Simulations of Concentrated Antibody Solutions and Comparison with Small-Angle Scattering Experiments

MAX WATSON, NICHOLAS CLARK, JOSEPH CURTIS, National Institute of Standards and Technology — We have performed atomically detailed Monte-Carlo simulations of hundreds of antibodies in concentrated solutions. In order to compare our simulations with experiments, we developed a novel method for explicitly calculating the scattering intensity of these large systems. At various salt conditions and pH levels, the simulations are found to be in good agreement with small-angle X-ray scattering measurements for antibody concentrations exceeding 100 mg/mL.