Subject: Change default structure copy option
Posted by helloWorld22 on Tue, 19 Dec 2023 15:36:40 GMT
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Hi,
I have created a plugin that retrieves data including structures from our internal database.
The structures are rendered in DW successfully.
However, when I try to copy all the data from the datatable including structures, the structures are copied as ID, that chemaxon for excel cannot parse.

When i copy 1 structure at a time, I get option to select MolfileV2 or smile or ID.
But when coping the full table that has data as well as structure, by default ID is selected.

Is it possible to change it MolfileV2 or V3 or smiles or Give an option while coping from the datatable?

Thanks

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

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...

Subject: Re: Change default structure copy option
Posted by helloWorld22 on Thu, 11 Jan 2024 09:06:58 GMT
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Thanks all for your reply.
Smiles work fine now.
