Abstract

[Index No.: 202/18/Chem./26]

Title: "Development of C–C Bond Forming Reactions Through $C(sp^3)$ –H Bond Functionalization: Approach for the Construction of Novel (Spiro)heterocycles"

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The thesis entitled "Development of C–C Bond Forming Reactions Through C(sp³)–H Bond Functionalization: Approach for the Construction of Novel (Spiro)heterocycles" is divided into five chapters. Chapters 1 and 4 consist of the introductory part about a brief overview of the hydride transfer reaction and indole-3-carboxylic acid derivatives respectively.

Chapter two deals with an atom economic redox neutral direct synthesis of 2-coumaranone bearing spirotetrahydro(iso)quinolines. A Lewis acid-free intramolecular C(sp³)–H bond functionalization has been described triggered by consecutive [1,5]-hydride shift /cyclization process, an approach for diastereoselective construction of novel spiroheterocycles in unprecedented cascade methods. The reaction proceeds through in-situ production of the olefin derivative from the corresponding aldehyde in one pot. We developed a cascade highly diastereoselective spirocyclization strategy without the help of any transition metal or oxidant. A reasonable reaction mechanism supported by control experiments has also been proposed to explain product formation.

Chapter three describes a Lewis acid catalyzed intramolecular C(sp³)–H bond functionalization, triggered by consecutive [1,5]-hydride shift /cyclization process, an approach for diastereoselective construction of novel pharmaceutically relevant spiroheterocycles. To explore substrate-scope diversity, several bioactive scaffolds such as benzofuran-3-one, 3-isochrommmanone, and the succinimide have been introduced for the preparation of *ortho* aminobenzylidene substrates through Knoevenagel or Wittig-type reaction which is the precursor of novel spiroheterocycles. These pharmacophore containing novel spirotetrahydro(iso)quinoline derivative has been made diastereoselectively utilizing hydride shift strategy in a straightforward, atom-economical oxidant free redox neutral process.

Chapter five reveals unorthodox cascade redox reactions of isatin using DMSO as a methine source for expeditious route to indole-3-carboxylic acids, and anthranilic acids. Switching the reaction condition this strategy enabled the access of indole-3-carboxylic acid (ICA) and anthranilic acid (AA) derivatives directly from isatin derivatives. The biggest advantages of methodology are the preparation of key intermediate ICA derivatives (an overall reduced product) without using any reducing agents, transition metal catalyst, Lewis acid, or employing an expensive directing group, and the same for AA (an overall oxidized product) employing none oxidant externally in economically viable and operationally simple conditions. The control experimental investigation study justified the mechanism of two different products described in detail in this chapter.

(Signature of the Supervisor and date) 29. 05. 2023

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