Subject: missing entry tautobase
Posted by nbehrnd on Wed, 12 May 2021 11:39:49 GMT
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Dear Thomas,

versions prior to 5.5.0 (Linux) of DataWarrior included the database about tautomers, tautobase.[1] At present, this entry is missing; neither the standard installation, nor the «fine print» / development version (by 2021-05-11) contain / retain it.

If the authors of this database agree, I would like to suggest that this either is a) re-added, or b) mentioned again on the site about the data files.[2]

Norwid

[1] https://github.com/WahlOya/Tautobase/blob/master/Tautobase.d war
[2] https://openmolecules.org/datawarrior/datafiles.html

Subject: Re: missing entry tautobase
Posted by thomas on Tue, 18 May 2021 18:22:23 GMT
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Dear Norwid,

which platform do you refer to. I checked the Linux installer, which contains it. The scripts for Windows and MacOS also seem to contain the file. I didn't actually make a fresh installation on Windows and MacOS to verify, though. The file was never on the https://openmolecules.org/datawarrior/datafiles.html page and in not part of the development update anymore, because it is supposed to be part of the 5.5.0 standard installation.

Best wishes,

Thomas

Subject: Re: missing entry tautobase
Posted by nbehrnd on Thu, 20 May 2021 21:10:07 GMT
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Dear Thomas,

indeed tautobase is present in the program (version 5.5.0 for Linux). My error was check along the GUI entry of Database only. However, the compilation is accessible via File -> Open Reference File -> tautobase_jan2020.dwar.

Thank you,