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

Subject: Re: Generate conformers - write to file does nothing
Posted by nbehrnd on Wed, 08 Jul 2020 22:58:47 GMT
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Hello Paul,

the generation of conformers may, but need not to, include the application of a force field. DW includes MMFF94s, MMFF94s+, and Indorsia; if used (which might be your default) some of the conformers may coalesce. The fourth option next to minimize energy is «don't minimize»; then retaining better the results of the parameters «Algorithm» and «Initial torsions» in display and file written.

Norwid

Subject: Re: Generate conformers - write to file does nothing
Posted by Paul on Thu, 09 Jul 2020 00:46:33 GMT
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Thanks - I have been able to use the various force fields with success, but only when generating a single conformer as new columns in the DWAR document.

Regardless of the force field, or choosing not to minimize, the output from generate conformers

Paul

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,

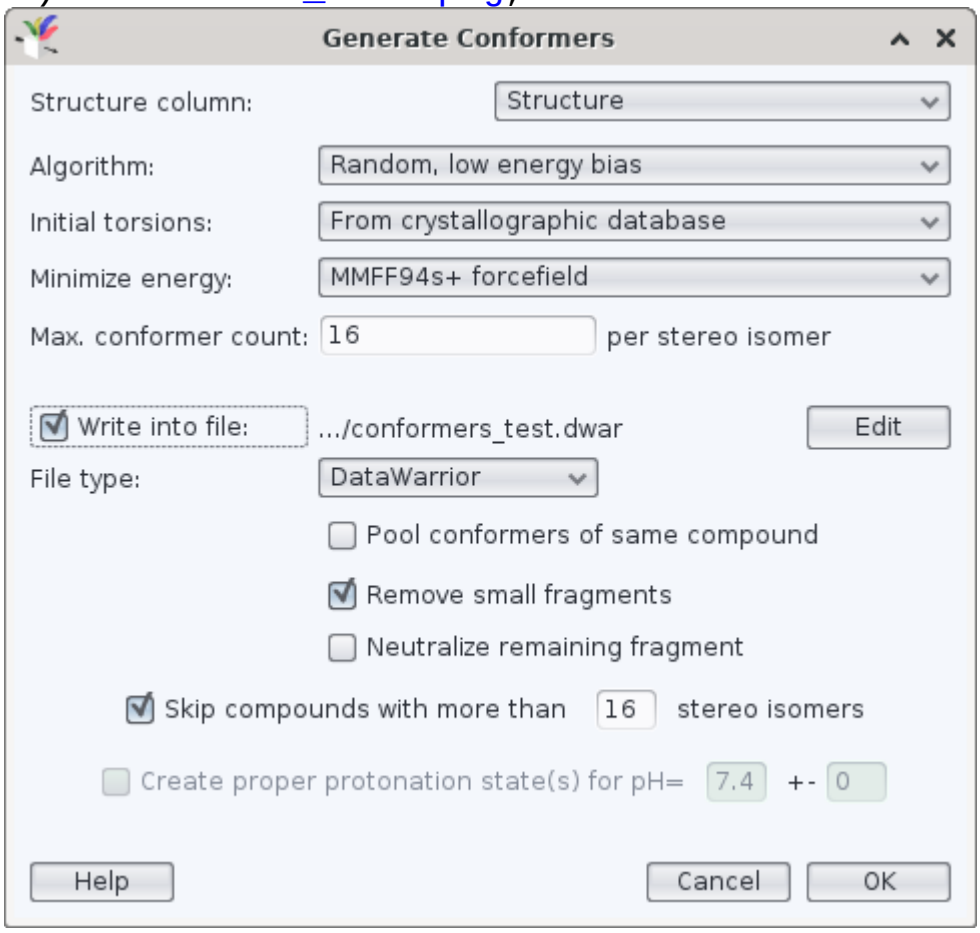
starting with the liquid_crystal.dwar file attached below, and using the parameters shown in the screen photo below

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 634 times
2) conformers_test.png, downloaded 1326 times



3) conformers_test.dwar, downloaded 665 times

Subject: Re: Generate conformers - write to file does nothing
Posted by Paul on Thu, 09 Jul 2020 16:23:45 GMT
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Thank you - your files helped me to determine the reason my attempts to write conformers to files have failed.

