Subject: Generating 2D Coords does not work with 3D structures
Posted by richards99 on Mon, 08 Mar 2021 10:56:47 GMT
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It seems that when I what to regenerate 2D coordinates for structures from Chemistry/Generate 2D Coordinates, and provide a Substructure to align too, this does not seem to work if the structures already have 3D coordinates.

Workaround currently, is I generated SMILES of these structures, do Name to Structure, and then generate 2D coordinates on these.

Simon.

Subject: Re: Generating 2D Coords does not work with 3D structures
Posted by thomas on Tue, 09 Mar 2021 16:20:18 GMT
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Thank you. There was an issue of not applying a template's 2d-atom-coordinates, if the template consisted of the same atoms that were later automatically discovered as part of a fragment coordinate rule within the coordinate inventor (e.g. a ring or a connecting chain. This is now fixed in the current development version. If you still have issues, please send me a reproducible example. Whether 3D-coordinates exist should not make a difference.

Thomas