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Subject: Re: Pentavalent carbonyl issue (urea formation?)

Posted by [padster](#) on Sat, 24 Jun 2023 21:45:29 GMT

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Hi Thomas, thanks for getting back to me. However, I still get the incorrect product when I run your macro. When I try to make it myself, it rearranges the mapping so that each nitrogen is 1, 6, 9 or 12 and the first carbonyl is 2-3, but the second one is 4-5 (see attached image). It is also strange how my old mapping does not work on Windows, but it worked perfectly fine on Mac. I'm getting the idea that the Windows version is reading the mapping different or automatically changes it somehow (if that's even possible).

Image:

Structure:

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### File Attachments

- 1) [Screenshot\\_1.png](#), downloaded 424 times
  - 2) [New library.dwar](#), downloaded 282 times
  - 3) [Screenshot\\_2.png](#), downloaded 514 times
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