Subject: .csv data input including SMILES Posted by nbehrnd on Thu, 13 Jun 2019 13:40:41 GMT View Forum Message <> Reply to Message

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 609 times

2) test\_LOC.csv, downloaded 590 times

3) headerless\_data\_cropped.png, downloaded 1078 times

4) data\_with\_header\_cropped.png, downloaded 982 times

Subject: Re: .csv data input including SMILES Posted by thomas on Thu, 27 Jun 2019 06:12:55 GMT View Forum Message <> Reply to Message

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.

Page 1 of 1 ---- Generated from openmolecules.org Forum