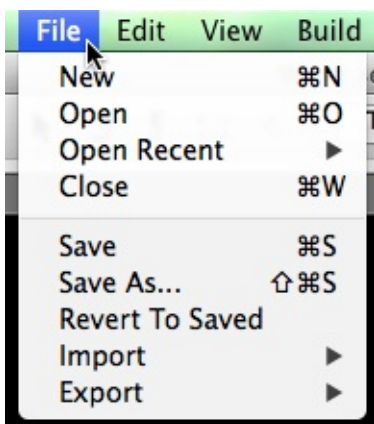
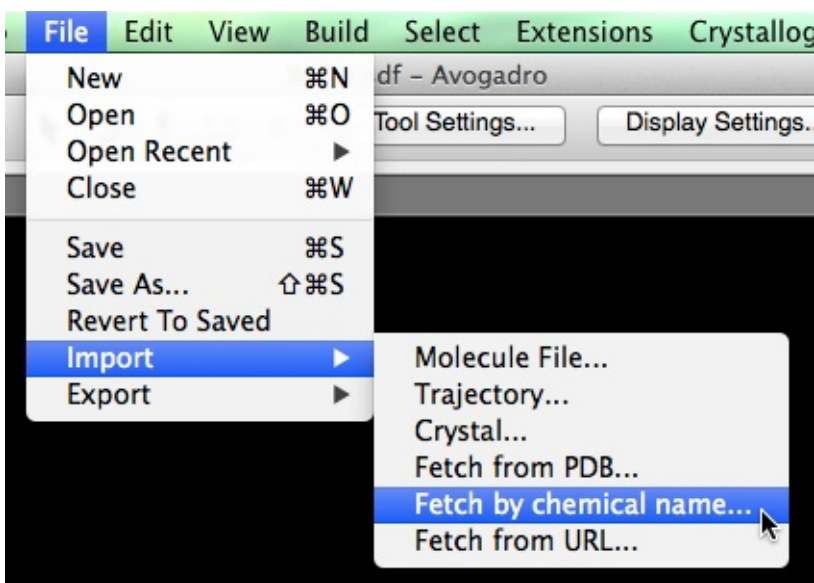


Importing Molecules by Name

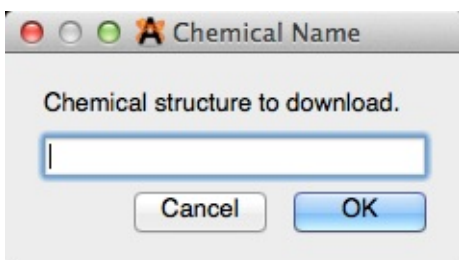
Select the "File" menu.



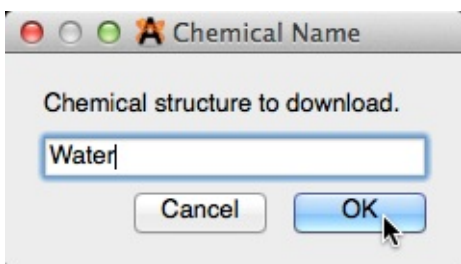
Then select "Import", and "Fetch by chemical name..."



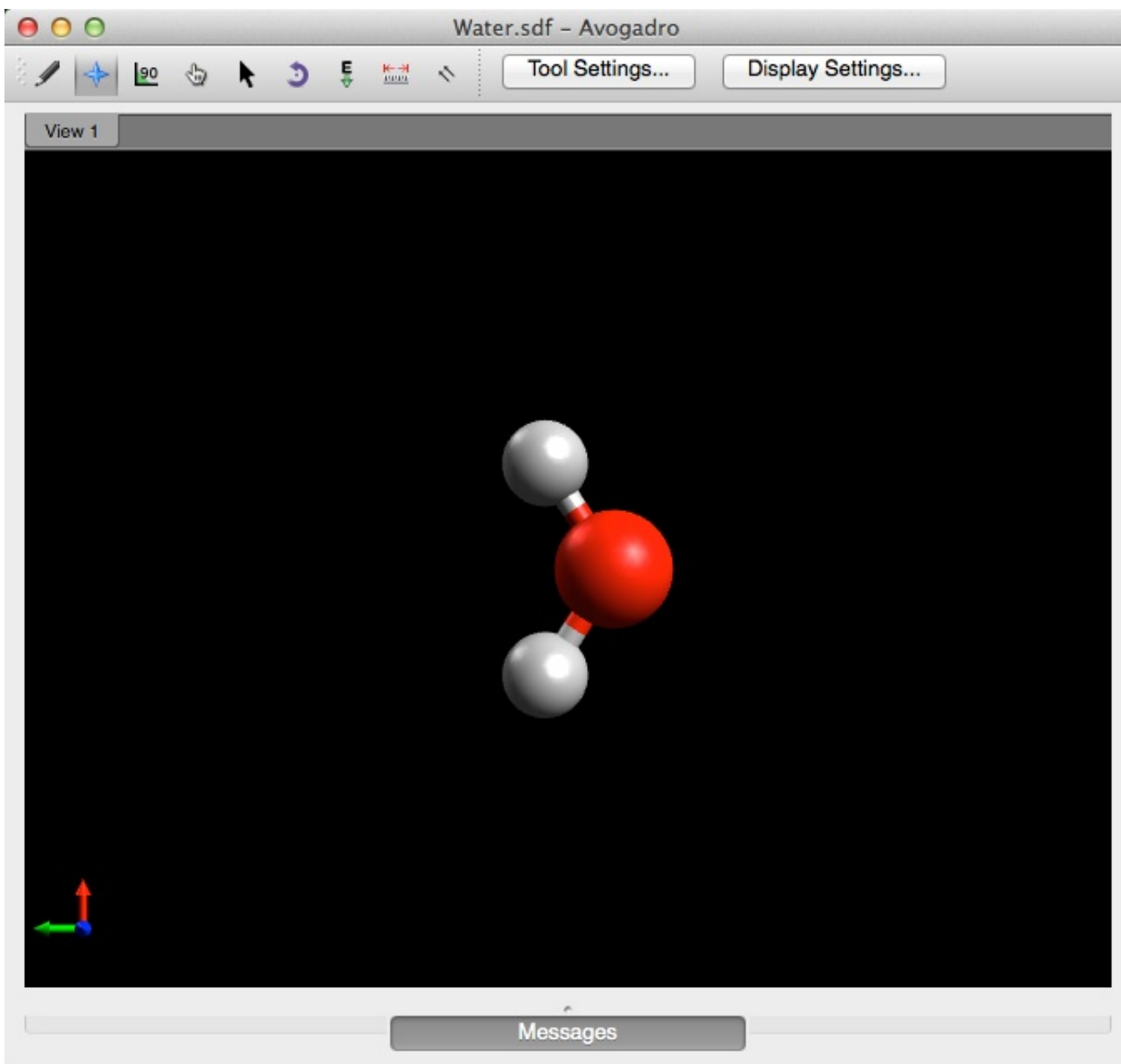
A dialog box will pop up (depicted below), where you can type in any chemical name.



Avogadro will import the molecule into the viewing screen after you click "OK".



It may take a few seconds or even a minute to download the molecule online. Avogadro uses the NIH "Chemical Resolver" <http://cactus.nci.nih.gov/chemical/structure> to convert the name into a molecular structure.

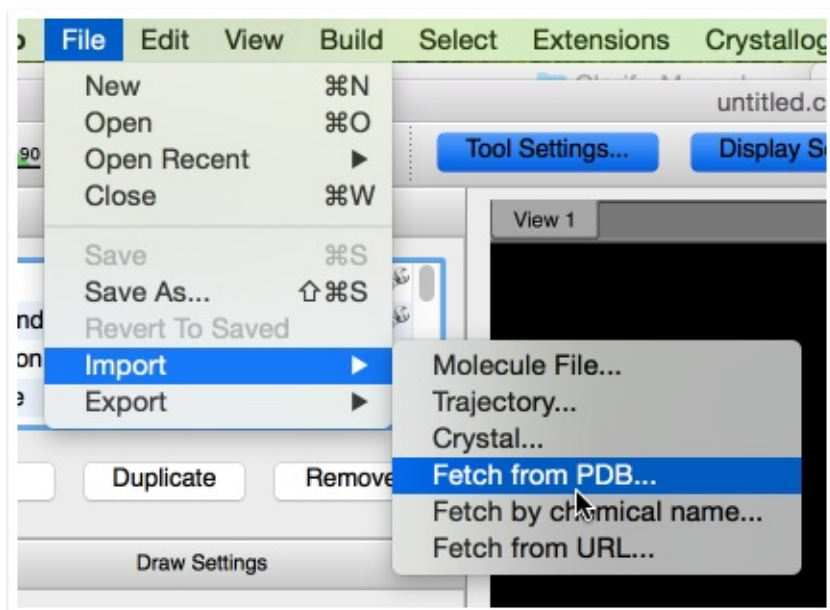


Importing from the Protein Data Bank (PDB)

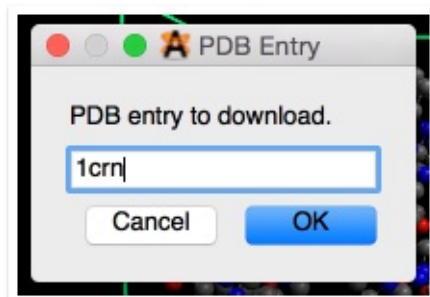
You can read PDB files that you download yourself from <http://www.rcsb.org/> or access the PDB code yourself.

Importing directly

Older versions of Avogadro have a bug with direct access to the PDB (since the website has moved) but using v 1.2.0, you can again use File > Import > Fetch from PDB... to download proteins.



A dialog will come up and allow you to enter a PDB code (e.g., 1CRN for crambin)

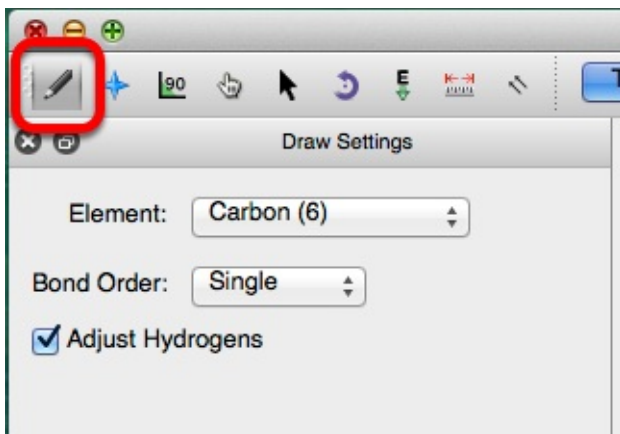


There it is... the PDB data direct from the website.

The Draw Tool

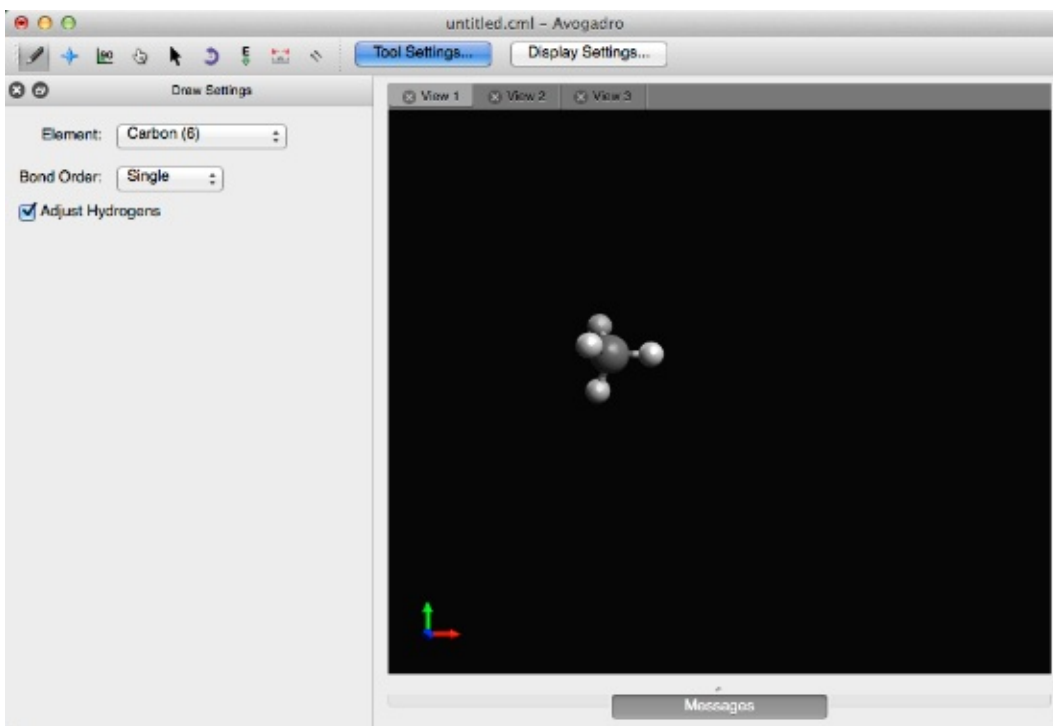
1. Creating a Molecule

Molecules can be built and edited with the draw tool.



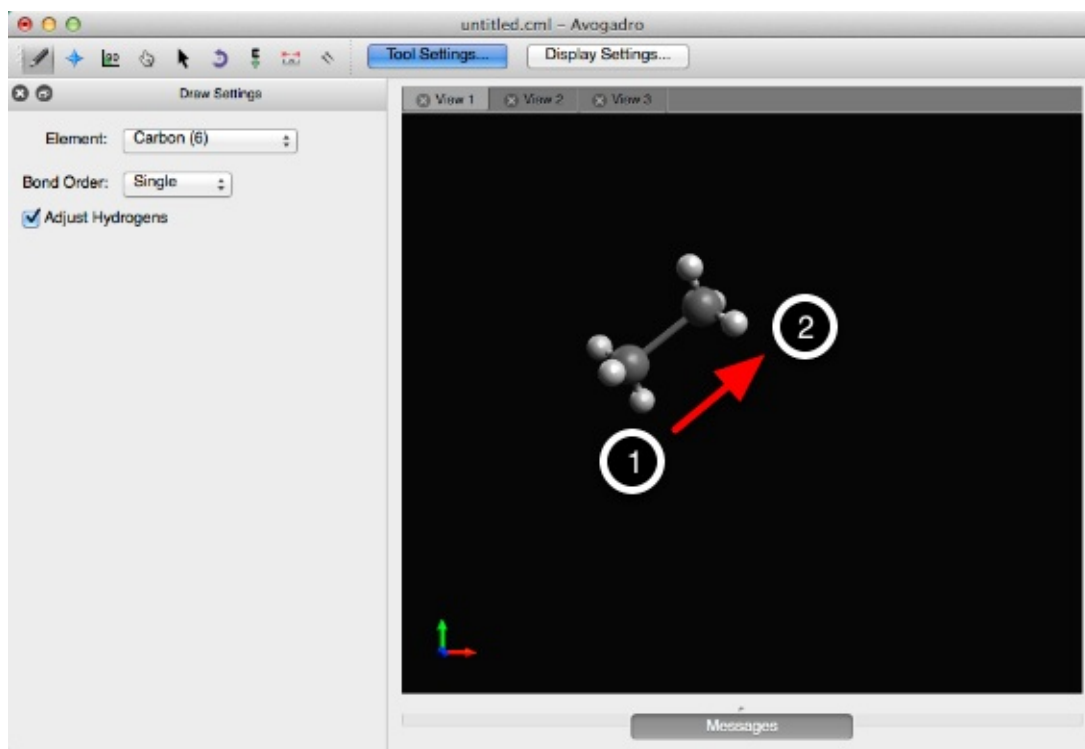
2.

You can begin creating a molecule by left clicking on the black display. This will generate a carbon atom. Right clicking on the atom will delete it.



