Subject: Re: Pentavalent carbonyl issue (urea formation?)
Posted by padster on Sat, 24 Jun 2023 21:45:29 GMT
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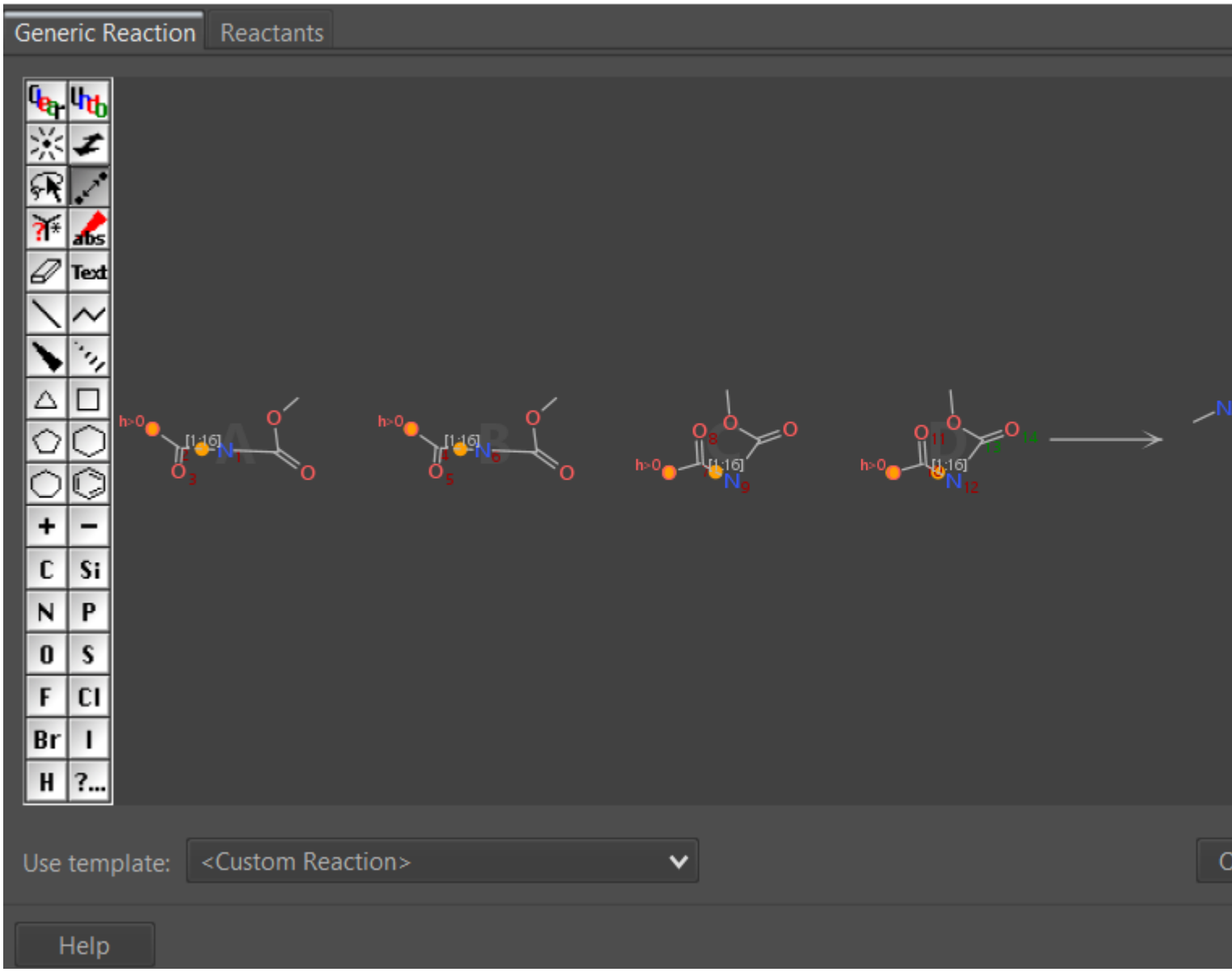
Hi Thomas, thanks for getting back to me. However, I still get the incorrect product when I run your macro. When I try to make it myself, it rearranges the mapping so that each nitrogen is 1, 6, 9 or 12 and the first carbonyl is 2-3, but the second one is 4-5 (see attached image). It is also strange 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).

