

# Vdraw Documentation

## What is Vdraw? What does it do?

WIP (Still needs to be written)

## How to Build a Molecule

### Workflow:

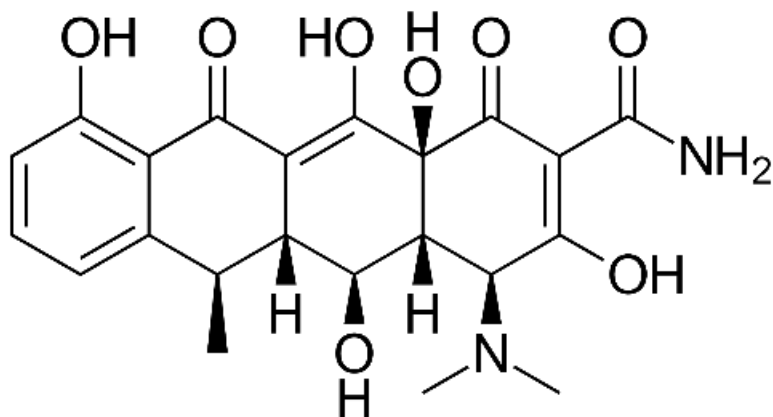
When building a molecule in Vdraw, it is best to follow this general order:

1. Build entire structure in carbons
2. Change carbons to appropriate elements (as needed)
3. Change bond orders to appropriate numbers
4. Edit charges to reflect proper formal charges (as needed)

**Note:** This is not a rigid order that must be followed, but it is the suggested way to use Vdraw

### Example Molecule:

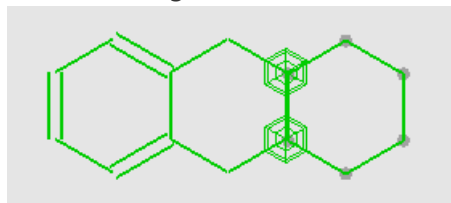
The following molecule will be used to demonstrate how to use Vdraw to build a molecule.




**Note:** Other molecules may require additional steps, using tools not explained in this demonstration. For more information of other tools available in Vdraw and how to use them, go to the "Other Vdraw Tools" section.

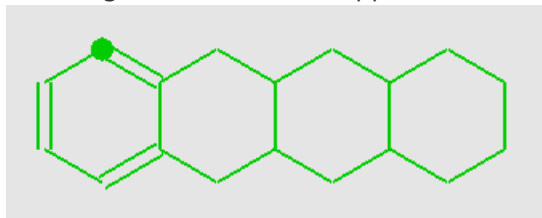
1. Build entire structure in carbons
  - a. To begin building, first click on the element that you want to build with
    - i. Carbon will be selected as the default

- ii. Pre-built pieces (e.g. rings) will always be built with carbons
- b. Different types of rings can be built by selecting one of the buttons on the lower right.
  - i. The "... " button beneath these pre-built rings can be clicked in order to view more pre-built ring options.
- c. To build four rings in the structure, we will use the pre-built ring buttons.
- d. In order to connect the rings:
  - i. Hover the new ring over the ring you would like it to bond with and click the left-mouse-button once it is in place.
  - ii. Small green hexagons will appear over the two bonding points (as shown below) indicating where the ring will attach

