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Subject: Bad Displaying of Complex Polycyclic Molecules

Posted by [yunforce](#) on Fri, 20 Sep 2024 02:56:17 GMT

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When working with complex polycyclic molecules in DataWarrior, it has come to my notice that the current visualization capabilities of the software sometimes struggle with accurately and effectively displaying the structure of these intricate molecules.

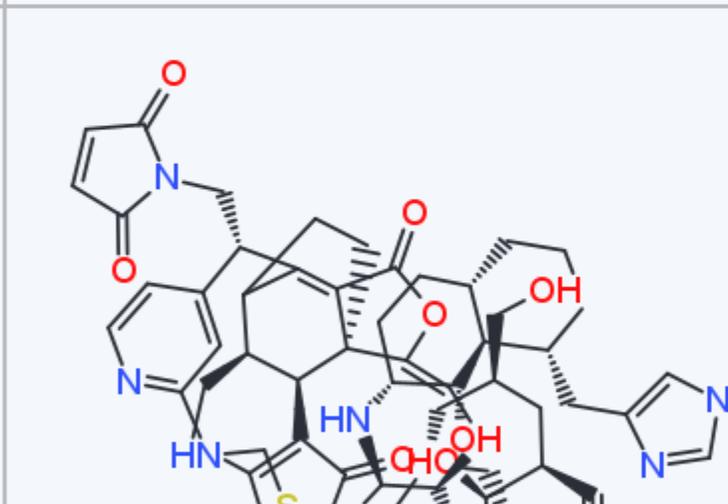
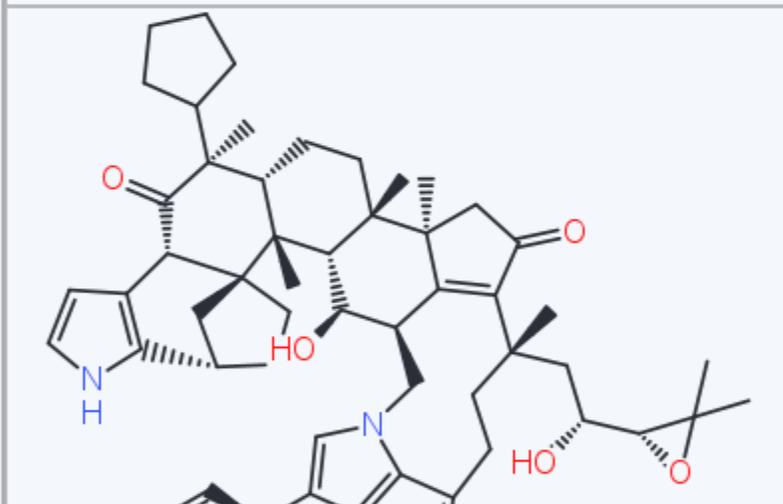
