Abstract

Solvent-free multicomponent reactions are very important tools to carry out organic synthesis and functional group transformations rapidly thus opening up the possibility of synthesis of a wide variety of organic compounds in a very clean and an efficient manner according to the postulates of Green Chemistry. There are several methods for the synthesis of Nitrogen Containing Heterocyclic Compounds but most of the methods suffer from various drawbacks like low yield, harsh reaction conditions, use of toxic solvents, long reaction time and tedious work up procedures. Taking all these facts into consideration, we have tried to synthesize few Nitrogen containing Heterocyclic Compounds in a clean and efficient manner using solvent free multi-component approach taking some of the Transition Metal Borates as catalysts.

The entire thesis has been segregated into 6 (six) broad chapters and many chapters are further divided into sections for better discussion of the outcomes of the research work.

Chapter-I includes a brief introduction to the concept of Solvent free multicomponent reactions and the postulates of Green Chemistry. An idea about the Nitrogen Containing Heterocyclic compounds which have been prepared in this work is given in the chapter along with the recent literature review and their various biological applications. This chapter also includes a brief introduction to the transition metal borates under study and their applications in various fields of science.

Chapter-II is the experimental section where the sources and purity of various chemicals used in this research work is documented. It also includes the details of the various analytical and spectroscopic techniques like Melting Point determination, FT-IR spectroscopy, NMR spectroscopy, X-Ray Crystallography, etc., used for physicochemical characterization of the synthesized compounds. This chapter also includes the details of the theoretical works carried out on the selected synthesized compounds like DFT, Molecular Docking and Pharmacokinetic studies.

Chapter-III has been divided into three sections. **Section-A** contains the multi-component green synthesis of 2,4,5-triaryl imidazole derivatives using Copper Borate (CuB_4O_7) as a catalyst wherein a variety of 2,4,5 triaryl imidazoles have been prepared using Benzil, aromatic aldehyde and ammonium acetate). The reaction proceeded in a milder way with excellent yield of the products. The products were characterized by FT-IR and ^{1}HNMR spectroscopic techniques. **Section-B** comprises of the Synthesis, X-ray Diffraction study, Hirshfeld surface analysis and catalytic activity of Bis[2-(4,5-diphenyl-1H-imizol-2-yl)-4-nitro-phenolato] copper (II) dihydrate complex. This chapter is also important from the view that the evidence of in-situ conversion of CuB_4O_7 into $Cu(OAc)_2.2H_2O$ in presence of NH_4OAc is discussed here. **Section-C** of the chapter mostly focusses on the DFT, Molecular Docking and Pharmacokinetic study of some selected synthesized 2, 4, 5-triarylimidazole derivatives.

Chapter-IV is divided into two sections. **Section-A** of the chapter deals with the green synthesis of 3,4-dihydropyrimidine-2-(1H)-ones (DHPMs) using Iron Borate as an efficient catalyst using substituted Benzaldehyde, Ethyl acetoacetate and Urea. The reaction provides a method for the synthesis of a variety of 3, 4-dihydropyrimidine-2-ones with good to excellent yields and the catalyst has been versatile for a wide range of aromatic aldehydes. The products were characterized by FT-IR and ^{1}HNMR spectroscopic techniques. **Section-B** of the chapter includes the DFT, Molecular Docking and Pharmacokinetic study of some selected 3, 4-dihydropyrimidin-2(1H)-one (DHPM) derivatives.

Chapter-V contains two sections. **Section-A** of the chapter includes an efficient and green protocol for the synthesis of 1-hydroxy-2-arylimidazole-3-oxide derivatives under solvent free condition using inexpensive Copper borate (CuB_4O_7) catalyst using a mixture of diacetyl monoxime, substituted benzaldehyde and hydroxylamine hydrochloride and the products were characterized by FT-IR and ^{1}HNMR spectroscopic techniques. **Section-B** includes DFT, Molecular Docking and Pharmacokinetic study of some selected 1-hydroxy-2-arylimidazole-3-oxide derivatives.

Chapter-VI deals with the solvent free green synthesis of 2-substituted benzimidazole and 1, 2-disubstituited benzimidazole derivatives using Nickel Borate as a catalyst with excellent yield of products. The synthesized products were characterized by FT-IR and ^{1}HNMR spectroscopic techniques.

Finally, the thesis ends with concluding remarks of the research work embodied in the thesis.