Subject: Re: feature suggest: array cleaning by delete button

Posted by nbehrnd on Sat, 04 Nov 2023 19:19:59 GMT

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Dear Thomas,

thank you for depicting a different logic to address the task. Beside the possibility to go back and forth between the original set of data and the entries to be removed, it offers to export the unwanted entries (and their data associated) for a later review -- and hence, an additional advantage to the «single click» approach suggested.

There then however is a (cosmetic?) issue. After the removal of the unwanted structures, the counter of selected entries reverts to zero, the counter of the total of structures decreased. So far, I assumed this integer equally should be the one shown as "structures visible", quite like the state prior to edit/removal of individual structures (even before their identification and selection).

The EL in question was generated with the default set of 8 motifs (two of them about (R)/(S) racemates, i.e. a total of 10 molecules), the creation of compounds like approved drugs with a sole fitness criterion (molecular weight equal or less equal than 400). This lead to 278 records, where 2 records contain one single stereogenic centre each which might be either (R), or (S). Plus 5 other records with a C=C double bond in either (E), or (Z) configuration.* This would lower the total count either by 7 (for a then total equal to 271), or by 14 (to then retain 264 structures) if one aims for a representation without either (E)/(Z), nor (R)/(S) flexibility. Application of the Data -> Delete Rows -> Invisible Rows however yields a "Selected: 0, Visible: 237, Total: 271". (Simultaneously to the edit applied, the slider "generation" turns red, too.).

The export of the results as .txt file contains 271 records. Saving the (edited) .dwar file as a new .dwar file, and subsequent reading of this new .dwar file still displays the reading "selected: 0, visible: 237, total 271" on the lower rim of the frame, too. Is there a discrepancy between the selection of individual entries of a row displayed vs eventual edit (i.e. the remove) of of every entry of their corresponding rows displayed? My intent was the remove of only the 7 potentially ambiguous entries.

Best regards,

Norwid

* Somehow the submission of this original EL .dwar file to DW's Generate Conformers with a constrain of maximal 1 conformer per stereo isomer is able to split/disentangle them, i.e. to provide one (R) and one (S) conformer; or one (E) and one (Z) conformer (DW for Linux, v05.06.00, 22-Sep-2023).

The centre's assignment by `&` and `or` in the array display, where applicable, is the same throughout the program, hence known.