

Abstract Submitted
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Ultrafast Dynamics of Leu-Enkephalin in Water and Membranes¹

SOOHWAN SUL, YUAN FENG, UYEN LE, NIEN-HUI GE, Department of Chemistry, University of California, Irvine — Ultrafast two-dimensional infrared (2D IR) spectroscopy has been applied to investigate the peptide-membrane interaction and conformational distribution of Leu-enkephalin (Lenk) in bilayer membranes. We compare the results from linear and 2D IR experiments on p-cresol in water, Lenk in water, and Lenk in membranes, focusing on the ring stretching mode of the Tyr side chain. Frequency-frequency correlation functions obtained from a series of waiting-time-dependent 2D IR spectra reveal a fast decaying component with a ~ 1 ps time constant that is common for all three systems. This spectral diffusion component is attributed to hydrogen-bond making-breaking dynamics of the Tyr side chain. Unlike p-cresol in water, both Lenk systems exhibit substantial spectral inhomogeneity that does not decay within the 4 ps window. The observed hydrogen-bond dynamics suggests that the Tyr side chain of Lenk in membranes is located at the water-abundant region at the water-membrane interface. The experimental results are compared with those from MD simulations and DFT calculations.

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