New Pd-catalyzed C-O and C-H activation reactions

Sara L. S. Gomes\(^1\) (PG), Victor Snieckus\(^2\) (PQ), Alcides J. M. da Silva\(^1\) (PQ)\(^*\)

\(^1\)Laboratório de Catálise Orgânica, Instituto de Pesquisa de Produtos Naturais, Centro de Ciências da Saúde, Bl. H, Cidade Universitária, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, 21941-902, Brasil. \(^2\)Department of Chemistry, Queen’s University, Kingston, Ontario, K7L 3N6, Canada.

Email: alcides@nppn.ufrj.br

Keywords: C-O activation, naphthoquinone, acrylates, catalysis.

**Introduction**

Transition metal catalyzed reactions constitute an important synthetic tool for the construction of new C-C bonds. The combination of C-O activation with cross-coupling reactions to achieve more complex molecules is a widespread methodology in organic synthesis. In this work we would like to highlight the use of O-carbamates for these transformations since they are known to be inert to Pd-catalysis.\(^1\)

**Results e Discussion**

Herein we report the reaction between 2-\(N,N\)-diethyl O-carbamate of lawsone (1) and ethyl acrylate (2) under Heck conditions, which, surprisingly, provided the anthraquinone (4) as the major product.

![Figura 1. Obtention of anthraquinone (4).](image)

The optimization of the reaction conditions was extensively studied and the best result is described below (50% yield). An experiment without palladium was conducted proving that the presence of the catalyst is essential for the reaction to occur.

![Tabela 1. Palladium source optimization.](image)

Different types of olefins were tested and less bulky electron withdrawing alkenes were found to give better results.

![Figura 2. Olefins tested on the study.](image)

Experiments are being done to clarify whether the reaction mechanism passes through a two-fold Heck reaction followed by 6π-electrocyclization and dehydrogenation\(^2\) or a C-H activation reaction followed by a Heck-type reaction.\(^3\)

**Conclusions**

Despite the low yields, the current reaction represents the first Pd-catalyzed C-O activation involving the O-carbamate moiety as a leaving group. Studies about the reaction mechanism are ongoing in our lab.

**Acknowledgement**

UFRJ, CAPES, CNPq and IPPN.

