Subject: feature suggest: array cleaning by delete button Posted by nbehrnd on Fri, 27 Oct 2023 10:33:54 GMT

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Dear Thomas,

I would like to suggest an extension to edit the structure array (presented after the generation of an evolutionary library); to delete selected entries by single press of the delete key.

While browsing an EL (attached), I noticed a few entries either with a &1 as place holder for (R)/(S) on stereochemical centres, or «crossed double bonds» to indicate an unassigned/flexible (E)/(Z) configuration. For small test down the road, my intent was to select these records (left mouse click) -- eventually multiple (left mouse click while holding the Ctrl key) -- and to remove them.

At present, this is possible by the subsequent Data -> Delete Rows [sic!] -> Selected Rows. This approach works to remove only the selected entries (thankfully: only the ones identified, and not the whole row of the entries). My suggestion is to offer a remove of the entries already marked by single press of the delete button as a shorter one.

The pulldown menu available for the array (right mouse button click on a cell) includes an entry «edit», but no delete. If the suggested functionality were provided here, it would again request a journey of three mouse clicks instead of a single key action. To change to the tab «table», to select whole rows then deleted is possible though this display does not offer as much a synopsis of the structures in question as does the tab «structures».

The observation refers to DW for Linux in version 05.06.00 by September 22nd.

Regards,

Norwid

File Attachments

- 1) structure_array.png, downloaded 172 times
- 2) Evolutionary_Library.dwar, downloaded 72 times
- 3) Evolutionary_Library_edited.dwar, downloaded 71 times