Subject: Generate conformers - write to file does nothing Posted by Paul on Wed, 08 Jul 2020 19:01:48 GMT

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Hello,

When I try to write conformers into file, a 1KB dwar file is generated, which contains only what appear to be the file markup tags, i.e <datawarrior-fileinfo> . . . </datawarrior properties>.

Conformers are generated successfully and get a new 3D molecule view pane when "write to File" is not selected, and Max conformer count per stereoisomer is set to 1.

When Max conformer count is set to 2 or larger, a single conformer is displayed. The appropriate number of energies is given in the new Energy column, but only 1 conformer is provided.

Best Regards,

Paul