Subject: Bad Displaying of Complex Polycyclic Molecules
Posted by yunforce on Fri, 20 Sep 2024 02:56:17 GMT
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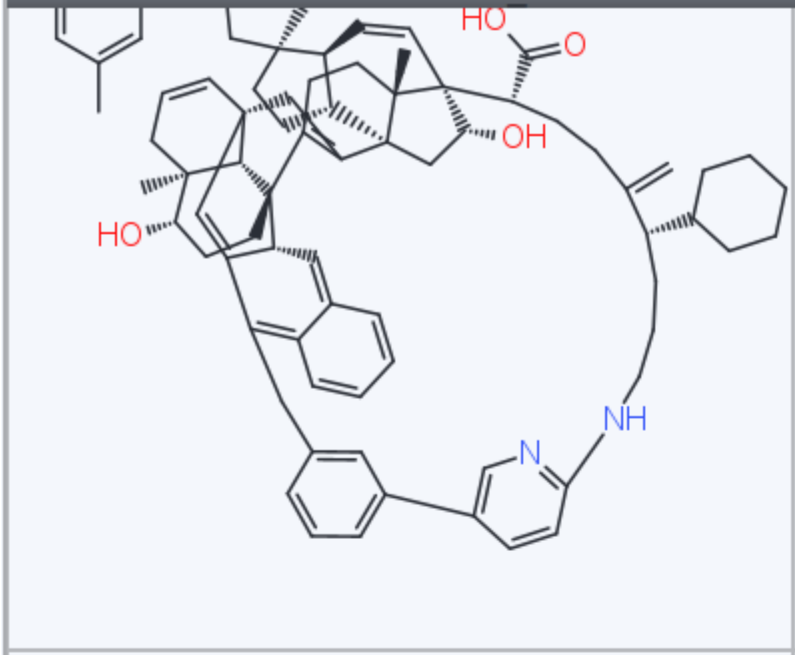
When working with complex polycyclic molecules in DataWarrior,It has come to my notice that the current visualization capabilities of the software sometimes struggle with accurately and effectively displaying the structure of these intricate molecules.

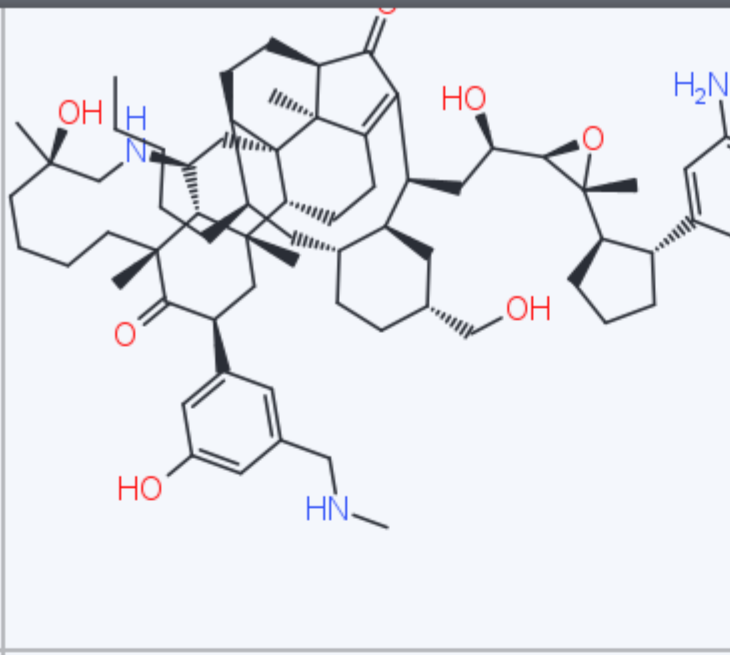
While DataWarrior is an invaluable tool for chemical data analysis, the display issue can significantly impact the user experience and the accuracy of our work. Specifically, when dealing with molecules that have multiple rings or complex bonding patterns, the visualization can become cluttered or distorted,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

