Subject: Mapping tool defective
Posted by timandrews on Fri, 12 Apr 2019 10:22:14 GMT
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Hi All. So I have the newest version of DataWarrior and everytime I try to create/enumerate a combinatorial library reaction the "atom mapping" tool doesn't work.

In the past I've never had an issue with it working but now, everytime I click on the mapping tool icon and then to an atom, a number for it isn't assigned.

Does anyone else suffer from this?

Subject: Re: Mapping tool defective
Posted by thomas on Sun, 14 Apr 2019 19:39:51 GMT
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when using the mapping tool, you are supposed to press the mouse over a reactant atom and then draw the mouse while still pressing over the respective product atom. When you release now, both atoms are assigned.

In you encounter bugs, you may also try to use the most recent development version, which should have all known bug fixed, but may introduce new functionality and (potentially) new bugs. You may download updated exe/jar files for Windows/OSX&Linux under these links: openmolecules.org/datawarrior/dw500win.zip and dw500x.zip. Just unpack the zip file and put the files it contains into you installation folder, where they should replace the original files.

Hope this solves the issue, Thomas