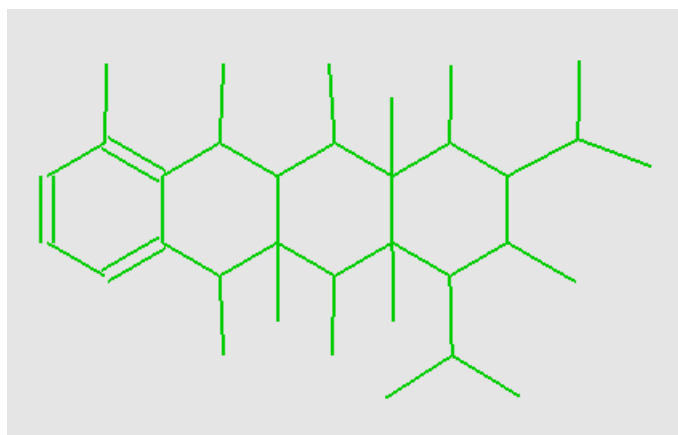
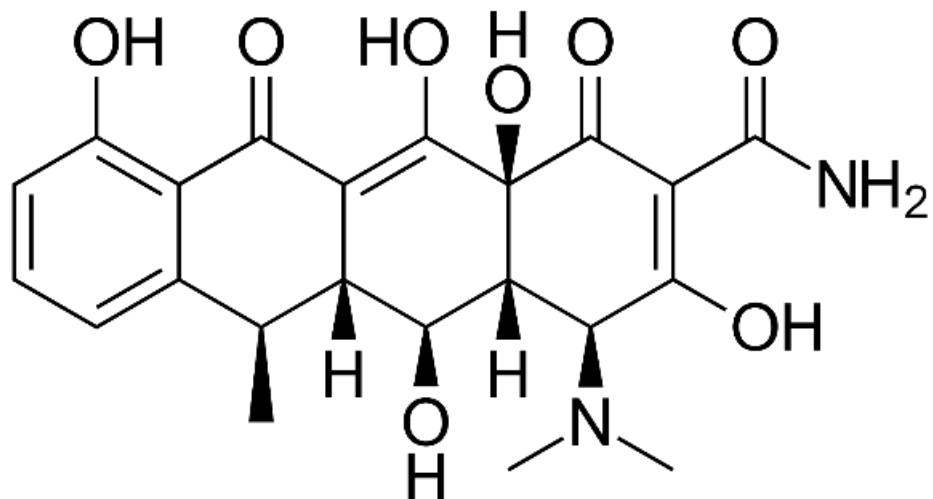


- e. Once the rings are in place, we can begin building the other parts of the structure
- f. To draw new bonds:


- i. Select draw mode (  ) from the upper left section of buttons
  - 1. Carbon will once again be the default element selected
- ii. Hover over the atom that will be the connection point for the new bond
  - 1. A small green circle should appear, indicating where the new bond will be formed.

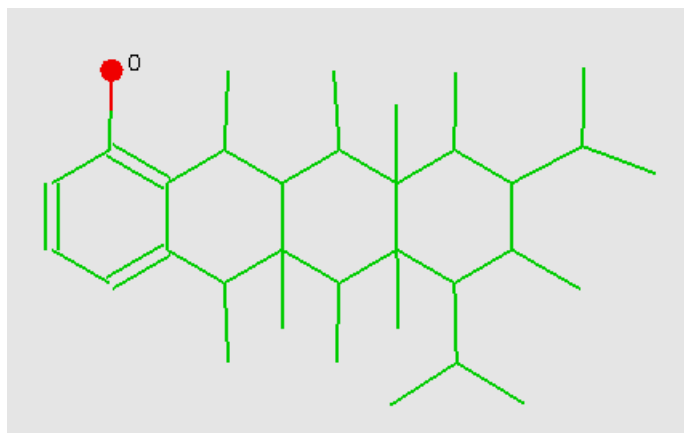


- iii. Click and hold down the left-mouse-button, then drag outwards to create the new bond.
  - 1. The angle of the new bond can be controlled by moving the left-mouse-button around after dragging outwards
  - 2. The angle of the bond can also be changed later by clicking on the atom that you would like to move and dragging the atom around
- g. Now the skeleton structure (built in all carbons) has been completed
  - i. Final Structure (left); Step 1 Structure (right)



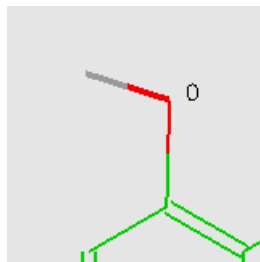
2. Change carbons to appropriate elements (as needed)

- a. First, we must select the element that we want to replace a carbon with using the element buttons of the left side
  1. The selected button will have a light blue square around it (ex: )
- b. Once the appropriate element has been selected, hover your mouse over the atom you would like to replace.
  - i. A small green circle will once again appear over the atom, indicating which atom will be replaced
- c. Click on the appropriate atom and it will be replaced with the selected element
  - i. Ex: The circled atom was clicked on after selecting the oxygen element; therefore, the carbon was replaced with an oxygen



