Subject: Re: Macro for evolutionary library (EL) in Datwarrior (DW)
Posted by nbehrnd on Tue, 06 Sep 2022 06:05:51 GMT
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Dear Jon,

the links following the penguin, the apple, the Windows symbol and before the «I have read and understood the disclaimer» which turn into green rectangles after your click: these are the links for the installers of DW for Linux, MacOS, and Windows respectively to provide the basic version of the program (at present, version 5.5.0) for major releases.

The address https://openmolecules.org/datawarrior/dw550win.zip only provides access to an archive to substitute the bits and bolts which changed since the release of the installer, version Windows. This sub set of data alone will not suffice to use DW. Without change of the address, the very same address is used for every update of the Windows version of DW. Speaking for the updates for MacOS/Linux I use, this either happens about once in 14 days (regular interval), or once a bug was identified and corrected. In the later case, uploads are updated as soon as possible (on occasion, multiple per day). This is why a keep a local copy of the installer, and of a few updater archives.

This allows to revert to an earlier minor version of DW should there be a need.[1] Then, deinstall DW completely, use the installer to install the major version 5.5.0 again, and eventually run the latest updater known to work well enough. Because the updater packages replace parts of DW's inner gear and I use only one installation directory for DW, there only is one version of DW installed (and most often working well). So far, there was no need for me to have multiple installations of DW (a minor release of June, and an other of August, etc.) to be present simultaneously. For one, the concurrent, simultaneous use of them would require additional guards to keep them separate in the computer's working memory (like in individual sandboxes,[2] or virtual machines[3]). For two, a user written macro should work regardless of the minor upgrade of DW used to write/record it, and irrespective if the underlying operating system was/is Windows, MacOS, Linux. Though only aware about two video recordings[4,5] I think Isabelle Giraud's workshop at RSC Open Chemical Sciences in 2020 set an other example of exchanging DW macros freely; they are meant to ease exchange among the interested. In case they do not work on more recent versions of DW, file a bug report; in case they don't work on an elder version of DW, perhaps the addressed functionality in DW wasn't yet implemented and you may get help here. Directory addresses -- if the macro uses them (many don't) -- may require an adjustment; yet because the macros are plain text, this requires a one-time edit already possible with a text editor.

Norwid

[1] example https://openmolecules.org/forum/index.php?t=msg&th=609&a mp;start=0&
[2] https://en.wikipedia.org/wiki/Sandbox_(software_development)
[3] https://en.wikipedia.org/wiki/Virtual_machine
[4] https://www.youtube.com/watch?v=mQCf9GakQW0
[5] https://www.youtube.com/watch?v=Is2hLqqSFvM