Subject: UI suggestions for Table and Form views Posted by Andrew0 on Mon, 10 Aug 2015 16:11:05 GMT

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Thomas,

First off, thank you for working so hard on this tool and releasing it to the public. I am very excited to have a free tool to use for chemistry-aware data analysis.

As I have been working on adapting DataWarrior for my needs, I have come across a few UI suggestions to improve the Table and Form views. I would be interested in hearing your thoughts about incorporating some of these into future versions of DataWarrior.

Option to freeze column(s) in Table view

When looking through the Table view, the option to freeze the first n columns of the table would be helpful. For example, freezing a structure and ID column would allow users to compare properties in large tables with less scrolling back and forth. Improved naming mechanism for "multiple values" columns in Table view

The mechanism to display multiple values is versatile and intuitive. When aggregating these values, however, column names become difficult to read. Prepending the aggregation type (average, median, etc.) becomes lengthy and confusing, especially when side-by-side columns use similar aggregation types. I see a few potential options to address this:

Allow word wrap and multiple lines in column names Append, rather than prepend, the aggregation type (e.g., "IC50 (median)") Remove the aggregation type from the column name altogether. Whenever values are combined, it is indicated in the table anyway, so the information may not be needed in the column header. Options to "Show" columns in Table view are limited by screen size

The table I am working with has a large number of columns, many of which are hidden. The menu to "Show" columns that pops up when right-clicking on a column header displays as many names as it can in the screen space available, but some column names can't be accessed. One way to address this would be by adding a scroll arrow at the bottom to access more column names. Option to ignore newline characters in Form views

I set up my dataset in a similar way to the "Table View" vendor example in the user guide, where a single structure has multiple values on multiple lines in each column. This is great for the Table View, but the newline characters don't interact well with the Form view - only the first line of each entry is shown. Is there a workaround for this, or could an option to ignore newlines in Form view be implemented? Enhanced formatting options for Form views

This one is a major undertaking, but I'll throw it out there as an idea. The Form views are nice, but as-is it can be difficult to distinguish one parameter from another. Enabling user formatting in forms would allow grouping of relevant parameters together so that users can quickly glance at the Form and find the information they are looking for. Some ideas for formatting options:

Adding separators or borders to group parameters together Adding plain, static text for headings or group labels Enabling user control of text size

These are just a few ideas, and I recognize that they aren't all easy (especially the last one). Thanks again for your work on this tool, and I look forward to all future updates.

Best regards, Andrew