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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](https://pubs.acs.org/doi/suppl/10.1021/jm301008n/suppl_file/jm301008n_si_002.xlsx)

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#### File Attachments

- 1) [table\\_S3.png](#), downloaded 1137 times
  - 2) [table\\_S3.dwar](#), downloaded 503 times
  - 3) [table\\_S3.pdf](#), downloaded 540 times
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Subject: Re: suggest: native .pdf export

Posted by [thomas](#) on Mon, 11 May 2020 18:51:53 GMT

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If you have a pdf printer driver installed (on Ubuntu you do that with "sudo apt-get install printer-driver-cups-pdf"), you can easily print as PDF, see attached file.

A comment to your openbabel conversion: DataWarrior can directly interpret SMILES. If you rename your .smi to .txt and open with DataWarrior, you should automatically get a structure column. An alternative is to copy the SMILES into the clipboard and just paste them into DataWarrior, which produces a new document with native chemical structures.

Best wishes, Thomas

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#### File Attachments

- 1) [DataWarrior\\_table\\_S3-1.dwar\\_\\_on-Linux-generated\\_files-job\\_91.pdf](#), downloaded 540 times
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Subject: Re: suggest: native .pdf export  
Posted by [nbehrnd](#) on Tue, 12 May 2020 14:03:44 GMT  
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It was possible to replicate the indicated method using the cups pdf printer.

As a closing comment:

Still interested to benefit more from the vector format I wrote a Python script that reads some of DW's .dwar file content and the retained list of SMILES strings, calls openabel to visualize the structures, and puts all in an .xlsx file. The manual work then left was to open this file in LibreOffice Calc, to adjust the images' sizes to fit the cell size, to apply conditional cell background colors and to save it as .ods. The file size of the then exported .pdf is slightly less than half of the one printing from DW with cups while still offering a searchable, crisply printed text layer, too.

### File Attachments

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- 1) [table\\_S3.smi](#), downloaded 480 times
  - 2) [table\\_S3.dwar](#), downloaded 483 times
  - 3) [spreadsheet\\_test.py](#), downloaded 549 times
  - 4) [test.ods](#), downloaded 497 times
  - 5) [test.pdf](#), downloaded 552 times
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Subject: Re: suggest: native .pdf export  
Posted by [nbehrnd](#) on Fri, 15 May 2020 11:11:21 GMT  
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There is a reason why the structure import used a .sdf generated from the .smi by openbabel, instead of reading the SMILES listing file directly.

Neither the direct read of the smiles from a file like 3entries.smi.txt, nor the special copy / paste from the clipboard (paste without header) kept the column about molecules' names with e.g., the PubChem number only. The attached .pdf documents this observation.

If file 3entries.smi.txt containing the annotated smiles starts with an explicit header line, e.g "structure SMILES", then DW reads the file as containing three structures; the annotating column then still contains both SMILES string and the PubChem number entry.

### File Attachments

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- 1) [SMILES\\_3entries.smi.txt](#), downloaded 429 times
  - 2) [3entries.sdf](#), downloaded 488 times
  - 3) [3entries\\_import\\_sdf.dwar](#), downloaded 465 times
  - 4) [3entries\\_import\\_smi.dwar](#), downloaded 442 times
  - 5) [data\\_read.pdf](#), downloaded 583 times
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Subject: Re: suggest: native .pdf export

Posted by [thomas](#) on Thu, 21 May 2020 22:25:28 GMT

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DataWarrior uses TAB or comma delimited text files. The smi File only contains spaces between Smiles and Name. If you replace all SPACES by a TABs in any Text-Editor before pasting into DataWarrior, you will correctly get three columns: Structure, Smiles, and Name

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