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Assortative mixing in Protein Contact Networks and protein folding kinetics

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▶ Abstract

Motivation: Starting from linear chains of amino acids, the spontaneous folding of proteins into their elaborate three-dimensional structures is one of the remarkable examples of biological selforganization. We investigated native state structures of 30 singledomain, two-state proteins, from complex networks perspective, to understand the role of topological parameters in proteins' folding kinetics, at two length scales - as "Protein Contact Networks (PCNs)" and their corresponding "Long-range Interaction Networks (LINs)" constructed by ignoring the short-range interactions.

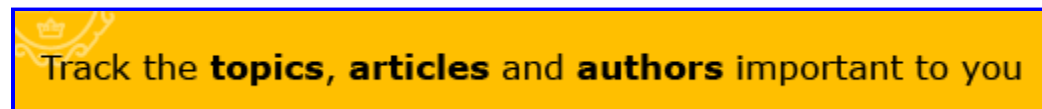
Results: Our results show that, both PCNs and LINs exhibit the exceptional topological property of "assortative mixing" that is absent in all other biological and technological networks studied so far. We show that the degree distribution of these contact networks is partly responsible for the observed

assortativity. The coefficient of assortativity also shows a positive correlation with the rate of protein folding at both short and long contact scale, whereas, the clustering coefficients of only the LINs exhibit a negative correlation. The results indicate that the general topological parameters of these naturally evolved protein networks can effectively represent the structural and functional properties required for fast information transfer among the residues facilitating biochemical/kinetic functions, such as, allostery, stability, and the rate of folding.

Supplementary Information: Supplementary data are available at *Bioinformatics* online.

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