
Subject: macro buildEvolutionaryLibrary from a mac terminal

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@HRYWmYUyWYgHh\JvNijZji`@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/Evolutionary_Library-coagulation.txt
</task>
<task name="closeWindow">
</task>
</macro>
```
