
Subject: Re: Batch convert .csv to .DWAR
Posted by [nbehrnd](#) on Tue, 22 Oct 2019 22:25:50 GMT
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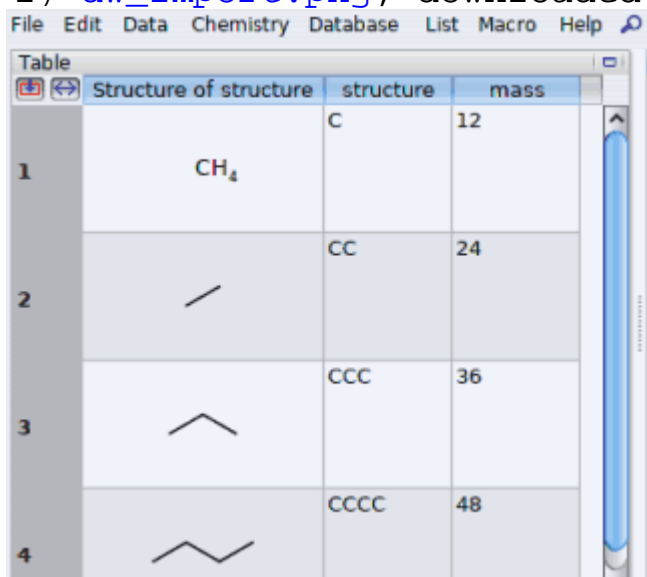
Assuming Thomas' script did the catenate the files, ensure that each of the columns has a header; for example "structure, mass" as in the example.csv attached below. (An extension .txt equally will be recognized sucessfully by DataWarrior. If working in Linux, DataWarrior will trade well with the file regardless if the line ending is encoded in dos, or unix convention, too.)

Then open either by shortcut Ctrl + O, or in the menue File -> Open the directory and eventually the .csv in question. While reading the file, DataWarrior converts automatically the structure string to populate an additional column.




Do not forget to explicitly instruct DataWarrior to save the read as .dwar.

File Attachments

1) [dw_import.png](#), downloaded 1110 times



The screenshot shows the 'Table' window in DataWarrior. It contains a table with three columns: 'Structure of structure', 'structure', and 'mass'. The table has four rows of data, each representing a different alkane. The first row shows the chemical formula CH₄, the second row shows a skeletal structure of ethane, the third row shows a skeletal structure of propane, and the fourth row shows a skeletal structure of butane. The corresponding 'structure' column contains the SMILES strings 'C', 'CC', 'CCC', and 'CCCC', and the 'mass' column contains the values 12, 24, 36, and 48.

	Structure of structure	structure	mass
1	CH ₄	C	12
2		CC	24
3		CCC	36
4		CCCC	48

2) [example.csv](#), downloaded 664 times

3) [example.dwar](#), downloaded 656 times
