
Subject: Incorrect dearomatization of indazole structures

Posted by [Andrievs](#) on Tue, 30 Nov 2021 10:48:26 GMT

[View Forum Message](#) <> [Reply to Message](#)

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 254 times
 - 2) [DataWarrior.png](#), downloaded 295 times
-