Project 2.4 Asymmetric reduction of prochiral ketones - designing new catalysts using artificial intelligence methods.

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Background:

Analysis of data collected in our team and analysis of literature data. Synthesis of catalysts. Performing catalytic reactions with zinc- and magnesium-based catalysts and discovery new catalytic reactions based on AI data analysis. Preparation of reports and manuscripts.

Aim:

The aim of the planned research is the artificial intelligence-assisted design and then experimental verification of new chiral Lewis acids containing zinc and magnesium ions as catalysts in selected organic reactions, in particular in the asymmetric reduction of the carbonyl group. Computer aided design of catalysts will require the analysis of data collected by our team during many years of work in the field of asymmetric synthesis and analysis of literature data. The aim of the research is also to implement a substantial database of results (both positive and negative) obtained in the course of previous research to solve the problems encountered at that time.

Requirements:

- MSc degree in chemistry,
- experience in organic synthesis and interpretation of spectral data,
- good communication skills in English