Subject: Saving columns with user data after conformer generation to new file
Posted by alex on Mon, 17 Mar 2025 14:40:53 GMT
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Dear Thomas,

Is it possible to save all columns with data from the parent dwar-file when running "Generate Conformers" with "Write into file" option?

To date, new file with generated conformers contains only ID, Stereo Isomer, Energy and Minimization Error columns regardless of the columns in parent file.

Data can be added manually by files merging after conformer generation, but perhaps there is an option to save the data automatically?

Best wishes,
Alex

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