
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 608 times
- 2) [2022-08-27_EL_attempt -- dw.png](#), downloaded 1404 times

Random_Molecules.dwar

File Edit Data Chemistry Database List Macro Help

Table

	Structure
1	
2	
3	
4	
5	

Build Evolutionary Library

1st generation compounds: From a structure column... Build at task execution

- Default
- Custom
- Random
- From the clipboard
- From a file...
- From a structure column...**
- From all selected rows...
- From a row list...

automatic Generations Create compounds like

128 Compounds per generation

8

Fitness Criteria

Help

OK

<To add fitness criteria select type and click 'Add Criterion'

273 of 840 MB Selected: Visible:5 Total:5