

Spectroscopic insights into the structural transitions of bovine serum albumin induced by sodium dodecyl sulfate

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Understanding the mechanisms of protein structural transformations induced by external factors is essential for elucidating fundamental molecular processes in living organisms. Surfactants are particularly useful in these studies because they induce conformational changes at millimolar concentrations, in contrast to the molar concentrations required by urea or guanidine. Protein–surfactant systems offer a unique opportunity to monitor simultaneous, time-dependent changes in secondary and tertiary structures, their coupling, and their dependence on solvent conditions. Early kinetic studies were initiated in the 1980s by Kunio Takeda and colleagues [1,2] and more recently continued by Daniel Otzen and collaborators [3].

In our study, we investigate SDS-induced unfolding of bovine serum albumin (BSA) by combining steady-state spectroscopy and kinetic stopped-flow measurements. Secondary structure changes are monitored by far-UV CD, tertiary structure by near-UV CD, and the local environment of aromatic residues by intrinsic fluorescence.

Steady-state CD shows far-UV signal saturation near ~ 12 mM SDS, while near-UV CD changes little over a wide SDS range. These observations suggest that major secondary-structure rearrangements are largely completed before tertiary packing, which converges to a relatively uniform aromatic environment once SDS binding is established. In contrast, fluorescence is highly sensitive below the CMC, indicating that SDS monomers disrupt tertiary packing even before detectable secondary-structure changes. Ionic strength has little effect on steady-state CD but significantly affects fluorescence kinetics. At constant SDS concentration, NaCl content alters reaction rates and amplitudes, maximally delaying slow relaxation phase at ~ 75 mM, which indicates the kinetic stabilization of a long-lived intermediate.

[1] K. Takeda and S. Takagi (1981) *Agric. Biol. Chem.* 45, 777-779.

[2] K. Takeda (1983) *Bull. Chem. Soc. Jpn.* 56, 1037-1040.

[3] G. V. Jensen, J. N. Pedersen, D. E. Otzen and J. S. Pedersen (2020) *Front. Mol. Biosci.* 7, 125.

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