

Research Summary

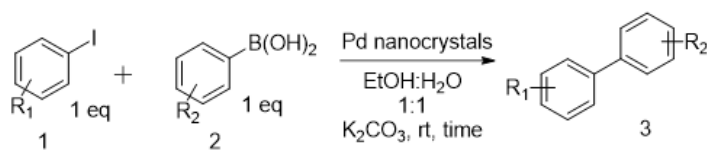
Soumyadip Das

I am Soumyadip Das, on the verge of completing my PhD studies at Vellore Institute of Technology, Vellore, India. My primary focus of research revolves around the intricate realms of heterocyclic molecule synthesis and organic synthesis. In the pursuit of my doctoral studies at Vellore Institute of Technology, I have dedicated my efforts to unravelling the methodologies and mechanisms involved in the creation of diverse heterocyclic structures. This exploration extends to the broader domain of organic synthesis, where I seek to contribute novel insights and methodologies to the synthesis of organic compounds with a particular emphasis on their applications in various scientific fields. In addition to that, I bring valuable work experience in Computational Chemistry to my research portfolio. I have actively engaged in Molecular Docking and Molecular Dynamics (MD) Simulation methodologies, applying them to investigate the potential of synthesized heterocyclic molecules as drug candidates. In the forthcoming discussion, I will provide concise overviews of each research endeavour, offering insights into the methodologies employed and the implications of these investigations.

1. Facet-Dependent Catalytic Activity of Palladium Nanocatalyst in C-C bond formation reaction

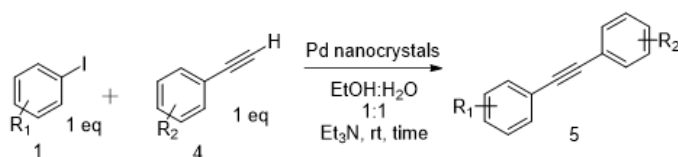
Palladium nanocubes, octahedra were synthesized and examined for facet dependent catalytic activity in C-C bond formation reaction. Herein, we have performed the synthesis and application of Pd nanocubes in the Suzuki-Miyaura cross-coupling reaction and Sonogashira coupling reaction. The Pd nanocubes with Pd(100) facet showed excellent catalytic activity, as it takes less reaction time than the Pd octahedra with Pd(111). The possible reason is that the Pd(100) facets have a lesser surface atom density and more degree of unsaturation of the nano crystal atoms than Pd(111) facets.

Suzuki-cross Coupling Reaction



Nanocrystals	Time
Cube	1-1.2 h
Octahedra	2-3 h

Sonogashira Coupling Reaction



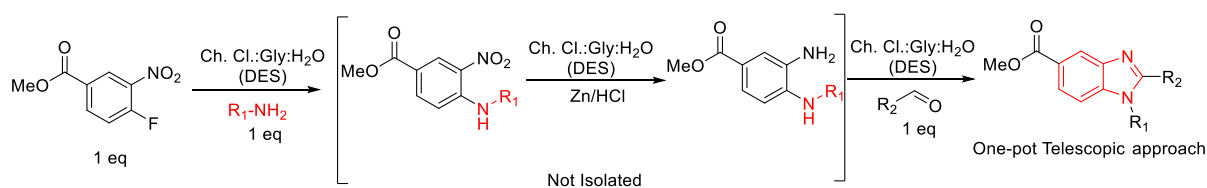
Nanocrystals	Time
Cube	1-1.2 h
Octahedra	2-3h

(This work communicated in ChemNanoMat)

Also, in this context we have published one review in ChenNanoMat.

