







PhD POSITIONS (2)

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Job Information

Organization: Université de Liège (ULiège, Belgium) Department: Center for Integrated Technology and Organic Synthesis - CiTOS Research Field(s): Organic chemistry, Computational chemistry, Chemical Engineering

Type of Contract: 2 PhD positions available, temporary (24 months, renewable) Job Status: Full-time Offer Starting Date: 1 Oct 2023 Application Deadline: 1 Sep 2023 - 12:00 (Europe/Brussels)

Offer Description

Overall context

This research proposal falls under the umbrella of a Wel-T advanced grant led by Prof. Jean-Christophe Monbaliu and strengthens current research efforts at the Center for Integrated Technology and Organic Synthesis (CiTOS).

The work will be carried out at the Center for Integrated Technology and Organic Synthesis (CiTOS, University of Liège, Belgium) in a competitive research environment and within a multidisciplinary team including synthetic chemists and chemical engineers. The candidates will have access to the most recent flow reactor technologies from Corning AFR and an internal analytical platform (LC, LC-MS, GC, GC-MS, benchtop NMR, IR, UV, etc.). Our large network of industrial collaborators stimulates research toward concrete industrial and/or societal challenges, making this a unique opportunity for candidates aspiring to continue either towards careers in academia or industry.

Research project

The goal of this project is to decrease the reliance on trial-and-error approaches to chemistry by using quantum mechanics computations to obtain a priori knowledge of a chemical reaction. This project brings together computational modeling to generate initial data, and machine learning to home in on an effective prediction model for reactivity. This model will be used to predict optimal reaction conditions, which will then be tested using a microfluidic flow reactor. Experiments will be conducted on an in-house automated platform equipped with inline monitoring. This approach will be applied to novel synthetic routes, for which there is no existing data, to showcase how novel, more efficient synthetic routes can be developed with a minimal number of experiments through the combination of these disciplines. The target compounds are active pharmaceutical ingredients.

Applicant's Profiles

There are 2 PhD positions available

The candidate should have a Master's degree in chemistry or chemical engineering and an interest in developing skills in organic synthesis, as well as in flow technology, automation. An interest for computational chemistry (DFT) is an asset. S/he will be tasked with the development of the synthesis and characterization of the targeted compounds. The candidate should be willing to learn how to operate the flow equipment and develop the automated setups. Two PhD students will be hired to work on this project to cover the entire scope of reactions that will be studied.

Application

Interested candidates please send electronic applications including (a) a cover letter, (b) a curriculum vitae, (c) a short statement on your motivation and career objectives, and (d) the names and contact details of 3 professional references. The motivation letter should emphasize any previous research experience that aligns with this project. The application files should be addressed to Prof. Jean-Christophe M. Monbaliu (admincitos@uliege.be) (ref. Wel-T_ADV_PhD_2023). Candidates will be selected based on scientific excellence and achievements in research. Review of applications will begin on September 1, 2023 and will continue until the position is filled. Selected candidates will be interviewed.

Additional information

Prof. Jean-Christophe Monbaliu, Center for Integrated Technology and Organic Synthesis (CiTOS) Email (for application files): <u>admincitos@uliege.be</u> CiTOS: <u>http://www.citos.uliege.be/</u> ULiège: <u>https://www.uliege.be/</u> Wel Research Institute: <u>https://welri.org/cms/c_16995060/en/welri-mission</u>