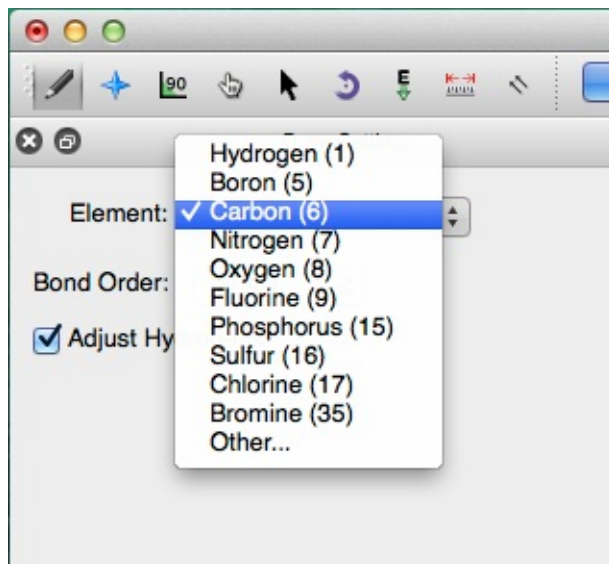
3.

Left clicking and dragging the mouse will generate a bond to another carbon atom.



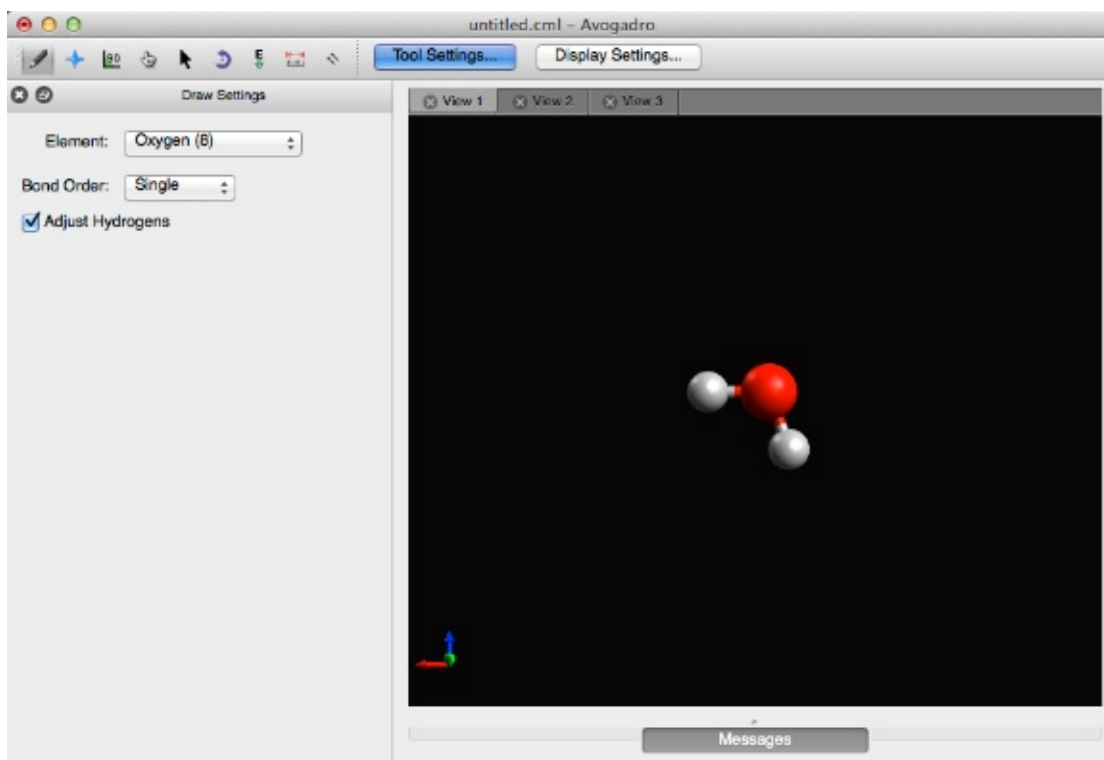
4.

Different elements can be selected from the Element drop down menu. Typing the atomic symbol (e.g., "A-s" for Arsenic) is a shortcut for changing the selected element.



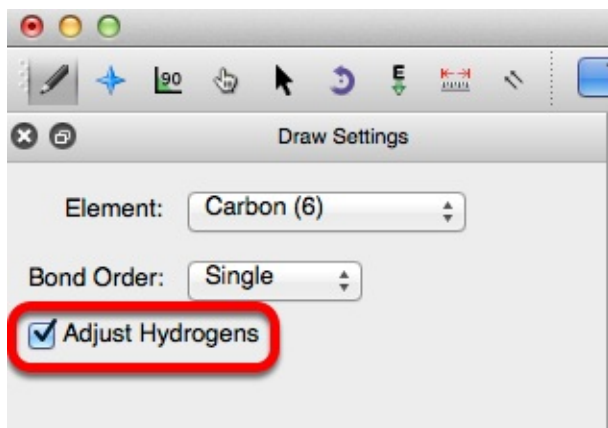
5.

For example, if you wanted to create water, you can type in "O", or select "Oxygen (8)" from the drop down menu and click on the black display.



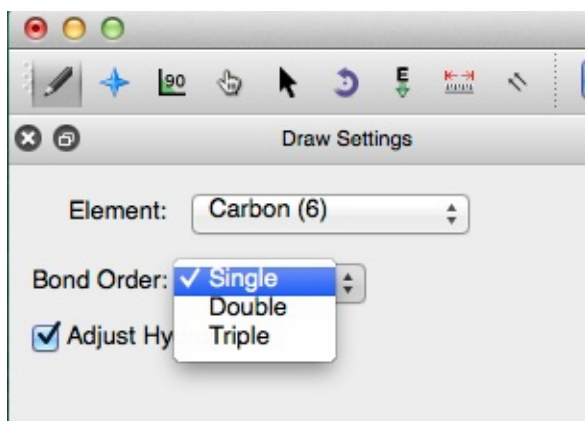
6.

If the "Adjust Hydrogens" box is checked, hydrogens in the molecule are automatically adjusted to satisfy valency (as shown above).



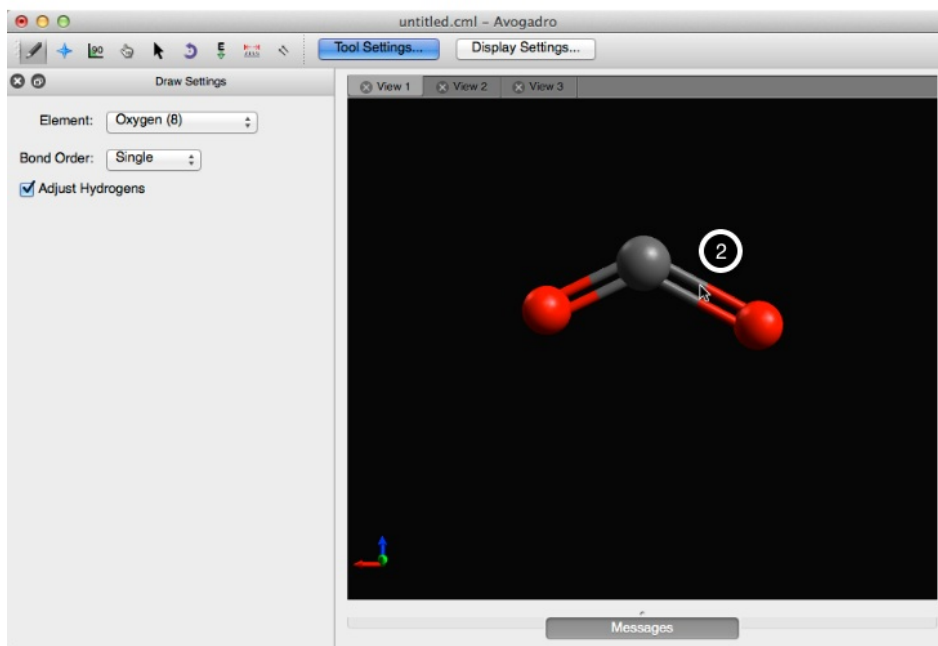
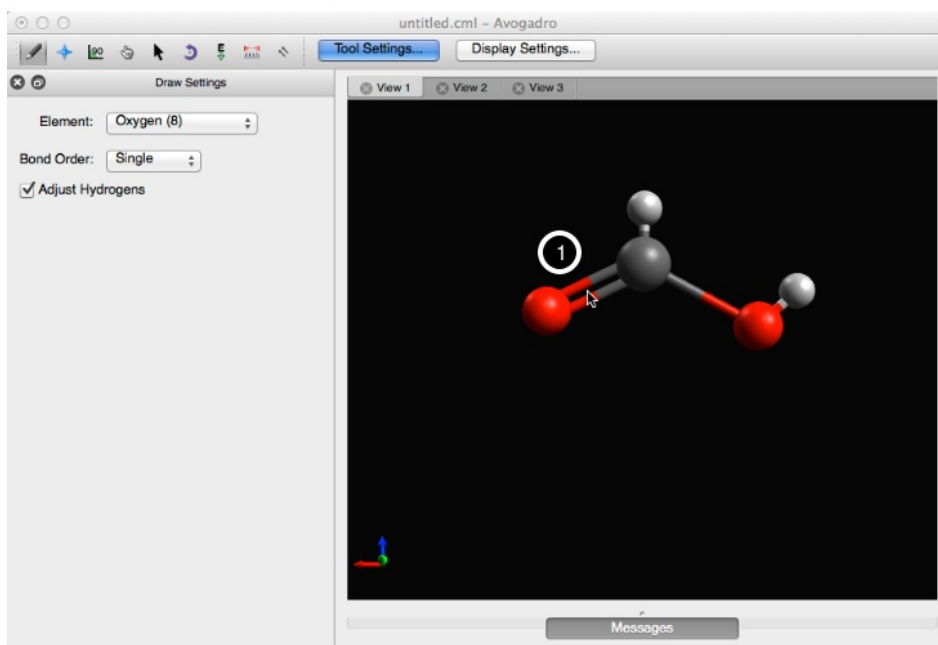
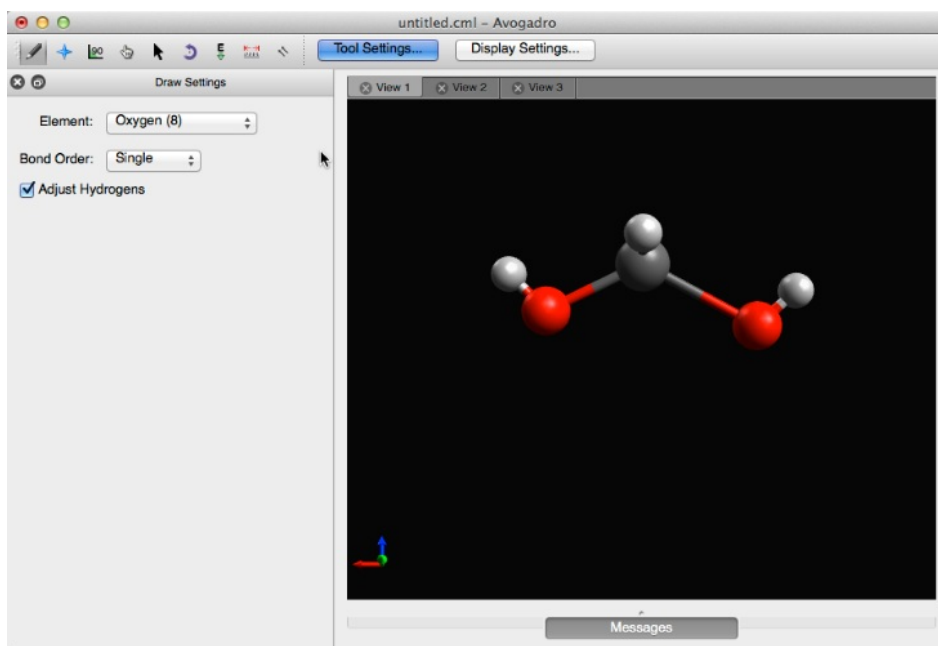
7.

Bond order can be changed through the Bond Order drop down menu, or by typing the numbers "1", "2", or "3". Bonds can also be added to a molecule by left clicking on a bond that has already been created (this process cycles through single, double, and triple bonds). Right clicking on a bond will delete the bond, and the atom it's bonded to.



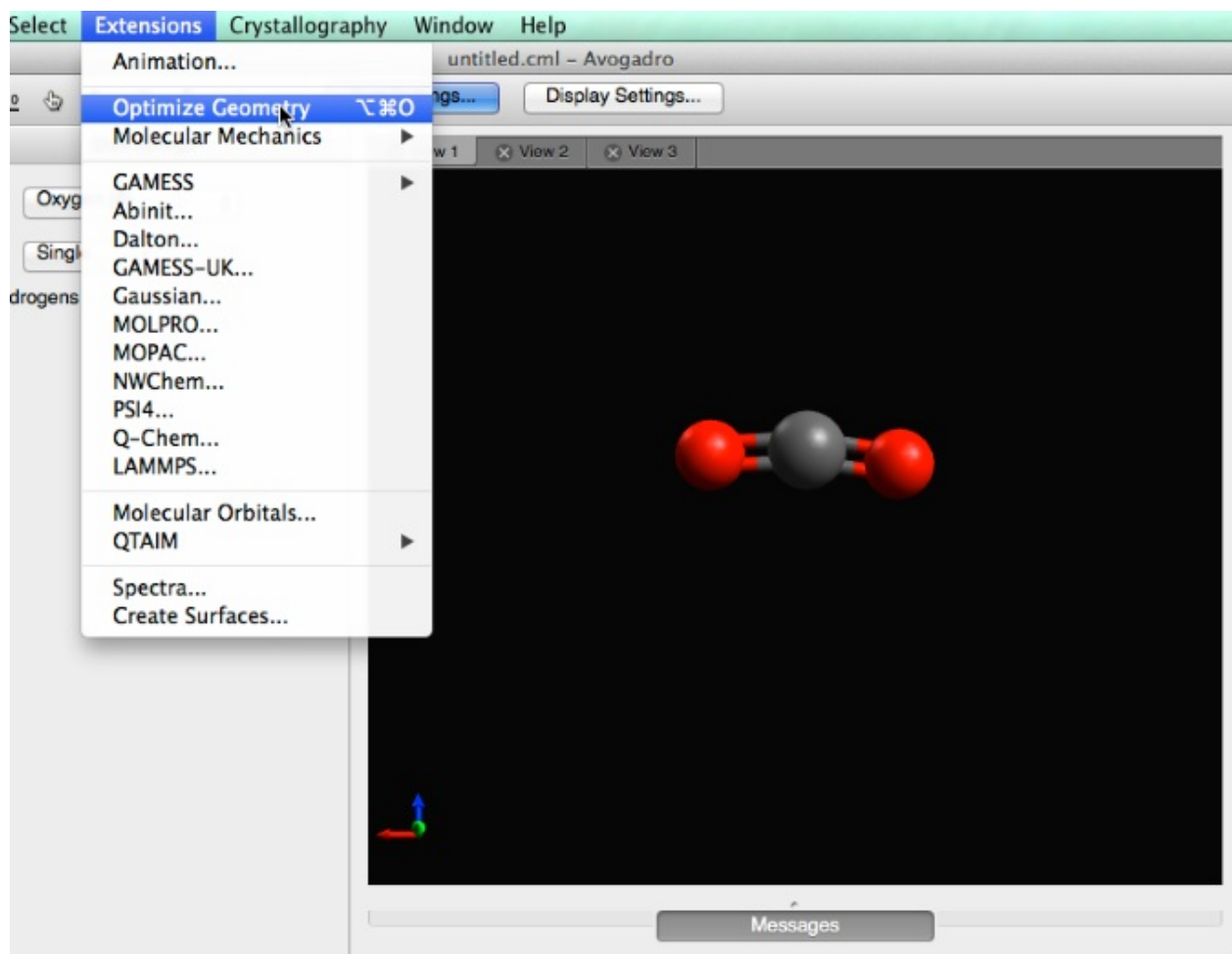
8.

For example, to create carbon dioxide, the general structure ("O-C-O") needs to be drawn, and then by left clicking the bonds in the molecule, double bonds will be created.



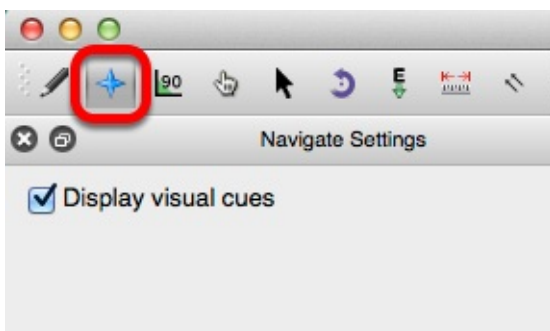
9.

