
Subject: Re: Merging files error

Posted by [thomas](#) on Wed, 22 Apr 2020 18:56:45 GMT

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sorry, I wasn't precise. A csv file is a text file with row entries separated by commas. If you, however, double click it on Windows, it often opens in a spreadsheet application (e.g. Excel), where you cannot see the commas anymore, because they are removed in the process of splitting up a line's content into individual cells.

To see the commas and add a column header you need to open the file in a text editor. On Windows, if you don't have anything better, you should be able to use Notepad for it.

What you could do alternatively is to just copy all relevant cells in Excel and paste it into DataWarrior (Edit->Paste). That way you get a new DataWarrior window with all the information. For every column that contains Smiles you automatically get a new structure column. If you have empty columns, you can delete them within DataWarrior. You may then save the file. Do that with the other file as well. Then you can merge both DataWarrior files. The only thing to make sure is that the first line of copied cells contains column names and that none of the copied cells in the first line is empty.

Hope this works,

Thomas

PS: for other questions you may also contact me privately on the e-mail in the openmolecules.org about.
