
Subject: Re: Generate conformers - write to file does nothing

Posted by [nbehrnd](#) on Thu, 09 Jul 2020 08:10:08 GMT

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Hello Paul,

starting with the liquid_crystal.dwar file attached below, and using the parameters shown in the screen photo below

the newly written conformers_test.dwar contains multiple models. Not 16 which was set as the maximum number, but at least four. May you share a minimal example, including the parameters you use, leading to the empty .dwar file?

Norwid

File Attachments

- 1) [liquid_crystal.dwar](#), downloaded 415 times
 - 2) [conformers_test.png](#), downloaded 920 times
 - 3) [conformers_test.dwar](#), downloaded 455 times
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