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.