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 190 times