

Poster Presentation

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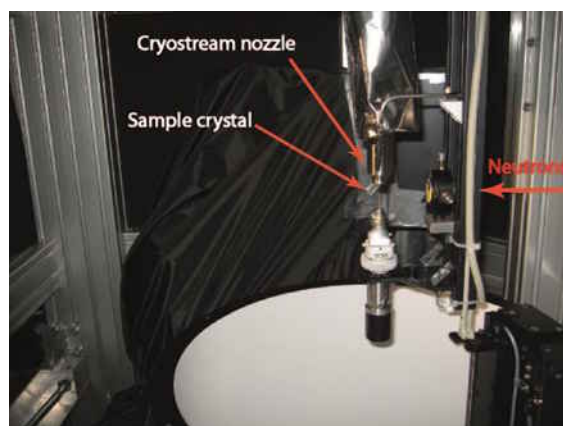
BioDiff - a neutron diffractometer for protein crystallography

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The research reactor Heinz Maier-Leibnitz (FRM II) is a modern high flux neutron source which feeds some 30 state of the art neutron beam instruments. Currently 24 are operational, others in commissioning or under construction. The newly built neutron single crystal diffractometer BIODIFF 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. Typical scientific questions addressed are the determination of protonation states of amino acid side chains (see e. g. [1,2]) and the characterization of the hydrogen bonding network between the protein active centre and an inhibitor or substrate. BIODIFF is designed as a monochromatic instrument. By using a highly orientated pyrolytic graphite monochromator (PG002) the diffractometer is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. Contaminations of higher order wavelengths are removed by a neutron velocity selector. 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. A fast Li/ZnS scintillator CCD camera is available for additional detection abilities. An optical CCD-camera pointing at the sample position is used to quickly align the crystal with respect to the neutron beam. The main advantage of BIODIFF is the possibility to adapt the wavelength to the size of the unit cell of the sample crystal while operating with a clean monochromatic beam that keeps the background level low. BIODIFF is equipped with a standard Oxford Cryosystem "Cryostream 700+" which allows measurements in the temperature regime from 90 K up to 500 K (see Figure underneath).

[1] S. J. Tomanicek, R. F. Standaert et al., *The Journal of Biological Chemistry*, 2013, 288, 4715-4722, [2] T. Bryan, J. M. González et al., *Acta Crystallographica Section F*, 2013, F69, 1015-1019



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