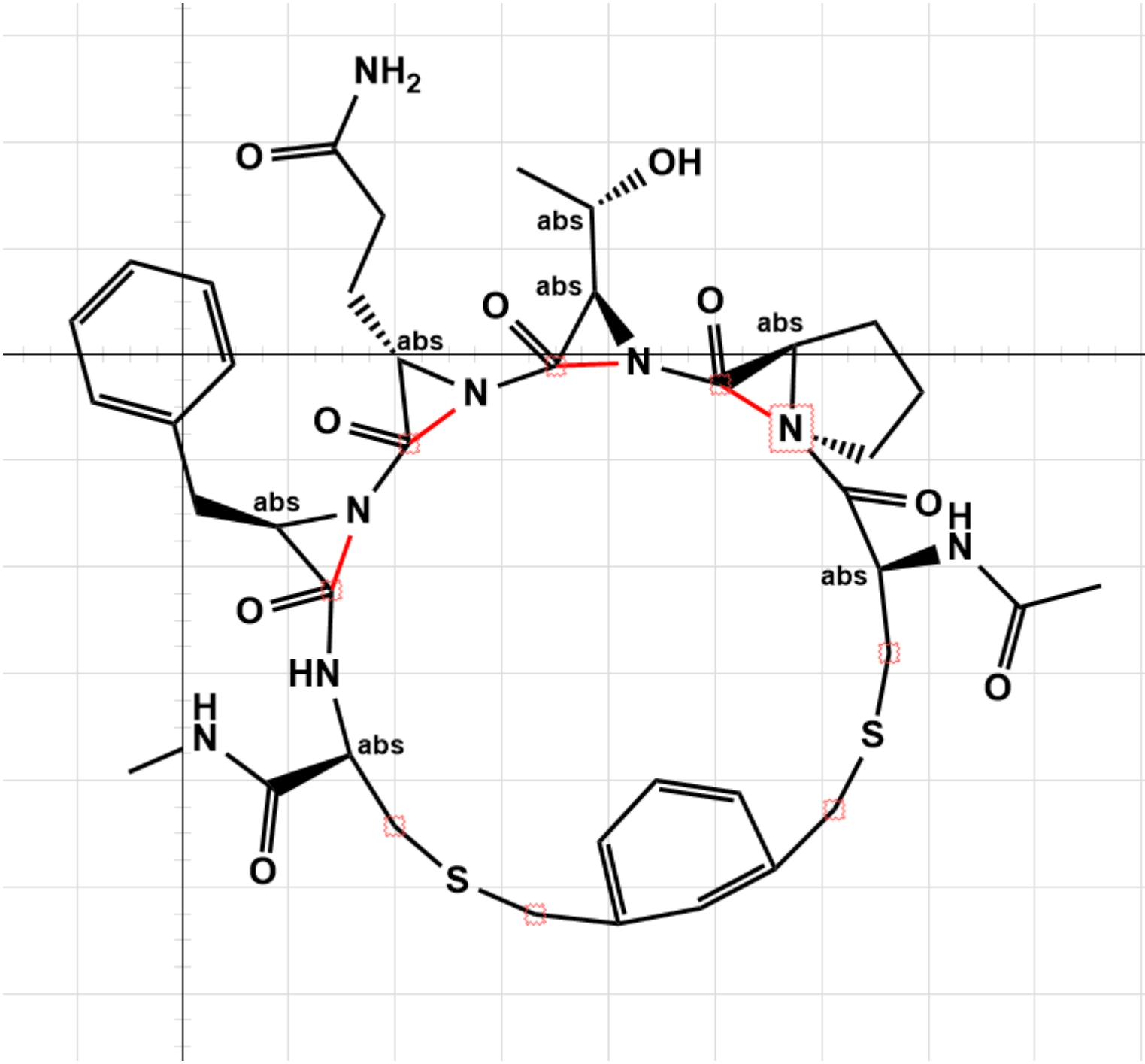
Image:
Structure:

File Attachments

1) Screenshot_1.png, downloaded 727 times



2) New library.dwar, downloaded 472 times
3) Screenshot_2.png, downloaded 813 times


NH2
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