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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 fuopyrazole, 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.

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#### File Attachments

- 1) [piperazine.png](#), downloaded 392 times
- 2) [piperazine.dwar](#), downloaded 1804 times

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