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.