**i Note:** There is now a zero next to the oxygen atom. This zero indicates the formal charge of the atom.

- d. Continue this process throughout the structure by selecting the proper element and clicking the carbon atom that needs to be replaced
- e. If you would also like to add hydrogens to the structure for clarity (such as those attached to an oxygen or nitrogen), that can be done by adding hydrogens directly.
  - i. Instead of replacing bonds in the carbon skeleton structure, a new bond can be created using hydrogen
  - ii. First, select the hydrogen by clicking on the hydrogen element button
  - iii. Then, just like creating new carbon bonds, click and drag away from the atom that you want the hydrogen to bond with
  - iv. This will create a new bond between the selected atom and the hydrogen

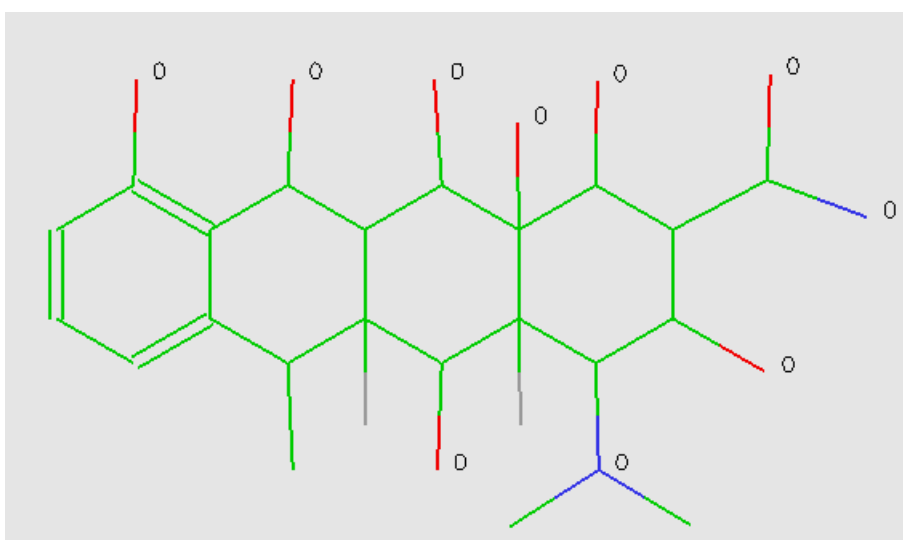
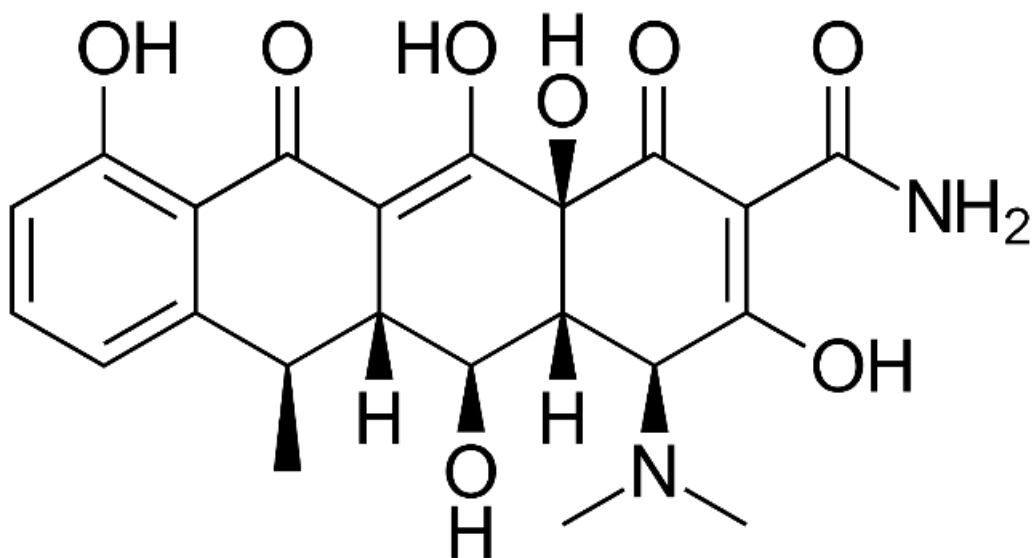



**i Note:** VeraChem software can infer where hydrogens are if the formal charges are correct. Therefore, there is no need to add them explicitly.

- f. In this demonstration molecule, only hydrogens with explicit stereochemistry (circled in blue below) were added to the molecule.

