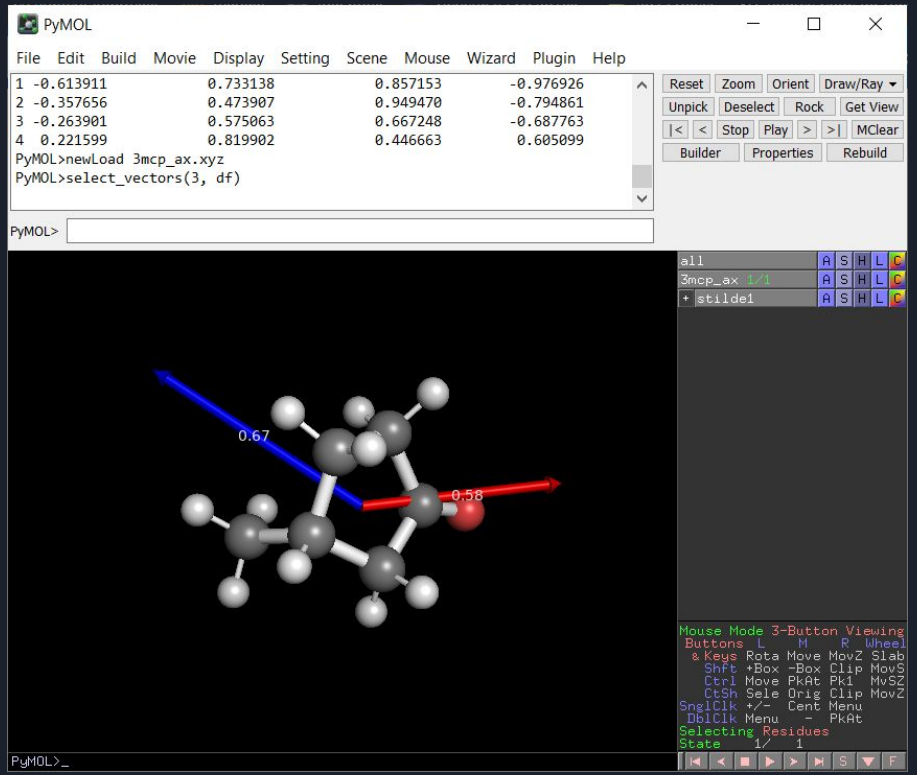
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PyMOL>
Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Builder Properties Rebuild
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0.58
all
3mcp_ax 1/1
stilde1
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
&Keys Rota Move MovZ SLab
Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
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Selecting Residues
State 1/ 1
PyMOL>_

Exporting the model as an image

- Use the ‘png’ command to export an image of the current view window
  - Only the section containing the molecule will be captured, not the surrounding toolbars
- Syntax: *png filename.png* or *png Desired/File/Path/filename.png*

Conclusion

- Following this guide, you should be able to effectively draw arrows representative of s-tilde values in PyMol and easily export them
- For more information on PyMol and it's various functions and settings, consult the PyMol wiki
- If you encounter errors that you can't solve, email me at zack_khaz@ku.edu, or post an issue on the program's Github page