ULTRAFAST HYDRATION DYNAMICS OF MELITTIN : HELIX FORMATION AND TETRAMER SELF-ASSEMBLY

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Elucidation of protein-water interactions at the local molecular level is critical to the understanding of protein folding and aggregation. Here, we report our systematic studies of hydration dynamics in three conformations of melittin from a random coil, to an α-helix, and to a self-assembled tetramer using intrinsic amino acid (W19) as a local optical probe. With femtosecond resolution, we observed distinct hydration dynamics in conformational transitions from 14 ps for the random coil to 100 ps for the α-helix and tetramer. These different time scales of water motions imply appropriate water mobility which is necessary to maintain structural stability as well as to keep certain flexibility. These studies reveal the critical role of hydration dynamics on peptide conformation changes.