Subject: Merge file failed
Posted by sim on Sat, 25 Oct 2025 20:28:33 GMT
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Hi,

The program froze at the end, had to close it via Task Manager. The objective of my work was to replace the fluorine atoms in a certain position with W atoms in the same position. Starting from "starting file.dwar", the sequence of operations is shown in the attached screenshots. The file "starting file.sdf" was exported from the dwar file and used for enumeration of the combinatorial library via "Add from file".

This story was preceded by another one. With a starting file containing the same structures but a greater number of columns (starting file _all columns.dwar) the program performed the substitution correctly and did not froze. However, the structure search in the obtained file found only part of the structures containing the W atom. I could not see any logic in its behaviour but I guess that both bugs have a common root. Unfortunately I did not save those files, will redo if required.

File Attachments

1) Bug report.zip, downloaded 163 times

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.