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Title: Bicyclic (Alkyl)(Amino)Carbene (BICAAC) as an Organocatalyst for Gomberg Bachmann Coupling Reaction: Unravelling Conventional Biaryl Synthesis Through

a Novel Approach

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Abstract:

Ever since the discovery of carbenes, they are known to be highly reactive transient intermediates in organic reactions due to their incomplete electron octet. Later, stable N- heterocyclic carbenes (NHCs) have emerged as powerful tools in organic, inorganic, and organometallic chemistry, owing to their remarkable stability and diverse applications. Here, in this work, we are focusing on one of the recently discovered carbene by Bertrand and co-workers having a bicyclic framework, bicyclic (alkyl)(amino) carbene or commonly known as BICAAC, which is more advanced compared to NHCs in terms of better electrophilicity as well as nucleophilicity. In this project, we have tried to explore the potential of BICAAC to function as an organocatalyst in the synthesis of biaryl scaffolds. In the first chapter, we have tried to present our efforts in Gomberg-Bachmann coupling reaction by using BICAAC as catalyst and K t BuO as base. We were successful in optimizing the reaction that concluded under ambient conditions with low catalyst loading and resulted in the synthesis of ~21 substrates ranging from reactants containing substituents that are electron donating to electron withdrawing in nature. All the substrates that were synthesized were isolated through column chromatography and fully characterized using 1 H and 13 C{ 1 H} NMR spectroscopy. In the second chapter, we have attempted to unravel plausible mechanistic pathway for this particular reaction. Various control experiments such as radical quenching experiments, competitive reactions and kinetic isotope effect experiments were conducted to get insights into the radical initiation stage and rate-determining steps. Drawing upon a thorough literature review and experimental data, we were successful in proposing a mechanistic pathway for the Gomberg- Bachmann coupling reaction mediated by BICAAC as an organocatalyst. The control experiments, at present, were supported by observations from spectroscopy and HRMS spectrometry. I 1 H and 13 C{ 1 H} NMR

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