Subject: Structure issues from smiles when opening text files
Posted by Andrew0 on Wed, 03 Jan 2018 20:24:35 GMT

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Thomas,

I have run into an issue after updating DataWarrior to the latest version when importing text files. When I import a text file that contains more than 500 rows, something happens with the SMILES data for each row. Many of the rows just display nothing where a structure should be present.

I have attached two text files, one with 500 rows and one with 501. The first file imports properly, while the second file has many empty structure cells.

For reference, I am using the 4.7.1 32-bit Windows installation, and I have previously imported larger files (3000 rows) without running into any similar issues.

As always, thanks for your work on this tool!
Andrew

File Attachments
1) vanillin_500.txt, downloaded 499 times
2) vanillin_501.txt, downloaded 504 times

Subject: Re: Structure issues from smiles when opening text files
Posted by thomas on Mon, 08 Jan 2018 21:35:14 GMT

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Dear Andrew,

thank you very much for the detailed bug analysis and report. I have found and corrected the problem in the source code. With more than 500 rows SMILES parsing switches from single thread to a multi-thread approach. Unfortunately, a molecule buffer was erroneously shared by those threads leading to unpredictable results. Since this is a severe problem, I will release an update in the next days...

Thomas