POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 41st cycle

THEMATIC Research Field: NOVEL BIOCATALYTIC STRATEGIES FOR ORGANOBORON CHEMISTRY

Monthly net income of PhDscholarship (max 36 months)
1500.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	The project aims to develop novel photo- and bio-catalytic methods for the sustainable synthesis of organoboron compounds (OBCs). OBCs are essential building blocks in modern organic synthesis and play an increasingly important role in pharmaceuticals and material science, yet their current production methods lack sustainability (DOI:10.1021/acs.chemrev.3c00663). The project aims to bridge this gap by developing a novel, sustainable, and efficient approach for their synthesis and functionalization. Biocatalysis, which uses enzymes to catalyze chemical reactions, is leading the green revolution in organic synthesis (DOI:10.1021/jacsau.3c00263). However, certain classes of compounds, such as OBCs, remain difficult to access through biocatalytic methods. This is because only a few natural enzymes are known to interact with organoborons, leaving their biocatalytic functionalization largely unexplored (DOI:10.1038/nature24996). The project focuses on engineering new-to-nature enzymatic transformations to form C-H, C-C and C-N bonds by harnessing the unique reactivity of organoboron compounds (DOI:10.1002/anie.202207067). This goal will be pursued through the discovery and development of novel enzymatic mechanisms (DOI:10.1021/jacsau.4c00247), via either polar or radical pathways, and leveraging the photoreactivity of either exogenous catalysts or flavin-

	dependent enzymes (DOI:10.1021/acs.accounts.4c00129). The development of a biocatalytic platform will allow the stereoselective synthesis of chiral organoborons with a focus on synthetic intermediates relevant for both pharmaceutical and natural product synthesis.
Methods and techniques that will be developed and used to carry out the research	A comprehensive prior art and literature survey will be conducted to delineate the relevant chemical space and identify existing methodologies and catalytic precedents. This foundational step will establish the conceptual and practical boundaries of the investigation and highlight opportunities for innovation. The preparation of building blocks and boron-containing substrates will be carried out in alignment with the most recent advances in transition-metal and photoredox catalysis. Particular emphasis will be placed on synthetic efficiency, scalability, and compatibility with downstream enzymatic transformations. Enzymes required for the study will either be obtained from commercial sources (e.g., enzyme screening kits) or produced in-house through heterologous expression in E. coli. The enzyme screening phase will involve the design and optimization of suitable experimental setups, including oxygen-free systems, glove-box manipulations, and custom photochemical reactors, to accommodate diverse catalytic requirements. An integrated analytical platform will support high-throughput evaluation of enzyme performance and reaction outcomes. Analytical methods based on spectroscopy and chromatography will enable the rapid identification of the most promising enzyme candidates and optimal reaction conditions, thereby streamlining the process of reaction optimization and mechanistic understanding. The newly developed biocatalytic methodologies will subsequently be applied to the synthesis of target molecules of interest, following the principles and strategies of modern organic synthesis. This translational approach aims to demonstrate the synthetic utility, selectivity, and sustainability of the developed systems. Analytical techniques to be employed include Nuclear Magnetic Resonance (NMR) spectroscopy, Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry

	(LC-MS), High-Performance Liquid Chromatography (HPLC) using chiral stationary phases, Polarimetry and Circular Dichroism (CD) for chiroptical characterization, Ultraviolet–Visible (UV-Vis) and Infrared (IR) spectroscopy for additional structural and mechanistic insights
Educational objectives	Training in organic chemistry research focused on photo- and biocatalysis, covering the full process from literature review and experimental design to data analysis and scientific writing. Emphasis will be placed on developing independence in experimental work and critical evaluation of results. The program promotes teamwork and collaboration through group meetings, problem-solving sessions, and literature discussions, fostering both technical expertise and scientific communication skills.
Job opportunities	The research and educational training will provide solid foundations for a Research &Development job in the chemical and biotech industry, particularly in the fine chemical sector (pharmaceuticals, agrochemical, flavours &fragrances). Also, the PhD will lay foundations for further academic research at postdoctoral level.
Composition of the research group	1 Full Professors 3 Associated Professors 3 Assistant Professors 3 PhD Students
Name of the research directors	Dr. Daniele Fiorito

Contacts
Telephone: 3516477628 Email: daniele.fiorito@polimi.it Web-pages of the research group: https://www.cmic.polimi.it/ricerca/elenco-gruppi-di-ricerca/biocatlab/ www.fioritoresearch.com

Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents	--

Scholarship Increase for a period abroad	
Amount monthly	750.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Educational activities (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student per year: 1st year: around 2.000 euros per student 2nd year: around 2.000 euros per student 3rd year: around 2.000 euros per student **Teaching assistantship**: availability of funding in recognition of supporting teaching activities by the PhD student:There are various forms of financial of for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.