Under the "Extensions" menu, the geometry of a molecule can be optimized by selecting "Optimize Geometry".

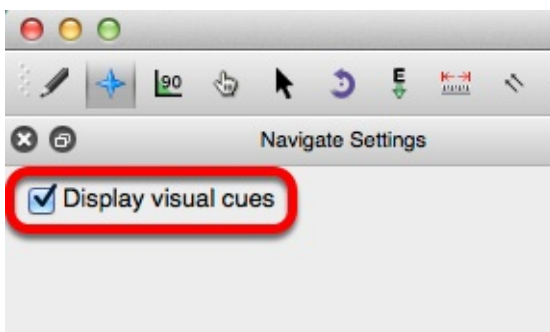


The Navigate Tool

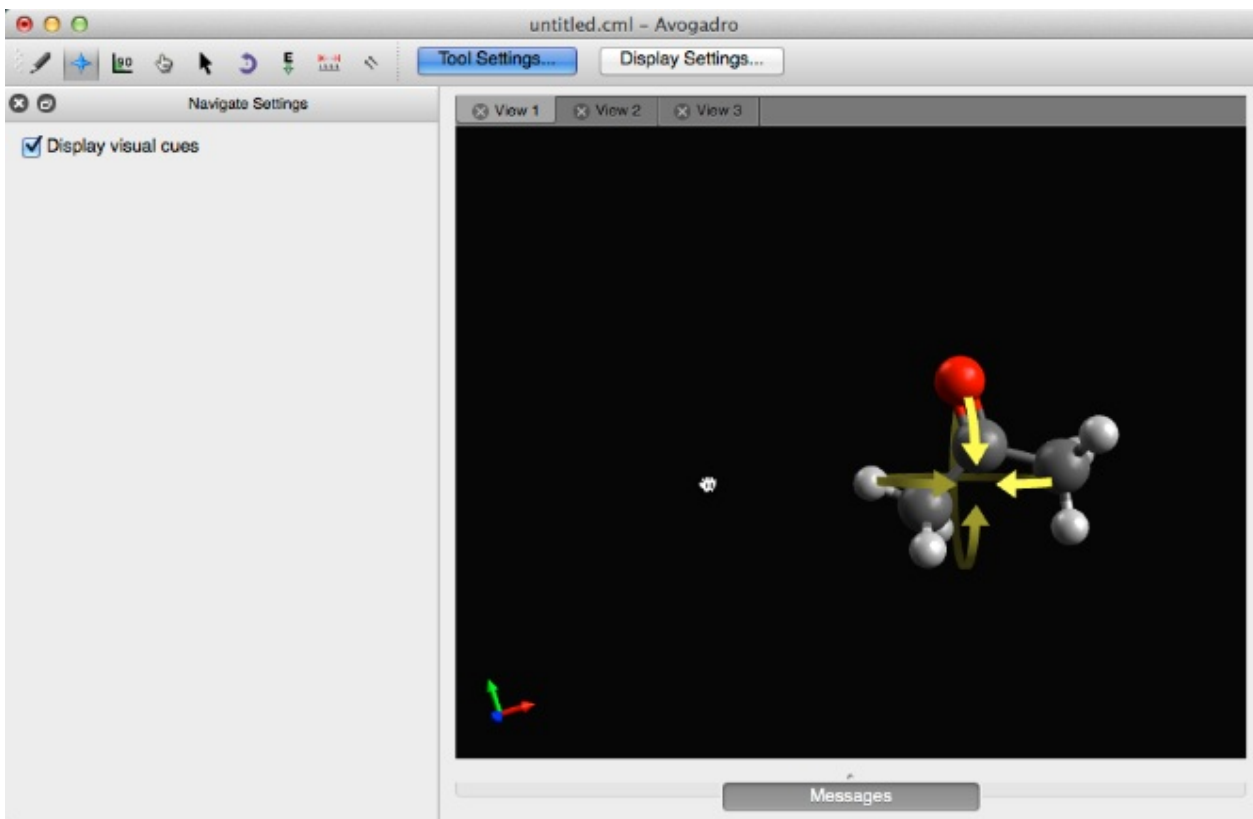
The navigation tool is used to pan, rotate, and scale the view of a molecule.



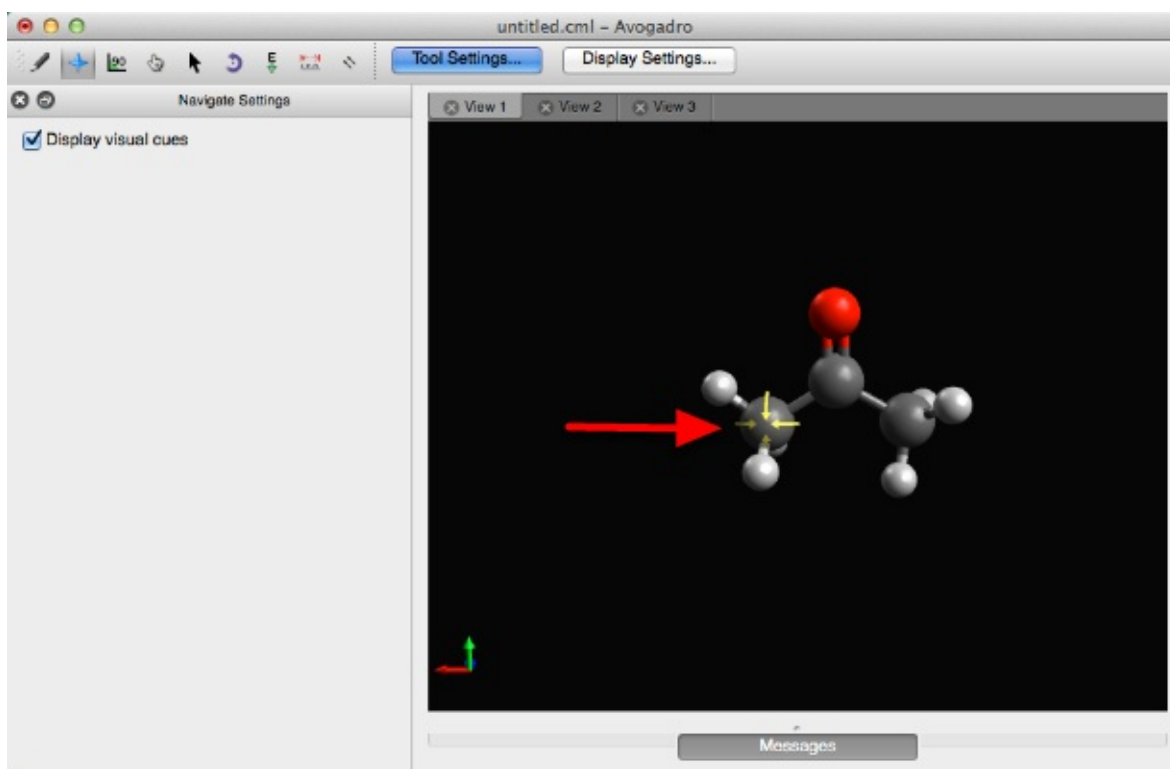
If the "Display visual cues" box is checked, yellow arrows will display what type of navigation is taking place.



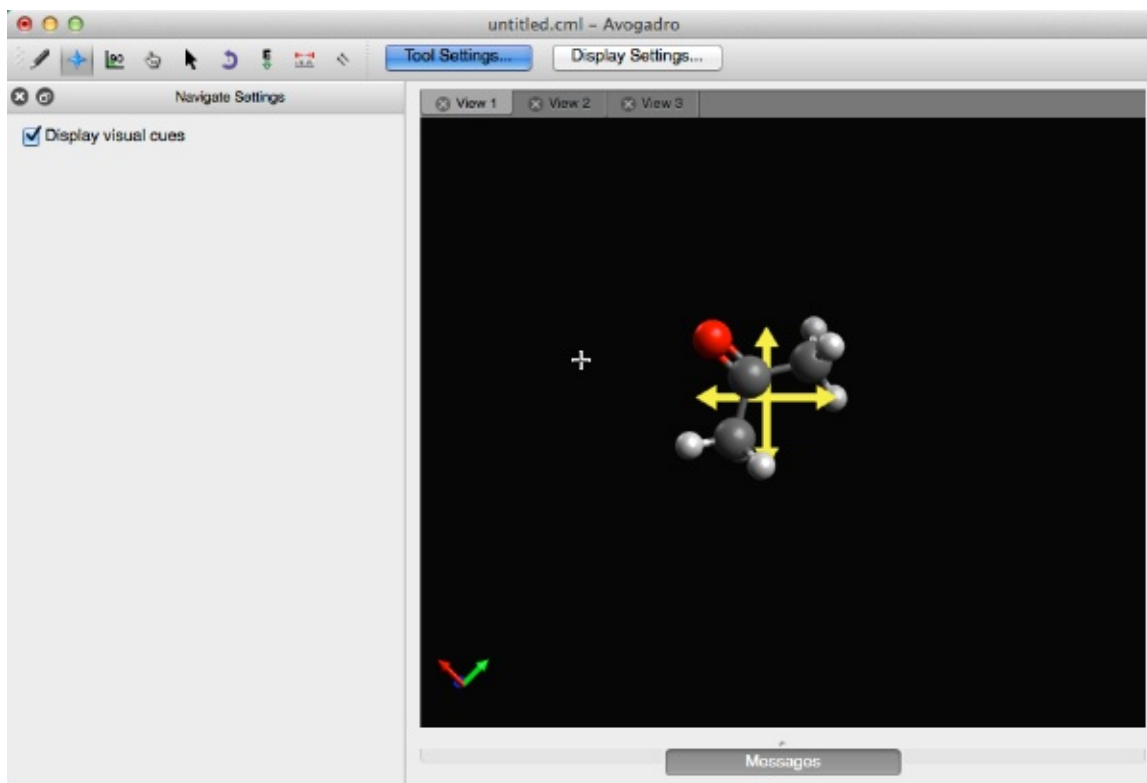
Clicking anywhere on the black display and dragging the mouse will tilt, and rotate the entire molecule (as shown below).



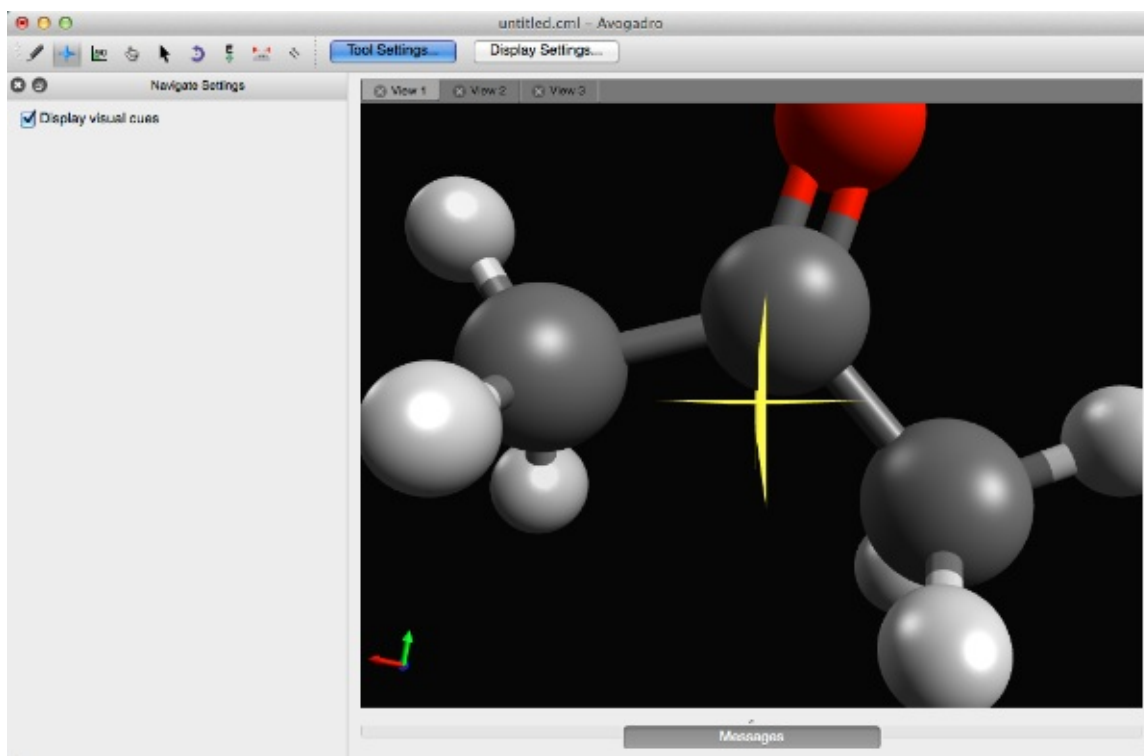
A molecule can also be rotated about an atom by clicking the atom and dragging the mouse. Depicted below, acetone is being rotated about it's initial carbon.



Right clicking allows you to change the molecules location on the display. Double clicking the molecule will reset the molecule's view.

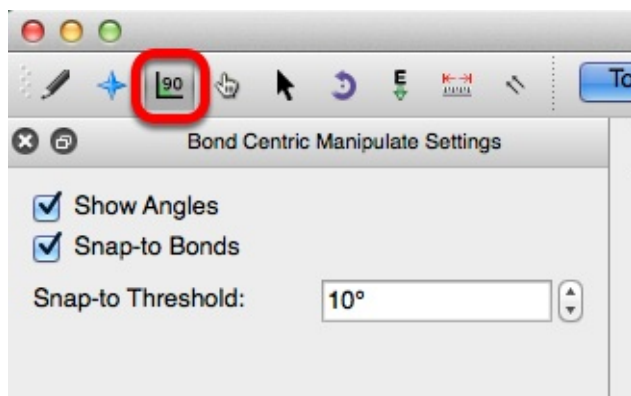


Using the middle scroll bar on a mouse will allow you to zoom in and out.

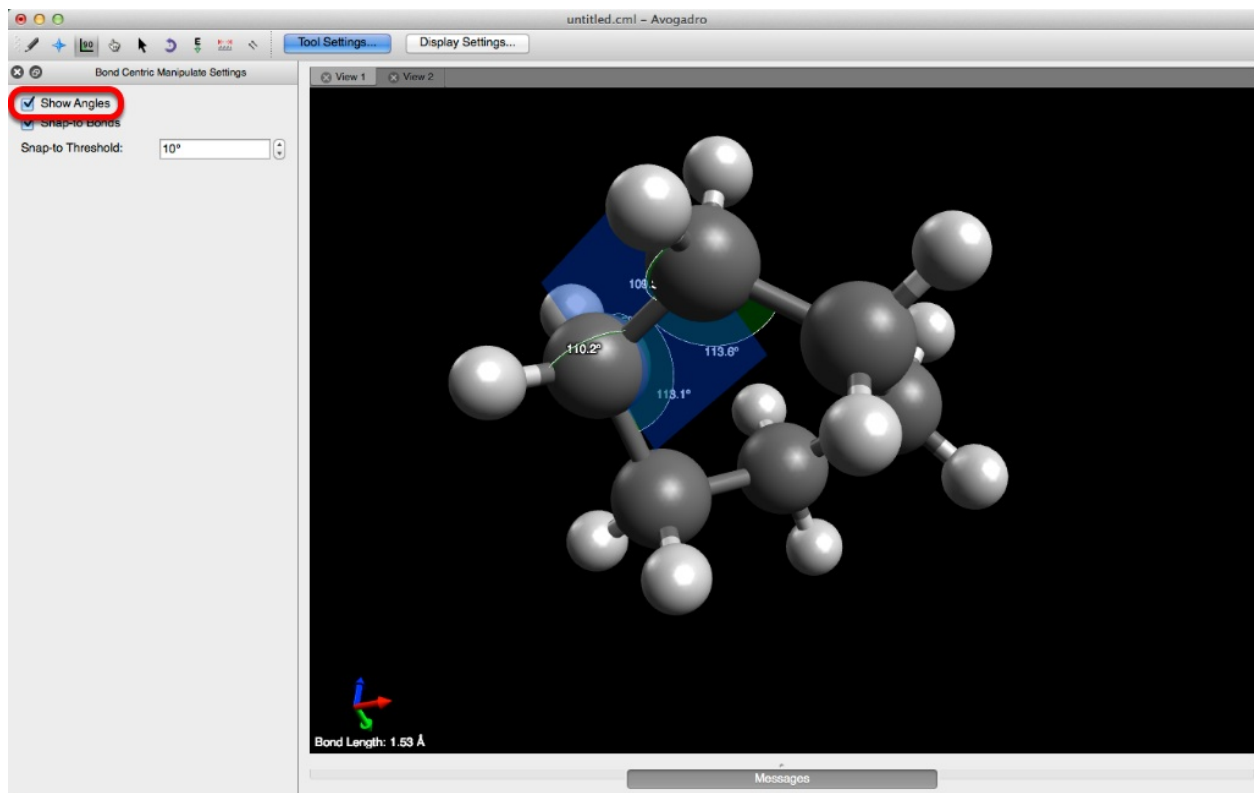


The Bond-Centric Manipulate Tool

The Bond-Centric Manipulate tool alters angles, bonds, and torsions of a molecule.

