Subject: Re: Merge file failed
Posted by thomas on Mon, 24 Nov 2025 18:02:53 GMT
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Sorry for the late response. I now tried to reproduce the freeze. I tried you complete procedure.
I tried loading the 'starting file.dwar' and merging with 'Combinatorial_Library.sdf'
I also tried with 'starting file.sdf' and my own generated combichem lib file and combinations.
The program never froze and the replacements of the 34 structures out of 90 seemed always correct.
I also tried with the all_column file with the same result.
I used DataWarrior v06.05.02 on Ubuntu for the tests. The OS should not make a difference, but if you use something else than Linux, I may retry.

And a tip: Instead of generating a combinatorial library, you may just use 'Perform Reaction...' from the Chemistry menu.