Subject: Unable to diaplay zwitterion structure correctly in both + and - sperately
Posted by SallyS on Fri, 02 Jun 2023 07:35:52 GMT
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Hi,

I was writing this message to report a display isuue for zwitterion structures.

For instance,

O=C([O-])c1cc(NS(=O)(=O)c2ccccc2Cl)cnc1N1CCC[C@H](C[NH+]2CCC C2)C1
This structure contains both N+ and O-, and the net charge is 0.

However this structure was displayed as attachments 'strcuturedisplay.jpg',

unlike what it could be correctly in attachment 'strcuturedisplay.jpg'

I am not sure its a bug or I could set any function to show the strcuture correctly.
Thank you for your time and I am looking forward to hearing from you soon.

Best regards,
Sally

File Attachments

1) strcuture_correct.jpg, downloaded 393 times
2) strcuturedisplay.jpg, downloaded 320 times

Subject: Re: Unable to diaplay zwitterion structure correctly in both + and - sperately
Posted by thomas on Sun, 04 Jun 2023 19:14:27 GMT
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When DataWarrior creates a new window from structures converted from an external format (typically SMILES or molfiles; from file or clipboard) then DataWarrior converts these structures into a normalized and canonical form (idcode), which is then stored in a dwar file. Part of the normalization is moving protons in order to remove charges. The canonicalization then classifies all atoms after detecting ring and stereo features for a unique numbering, which allows to create a compact and canonical molecule encoding.

The idea of this is that input structures, which just differ because different atoms are (de-)protonated, are recognized as the same thing.

Admittedly, there are applications, where one needs to dinstinguish different protonation states or zwitter ions from the neutral molecule. If you edit an existing structure within DataWarrior, then the normalization is not done, because DataWarrior assumes that you know what you are doing and that you really intended the drawn protonation state. It just writes the canonicalized drawn

structure into the cell. The same happens, if you paste one or multiple structures or SMILES into a structure column: protonation states are retained. (right mouse click on a structure within the table and 'Paste Into Table')

Thus, a solution to you problem is: If you have one or multiple SMILES in the clibboard, then do 'File-Paste'. A new window is created with normalized structures. Press the right mouse button in the first structure cell and choose 'Paste Into Table'. The normalized structure(s) are now replaced by the non-normalized ones retaining the original protonation state.