ONE-POT PREPARATION OF 1,2,3-BENZOTRIAZIN-4(*3H*)-ONES AND ACETYLBENZOTRIAZOLES USING A KEY Cp*Co(III)-CATALYZED C−H AMIDATION STEP

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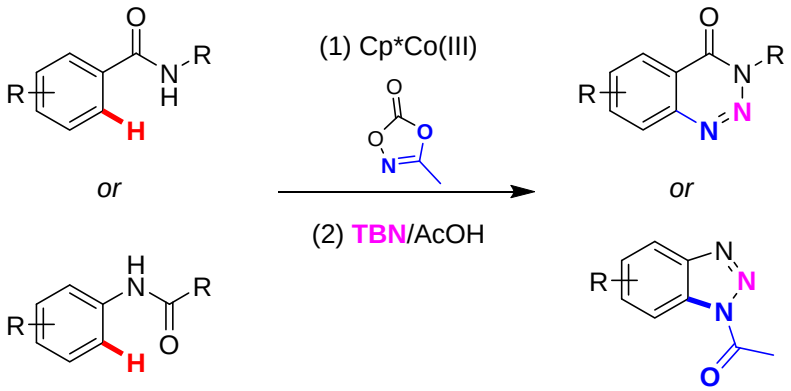
1,2,3-benzotriazin-4(*3H)*-one and benzotriazoles derivatives have been recognised for their potential application as pesticides and pharmaceuticals thus new facile methodologies for their preparation, starting from readily accessible reagents would an attractive proposition.[1,2]



In our recent research, we have focused on developing efficient routes to valuable heterocyclic compounds starting from inexpensive, readily available, benzamide and acetanilide substrates. In this context, we report the use of a Cp*Co(III) catalyst for the amidation of these substrates using 1,4,2-dioxazol-5-ones as amidating agent. The isolable amidated products can thereafter be readily converted to the desired 1,2,3-benzotriazin-4(*3H*)-one and *N*-acetylbenzotriazole derivatives through the use of *tert*-butyl nitrite (TBN) under mild conditions.[3]

It was found to be possible to perform the second step with the crude reaction mixture obtained from the initial C-H amidation step, leading to the overall development of a facile one-pot sequential procedure for the preparation of a range of substituted derivatives. In addition, the key Cp*Co(III)-catalyzed C-H amidation step has been studied by DFT calculations in order to fully elucidate the reaction mechanism of the C-H amidation reactions for both benzamide and acetanilide substrates.

[1] Z. Khalid, H. A. Ahmad, M. A. Munawar, M. Khan, S. Gul, Heterocycles, 2017, 94, 3.

[2] I. Briguglio, S. Piras, P. Corona, E. Gavini, M. Nieddu, G. Boatto, A. Carta, Eur. J. Med. Chem., 2015, 97, 612.

[3] P. G. Chirila, L. Skibinski, K. Miller, A. Hamilton, C. J. Whiteoak, Adv. Synth. Catal., 360, 2324.