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

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