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An unprecedented exocyclic n-acyliminium ion (nai) cyclization: Access to fully substituted oxazoles and furocoumarins

Venkata Nagarjuna Babu

Indian Institute of Technology, India

N-acyliminium ions (NAIs) are well recognized as potent or highly reactive intermediates in C-C and C-heteroatom bond forming reactions, and extensively explored for the synthesis of diverse natural-products and bioactive molecules due to their highly electrophilic nature. Chemists have developed N-acyl iminium ion based biomimetic approaches for the synthesis of various alkaloids inspired by nature's design principles. The development of a direct route to access NAI precursors and their further transformations toward diverse scaffolds in single pot is a daunting challenge. The reason is the formation of NAI ion species prerequisite is a good leaving group at the α -position to the nitrogen atom. In order to bring leaving groups at desired position in substrates involves multistep syntheses and which are highly difficult to operate in single pot. These challenges led us to examine a direct synthetic route to access NAI precursors and their further efficient transformations through a cascade process.

Herein, we report a novel super-acid-promoted tandem cyclization strategy to synthesize diversified fully substituted Oxazoles and Furocoumarins from readily available starting materials via insitily generated exocyclic NAI precursor in

one pot. The key step in this transformation involves insitu generation of N-acyliminium ion (NAI) precursor under catalyst and solvent-free conditions, and their further transformations promoted by superacid in the same pot. We have also presented the experimental evidence for the involvement of proto-solvated novel exocyclic N-acyliminium ion. Further, we have examined the photophysical properties of some of the synthesized Furocoumarins and Pyrid-oxazole derivatives.

The important features of the present protocol are transition-metal free, robust, H_2O as sole byproduct, and cleaner reaction profile, and practical method for the synthesis of diverse fused Oxazole's and Furocoumarins.

Speaker Biography

Venkata Nagarjuna Babu obtained his bachelor's degree (B.Sc.), in 2009 and master's degree (M.Sc.) in Organic Chemistry from Osmania University, Hyderabad, Telangana, in 2011. Then he worked as a Lecturer on contract basis in Narendra Degree & PG College, Armoor, Telangana in 2012 to 2013. After securing CSIR-UGC-JRF (2013), he joined the research group of Dr. Sharada's Catalysis and Chemical Biology Lab in the Department of Chemistry as a Doctoral Fellow at Indian Institute of Technology Hyderabad (IITH), in Jan-2014. He has publications on the topic of organo-iodine reagents promoted C-H functionalization, acid catalysed cyclization's and catalyst-free & solvent-free sustainable organic transformations.

e: nag8289@gmail.com



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