

Modeling ensembles of beta-sheet folds

Determining the physical structure of a protein or protein complex is one of the best ways to understand its mechanism and function. To assist in this goal, software structure modeling tools typically use sequence data (only) to predict a single most likely protein conformation. We present here algorithmic techniques for the prediction of a Boltzmann ensemble of protein structures, that is, the statistical mechanical set of all likely protein conformations that may exist at once. This is achieved by a hypothesis-driven strategy, incorporating experimental knowledge and allowing for an exhaustive search of conformational space.