Subject: Batch conversion of dwar files
Posted by jeremy on Wed, 21 Oct 2020 15:19:10 GMT
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Hello,
I have to convert a bunch of dwar files into csv (or SDF) files.
I can open them one at a time and export; but I would prefer a more automated way. I can read the dwar file as tab delimited files (ignoring top lines), but I don't know how to convert the structure string into a molecule. Is there a way to convert the structure string into a molecule outside DW?
Thank you

Subject: Re: Batch conversion of dwar files
Posted by thomas on Thu, 22 Oct 2020 15:47:24 GMT
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Hello,

with the current development patch you can run a macro loop over all files within a given directory. You can also create a new macro from a text macro representation as the following. If you copy the following macro text without any empty lines and select the 'Paste Macro' in the DataWarrior 'Macro' menu, and then select 'Run Macro->convertAllFilesToSDF', then DataWarrior asks you to select a directory and then writes an SD-File from every dwar file it finds in the directory.

(the needed DataWarrior files can be downloaded on the download page after selecting the 'Read and understood' checkbox. Look carefully, the download link is in the fineprint!

```
<macro name="convertAllFilesToSDF">
<task name="repeatNextTasks">
dir=#ask#
filetype=datawarrior
all=true
</task>
<task name="openFile">
fileName=$FILENAME
</task>
<task name="saveSDFile">
version=v3
idColumn=<idColumn>
structureColumn=Structure
coordinates=2D
fileName=$FILENAME.sdf
</task>
<task name="closeWindow">
</task>
</macro>
```