Subject: running a DW macro in batch
Posted by SM2020 on Thu, 30 Nov 2023 15:36:56 GMT
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Hi,
I would like some help with running a DW macro over multiple .dwar files in a folder, please.
I am running DW version 5.5.0.

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

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

I tried to use a previous post describing looping a macro over multiple dwar files to get started (see below) but I am getting stuck.
https://openmolecules.org/forum/index.php?t=msg&goto=109 3&&srch=loop#msg_1093

My macro attempt is given below.

<macro name="batch-conformers">
<task name>="repeatNextTasks"
dir=C:\PATH #path is specified when run
filetype=datawarrior
all=true
<task>
<task name="openFile">
fileName=$FILENAME
<task>
<task name="generate2DAtomCoordinates">
scaffoldMode=centralRing
structureColumn=Structure
automatic=true
colorizeScaffolds=false
</task>
<task name="generateConformers">
poolConformers=false
neutralize=false
fileName=$FILENAME_conf.dwar
torsionSource=crystallDB
largestFragment=true
stereoIsomerLimit=16
minimize=mmff94+
algorithm=lowEnergyRandom
maxConformers=16
structureColumn=Structure
fileType=dwar
<task>

<task name="closeWindow">
</task>
</macro>

When I try to run the macro, I get the following error-
“macro ‘batch conformers’ does not have any tasks”

If someone can help, it would be very much appreciated.

Thanks.

Subject: Re: running a DW macro in batch
Posted by thomas on Wed, 06 Dec 2023 16:31:30 GMT
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Hi SM2020,

It seems that your macro has some syntax errors, e.g. '<task>' are task end tags and should always look be '</task>'. The second line should end with '>'.

A working macro should be the following:

<macro name="batch-conformers">
<task name="repeatNextTasks">
dir=#ask#
filetype=datawarrior
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=mmff94+
algorithm=lowEnergyRandom
maxConformers=16
structureColumn=Structure
fileType=sdf2
</task>
<task name="closeWindow">
saveChanges=no
</task>

</macro>

Subject: Re: running a DW macro in batch
Posted by SM2020 on Thu, 28 Dec 2023 12:27:44 GMT
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Thank you for helping with the Syntax - seems to work now.

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.
