Subject: Re: Generate 2D atom coordinates gives overlapping atoms
Posted by nbehrnd on Thu, 02 Feb 2023 19:37:30 GMT
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Hello mcmc,

your question does not describe how the piperazines on the left are generated in first place. Is it a SMILES string, a .sdf file you import? Do you draw them with DW's sketcher? Opting for the latter, starting to draw the molecule from the right, the furopyrazole, to which I added piperazine, and lastly, the bridge to piperazine, I did not observe the overlap you describe.
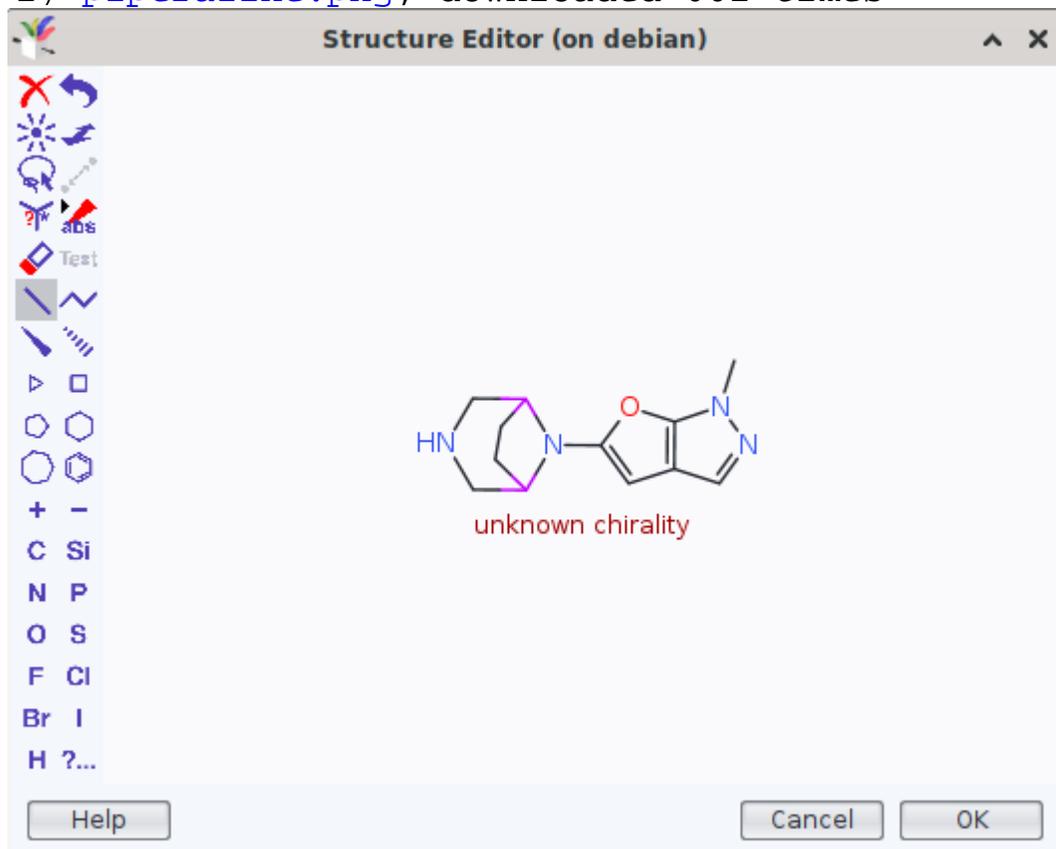
Regards,

Norwid

DW for Linux/MacOS version 5.5 with updates published by 2023-01-18 in Linux Debian 12/bookworm.

File Attachments
1) piperazine.png, downloaded 601 times

2) piperazine.dwar, downloaded 1880 times