Subject: Re: Comparing Structure Files Posted by thomas on Tue, 05 Apr 2022 14:47:59 GMT

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Dear Olivier and Norvid,

I am sorry that it took such a long time for me to realize the issue here. When comparing an open window against an SD-file and if columns shall be copied from the SD-file into the open window, then DataWarrior used to parse the SD-file to the end in order to create a list of existing columns. When then starting comparing molecules, it didn't find any molecules, because it was already at the end of the SD-file and, therefore, it never found matching molecules in this case. This should now be fixed in the current dev version.

Thomas