Subject: Pentavalent carbonyl issue (urea formation?)

Posted by padster on Thu, 22 Jun 2023 19:14:13 GMT

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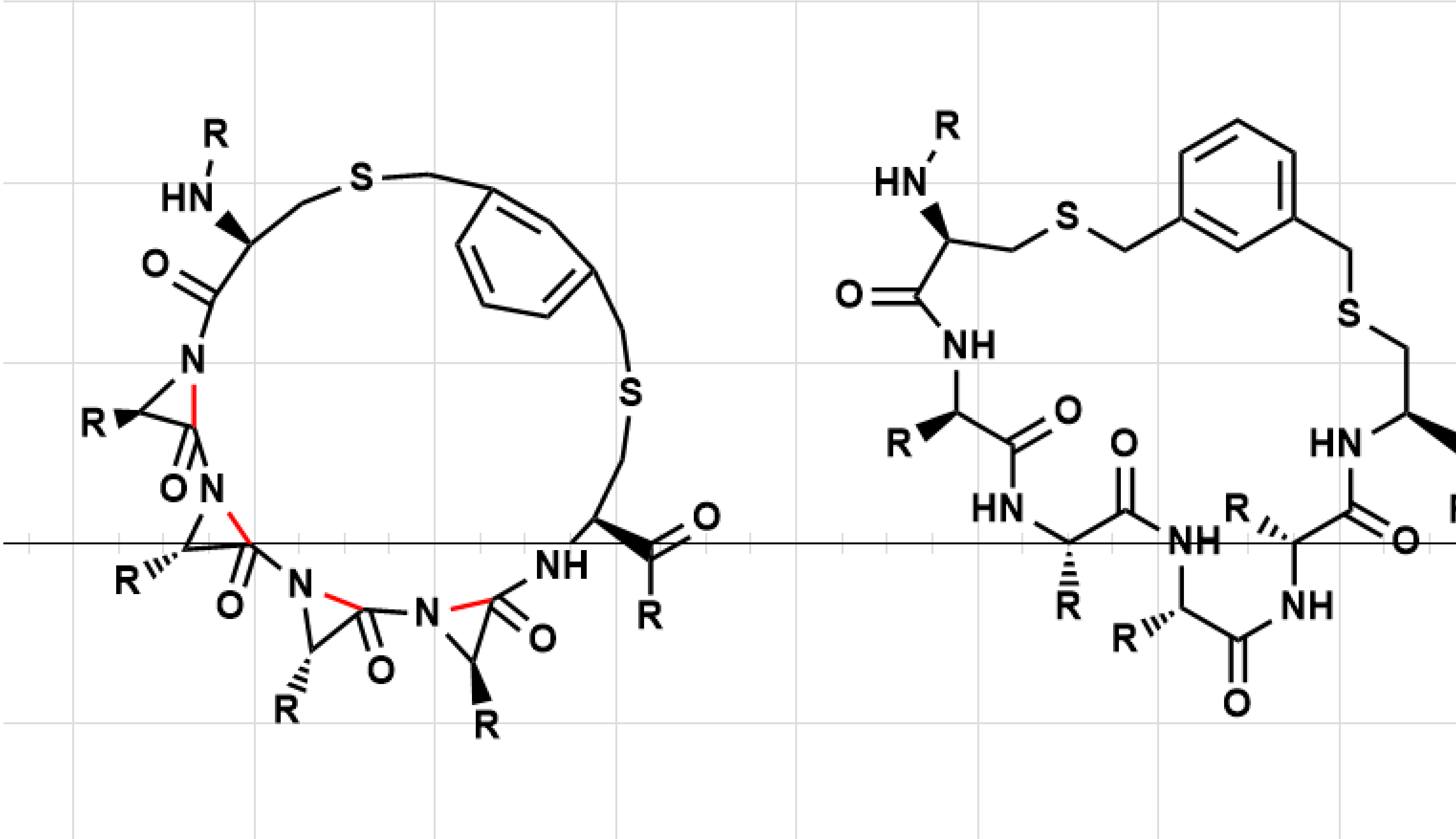
Hi, I am trying to create a combinatorial library (macrocyclic peptide) in DataWarrior. The issue I run into however is that every amide bond forms correctly with the next amino acid, but for some reason it also forms a bond (red bond in image) between the N and C=O of the same amino acid, creating a urea-like motif (refer to image attached). If the red bond is deleted, it forms the correct structure. Curiously, this issue does not happen when running DW on Mac. Is there a way to fix this on Windows so that it runs correctly as well, or is there some sort of setting that changes this? I reinstalled DW, but still run into the same issue.

