
Subject: Updating Merged Columns

Posted by [ELFritzen](#) on Thu, 19 Nov 2020 15:09:47 GMT

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I've created a number of merged columns in a DataWarrior file. As an example, the merged column might have data for the same assay from two different vendors. When I add new data to the source columns, I noticed the merged columns are not updated. Is there a way to update merged columns when data is added to the source columns? I know you can re-calculate columns that are calculated values, so this would be similar for updated merged columns.

Thanks,
Ed

Subject: Re: Updating Merged Columns

Posted by [nbehrnd](#) on Thu, 19 Nov 2020 16:48:19 GMT

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I would suggest to continue on the path mentioned by you, i.e. starting with two columns of raw data and a third column based on calculated data offering the quick re-calculate option (yielding the update).

To illustrate, I set up a small set of molecules and randomly attributed data. To simulate data missing, I kept some of the cells empty, or used as entries the strings "0" .or. "NaN". The column to pick data from either one of the two previous columns then used the if-clause

```
if((vendor_1!=0), vendor_1,vendor_2)
```

which works reasonably well in terms of an update in the new column.







This however assumes the absence of a row, where both columns contain disagreeing entries ...

File Attachments

1) [example_update.png](#), downloaded 1207 times

update_from_two_columns.dwar

File Edit Data Chemistry Database List Macro Help

Table	Structure	vendor_1	vendor_2	vendor_1_2
1		NaN	NaN	NaN
2		2	0	2
3		3.5	0	3.5
4		12		12
5		0	13	13
6		0	12	12

Add Calculated Values

Please enter a formula:
`if((vendor_1!=0), vendor_1,vendor_2)`

Add Variable Structure

Overwrite existing column
 Column to overwrite: vendor_1_2

Help Cancel OK

2) [update_from_two_columns.dwar](#), downloaded 620 times

Subject: Re: Updating Merged Columns

Posted by [ELFritzen](#) on Thu, 19 Nov 2020 19:53:55 GMT

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Thank you for the prompt reply, nbehrnd,

I understand what you're saying, however, how would the formula change if there were values for both vendor_1 and vendor_2, and you wanted to show both values in the "merged" column. In the attached file, how could I get the vendor_1_2 column (the calculated column) to look like the merged column? Can that be done with a calculated expression?

Thanks for the help.

Ed

File Attachments

1) [update_from_two_columns_mergedcolumn.dwar](#), downloaded 643 times

Subject: Re: Updating Merged Columns
Posted by [nbehrnd](#) on Thu, 19 Nov 2020 20:51:32 GMT
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Dear Ed,

based on your reply, I understand that my initial reading of your question does not fit your needs. I wrongly assumed you wish to display in column C at either the result of column A, or of column B. But you want to display both values simultaneously in one column of recalculated values.

This is possible using an expression in the following pattern

```
str(if(vendor_1!=0,vendor_1,"NaN")) + str("; ") + str(if(vendor_2!=0,vendor_2,"NaN"))
```

The expression asks both columns independently for a value -- if there is no value, these if clauses will explicitly state the absence by issuing an «NaN» string. These results, regardless if a numeric result, or some text, will be converted into a string. These are separated by a third string comprising a semi-colon and an explicit space (but it could be any other separator character, too [.csv files]). Eventually, the plus signs are used to concatenate the parts into the string displayed in the table.

Et voilà, in the sixth column (an example .dwar file is attached, too):

Norwid

File Attachments

- 1) [adjust.dwar](#), downloaded 642 times
- 2) [adjust-or8.png](#), downloaded 1287 times

The screenshot shows a software window titled "adjust.dwar" with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help). Below the menu is a table with the following columns: Structure, vendor_1, vendor_2, vendor_1 2, Merged Data, and Calculated Column. The table contains five rows of data, each with a chemical structure icon. A dialog box titled "Add Calculated Values" is overlaid on the table. The dialog contains the following text and controls:

Please enter a formula:
`str(if(vendor_1!=0,vendor_1,"NaN*)) + str("; ") + str(if(vendor_2!=0,vendor_2,"NaN*))`

Buttons: Add Variable, CalculatedColumn (dropdown)

Overwrite existing column
Column to overwrite: CalculatedColumn (dropdown)

Buttons: Help, Cancel, OK

	Structure	vendor_1	vendor_2	vendor_1 2	Merged Data	Calculated Column
1		NaN	NaN	NaN	NaN; NaN	NaN; NaN
2		2	5	2	2; 5	2; 5
3		3.5	0	3.5	3.5; 0	3.5; NaN
4		12		12	12	12; NaN
5		0	13	13	0; 13	NaN; 13

Subject: Re: Updating Merged Columns

Posted by [ELFritzen](#) on Fri, 20 Nov 2020 15:00:28 GMT

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Thanks, Norwid,

That's exactly what I need. I know very little about writing such expressions. This will be a big help.

Ed
