Prediction of Peptide Conformation by Multicanonical Algorithm: New Approach to the Multiple-Minima Problem

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We apply a recently developed method, the multicanonical algorithm, to the problem of tertiary structure prediction of peptides and proteins. As a simple example to test the effectiveness of the algorithm, met-enkephalin is studied and the ergodicity problem, or multiple-minima problem, is shown to be overcome by this algorithm. The lowest-energy conformation obtained agrees with that determined by other efficient methods such as Monte Carlo simulated annealing. The superiority of the present method to simulated annealing lies in the fact that the relationship to the canonical ensemble remains exactly controlled. Once