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Title: Water Rearrangements upon Disorder-to-Order Amyloid Transition

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Water plays Critical role

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Abstract:

Water plays a critical role in governing the intricate balance between chain-chain and chain-solvent interactions during protein folding, misfolding, and aggregation. Previous studies have indicated the presence of different types of water in folded (globular) proteins. In this work, using femtosecond and picosecond time-resolved fluorescence measurements, we have characterized the solvation dynamics from ultrafast to ultraslow time scale both in the monomeric state and in the amyloid state of an intrinsically disordered protein, namely κ -casein. Monomeric κ -casein adopts a compact disordered state under physiological conditions and is capable of spontaneously aggregating into highly ordered β -rich amyloid fibrils. Our results indicate that the mobility of "biological water" (type I) gets restrained as a result of conformational sequestration during amyloid formation. Additionally, a significant decrease in the bulk water component with a concomitant increase in the ultraslow component revealed the ordering of trapped interstitial water (type II) upon disorder-to-order amyloid transition. Our results provide an experimental underpinning of significant water rearrangements associated with both chain desolvation and water confinement upon amyloid formation.

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