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Subject: Re: Incorrect dearomatization of indazole structures

Posted by [thomas](#) on Tue, 30 Nov 2021 13:53:31 GMT

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Hi Andrievs,

Your SD-File includes a non-standard Marvin extension that is not understood by DataWarrior:

MRV\_IMPLICIT\_H

Marvin uses that feature to define explicit hydrogen atoms, which usually is not needed, because molfiles

usually are in a kekulized form. If, however, molfiles just contain bonds marked to be aromatic, the Kekulizer needs more information, if multiple potentially protonated nitrogen atoms are present.

Standard molfiles simply don't have a place to store that information. The only way to make your SD-files compatible would be to extend DataWarrior's molfile parser to support Marvin's non-standard extensions.

Hope this explains it, Thomas

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