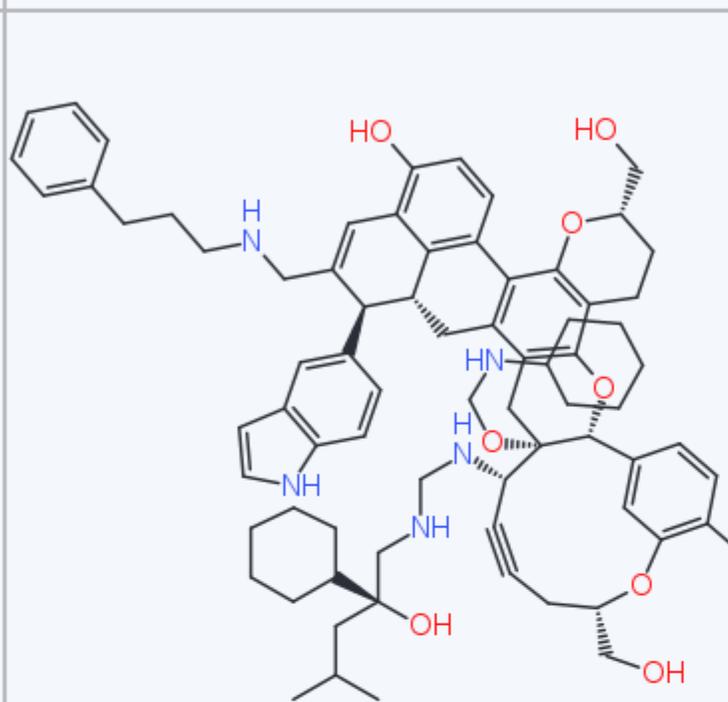
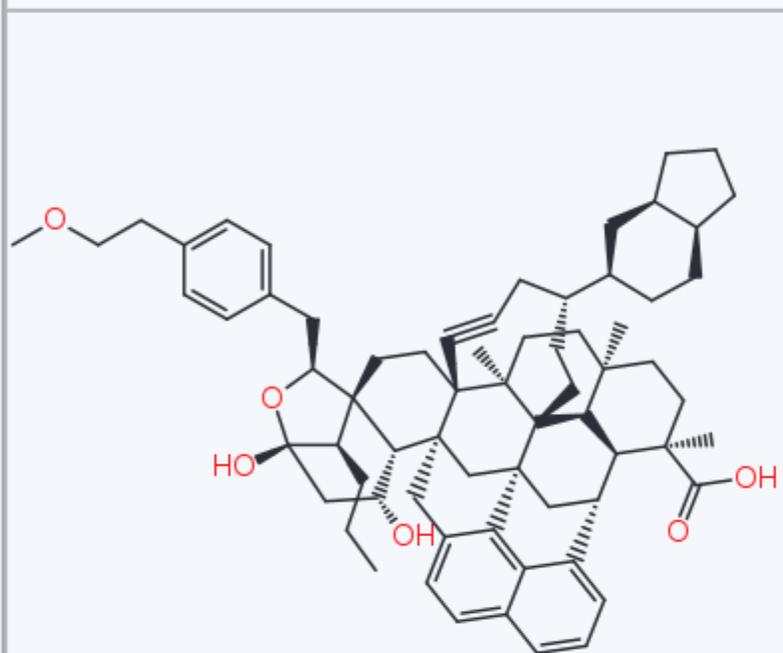
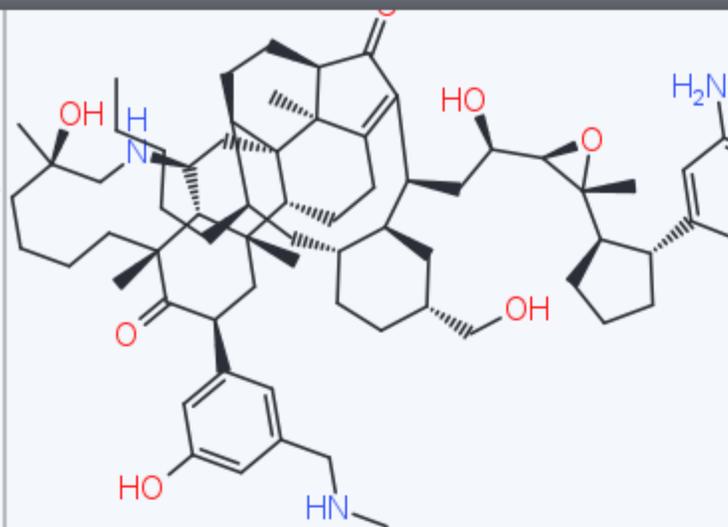
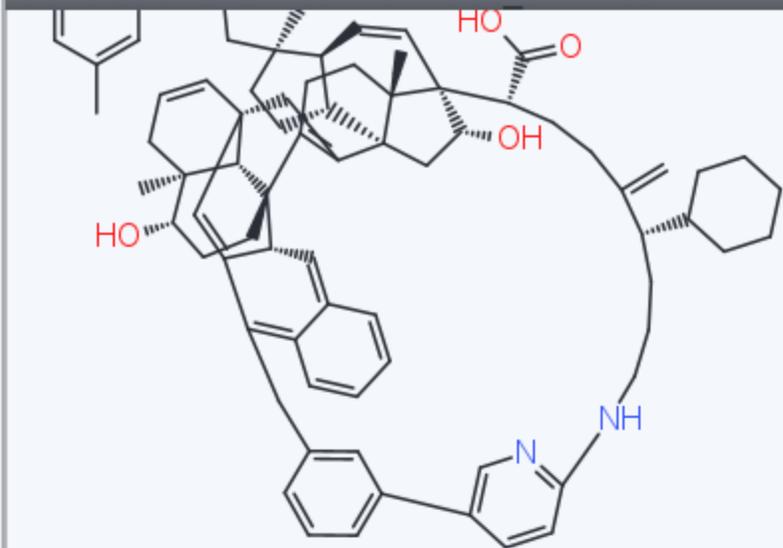
While DataWarrior is an invaluable tool for chemical data analysis, the display issue can significantly impact the user experience and the accuracy of our work. Specifically, when dealing with molecules that have multiple rings or complex bonding patterns, the visualization can become cluttered or distorted, making it difficult to discern important structural details.

