223a Adsorption Simulations and Biology: Grand Canonical Monte Carlo Calculations of Binding Locations, Occupancy, and Free Energies of Xenon in Comp and Mutant Phage T4 Lysozyme L99a

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The binding of xenon with the oligomerization domain of rat cartilage oligomeric matrix protein and with an engineered mutant of phage T4 lysozyme has been studied by Grand Canonical Monte Carlo simulations. In both proteins, the xenon sites determined by previous X-ray diffraction studies were found via analysis of the simulation results. A novel clustering algorithm facilitated the rapid identification of binding sites and enabled the calculation of site occupancies, binding equilibrium constants, and binding free energies from the simulation data.