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by

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Effect of Packing Density on Protein Dynamics

ABSTRACT

The function of a protein is influenced not only by the amino acid specificity, but also by its shape and its packing density. These latter properties are embedded in the recently developed elastic network models in a simple way to predict how proteins move to perform their function. Although simulation tools, such as Molecular Dynamics, are very useful to analyze localized, high-frequency motions, they cannot reach time scales large enough to capture low-frequency motions, e.g. domain motions, to relate dynamics to protein functionality. Elastic network models prove very successful in deriving domain motions: comparison of elastic network models' results with experimental data from X-ray crystallography, NMR, and hydrogen-exchange experiments shows high correlation. Although successful, the elastic network models may benefit from more complex expressions of packing density to provide an improved reproduction of X-ray crystallographic data. In this work, we utilized a non-redundant dataset of 113 proteins to find the optimal cut-off radius that captures the protein packing density and compare our results with experimental B-factors for different protein folds. We also plan to include various forms of spring constants to elastic network models to test whether these models can be further improved.