

ACCESS TO UNUSUAL HETEROCYCLIC COMPOUNDS UTILIZING A KEY COBALT-CATALYZED C-H FUNCTIONALIZATION APPROACH

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Since the publication of Matsunaga and Kanai in 2013 demonstrating the potential of Cp*Co^{III}-type catalysts in C-H functionalization protocols[1], the field has rapidly expanded and engaged the interest of a large number of researchers[2]. In general, these reports can be divided into two key areas; (a) linear couplings and (b) new/efficient routes to heterocycle formation. The latter of these areas is of significant interest as most of the small molecule drugs approved by the FDA in 2017 contained complex heterocyclic motifs[3] and as a result novel, improved methods for their synthesis is likely to be an important innovation. In this context, we have engaged in the use of Cp*Co^{III} catalysts, with readily available benzamide substrates, for the preparation of some more unusual heterocyclic compounds through either a cascade reaction[4] or a two-step sequential one-pot protocol[5] using C-H functionalization as the key step in both cases. In addition to these synthetic results, studies of their mechanisms using DFT have revealed key aspects of the catalytic cycles, allowing for a fuller understanding of the observed selectivities and reactivities. In summary, this contribution showcases the potential for rapidly building up molecular complexity exploiting efficient and sustainable first-row transition metal catalysis as the key tool.

[1] T. Yoshino, H. Ikemoto, S. Matsunaga, M. Kanai, *Angew. Chem. Int. Ed.*, **2013**, 52, 2207.

[2] For an overview see: P. G. Chirila, C. J. Whiteoak, *Dalton Trans.*, **2017**, 46, 9721.

[3] L. M. Jarvis, *Chem. Eng. News*, **2018**, 96, 26.

[4] P. G. Chirila, J. Adams, A. Dirjal, A. Hamilton, C. J. Whiteoak, *Chem. Eur. J.*, **2018**, 24, 3584.

[5] P. G. Chirila, L. Skibinski, K. Miller, A. Hamilton, C. J. Whiteoak, *Adv. Synth. Catal.*, **2018**, 360, 2324.