Molecular Movies and Really Pretty Pictures

A basic tutorial on use of PyMol by M. Pitt which comes with no guarantee or support on my part.

PyMol is a very cool molecular graphics package for Mac, Linux, and Windows. It's really good for structure viewing and is under constant development, so sometimes the commands will change when you get a new version. Caveat Emptor. There is a reasonably well-maintained wiki, as well as tons of other resources on the web. Consult them frequently.

Useful resources:

http://www.rubor.de/anlagen/PyMOL_Tutorial.pdf
http://www.pymolwiki.org/index.php/Main_Page

What you need:

1. A computer. Preferably a Mac or Linux box, because I think PyMol is easier to run on them. This might be my own prejudice.
2. PyMol (http://delsci.com/rel/). A free educational version is available, just email Warren deLano for download credentials.
3. A Python interpreter (from http://www.python.org)
4. The rtools package. (http://www.rubor.de/bioinf/pymol_extensions.html). There are some great resources for movie commands available there. Also see:
5. A .PDB file (A crystal structure, molecular model, or otherwise)
6. Quicktime or some other software that can assemble individual images into a movie. (Optional on Mac)

Getting Started:
First, make a folder with a copy of your PDB file and the `movie.py` file. Open your copy of PyMol (on Windows, make sure you open the version including the graphical user interface).

Here are some basic commands you'll want to know.

`PyMol>` Here's the command prompt

`cd ..` Change directory (move up one level)
`cd directory_name` Move to a different directory
`ls` Show contents of current directory
`run movie.py` Runs the script "movie.py"
`load molecule.pdb` Opens the file "molecule.pdb"

With newer versions, you can open .pdb files directly from a drop-down menu.

Hint: Pressing TAB after entering a few letters will often autocomplete your entry. Some syntax may be different depending on your OS!

Now, from the PyMol command line, navigate to the folder containing your PDB file, run the movie script, and load your molecule file. You will see your molecule displayed as a collection of colored lines.

Mouse actions: Left click and drag moves; right click and drag zooms. There are many more in the manual.

Making your molecule pretty:

Atoms can be represented by many different symbols such as

`Lines` `Sticks` `Spheres` `Ribbons`

You can `show` or `hide` these representations based on selection parameters such as atom types:

```
Pymol> show sticks, elem c+n+o+s
Pymol> hide everything, elem h
```

This show the `sticks` representation of carbon, nitrogen, oxygen, and nitrogen, while hiding *all* representations of hydrogen. This means you won't see the hydrogens anymore.

You can also change the colors of certain atoms:

```
Pymol> color gray, elem c
```

The reference files have a complete listing of predefined colors.

From the drop down menus, you can change the background to different colors. Or just type:

```
Pymol> bg_color white
```

Specific Selections:

You can also collect any combination of atoms into a named selection to make commands a bit simpler:

```
Pymol> select ligand, elem c+n+o+h+s
```

Here, I have told Pymol that "ligand" consists of all the named atoms. This way they can all be changed at once.

```
Pymol> show sticks, ligand
```

Ray-Tracing:

At any time you can type the command `ray` to produce a very nice, smooth picture. You can copy this and paste it into documents or presentations. Or export it as a .png file from the drop-down menus.

Movies:

Since you've already run the movie script, this is *easy!*

`movie -` plays a movie
`mvClear –` clears the frames
`mvMove 1-100,x,10 –` moves10 units to the right over the first 100 frames
`mvRot 101-150,y,180 –` rotates 180 degrees around y axis, next 50 frames
`mvSinrot –` Same as mvRot, but smooths the motion
`mvSinmove –` Same as mvMove, but smooths motion

Updated movie commands (with all the right places to include arguments) are here:
http://www.weizmann.ac.il/ISPC/rTools_doku.htm

Decide what motions you want to incorporate, how many frames you want to use, etcetera. Issue your commands to Pymol, then issue the `movie` command to watch your movie. Once you have it how you like it, make sure to check the "Cache Frames" option, because it will run a lot faster. Especially when you ray-trace the frames.

Getting the Movie out of PyMol:

If you want each frame to be ray-traced, make sure that you click "Movie," then "Render Frames." This will take longer, use more file space, but the images will be prettier.

On Windows: Once your movie is prepared, go to the file menu and save the movie as numbered PNG files. Then run VideoMach, click File => Open, select Just the First Image, and click Open. At the prompt, select open series of images. Click File => Save as, enter the output name movie.avi (you can change "movie" to whatever you want). Then click the Video tab and the Codec Settings button. Choose any codec with a green dot next to it. Now click the Start button to make your movie! You should be able to watch it in Windows Media Player or Quicktime.

On a Mac: Your life is much easier. All you have to do once the movie frames are prepared is

click File => Save Movie As => Quicktime. If you really want to, you can save the frames as images and compress them on your own.

PyMol has many, many other features that you might find useful. You can:

1. Select by molecule in your model, so you can selectively manipulate (for example) a guest molecule.
2. Use the "Measurement" wizard to measure distances, then show/hide the related dashed line and measurement. Really handy for showing hydrogen bonds.
3. Make spheres bigger or smaller. If you want to make your metal atoms a certain size, for example, type "alter elem As, vdw=1.5", then "rebuild." This will make the van der Waals radius of all arsenic atoms 1.5 angstroms.
4. Check out the ray-tracing options – there are some really fun ways to render the molecules. Explore and find out.