Subject: Re: Generate conformers - write to file does nothing
Posted by thomas on Fri, 10 Jul 2020 11:22:41 GMT
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I cannot reproduce this. If I generate 10 random molecules with otherwise default settings, and if I then generate conformers (Max conformer count: 2, otherwise default), I get two conformers for most molecules:

I tried with V5.2.1 as well as with the most recent dev version. Writing 16 conformers per structure into a file also worked. Maybe it somehow is related to your input structures? Could you share a problematic structure?

File Attachments
1) t.png, downloaded 1254 times