Algorithms for Proteins Folding Prediction: 3D Cubic Lattice in HP Model

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Proteins are important biological molecules which play a key role in almost all bio-logical processes. The tertiary structure of the proteins determines their functions. Therefore, the predicting of protein's tertiary structure, based on the primary amino acid sequence from long time is the most important and challenging subject in bio-chemistry, molecular biology and biophysics.

Here, we will present extension of the heuristic algorithm for 2D HP models de-scribed by Traykov et al. to solve the 3D HP lattice model for protein folding prob-lem. The algorithm divided the protein sequence S of k non intersected segments S1,..., Sk which are supposed to be small. On the first step the algorithm finds the opti-mal fold for segment S1. After that, the algorithm finds optimal folding for S1 S2 taking into account the saved fold, and so on. We compare the obtained results with the results of well-known in the literature algorithms for solving the 3D HP lattice model as genetic algorithms, ant-colony algorithms, and Monte Carlo algorithms.

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References

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