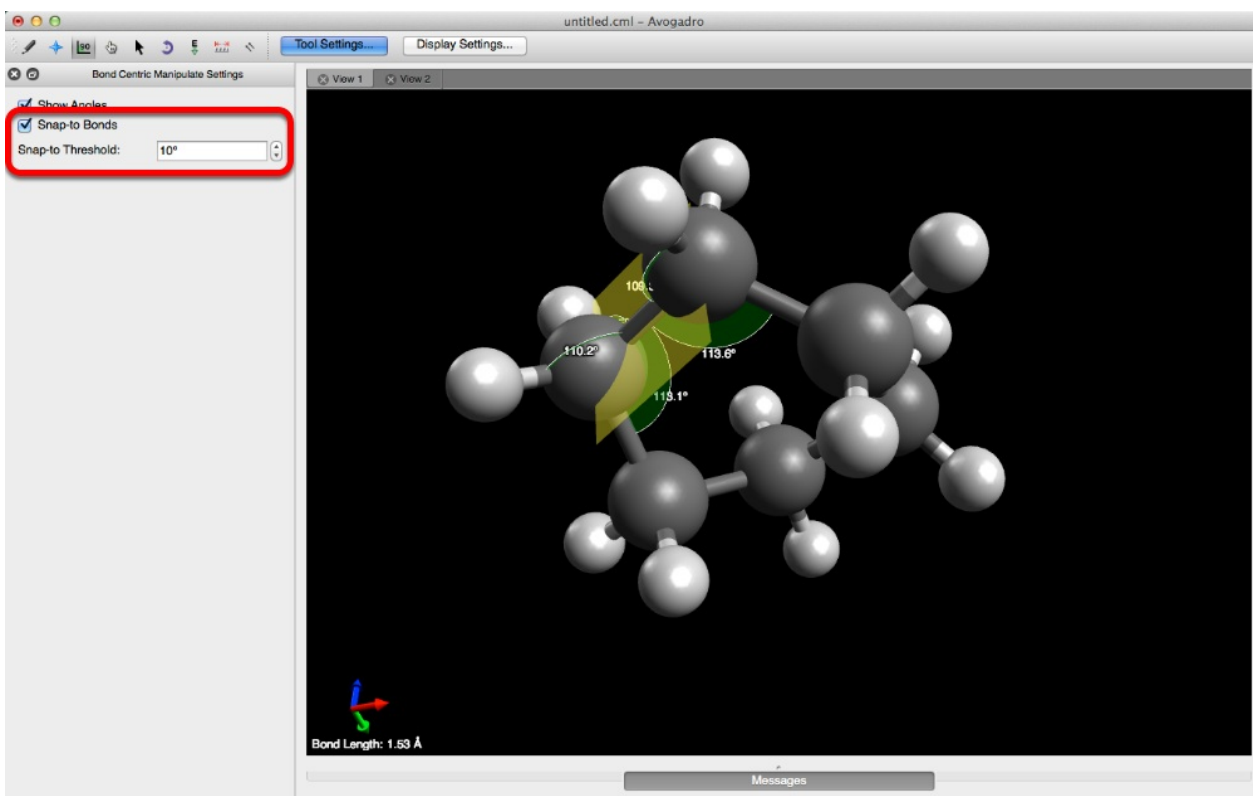


Left clicking on a bond and dragging your cursor allows you to adjust the plane. If the "Show Angles" box is checked, the angles from the selected bond to all adjacent bonds are displayed.

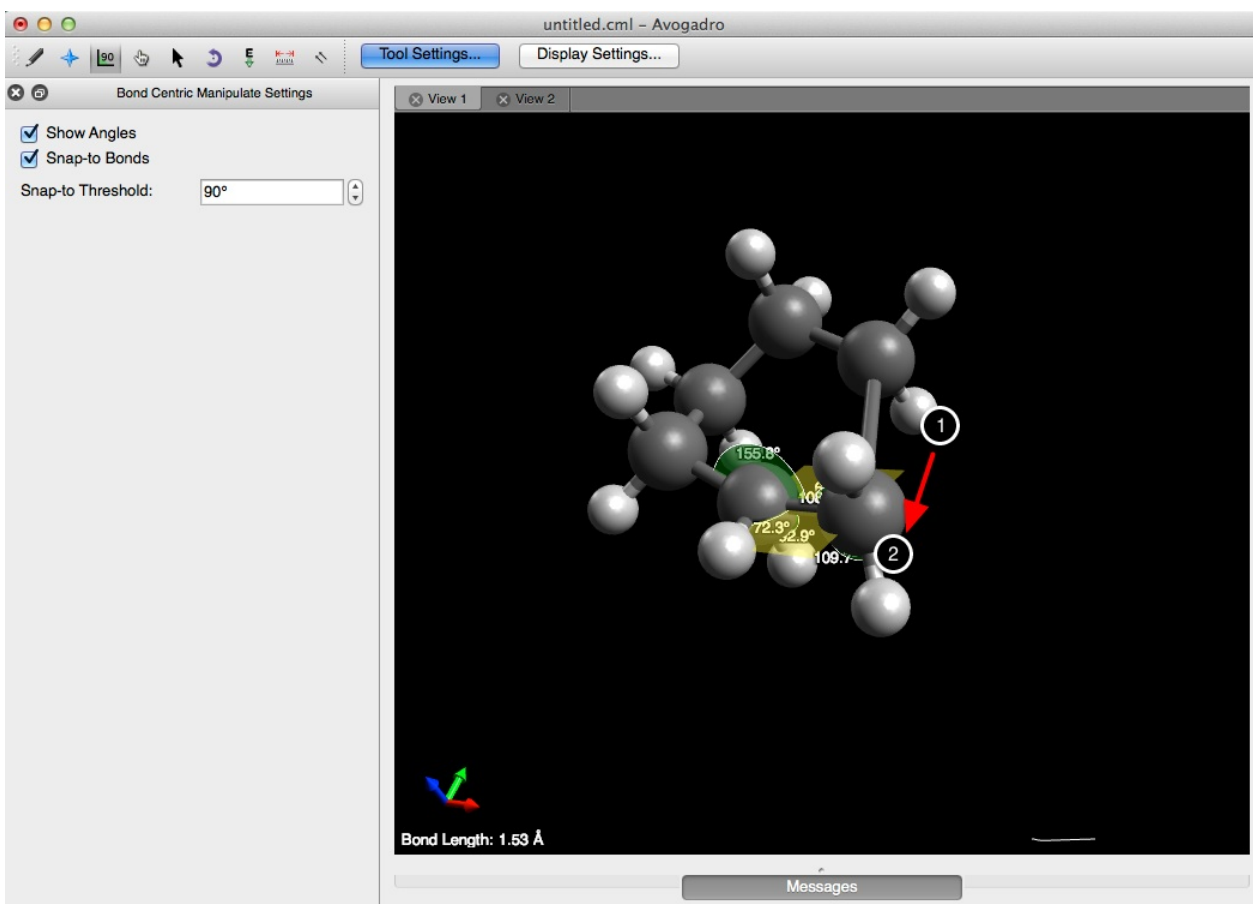


As you're rotating the plane you'll notice that if the "Snap-to Bonds" box is checked, the plane will change colors between yellow and blue. If the plane depicted is yellow then the plane *is* in line with an adjacent bond. If the plane depicted is blue the plane *is not* in line with any adjacent bonds.

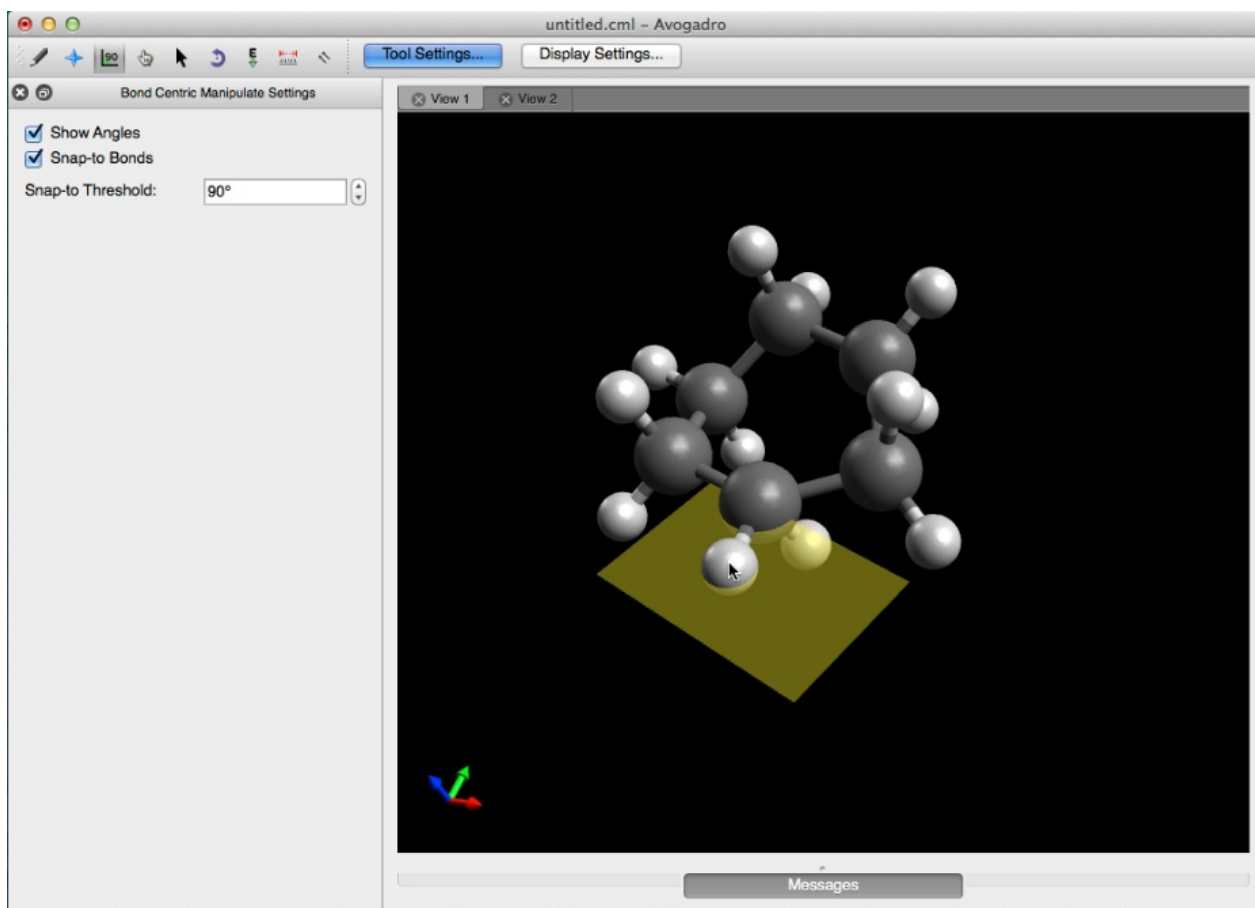
The "Snap-to Threshold" determines how far away a plane has to be to *snap* to an adjacent bond plane. For example, below the Snap-to Threshold is 10 degrees. If the plane being rotated comes within 10 degrees of an adjacent bond, that plane will snap to the adjacent bond plane. If the Snap-to Threshold is changed to 90 degrees, the rotating plane will only snap to adjacent bond planes.



Once a plane is selected the atoms on either end of the plane can be manipulated, by left clicking on the atom and dragging. The displayed angles will automatically adjust, and the selected bond will *not* change in length.

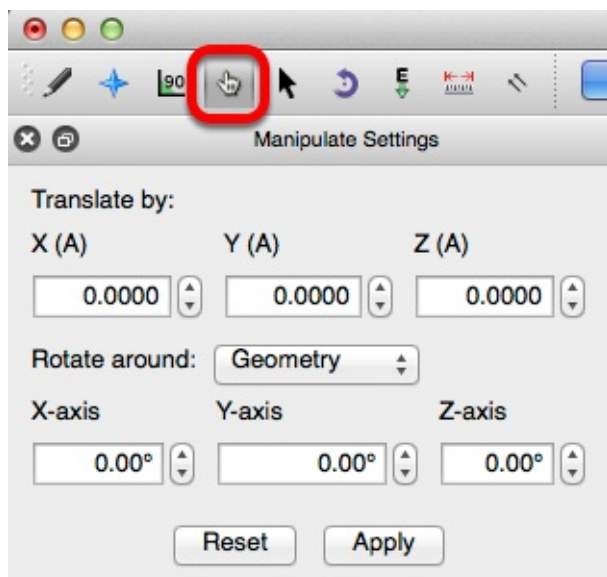


Left clicking on a substituent, or in this case a hydrogen bonded to one of the selected carbon atoms will allow you to adjust the torsion angle.



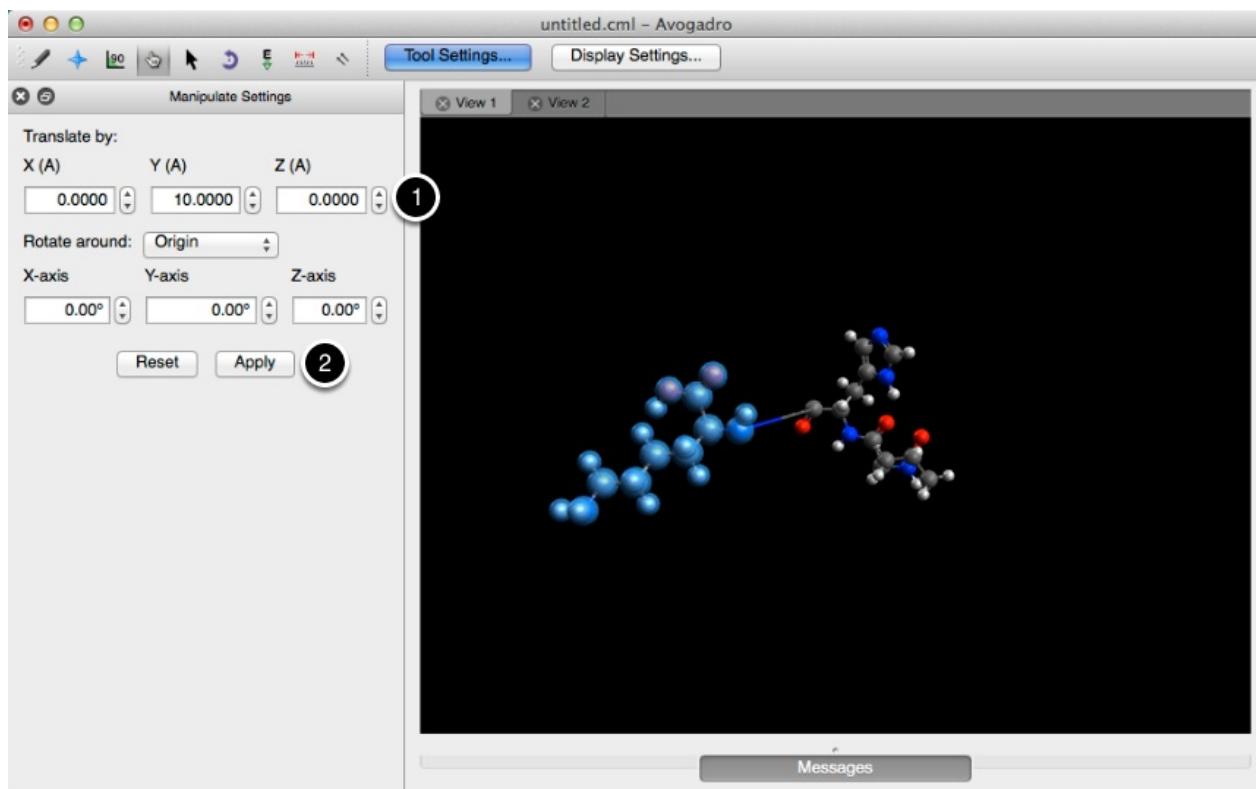
The Manipulate Tool

The manipulate tool allows you to move atoms and selected fragments.

