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ACCEPTED MANUSCRIPT

An isocyanide based multi-component reaction under catalyst- and solvent-free conditions for the synthesis of unsymmetrical thioureas

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Abstract: A new and efficient method for the synthesis of thiourea derivatives by a sequential one-pot, three-component reaction between aromatic isocyanides, amines, and 1,2-di-*tert*-butyldisulfane (DTBS) was developed and **27** different examples were synthesized in good to excellent yields. DTBS was identified as an effective sulfur surrogate without the use of both catalysts and solvents. This protocol does not employ any transition metal catalyst or special experimental setup.

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Catalyst- and solvent-free approaches towards organic synthesis have attracted an immense interest from the organic chemistry community over recent decades.[1-2] The avoidance of catalysts and solvents in well established chemical processes, or the replacement of toxic solvents with more environmentally-benign solvents, has become a major focus in the pharmaceutical industry. Also, multicomponent reactions (MCRs) have become an effective approach for rapid assembly of complex molecules from simple precursors in a one-pot procedure *via* the formation of carbon-carbon and carbon-heteroatom bonds.[3] These domino-type reactions involve multiple intermediate reactions where the product of the first is the starting substrate for the subsequent and can also incorporate "green chemistry" values such as atom economy, time, and labour economies.

Thiourea containing molecules have been reported to possess a plethora of biological properties such as anti-bacterial, anti-fungal, anti-inflammatory and anti-cancer.[4] In addition, they are used as supramolecular assemblies, and anion sensing.[5] On the other hand, the area of organocatalysts has been dominated by the cinchona-thiourea based catalysts for variety of organocatalytic transformations.[6] These intrinsic qualities of thioureas, in combination with

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