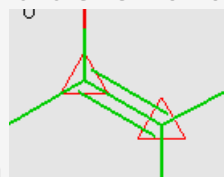
### 3. Change bond orders to appropriate numbers

- Final Structure (left); Step 2 Structure (right)



- Select the draw mode button () in order to change bond orders
- Hover the mouse over the bond you would like to change and click on it to change the bond order.
  - One click will increase the bond order to a double bond
  - Another click will change the bond order from a double to a triple bond
  - A third click will change the bond order from a triple to a single bond


**Note:** If the number of bonds is not compatible with the normal valence of the atom, a small red triangle will appear over that atom

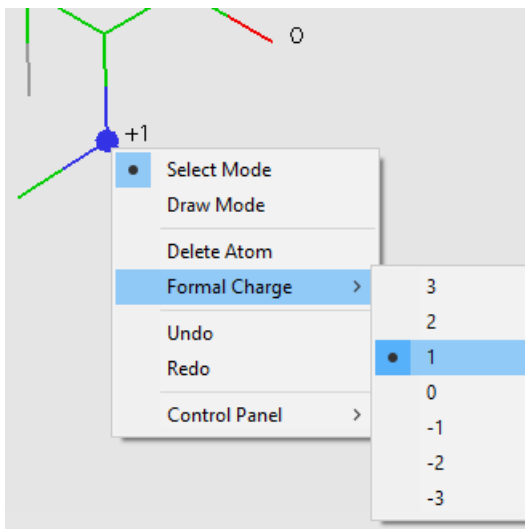


- Once all bond orders have been changed appropriately, continue to step four.



#### 4. Edit formal charges and stereochemistry as needed

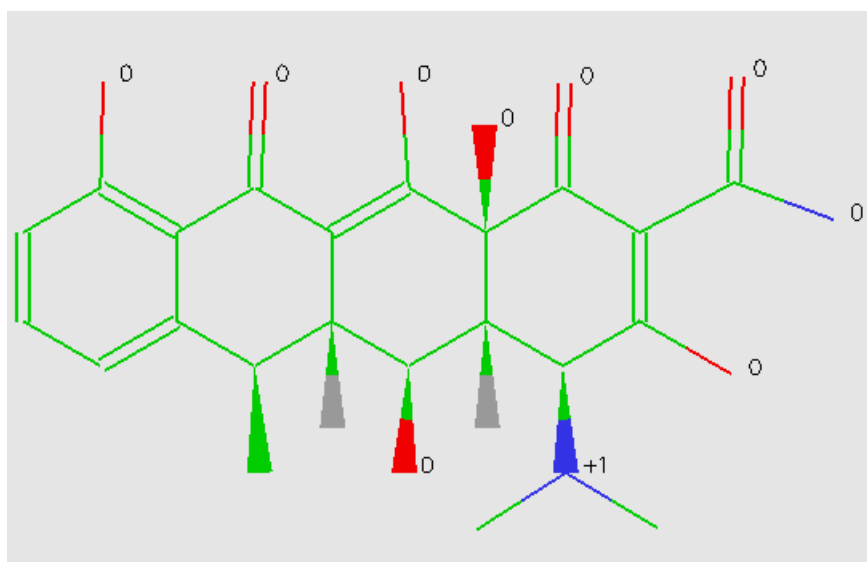
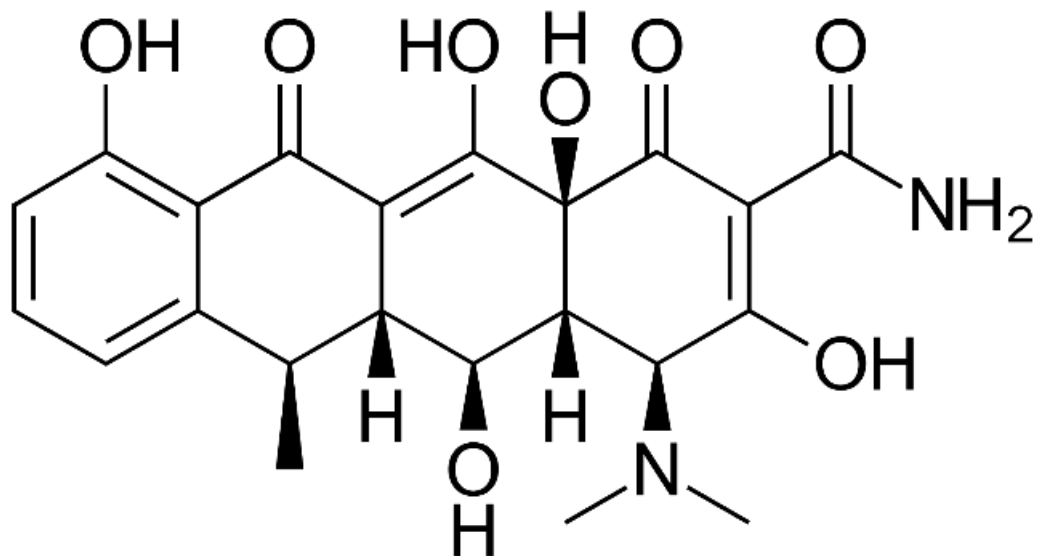
a. To edit formal charges:

