Access Highlights - Martin Weik

The coupling between hydration-water and protein dynamics as assessed by neutron scattering and perdeuteration

Institut de Biologie Structurale CEA-CNRS-UJF, 41 rue Jules Horowitz, 38027 Grenoble Cedex 1, France

The thin film of water around proteins, their hydration water, is vital to the macromolecule's biological activity. Without hydration water, proteins would not only be incorrectly folded but also lack the conformational flexibility that animates their 3D structures and brings them to life. Consequently, protein dynamics is thought to be slaved to hydration-water dynamics. One way of exploring the coupling exploits so-called dynamical transitions, characteristic changes in atomic fluctuations that appear in both water and proteins at certain cryo-temperatures. Do both dynamical transition temperatures coincide? In other words, does a transition in the water trigger one in the protein at the same temperature? If the coupling is indeed tight, one would assume so.

We addressed the dynamical coupling of globular, membrane and intrinsically unfolded proteins with their hydration water by incoherent neutron scattering experiments. The experimental trick played to directly access the water behaviour was perdeuteration of the proteins, which almost completely masked the protein's contribution to the neutron scattering signal. In the case of the globular maltose binding protein (MBP), a hydration-water transition was observed at 220 K, coinciding with the dynamical transition of the protein [1]. The latter was measured on a hydrogenated MBP sample hydrated in D2O. MD simulations reproduced the coincidence of transitions and revealed that both originate from the onset of translational diffusion of water molecules at the protein's surface. The combination of neutron scattering, perdeuteration and MD simulations, carried out on the same protein, paints a coherent picture in which the dynamics of soluble globular proteins and their hydration-water are strongly coupled. The observation is in sharp contrast with the case of the purple membrane, a biological membrane composed of the protein bacteriorhodopsin and several lipid species. The hydration-water transition and the membrane transition appeared at temperatures that differ by 50 K [2], suggesting that the dynamics of membrane proteins is controlled by their lipid environment, rather than by the membrane hydration water. First experiments on the intrinsically unfolded protein tau that is involved in Alzheimer disease suggest that protein flexibility is increased with respect to globular and membrane proteins and that the dynamical coupling to hydration water is much tighter [3].

The studies have been carried out at the backscattering spectrometers IN16 at the ILL in Grenoble and SPHERES at FRMII in Munich. Protein perdeuteration has been largely carried out in the DLAB laboratory in Grenoble. NMI3 funded the deuteration experiments at the DLAB and travel, accommodation and living costs related to experiments at SPHERES.

[1] Wood, K., Frolich, A., Paciaroni, A., Moulin, M., Hartlein, M., Zaccai, G., Tobias, D. J. & Weik, M., J Am Chem Soc 130, 4586 (2008).

[2] Wood, K., Plazanet, M., Gabel, F., Kessler, B., Oesterhelt, D., Tobias, D. J., Zaccai, G. & Weik, M., Proc Natl Acad Sci U S A. 104, 18049 (2007).

[3] Gallat, Wood, Colletier, Laganowski, Schneider, Wuttke, Moulin, Härtlein, van Eijk, Blackledge, Eisenberg, Zaccai & Weik, unpublished

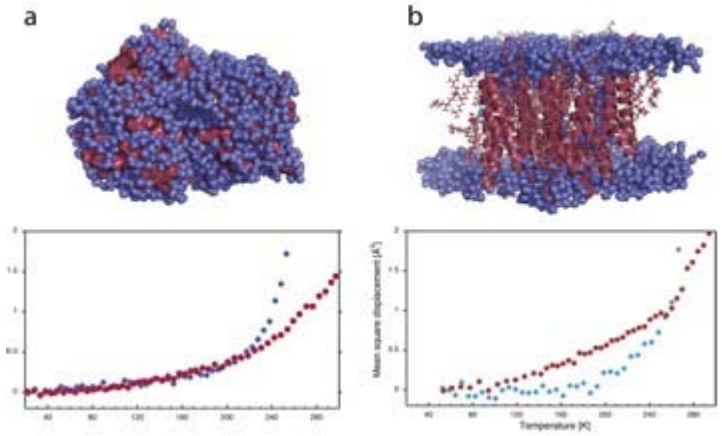

Figure: Mean square displacement of hydrogens in the hydration-water (blue) and the protein (red) as a function of temperature as determined from elastic scans for a globular protein (a; [1]) and a membrane protein (b; [2]).