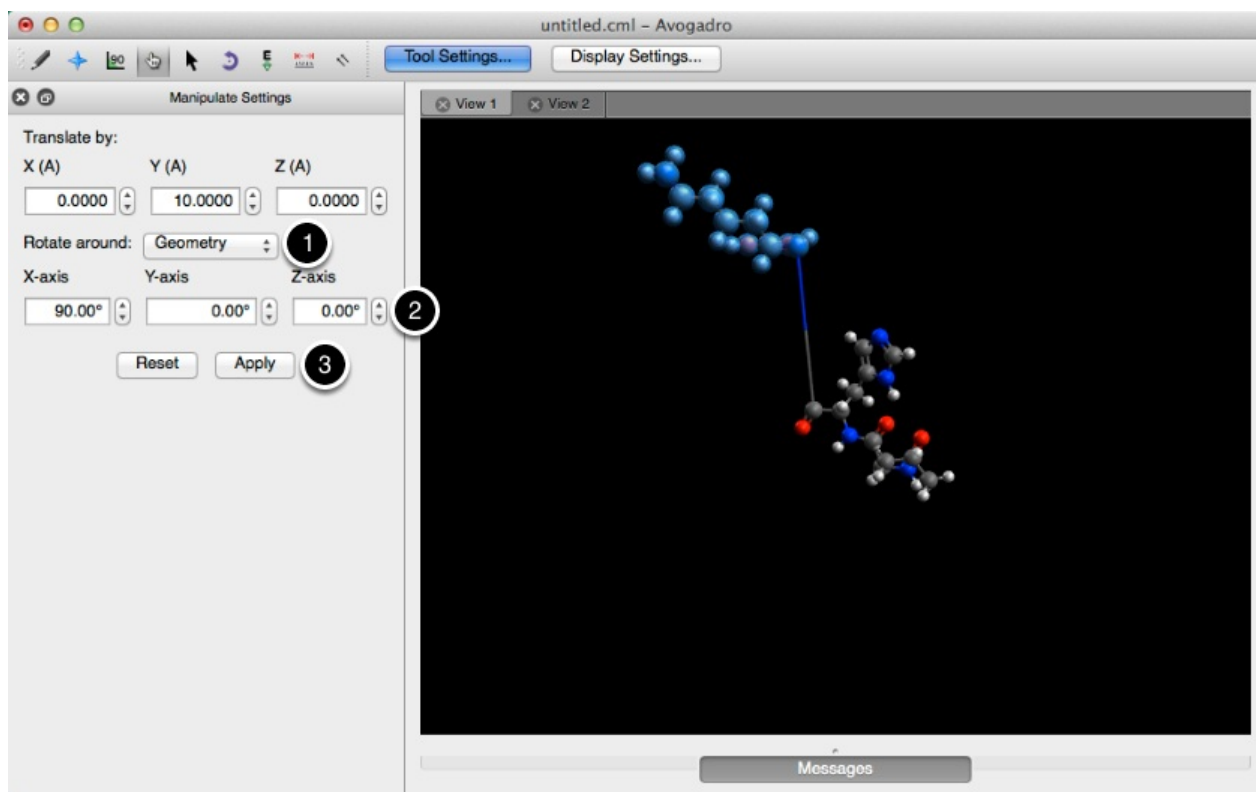


If inserting a fragment, the manipulate tool is automatically selected so that the fragment can easily be rotated into position.

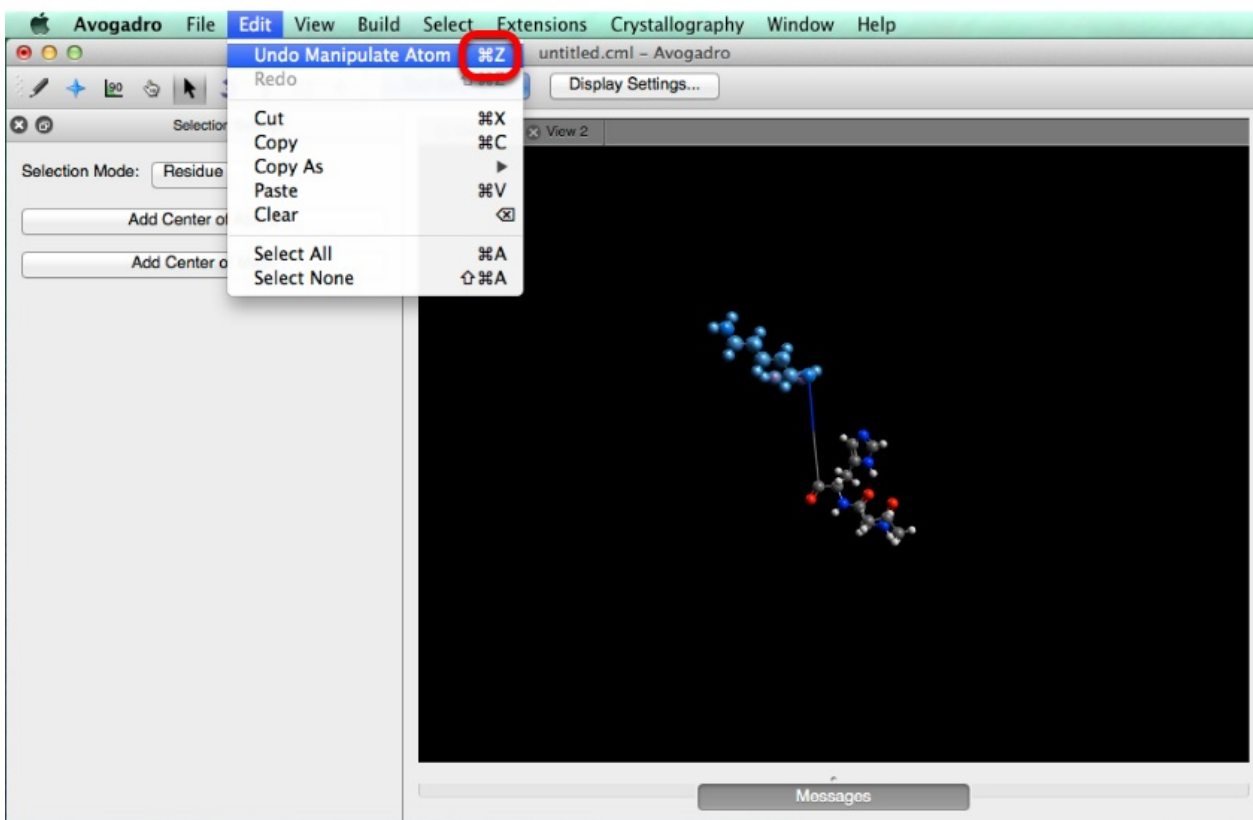
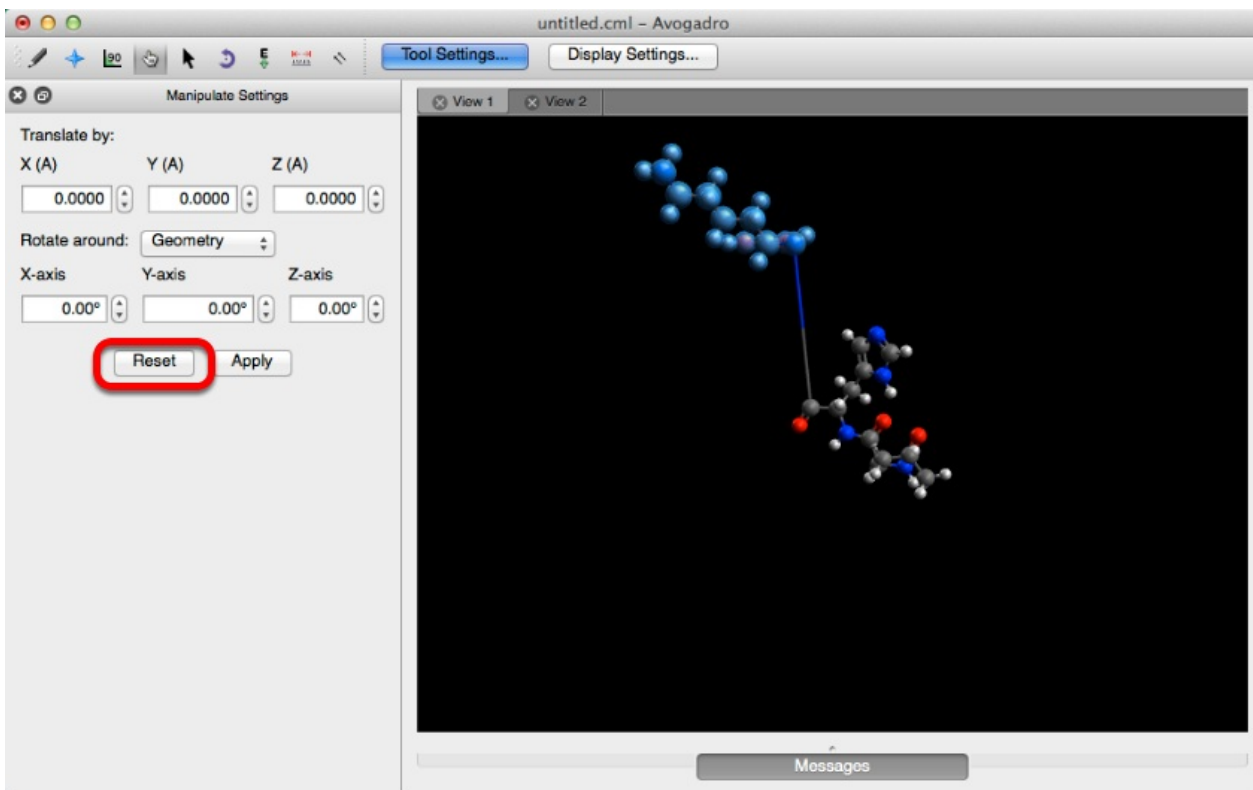
The "Translate by:" section allows you to easily translate the length of a bond (to a fragment or atom) into the desired position. For a translation to take place, enter in the desired translation and then click "Apply".



The "Rotate around:" section allows you to rotate your selection around the geometry, or the origin. This section then gives you the ability to choose how many degrees to rotate the fragment. Click "Apply" once you've made your selection.

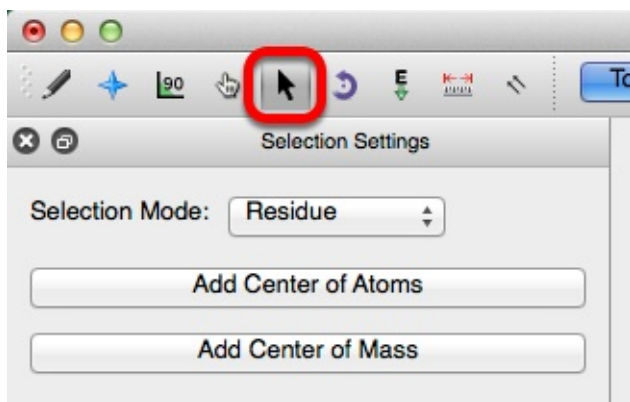


Clicking "Reset" will reset all of the information in the translation, and rotation boxes. This does not reset the molecule, if you want to undo your adjustments go to the "Edit" menu in the top bar and select "Undo Manipulate Atom".



The Selection Tool

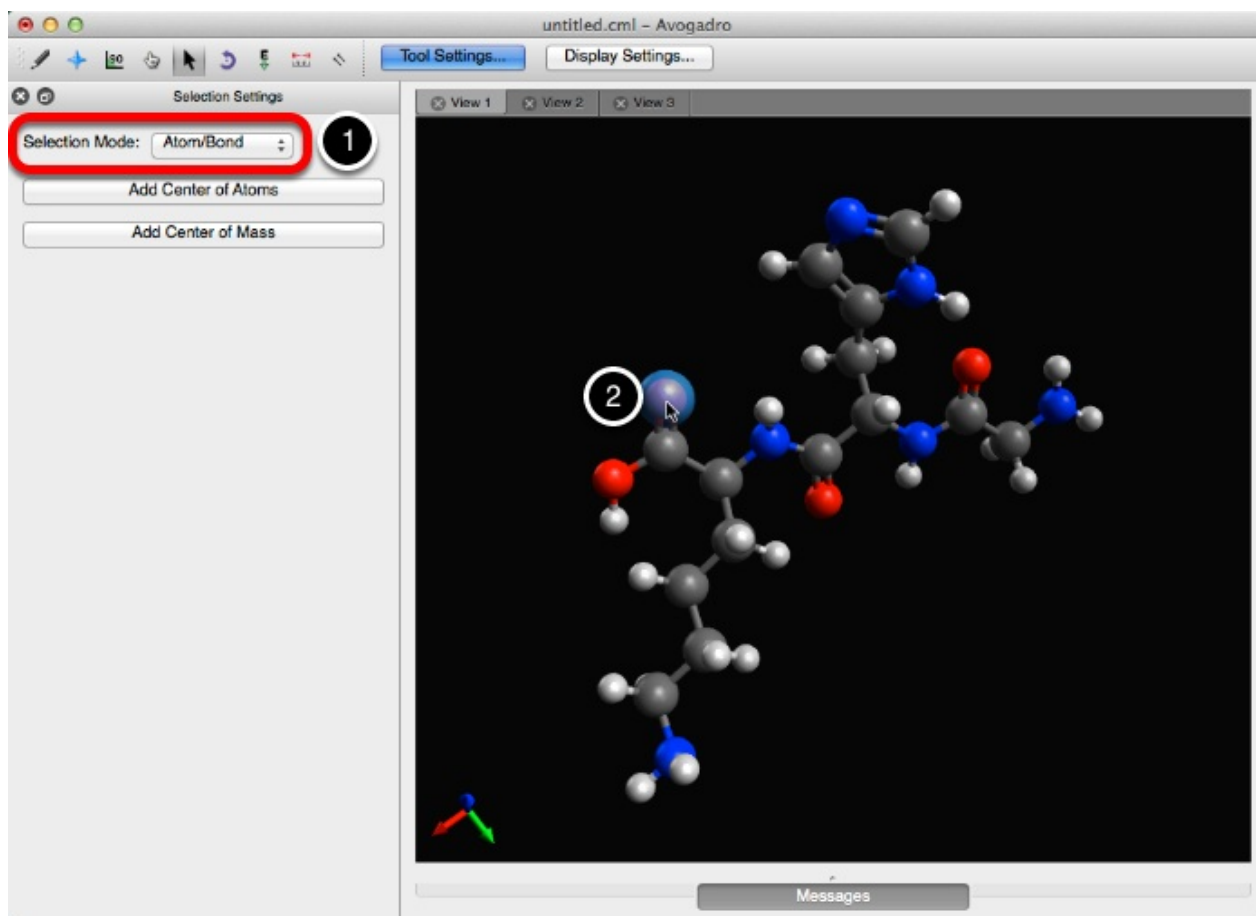
The selection tool allows the individual selection of atoms, bonds, or fragments.



