Subject: Re: running a DW macro in batch
Posted by SM2020 on Tue, 18 Nov 2025 14:40:28 GMT
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Hi,
This is a follow up to a previous forum support request.

I would like some help with running a DW macro over multiple .sdf files in a folder, please.
I am running DW version [6.05.02] on Windows 11 – the macro (see below) used to work in earlier versions of DW, but which I now can't reproduce.

Aim: To generate 3D conformers for each molecule represented in a list of individual .sdf files in a specified directory

Intended result: an output of multiple .sdf files of molecule conformers from each original .sdf input file.

The previous working macro is given below.

```
<macro name="batch-conformers">
<task name="repeatNextTasks">
dir=#ask#
filetype=sd
all=true
</task>
<task name="openFile">
fileName=$FILENAME
</task>
<task name="generateConformers">
neutralize=false
fileName=$FILENAME_conf.sdf
torsionSource=crystallDB
largestFragment=true
stereoIsomerLimit=16
minimize=mmff94s+
algorithm=lowEnergyRandom
maxConformers=16
structureColumn=Structure
fileType=sdf3
</task>
<task name="closeWindow">
saveChanges=no
</task>
</macro>
```

Result when running the macro: When I try to run the macro, it seems to run but displays transient error/dialog messages (which are not left on the screen long enough to read) and the require output files are not created in the output directory.

When I have tried to re-run the macro on an older version of DW (on ubuntu), the macro will run but need to manually 'hit a key' type of operation to move onto the next conformer generation...

If someone can help – and suggest where the syntax in the macro is at fault - it would be very much appreciated.

Thanks.
