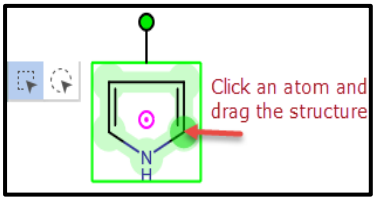
Tips for using ChemAxon MarvinJS in Reaxys

MarvinJS is a version of **ChemAxon MarvinSketch** that does not require an installation of Java on your computer. You can find lots of information about it on the ChemAxon website, including a MarvinJS User's Guide. Here are a few tips for using MarvinJS in Reaxys.

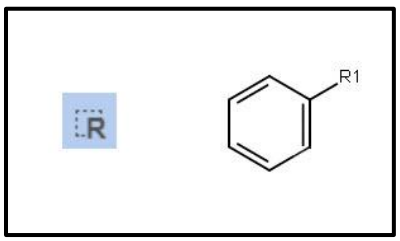
Select/Move a Molecule

1. Click a **Select** tool.
2. Press and hold the mouse button while dragging to select the structure.
3. Click an atom in the structure and drag to move the structure.



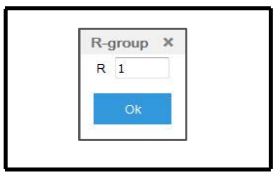
R-groups

1. Draw the parent structure.
2. Add R-group labels by clicking the "**R**" button and then clicking the appropriate atom(s).

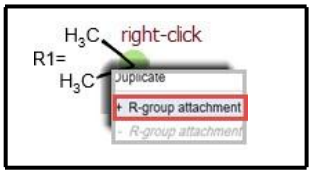


Then,

1. Draw the members of the R-group.
2. Select the members and click the "**R**" button.
3. In the R-group dialog window, type the appropriate R-group number.

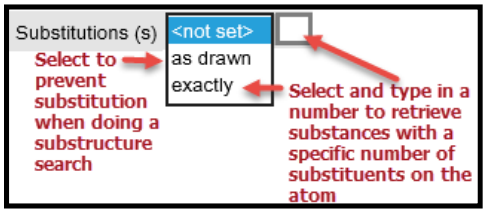


4. Optional: Add attachment points to the fragments (R-group members) by right- clicking an atom and selecting *R-group attachment*.



Substitution

1. Right-click an atom
2. Click **Atom Properties** and click the **Advanced** tab.
3. Look for the Substitutions(s) box.
   - Select **as drawn** to prevent substitution when doing a substructure search
   - Select **exactly** and **type in the number** to retrieve substances with a specific number of substituents on the atom.

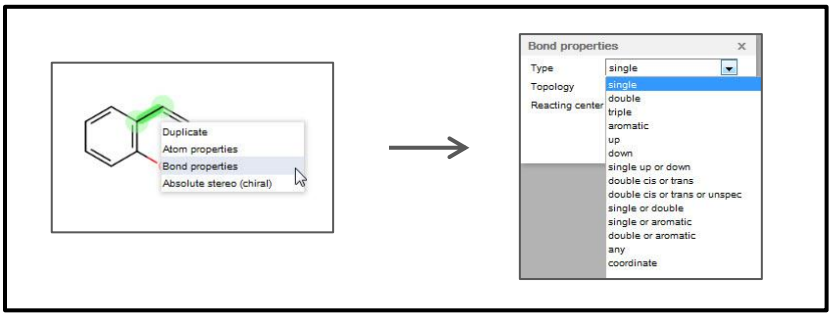


Alternatively,

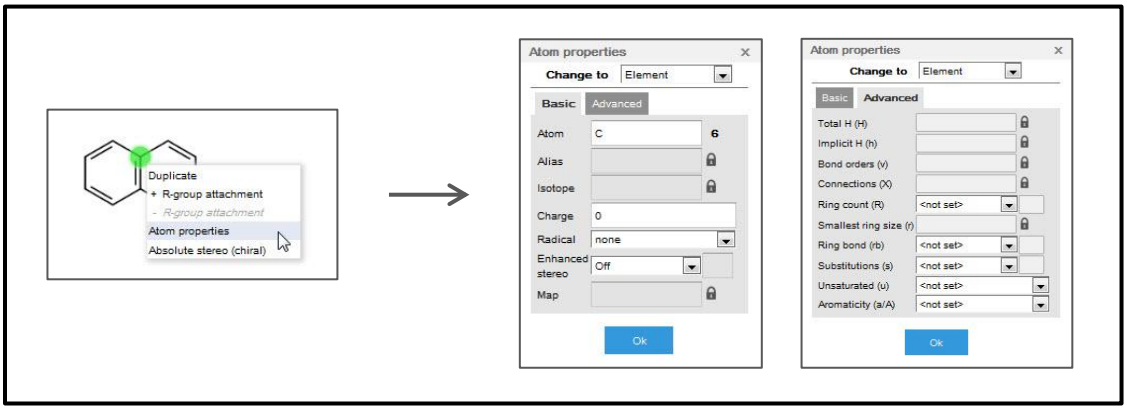
1. Click in the white space and type "." key on your keyboard
2. From the “Atom Query Properties” menu select “.s+”
3. Click the atoms that should have a substitution count until the count has reached the desired number.

