

Project 2.4 The self- or directing group-aided remote C-H functionalization of bifunctional compounds initiated by alkoxy radical species

Supervisor: Dr Sebastian Stecko, Assoc. Professor

Institute: Institute of Organic Chemistry Polish Academy of Sciences

Unit: The Stecko Research Group (Research Group XXI)

www: www.steckogroup.pl

Background:

The PhD candidate will be responsible for:

- synthesis of the selected model starting materials;
- optimization of self-C-H functionalization reaction of the selected model bifunctional compounds initiated by alkoxy radicals;
- optimization of directing group-aided C-H functionalization reaction of the selected model bifunctional compounds initiated by alkoxy radicals;
- evaluation of reaction scope and limitations of the both strategies, including reagents scope, chemoselectivity and enantioselectivity of the process;
- computational studies of reaction mechanism;
- application of the developed method for synthesis of the selected bioactive compounds and medicinals;
- full characterization of the obtained compounds by spectroscopic techniques;
- data analysis, report preparation, manuscript draft preparation.

Aim:

The announced research project, funded by Polish National Science Center, is devoted to develop novel methods for self- and a directing group aided C(sp³)-H functionalization of simple bi- and polyfunctional organic molecules. Most of the efforts will be put on the development mild and versatile protocols under modern radical photoredox or electrochemical conditions. Previous experience with organic photochemistry and/or electrochemistry will be an additional asset.

The PhD candidate (PDC) will be responsible for synthesizing, depositing, and characterizing of the starting materials and intermediates, followed by an optimization of reaction conditions for model transformations of alkoxy radical initiated remote C(sp³)-H functionalization of bi- and polyfunctional organic compounds. In extension, the PDC will investigate a scope of the developed protocols, including starting material variations, reaction condition variation (photoredox, electrochemical, transition-metal catalyzed process). Key efforts will be put on an investigation of asymmetric mode of the investigated C-H functionalization along with application studies devoted to synthesis of the selected bioactive or medicinally important molecule by using investigated process. Complementary theoretical studies on reaction mechanisms may be performed by the PDS or as part of a collaboration, depending on the scholar's interests. To a certain degree, the PDC will be given intellectual freedom in defining their research.

The PhD candidate will also participate in the Institute scientific life by attending to group and institute seminars and lectures. The PhD candidate will also attend to advanced course devoted to modern organic chemistry and spectroscopy.

Requirements:

- MSc degree in chemical science (or related areas) or the expected date of obtaining the master degree before starting work;

- good knowledge in organic synthesis and spectroscopy,
- communicate well in English in writing and in oral and visual presentation, and be able to write reports and manuscripts for publication in scientific journals;
- be highly motivated and have a strong commitment to research; curiosity, creativity and passion;

Optional requirements:

- experience in synthetic organic chemistry;
- previous experience catalysis, organometallic chemistry, radical chemistry, safe handling of air/water sensitive materials, Schlenk techniques;
- expertise and interest in photochemistry and electrochemistry will be an additional asset;
- creativity, responsibility, independence, as well ability to work in team;