

Supervisor Expression of Interest MSCA-IF Marie Sklodowska Curie Action-Individual Fellowship 2020

Supervisor name:	Mónica H. Pérez Temprano
e-mail address: Research Group webpage:	<u>mperez@iciq.es</u> <u>http://www.iciq.org/research/research_group/dr-monica-h-</u> perez-temprano/
Research Topic:	Rational Design of First-Row Metal-Catalyzed Transformations

Brief description of the research project idea:

Rational Design of First-Row Metal-Catalyzed Transformations

The Pérez-Temprano lab is an emerging research group at the Institute of Chemical Research of Catalonia (ICIQ) whose main goal is the development of knowledge-driven approaches for the rational design of chemical transformations.

The groundbreaking nature of our research strategy relies on the use of key reaction intermediates as knowledge building blocks (kBBs) to uncover the underlying mechanism of transition metal-catalyzed transformation in order facilitate the bottom-up design of innovative and more efficient processes (<u>http://bit.ly/2J9BEni</u>). Our approach is based on a very simple concept: the success or failure of chemical reactions relies on the performance of the reactive intermediates involved in the elementary steps of the catalytic cycles. This idea may seem very obvious, yet overlooked, and it can be a completely game-changer for non-efficient transformations. Therefore, uncovering the factors that determine reaction success or failure, allows us to propose knowledge-driven tailored made solutions for resolving the main bottlenecks that hinder the efficiency of chemical reactions.

In particular, we apply our approach to the optimization and creation of site-selective C–H functionalization reactions-catalyzed by cheap, earth-abundant first-row transition metals using readily available starting materials. To fulfill this goal, we have established a synergistic and effective collaboration between fundamentals and catalysis, merging synthetic organic and organometallic chemistry, with a wide variety of analytical techniques and physical organic tools. In particular, the following objectives are pursued:

- 1. Investigating C–H bond activation mechanisms in first-row-based systems
- 2. Development of carbon–carbon bond-forming reactions for the synthesis of druglike molecules
- 3. Creation of new catalytic reactivity patterns: exploration of carbon-heteroatom bond-forming reactions

We are looking for highly motivated, independent and creative researchers with excellent interpersonal skills. The candidates shall have experience in organometallic chemistry and/or transition metal-catalysis. Experience on mechanistic studies would be highly appreciated. High oral and written communications skills in English are required.