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
Page 1 of 1 Generated from openmolecules org Forum