Posted by Bruno on Sat, 04 Jun 2022 10:17:31 GMT
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Dear Thomas
I am trying to run a macro directly from the terminal on a MAc (i haven t tried yet on Linux)... The content of this test macro is below.
When i open it in DataWarrior it runs fine. When i run from the Terminal, it doesn t. Would you have some advice ?
many thanks
Bruno


```
<macro name="TestMacro">
<task name="buildEvolutionaryLibrary">
paramConfig2=rotatableBonds 15 0
paramConfig1=cLogP 8 0
paramConfig0=molweight 350 750 0
kind=drugs
generationCount=automatic
survivalCount=32
 startSet=ek`\JD@AGFnMOIc`Ha@HRYWmYUyWYgHhl\JjvNijZji`@jZfJAQ @@
generationSize=256
paramCount=3
</task>
<task name="selectWindow">
viewName=Evolutionary Library
</task>
<task name="selectView">
viewName=Table
</task>
<task name="deleteColumns">
defCriterion=
columnList=Child No cLogP cLogP Fitness Fitness Generation Molecular weight Molecular weight
Fitness Parent Generation Parent ID Rotatable bond count Rotatable bond count Fitness
columnDefMode=list
</task>
<task name="findAndReplace">
isStructure=false
column=ID
isRegex=true
what=$
with=-coag
</task>
<task name="addSmilesCodes">
structureColumn=Structure
</task>
```

```
<task name="calculateCompoundProperties">
propertyList=nasty
structureColumn=Structure
</task>
<task name="deleteColumns">
defCriterion=
columnList=Structure
columnDefMode=list
</task>
<task name="saveTextFile">
 fileName=/Users/Test/Desktop/Test-collection.dir/Evolutionar y_Library-coagulation.txt
</task>
<task name="closeWindow">
</task>
</macro>
```

Subject: Re: macro buildEvolutionaryLibrary from a mac terminal
Posted by thomas on Mon, 06 Jun 2022 08:17:47 GMT
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Hi Bruno,

I tried to reproduce, but had many problems with your macro:
- all TABs seem to be replaced by SPACEs
- the startset of the first task contains a SPACE close to the end that does not belong there
- the first double quote is a wrong double quote character
- the column list in deleteColumns task contains lots of duplicates

It seems that you used a text editor that does funny things on its own. Maybe the problems are related to that. Otherwise, please send me a fresh copy of the working macro and I will try again...

Subject: Re: macro buildEvolutionaryLibrary from a mac terminal
Posted by Bruno on Mon, 06 Jun 2022 09:21:39 GMT
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Thanks Thomas
yes it was a copy and paste, but here is a similar macro directly saved from Datawarrior (dwam).
It runs fine when started with the app, but not from my terminal, with the terminal it opens the
Osiris window but does not start the process as if i was missing a command.
Best
Bruno

File Attachments

1) `test_Macro_Mac_june6.dwam`, downloaded 476 times

Subject: Re: macro buildEvolutionaryLibrary from a mac terminal
Posted by thomas on Mon, 06 Jun 2022 15:37:10 GMT

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Hi Bruno, thank you for the update. I have experimented a little bit and found that the appbundler, which I use to build the Macintosh DataWarrior application (/Applications/DataWarrior.app/Contents/MacOS/DataWarrior) has a bug, which prevents command line arguments from being passed to the main() function of the DataWarrior Java bytecode. It seems that there is a fork, that solves this issue. I will verify that and possibly use that fork for the next full Macintosh version. For the time being you may use another mechanism to launch DataWarrior from the command line if you have a JRE8 installed. If you don't have one, then I recommend liberica (full version is important, because only that has JavaFX included). If you type 'java -version' in a terminal and if it gives you a version 1.8... then you can use the following to solve your issue, i.e. to run datawarrior with parameters from the command line:

Copy the attached batch file 'datawarrior' to launch the DataWarrior application.
You may need to type and run 'chmod 755 datawarrior' to make the file executable.

Then you may execute the macro with 'datawarrior mymacro.dwam'.

I also attach a working macro file t.dwam in the following. Please notice that the macro exits without a dialog 'Do you want to save...'. I just noticed that it is the forum software that does the funny things to the macro, if you disable SMILIES.

File Attachments
1) `t.dwam`, downloaded 479 times
2) `datawarrior`, downloaded 458 times

Subject: Re: macro buildEvolutionaryLibrary from a mac terminal
Posted by Bruno on Wed, 15 Jun 2022 10:09:36 GMT

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thanks a lot Thomas
i got this error now when running ./datawarrior t.dwam
Error: Could not find or load main class
com.actelion.research.datawarrior.DataWarriorActelionLinux

Subject: Re: macro buildEvolutionaryLibrary from a mac terminal
Posted by thomas on Sat, 25 Jun 2022 10:55:49 GMT
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sorry, in the datawarrior batch file you should replace DataWarriorActelionLinux by DataWarriorLinux or DataWarriorOSX.