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Abstract:

Ram Vanam M.S., Indiana University, December 2004. Electrostatic modeling of protein aggregation. Research Advisor: Paul L. Dubin Electrostatic modeling was done with Delphi of insight II to explain and predict protein aggregation, measured here for β-lactoglobulin and insulin using turbidimetry and stopped flow spectrophotometry. The initial rate of aggregation of β-Lactoglobulin was studied between pH 3.8 and 5.2 in 4.5mM NaCl; and for ionic strengths from 4.5 to 500mM NaCl at pH 5.0. The initial slope of the turbidity vs. time curve was used to define the initial rate of aggregation. The highest initial rate was observed near pH < pI i.e., 4.6 (< 5.2). The decrease in aggregation rate when the pH was increased from 4.8 to 5.0 was large compared to its decrease when the pH was reduced from 4.4 to 4.2; i.e., the dependence of initial rate on pH was highly asymmetric. The initial rate of aggregation at pH 5.0 increased linearly with the reciprocal of ionic strength in the range I = 0.5 to 0.0045M. Protein electrostatic potential distributions are used to understand the pH and ionic strength dependence of the initial rate of aggregation. Similar studies were done with insulin. In contrast to BLG, the highest initial aggregation rate for insulin was observed at pH = pI. Electrostatic computer modeling shows that these differences arise from the distinctly different surface charge distributions of insulin and BLG.

Description:

Submitted to the faculty of Indiana University in partial fulfillment of the requirements for the degree Master of Science in the Department of Bioinformatics in the School of Informatics of, Indiana University December, 2004

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