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by

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The application of the transfer matrix method to compact lattice conformations - cyclic conformations of larger sizes, non-cyclic conformations, and irregular conformations

ABSTRACT

Enumerating all protein conformations in a compact lattice is a biologically important yet computationally challenging process. The challenge arises when using traditional methods (especially with larger conformations) because of attrition – many conformations end up terminating at dead ends. We've developed a superior method, the transfer matrix method, which is far less computationally expensive. Our method overcomes the problem of attrition by enumerating all possible conformations in a row-by-row process. In previous works we've applied the transfer matrix method 2-D square and 3-D rectangular matrices and analyzed the effect of HP model potentials on the average statistical properties based on all cyclic conformations on the 4 x 10 square lattice. Here, we apply our method to all cyclic conformations on the 5 x 10 square matrix, show ways of including non-cyclic conformations, and expand our method to more irregular conformations that contain sequential configurations of various $m \times n$ square and $m \times n \times l$ cubic lattices. All of the above directions would be steps towards more closely modeling real proteins in the hopes of further understanding the energetics of the protein folding problem.