[3] X.J. Yang et al., *Structure* 23, 1179-1189 (2015)
[4] E.S. Burgie et al., *Structure* 24, 448-457 (2016)

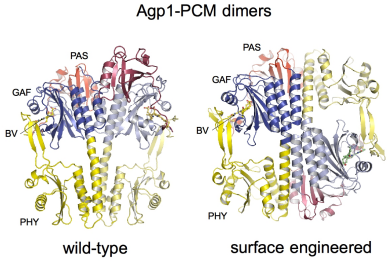

Figure 1. Structures of parallel (left) and anti-parallel dimers (right) of the photosensory core modules (PCMs) of wild-type Agp1 and a surface-engineered mutant, respectively. The domains of the PAS-GAF-PHY tridomains are shown in different colours.

Keywords: phytochrome, histidine kinase, dynamic quaternary structure

MS9-P6 Neutron macromolecular crystallography at the FRM II - Or: what can neutrons do for you

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The research reactor Heinz Maier-Leibnitz (FRM II) is a modern high flux neutron source which feeds at the present 27 state of the art instruments. The newly build neutron single crystal diffractometer BIODIFF is especially designed to collect data from crystals with large unit cells. The main field of application is the structure analysis of proteins, especially the determination of hydrogen atom positions. BIODIFF is a joint project of the Forschungszentrum Jülich (FZJ/JCNS) and the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II). Typical scientific questions addressed are the determination of protonation states of amino acid side chains in the active center of enzymes and the characterization of the hydrogen bond network between the protein 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 and thus to minimize the data collection time the main detector of BIODIFF consists of a neutron imaging plate system in a cylindrical geometry. A Li/ZnS scintillator CCD camera is available for additional detection abilities. 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. BIODFF is equipped with a standard Oxford Cryosystem “Cryostream 700+” which allows measurements in the temperature regime from 90K up to 500K.

Keywords: Protonation states, enzyme function, neutron macromolecular crystallography, water structure