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A novel canonical dual computational approach for prion AGAAAAGA amyloid fibril molecular modeling

Jiapu Zhang, David Y. Gao, Johh Yearwood

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Many experimental studies have shown that the prion AGAAAAGA palindrome hydrophobic region (113-120) has amyloid fibril forming properties and plays an important role in prion diseases. However, due to the unstable, noncrystalline and insoluble nature of the amyloid fibril, to date structural information on AGAAAAGA region (113-120) has been very limited. This region falls just within the N-terminal unstructured region PrP (1-123) of prion proteins. Traditional X-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy experimental methods cannot be used to get its structural information. Under this background, this paper introduces a novel approach of the canonical dual theory to address the 3D atomic-resolution structure of prion AGAAAAGA amyloid fibrils. The novel and powerful canonical dual computational approach introduced in this paper is for the molecular modeling of prion AGAAAAGA amyloid fibrils, and that the optimal atomic-resolution structures of prion AGAAAAGA amyloid fibils presented in this paper are useful for the drive to find treatments for prion diseases in the field of medicinal chemistry. Overall, this paper presents an important method and provides useful information for treatments of prion diseases. Overall, this paper could be of interest to the general readership of Theoretical Biology.

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