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

1) SMILES_3entries.smi.txt, downloaded 829 times
2) 3entries.sdf, downloaded 856 times
3) 3entries_import_sdf.dwar, downloaded 788 times
4) 3entries_import_smi.dwar, downloaded 811 times
5) data_read.pdf, downloaded 965 times