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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.

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### File Attachments

1) [Snipaste\\_2024-10-29\\_17-02-01.png](#), downloaded 468 times

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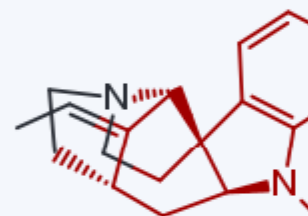
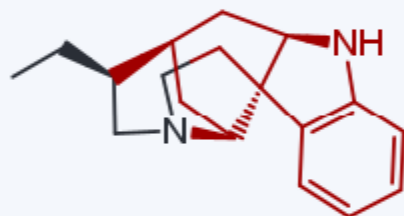
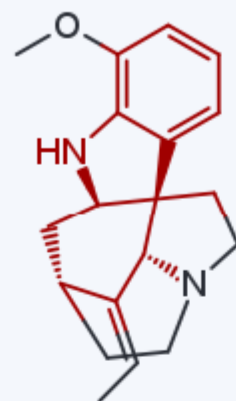
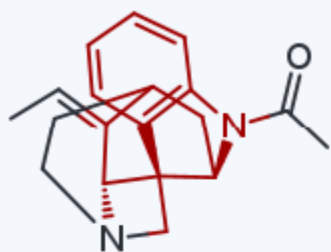
Smiles: CC[C@@]12CCC(=O

When copy to DataWarrior  
(hard to read the real structure)



2) [Snipaste\\_2024-10-29\\_17-10-46.png](#), downloaded 601 times

# Structure of canonical\_smiles



3) [examples.dwar](#), downloaded 367 times

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