
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 1189 times

2) [benazepril_wrong.mol](#), downloaded 1167 times

Subject: Re: Stereo issue?

Posted by [thomas](#) on Thu, 18 Jun 2015 18:50:41 GMT

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Hi Bruno,

I am sorry for answering so late. My intention is to answer within 24 hours after being aware of a question. If you don't get a quick answer, you may assume, that I simply didn't see your question (as in this case). Then please send me an e-mail...

I checked your source code, which seem perfectly correct. With the current SmilesParser it also works fine. The problem is that Smiles were not used at Actelion and therefore I didn't notice that the stereo recognition was not working well. Recently, we published a paper and a website with structure search on all Wikipedia structures. Since this requires parsing the Smiles strings from the Wikipedia database, I enhanced the SmilesParser and fixed lots of stereochemistry related and other issues. You can find the up-to-date version on GitHub in the OpenChemLib project. It will also arrive as part of the source code of the upcoming new DataWarrior release in hopefully early June.

Thomas

Subject: Re: Stereo issue?

Posted by [bruno.b](#) on Thu, 05 Nov 2015 09:23:45 GMT

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It is indeed improved.

I tested further the SMILES to structure generator, Here is a SMILES that does not give good 2D coordinates: c1ccc(C23C(N(c4ccc(cc4)C)C(C2C2c4c(C3c3c2cccc3)cccc4)=O)=O)c c1

This is not an easy case.

Best regards,

Bruno

Subject: Re: Stereo issue?

Posted by [thomas](#) on Tue, 10 Nov 2015 14:54:21 GMT

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This is indeed a little tricky. But it is a problem of the CoordinateInventor and not of the SmilesParser.

Generating coordinates is a never ending story. Paul Labute has once written a nice paper about it...

Best wishes,

Thomas
