Subject: Merging files error
Posted by Adk2020 on Tue, 21 Apr 2020 22:21:22 GMT

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Hello again,

Not sure why my original and first post is not showing. So i'll try it again. Being new to data warrior and this messaging board my goal is to become well versed in its power to visualize data for streamlining analysis and group presentations.

My first question involves the use of the merge file option. I am trying to merge two sets of data - one data file represents the initial primary screen, the other the confirmation (hit confirmation of the original primary screen - within these files are columns highlighting molecular name, structure , smiles, Tm values, electrophile type etc. The goal of this exercise is to find out what makes a hit verse a non hit based on the electrophile type to better understand how molecular composition affects binding and generate the corresponding file.

Unfortunately, when I try to merge the files I receive a "source column not defined" error message (see attached file). I am not sure what this means being a novice, but I see no difference in the files - both are csv. As you can see, I've set the merge key to assign the molecular name between files and the rest of the merge options to append except for the smiles

What is the source of this error with respect to the files and how do I go about correcting this error and what else should I be aware of when merging files in general?

Thank you for your time and consideration.
Sincerely,
Frank

File Attachments
1) merge file error.jpg, downloaded 683 times

Merge File

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

Incoming Columns		Existing Columns		M
Assign Molecule Name	to	Molecule Name ⌄		a
Assign Structure	to	Structure ⌄		a
Assign Structure of SMILES	to	Structure of SMILES ⌄		re
Assign SMILES	to	SMILES ⌄		a
Assign Delta Tm (C)	to	⌄		a
Assign Melting temperature (average) (C)	to	⌄		a
Assign Delta Tm (Std Dev) (C)	to	⌄		a
Assign Transition	to	transition ⌄		a
Assign Electrophile 1	to	Electrophile 1 ⌄		a
Assign Electrophile 2	to	Electrophile 2 ⌄		a
Assign	to	<don't use it> ⌄		

Merge File ✕

🚫 Source column not defined.

OK

☐ Append rows not existing in current data

Help