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A residue level protein-protein interaction model in electrolyte solutions XUEYU SONG, Iowa State University — The osmotic second virial coefficients B_2 are directly related to the solubility of protein molecules in electrolyte solutions and can be useful to narrow down the search parameter space of protein crystallization conditions. Using a residue level model of protein-protein interaction in electrolyte solutions B_2 of bovine pancreatic trypsin inhibitor and lysozyme in various solution conditions such as salt concentration, pH and temperature are calculated using an extended Fast Multipole Methods in combination with the boundary element formulation. Overall, the calculated B_2 are well correlated with the experimental observations for various solution conditions. In combination with our previous work on the binding affinity calculations of protein complexes it is demonstrated that our residue level model can be used as a reliable model to describe protein-protein interaction in solutions.

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