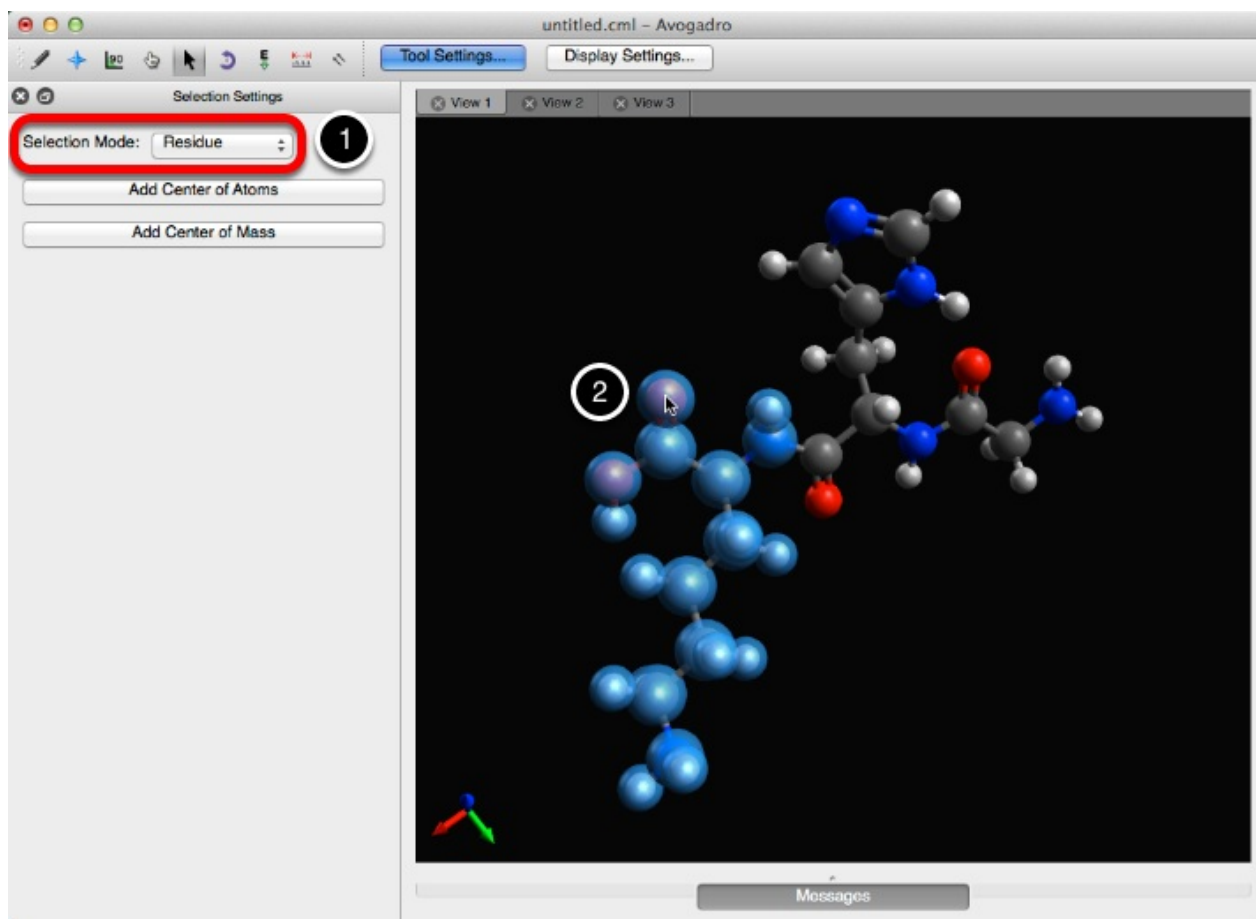
There are three types of selection modes: "Atom/Bond", "Residue", and "Molecule".

The "Atom/Bond" selection mode provides you with the ability to select a single atom within a molecule. This is achieved by left clicking the atom. Pressing down the "Shift" button on your keyboard allows the selection of multiple atoms.

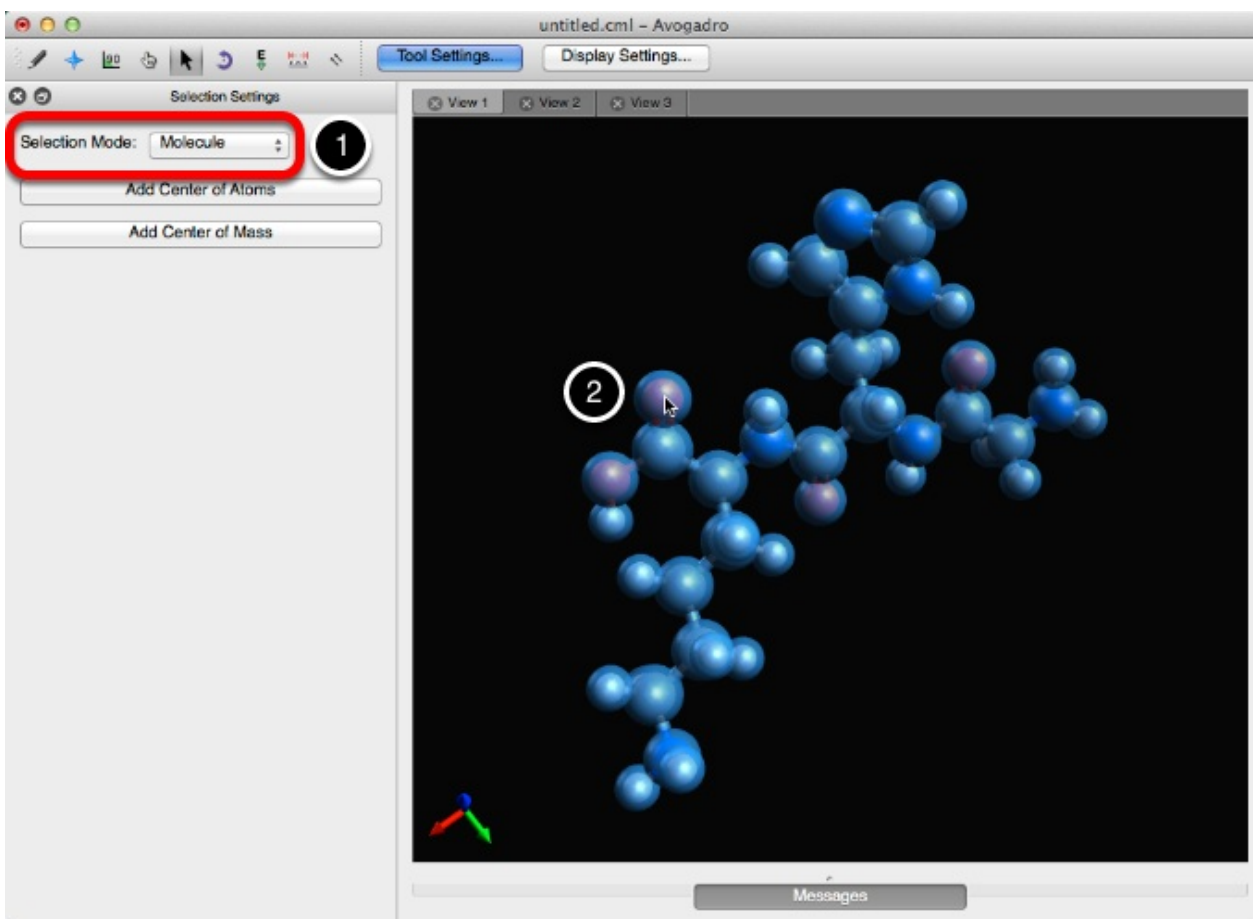
Right clicking on the black display will clear the selection made.



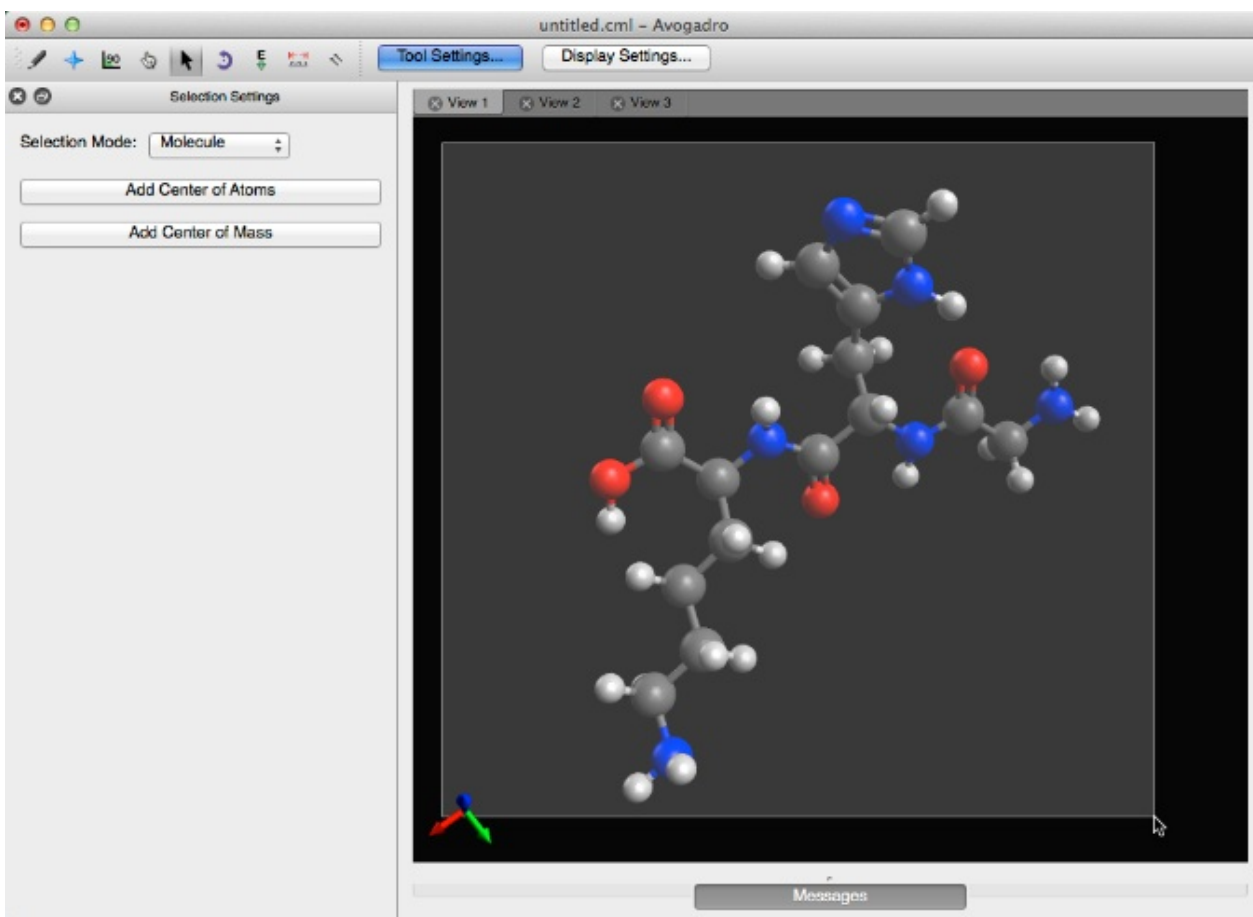
The "Residue" selection mode will select an entire residue within the molecule, by clicking on a single atom in the residue.



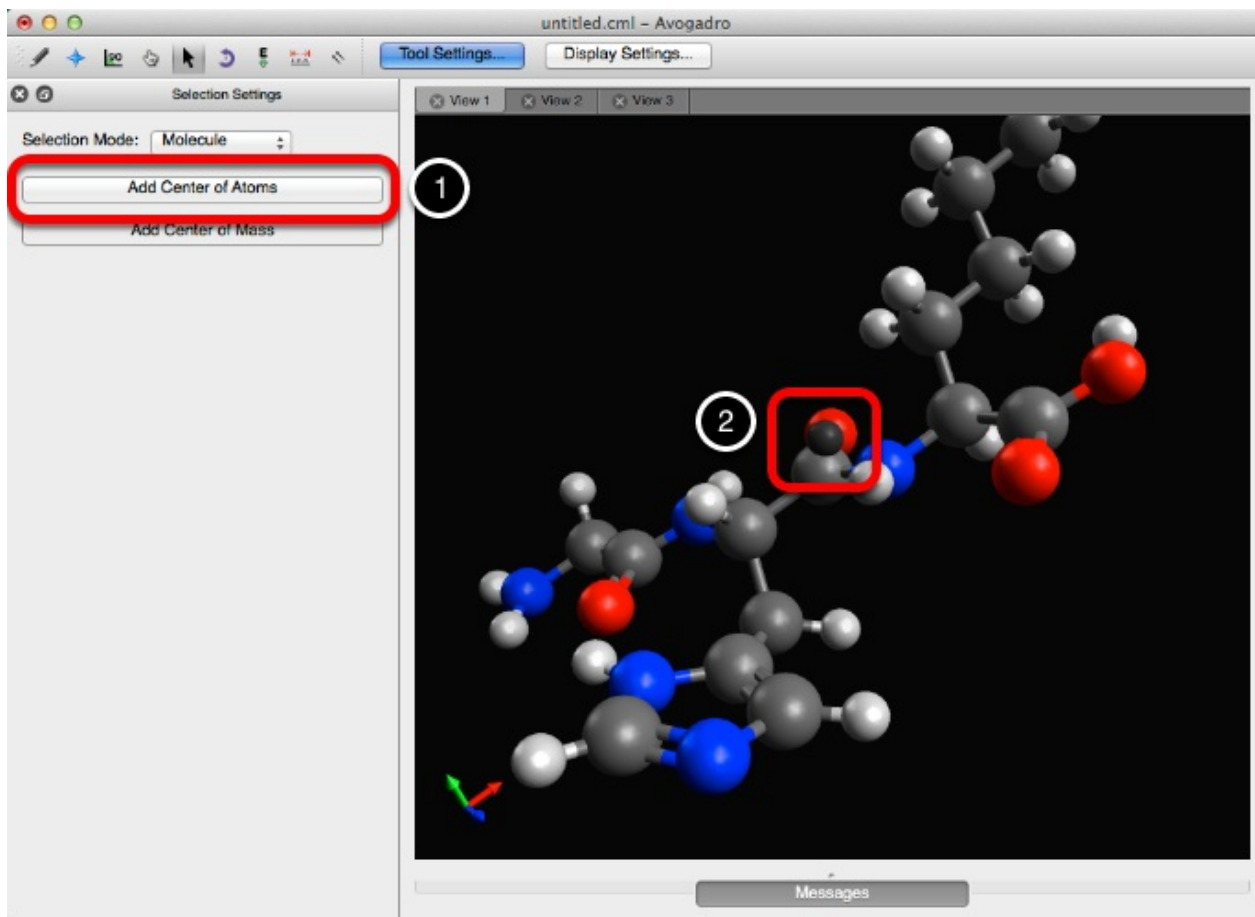
The "molecule" selection mode will select the entire molecule by clicking on an atom. Double clicking the molecule will also select the entire molecule.



