Subject: Re: Faulty SDF import
Posted by nbehrnd on Thu, 22 Oct 2020 10:28:02 GMT
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Affirmative. The pristine installation of DW for Linux using the stable release (last edit 23 Feb 2020) loads your .sdf file and then displays the single protonated pyridinium, as described in my initial post. But the substitution of elder / original datawarrior.jar file by the one obtained from the development branch for Linux (1), deposit into the /opt/datawarrior directory (last edit 13 Sep 2020), then yields the questionable double-protonation on the pyridine; which matches 1:1 your initial observation.

Because rebuilding DW today (22 Okt 2020) from its public sources (2, last edit 13 Sep 2020) in Linux equally yields an executable displaying again the erroneous «double pyridine protonation», possibly the issue spreads out to the development version for Windows,(3) too.

Norwid

(1) http://www.openmolecules.org/datawarrior/dw521x.zip
(2) http://www.openmolecules.org/datawarrior/dw521source.tar.gz
(3) http://www.openmolecules.org/datawarrior/dw521win.zip