
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

[View Forum Message](#) <> [Reply to Message](#)

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
-