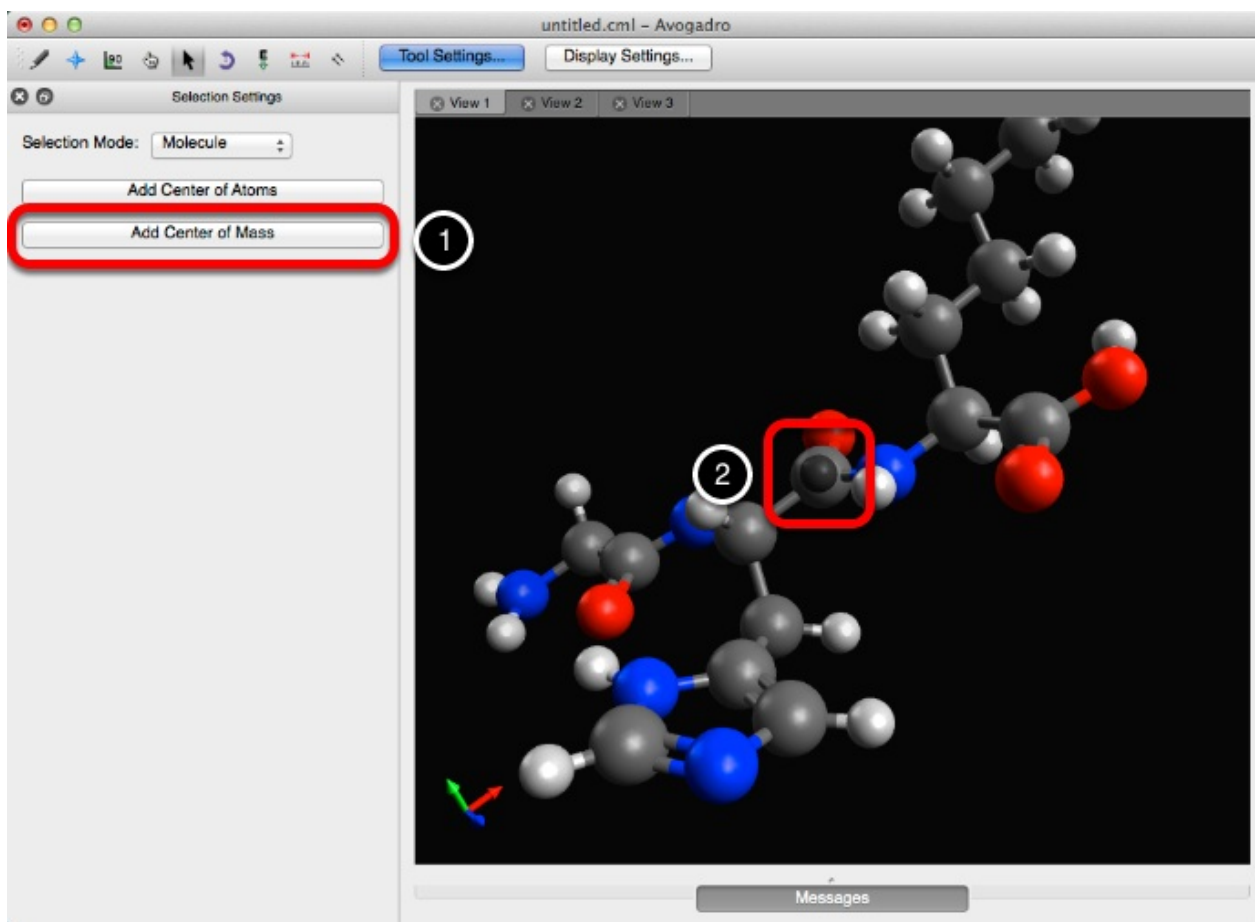
Molecules can also be selected by clicking and dragging your cursor across the display.



Clicking on "Add Center of Atoms" will display a black ball where the center of the atoms is found.

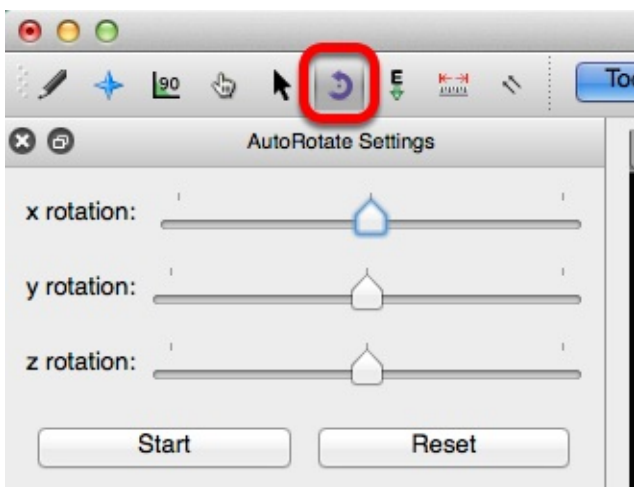


Clicking on the "Add Center of Mass" will display a black ball where the center of mass of the molecule is found.

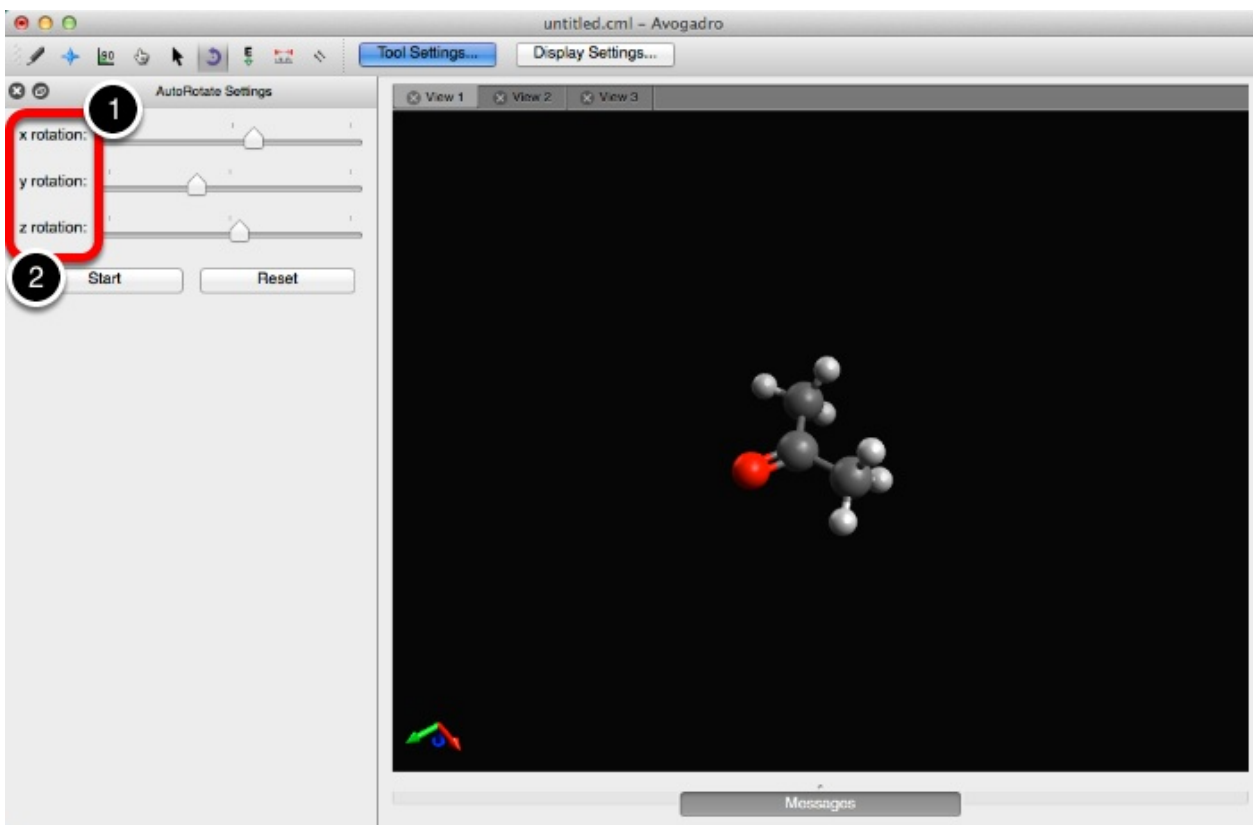


The Auto-Rotate Tool

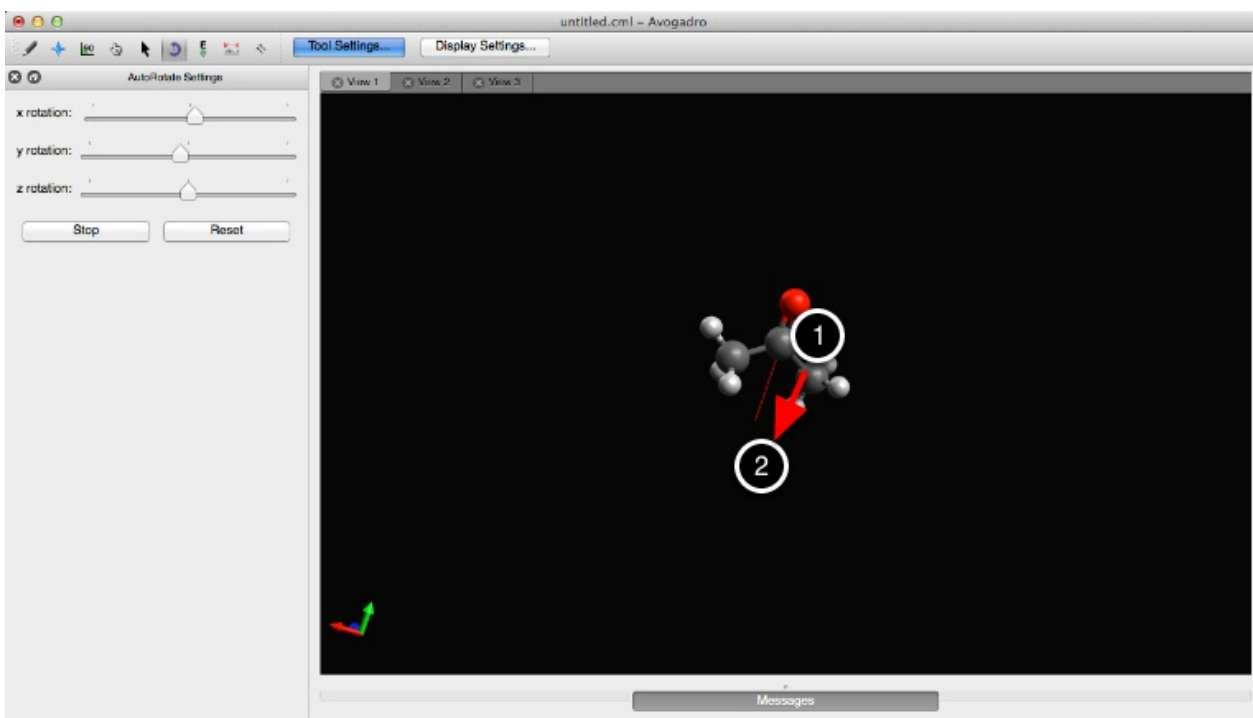
The auto rotate tool allows for the continuous rotation of a molecule.



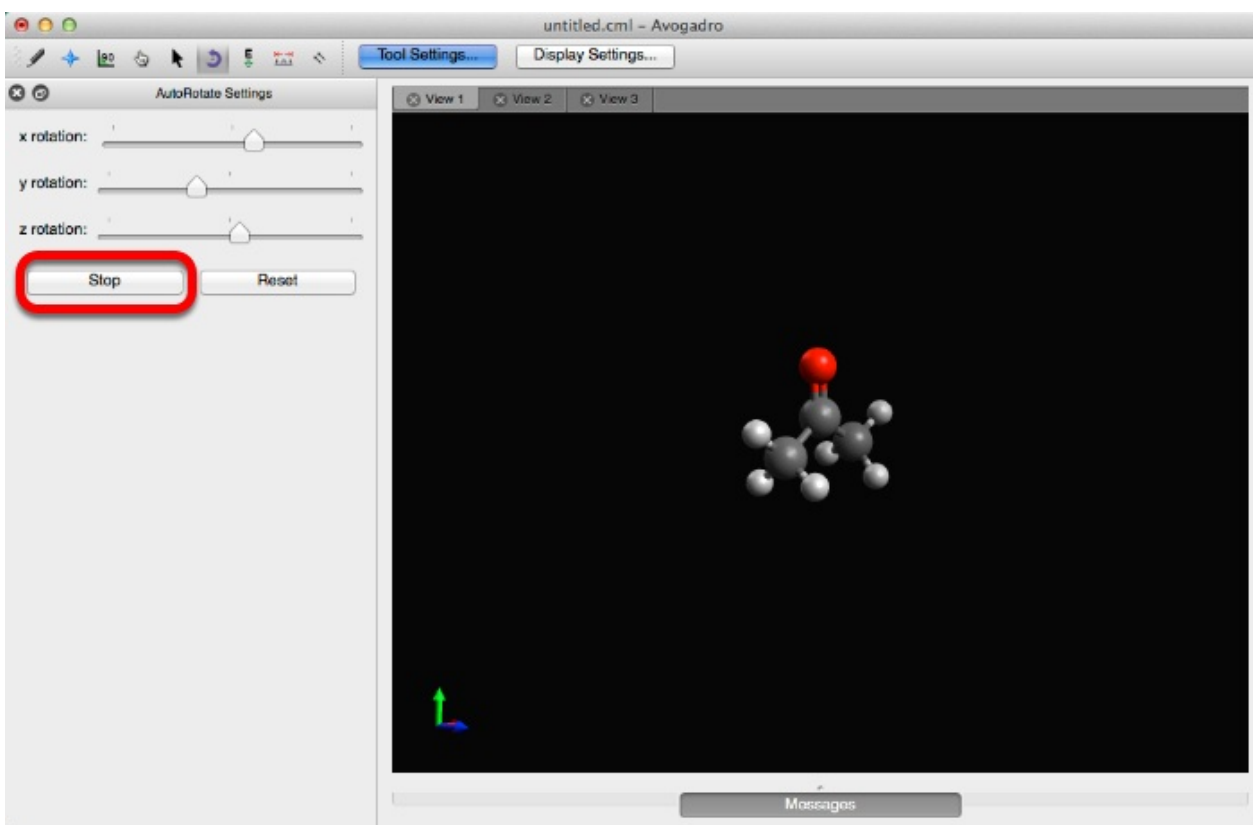
To rotate the molecule, adjust the x, y, and z rotation scales as desired. Then select "Start".



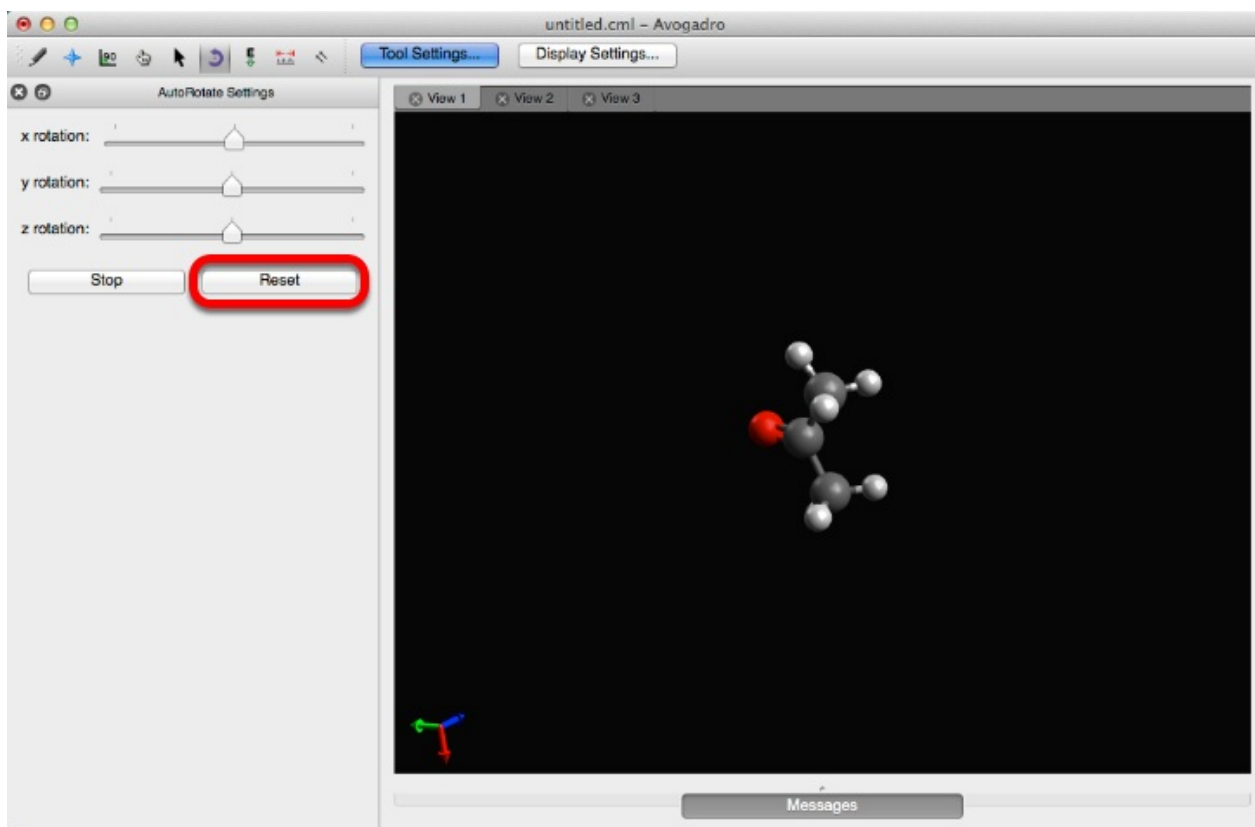
You can also click and drag from an atom to rotate the molecule in a specific direction.