2. One-pot telescopic approach to synthesize disubstituted benzimidazoles in deep eutectic solvent

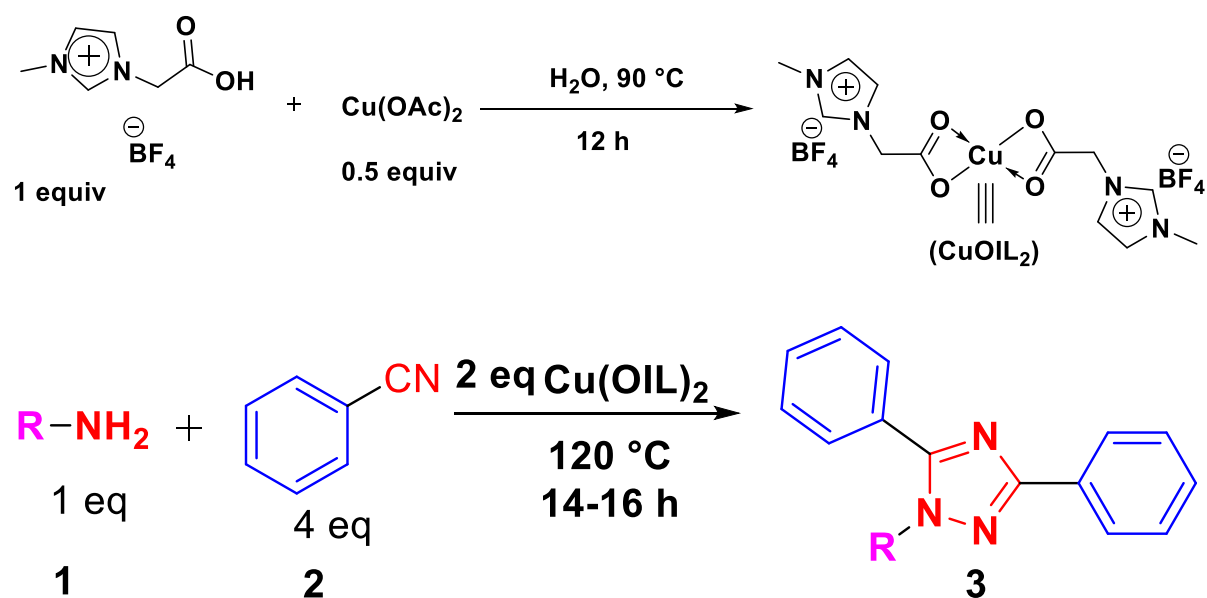
This work deals with an ongoing challenge in the pharmaceutical sector is the need to find and implement novel synthetic approaches because traditional methods sometimes violate the principles of green chemistry. While benzimidazoles are of great importance as building blocks for the creation of molecules having pharmacological activity, the development of methods for their sustainable synthesis has been a challenge for organic synthesis. Herein, we have carried out a one-pot telescopic approach to the synthesis of disubstituted benzimidazole derivatives in a deep eutectic solvent (DES) medium to investigate an alternate synthetic technique. Starting with methyl 4-fluoro-3-nitrobenzoate, S_NAr reaction, reduction, and cyclization were performed with choline chloride/glycerol/ H_2O as DES medium, which gave the best performance out of the five DESs examined.



(This work published in *Synthesis*)

