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Quasi-physical Algorithm for Protein Folding in an Off-Lattice Model

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Abstract: We study a three-dimensional off-lattice protein folding model, which involves two species of residues interacting through Lennard-Jones potentials. By incorporating an extra energy contribution into the original potential function, we replace the original constrained problem with an unconstrained minimization of a mixed potential function. As such an efficient quasi-physical algorithm for solving the protein folding problem is presented. We apply the proposed algorithm to sequences with up to 55 residues and compare the computational results with the putative lowest energy found by several of the most famous algorithms, showing the advantages of our method. The dynamic behavior of the quasi-physical algorithm is also discussed.

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