Subject: Export Superimposed structures
Posted by sbembenek18 on Thu, 14 Apr 2022 03:11:42 GMT
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I have aligned my molecules to a 3D reference using 'Superimpose Conformers'. Can I now write an SDF file with these new aligned (updated) coords for each molecule rather than the original 3D coords?

Subject: Re: Export Superimposed structures
Posted by thomas on Sun, 15 May 2022 15:08:53 GMT
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Yes. Admittedly, it is not really obvious. The Superimpose method creates a new (hidden) column 'Best Match'. It is hidden, because in most cases it contains just the same structure from the 'Structure' column. The new aligned 3D-coordinates are stored as another hidden column assigned to 'Best match'. Thus, use 'File->Save Special->SD File'. In the dialog choose 'Best match' as structure column and 'Superposition' as coordinates. Then you may also choose 'Include Reference Molecule' to also include the superposition target molecule oin the SD-file.

File Attachments
1) temp.png, downloaded 662 times