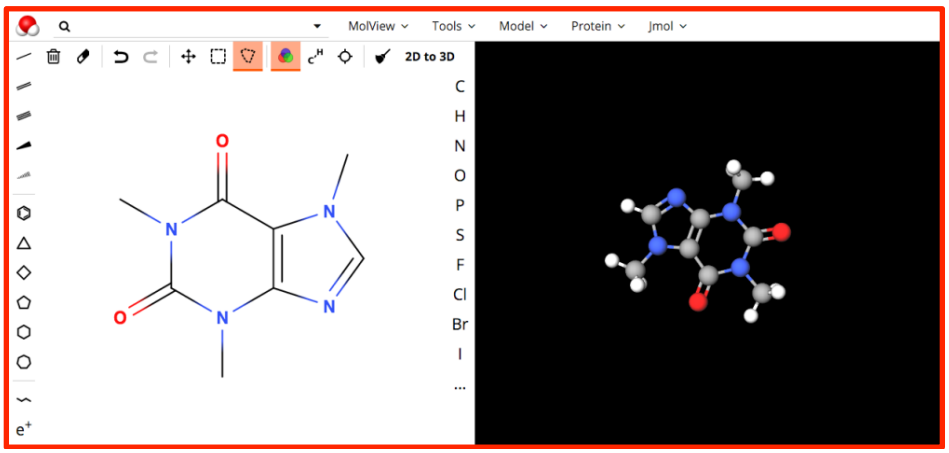
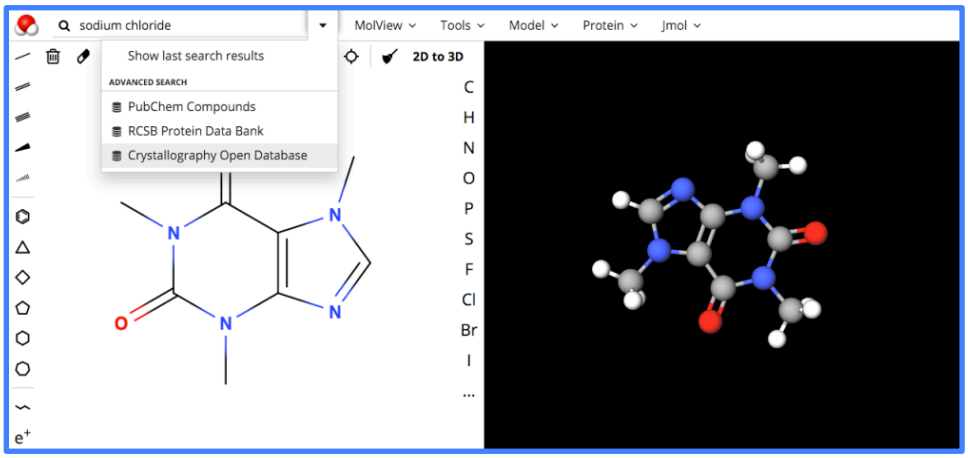
Go to molview.org and get started!

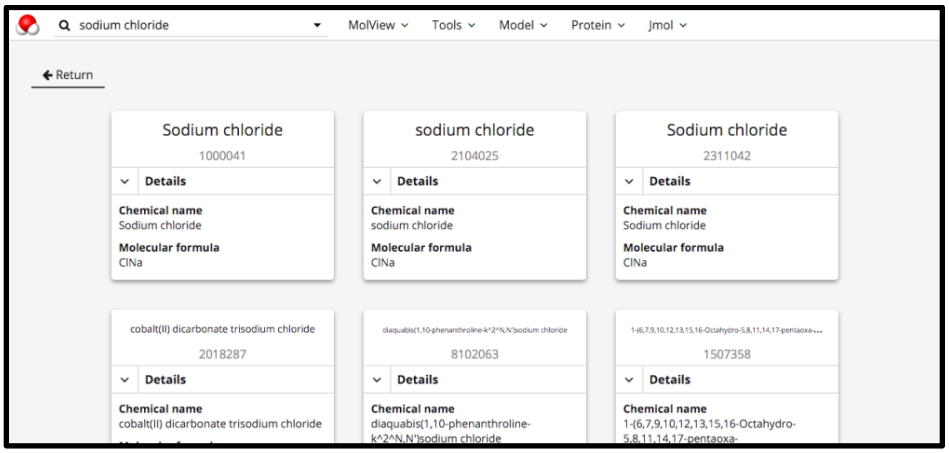
Does your screen look like this (maybe with a different compound)? Good!



