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Design Optimization of Protein Tertiary Structure using Three-Residue Fragments

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Summary

Optimization of the unique tertiary structure of a protein from its amino acid sequence alone is one of the important challenges in science and technology. It is because the tertiary structure itself and the folding mechanism toward it are indispensable for understanding the function and biological role of the protein. One of the computational methods often used for protein structure design is a fragment assembly method. It shows good native-like structure designs in many cases. There are limitations, however, in the conventional fragment assembly methods. Arguments for uses of energy functions and global optimization to design the structures are in progress for example.

In this study, a new design optimization method for protein structures is proposed. The proposed system mainly consists of two methods. The first one is a fragment assembly where 3-residue fragments of representative protein chains are used to produce initial structures of a given sequence of amino acids. The second one is a global optimization which uses folding optimization to construct optimized structures. Numerical examples show that one of our optimized structures was gauged 5.2 Å of α-carbon RMSD (root mean square deviation) on its native tertiary structure.

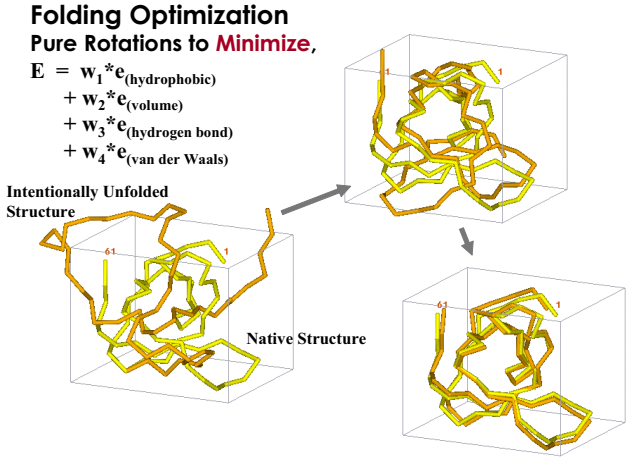

Figure 1: Numerical experiment to verify the proposed folding optimization and its energy function

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