Subject: Incorrect dearomatization of indazole structures
Posted by Andrievs on Tue, 30 Nov 2021 10:48:26 GMT
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I am having issues with SD files where the structure is an indazole superstructure.
I have attached a SD-file as examples with 3 structures.

The problem is that during the dearomatization process DataWarrior incorrectly places the double bonds resulting in a formation of s stereocenter.

See attached image for visual differences.

Is there a way to have the dearomatization be done correctly with out using additional software?

P.s. I am using DataWarrior version 5.5.0

Sincerely, Andrievs

File Attachments
1) indazole_aromatized.sdf, downloaded 164 times
2) DataWarrior.png, downloaded 258 times

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 extentions.

Hope this explains it, Thomas