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Neutron protein crystallography at the Heinz Maier-Leibnitz Zentrum (MLZ): New developments and recent application examples

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The neutron single crystal diffractometer BIODIFF at the research reactor Heinz Maier-Leibnitz (FRM II) is especially designed to collect data from crystals with large unit cells. The main field of application is the structural analysis of proteins, especially the determination of hydrogen atom positions. BIODIFF is a joint project of the Jülich Centre for Neutron Science (JCNS) and the FRM II. BIODIFF is designed as a monochromatic instrument with a narrow wavelength spread of less than 3 %. To cover a large solid angle the main detector of BIODIFF consists of a neutron imaging plate in a cylindrical geometry with online read-out capability.
BIODFF is equipped with a standard Oxford Cryosystem "Cryostream 700+"which allows measurements at 100 K. A new kappa goniometer head was added recently. This allows an automated tilting of the crystal in order to increase the completeness of the data set when recording another set of frames in the tilted geometry. Typical scientific questions addressed are the determination of protonation states of amino acid side chains in proteins and the characterization of the hydrogen bonding networks between the protein active centre and an inhibitor or substrate.
Picking out some recent highlights from measurements at BIODIFF it will be shown how the method of neutron protein crystallography could be used to answer mechanistic questions in enzymatic processes or help to improve inhibitor fragment screening. New developments at the instrument will also be presented: A new collimation for the primary beam should lead to a reduction in background. It should also make it easier to align the neutron beam with the centre of the neutron imaging plate detector. Furthermore, a new single crystal x-ray diffractometer has been installed in the new MLZ lab building. It features a Molybdenum and a Copper Microfocus x-ray source and a 150° (2 ⊠) x-ray detector. It also features also an Oxford Cryosystems 800 series Cryostream for sample temperatures between 80-400K. This x-ray diffractometer can be used to record an x-ray data set of the protein crystal after having been measured at the BIODIFF instrument. It may also be used to pre-scan the diffraction quality of the crystals the user brings for neutron beam times at MLZ instruments.

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