Abstract

Palladium Catalyzed Heteroannulations for Easy Accessing the Compounds of Biological Importance

Submitted by: Debasmita Mondal **Index No: 40/19/Chem./26**

In the view of immense importance of heterocycles which serve as core structure of many drugs, biologically active substrate and naturally occurring compounds, the development of new methodology for their synthesis appears to be important. In this thesis, few elegant methods are reported for the general synthesis of nitrogen and oxygen containing heterocycles of biological importance via palladium-catalyzed cyclizations of acetylenic or allenamide substrates as described briefly below.

Chapter-1 describes the Pd(0) catalysed cyclisation reactions between *tert*-butyl propargyl carbonates and 2-aminotosyl benzamides or sulphonamides to deliver 1, 4-benzodiazepin-5-ones or sultam derivatives. On the other hand, 2-amino benzamides/sulphonamides require propargyl carbonates substituted at acetylenic carbon to undergo the reaction resulting in the stereoselective formations of 3-ylidene-[1,4]benzodiazepin-5-ones/benzo[*f*][1,2,5]thiadiazepine-1,1-dioxides.

Chapter-2 describes facile method for the general synthesis of δ-carbolines or benzofuro[3,2-*b*]pyridines via palladium(0)-catalyzed reactions between allenamides and aryl iodides/bromides. The reaction constitutes a fast intermolecular assembly that takes place in one pot, and the choice of the phosphine ligand is critical for success. A plausible reaction mechanism has been proposed. The reaction is also amenable to the synthesis of bis-heteroannulated products.

Chapter-3 deals with a direct and straightforward method to gain access benzofuro[3,2-*b*]pyrroles or benzofuro[3,2-*b*]indoles through palladium(0)-catalyzed reaction between (benzofuran-3-yl)-*N*-(but-2-yn-1-yl)-4-methylbenzenesulfonamide and aryl iodide followed by a base (DBU) mediated isomerization or DDQ-mediated *Diels-Alder* reaction. The mechanistic rational has been provided. Besides, this reaction is also found to be compatible to polyheteroannulation carried out under one-pot.

Debasmita Mondal
Signature of Candidate
Date: 1/8/2023

Signature of Supervisor with seal
Date: 1/8/2023

Dr. Chinmay Chowdhury
Chief Scientist & Deputy Head
Organic & Medicinal Chemistry Division
Indian Institute of Chemical Biology
4, Raja S. C. Mullick Road
Kolkata - 700 032