
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).