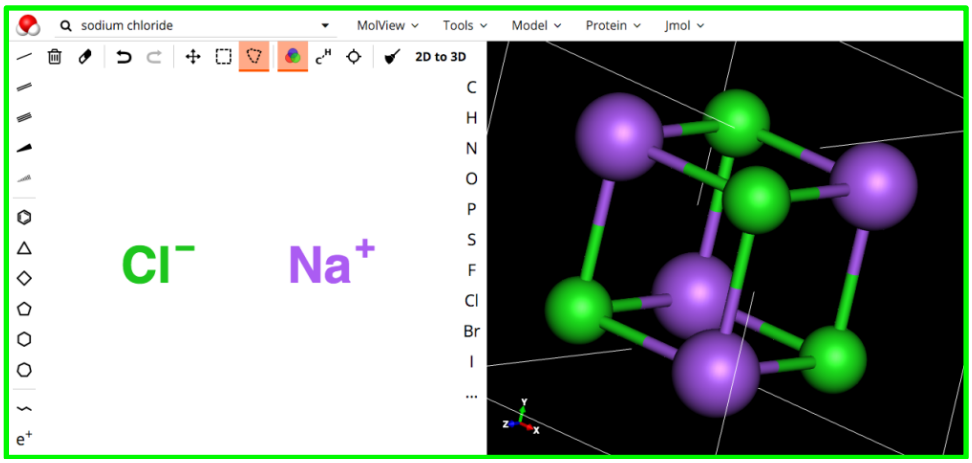
Now find your search bar, type in “sodium chloride” but don’t press “Enter”! See that little arrow next to your search box? Click it to get a drop-down menu like this:



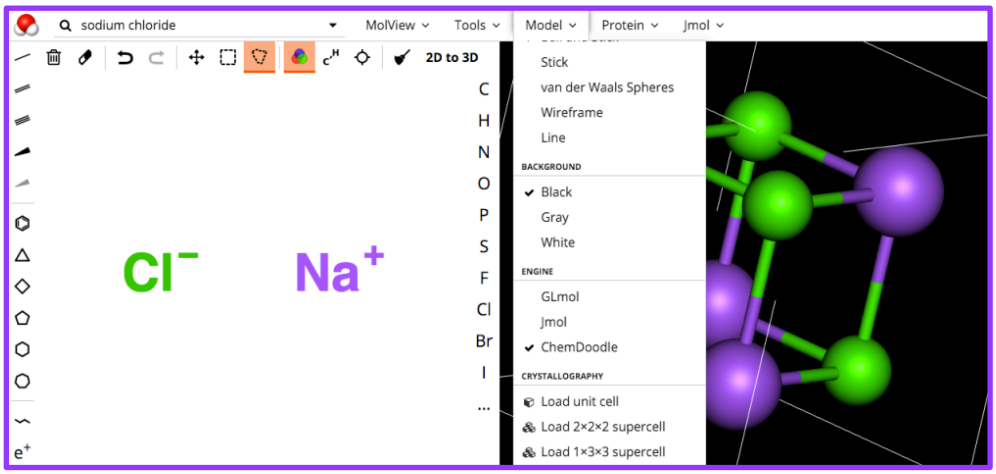
Select “Crystallography Open Database.” That will give you some options like this:



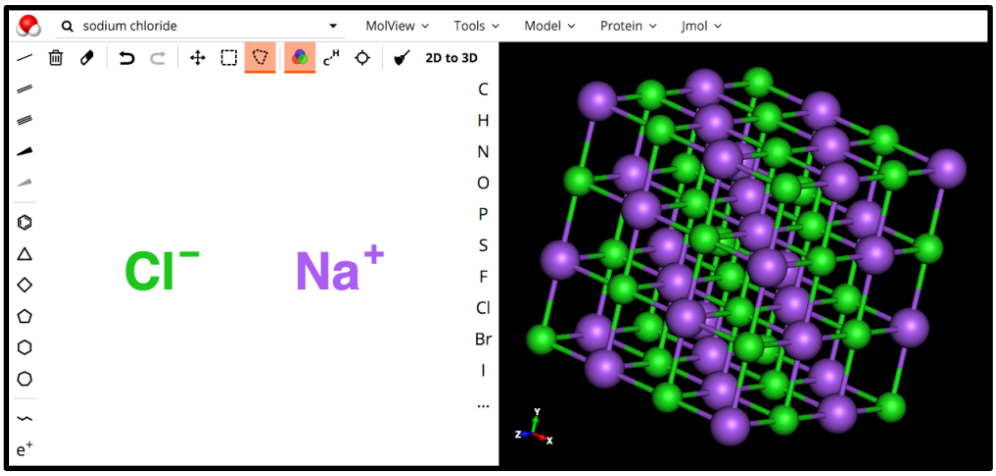
From what I have found, you can just click the first one and it will give you what you need. Now you should have a unit cell of sodium chloride. You can hold down your mouse clicker and drag over the structure to rotate the structure like this:



Want a bigger crystal? We can do that. Click the “Model” drop-down menu and scroll to the bottom where you should see the options, “load 2x2x2 supercell” and “load 1x3x3 supercell.” Like this:



Let’s try a “2x2x2 supercell.”



Look how pretty that is! Go ahead and repeat with any other molecular, ionic or atomic substance. For some substances, like copper, you can just type in the name of the element, press “Enter” and the unit cell will pop up! If you try that and it doesn’t work, just search the crystallography database and it should be there.

These directions were originally published on Lauren Stewart’s post, Switching from Mercury to MolView, on her personal blog, The Model So Far.