Subject: Re: Linux version bugs
Posted by nbehrnd on Fri, 14 Jan 2022 09:37:14 GMT
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Dear zhentg,

attempting the export of a .dwar file as a .sdf with DataWarrior, I received an error as shown in the attachment below for the Linux version of DW. It may be replicated by
+ running the native Linux installer in Debian 12 (datawarrior550.tar_gz, md5sum 1feb7bff2ad7129ac677973186436ee8), followed by
+ running the nightly update, apparently packaged on December 8th, 2021 (md5sum d4b262e803117dbbb3bc4dfb5c4d8bf1), followed by
+ running the nightly update, apparently packaged on January 6th, 2022 (md5sum 780819003b519e34586c0d32678b2f27).

This pattern is an update on top of an other/others already existing.

The export I aimed for was however possible again by starting from scratch. Let me suggest the following:
+ remove DW. The bash script unistall.sh is is provided in /opt/datawarrior as well in the .tar_gz of the installation archive. This is followed by
+ pristine installation of DW 5.5.0/April 2021, followed by
+ direct installation of the nightly update packaged by January 6th, 20222.

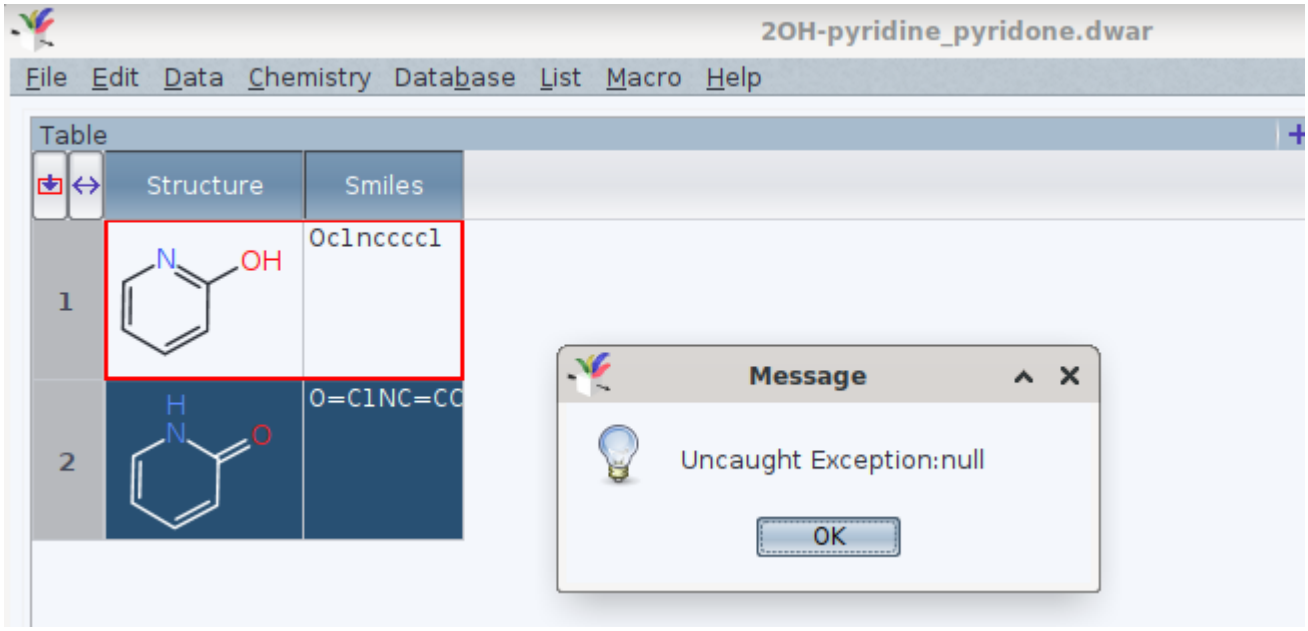
Without analysis of the updates provided by December 2021 and January 2022, it would be speculation where/why the two differ. As long as there is no major release update of DW (as pointed out in the right hand side column «recent changes»[1]), it appears safest to i) download once the installer archive, and ii) archives of the nightly updates separately in a local backup prior to an update of the local installation. To retain the archives doesn't cost much space either (as archives, the updates are about a seventh of the volume of the installer).

Norwid

[1] https://openmolecules.org/

File Attachments

1) 2022-01-14_export_error.png, downloaded 609 times


2OH-pyridine_pyridone.dwar
File Edit Data Chemistry Database List Macro Help
Table
Structure
Smiles
1
Oc1nccccl
2
O=C1NC=CC
Message
Uncaught Exception:null
OK