Subject: Re: Creat macro file and run, but cant open the created dwar file
Posted by thomas on Wed, 09 Oct 2019 21:42:08 GMT

Dear Kelly,

sorry for the late reply. Would it be possible to send me a small example macro, such that I can reproduce the issue. And also may an example of the SMILES file that is causing the trouble? DataWarrior should never crash, when reading SMILES, even if the SMILES are invalid. Invalid SMILES should simply be ignored.

Thanks in advance, Thomas