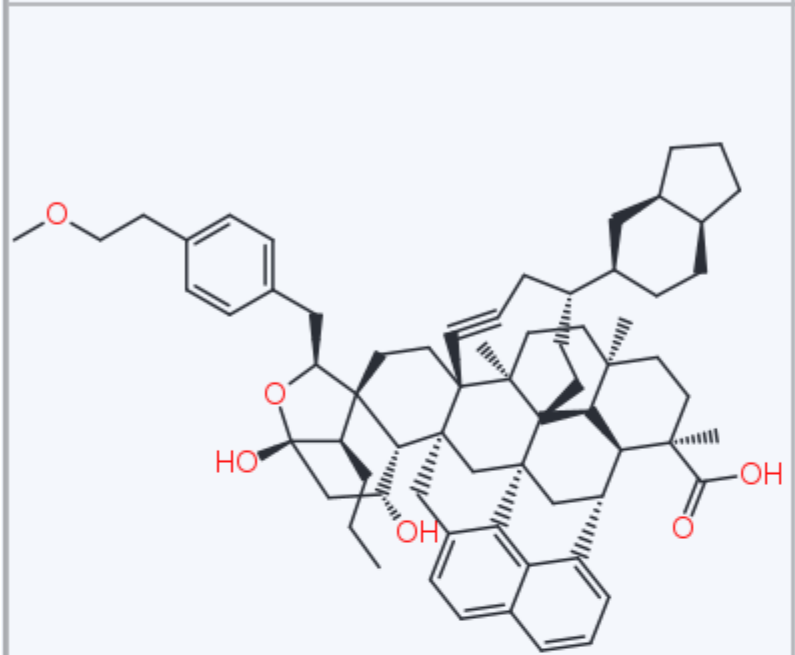
## File Attachments

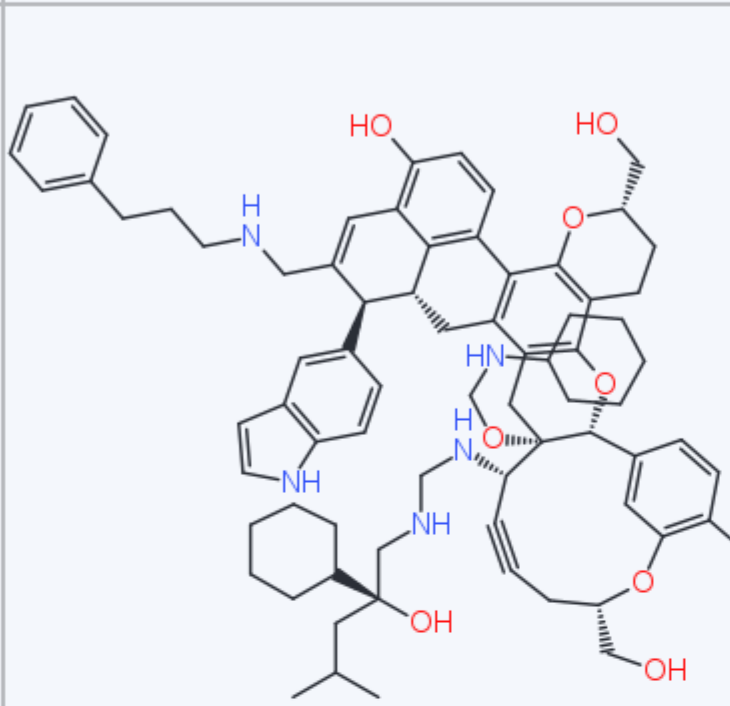
1) Snipaste_2024-09-20_10-50-09.png, downloaded 458 times

