

Progetto PRIN 2022 PNRR - P2022RHMCM

LIGHT-CAT: Light-driven Catalytic Technologies for the Selective Functionalisation of C(sp³)-H Bonds

The LIGHT-CAT project, which is granted by PRIN2022 (grant number P2022RHMCM), aims to develop innovative light-driven processes that selectively functionalise C(sp³)-H bonds, thus offering new ways to prepare complex relevant molecules directly from natural products and abundant C(sp³)-H rich substrates. The research tackles challenges in aliphatic C-H functionalisation chemistry. The overarching goal is to combine Hydrogen Atom Transfer (HAT) mechanisms and advanced catalytic techniques to selectively couple alkanes and other aliphatic derivatives with abundant substrates, including carboxylic acids, amines, or even other alkanes and pyridines. To achieve this, we will use photocatalytic Hydrogen Atom Transfer (HAT) processes to selectively target strong unactivated C(sp³)-H bonds. For example, we will use the rich photochemistry of tetrabutylammonium decatungstate (TBADT), a polyoxometalate widely used as an efficient HAT photocatalyst. Upon light excitation, TBADT can form radicals upon H-abstraction from unactivated C-H bonds. The new methods will offer innovative tools for unlocking inaccessible reaction pathways, thus enabling the preparation of previously difficult-to-make molecules. To test their utility, the photochemical protocols developed will be applied to the late-stage diversification of natural molecules, pharmaceuticals and agrochemicals. We will also develop appropriate conditions for continuous processing of our photochemical strategies through flow chemistry, with an emphasis on improving catalyst loading, product purity, waste reduction, and energy efficiency.

For the research position, we are seeking candidates with a strong foundation in radical chemistry, especially in Hydrogen Atom Transfer (HAT) processes, and in particular flow chemistry. Experience in photochemistry and radical mechanistic investigations will be highly regarded. These competencies are crucial for effectively achieving milestones 4 and 5 of the LIGHT-CAT project, which focus on **Flow Chemistry and Process Intensification, and Mechanistic Studies**. This project will be conducted in close collaboration with the University of Pavia, leveraging their extensive expertise in HAT chemistry and flow photochemistry. This knowledge will be crucial in successfully transitioning a batch reaction into a continuous flow method, a goal that the research team at UNIBO must achieve for the project. It is specified that the research activities will be conducted in the laboratories of the University of Pavia.