Subject: Re: Generate 2D atom coordinates gives overlapping atoms
Posted by mcmc on Fri, 03 Feb 2023 09:51:31 GMT
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Ah, no I didn't. They were either uploaded as SDF (V3000), or as SDF coming out of Chemdraw drawings.
I should also add, I modified the right-hand side from a different fused bicycle, for the purpose of this post. I did not want to disclose the actual molecules we are working on.

Also, the bridged piperazine is treated as substituent in generating the coords. The core (bicycle) is the constant part

I am surprised that this matters, as this module generates new 2D coords. But your observation is interesting, and I'll see if I can tune things a little. Maybe the size/depth of the bridge decides whether the 6- or 5-membered ring gets prioritised.

At any rate, it's a pity that overlapping atoms are generated in the first place, but maybe that's anyway not due to Datawarrior code.