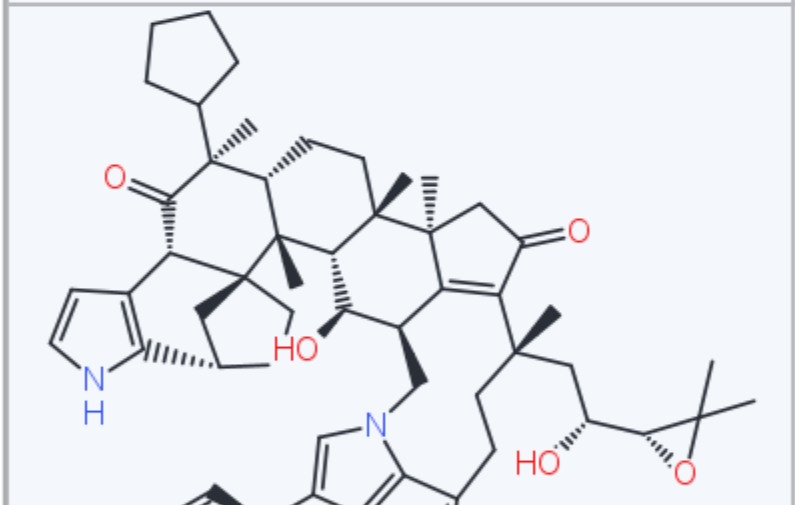
Structure of canonical_smiles

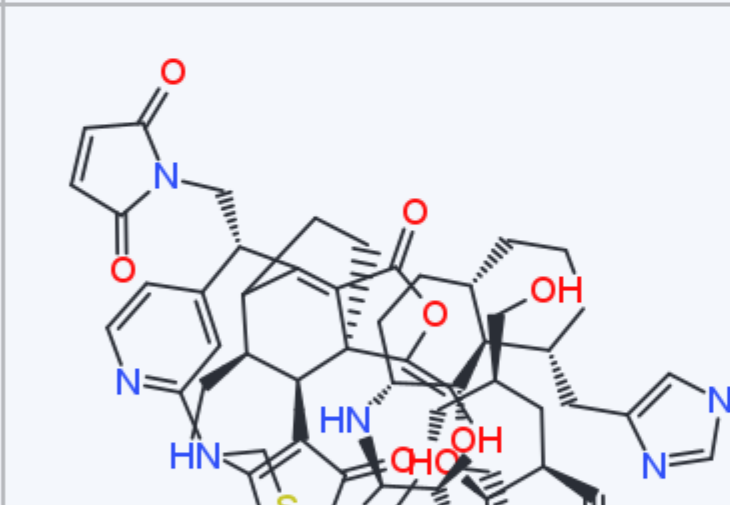


2) examples.dwar, downloaded 335 times

Subject: Re: Bad Displaying of Complex Polycyclic Molecules
Posted by nbehrnd on Fri, 20 Sep 2024 05:38:02 GMT
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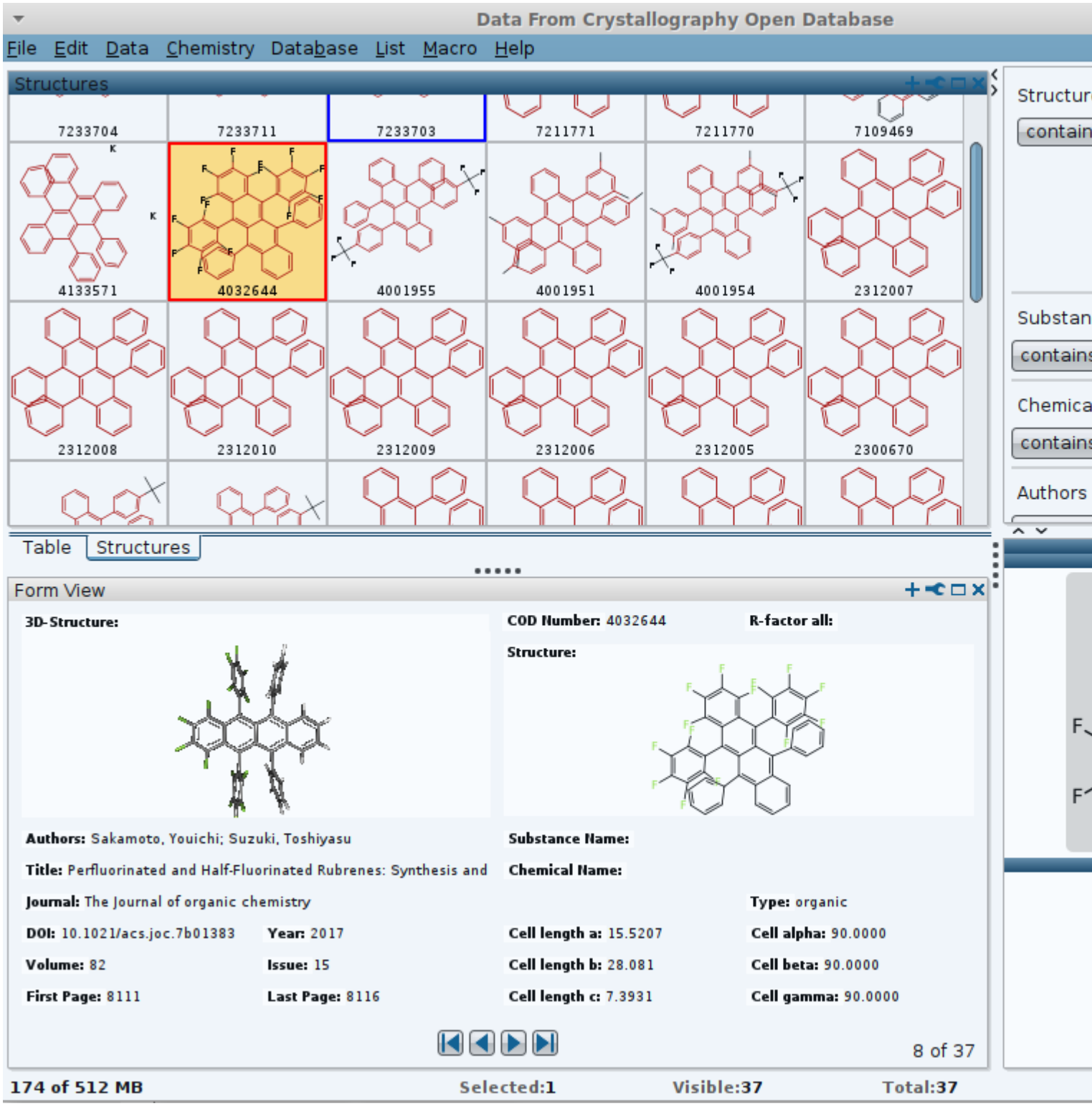
Hell yunforce,

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

File Attachments
1) search_ruberene.png, downloaded 412 times


Data From Crystallography Open Database
File Edit Data Chemistry Database List Macro Help
Structures
7233704
7233711
7233703
7211771
7211770
7109469
4133571
4032644
4001955
4001951
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2312007
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2312010
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2312006
2312005
2300670
Table Structures
Form View
3D-Structure:
COD Number: 4032644
R-factor all:
Structure:
Authors: Sakamoto, Youichi; Suzuki, Toshiyasu
Substance Name:
Title: Perfluorinated and Half-Fluorinated Rubrenes: Synthesis and
Chemical Name:
Journal: The Journal of organic chemistry
Type: organic
DOI: 10.1021/acs.joc.7b01383
Year: 2017
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Issue: 15
Cell length b: 28.081
Cell beta: 90.0000
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Last Page: 8116
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8 of 37
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