Subject: Re: Change default structure copy option
Posted by nbehrnd on Tue, 19 Dec 2023 22:20:39 GMT
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Hello,

if a SMILES string is sufficient to serve as an «anchor» for your work after DW, Chemistry -> From Chemical Structure -> Add SMILE Code allows you to assign all entries in the array this descriptor. (It is an action you equally can store in a DW marco file, file extension .dwam). Export then the array via File -> Save Special -> Text File as a plain ASCII text file with one header line and columns separated by tabulators. This will transfer the whole array into the new format.

Though one can alter the sequence of columns in a dwar array by drag-and-drop, the export as text file always starts by the column about the structure / ID as the first one. At level of the text file, this can be changed by a script (e.g., AWK), or a spread sheet (gnumeric, LibreOffice Calc, etc.). The later however can impose some limitations (e.g., 65000 rows maximum in MS Excel) not every time visible.

Regards,

Norwid