

Abstract

Pd-Catalyzed Cycloaddition of Bicyclic Aziridine with Isocyanates [†]

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Abstract: Nitrogen-containing heterocycles can have several applications in the pharmaceutical industry since they contain a wide spectrum of biological activities. Imidazolidinones have shown activity against leukemia, lung cancer, and metabolic disorders. These cyclic urea frameworks can be obtained through transition-metal-catalyzed intermolecular cycloaddition using an aziridine moiety as the starting material. These reactions often provide effective one-step procedures that result in heterocyclic derivatives that are challenging to access through conventional approaches. We have previously described the photoreaction of butyl pyridinium salt with the corresponding bicyclic aziridine in continuous flow. Additionally, we reported that the palladium-catalyzed ring opening of bicyclic aziridines with active methylenes exhibited a new S_N2' selectivity. In this study, the reaction between bicyclic aziridines and several isocyanates, in the presence of Pd(0)-catalyst is presented. The reactions proceed through ring opening of the aziridine moiety, with the formation of the π -allylpalladium complex, followed by cyclization via nucleophilic addition of nitrogen to the isocyanate, affording regioselectively imidazolidinones.

Keywords: pd-catalysis; imidazolidinones; bicyclic aziridines; continuous flow

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