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Subject: Re: Faulty SDF import

Posted by [nbehrnd](#) on Wed, 21 Oct 2020 07:15:38 GMT

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My observation differs:

1) First I pasted the SMILES string into DW (5.2.1, natively Linux version [used in Debian 10 / unstable]) and obtained a pyridinium:

2) Then the .sdf provided by you (as generated by Marvin) was read by a separate, newly started instance of DW, again yielding a pyridinium:

which seems chemically plausible, matches (by constitution) both the former and the visual output when requesting OpenBabel (3.1.0) to visualize the .sdf as a .png:

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#### File Attachments

- 1) [test.dwar](#), downloaded 240 times
  - 2) [test\\_in\\_DW.png](#), downloaded 560 times
  - 3) [untitled\\_molecule\\_file.dwar](#), downloaded 243 times
  - 4) [test\\_import.png](#), downloaded 434 times
  - 5) [untitled\\_molecule\\_file.png](#), downloaded 549 times
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