Subject: Canonical codes do not distinguish stereoisomers
Posted by wsmts on Fri, 29 Aug 2025 13:32:49 GMT
View Forum Message <> Reply to Message

Hi,

I noticed that for some molecules the Canonical codes don't distinguish stereoisomers even though the box was selected in the calculation dialog. (I had also deselected distinguish tautomers).

I was expecting the canonical codes to follow the pattern of the InchiKeys but they ignored the stereochemistry for these examples. (dwar attached)

v06.05.01 (Windows 11)

Best,

--
Wim

File Attachments

1) Canonical Codes.dwar, downloaded 333 times

Subject: Re: Canonical codes do not distinguish stereoisomers
Posted by thomas on Thu, 04 Sep 2025 09:20:14 GMT
View Forum Message <> Reply to Message

I agree that this is disturbing at the first glance. However, here we have a situation, were the set of tautomers contain multiple stereo isomers. The canonical code of your different stereo isomers correctly differs for your different stereo isomers if it shall also distinguish tautomers. However, if you ask for different tautomers to create the same code, then this is what you get. The upper part of the image shows three tautomers of a part of your structure where from left to right a stereo center inverts its configuration, but all three structures are just different tautomers of the same thing. The bottom part of the image shows the same situation for the other stereo center.

File Attachments

1) tautomers.jpeg, downloaded 967 times

