Neutron macromolecular crystallography at the FRM II
The neutron single crystal diffractometer BIODIFF
or: What can neutrons do for you?

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Neutron structure determination:
Hydration structure analysis:
Example: myoglobin

H₂O/ D₂O exchange: as measure of flexibility and accessibility
Hydration structure analysis:
- Deuterium exchange as a measure of flexibility and accessibility (discrimination between H/D)
- Solvent structure including hydrogen atoms can be analyzed
- Discrimination between neighbors in the periodic table is possible: e.g. N and O, Fe and Mn

B-factors (σ²) of the hydrogen atoms can be compared with data of other techniques.

The diffractionometer BIODIFF:

First “user data-sets”:

β-lactamase with bound BZB inhibitor
S.J. Tomarsick, R.F. Stander, K.L. Weiss, J.D. N., L. Coates (Group of P. Laragen)

Human farnesyl pyrophosphate synthase with risedronate
T. Yokoyama, M. Wizgult, N. Nishimura, S. Tanaka

Compound I of cytochrome c peroxidase @100K
Sauer et al. (2005) Science 308: 150

Analysis of H/D-exchange:

Sample environment:

NIP and CCD detector system:

Examples of user experiments:

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