Subject: Re: Change default structure copy option
Posted by thomas on Sun, 31 Dec 2023 13:47:53 GMT
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Hello

if your plugin creates two columns, which both receive the same SMILES, but are defined with different types (COLUMN_TYPE_STRUCTURE_FROM_SMILES and COLUMN_TYPE_ALPHANUMERICAL), then your DataWarrior table will contain one column with visible chemical structures and another with your original SMILES codes. When copying parts of the table you might include the SMILES column, but not the one with chemical structures, ChemAxon should happily parse...

The advantage will be that you don't convert from Smiles to IDCode and back to SMILES, which always poses the danger to change the structure, because of different aromaticity and stereo chemistry concepts...