After I downloaded your files, I was able to write conformers to file from those dwar files.

Immediately noticeable was that your file contained only an option "Structure" in the Structure Column dropdown menu in the generate conformers dialog.

My files contained only an option "Structure of SMILES" in the same dialog, even though they also contain 3D structures (data column 3-D structure of SMILES) that are clearly visible in Datawarrior's 3D-Structure pane. With this option, writing conformers to file generates an empty DWAR container.

When I Delete the SMILES and/or structure of SMILES column(s), the image in the 3D-Structure pane disappears. This suggested that the conformer displayed in the 3D viewer pane was somehow dynamic, but when I edit the SMILES, neither the structure of SMILES nor the previously generated conformer update to the new SMILES.

Since you had shown me that writing conformers to file could work, I then continued to try different approaches to obtaining a file without a Structure of SMILES column, but instead a Structure column.

I saved my file as SDF, choosing 3D structure if available. When I opened the new SDF, I then had the desired "Structure" column (not "Structure of SMILES). The SDF still contained a SMILES column, but DWAR used the 3D structure instead of generating structures from SMILES. Writing conformers to file now works!

However, if a DWAR file contains both SMILES and 3D structures, Datawarrior uses the SMILES > Structure of SMILES and will not write conformers to file.

At last, I successfully wrote conformers to file (either from the SDF or after saving it back to DWAR, so long as the SDF did not contain a SMILES column)! The SMILES column must be deleted after opening the SDF, not from the DWAR file, then saved to a DWAR file.

So then, I am thinking that there must be a better way to accomplish these ends without (1) generating a conformer from structure of smiles in Datawarrior, (2) Saving it to SDF, and (3) Using the new SDF to generate conformers (or deleting the smiles column then saving it back to DWAR).

On further exploration, I determined that I can write conformers to file without the SDF intermediate if I generate 2D atom coordinates (from Structure of SMILES, of course).

The generate conformers dialog does not change - the only structure available in the dropdown menu is still Structure of SMILES (even though I now have columns for 3D-structure of smiles, Structure of SMILES [2d coordinates], and Structure of SMILES).

Conclusions:

Datawarrior's Generate Conformers > Structure Column dropdown menu lists only one structure column, even when more are available.

Datawarrior will generate conformers from Structure of SMILES within a current document (SDF or DWAR), but not to a new document. Attempts to write to file generate empty DWAR containers.

Datawarrior will write conformers to file when the DWAR-generated Structure of SMILES [2D coordinates] data column exists, even though there is no apparent difference between the generate conformers dialog (it indicates conformers are generated from Structure of SMILES).

Thank you very much for helping me work this out.

Now I'm wondering - does the Structure dropdown menu ever populate with more than one option?

Best Regards,

Paul

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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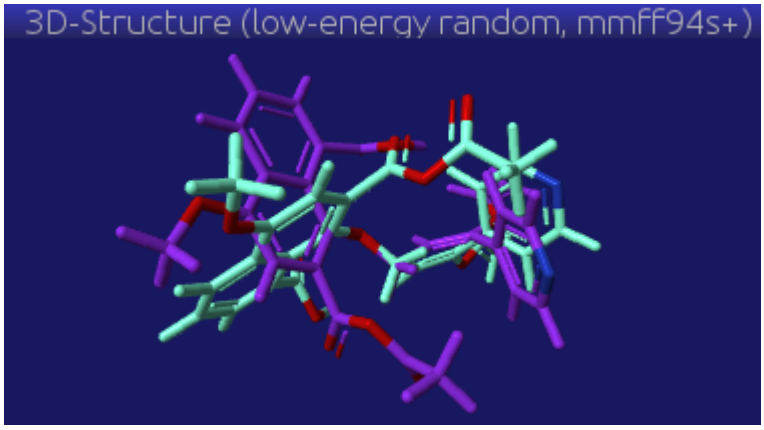
I cannot reproduce this. If I generate 10 random molecules with otherwise default settings, and if I then generate conformers (Max conformer count: 2, otherwise default), I get two conformers for most molecules:

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 1159 times


3D-Structure (low-energy random, mmff94s+)