3. Solvent-free synthesis of 1,2,4-triazole by using ionic liquid supported Copper catalyst

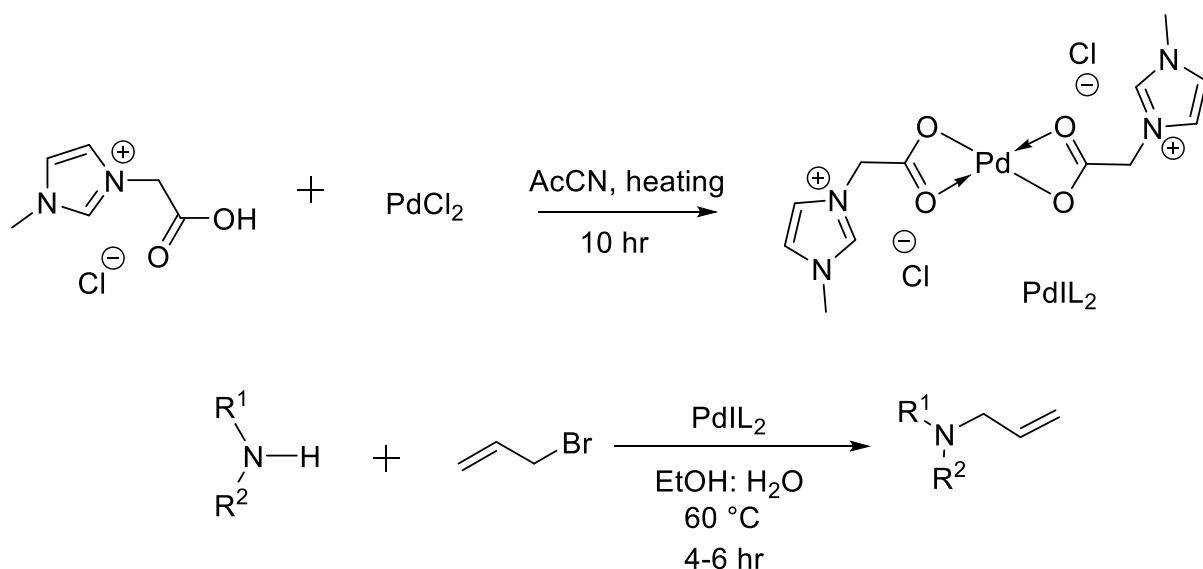
This work deals with the synthesis of a series of 1,2,4 triazole using Ionic Liquid supported copper catalyst in solvent free condition. Main goal of this work is to improve the yield and decrease the reaction time by following the Green Chemistry principle.



(This work recently communicated in *Organic Chemistry Frontiers*)

4. Ionic Liquid supported Palladium catalyzed Tsuji-Trost Allylic Amination reaction

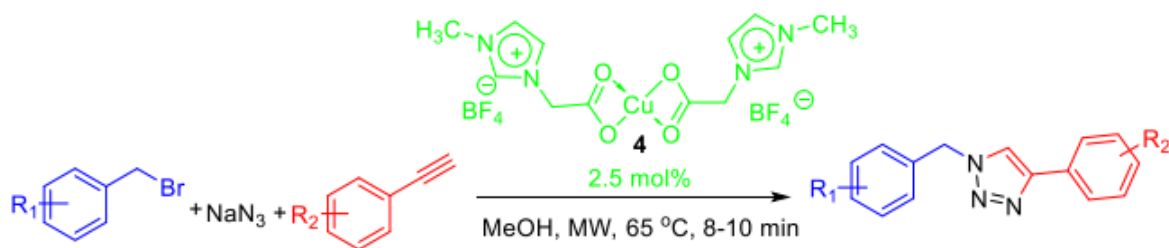
In this work, we have performed the Tsuji-Trost coupling reaction using Ionic Liquid supported Palladium catalyst.



(This project is ready for communication)

5. Sequencing [3+2]-cycloaddition and multicomponent reactions: A regioselective microwave-assisted synthesis of 1,4-disubstituted 1,2,3-triazoles using ionic liquid supported Cu(II) precatalysts in methanol

Heterocyclic compounds with two to three nitrogen atoms play a pivotal role in the normal life cycle of a cell. Further the design and synthesis of a quality heterocyclic compound library with N-atoms as new chemical probes active, is vital in drug discovery. In this context, an efficient one-pot multicomponent strategy for the synthesis of a mini library of 1,4-disubstituted 1,2,3-triazoles is described. This new multicomponent one-pot method features a combination of ionic liquid supported Cu(II) precatalysts in methanol catalyzed [3+2]-cycloaddition with microwave irradiation reactions. The synthetic manipulation involved the efficient reduction of ionic liquid supported Cu(II) catalyst by methanol followed by [3+2] cycloaddition with alkynes using in situ generated azides to obtain 1,2,3-triazoles regioselectively.



(This work published in Tetrahedron Letters)