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 749 times
2) test_LOC.csv, downloaded 727 times
3) headerless_data_cropped.png, downloaded 1322 times

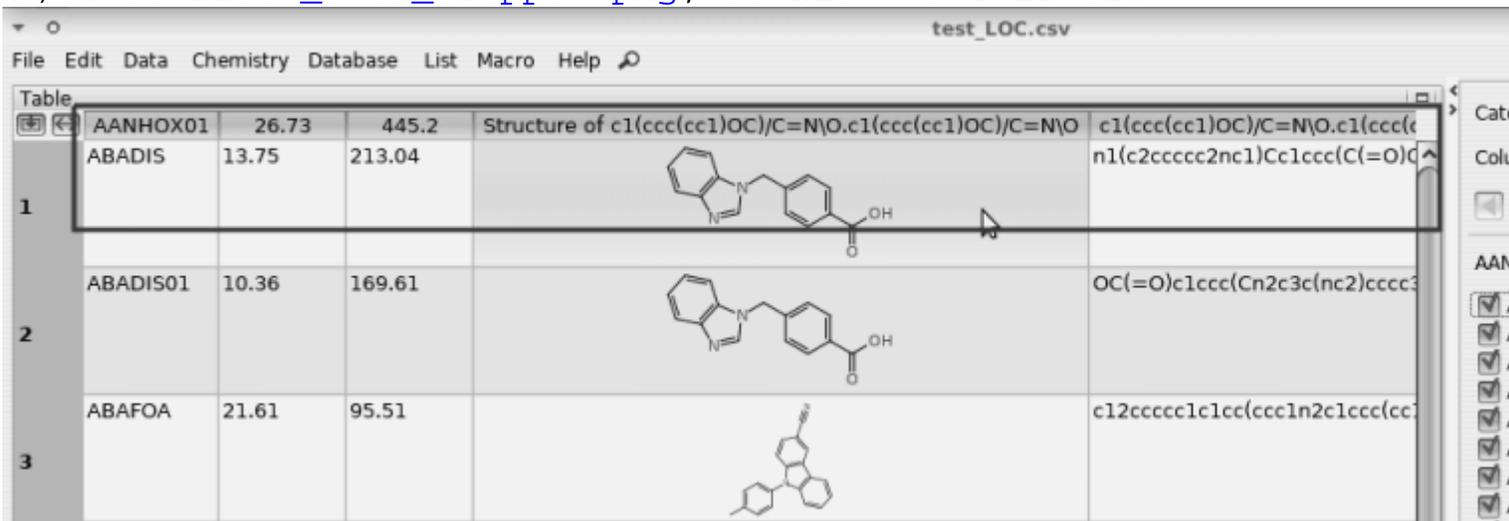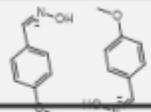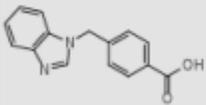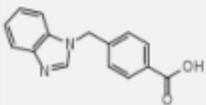4) data_with_header_cropped.png, downloaded 1216 times

Marcus_parameters_and_smiles.csv

File Edit Data Chemistry Database List Macro Help

Table

	CCDC code	|Hab|	lambda	Structure of Smiles	Smiles	CODE check
1	AANHOX01	26.73	445.20		c1(ccc(cc1)(	AANHOX01
2	ABADIS	13.75	213.04		n1(c2ccccc2	ABADIS
3	ABADIS01	10.36	169.61		OC(=O)c1cc	ABADIS01

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.