

Research Project

C-H Bond Functionalization via Catalytic Migrative Cross-Coupling

Third-party funded project

Project title C-H Bond Functionalization via Catalytic Migrative Cross-Coupling

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Organisation / Research unit

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Department

Project start 01.04.2016

Probable end 31.03.2019

Status Completed

This proposal is dedicated to the development of a new C-H functionalization strategy allowing to selectively create a C-C bond at the terminal position of an alkane fragment. This strategy is based on the ability of group 10 metals to migrate along an alkyl chain via the β -H elimination/p-complex rotation/insertion mechanism and undergo reductive elimination at the least substituted terminal position. This proposal features 3 Work Packages (WP) of progressively more challenging character. In WP1, the palladium(0)-catalyzed ligand-controlled regioconvergent coupling of organozinc compounds, obtained from mixtures of alkyl bromides, is proposed. Coupling this migrative cross-coupling with an initial C-H bromination step would allow to selectively functionalize alkanes in two-steps at the terminal carbon. WP2 features the development of a nickel-catalyzed version of the preceding migrative coupling, which would offer a useful complementarity both in terms of scope and mechanism. The main purpose of WP3 is to replace organozinc reagents employed in the Ni-catalyzed process (WP2) with photoredox-generated radicals, such as those generated from carboxylic acids or amines in combination with an Ir-based photocatalyst. This modification would allow to significantly expand the scope and practicability of this C-H functionalization strategy.

Keywords cross-coupling, organotransition metal catalysis, C-H functionalization

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Published results

3692713, Dupuy, Stéphanie; Zhang, Ke-Feng; Goutierre, Anne-Sophie; Baudoin, Olivier, Terminal-Selective Functionalization of Alkyl Chains by Regioconvergent Cross-Coupling, 1433-7851 ; 1521-3773, Angewandte Chemie International Edition, Publication: JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)

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