
Subject: Creat macro file and run, but cant open the created dwar file

Posted by [dongkeke](#) on Wed, 18 Sep 2019 09:16:44 GMT

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Dear Thomas,

I create a macro file that import txt-file with chmical smiles to datawarrior, and creates the imageand then closes the datawarrior application. Then I open the macro file in windows, and I get a dwar file. But when I open the created dwar file, it occured a message like the attached picture.

I checked the dwar file, and found there are some settings. When I modify the three number as 0.5, the dwar file could be opened normally. But the seeting would not be recorded in the macro file. How can I open the dwar file in a correct way.

```
"<mainViewCount="5">  
<mainViewDockInfo0="root">  
<mainViewDockInfo1="Table bottom -0.006">  
<mainViewDockInfo2="2D View center">  
<mainViewDockInfo3="Table right -0.005">  
<mainViewDockInfo4="3D View_raw right -0.005">"
```

Another question is that I can not import the file with chemical smiles in Linux. It is stucked in the process of converting smiles.

Thanks,
kelly

File Attachments

1) [message.PNG](#), downloaded 917 times

Subject: Re: Creat macro file and run, but cant open the created dwar file

Posted by [nbehrnd](#) on Wed, 18 Sep 2019 21:26:29 GMT

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Dear Kelly,

in my experience, there is more than one form of «SMILES». Just today I faced this again with SMILES exported from the CCDC database' Python API where a few of them were not compatible with DW. Most of them were curated successfully with openbabel, translating these into its default SMILES format accessible for DW. This may be done in babel's GUI, but if you have many SMILES codes to convert and already in a file, it is often more convenient to perform this on the terminal. If this does not help, it still is possible to try openbabel's translation into «canonical SMILES». While the two SMILES differ, depending on using either default or canonical SMILES, DW typically understands at least one of them smoothly. So I would suggest to check if the import

of your structures into DW with «reformatted SMILES» still stalls.

As example I attach the list of SMILES originally generated from the CCDC API and its subsequent import in DW, which did not work completely. But both openbabel's SMILES worked fine (two SMILES lists and one almost complete DW import.) The machine where the CCDC database was installed was running Windows, the one eventually passing the data to DW was Linux. While this was a smooth transition, maybe yours got malformed for the different line endings in the operational systems. In many Linuxes, there is the dos2unix utility allowing to curate this while passing from Windows to Linux / Mac to Linux and back.

Norwid

http://openbabel.org/wiki/Main_Page

<http://dos2unix.sourceforge.net/>

File Attachments

- 1) [CCDC_generated_with_header.dwar](#), downloaded 481 times
 - 2) [CCDC_generated.txt](#), downloaded 493 times
 - 3) [babel_default.txt](#), downloaded 458 times
 - 4) [babel_canonical.txt](#), downloaded 482 times
 - 5) [babel_default_with_header.dwar](#), downloaded 490 times
-

Subject: Re: Creat macro file and run, but cant open the created dwar file

Posted by [dongkeke](#) on Thu, 19 Sep 2019 14:13:33 GMT

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Thanks, Norwid. I will have a try.

Subject: Re: Creat macro file and run, but cant open the created dwar file

Posted by [dongkeke](#) on Thu, 19 Sep 2019 14:21:21 GMT

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Thanks, Norwid,

But the another key question is that How I can set the "mainViewDockInfo" information in the macro file? Or it just only support the defalut setting?

Thanks,

Kelly

Subject: Re: Creat macro file and run, but cant open the created dwar file

Posted by [nbehrnd](#) on Thu, 19 Sep 2019 17:47:22 GMT

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Dear Kelly,

so far, I used DW's option to record macros just a few times. Reading the .dwam files with a text editor did not show me an occurrence of the keyword «mainViewDockInfo» you mention. I just put a very elementary marco together which, if run after importing the file with babel-generated canonical SMILES by yesterday will a) determine the molecular mass of the molecules encoded in these strings and b) subsequently interchange the table and the array with each other.

I speculate the addition of a typical test file and the DW macro file written by you as minimal working example might help in finding a solution for your problem.

Norwid

File Attachments

1) [molar_mass.dwam](#), downloaded 589 times

Subject: Re: Creat macro file and run, but cant open the created dwar file

Posted by [thomas](#) on Wed, 09 Oct 2019 21:42:08 GMT

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Dear Kelly,

sorry for the late reply. Would it be possible to send me a small example macro, such that I can reproduce the issue. And also may an example of the SMILES file that is causing the trouble? DataWarrior should never crash, when reading SMILES, even if the SMILES are invalid. Invalid SMILES should simply be ignored.

Thanks in advance, Thomas
