Subject: New feature request: align structures
Posted by mvamos on Wed, 18 Sep 2019 22:47:26 GMT
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Hello. Would it be possible to add a feature where the user can align all (related) structures/analogs in a dataset for easy viewing to determine SAR trends?

Subject: Re: New feature request: align structures
Posted by thomas on Wed, 09 Oct 2019 21:27:46 GMT
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You can generate new atom coordinates with:

"Chemistry -> Generate 2D Atom Coordinates"

Then check

"Automatically detect scaffolds and unify their orientation"
and select a scaffold detection method: "most central" should be fine

When clicking OK, DataWarrior will rearrange your 2D-structures such that the most central ring system, where multiple molecule share the same scaffold, this scaffold is always drawn the same way.

For more flexibility, you may provide scaffolds with defined coordinates in the same dialog.

Subject: Re: New feature request: align structures
Posted by sbembenek18 on Fri, 11 Oct 2019 16:46:24 GMT
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thanks!