Subject: Macro for evolutionary library (EL) in Datwarrior (DW)
Posted by Jo W on Tue, 09 Aug 2022 12:42:22 GMT
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I want to be able to copy a (any) structure from an existing table in DW into EL using a macro.

when I create a macro to do this it works fine.

However when I try to use this same macro on a new structure, it doesn't work. The macro just uses the previous structure and ignores the new one.
How do you get around this?

Ultimately I want to be able to run several EL's in a "chain" using a macro starting ideally from any structure to help towards creating a virtual library of new compounds.
Many thanks in advance
Jon