The relation between protein and solvent dynamics as studied by neutron scattering and temperature-controlled X-ray crystallography

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The degree of coupling between protein and solvent dynamics is still a debated issue. In particular, it remains unclear whether dynamical changes in a protein's environment, such as a glass transition, trigger dynamical transitions in proteins which have been revealed and studied by numerous experimental and simulation techniques. Since specific flexibility is vital to protein function, the study of dynamical aspects of proteins and their environment is highly relevant to the understanding of structure-function-dynamics relationships in biology.

We are employing two complementary techniques, neutron scattering and temperature-controlled X-ray crystallography, to address the issue of the dynamical coupling of proteins and their environment. Elastic incoherent neutron scattering allows the determination of atomic mean-square fluctuations on the ns-ps time scale averaged over all hydrogen atoms present in the sample. Consequently, global protein dynamics are assessed if a hydrogenated protein is investigated in D_2O and solvent dynamics is probed if deuterated proteins in H_2O are employed. In particular, temperature-dependent experiments inform about dynamical transitions from harmonic to anharmonic motions in either the protein or the solvent and their relation can be studied. X-ray crystallography, on the other hand, informs about spatially-resolved structural changes as a function of temperature. In this context, intense synchrotron radiation has been discovered to produce specific chemical damage to crystalline proteins that proves to be a valuable tool to monitor structural flexibility. Temperature-dependent structural radiation damage, determined at and below the glass transition of the protein-crystal solvent, suggests that solvent and local protein dynamics are coupled.

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