

**PLEASE USE THIS ABSTRACT TEMPLATE, one single A4 PAGE only!**

### Title

Design and synthesis of paramagnetic tags for protein dynamic studies in NMR

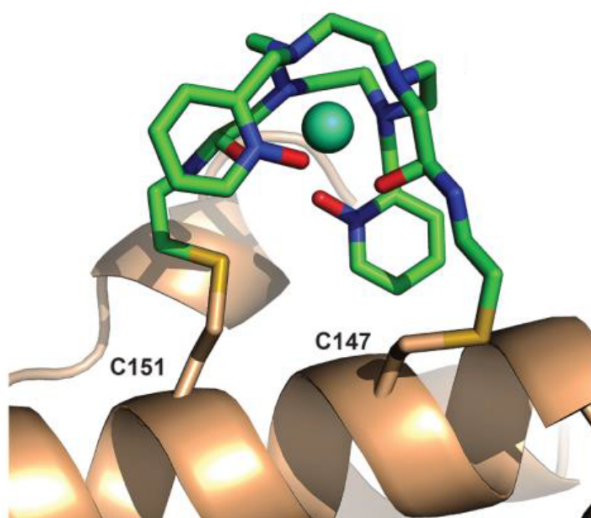
### Authors

René Dekkers, Qing Miao, Marcellus Ubbink, Mark Overhand

### Abstract poster presentation

To understand the functioning of macromolecules such as proteins, it is important to study their dynamics. While low energy states (LES) are well-known and extensively studied with commonly used techniques (e.g. crystallography or Cryo-EM), high energy states (HES) are more difficult to observe due to their short time of existence. Nevertheless, it is hypothesized that HES are crucial for understanding macromolecular functioning. In this project, we aim to study these HES using NMR, making use of paramagnetic effects. These effects are obtained using a paramagnetic metal, which we introduce by attaching a paramagnetic tag to the protein. One such tag needs to be chemically synthesized after which the paramagnetic metal can be included upon complexation, followed by covalently binding the tag to a protein. With my poster I would like to present a briefly some background, latest results and future prospects but would like to focus and emphasize the synthesis of these paramagnetic tags.

### Figure



### References

1. Miao, Q. et al., *Rigidified and Hydrophilic DOTA-like Lanthanoid Ligands: Design, Synthesis, and Dynamic Properties*. Inorg. Chem., 2023. **62**: p. 3776-3787.
2. Miao, Q. et al. *Paramagnetic Chemical Probes for Studying Biological Macromolecules*. Chemical Reviews, 2022, **122**: p. 9571-9642.
3. Hass, M. *A minor conformation of a lanthanide tag on adenylate kinase characterized by paramagnetic relaxation dispersion NMR spectroscopy*. J. Biomol. NMR, 2015. **61**: p. 123-136.