Select "Stop" to end the molecule's rotation.

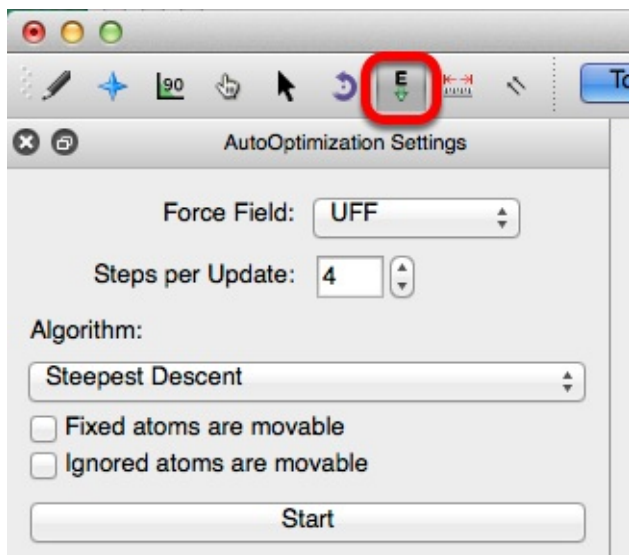


Clicking "Reset" will zero out the rotation scales and stop the rotation.

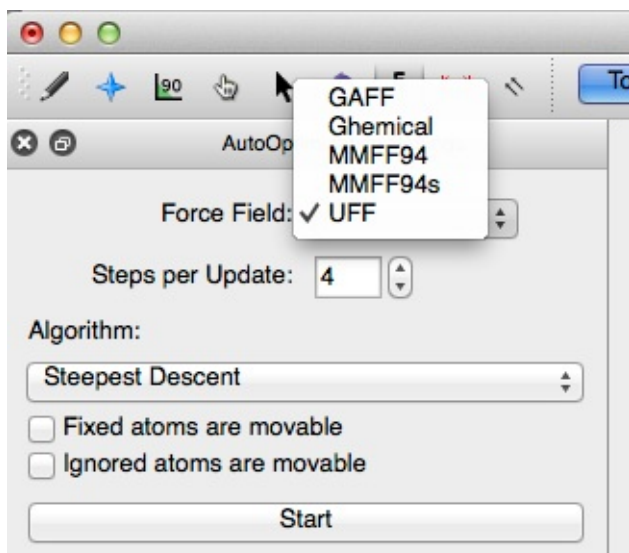


The Auto-Optimize Tool

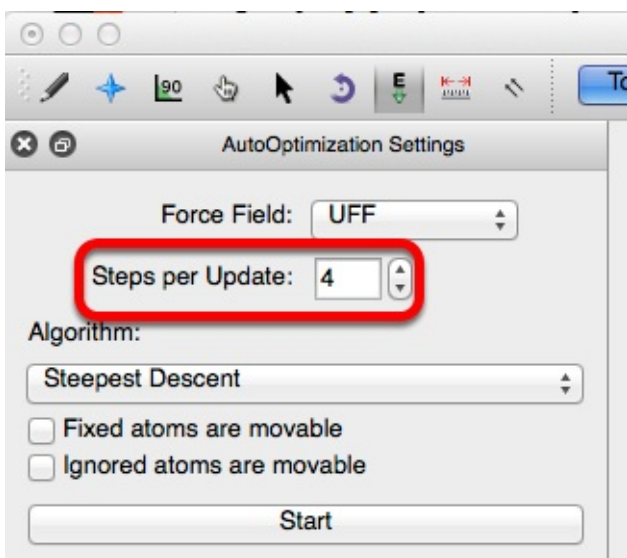
The Auto Optimize tool continuously optimizes molecular geometry through molecular mechanics. This tool also gives you the ability to manipulate the molecule while the molecular geometry is being minimized.



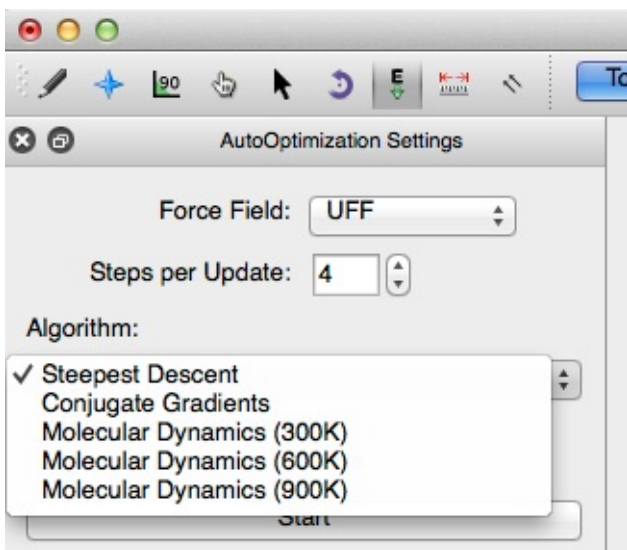
The Auto-Optimization settings provide several force field options. The default force field is UFF or the Universal Force Field. This force field is capable of reproducing the most structural features across the periodic table. However, depending on the molecule being tested, the other force fields may be better suited to optimize the molecular parameters. The force field options are shown below. For more information on force fields refer to the optimizing geometry section of this lab manual.



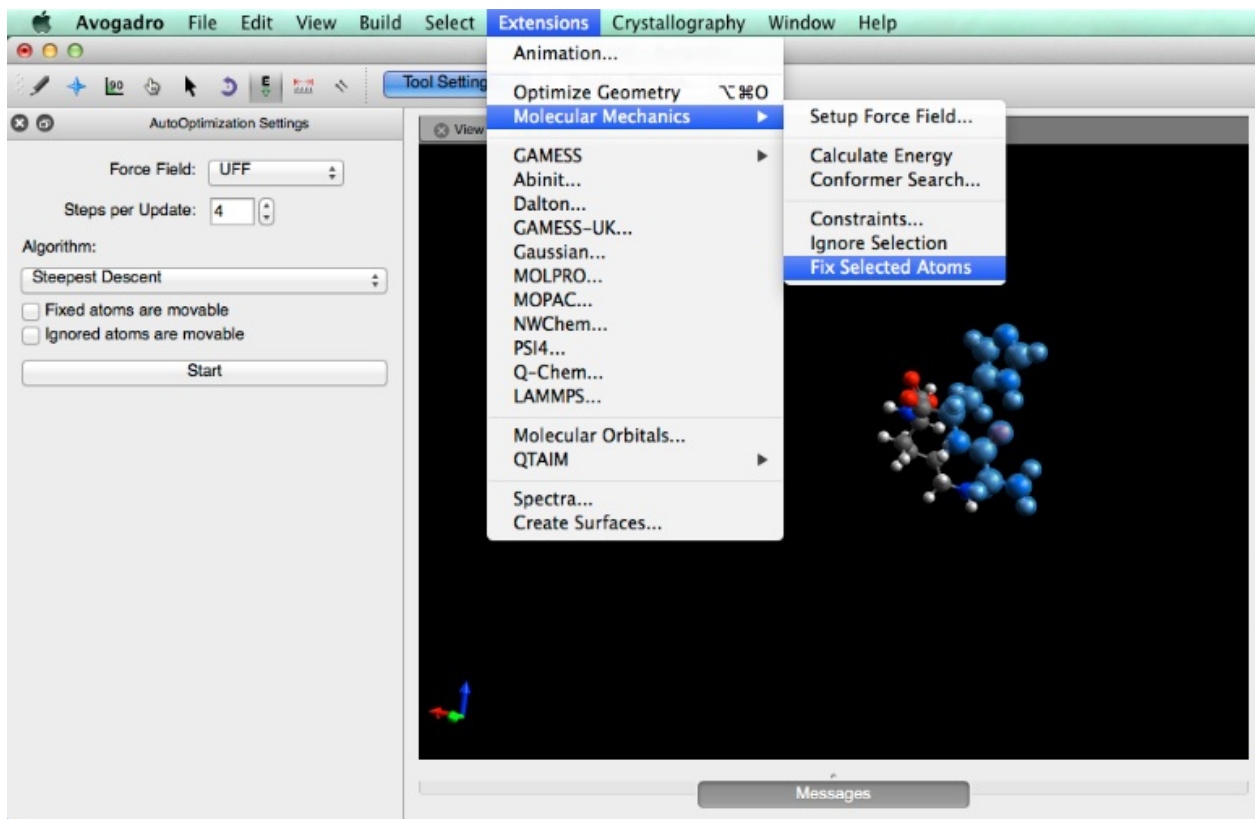
The default setting for "Steps per Update" is 4. This number can be increased or decreased, if you have a slower computer consider decreasing this number.



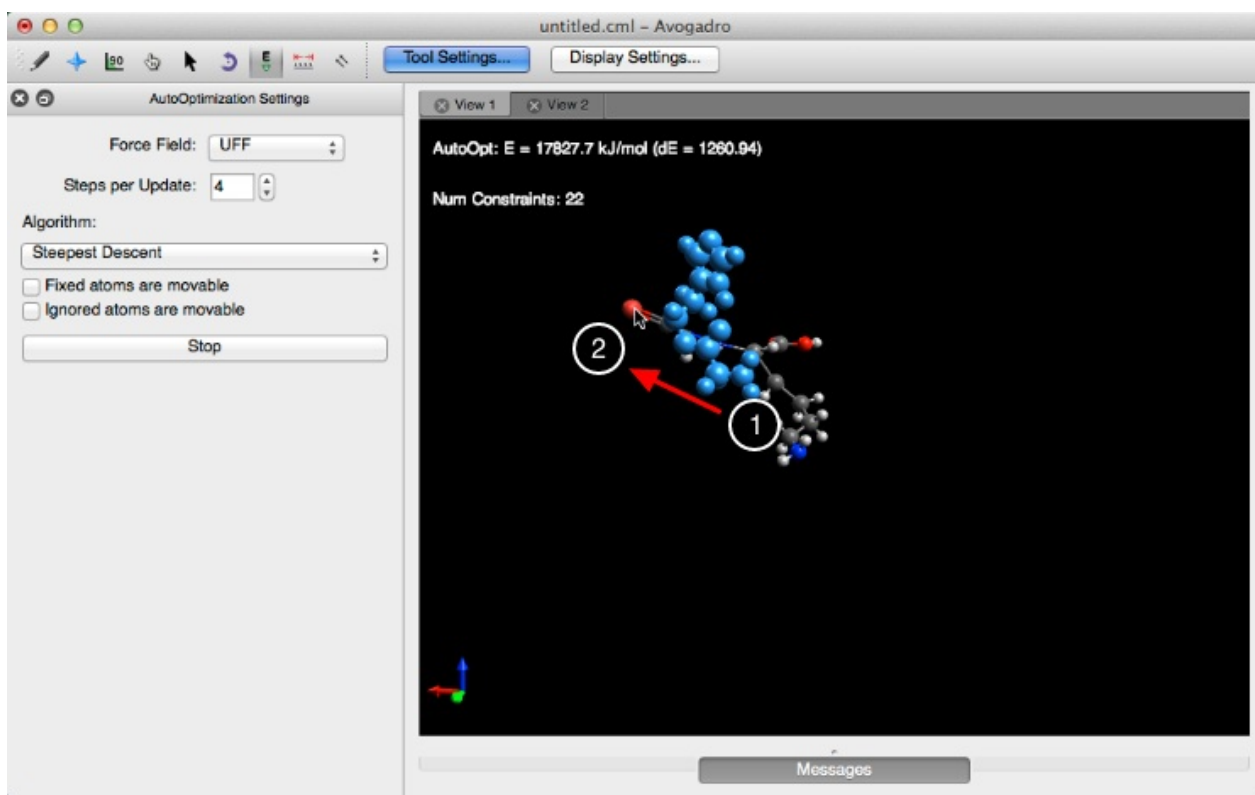
Avogadro can also apply specific algorithms dependent on your need. Steepest descent is the most fluid and interactive system, and is the default algorithm.



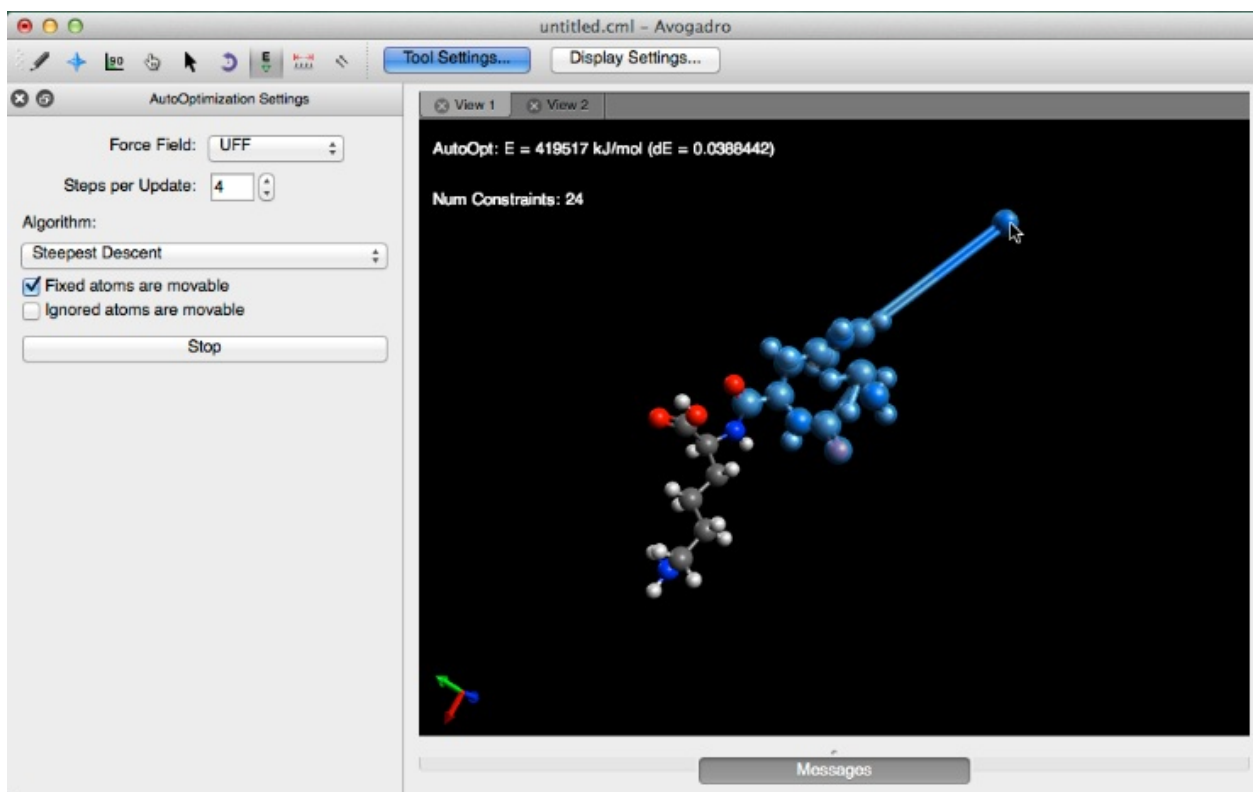
If necessary, atoms can be fixed into place before optimization so that they don't move. This is done by going to the "Extensions" menu, holding your cursor over "Molecular Mechanics" and selecting "Fix Selected Atoms".



Clicking on "Start" will allow you to manipulate the molecule by left clicking on an atom and dragging your cursor. Notice that the fixed atoms don't bend with the manipulation of the molecule.



If the "Fixed atoms are movable" box is checked, the bonds between atoms can be manipulated but are constrained. In this instance the selected atom does not reoptimize once it's dragged.



Essentially, the same thing takes place if the "Ignored atoms are movable" box is checked. However, ignored atoms (if the box is checked) *will* reoptimize once dragged. To ignore a selection select the "Extensions" drop down menu, hold your cursor over "Molecular Mechanics" option, and select "Ignore Selection".

The molecule will reoptimize until $dE=0$ or "Stop" is clicked.

