
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=crystalIDB  
largestFragment=true  
stereoisomerLimit=16  
minimize=mmff94+  
algorithm=lowEnergyRandom  
maxConformers=16  
structureColumn=Structure  
fileType=sdf2  
</task>  
<task name="closeWindow">  
saveChanges=no  
</task>  
</macro>
```