Investigation of the Wrapping Mechanism of β-Lactoglobulin Around SDS Micelles by Time-Resolved VUVCD and Molecular Dynamics Simulation

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Water-soluble proteins often undergo structural transitions induced by interactions with membrane interfaces, expressing biological functions such as drug transport and amyloid fibril formation[1,2]. Surfactants have been widely used as membrane mimics and adapted as a practical model for studying these interactions. In this study, we investigated the interaction between β-lactoglobulin (bLG), a model membrane-binding protein, and sodium dodecyl sulfate (SDS), an anionic surfactant, using time-resolved (TR-) VUVCD to elucidate the structural transition mechanism from the native (N-) to micelle-bound (MB-) state[3,4].

TR-VUVCD spectra of bLG were recorded in the 0.2–120 s range with 0.2 s resolution, revealing a transition from β-strand–rich to α-helix–rich structures (corresponding to N- and MB-states, respectively) (FIGURE). Kinetic analysis identified two intermediates, showing a stepwise increase in helical content. Molecular dynamics (MD) simulations based on these data further clarified the interaction mechanism, where initial electrostatic attraction facilitates approach to the micelle surface, followed by hydrophobic stabilization. These findings enabled us to propose a model for SDS micelle wrapping by bLG.

Our study demonstrates that combining TR-VUVCD and MD simulation is a powerful approach for probing protein–surfactant interactions and membrane-associated protein dynamics.

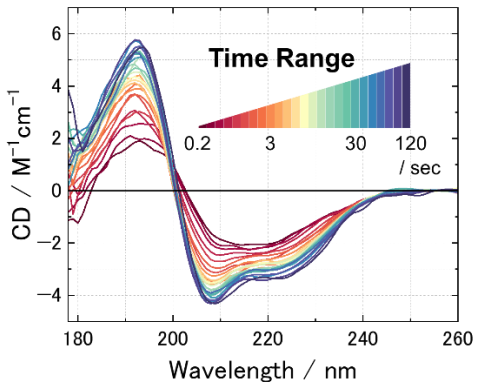

FIGURE. TR-VUVCD spectra of bLG during the interaction with SDS micelles, measured from 0.2 to 120 s.

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