

A DISCRETE APPROACH FOR THE DETERMINATION OF PROTEIN STRUCTURES USING NMR DATA

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ABSTRACT

We consider the problem of finding the three-dimensional conformation of a protein from a subset of inter-atomic distances provided by Nuclear Magnetic Resonance (NMR) experiments. The basic approach to this problem is to reformulate it as a continuous global optimization problem, where a penalty function is employed in order to measure the satisfaction of the constraints based on the known distances. Many methods have been proposed for the solution of this problem, and most of them are based on a search in a continuous space and/or on heuristic approaches to optimization. We work on a discrete approach to this problem, where the search domain is reduced from a continuous to a discrete set which has the structure of a tree. Based on this combinatorial structure, we developed an efficient branch-and-prune (BP) algorithm. Differently from other algorithms, BP can enumerate all the possible mathematical solutions to the problem. In this work, we explain how this discrete approach, previously applied to protein backbones, can also be applied to entire protein conformations, including the side chains of the amino acids composing the molecule. Support: French Embassy in São Paulo, UNICAMP, FAPERJ, FAPESP, CAPES, CNPq.

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