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Beginning to understand light-mediated Ni catalysis using physical organic techniques and data science

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Abstract: The Bahamonde group harnesses the distinct one-electron chemistry and photochemical reactivity of Ni complexes to generate and trap C-centered radicals enantioselectively and promote C–N reductive eliminations at room temperature. Our excitement for studying these systems stems from the fact that these two apparently unrelated processes are facilitated under almost identical conditions, but to date the ligand features, photocatalyst properties, and subtle reaction condition variations that favor one pathway over the other are not yet understood. Additionally, to expedite reaction optimization, the group develops multivariate linear regression models correlating observed enantioselectivity to computed molecular descriptors.

Biography: Ana was born and raised in the north of Spain. She obtained her B. Sc. in Chemistry at the Universidad de Oviedo in 2012. Subsequently, during her PhD she studied photoredox reactions promoted by organocatalysts at the Institute of Chemical Research of Catalonia (ICIQ) under the supervision of Paolo Melchiorre. Afterwards she moved away from her home country to work in the Sigman lab at the University of Utah as a postdoctoral researcher (2017-2020). During this time, she worked on Pd-catalyzed aza-Wacker reactions and the development of multivariate linear regression models to explain the rates of amide coupling reactions. Since 2020 she is an Assistant Professor at the University of California Riverside where her group uses a mechanistically guided approach to reaction development utilizing first row transition metals.