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Towards time-resolved protein dynamics on nanoscopic scales

Content

Protein function is realized by an interplay of molecular structure and dynamics.
Various methods have been established to study the evolution of macromolecular conformation after trigger events. The time-resolved evolution of protein dynamics on molecular length scales, however, still presents experimental challenges, in particular when considering proteins in the native environment, i.e. in solution [1].

Here, we present a case study by quasi-elastic neutron scattering that addresses the evolution of nanoscopic protein dynamics during thermal denaturation [2]. Using so-called elastic and inelastic fixed window scans, we obtain time-resolved information on the change of dynamics and the related dynamical confinement on length scales of nanometers and time scales of nanoseconds.

As intuitively expected, upon heating the protein solution, the dynamics first increase due to thermal activation, and then dramatically drops down upon unfolding and cross-linking. The slower dynamics is also preserved when cooling back, due to the formed protein gels. Interestingly, the comparison between dynamics and related confinement suggests that the main determinant of the decrease stems from changes of dynamics. The emerging picture thus includes a flexible motion of the protein network on nanosecond time scales, which is simply slowed down by the presence of the cross-linked neighbors.

The experimental approach allows to follow nanoscopic dynamics with a sampling time below one minute, which opens interesting opportunities for dynamical changes e.g. driving protein assembly.

[1] M Grimaldo, F Roosen-Runge, F Zhang, F Schreiber, T Seydel: Dynamics of proteins in solution, Quart. Rev. Biophys. 2019, 52, e7
[2] O Matsarskaia, L Bühl, C Beck, M Grimaldo, R Schweins, F Zhang, T Seydel, F Schreiber, F Roosen-Runge: Evolution of the structure and dynamics of bovine serum albumin induced by thermal denaturation, Phys. Chem. Chem. Phys. 2020, 22, 18507-18517

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