# Build-a-Molecule with IQMol

## Step 1: Download and install IQMol

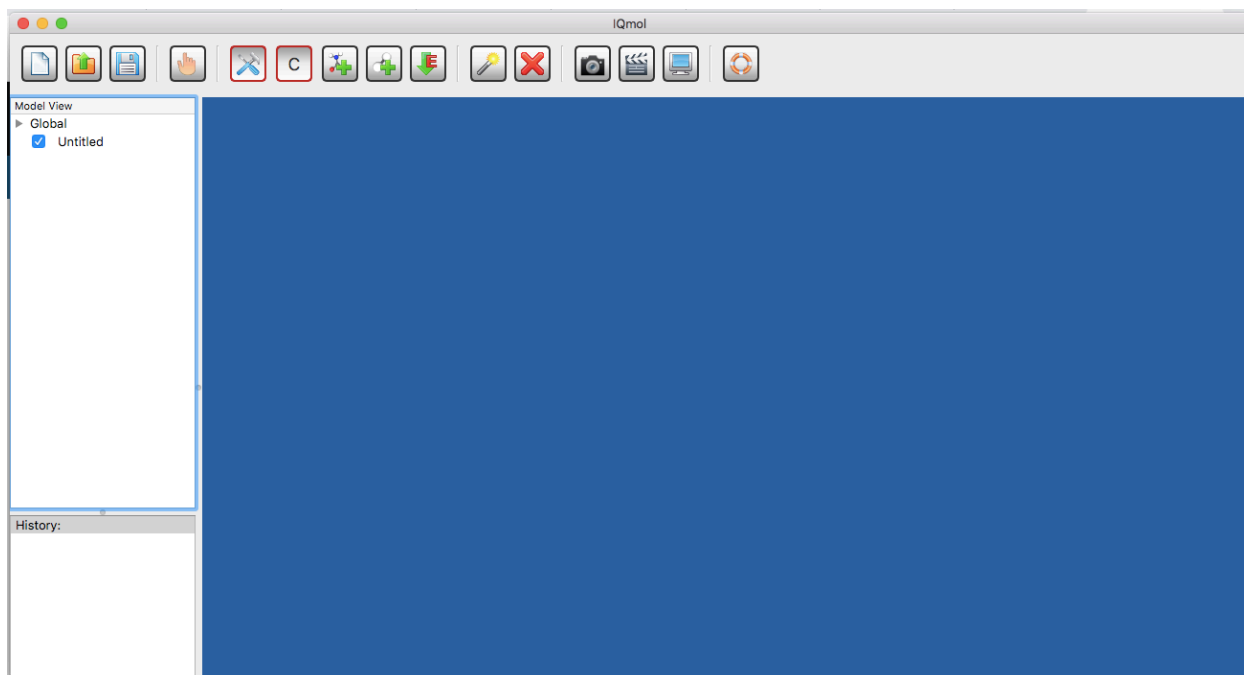You only need to do this once!

Go to: http://www.iqmol.org/downloads.html

Download and click on the installer (for example, in Mac, it is 'IQMol-2.14.dmg')

This will automatically install the software

## Step 2: Click on the IQMol icon
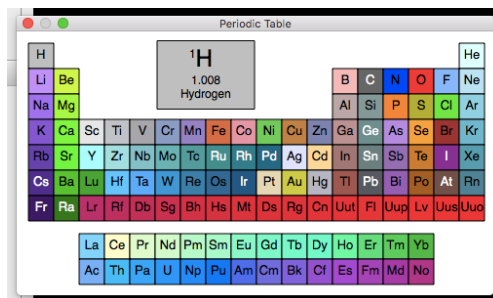
This will open a window that looks like this



You're all set 👍 Let's start building!

## Step 3: Draw a molecule

Name one greenhouse gas.

The  button indicates you are on draw mode. Click on the 'Element' dropdown and select 'Other'. Voila! It's the Periodic table!

Let's find oxygen on the periodic table.

Click on 'O' and close the periodic table box (red x on the top left corner) and you are ready to draw.

Click anywhere inside the black window. Do you see an oxygen atom or something else entirely?

We did not create oxygen but we did create water – $H_2O$.

This is because in the 'Draw Settings' the 'Adjust Hydrogens' is ON by default.

When you create an atom with this option, if it can complete its valence shell with an octet configuration, that is satisfied using hydrogens.

Let's see what happens if we turn off 'Adjust Hydrogens'.

Click on the check mark next to it so it is turned off.

Now go back to the black window and click anywhere. A red oxygen atom is created.

**Step 4: Delete atoms**

Click on the  button. Click on the oxygen atom and hit 'delete.' This should delete the oxygen atom.

**Step 5: Draw more molecules**

Click again on . Turn the 'Adjust Hydrogens' back to ON.

Click on the dropdown next to 'Element.' Choose carbon this time.

Click anywhere on the screen, but a little far away from the water molecule. What molecule do you see this time?

Repeat this step for nitrogen. What molecule do you see now?

In the periodic table, as we go from left to right from carbon to oxygen, the number of hydrogen atoms needed to create a molecule (methane – $CH_4$, ammonia – $NH_3$, water – $H_2O$) decrease.


**More things to try**

**Step 6: Make molecules funky!**

Click on [cursor icon]. Place the mouse pointer on the O-H bond in the water molecule. Now click and drag it anywhere.

Can water have one O-H bond very long and another very short?

One way to answer this question is to find the bond lengths that give the most stable structure.

This is usually determined by the energy of the molecule.

Find the [E icon] button and click on it. On the left side of the Avogadro window, you will see something like this.
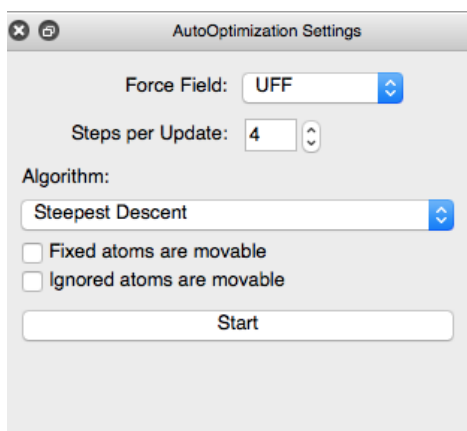


Click 'Start' and watch the water molecule find its stable structure.


**Supercomputing with molecules**

What you just did with this exercise is the starting point for most chemists doing simulations with supercomputers.

We draw molecules (big and small), find their stable structure, and feed these structures to supercomputers to calculate interesting chemical properties.

You just cleared the first step to becoming a computational scientist. **Good job!!**