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Variation of Structural and Dynamical Flexibility of Myelin Basic Protein in Response to Guanidinium Chloride

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Myelin basic protein (MBP) is intrinsically disordered in solution and is considered as a conformationally flexible biomacromolecule. Here, we present a study on perturbation of MBP structure and dynamics by the denaturant guanidinium chloride (GndCl) using small-angle scattering and neutron spin–echo spectroscopy (NSE). A concentration of 0.2 M GndCl causes charge screening in MBP resulting in a compact, but still disordered protein conformation, while GndCl concentrations above 1 M lead to structural expansion and swelling of MBP. NSE data of MBP were analyzed using the Zimm model with internal friction (ZIF) and normal mode (NM) analysis. A significant contribution of internal friction was found in compact states of MBP that approaches a non-vanishing internal friction relaxation time of approximately 40 ns at high GndCl concentrations. NM analysis demonstrates that the relaxation rates of internal modes of MBP remain unaffected by GndCl, while structural expansion due to GndCl results in increased amplitudes of internal motions. Within the model of the Brownian oscillator our observations can be rationalized by a loss of friction within the protein due to structural expansion. Our study highlights the intimate coupling of structural and dynamical plasticity of MBP, and its fundamental difference to the behavior of ideal polymers in solution.

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