Subject: Re: Faulty SDF import
Posted by nbehrnd on Wed, 21 Oct 2020 07:15:38 GMT
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My observation differs:

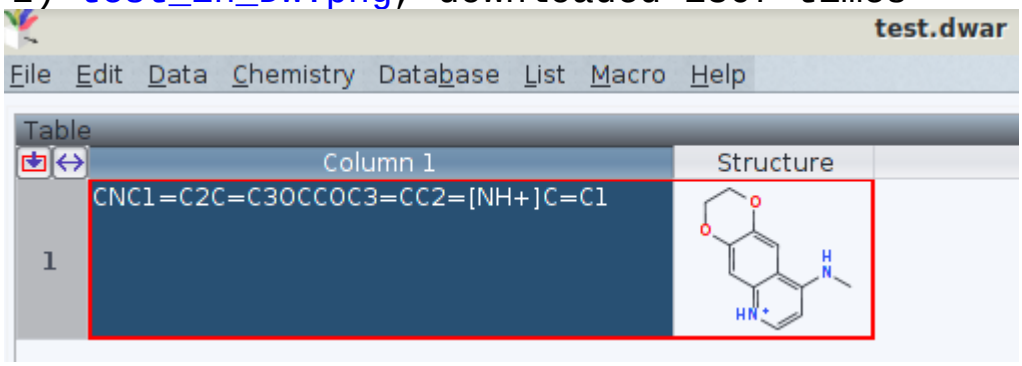
1) First I pasted the SMILES string into DW (5.2.1, natively Linux version [used in Debian 10 / unstable]) and obtained a pyridinium:

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:

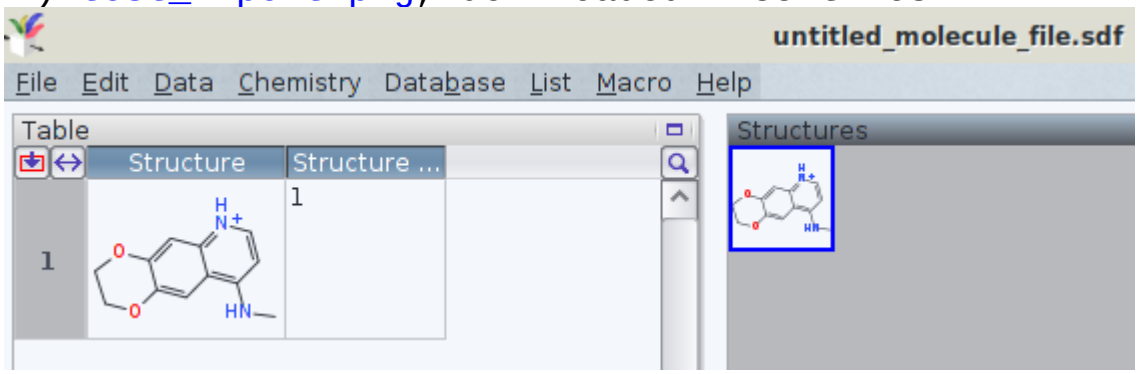
which seems chemically plausible, matches (by constitution) both the former and the visual output when requesting OpenBabel (3.1.0) to visualize the .sdf as a .png:

File Attachments

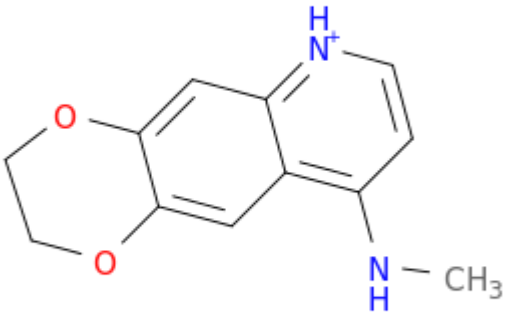
1) test.dwar, downloaded 701 times
2) test_in_DW.png, downloaded 1367 times



3) untitled_molecule_file.dwar, downloaded 706 times
4) test_import.png, downloaded 1235 times



5) untitled_molecule_file.png, downloaded 1449 times


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