Subject: bug: 3D coordinate saving causes crash
Posted by richards99 on Sat, 30 May 2020 21:56:48 GMT
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Hi,
If the data table of structures have 3D coordinates available, except for a couple of structures, if you then go to save the structures out as an SDF and in the export box choose to use 3D coordinates if available, it causes DataWarrior to crash.

Simon.

Subject: Re: bug: 3D coordinate saving causes crash
Posted by thomas on Fri, 05 Jun 2020 14:18:31 GMT
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Thank you for reporting precisely. This will be fixed in the next release.

Thomas

Subject: Re: bug: 3D coordinate saving causes crash
Posted by mpilipp on Mon, 24 Aug 2020 20:12:05 GMT
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It would also be very good if all of the compounds in the database could be saved in the 3D format, as sdf files.

Subject: Re: bug: 3D coordinate saving causes crash
Posted by thomas on Wed, 26 Aug 2020 10:09:38 GMT
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I am not sure, whether I understand correctly. If you save as SD-File with 3D-coords, then all compounds are saved, aren't they?