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.

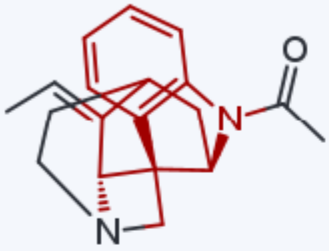
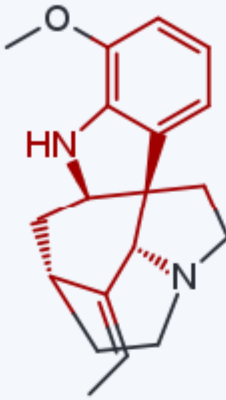
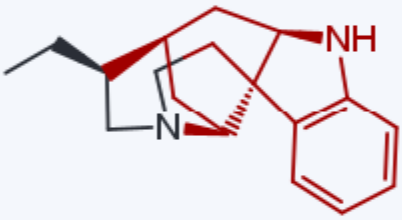
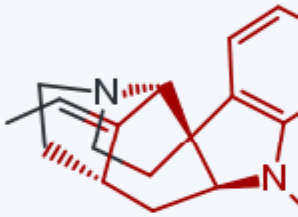
File Attachments

1) Snipaste_2024-10-29_17-02-01.png, downloaded 390 times

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

When copy to DataWarric
(hard to read the real stru

2) Snipaste_2024-10-29_17-10-46.png, downloaded 497 times

Structure of canonical_smiles	
	
	

3) examples.dwar, downloaded 342 times

Subject: Re: polycyclic molecule displaying issue
Posted by nbehrnd on Tue, 29 Oct 2024 21:35:40 GMT
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Hello,

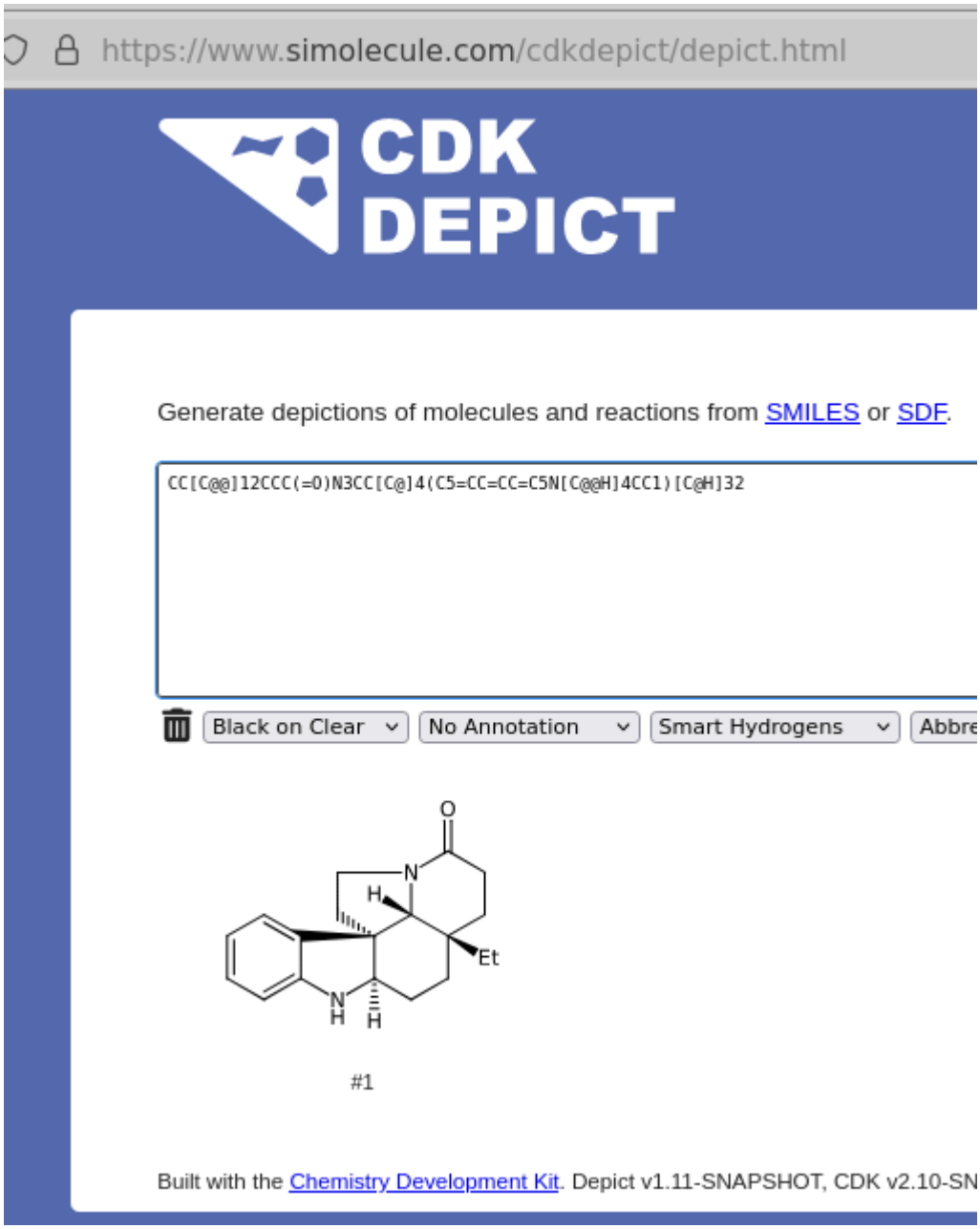
With DW you don't have leverage to alter DataWarrior's attempt to identify by itself the best 2D projection of a 3D molecule. If you copied the SMILES string to the clipboard memory of the computer, then double clicked into a field of the DW spreadsheet, a click with the right mouse button allows to paste the SMILES string already as structure. With the lasso, it is possible to move a little bit the atoms and bonds (as in the video attached), or iron out some oddities with the star button; but that's all. In this regard, DW is not like ChemDraw or Marvin where you can somewhat optimize and reorient the structure formula, or toggle on/off the descriptors of stereochemistry.

An idea for future versions of DataWarrior could be to let the user choose for each .dwar file for structure formulae either with the current 3D projection approach, or a "flattened" one as e.g., by CDKDepict (example attached). But I have no idea how much work this were to provide this choice.

Best regards,

Norwid

File Attachments
1) example_DW.mp4, downloaded 278 times
2) example_marvin.mp4, downloaded 293 times
3) example_CDKDepict.png, downloaded 383 times



Subject: Re: polycyclic molecule displaying issue
Posted by yunforce on Thu, 31 Oct 2024 01:22:54 GMT
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Dear Norwid, thanks for your reply! I'm looking forward to the new function of the "flattend" option.