Department of Chemistry Departmental Seminar Series

You are cordially invited to a lecture presented by



Prof Jan Korvink



Neil MacKinnon



Dilara Faderl

Institute of Microstructure Technology, Karlsruhe Institute of Technology, Karlsruhe, Baden-Württemberg, Germany

Date:	17 February 2023
Time:	11:30
Venue:	The Orbital (Room 3-1 Chemistry Building)

NMR spectroscopy for ligand screening

Nuclear magnetic resonance is a powerful analytical technique, capable of revealing molecular structure and dynamics with atomic resolution. This information is useful in many contexts, from understanding structure-function relationships, molecular transport under various conditions, to extracting the thermodynamics and kinetics of a process. Ligand screening falls under this application space, and NMR has found an important role in clarifying ligand binding interactions. A key drawback is in the speed at which screening by NMR can be done: as NMR is a rather slow measurement method, substantial time is needed to screen large ligand libraries as might be needed in a drug discovery effort.

Our group aims to tackle the measurement efficiency challenge, specifically in the case of ligand-protein screening. Our approach aims to address each step in an NMR-based screening protocol, including sample preparation, sample transfer, NMR signal enhancement, and measurement parallelization, all under some degree of automation. In this seminar we will discuss our efforts, with the ambitious goal of achieving a factor of 10'000 increase in measurement throughput.

Contact person:

E-mail: madelien.wooding@up.ac.za