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 439 times