Subject: Issues with multiple columns of smiles in 5.0.0
Posted by MarkG on Tue, 15 Jan 2019 15:54:59 GMT
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It looks like 5.0.0 has issues opening text files with multiple smiles columns. At least, I'm having an issue with the below.

SMILES smiles2
Cc1ccccc1 OCCC
Cc1ccccc1 OCC
Cc1ccccc1 OC

If I copy/paste 'with header row', 5.0.0 hangs on my machine.

Subject: Re: Issues with multiple columns of smiles in 5.0.0
Posted by thomas on Wed, 16 Jan 2019 22:41:10 GMT
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this is already fixed in the source code. An update is in preparation...

Subject: Re: Issues with multiple columns of smiles in 5.0.0
Posted by thomas on Thu, 17 Jan 2019 17:51:55 GMT
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Until there will be a full new version upgrade, I publish frequent intermediate DataWarrior builds with fixes of known bugs, which can be downloaded from this website. These are just the DataWarrior.exe file for Windows and the datawarrior.jar file for Linux and MacOS. To update, just replace these files. The links to these files are: openmolecules.org/datawarrior/dw500win.zip and openmolecules.org/datawarrior/dw500x.zip, respectively.

The current files include fixes for this two-column-smiles bug and some other small issues. It also contains a new column filter hiding columns instantly based on column names.

Thomas