

Nuclear magnetic resonance studies of chiral hemicucurbituril and oxacalixarene macrocycles

Summary

The PhD project focuses on NMR studies of chiral hemicucurbituril and oxacalixarene macrocycles. The undertaken experiments include structure elucidation of new macrocycles, NMR titration experiments to determine binding strengths with guest molecules and variable temperature NMR to derive the macrocycles' and their „host-guest“ complexes' thermodynamic and kinetic parameters.

Research field:	Chemistry and biotechnology
Supervisors:	Jasper Adamson Prof. Dr. Riina Aav
Availability:	This position is available.
Offered by:	School of Science National Institute Of Chemical Physics And Biophysics
Application deadline:	Applications are accepted between June 01, 2020 00:00 and July 03, 2020 23:59 (Europe/Zurich)

Description

Macrocycles are cyclic oligomers that are widely investigated in modern supramolecular science due to their broad capacity for molecular recognition – they form a pillar in supramolecular applications and have been a basis for a Nobel Prize in Chemistry in 1987 and 2016. We focus our work towards the synthesis and characterization of chiral hemicucurbituril and oxacalixarene based macrocycles. The PhD project will use nuclear magnetic resonance (NMR) spectroscopy as a tool to understand the behavior of these macrocycles in solution. Firstly, the PhD project will include structure elucidation of the as-synthesized macrocycles to provide information to the synthetic chemists in the group on the structures of the macrocycles and secondly will include more elaborate NMR characterization of the binding properties of the macrocycles. Namely, complexation strengths of the macrocycles will be investigated with ¹H NMR titration experiments to obtain binding affinities with a range of guest molecules and variable temperature ¹H and ¹³C NMR measurements will be undertaken to understand the dynamics of the macrocycles as well as the dynamics of their complexes in solution.

Qualifications

The applicants should fulfill the following requirements:

- The applicant should hold or be in the process of defending a Master's degree in Organic Chemistry or NMR with an understanding of Supramolecular Sciences.
- The applicant should be fluent in written and spoken English.
- Personal qualities, such as punctuality, conscientiousness and motivation, are essential for embarking upon the PhD degree.



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