Subject: Error on attempting to generate conformers
Posted by Paul on Wed, 24 Aug 2022 22:08:05 GMT
View Forum Message <> Reply to Message

Hello Everyone

In the midst of attempting to solve one problem, I discovered this one.

After downloading and installing the most recent official release and development versions of DataWarrior, I receive the error

"Uncaught Exception:chemaxon/formats/MolFormatException" on attempting to generate conformers.

This error occurs on files for which conformers were successfully generated earlier today (using an earlier Data Warrior version) on Windows 10 64-bit.

I tried several variations without success, e.g. structures from a smiles.txt file, an SDF with no smiles but a 2D structure table, and DWAR files for which conformer generation succeeded earlier today.

Conformer generation performs as expected using the most recent official release version of Data Warrior (to which I've returned).

Best Regards and Thanks,

Paul

Subject: Re: Error on attempting to generate conformers
Posted by thomas on Sat, 27 Aug 2022 10:14:48 GMT
View Forum Message <> Reply to Message

Hi Paul,

many thanks for reporting this serious issue. I was not aware of it, because I always tested with the capka.jar file in my classpath, which provides chemaxon pKa calculation. I had slightly changed the way, how that file would be recognized and used, which caused the problem. I have fixed and tested now with and without capka.jar.

Now conformer and property calculation work again in the newest dev version...

Thomas

Subject: Re: Error on attempting to generate conformers
Posted by Paul on Mon, 29 Aug 2022 15:18:45 GMT

Thanks to you and to all who improve and make DataWarrior available.

Paul