
Subject: Re: Datawarrior Commandline Option to Use Template

Posted by [nbehrnd](#) on Mon, 23 Dec 2024 22:08:54 GMT

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From your comment, I sense you are comfortable with the command line. Hence I feel comfortable to suggest DataWarrior's mode of action need not to be "file based" only, perhaps additionally could be "stream based" (as so many unix/linux utilities).

An illustration: OpenBabel reads many more file formats than e.g., .sdf DataWarrior accepts as input. While converting these files into a suitable syntax, OpenBabel can apply numeric, or (sub) structure related criteria as a filter. Hence, why not allow openbabel's results (via stdout) as one form of input (stdin) for DataWarrior (in unix' parlance, via a pipe)? Second, if DataWarrior's results are not an illustration, a 2D/3D diagram, they mostly are human readable plain text written into the .dwar file. While often useful, I think a permanent output file needn't be DataWarrior's only mode of operation -- there equally could be an optional output by DataWarrior itself as an output stream to redirect (>) or append (>>) to a permanent record, or to relay to a subsequent tool living in the command line.

Norwid

<https://open-babel.readthedocs.io/en/latest/Descriptors/descriptors.html>

[https://en.wikipedia.org/wiki/Pipeline_\(Unix\)](https://en.wikipedia.org/wiki/Pipeline_(Unix))
