Monte Carlo Simulations of Protein Folding using Lattice Models

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Understanding the so-called native state conformation of protein molecules is of great importance due to the direct relationship between their structure and biological function. However, this native conformation is typically adopted at the global free energy minimum located among an enormous number of local minima on a complex energy landscape. As a result, locating the global minimum through heuristic optimization techniques and simplifying models has attracted considerable attention. This study involved the use of simulated annealing (Kirkpatrick et al, 1983) and the Metropolis method (Metropolis et al, 1953), which utilized the Verdier-Stockmayer algorithm (Verdier et al, 1969). Additionally, the problem was greatly simplified through the use of a two-dimensional lattice model and the Hydrophobic-Polar model (Dil et al, 1985). Results from this study provided insight on protein folding and more realistic models that have since been developed.