Subject: Re: Saving columns with user data after conformer generation to new file
Posted by thomas on Mon, 17 Mar 2025 16:25:14 GMT
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Dear Alex,

currently, you cannot export other columns to the new created file, which means you import columns from the old file by merging using the structure as key.

Logically, another two step solution could be an alternative: generating multiple conformers in the same file (not 'write into file') and splitting rows with multiple conformers afterwards. Unfortunately, this does not work currently, because the conformer column is not available for selection, and because additional columns like 'MMFF Energy' are not grouped. Maybe, an option for the future...

Best wishes,

Thomas