Subject: Re: entering IC50s (or other data row by row)
Posted by thomas on Thu, 29 Jan 2015 20:59:53 GMT
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Hallo,

first my appologies for the late answer. For some reason I sometimes don't get notification mails.

The easiest way to get data from Excel into DW is to select and copy rows and columns of an Excel sheet and choose then
choose 'Paste' in DataWarrior. That should create a new DataWarrior window with the data as content. DataWarrior tries to
recognize, whether the first column is a title column, e.g. by checking for every column whether all except the first column can be interpreted numerically. Ideally the Excel data contains a column with structure identifiers, which are also available
in the SD-File. If the SD-File contains every structure only once, then you can directly read the structures from the SD-file
into the data from Excel. If the SD-file contains the same structure multiple times, then you need to open the SD-file
separately, remove redundant (based on the structure) rows from the Data menu and save as a dwar file. Now you should be able
to merge this file from the window with the excel data.

The opposite order should work as well, provided that the Excel data contains every structure identifier only once:
Create a dwar file from the excel data with copy/paste. Open the SD-file and merge the excel.dwar file into it by
assigning the identifier column of the excel file to the one of the open sd-file and using it as merge key.

Important: For numerical columns to be perceived numerical, none of the cells should contain starting or trailing spaces or
other content that is not numerical. Allowed are empty cells, values starting with modifiers (<, <=, >, >=), multiple values separated by '; ' (semicolon plus one space), 'NaN' and '?'

I hope I could help. Otherwise, you may send me small demo files, which don't work that I can learn what the problem is.

Kind regards,

Thomas