
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 c1cccc1    c1cccc1F
line2 n1cccc1    n1cccc1F
line3 [nH]1cccc1  [nH]1cccc1C
```

attached as test3.txt

Just hangs at 'processing records', then fails to finish 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 534 times
 - 2) [test5.txt](#), downloaded 507 times
 - 3) [test4.txt](#), downloaded 562 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

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Downloaded version works fine, thanks for the quick response.
