Subject: Stereo issue?
Posted by bruno.b on Sun, 31 May 2015 23:49:21 GMT
View Forum Message <> Reply to Message

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 1348 times
2) benazepril_wrong.mol, downloaded 1328 times

Subject: Re: Stereo issue?
Posted by thomas on Thu, 18 Jun 2015 18:50:41 GMT
View Forum Message <> Reply to Message

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
View Forum Message <> Reply to Message

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
View Forum Message <> Reply to Message

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