Subject: 2D coordinates in the template
Posted by richards99 on Wed, 27 Jan 2021 10:32:16 GMT
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Hi,
It would be great if when you set up 2D coordinates, using the "Generate 2D Atom Coordinates" and a drawn substructure, that when you save out the session as a Template (Save Special/Template) that this is remembered, so that when you apply the template to a dataset the 2D coordinates are generated for you.

This is really useful so you can have all the structures aligned in a way you want them right way.

Thanks,

Simon.

Subject: Re: 2D coordinates in the template
Posted by thomas on Thu, 28 Jan 2021 09:03:57 GMT
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Hi Simon,

thank you for the suggestion. Templates are meant to define views and filter settings. Applying a template should not modify the data itself. Therefore I suggest that you use a macro with just one "Generate 2D Atom Coordinates" task for that purpose. You could store it in the macro folder, then it would be generally available in all your DataWarrior files.

Thomas