Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)
Posted by thomas on Fri, 26 Aug 2022 13:25:18 GMT

I just released an update that allows deferred 1st generation building: In the e-lib dialog you can select to build the 1st generation at macro execution time using various option, e.g. molecules from clipboard, a file, a structure column from the current window optionally defining a subset by the selection or a row list. I have tested a lot of things, but the implementation involved a lot of code and changes. Thus, please test and let me know, if you experience unexpected behaviour. Have fun, Thomas