Subject: 3-D structures vs descriptors
Posted by Christophe on Tue, 04 Jan 2022 14:13:27 GMT
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Hello everyone,

I am a new user of DataWarrior and I really enjoy it, so many thanks for providing the scientist community with such an advanced tool.

Question: Is generating conformers from 2D structures, or smiles, a prerequisite in the calculation of molecular descriptors such as skelspheres or flexophores or can we do without it? More precisely, If I want to run a similarity/Activity cliff analysis for example, do I need first to compute optimized 3D structures from my 2D .sdf file?

Thanks a lot
All the best
C.

Subject: Re: 3-D structures vs descriptors
Posted by thomas on Tue, 11 Jan 2022 16:00:25 GMT
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Hallo Christophe,

you don't need conformers for any of the descriptors or any descriptor based calculations. The only descriptor that needs 3D-structures is the flexophore, but it generates them internally. Typically, if a functionality requires 3D-atom-coords, which are not there,then it will show a dialog asking you to generate conformers.

Thomas