
Subject: Re: Asses Prediction Quality bug
Posted by [nbehrnd](#) on Tue, 23 Apr 2024 20:40:39 GMT
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Hello Christophe,

affirmative, I can replicate the observation: though the file is saved (as .dwar file), the plots are gone if the file is then closed and opened again.

Because a .dwar file is plain text (though DW's structure IDs are not not necessarily human readable, in comparison to a SMILES strings), I started all over: a pristine copy of test.dwar was monitored by git version control. After the analysis, but prior to closing, the saved file is different: a good amount of lines are «reorganized» (old swapped for new ones, and a few truly new ones). Then, once opened again (and for the sake of git saved again), there are again differences in this .dwar file (in comparison to the state just after the analysis). Now git's notes about lines deleted are much larger in number, than about lines updated/swapped.

I think these observations indeed would support your line of thought the results of the Machine Learning analysis are not fully saved. A pattern different from panels (reversibly) hidden by click on the chevrons and possibly a bug.

Norwid
