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Effects of Trimethylamine-N-oxide on the Conformation of Peptides and Proteins ZHAOQIAN SU, FARBOD MAHMOUDINOBAR, CRISTIANO DIAS, New Jersey Institute of Technology — To provide insights into the stabilizing mechanisms of trimethylamine-N-oxide (TMAO) on protein structures, we perform all-atom molecular dynamics simulations of peptides and the Trp-cage miniprotein. Effects of TMAO on the charged residues of peptides are found to stabilize compact conformations, whereas effects of TMAO on nonpolar residues lead to peptide swelling. This suggests competing mechanisms of TMAO on proteins which would accounts for swelling of hydrophobic cores and stabilization of charge-charge interactions. These mechanisms are studied from replica exchange molecular dynamics simulations of the Trp cage miniprotein.

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