Subject: Rendering structures from SMILES
Posted by jwfeng on Wed, 05 Apr 2017 17:28:01 GMT

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Hi,

My SD file contains SD tag with SMILES strings as values. Is there a way to render them as structures in DW? Attached is a simple example of what I want to do. The Structure column display what's in the MOL block, the r-group smiles column should render the SMILES string as a structure instead of displaying it as text.

Thanks,

JW

File Attachments
1) Screen Shot 2017-04-05 at 10.26.34 AM.png, downloaded 719 times

Subject: Re: Rendering structures from SMILES
Posted by thomas on Wed, 05 Apr 2017 19:13:27 GMT

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Hi JW, if you open a text file (TAB or comma delimited) then DataWarrior automatically analyses all columns, whether they contain SMILES and adds structure columns for every valid SMILES column. SD-Files typically contain only one structure, which is shown as structure column. It would be possible to use the SMILES recognition mechanism also for SD-files, but currently, there is no straight-forward way. What you coulr do, however, is to create a macro, that after opening the SD-file does these tasks:
- (if you don't have any unique compound-IDs, then create a new column with row-numbers
- saves the file
- removes the structure column
- save as text file (TAB delimited)
- open the text file to automatically create structure columns for your SMILES columns
- save again as dwar
- open the original file
- merge with the new dwar that contains structure column for every SMILES using the compound-IDs as merge-keys
Does that solve the issue?

Thomas

Subject: Re: Rendering structures from SMILES
Posted by jwfeng on Mon, 01 May 2017 05:25:07 GMT

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Hi Thomas,

Thanks for the different options. I will convert my SD file into a tab separated file where the first column stores SMILES string of the SD structure. The remaining columns will store SD fields.

I like to store SMILES strings in SD tag where those SMILES could be substructures, near neighbors, or molecular match pairs.

JW