### File Attachments

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1) [Snipaste\\_2024-09-20\\_10-50-09.png](#), downloaded 460 times

# Structure of canonical smiles



2) [examples.dwar](#), downloaded 337 times

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Subject: Re: Bad Displaying of Complex Polycyclic Molecules

Posted by [nbehrnd](#) on Fri, 20 Sep 2024 05:38:02 GMT

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Hell yunforce,

I think your observation refers to a general problem for every program to provide a 2D projection of a 3D molecule. Partial overlap already can be observed for smaller molecules, perhaps especially if DW is used as an interface to access databases with experimentally determined coordinates. The example attached documents a query for rubrenes in the crystallographic open database. For large rings, it can become difficult/impossible to count the number of atoms building this cycle. The depiction can become very busy with if there are «too many» stereochemistry labels ([abs] R/S, P/M, E/Z) per area unit of the array of the structure previews (for which I think there is no toggle-on/off, either), too.

If your sdf data are associated with conformers, the 3D structure window allows to rotate the model of the molecule (dragged right hand mouse button), and change its scale (mouse wheel). This often is helpful when browsing through a stack of structures on a on-by-one basis, complementary to the preview provided by the array.

Norwid

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### File Attachments

1) [search\\_ruberene.png](#), downloaded 414 times

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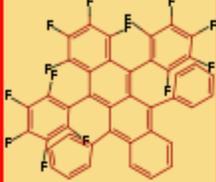
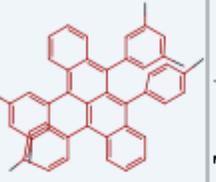
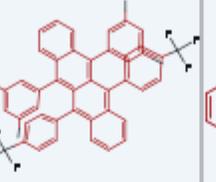
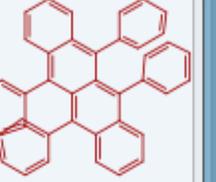
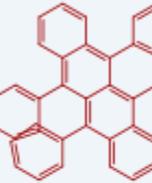
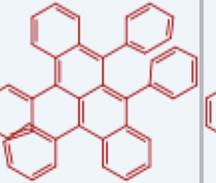
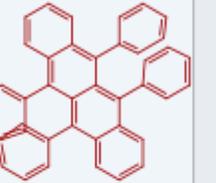
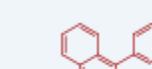
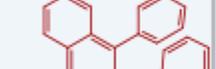
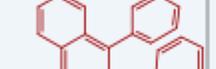
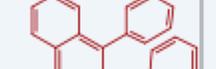
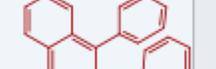
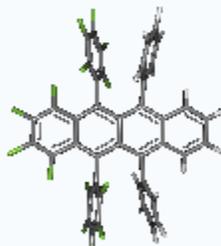
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 2312008	 2312010	 2312009	 2312006	 2312005	 2300670
 2312008	 2312010	 2312009	 2312006	 2312005	 2300670

Table Structures

Form View

3D-Structure:



Authors: Sakamoto, Youichi; Suzuki, Toshiyasu

Title: Perfluorinated and Half-Fluorinated Rubrenes: Synthesis and

Journal: The Journal of organic chemistry

DOI: 10.1021/acs.joc.7b01383

Year: 2017

Volume: 82

Issue: 15

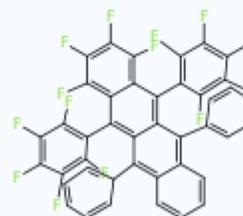
First Page: 8111

Last Page: 8116

COD Number: 4032644

R-factor all:

Structure:



Substance Name:

Chemical Name:

Type: organic

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Cell alpha: 90.0000

Cell length b: 28.081

Cell beta: 90.0000

Cell length c: 7.3931

Cell gamma: 90.0000



8 of 37

174 of 512 MB

Selected:1

Visible:37

Total:37