

## **Project 2.1 Autonomous discovery, development and optimization of organocatalytic reactions through intelligent chemical robots**

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**Unit:** Team VIIIb

**www:** <https://www.icho.edu.pl/en/zespol/janusz-jurczak-research/jaroslaw-granda-research/>

### **Background:**

Chirality plays an important role in nature, as molecules of different chirality can exhibit vastly different properties. A large part of the field of chemical catalysis, and in particular of organocatalysis, is devoted to the selective synthesis of chiral molecules. However, despite the huge progress made in recent decades, we are still far from being able to efficiently design the synthesis of any chiral molecule. Usually, the development of new (organo)catalytic methods requires extensive and time-consuming optimization, which is usually performed manually. Therefore new enabling technologies are needed to speed up this process. Automation and robotic approaches have started to play an important role in the chemical sciences. The use of automated approaches can speed up the research process, make the experiments more repeatable and free researchers from repetitive tasks, so they can focus on the design of new transformations.

### **Aim:**

In this project, we aim to investigate the field of organocatalysis with chemical automation and robotics that will ultimately be guided by artificial intelligence methods. The successful candidate will work on several goals:

- the design and construction of high-throughput automated robotic platform
- automated optimization of selected transformations
- autonomous searching for new transformations with robotic platform
- synthesis of starting materials, catalysts, and building blocks
- mechanistic investigation of selected transformations as well as probing their scope and limitations

During the project the student will gain skills necessary in chemical robotics, which are essential in pharmaceutical and fine-chemical industry.

### **Requirements:**

- analytical, methodological problem-solving skills and logical, objective thinking,
- completed master's studies in chemistry,
- good knowledge of organic chemistry,
- experience in research work will be an asset,
- any programming skills is a plus and/or experience with DIY