

Research Project

Mechanistic and structural investigations by NMR spectroscopy on a wide scope of compounds - from natural products and proteins to artificial enzymes, organometal catalysts and supramolecular materials

Third-party funded project

Project title Mechanistic and structural investigations by NMR spectroscopy on a wide scope of compounds - from natural products and proteins to artificial enzymes, organometal catalysts and supramolecular materials

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Organisation / Research unit

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Project start 18.11.2010

Probable end 30.11.2011

Status Completed

Determination of the three-dimensional structure of proteins in solution is a stronghold of modern bio-molecular NMR spectroscopy. Even more important for understanding processes in the living cell is the characterization of interaction sites and surfaces of protein-protein and protein-ligand complexes. NMR can provide not only structural but also dynamic information on this subject. Pseudo contact shift (PCS) NMR spectroscopy has a unique property as it is a long-range method that can cover distances of

more than 50 Å, in combination with precise angle information. The very sensitive 2D-NMR experiments can be performed even on larger proteins, provided a state of the art spectrometer is available. We have recently presented a new lanthanide chelating tag "M8", based on a sterically overcrowded DOTA framework

that shows PCS of unprecedented size when linked to ubiquitin. This project is aimed at further improving

the properties of the new ligand by systematically optimizing the linker between the DOTA core and the protein and by variation of the donor atom set of the chelator.

Financed by

Swiss National Science Foundation (SNSF)

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