Subject: Conformers and xyz
Posted by lutek14 on Thu, 10 Oct 2019 20:15:04 GMT
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Hello!
DataWarrior looks pretty awesome, however I'd like to know two things:
a) is it possible to generate chosen number of conformers (e.g. 10 instead of 2)?
b) is it possible to export CONFORMERS (as .xyz or .mol format), so they can be used in other programs?
Thank You

Subject: Re: Conformers and xyz
Posted by thomas on Fri, 11 Oct 2019 17:06:03 GMT
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Yes to both questions. When generating, you may define any number of conformers and choose an SD-file as output format. This is explained here:
http://www.openmolecules.org/help/conformers.html#Generate

In the upcoming update one may also generate and store conformer sets within one row. When such a DataWarrior window is exported into an SD-file, then the conformer ensemble is stored as individual conformers. The currently downloadable beta version already contains that functionality (download link for replacement files: openmolecules.org/datawarrior/dw500win.zip for Windows, dw500x.zip for Linux/Mac).