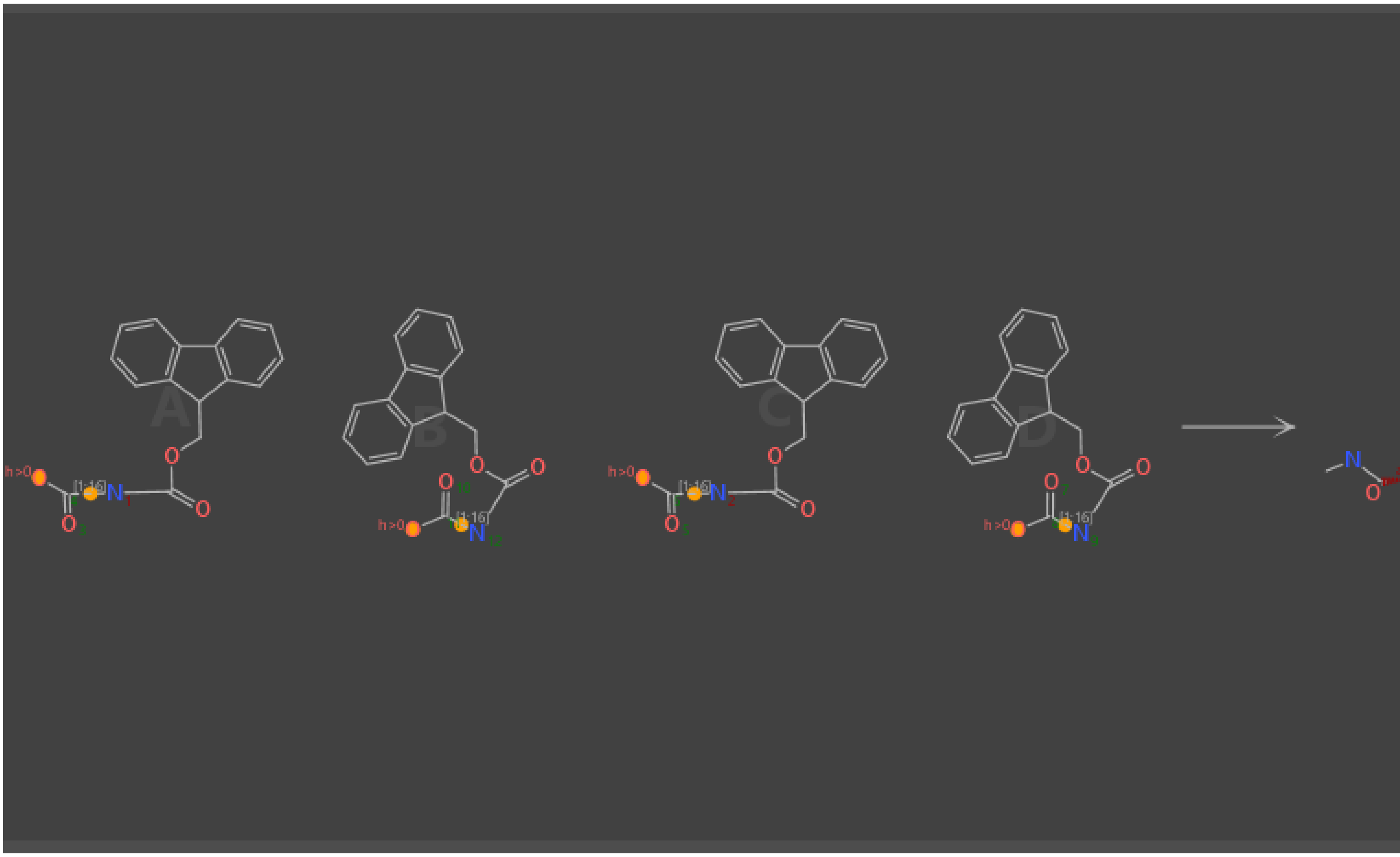
Macrocycle:
Reaction:

File Attachments

1) Screenshot_1.png, downloaded 835 times



2) Screenshot_2.png, downloaded 807 times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