REGIOSELECTIVE C-H ARYLATION OF NITRO HETEROCYCLES AND FURTHER TRANSFORMATION OF MANIPULABLE NITRO GROUP

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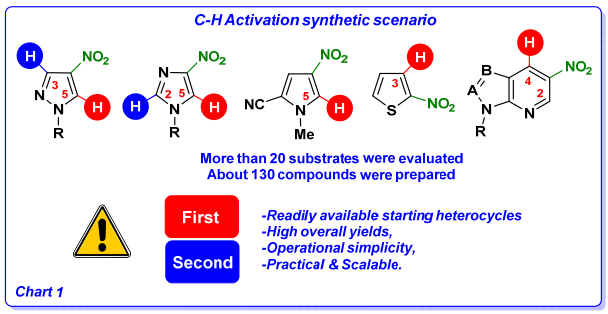
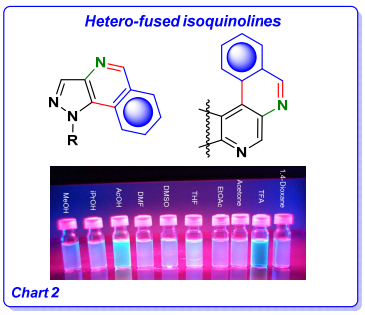
In recent years, transition metal catalysed C-H activation emerged as one of the most important methodologies of modern organic chemistry. The issue of selectivity in C-H activation of complex organic substrates containing two or more reactive C-H bonds, in particular drug-like heterocyclic scaffolds, is a pivotal topic to contemporary organic synthesis.





The Pd and Ni catalysed, guided and regioselective C-H arylation protocols for series of 4-nitropyrazoles, 4-nitroimidazoles, annulated 3-nitropyridines and several other nitro heterocycles were developed (*Chart 1*). The method described here is a facile tool for chemical functionalization of drug-like 5- and 6-membered nitro heterocycles. Scope and limitations of the developed methodologies and putative reaction mechanism were studied. Quintessential, the elaborated route had been utilized for construction of several hetero-fused isoquinolines – scaffolds with materials relevant photoelectronic properties (*Chart 2*) [1-3]. Furthermore, TM-catalysed C–H arylselenation of the title heterocyclic substrates was also successfully elaborated [4]. Finally, we demonstrated the chemical potential of manipulable nitro group transforming it into different functionalities [5]. Part of this work was supported by NCN SONATA 10 grant no. 2015/19/D/ST5/02774.

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