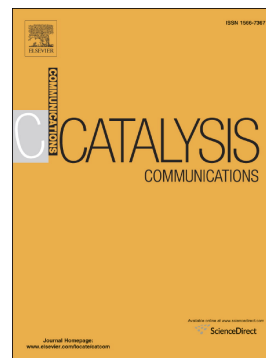


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Palladium-catalysed direct arylation of heteroarenes using 1-(bromophenyl)-1,2,3-triazoles as aryl source

Halima Hadj Mokhtar,^{a,b} Nouria Laidaoui,^{a,b,c} Douniazad El Abed,^{b,*} Jean-François Soulé,^{a,*} Henri Doucet^{a,*}

^a Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes "Organométalliques : Matériaux et Catalyse", Campus de Beaulieu, 35042 Rennes, France. Fax: (+33)2-23-23-63-84 E-mail: jean-francois.soule@univ-rennes1.fr; henri.doucet@univ-rennes1.fr.

^b Laboratoire de Chimie Fine, Département de Chimie, Faculté des Sciences Exactes et Appliquées, Université d'Oran 1 Ahmed BenBella, BP. 1524, EL M'naouer Oran 31100 Algérie.

^c Université des Sciences et de la Technologie d'Oran BP. 1505 El M'naouer Oran 31000 Algérie.

Abstract— A variety of 1-aryl-1,2,3-triazoles containing heteroarenes at C2-, C3- or C4-positions on the aryl ring was successfully prepared via palladium-catalysed direct arylation. These couplings were performed employing 1 mol% of phosphine-free Pd(OAc)₂ catalyst with 1-(bromophenyl)-1,2,3-triazoles and heteroarenes as coupling partners. A wide variety of heteroarenes such as thiazoles, thiophenes, furans, pyrroles or isoxazoles was tolerated. © 2016 Elsevier Science. All rights reserved

Keywords: palladium, C-H bond functionalization, heteroarenes, triazoles, aryl bromides

1. Introduction

1-Aryl-1,2,3-triazoles bearing heteroarenes on the phenyl ring are of considerable interest for pharmaceutical chemistry as they are employed as building blocks for access to biologically active compounds [1-5]. Therefore, the development of simple and convenient processes using readily accessible 1-aryl-1,2,3-triazole derivatives for the synthesis of such compounds is highly desirable.

Currently, heteroarylated 1-aryl-1,2,3-triazoles can be prepared by reaction of an azide functionalized benzene with a terminal alkyne in the presence of CuSO₄ as catalyst [3,6,7] (Scheme 1, a), or via Pd-catalysed Suzuki coupling using a 4-(bromophenyl)-1,2,3-triazole and benzofuran-2-ylboronic acid [8] (Scheme 1, b). An example of Ru-catalysed direct arylation using a 1-phenyl-1,2,3-triazole and a 5-bromofuran derivative as heteroaryl source has also been reported by Ackermann et al. [9] (Scheme 1, c). For this coupling reaction, the triazole moiety acts as a directing group to promote the arylation at C2-position of the phenyl ring. Therefore, this procedure is limited to the heteroarylations at C2-position of the phenyl unit of the 1-phenyl-1,2,3-triazole.

The Pd-catalysed direct arylation of several heteroarenes [10-23], including triazoles [24-26] via a C-H bond activation, using aryl halides as aryl source has led to successes in recent years. Compared to classical Pd-catalysed reactions such as Suzuki, Stille, or Negishi couplings, [27,28] C-H bond functionalization reactions are very attractive, as they do not require the preliminary synthesis of organometallic derivatives. However, to our knowledge, so far no examples of metal-catalysed direct arylations of heteroarenes using 1-(bromophenyl)-1,2,3-triazoles as aryl sources have been described. Here, we wish to report on the access to a wide variety of 1-phenyl-1,2,3-triazoles bearing a heteroarene on the phenyl ring, using Pd-catalysed direct arylation reaction.

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