
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 a stereocenter.

See attached image for visual differences.

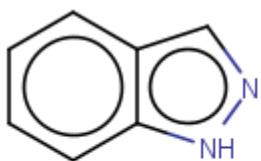
Is there a way to have the dearomatization be done correctly without using additional software?

P.s. I am using DataWarrior version 5.5.0

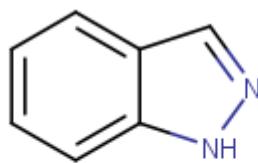
Sincerely, Andrievs

File Attachments

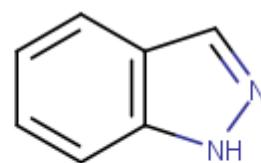
- 1) [indazole_aromatized.sdf](#), downloaded 530 times
- 2) [DataWarrior.png](#), downloaded 650 times



**Original
aromatized form**



**Possible kekule
form I**



**Possible kekule
form II**