
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:

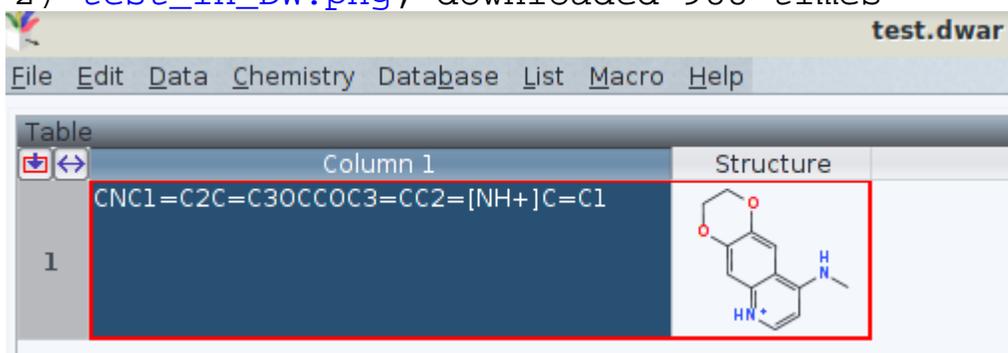
2) Then the .sdf provided by you (as generated by Marvin) was read by a separate, newly started instance of DW, again yielding a pyridinium:

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:

File Attachments

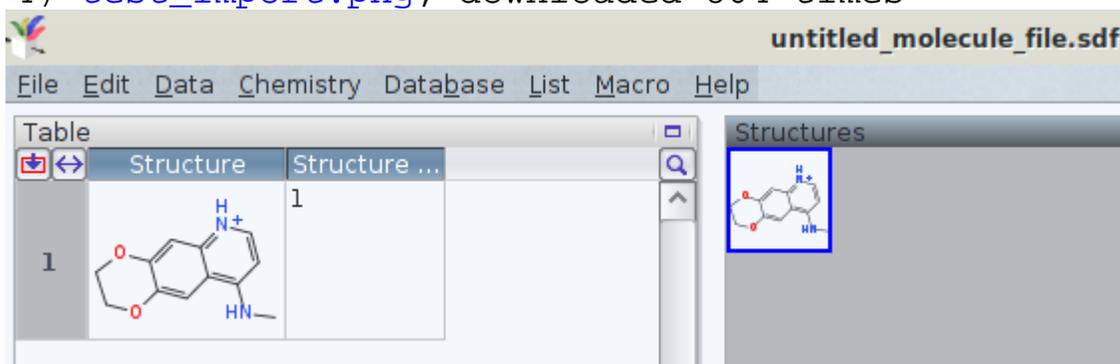
1) [test.dwar](#), downloaded 579 times

2) [test_in_DW.png](#), downloaded 988 times



3) [untitled_molecule_file.dwar](#), downloaded 593 times

4) [test_import.png](#), downloaded 864 times



5) [untitled_molecule_file.png](#), downloaded 1064 times

