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',

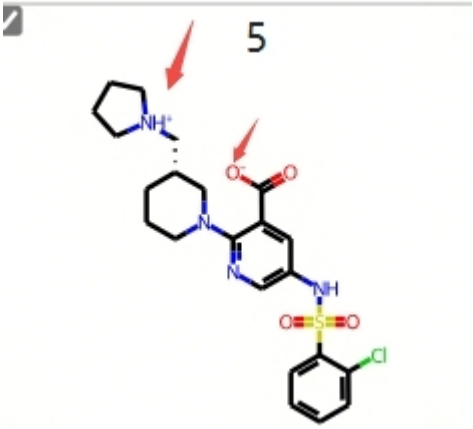
unlike what it could be correctly in attachment 'strcuturedisplay.jpg'

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 1532 times



2) strcuturedisplay.jpg, downloaded 1492 times