- i. Click on the select mode button ()
- ii. Right-click on the atom that you would like to change the formal charge of
- iii. Click on the **Formal Charge** option in the drop-down menu and select the appropriate formal charge



b. To edit the stereochemistry:

- i. Select either the wedge draw-mode button () or the hatched draw-mode button () to draw the the appropriate stereochemistry
- ii. Hover the mouse over the bond you would like to change and click once to apply the stereochemistry
  1. Clicking a second time will flip the wedge around
  2. If you want to flip the wedge back to the original position, click it one more time.
- iii. Continue this process throughout the entire molecule by selecting the appropriate draw button and changing bonds as needed.



## Other Vdraw Tools: Buttons

### **Vcharge**

The Vcharge button provides the partial electrostatic charges for each atom on the molecule.

### **Vconf**

The Vconf button uses the 2D structure to find and display the lowest energy 3D structure

### **Center**

This button will center the molecule on your screen

### **Select All**

This button selects all the atoms that are in the window

### **Copy Selection**

This button will copy whatever has been selected to the clipboard

### **Paste Selection**

This button will paste whatever has been copied to the clipboard

### **Delete Selection** ✕

This button will delete whatever atoms have been selected

### **Flip Selection** ↕

This button will flip whatever atoms have been selected over a horizontal line

### **Mirror Selection** ↔

This button will mirror whatever atoms have been selected over a vertical line

### **Undo** ↶

This button will undo the previous action

### **Redo** ↷

This button will redo the most recently undone action.

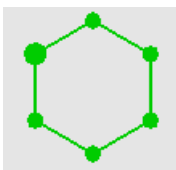
## Other Vdraw Tools: The Edit Tab

The Edit tab contains many of the same functions as the buttons in the upper right:

- **Select All** - Ctrl + A
- **Copy Selection** - Ctrl + C
- **Cut Selection** - Ctrl + X
- **Paste from Clipboard** - Ctrl + V
- **Delete Selection** - Delete
- **Flip Vertically** - Ctrl + F
- **Flip Horizontally** - Ctrl + G
- **Undo** - Ctrl + Z
- **Redo** - Ctrl + Y

The Edit tab also contains other functions:

- **Periodic Table** - brings up a periodic table; allows you to select elements to build with
- **Check Valences** - will check the valences of all atoms
- **Mark Atoms** - will mark each atom with a circle (see image below)




