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