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

File Attachments

1)

DataWarrior_table_S3-1.dwar__on-Linux-generated_files-job_91.p
df, downloaded 679 times