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

Posted by [Jo W](#) on Tue, 23 Aug 2022 21:28:43 GMT

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Hi Norwid (and Thomas)

I have been using Notepad to edit the macro and found that DataWarrior saves the structure in the Macro as an Idcode.

The reason the Evolutionary Library appears three times as I am attempting to make it recursive and a minimum of two evolutionary libraries would be necessary, the third was just a demonstration of it not working. The SkelSpheres may be too high but in this example, the focus is on having the Macro "Copy and Paste" into the "startSet=...". The specifics of Weighting can be focused on at a later date.

Thanks for bringing to light the restriction of molecules I am generating and the fact that the target fitness is the same as the original. However, in the future, the objective is still to get "Copy and pasting" working inside the Macro's view of the evolutionary window.

Even if SkelSpheres structure similarity was at '60' and the parameters for the desired structure were different I would still have the same issue as I have tried configuring these in multiple ways before.

So any further help from you and Thomas on enabling copying and pasting in EL using a macro would be appreciated.

Thanks, Jon

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