



CHRIST
(DEEMED TO BE UNIVERSITY)
BANGALORE · INDIA

Notice for the PhD Viva Voce Examination

Mr Venkata Chandrasekhar K (Registration Number: 2071402), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend his PhD thesis at the public viva-voce examination on Thursday, 13 February 2025 at 11.30 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis	:	Strategies for C-N Bond Formation toward One-Pot Regioselective Synthesis of N-Heterocyclic Compounds
Discipline	:	Chemistry
External Examiner - I	:	Dr N G Ramesh Professor Department of Chemistry Indian Institute of Technology Delhi Hauz Khas New Delhi-110016
External Examiner - II	:	Dr N Manoj Professor Department of Applied Chemistry Cochin University of Science and Technology Kochi - 682022 Kerala
Supervisor	:	Dr Ajesh Vijayan Assistant Professor Department of Chemistry School of Sciences CHRIST (Deemed to be University) Bengaluru – 560029 Karnataka

The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Place: Bengaluru
Date: 04 February 2025

Registrar

ABSTRACT

Nitrogen-based heterocyclic aromatic compounds and their derivatives are prevalent motifs in many fields, including natural products, medicinal chemistry, material science, agrochemicals, polymer chemistry, and drug development. We have explored a simple, environmentally friendly, ligand-free copper-catalysed system for synthesizing N-aryl/heteroaryl derivatives of pyrimidine, pyrazine, and 6-bromoquinazolin-4-amine. The broad applicability of this reaction was demonstrated by achieving high yields of novel functionalized N-arylated compounds. We have also developed a one-pot, straightforward, regioselective copper-catalysed method for synthesizing pyrido[1,2-*a*]benzimidazole derivatives. Utilizing CuBr as the catalyst, 1,10-phenanthroline as the ligand, and K₃PO₄ as the base in DMSO solvent at 110°C for 12 hours, we efficiently produced a range of functionalized pyrido[1,2-*a*]benzimidazole compounds with excellent yields.

The regioisomeric structures were confirmed through single-crystal X-ray diffraction analysis. Furthermore, we introduced a metal-free, base-catalysed one-pot synthesis for 11H-dipyrido[1,2-*a*:3',2'-*d*]pyrimidin-11-imine. This approach involves a domino process with simultaneous C-N bond formation. We explored the reaction's substrate scope with various electron-withdrawing and electron-donating groups, leading to the successful preparation of stable 11H-dipyrido[1,2-*a*:3',2'-*d*]pyrimidin-11-imine derivatives with high yields. A plausible reaction mechanism for this synthesis was also proposed.

Keywords: Ligand-free reactions, copper catalyst, C-N bond formation, Ullman coupling, one-pot synthesis, intermolecular cyclization, and ligand.

Publications:

1. **Venkata Chandrasekhar Kommuri**, Krishnaji Tadiparthi, Lokesh Pawar & Athimoolam Arunachalampillai, "A Simple and Efficient Ligand-Free Copper Catalyzed C-N Bond Formation of Aryl (Hetero) Halides and N-Heteroaryl Amines", *Polycyclic Aromatic Compounds*, 2021, 43 (3):1-9. DOI:10.1080/10406638.2021.2019802.
2. **Venkata Chandrasekhar Kommuri**, Ajesh Vijayan, Lokesh Pawar, and Athimoolam Arunachalampillai, 'An Efficient Copper-Catalyzed Regioselective One-Pot Synthesis of Pyrido[1,2-*a*]benzimidazole and Its Derivatives' *Chemistryselect*. 2023, 8, (39); DOI:org/10.1002/slct.202303000.
3. **Venkata Chandrasekhar Kommuri**, Ajesh Vijayan, Metal and Ligand-Free Approach towards the efficient one-pot synthesis of stable 11H-dipyrido[1,2-*a*:3',2'-*d*]pyrimidin-11-imine derivatives. *Chemistryselect*. 2024, 9, (19); DOI:org/10.1002/slct.202401205.