Subject: Version 5.0 does not open file with 2 columns of SMILES
Posted by edgriffen on Mon, 21 Oct 2019 12:31:22 GMT
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Using DW version 5 , on Mac running Mojave 10.14.5, Java updated to 8 Update 231.

this file is not read:

name	SMILES1	SMILES2
line1	c1ccccc1	c1ccccc1F
line2	n1ccccc1	n1ccccc1F
line3	[nH]1cccc1	[nH]1cccc1C

attached as test3.txt

Just hangs at 'processing records', then fails to finnish cleaning up.

Just reading the 1st and 2nd or 1st and 3rd columns, both read in fine.

Files attached as test4.txt and test5.txt

Double structure column reads fine on DQ v 4.7.2 - if only I could go back....

Thanks,

Ed

File Attachments

1) test3.txt, downloaded 866 times
2) test5.txt, downloaded 767 times
3) test4.txt, downloaded 852 times

Subject: Re: Version 5.0 does not open file with 2 columns of SMILES
Posted by thomas on Mon, 21 Oct 2019 18:58:06 GMT
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thanks for the report. This is fixed in the update due later this year.
You may download a not yet finished early access version on
openmolecules.org/datawarrior/dw500x.zip.
This archive contains a few files, which (on the Macintosh) must be copied into
/Applications/DataWarrior.app/Contents/Java

Subject: Re: Version 5.0 does not open file with 2 columns of SMILES
Posted by edgriffen on Tue, 22 Oct 2019 09:25:42 GMT

Downloaded version works fine, thanks for the quick response.