





EUROPEAN UNION

Seminar Speaker Series

in the framework of Interreg V-A project CAPSID

presents

Prof. Daniel Häussinger

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Lanthanide Chelating Tags in Structural Biology

11.03.2021 at **14:00**

Online virtual talk via Zoom

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RESEARCH FOCUS

Nuclear magnetic resonance spectroscopy provides an ideal toolbox for elucidating structure, dynamics and interactions of biomacromolecules in solution, since the offered possibility to tune and adjust the experimental conditions, i.e. buffer components, salt concentration, additives, temperature and pH, yields realistic and atomic-resolution structures of biomacromolecules under physiological conditions. In order to study protein-protein or protein-ligand interactions as well as the positioning and conformation of flexible domains within proteins in solution, long-range structural restraints are urgently needed. Paramagnetic nuclear magnetic resonance spectroscopy, more specifically pseudo-contact shifts and residual dipolar couplings generated by lanthanide chelating tags, can deliver such long-range restraints and thereby render amenable the structural analysis of large protein complexes as well as protein-ligand binding in solution.

RESEARCH HIGHLIGHT

"Design of next-generation lanthanide chelating tags"

In order to generate strongly paramagnetic lanthanide chelating tags that are sufficiently immobilized on the surface of the protein and generate thereby large paramagnetic effects, i.e. large pseudo-contact shifts and residual dipolar couplings, we synthesize sterically overcrowded DOTA-derived lanthanide chelating tags with different linker systems. More specifically, the introduction of sterically demanding substituents, e.g. isopropyl groups, as well as the introduction of novel, reduction-stable linker moieties, e.g. pyridinethiazole derivatives, proved to be highly beneficial in order to generate lanthanide chelating tags with optimal properties and general applicability.

REFERENCES

"Design and application of lanthanide chelating tags for pseudocontact shift nuclear magnetic resonance spectroscopy on biomacromolecules."

Joss & <u>Häussinger</u>, Progress in Nuclear Magnetic Resonance Spectroscopy, **2019**, 114-115, 284-312.

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