Atom/Bond Properties

1. Right-click an atom or a bond and select **Atom properties** or **Bond Properties** as required.
   - Bond: Ring, Chain, Reacting Center, Up/Down, Cis/Trans, Single/Double/Triple

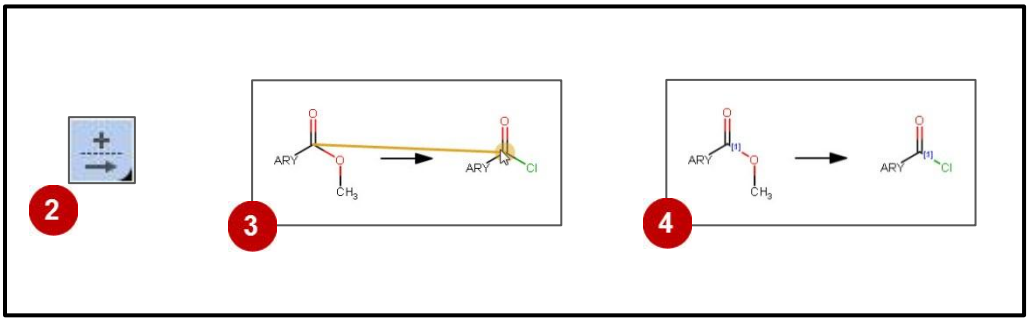


   - Atom: Charge, Radical, Substitution



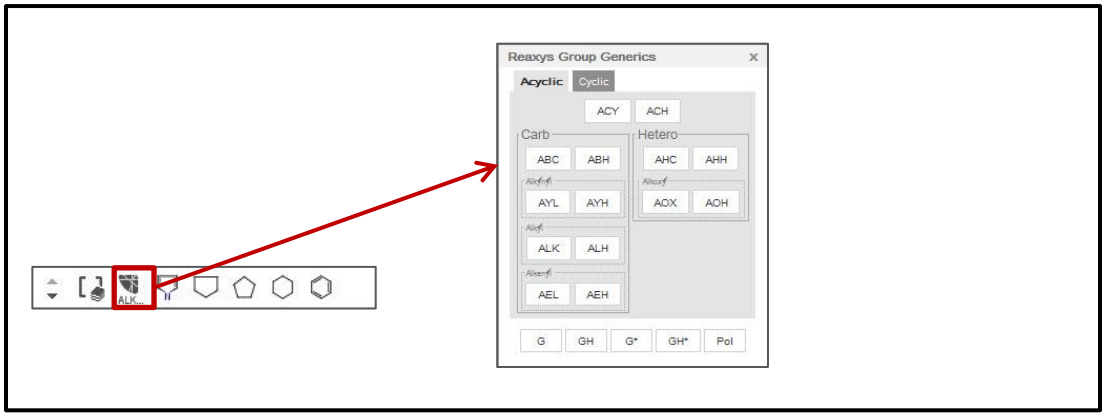
Atom Mapping

1. Draw the reaction.
2. Click the **reaction arrow button**
3. Click an atom in the reactant and drag to an atom in the product.
4. The mapped atoms are labeled.



Reaxys Predefined Generic Groups

1. Click the "**ALK…**" icon
2. Select from the **Acyclic** or **Cyclic** tab.



Position Variation Bond

1. Click a **Select** tool.
2. Press and hold the mouse button while dragging to select the appropriate atoms.
3. Click the **Bond** tool and select the **Position Variation Bond** icon.
4. The atom on the new bond can be changed to another atom, predefined generic group, or atom list.