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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 solvation 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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