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Subject: Re: Filter out nasty functions

Posted by [nbehrnd](#) on Tue, 06 Jun 2023 21:10:42 GMT

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Dear Julio,

at present I understand the task ahead as you want to retain both sets of molecules as eventual separate files. With DataWarrior 5.5.0 including the updates packaged by 2023-05-18 (just downloaded again), I'm unable to write a .dwam macro which would save them directly as .sdf. Apparently, the filter -- here, to display either set «retain entry», or «skip» only acts to display. File -> Save Special -> SD-File, which would open the menu to .sdf file still exports molecules which fits either criterion. Coherent with this observation, the entry in Macro Editor annihilates the effort to filter the molecules, too.

This is the reason why the current bypass is to simulate a File -> Save Visible As with the .dwam macro to save the sets separately, however in DataWarrior's native .dwar format. Altogether with a test library, the edited .dwam macro, the two resulting sub sets; and a brief silent are attached. Obviously, this leaves the separate (not macro driven) action to open the .dwam files for a Save -> Save Special -> SD-File still on the table.

Norwid

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#### File Attachments

- 1) [10Random\\_Molecules.dwar](#), downloaded 101 times
  - 2) [sucoco\\_edit.dwam](#), downloaded 97 times
  - 3) [10Random\\_Molecules\\_good.dwar](#), downloaded 99 times
  - 4) [10Random\\_Molecules\\_bad.dwar](#), downloaded 104 times
  - 5) [record.mp4](#), downloaded 103 times
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