Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)
Posted by nbehrnd on Sat, 27 Aug 2022 12:12:51 GMT
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Dear Thomas,

with the current update of DW (packaged 2022-08-27 12:08 for Linux/MacOS) the «self-reference» is unable to start. As a test, I let DW generate 5 random molecules in first place and saved the result as .dwar. Subsequently, and still with the same file, the aim to pick these structures as start for an EL fails:

However one may argue to populate the window «1st generation molecules» right away would be at least as valuable than the pick from an external/other .sdf or .dwar file (which are accepted input).

To mark every in the structure column by individual click (in my installation, the cell's background then darkens) and attempt again to use these entries of the same file just open and running via «structure column» equally fails.

Norwid

File Attachments
1) Random_Molecules.dwar, downloaded 383 times
2) 2022-08-27_EL_attempt -- dw.png, downloaded 908 times