- **Check Chirality** - will check the chirality of all atoms

- Chirality has successfully been calculated for atoms marked with



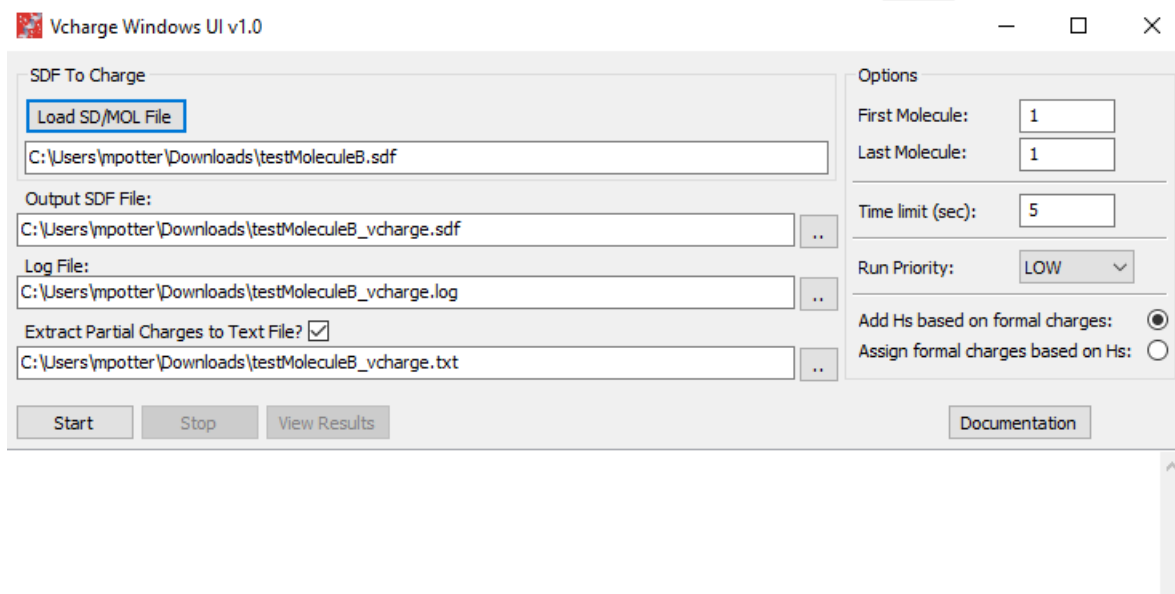


- There is not enough information to determine chirality for atoms marked with 
- **Check Overlaps** - will check for atoms that overlap or on top of each other
- **Background** - allows you to change the background color
- **Control Panel** - allows you to change which side the control panel (buttons) appear on

