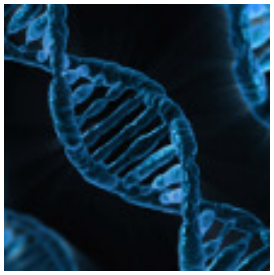

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Virtual Cell Model For Osmotic Pressure Calculations In Protein Solutions

The osmotic pressure of protein solutions is an important measure of intermolecular interactions and can be used to predict stability and phase separation. Computationally, the osmotic pressure due to a single, spherical charged macromolecule can be obtained, from a purely structural force-free calculation of the counter-ions density at the boundary of the simulation box, via the cell-model. However, protein shape anisotropy and the surface charge distribution are ignored in the original cell model, as are specific ion-residue and ion-ion interactions. In this study, we first revisit the original cell model for a spherical cell and use it to calculate the osmotic pressure of an aqueous plectasin solution using coarse grained Monte Carlo (MC) simulations. To assess the validity of the cell-model approximations, we compare with two-body MC simulations that explicitly account for direct protein-protein interactions. Next, we extend the cell model to all-atom molecular dynamics (MD) simulations, which account for explicit solvent solvatation and internal protein flexibility, and show that protein concentration dependent osmotic pressures can be obtained by confining counter-ions in a virtual spherical subspace defining the protein number density. We also show the possibility of using specific interaction parameters for the protein-ion and ion-ion interactions, which would provide a more accurate description of osmotic pressures of protein solutions.

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