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 505 times
- 2) vanillin 501.txt, downloaded 510 times