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