Subject: Linux version bugs
Posted by zhentg on Fri, 07 Jan 2022 06:42:36 GMT
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Hi Thomas,

I used to run Datawarrior on my Linux box smoothly.
I updated the files by unzip the downloaded dw550x.zip(2022/1/6 nightly build).
Then I got the following error and DataWarrior exit. Could you help to check?

Exception in thread "AWT-EventQueue-0" java.lang.NoSuchMethodError:
com.actelion.research.datawarrior.DEMainPane.addDividerChang
eLister(Lcom/actelion/research/gui/dock/DividerChangeListene r;)V
 at com.actelion.research.datawarrior.DEParentPane.<init>(DEParentPane.java:60)
 at com.actelion.research.datawarrior.DEFrame.<init>(DEFrame.java:65)
 at com.actelion.research.datawarrior.DataWarrior.createNewFrame (DataWarrior.java:692)
 at com.actelion.research.datawarrior.DataWarrior.<init>(DataWarrior.java:208)
 at com.actelion.research.datawarrior.DataWarriorLinux.<init>(DataWarriorLinux.java:29)
 at com.actelion.research.datawarrior.DataWarriorLinux.lambda$ma
in$3(DataWarriorLinux.java:161)
 at java.awt.event.InvocationEvent.dispatch(InvocationEvent.java :311)
 at java.awt.EventQueue.dispatchEventImpl(EventQueue.java:758)
 at java.awt.EventQueue.access$500(EventQueue.java:97)
 at java.awt.EventQueue$3.run(EventQueue.java:709)
 at java.awt.EventQueue$3.run(EventQueue.java:703)
 at java.security.AccessController.doPrivileged(Native Method)
 at java.security.ProtectionDomain$JavaSecurityAccessImpl.doInte
rsectionPrivilege(ProtectionDomain.java:74)
 at java.awt.EventQueue.dispatchEvent(EventQueue.java:728)
 at java.awt.EventDispatchThread.pumpOneEventForFilters(EventDis patchThread.java:205)
 at java.awt.EventDispatchThread.pumpEventsForFilter(EventDispat chThread.java:116)
 at java.awt.EventDispatchThread.pumpEventsForHierarchy(EventDis patchThread.java:105)
 at java.awt.EventDispatchThread.pumpEvents(EventDispatchThread. java:101)
 at java.awt.EventDispatchThread.pumpEvents(EventDispatchThread. java:93)
 at java.awt.EventDispatchThread.run(EventDispatchThread.java:82)

Subject: Re: Linux version bugs
Posted by nbehrnd on Tue, 11 Jan 2022 05:44:14 GMT
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Dear zhentg,

departing from default native Linux installation running in Linux Debian 12/bookworm (branch
testing), which I previously was updated (December 8th, 2021), I unzipped the currently available
dw550x.zip (md5sum 780819003b519e34586c0d32678b2f27) you mention. After copy-paste of
the three files extracted (cp -arvx * /opt/datawarrior/), I was able to start DataWarrior as usual. A

few functions tested (e.g., compute smiles for a structure, search in Google Patents) work as anticipated.

Norwid

Subject: Re: Linux version bugs
Posted by thomas on Tue, 11 Jan 2022 15:54:50 GMT
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Hi zhentg,

I just tested and can also confirm that the dw550x.zip with md5sum 780819003b519e34586c0d32678b2f27 unpacks and starts well with JRE 8 on Ubuntu. Can you check the md5sum? The error sounds like a damaged jar file.

Thomas

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
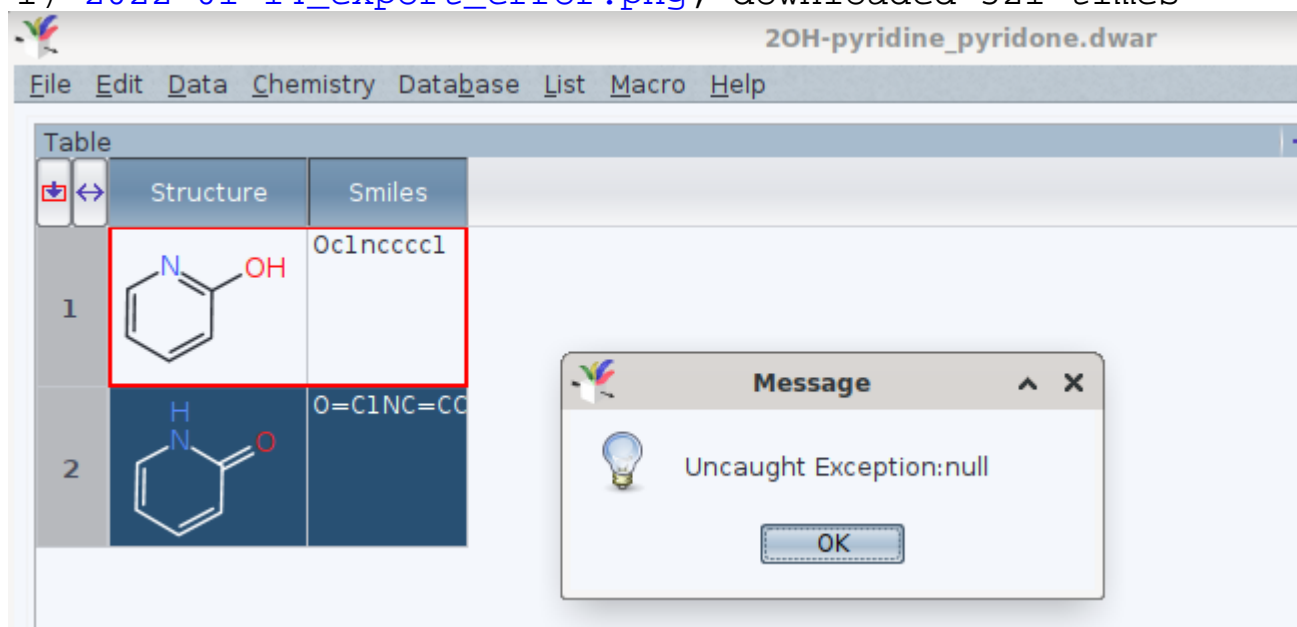
once the installer archive, and ii) archives of the nightly updates separately in a local backup prior to an update of the local installation. To retain the archives doesn't cost much space either (as archives, the updates are about a seventh of the volume of the installer).

Norwid

[1] https://openmolecules.org/

File Attachments
1) 2022-01-14_export_error.png, downloaded 521 times

Subject: Re: Linux version bugs
Posted by thomas on Thu, 20 Jan 2022 10:03:50 GMT
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Dear Norwid,

Unluckily, I have introduced a bug into the dev-version when updating the SD-file export early January to allow choosing one of multiple 3D-coordinate columns and to include structures defines as column properties (e.g. a superposed conformer or cavity or natural ligand being shown on any row's 3D-strucure). That bug caused exceptions in case of normal 2D-SD-file exports. The bug is fixed in yesterdays dev-version update.

The bug does not explain zhentg's issue.

Thomas

Subject: Re: Linux version bugs
Posted by nbehrnd on Mon, 24 Jan 2022 08:48:54 GMT

Dear Thomas,

the problem exporting the .sdf was noticed (yet not reported) because it still was possible to assign SMILES to the structures then exported in a text file. After accessing the column in question (via awk), OpenBabel provided external regeneration of the .sdf.

Norwid