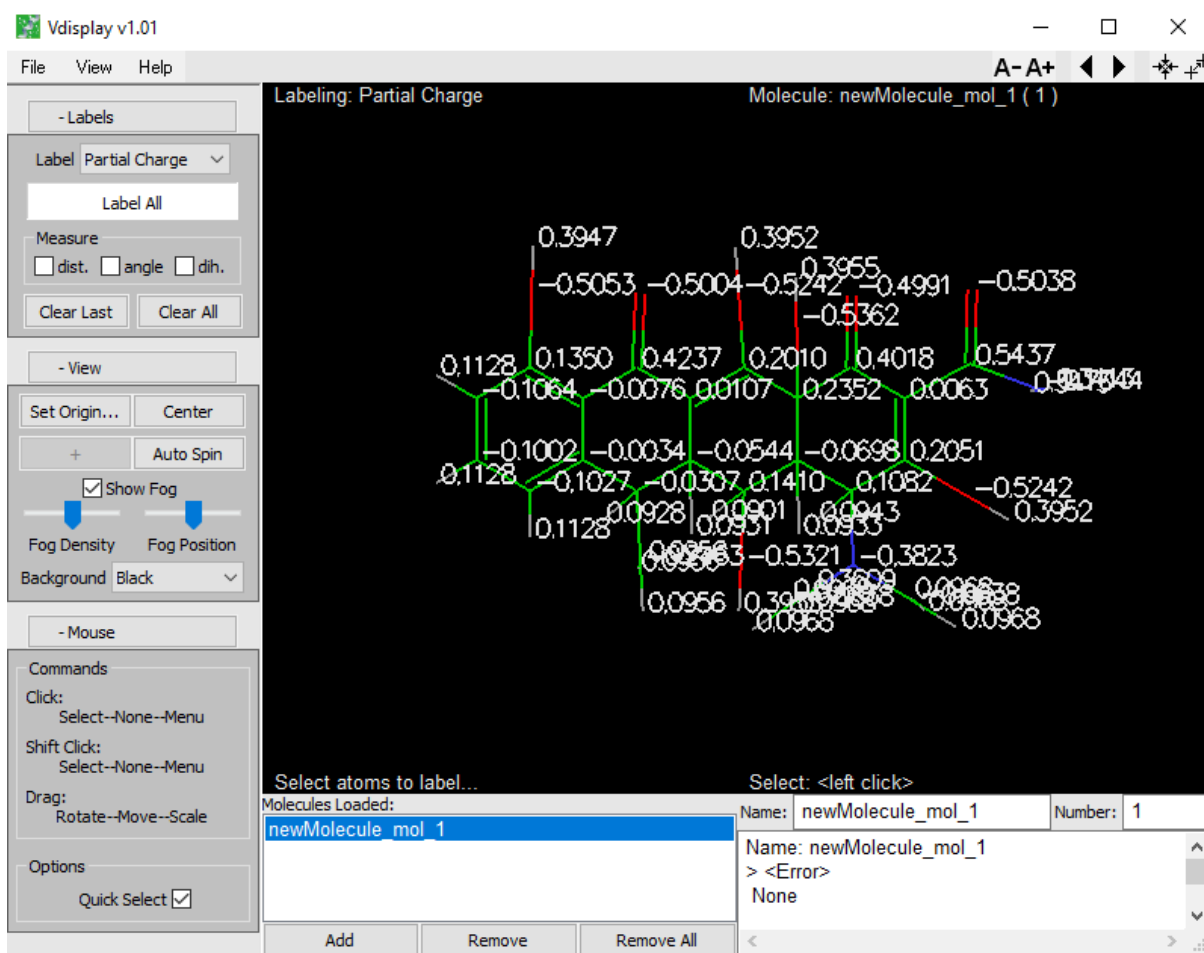
## Using Vcharge and Vconf

### Vcharge:

1. Click the Vcharge button
2. It will require you to save the molecule as an sdf, regardless of whether or not you have saved it before.
3. The interface window for Vcharge will open, allowing you to run the program
  - a. You usually will not have to change anything on the interface, just click **Start**

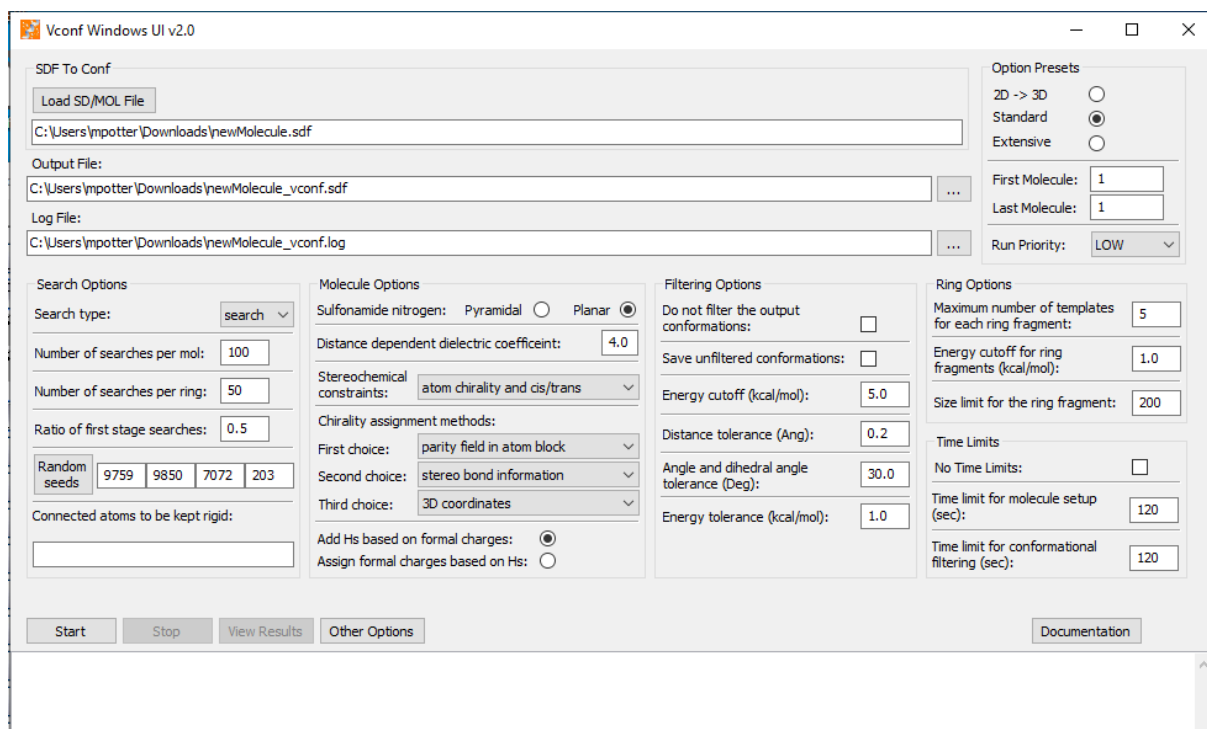


4. After pressing start and letting the program run, click **View Results**
5. This will open a new Vdisplay window, showing the molecule with the partial electrostatic charges for each atom.
  - a. This window may take a few seconds to open after pressing **View Results**

