
Subject: Re: Export Superimposed structures

Posted by [thomas](#) on Sun, 15 May 2022 15:08:53 GMT

[View Forum Message](#) <> [Reply to Message](#)

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 in the SD-file.

File Attachments

1) [temp.png](#), downloaded 581 times
