
Subject: suggest: native .pdf export

Posted by [nbehrnd](#) on Mon, 11 May 2020 10:29:36 GMT

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Based on a .smi derived from elsewhere,[1] which was converted with openbabel into a .sdf I let DataWarrior screen the structures for a few characteristics.

Aiming to share it with one who does not use DataWarrior, I miss a built-in function to print the table as a .pdf file as a vehicle of discussion.

This could be useful, especially if -- as here -- the cell's background colour has a significance.

So far, I printed the table via an installed HP printer as a postscript into a file (of very large file size) and converted it with ps2pdf into a .pdf like the example file attached. At page breaks, however, lines seem to be broken (table headings). If exported directly from DW as .pdf, their file size could be considerably smaller than now (containing an image in the .pdf as a container) and possibly retain a searchable text-layer.

[1] https://pubs.acs.org/doi/suppl/10.1021/jm301008n/suppl_file/jm301008n_si_002.xlsx

File Attachments

1) [table_S3.png](#), downloaded 1803 times

Table	Structure	Molecule Name	Druglikeness	Mutagenic	Tumorigenic	Reproductive Effective	Irritant	Nasty Functions
5		MERREM	6.4914	none	none	none	none	
6		NASONEX	3.0117	low	high	high	none	
7		PULMICORT	1.6963	none	none	none	none	
		TAMIFLU	-1.4998	none	none	none	none	

2) [table_S3.dwar](#), downloaded 791 times

3) [table_S3.pdf](#), downloaded 802 times
