Synthesis and application of conformationally flexible multifunctional organocatalysts

Summary

The PhD project will focus on the design, synthesis and application of multifunctional enantiomerically pure organocatalysts. New catalysts possess several halogen bonding, hydrogen bonding and Lewis basic sites mimicking active sites of enzymes.

Research field:	Chemistry and biotechnology
Supervisor:	Prof. Dr. Tõnis Kanger
Availability:	This position is available.
Offered by:	School of Science Department of Chemistry and Biotechnology
Application deadline:	Applications are accepted between June 01, 2022 00:00 and June 30, 2022 23:59 (Europe/Zurich)

Description

Asymmetric catalysis has become a major tool for the synthesis of enantiomeric compounds and at present catalytic reactions have surpassed the auxiliary-based approaches. The project deals with asymmetric organocatalysis that is one of the top ten emerging technologies in chemistry listed by IUPAC experts in 2019. New multifunctional catalysts that consist of halogen bonding and hydrogen bonding Lewis basic or carboxylic site will be designed and synthesized. Coupling of these catalytic moieties with amino acids is a tool for the construction of the chiral skeleton of the catalyst. The modular nature of amino acids allows developing different chiral environment of the catalyst mimicking enzymes. Conformational flexibility of enzymes often leads to the preorganization of the active site (due to stabilizing non-covalent interactions) and remarkable rate accelerations and selectivity is achieved. To address the problem of the conformational rigidity vs flexibility of the catalyst quantum chemical calculations will be used. The optimal structure of the catalyst will be calculated and according to obtained results, new catalysts will be synthesized. Thus, the project connects basic organic chemistry, asymmetric synthesis, supramolecular and computational chemistry. Synthesized catalysts will be applied in various reactions leading to precursors or intermediates of biologically active compounds. The PhD student will gain extensive experience in asymmetric synthesis and analysis.

PhD candidates must have a master's degree in a relevant scientific discipline and a strong interest in organic chemistry. The successful candidate will be a highly motivated and proactive individual with excellent communication skills. Strong experience in organic synthesis, analytical (NMR, MS) and chromatographic methods (HPLC, GC) needed for characterizing synthesized compounds are desirable.

To get more information or to apply online, visit https://taltech.glowbase.com/positions/492 or scan the the code on the left with your smartphone.

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