Subject: Error when calculating largest fragment from macro
Posted by wsmts on Tue, 16 Apr 2024 09:59:30 GMT

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Hi,

When I try to extract the largest fragment of a structure via a macro I get the following error message:
java.lang.NullPointerException: Cannot invoke "javax.swing.JComboBox.getSelectedIndexO" because "this.mComboBoxExtractFragment" is null

Calculating the largest fragment via the menu works fine. It's only when I run the calculation from a macro.
(example file w/ macro attached)

I'm using v6.1.3 on windows 10.
Is this just my installation or can you replicate the error? [or am i missing something?]

Best,

--
Wim

File Attachments
1) largest_fragment_macro_error.dwar, downloaded 482 times
2) error message 2024-04-16 114715.jpg, downloaded 823 times

Unexpected Macro Error

! java.lang.NullPointerException: Cannot invoke "javax.swing.JComboBox.getSelectedIndex()" because "this.mComboBoxExtractFr...

OK

Subject: Re: Error when calculating largest fragment from macro
Posted by nbehrnd on Tue, 16 Apr 2024 19:53:24 GMT

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Hello Wim,

affirmative, I'm able to replicate your observation with DW 6.1.3 in Linux Debian. Initially, I presumed the cause would be to carry both the data, as well as the macro in one file and hence wrote a separate macro file (largest_fragment.dwam, attached in the .zip archive below) to process a small library of random molecules (Macro -> Import Macro, then Macro -> Run Macro ->

largest_fragment [note the underscore]). However no, I encounter the same observation as reported by you with either approach. It still is possible to launch the extraction manually (Chemistry -> From Chemical Structure -> Extract Fragment).

The issue possibly does not affect everything; processing the same library to assign Hill formula and molecular mass (Hill_formula_and_mass.dwam) worked just fine.

Perhaps helpful for Thomas, the first attempt to update DW to version 06.01.03 briefly yielded the note of a mismatch of the update package by the md5sum check though «now» DW reports a splash screen which isn't out of the anticipated pattern.

Norwid

File Attachments
1) 2024-04-16_dw_test.zip, downloaded 487 times

Subject: Re: Error when calculating largest fragment from macro
Posted by thomas on Mon, 22 Apr 2024 08:52:08 GMT
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Hi Wim and Norvid,

many thanks for reporting and confirming. I have fixed the issue. The fix will be part of the next automatic update.

Thomas