Subject: polycyclic molecule displaying issue
Posted by yunforce on Tue, 29 Oct 2024 09:11:55 GMT
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I copied the same SMILES string (CC[C@@]12CCC(=O)N3CC[C@]4(C5=CC=CC=C5N[C@@H]4CC1)[C@H]32) into both DataWarrior and ChemDraw. In DataWarrior, the structure displayed had many overlapping bonds, making it difficult to discern the true structure of the molecule. However, when I pasted this SMILES into ChemDraw, it displayed a clearer structure. I wonder if this is due to an issue with the software itself or differences in the structure generation algorithms. If improvements could be made in this area, it would certainly make DataWarrior more popular.

File Attachments

1) Snipaste_2024-10-29_17-02-01.png, downloaded 106 times
2) Snipaste_2024-10-29_17-10-46.png, downloaded 135 times
3) examples.dwar, downloaded 105 times