Development of Computational Methods for Predicting Binding Properties of Chiral Hemicucurbiturils

Summary

The PhD project is part of a broader research effort focused on sensing, capturing, and separating enantiomers using hemicucurbiturils. Chiral compounds appear frequently in agricultural chemistry, cosmetics, and drug design and using hemicucurbiturils could be a cheap and green option to work with such molecules. The combinations of potential monomers, oligomers, and templates is virtually limitless; thus, optimizing the reactants for a macrocycle with specific binding properties can be a long and costly endeavor. Due to that, there is a need for accurate in silico models that could accurately screen thousands of combinations of monomers, oligomers, and templates in a relatively short time-span. To achieve this, the project will combine knowledge gained from experiments and ab initio calculations with semi-empirical and/or machine learning approaches to build models that predict binding properties of chiral hemicucurbiturils.

Research field:	Chemistry and biotechnology
Supervisors:	Prof. Dr. Riina Aav Dr. Mario Öeren
Availability:	This position is available.
Offered by:	School of Science Department of Chemistry and Biotechnology
Application deadline:	Applications are accepted between June 01, 2024 00:00 and June 30, 2024 23:59 (Europe/Zurich)

Description

The PhD project is part of a broader research effort focused on sensing, capturing, and separating enantiomers using Hemicucurbiturils. Chiral compounds appear frequently in agricultural chemistry, cosmetics, and drug design and using Hemicucurbiturils could be a cheap and green option to work with such molecules. Hemicucurbiturils are obtained through a single-step, templated, mechanochemical synthesis and due to the absence of bulk solvent the self-organizing efficiency is amplified and there is less waste. The combinations of potential monomers, oligomers, and templates is virtually limitless; thus, optimizing the reactants for a macrocycle with specific binding properties can be a long and costly endeavor. Due to that, there is a need for accurate *in silico* models that could accurately screen thousands of combinations of monomers, oligomers, and templates in a relatively short time-span. To achieve this, the project will combine knowledge gained from experiments and *ab initio* calculations with semi-empirical and/or machine learning approaches to build models that predict binding properties of chiral Hemicucurbiturils.

We are seeking a highly motivated PhD student to join our team and contribute to the development of innovative approaches to help synthesize novel Hemicucurbiturils. The successful candidate will develop a theoretical understanding of the forces and interactions leading to the self-assembly of Hemicucurbiturils and build and/or train models for predicting necessary monomers and reaction conditions to form macrocycles with the desired properties.

Computational chemistry work will be conducted using programs such as Gaussian and xTB. In addition, the data will be analyzed using various Python packages (e.g., NumPy, SciPy, and Matplotlib). The PhD student will have access to the TalTech HPC Centre.

Responsibilities and (foreseen) tasks

- Development of new computational approaches to predict binding properties of macrocycles.
- Publication of scientific results.
- Supervision of undergraduate students in the group.

Applicants should fulfil the following requirements:

- a master’s degree in computational chemistry or in a relevant field
- strong knowledge of computational chemistry methods
- a clear interest in the topic of the position

- excellent command of English
- strong and demonstrable writing and analytical skills
- capacity to work both as an independent researcher and as part of an international team
- capacity and willingness to provide assistance in organizational tasks relevant to the project

(The following experience is beneficial:)

- experience with the Python programming language.

The candidate should submit a research plan for the topic, including the overall research and data collection strategy. The candidate can expand on the listed research questions and tasks, and propose theoretical lenses to be used.

We offer:

- 4-year PhD position very strong research group
- The chance to do high-level research in very attractive research fileld
- Opportunities for conference visits, research stays and networking with globally leading universities and research centers

About the department

The **department of Chemistry and Biotechnology** is divided to three Divisions. The main research areas of Division of Chemistry n include analytical, computational, industrial, organic, supramolecular, and wood chemistry. The Division of Chemistry is responsible for education in these fields at the bachelor's, master's, and doctoral levels, thus ensuring the ongoing cultivation of proficient specialists in chemistry. In our research and teaching, we put emphasis on the development and implementation of sustainable and green thinking.

The research and teaching facilities at the Division of Chemistry are furnished with modern equipment, supporting high-level research and education. A total of 10 research groups operates within our division, with approximately 80 academic staff members, including 4 professors and 25 doctoral students. Our researchers are engaged in international networks and cooperations, making their research worldwide visible.

Supramolecular Chemistry research group, lead by Riina Aav, is focusing on intermolecular interactions in order to understand complex systems of molecules and find greener approaches in chemistry. We are developing sustainable synthetic methods and designing new chiral supramolecular receptors for sensing chirality and chiral separation. We are also looking for methods to recycle and valorize waste in order to decrease pollution.

(Additional information)

For further information, please contact Prof Riina Aav riina.aav@taltech.ee and Dr. Mario Öeren mario.oeren@taltech.ee or visit https://riinaaav.wixsite.com/grouppage/group-news

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