

Multicanonical methods for protein folding

B. Berg, G. La Penna, V. Minicozzi, S. Morante, G. Rossi

Universita' di Roma Tor Vergata
Via della Ricerca Scientifica 00133 - ROMA

We present a variant of the Multi-canonical Monte Carlo method which allows to deal with fully flexible chains of bonded monomers, thus opening the way to the possibility of modelling the presence of a solvent at the fundamental atomic level in the context of folding processes. These results represent an important preliminary step in the direction of simulating folding in realistic conditions.