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>