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