
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 343 times
 - 2) [Screenshot_2.png](#), downloaded 323 times
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