

Exploring the formation of nitrogen-rich, six-membered polycyclic compounds

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ABSTRACT

Nitrogen-rich polycyclic compounds are widespread in nature, have interesting biological activities and are privileged scaffolds among pharmaceuticals. The cyano-Schmitt cyclization (or, as it can also be called, the tridehydro-Diels-Alder – tri-DDA – reaction) is an intramolecular cyclization reaction and, formally, the equivalent of an oxidized Diels-Alder reaction that can afford these kinds of compounds under reaction conditions free of metals and complex reagents.

To further probe the scope of this reaction, we synthesized a substrate that would hypothetically undergo tri-DDA reaction and form novel polycyclic, nitrogen-rich six-membered compounds. The reaction gave the desired compound with four fused six-membered rings, two of them being pyridines (**A**), and its fully aromatized analog (**B**). We were able to isolate both in moderate yields. Decomposition of the starting material and formation of unidentified side products were also observed. Control experiments were also conducted to gain insight about the mechanistic pathway of the reactions.

From ¹H-NMR spectroscopy it was determined that both compounds were formed simultaneously (**A**:**B** in a 2:1 yield), quickly, and from the same starting material. Control experiments showed that base is needed for the cyclization to proceed to form **A**, but it is still not known how **B** was formed. To our knowledge, there is no literature data on either of these compounds and so it is interesting to explore this reaction in further detail. Future directions include optimizing the reaction by using bulkier bases and repeating the synthesis at lower temperatures.