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 243 times
2) example_marvin.mp4, downloaded 256 times
3) example_CDKDepict.png, downloaded 292 times

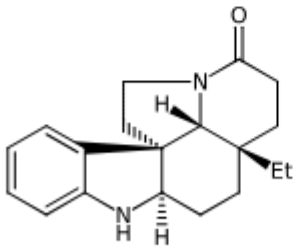
https://www.simolecule.com/cdkdepict/depict.html

CDK DEPICT

Generate depictions of molecules and reactions from SMILES or SDF.

```
CC[C@@]12CCC(=O)N3CC[C@]4(C5=CC=CC=C5N[C@@H]4CC1)[C@H]32
```

Black on Clear | No Annotation | Smart Hydrogens | Abbre



#1

Built with the Chemistry Development Kit. Depict v1.11-SNAPSHOT, CDK v2.10-SN