
Subject: Issues with multiple columns of smiles in 5.0.0

Posted by [MarkG](#) on Tue, 15 Jan 2019 15:54:59 GMT

[View Forum Message](#) <> [Reply to Message](#)

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

Cc1cccc1 OCCC

Cc1cccc1 OCC

Cc1cccc1 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

[View Forum Message](#) <> [Reply to Message](#)

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

[View Forum Message](#) <> [Reply to Message](#)

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
