Reg. No: 2019/32/C/ST4/00235; Principal Investigator: dr Jakub Szyling

## **Research objective**

The aim of the project is to develop new methods for the synthesis of organoboron compounds *via* catalytic hydroboration of  $\pi$ -conjugated C-C bonds under repetitive batch reaction system, and in the final stage of the proposal, in a continuous-flow regime. The application of unconventional reaction media will allow the elimination of toxic organic solvents, recycling of expensive catalysts, simplify and at the same time increase the effectivity of the separation of the product from the post-reaction mixture.

## **Research within project**

The project will be focused on the hydroboration of unsaturated bonds in  $\pi$ -conjugated compounds in divines, envnes and dienes, which functionalization due to the possibility of the formation of various products is difficult. Therefore within this project the new catalytic systems will be discovered to carry out the reaction with high selectivity and applying environmentally friendly, unconventional reaction media: poly(ethylene glycols) (PEGs) and supercritical  $CO_2$  (scCO<sub>2</sub>) to make the process greener. The first stage of the project is to develop an active and selective catalytic system and to optimize reaction conditions. An important step in the implementation of the project will be the development of an effective method for catalyst immobilization through i) physical or chemical interactions with the solvent (PEG), ii) physical or chemical sorption of the thin layer of PEG on the solid support surface, and iii) creation of Augustine-type systems. Likewise, an important element of the project will be the development of an effective method of product separation from the post-reaction mixture. For this purpose, two strategies will be used: i) extraction with an organic solvent and ii) extraction with supercritical CO<sub>2</sub>. The development of a stable, active and selective catalytic system and the effective method of products isolation from the post-reaction mixture is an indispensable step for the catalytic hydroboration of  $\pi$ -conjugated C-C bonds under repetitive batch mode. At the final stage of the project, an attempts will be made to transfer the processes carried out under periodical systems to the system operated under continuous-flow conditions. It is possible due to the cooperation with ITMC RWTH, which is one of the leading research centers working on the application of neoteric solvents in the discovery of continuous-flow processes.

## Justification of the research

Issues addressed in the project: usage of unconventional reaction media, multiple uses of expensive catalysts, simple and effective separation of the product from the reaction mixture, have become a very important area of research of leading research institutions and industry. However, the synthetic protocols of organoboron compounds with the respect of green chemistry rules are almost unexplored. Therefore, undertaking this task within the project is fully justified. Its implementation will bring real benefits at the level of: (i) ecological - elimination of volatile and toxic organic solvents, (ii) economic - recycling of expensive catalysts and shortening the process time by one-step isolation methods, (iii) scientific - the obtained results will bring an important contribution to fundamental knowledge, allowing a comprehensive understanding of these processes and give a chance to propose new solutions for modern organometallic chemistry with organoboron compounds. Such compounds are useful building blocks in the synthesis of advanced *fine chemicals*.