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The relevance of protein dynamics for protein folding: The case of apomyoglobin

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Dynamics of different folding intermediates and denatured states might have implications in understanding protein folding. Apomyoglobin (apoMb) has been investigated using neutron spin-echo spectroscopy (NSE) and SANS [1] and quasielastic neutron scattering (QENS) [2,3] in different states: native-like, partially folded and completely unfolded. Mean square displacements obtained by QENS showed a correlation with the secondary structure content of apoMb [2,3]. However, recent NSE & SANS data offered a detailed picture on the physical nature of slow collective dynamics and different dynamics behavior was observed [1]. While the internal dynamics of the native-like state can be understood using normal mode analysis based on high resolution structural information of myoglobin, for the unfolded and even for the molten globule states, models from polymer science are employed. The Zimm model accurately describes the slowly-relaxing, expanded GdmCl-denaturated state. Dynamics of the acid unfolded and molten globule state are similar in the framework of the Zimm model with internal friction. Transient formation of secondary structure elements in the acid unfolded and presence of α-helices in the molten globule state lead to internal friction to a similar extent, which demonstrates the importance of secondary structure elements as source of internal friction in partially folded proteins.

1. Balacescu et al. Scie Rep, 2020
2. Stadler et al. JPCB, 2015
3. Stadler et al. PCCP, 2016

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