Posted by Adk2020 on Tue, 21 Apr 2020 20:45:32 GMT

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Hello All,

I both new to data warrior and this form, so forgive the naivety of the question. When I try to merge two files (both of which are csv files) I get the following error- source column not defined - see attached file. The incoming file has two more columns than the file I want to merge with. What am I missing?

While I have your attention, these two files represent a primary screen of 262 molecules and a confirmatory screen (hits) of 111 cmpds. The data file for the primary screen will eventually ave the same number of column descriptors as hit confirmation file. What I'd like to use data warrior is to compare both files across all descriptors and determine which/why molecules didn't confirm. For example, if the only 5 out of 50 aryl halides confirmed, how do the hits differ from the non hits.

I think this software is really cool and has lots of potential for visualizing analyses of this type and more. Thank you for your time and consideration.

Frank

File Attachments
1) merge file error.jpg, downloaded 779 times

Merge File

File: ...\DW confirmatory small molecule screen 111 cmpds CDD Excel Export w_transition.csv

Incoming Columns		Existing Columns		☑ Me
Assign Molecule Name	to	Molecule Name ⌄		as
Assign Structure	to	Structure ⌄		ap
Assign Structure of SMILES	to	Structure of SMILES ⌄		re
Assign SMILES	to	SMILES ⌄		ap
Assign Delta Tm (C)	to	Delta Tm (C) ⌄		ap
Assign Melting temperature (average) (C) to		Melting temperature (average) (C) ⌄		ap
Assign Delta Tm (Std Dev) (C)	to	Delta Tm (Std Dev) (C) ⌄		ap
Assign Transition	to	transition ⌄		ap
Assign Electrophile 1	to	<new column> ⌄		
Assign Electrophile 2	to	<new column> ⌄		
Assign	to	<new column> ⌄		

☑ Append rows not existing in current data

Merge File ✕

🚫 Source column not defined.

OK

Help