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Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)

Posted by [thomas](#) on Fri, 26 Aug 2022 13:40:32 GMT

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Hi JonW,

One more remark: when after sorting a generated e-lib by fitness and before feeding those compounds into a new start generation, it would probably be useful to use just the best n compounds for the new start set. I didn't see a task to achieve that in you macro. One way of doing that would be to add row numbers after sorting and then applying a filter on the row number column e.g. from 1-32, then save visible rows as the file to be used for the next start set. Alternatively, you could select the table view, select all (visible) rows, copy view content (which in this case would be the entire TAB-delimited table) and use the selection as new 1st generation.

I noticed that a task to copy the n best molecule, providing n and the column to decide what is best, would be very handy here...

Hope this was more or less clear...

Thomas

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