CATMETGOLD

Catalytic methods based on gold or other electrophilic metals

Timeline | 06/2020 to 05/2023

ICIQ People | A. Echavarren Research Group

Budget | 399,300 €

Call | Proyectos I+D - Excelencia 2019

SUMMARY

We propose to synthesize chiral gold catalysts based on new designs and to develop new synthetic methods based on the homogeneous catalytic chemistry of gold, and area in which our research group has been one of the pioneers. We will also study the potential use of other electrophilic metal complexes as alternative catalysts to gold, particularly in the context of the generation of reactive metal carbenes. To demonstrate the synthetic potential of these new developed reactions, we will apply these methodologies in the context of the synthesis of biologically active natural products and for the direct, late stage functionalization of complex molecules. Methodologically, new reaction discovery will follow a comprehensive approach, which includes the routine implementation of experimental physical organic studies and DFT calculations, reinforced by high throughput screening methods.

The new chiral catalysts will be designed with the chiral element close to where the key carbon-carbon bond formation takes place, to circumvent the limitations imposed by the linear coordination of gold(I). In addition, in an enzyme-mimetic manner, the new ligands will maximize the attractive aromatic interactions with the substrate to achieve the desired high enantioselectivities. Other catalysts based on supramolecular binding of a metal cation with a chiral anion, through hydrogen bonds, will be prepared. These catalysts will be applied for the biomimetic cyclization of unsaturated substrates, for the synthesis of complex chiral biaryl systems, and for the activation of acetylene, an abundant commodity gas. A method for the polymerization of acetylene will be also developed based on a new type of metal-catalyzed metathesis reaction.

Finally, new catalysts and methods will also be developed for the late stage functionalization of biologically relevant compounds, including pharmaceuticals and agrochemicals. These methods will be based on the metal-catalyzed alkynylation of C-H bonds assisted by weak coordination with functional groups commonly found in this type of molecules.

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