

Abstract Submitted
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A Mean Field Model for Studying the Crowding Effect of TMAO in the Protein Hydration Shell ANTHONY COOPER, LUCA LARINI, Rutgers University Camden — Studying the local dynamics of the water molecules closest to a protein has been a long-standing challenge. As the surface of a protein is not uniform, the solvent binds to a varying degree across different points along the surface. Additionally, other solutes may change the local properties of the hydrogen bond network, which in turn may stabilize or destabilize the protein itself. TMAO is a well-known crowding agent that is believed to stabilize a proteins secondary structure not by direct contact with the backbone, but by an effect that is mediated by altering the hydrogen bond network of the water surrounding the protein. The exact nature of this effect is not fully understood. Here, we propose a mean field model that describes the interaction of TMAO with the water surrounding the protein and we will test our prediction through comparison with existing 2D IR spectroscopic data. Our mean field model correctly predicts the shift of the resonance frequency and the dependence on the concentration of solute while establishing a connection between the decay of the frequency-frequency correlation function and entropy of the system.

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