BioDiff - a neutron diffractometer optimized for crystals with large unit cell dimensions

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Neutron structure determination:

Hydration structure analysis:

The hydrogen atoms can be resolved even at a resolution of d_{min} = 2.5 Å.

<table>
<thead>
<tr>
<th>Comparison of form factors (X-ray) and scattering lengths (neutrons):</th>
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<tbody>
<tr>
<td><strong>H</strong></td>
</tr>
<tr>
<td>X-ray</td>
</tr>
<tr>
<td>Neutron</td>
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Amino acid protonation states:

- Protonation states of amino acid side chains
- Deuterium exchange as a measure of flexibility and accessibility (dissociation between H/D)
- Solvent structure including hydrogen atoms can be analysed
- Discrimination between neighbors in the periodic table is possible: e.g. N and O, Fe and Mn
- B factors (σ²/σ²) of the hydrogen atoms can be compared with data of other techniques
- No radiation damage compared to measurements at synchrotrons

**The diffractometer BIODIFF:**

**First “user data-sets”: β-lactamase with bound BZB inhibitor**

**Publication:** Domonicki et al., J. Biol. Chem., 288, 4751 (2013)

**Experimental Team:** S. Tomaszek, R. Standhard, K. L. Weiss, J. D. Ng, L.

**Coates:** [Group of F. Langen]

**Structure of Compound I of Cytochrome C Peroxidase:**

**Publication:** Science 311 July 2006 vol. 311 no. 5766 pp. 166–170 DOI: 10.1126/science.1123679

**Experimental Team:** Cecilia M. Casadei, Andrea Gumiero, Clive L. Metcalfe, Emma J. Murphy, Jaswir Basran, Maria Grazia Concilio, Susana C. M. Tei, Tobias E. Schrader, Alain J. Fielding, Andreas Ostermann, Matthew P. Blakeley, Emma L. Raven, and Peter C. E. Moody

**Neutron diffraction (100 K) at BioDiff:**

**X-ray diffraction:**

**The structure of compound I of CIP in the region of the heme.** Nuclear scattering density (2Fo-Fc contoured at 2.2 RMS) in the (A) distal and (B) proximal heme pocket. Electron density (2Fo-Fc contoured at 2.6 RMS) in the (C) and (D).

**Web-pages to hand in proposals:** user.frm2.tum.de

**Next Proposal Deadline:** January, 16th 2015!