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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

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