DIGITAL TOTAL

Studying protein 3D structures using network science

Understanding protein 3-dimensional (3D) structures is important because functions of proteins depend on them. We proposed (static or dynamic) network approaches to model protein 3D structures as protein structure networks (PSNs). Static PSNs model the whole 3D structure of a protein as a single-layer PSN. Because the folding of a protein entails some protein parts folding before others, we additionally proposed to model a protein as a dynamic (i.e., multi-layer) PSN. Using 44,000 proteins, we evaluated our PSN models in the task of protein structural classification (PSC); a supervised problem of assigning proteins into pre-defined structural classes. We showed that our models outperformed state-of-the-art PSC approaches, showing our models' promising application in understanding 3D structures of proteins.

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Keywords

Protein 3D structures
Protein structure networks
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TentID

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