311e Adaptive Neuro-Fuzzy Modeling of Protein Crystal Nucleation Kinetics

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Formation of stable, biologically active crystals and nanoparticles of protein and protein/nucleic acid complexes from solution is dominated by the kinetics of nucleation of these clusters. Nucleation of these protein crystals is the necessary first step in crystallization of proteins and protein complexes for isolation and purification of a protein solid phase and for X-ray crystallographic structure determination at atomic resolution. Prediction of crystal nucleation plays a critical role in the control and optimization of crystal formation and particle size distribution.

In the present work Adaptive Neuro-Fuzzy Logic has been used to obtain a predictive model to estimate the nucleation kinetics of protein at various conditions. The nucleation kinetic data at various conditions that consist of range of pH, temperature, precipitant concentration and additive concentration was used as the training data for the fuzzy logic system. A comparison between the nucleation rate model obtained through non-linear regression techniques (Bhamidi et. al., 2002) and that obtained by fuzzy logic was made.

Reference: V. Bhamidi, S. Varanasi, C. A. Schall. "Measurement and Modeling of Protein Crystal Nucleation Kinetics", Crystal Growth & Design, 2(5), 395-400, (2002).