Simple Model for Phase Diagram of Lysozyme as a Function of Salt Type and Salt Concentration

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TON, Lehigh University — The liquid-liquid phase separation curves for lysozyme are known to depend on the salt type and salt concentration. For the case of monovalent cations, the cloud point temperature typically increases with increasing salt concentration, for fixed lysozyme concentration. For the case of divalent cations, however, a maximum in the cloud point temperature is observed that has been interpreted as being due to ion binding to the protein surface and subsequent water structuring. In this paper we use a simple square well model due to Grigsby et al (Biophys. Chem. 91, 231 (2001)), whose well depth depends on salt type and salt concentration, to determine the phase diagram for both monovalent and divalent cations. The phase diagrams are calculated using standard Monte Carlo simulations and compared with known experimental results.