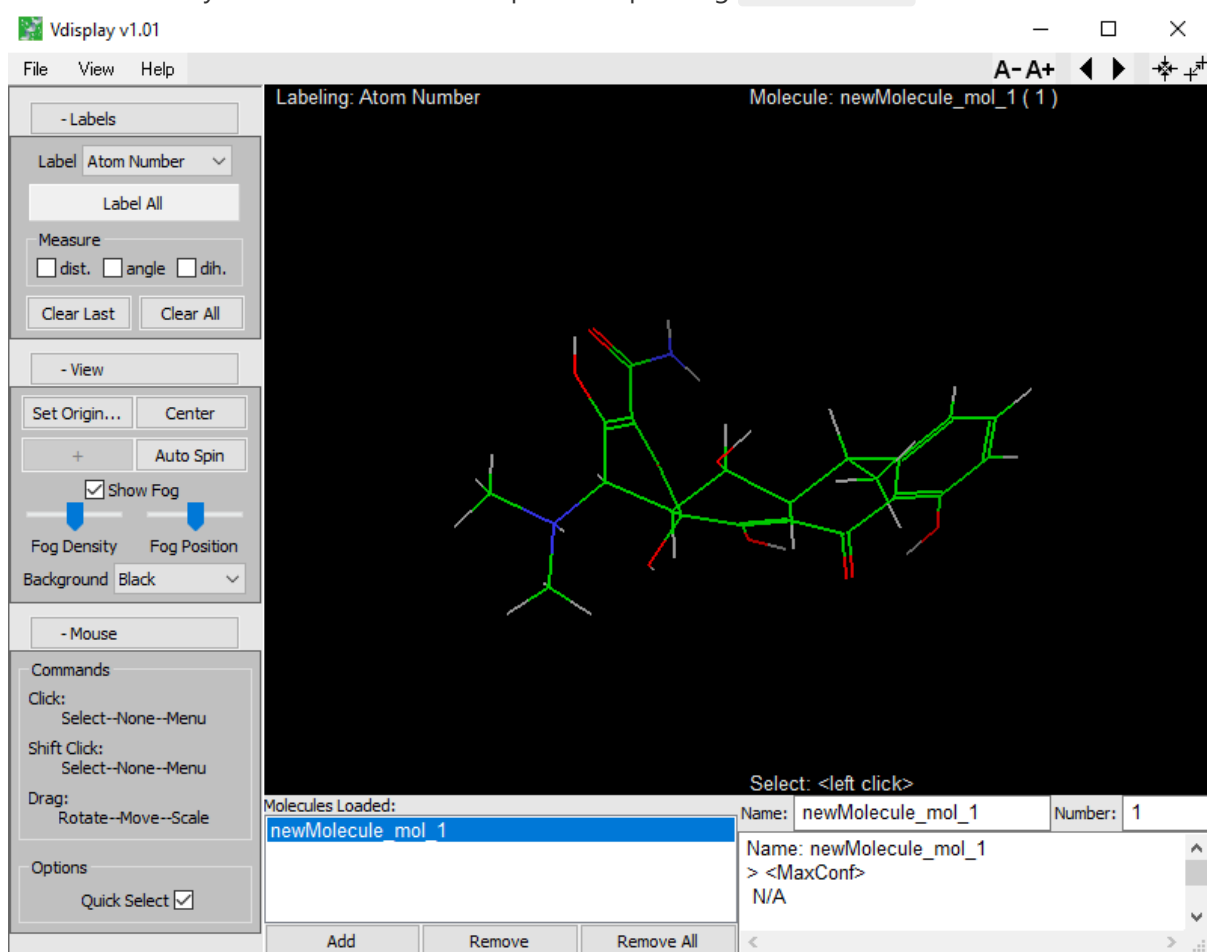


## Vconf:

1. Click the Vconf button
2. It will require you to save the molecule as an sdf, regardless of whether or not you have saved it before.
3. The interface window for Vconf will open, allowing you to run the program
  - a. You usually will not have to change anything on the interface, just click **Start**



4. After pressing **Start** and letting the program run, click **View Results**
5. This will open a new Vdisplay window, showing the lowest energy 3D confirmation of the molecule
  - a. This window may take a few seconds to open after pressing **View Results**



# Thanks for Reading!

