

Bayesian Structural Alignment of Proteins

The analysis of the three dimensional structure of proteins is an important topic in structural biology since fold plays a decisive role in defining the function of proteins, and therefore it tends to be more conserved in evolution than sequence. A particularly important aspect is the identification and evaluation of structural similarities between proteins because this can help in understanding the function of new proteins or lead to the discovery of new active agents for drugs. In this work we present a Bayesian model for pairwise structural comparison of proteins which allows to identify possible alternative alignments and provides a clear measure of the significance of the matches while allowing the estimation of parameters that are usually subjectively fixed. We illustrate the model with different examples taken from the literature and compare our results with those obtained through the widely used Combinatorial Extension (CE).