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

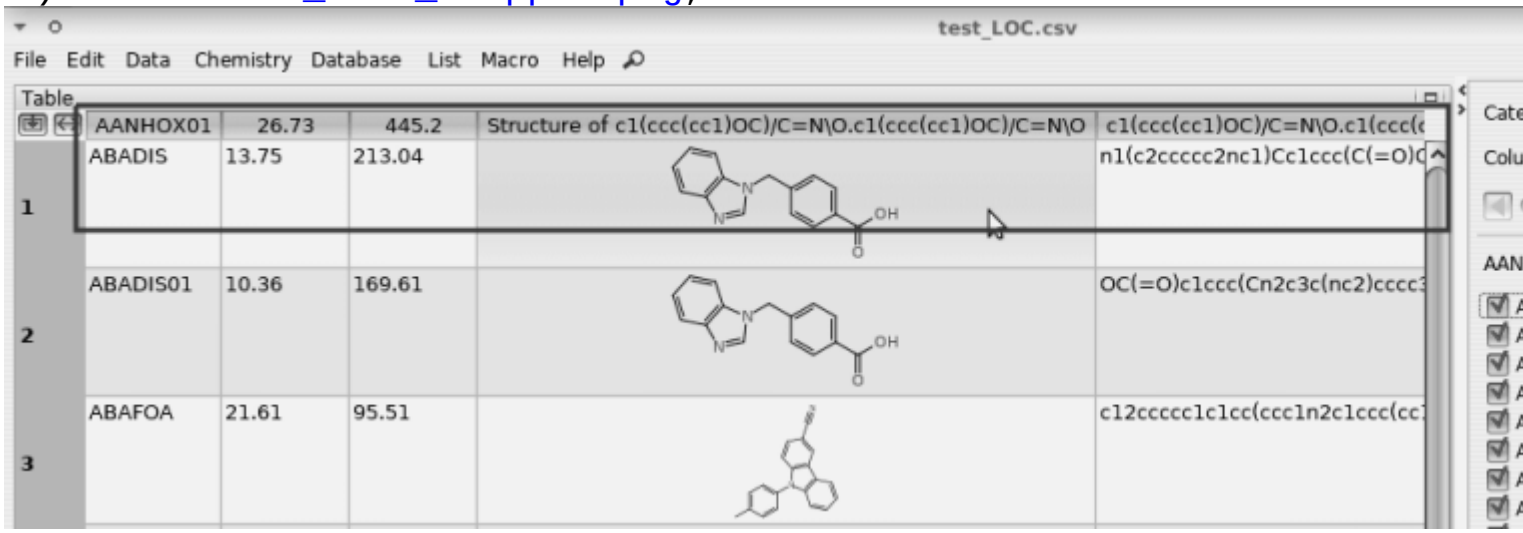
while importing comma-separated tables including a column containing SMILES,
I noticed DataWarrior (version 5.0.0; running in Linux) appears to work well
starting with the second line of the table only. It is not an issue related
to file endings which could be resolved by the user by unix2dos. Apparently,
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:

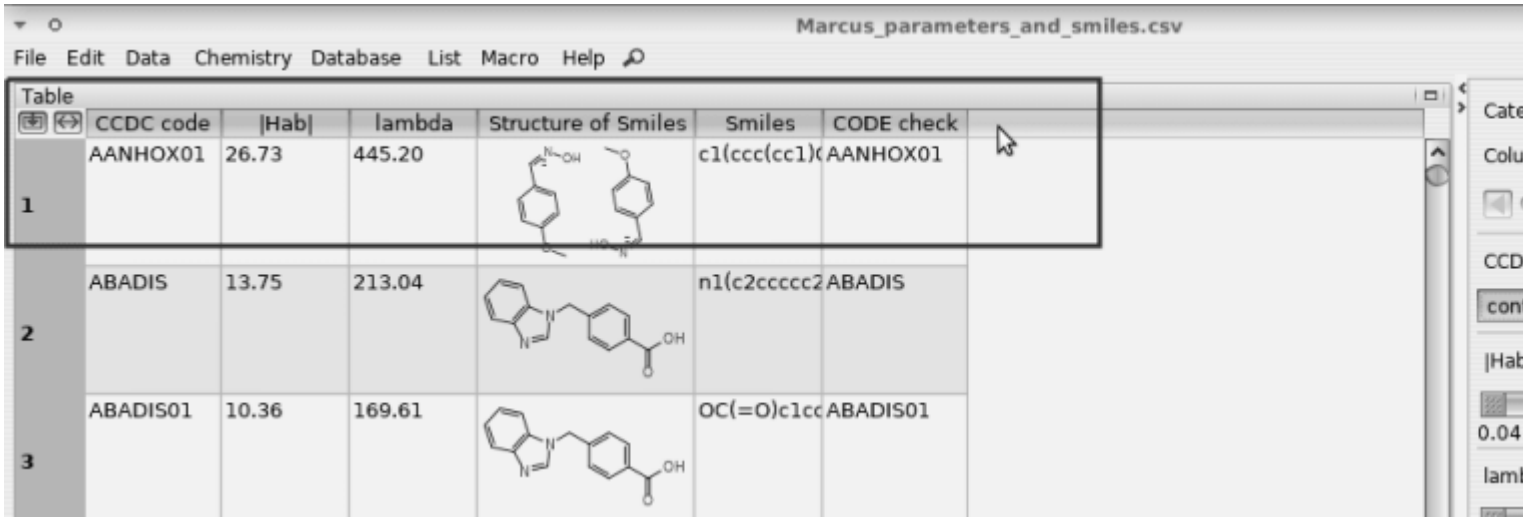
Example of reading a .csv file containing explicit header:

File Attachments

1) test_data_with_header.csv, downloaded 882 times
2) test_LOC.csv, downloaded 846 times
3) headerless_data_cropped.png, downloaded 1712 times



4) data_with_header_cropped.png, downloaded 1581 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