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## Neutron macromolecular protein crystallography – shedding light on the structure-function relationship in proteins and enzymes

*Thursday, May 25, 2023 10:20 AM (40 minutes)*

Proteins play a crucial role in many biological processes. For example, all chemical reactions in living cells are accelerated by many orders of magnitude by enzymes, which are proteins that are responsible for catalyzing selectively one specific chemical reaction. Proton transfer is a fundamental mechanism at the core of many enzyme-catalyzed reactions. That is why the knowledge of protonation states and H-bonding networks in the active center of enzymes is essential to understand their ligand specificity and reaction mechanism. In addition, information about orientation of water molecules and the protonation state of ligands in the active center can further aid in revealing the underlying reaction mechanism. This knowledge is often the starting point for developing tailor-made inhibitors for so-called drug-target enzymes.

Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen atoms in biological macromolecules. This talk will use selected examples from the neutron single crystal diffractometer BIODIFF at the Heinz Maier-Leibnitz Zentrum to show how neutrons can help to gain information about reaction mechanisms in enzymes.

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