Subject: .csv data input including SMILES Posted by nbehrnd on Thu, 13 Jun 2019 13:40:41 GMT

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Dear Thomas.

while importing comma-separated tables including a column containing SMILES, I noticed DataWarrior (version 5.0.0; running in Linux) appears to work well starting with the second line of the table only. It is not an issue related to file endings which could be resolved by the user by unix2dos. Apparently, DataWarrior expects the first line to be a header; which currently is not described-as-such in the online manual pages "Loading Data into DataWarrior".

Example of hampered reading of a .csv file lacking an explicit header:

Example of reading a .csv file containing explicit header:

File Attachments

- 1) test data with header.csv, downloaded 684 times
- 2) test_LOC.csv, downloaded 670 times
- 3) headerless_data_cropped.png, downloaded 1179 times
- 4) data with header cropped.png, downloaded 1074 times

Subject: Re: .csv data input including SMILES Posted by thomas on Thu, 27 Jun 2019 06:12:55 GMT

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Dear Norwid, thank you for the hint. DataWarrior does a minimum data analysis trying to figure out whether there is a header line or not. I will improve this check and also update the manual to explain.