A Mesoscopic Model for Protein Interactions

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Abstract. Proteins in the living cell can interact with a wide variety of solutes, ranging from other proteins, small peptides, ions, DNA, and membranes. Charged groups play a major role and solution conditions such as pH and ionic strength can modulate the interactions significantly. Describing these systems in a statistical mechanical framework envolves thousands of pair-interactions and therefore a certain amount of coarse graining is often required. We here present a conceptually simple "mesoscopic" protein model [1] where the detailed charge distribution and surface topology is well preserved but is much faster than a full atomistic description. Using Monte Carlo simulations the model can be used to accurately reproduce second virial coeffients, pH titration curves and binding constants. Special attention will be given to *proton fluctuations* that – under certain circumstances – can give rise to an increased attraction between bio-molecules [2].

References

1. Lund, M., Jönsson, B.: A Mesoscopic Model for Protein-Protein Interactions in Solution. *Biophysical Journal* (2003)
2. Lund, M., Jönsson, B.: On the Charge Regulation of Proteins. *Biochemistry* (2005).