
Subject: Stereo issue?

Posted by [bruno.b](#) on Sun, 31 May 2015 23:49:21 GMT

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Hi Thomas,

I wrote a small Java program that uses the open source Datawarrior library. This program converts the smiles of the drug benazepril into a MOL file. I used the smiles from Pubchem. The generated MOL has only one stereo center instead of two. I have attached the MOL output and the java code to this post.

I am not sure that the Java program I wrote is correct.

Thank you for providing the library,

Bruno

File Attachments

- 1) [smiles2mol.java](#), downloaded 1244 times
 - 2) [benazepril_wrong.mol](#), downloaded 1227 times
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