

The development of green multi-component reactions as an efficient synthetic methodology for the construction of biologically active molecules have received great attention in the last couple of decades. However, organic scaffolds such as 2,3-dihydrofurans and 2,3-dihydrofuro[3,2-*c*]coumarins (DHFC), despite possessing an extremely wide range of biological activities were yet to be succumb in greener way. Following the nature's footsteps, herein we reported an eco-friendly, inexpensive, and efficient one-pot green multicomponent approach to synthesize *trans*-2,3-dihydrofuro[3,2-*c*]coumarins (DHFC) catalyzed by imidazole in water under mild conditions. Applications of the developed catalytic process under a multicomponent strategy in a greener medium revealed the outstanding activity, productivity, and broad functional group tolerance, affording a series of newly designed DHFC in excellent yields. In addition, the biological study that was carried out by the collaborative group demonstrates the ability of the synthesized DHFC derivatives to bind to human serum albumin (HSA). Detailed *in silico* and *in vitro* structure-activity analysis has been performed, covering all the bases of this biological investigation. Furthermore, the developed strategy was implemented to synthesize bioactive heterocycles, namely dimedone fused 2,3-dihydrofuran derivatives, under mild conditions with excellent yields, using imidazole and water as green catalyst and solvent, respectively. The synthesized dimedone based 2,3-dihydrofuran derivatives have been found to inhibit SaTR *in vitro* at low to medium micromolar concentrations. On the other hand, the indole alkaloids are known as an epic family of natural products with structurally diverse architecture and a wide range of biological activities. In line, a BF₃.OEt₂ catalysed cascade strategy for the synthesis of highly substituted pyrrolo[1,2-*a*]indole core with high diastereoselectivity has been developed. Further, biological evaluation of synthesized derivatives was reflected in their excellent bioactivity. Further, oxidation of polycyclic aromatic hydrocarbons (PAHs) found to be an important area belongs to the biochemistry, astrochemistry, and chemical industries. In line, we have developed the one-pot oxidation of naphthalene, anthracene, pyrene and substituted PAHs in the presence of H₂O₂ and newly designed [Cu^{III}L] complex derived from non-toxic transition metal and ligand based redox-active PLY backbone, that provided a route for their detoxification and conversion into industrially important compounds. Furthermore, transforming the alcohols and aldehyde groups to esters via oxidative coupling with alcohols has become an attractive target for organic chemists, due to the significance and omnipresence of ester group in chemistry. Thus, a new-designed V-catalyst [(L₂)V^{IV}O](ClO₄) was synthesized and utilized for its potential catalytic activity towards direct oxidation of two different functionalities, alcohols and aldehydes to their corresponding esters in one-pot procedure using H₂O₂ and alcoholic medium. Moreover, cinnamate esters transformed to ester (via C=C bond breaking followed by oxidation of in-situ generated aldehyde) in single-step, which is found to be the first ever report to this end.

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