Subject: Re: Comparing Structure Files

Posted by biolive31!! on Tue, 08 Mar 2022 14:37:26 GMT

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Dear Norwid,

Thank you to keep inform about this problem. Where the development version is downable? In addition in the version I used there is an other bugg in the fine similarity function when you slect Structure[FragFp] tools.

When you are using this tool to find similar compound in an other SDF file it work well only when you are not selecting colomuns to be copied into the file. When you select a column to copy into the file the similarity tool doesn't work.

Thank you for your help

Olivier