Subject: Tagging Data to a Particular Assay
Posted by ELFritzen on Thu, 06 Aug 2020 18:06:23 GMT
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I'm not sure this can be done in DataWarrior or not, but I thought I'd ask. In adding ADME data to a Datawarrior file, I need to add data for the same assay run at different test sites. For example I might have solubility data for the same compound run at two or three different CRO's. I'd like to keep that data in a column labeled solubility, for example, but have some way of tagging which value was done at which CRO. Currently the only way I know of doing this is to create separate columns labeled Solubility CRO1, Solubility CRO2 etc. This works, but will be very cumbersome when done for some of the other assays we're doing. It would be nice to keep all the data for the same assay in just one column. Notating the data with an asterisk and placing a comment in a the comment column would also work, but that brings up some other problems when it comes to sorting or exporting data. Does anyone else face a similar challenge?
Thanks.
Ed Fritzen
VincereBio

Subject: Re: Tagging Data to a Particular Assay
Posted by thomas on Fri, 07 Aug 2020 07:49:44 GMT
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The proper alternative would be having the solubility data all in one column and a second column containing the source. If a row contains multiple measurements from different (or same) sources, then both columns should contains the same number of entries separated by '; ' or in separate lines. In dwar files line breaks are encoded as '<NL>'. You may tell DataWarrior that both columns are logically connected and the order of cell entries in both columns match. For that both columns must have the same group name defined in the column properties section. If your column titles would be 'Solubility Value' and 'Solubility Source' and the group name would be 'solubility' then the column properties section should look like this:
(Note: the white space in the column properties line must be a TAB)

<column properties>
<columnName="Solubility Value">
<columnProperty="groupName solubility">
<columnName="Solubility Source">
<columnProperty="groupName solubility">
...
</column properties>

Subject: Re: Tagging Data to a Particular Assay
Posted by ELFritzen on Fri, 07 Aug 2020 11:59:48 GMT
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Hi Thomas,
Thank you for the prompt reply. That's exactly what I would like to do. I could repeat the process for each assay that has been done by multiple sources. I just am not familiar with how to actually set up the columns. How do you set columns like you've shown? If I add a new column, I only get options to set "column type" and "column name". Is there another way to add columns?
Thanks,
Ed

Subject: Re: Tagging Data to a Particular Assay
Posted by thomas on Fri, 07 Aug 2020 15:46:25 GMT
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sorry I wasn't clear. The problem is that DataWarrior has no GUI elements to define that. These settings are done automatically, when retrieving data from e.g. the Idorsia drug discovery database.

You basically have two options of how to set the column properties:
- open a dwar files with a text editor and type or paste the four lines just after the <column properties> line.
  If there is no <column properties> line, you have to add that as well followed by a </column properties> line
  after the four pasted lines.
- alternatively you can run a macro that adds the column properties. I have attached an example macro file.
  You can also edit the macro file in a text editor to match your column names.

Thomas

File Attachments
1) t.dwam, downloaded 615 times