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 1252 times
2) benazepril_wrong.mol, downloaded 1233 times