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Synthesis of substituted benzazoles and computational evaluation of their mechanism

Ashok Kumar, Pratibha Sharma and **Ujla Daswani**
Devi Ahilya Vishwavidyalaya, India

In organic synthesis, fused azoles display ample of applications as protecting groups, reagents, ligands, synthetic intermediates, organic materials, and polymers. Thus, there has been a proliferation of new synthetic strategies, photoredox reactions, solvent-free reactions, and cross-coupling for their synthesis. Thus in view of the ever pressing demand of fused azoles, it was thought worthwhile to design and develop a sustainable, environmentally compassionate protocol for the synthesis of these heterocyclic scaffolds. In particular, benzazoles are found to play a noteworthy role as core motif in many anti-microbial, anti-inflammatory, and anti-tumour agents. The present paper elicits a greener, facile and an efficient transition metal-free pathway for the synthesis of 2-substituted benzazoles. Use of cyclohexanone and guanidine/urea derivatives in the presence of N-bromo succinimide (NBS) and oxone, afforded the 2-aminobenzimidazoles (2-ABI)/2-aminobenzoxazoles (2-ABO). Structures of all the synthesized compounds were substantiated on the basis of FTIR, ^{1}H and ^{13}C-NMR, mass spectroscopy, and elemental analyses data. Purity of all the synthesized compounds was ensured on the basis of column and thin layer chromatographic elution using appropriate binary eluting systems. Present strategy deals with a green laboratory platform embracing several advantages such as the better selectivity, mild reaction conditions, clean reaction profiles, simple product filtration to furnish excellent yields. The combination of NBS and oxone are the tools lying underneath of umbrella of green chemistry. Moreover, the synthetic strategy was analyzed on the basis of certain ecological parameters *viz*., ecoscale score and *E*-factor. Furthermore, the mechanism has been computationally authenticated using density functional theory (DFT) with 6-311++G(d) basis sets available in Gaussian 09 program suite.

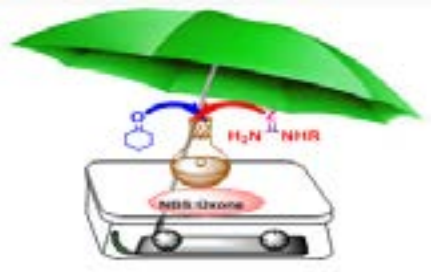

Fig.1 A Greener Synthetic Pathway for benzo fused heterocycles

Recent publications

1. Gagandeep Kour Reen, Monika Ahuja, Ashok Kumar, Rajesh Patidar and Pratibha Sharma (2017) ZnO nanoparticle-catalyzed multicomponent reaction for the synthesis of 1,4-diaryl dihydropyridines. Organic Preparations and Procedures International 49:273-286.
2. Ujla Daswani, Nitin Dubey, Pratibha Sharma and Ashok Kumar (2016) A new NBS/oxone promoted one pot cascade synthesis of 2-aminobenzimidazoles/2-aminobenzoxazoles: A facile approach. New Journal of Chemistry 40:8093-8099.
3. Monika Ahuja, Gagandeep Kour Reen, Ashok Kumar and Pratibha Sharma (2016) A typical NEDDA cycloaddition strategy between C-3- and N-substituted indoles and butadienes using silica-supported copper triflate as an efficient catalytic system: A correlative experimental and theoretical study. Chemistry Letters. 45:752-754.
4. Ujla Daswani, Pratibha Sharma, and Ashok Kumar (2015) A comprehensive account of spectral, Hartree Fock, and Density Functional Theory studies of 2-chlorobenzothiazole. Journal of Molecular Structure 1079:232–242.
5. Bandyopadhyay P, Prasad G K, Sathe M, Sharma P, Kumar A and Kaushik M P (2014) Titania nanomaterials: Efficient and recyclable heterogeneous catalysts for the solvent-free synthesis of poly-substituted quinolines via Friedlander hetero-annulation. RSC Advances 4:6638-6645.

Biography

Ashok Kumar, maintaining an active research laboratory, has expertise in synthesis, spectroanalytical characterization and structure-biological activity evaluation of synthesized compounds and also, the role of nanoparticles catalyzed heterogeneous synthetic routes was envisaged to develop and optimize the synthetic protocols. He explores the computational Gaussian 09 program suite as the theoretical tool to ascertain the mechanistic aspects of their formation. Besides, he tries to evaluate the redox behavior of the compounds using computer controlled potentiostatic devices. To date a number of heterocyclic categories ranging from three-membered aziridines to eight-membered azocins and supramolecular macrocyclic calixarenes were designed and developed in his laboratory.

drashoksharma2001@yahoo.com