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WITHDRAWN (G) (POS-47) Effects of Macromolecular Crowding on Protein Folding in the Presence of Nonnative Interactions

The high total concentration of macromolecules inside living cells leads to the emergence of a phenomenon called macromolecular crowding which affects various protein processes including folding. In general, interactions between a protein and surrounding crowder molecules can involve both attractions and repulsive excluded volume forces. Here we revisit the effect of purely repulsive crowders on protein folding and stability with a sequenced-based coarse-grained model. The crowders are modelled as spheres with two independent parameters representing size and softness. Using simulated tempering Monte Carlo, we determine the thermodynamic behaviours of two amino acid sequences with 35 amino acids folding into a helical hairpin and a 5-stranded β-barrel, respectively, over a range of crowder concentrations $\phi_c = 0$ and crowder sizes. These behaviours are analyzed in the terms of stability of the folded state, radius of gyration, and non-native interactions. For the α-helical protein, we find that the native state stability increases monotonically with $\phi_c = 0$. However, the crowders induce a destabilization of the β-barrel protein at low temperature and low $\phi_c = 0$. Our analysis shows that this destabilization arises from two factors: A compact state characterized by non-native interactions and a population of approximately 2% at $\phi_c = 0$, and a relatively compact unfolded state, which is therefore only weakly disfavored entropically by the crowders.

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