

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 800 times
- 2) [test_LOC.csv](#), downloaded 771 times
- 3) [headerless_data_cropped.png](#), downloaded 1473 times

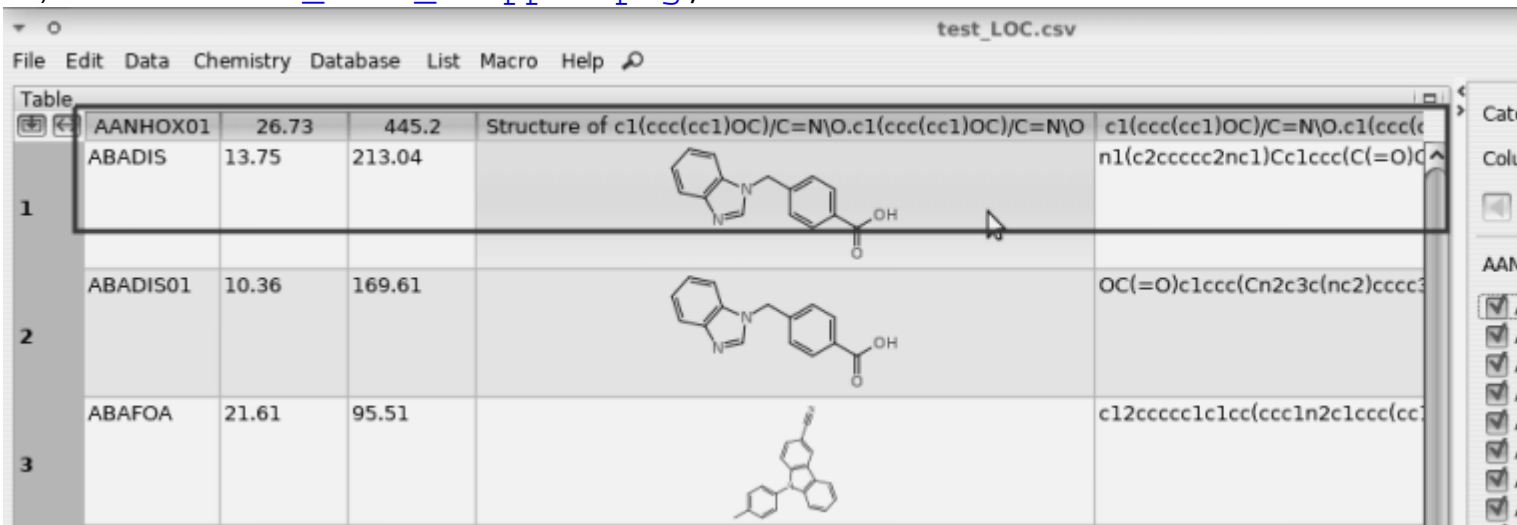
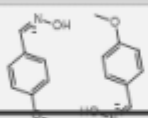
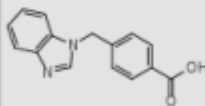
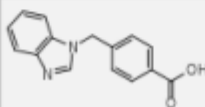


Table				
1	AANH0X01	26.73	445.2	Structure of <chem>c1(ccc(cc1)OC)/C=N\O.c1(ccc(cc1)OC)/C=N\O</chem>
2	ABADIS	13.75	213.04	<chem>c1(ccc(cc1)OC)/C=N\O.c1(ccc(cc1)OC)/C=N\O</chem>
3	ABADIS01	10.36	169.61	<chem>OC(=O)c1ccc(Cn2c3c(nc2)cccc3)</chem>
	ABAFOA	21.61	95.51	<chem>c12cccc1c1cc(ccc1n2c1ccc(cc1))</chem>

- 4) [data_with_header_cropped.png](#), downloaded 1359 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	AANH0X01	26.73	445.20		<chem>c1(ccc(cc1)C</chem>	AANH0X01
2	ABADIS	13.75	213.04		<chem>n1(c2ccccc2</chem>	ABADIS
3	ABADIS01	10.36	169.61		<chem>OC(=O)c1cc</chem>	ABADIS01