Subject: Error on attempting to generate conformers
Posted by Paul on Wed, 24 Aug 2022 22:08:05 GMT
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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