

Clustering and Diversity of Fluctuations for Proteins

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Abstract:

We have studied the fluctuations of proteins employing a new approach. An annealing algorithm is used to generate a 3-dimensional protein structure from the contact map. First, we study the building diversities of structural elements by adding individual structures (domains or sub-domains). Thereafter, we focus on the properties of structural elements based on fluctuations. Low and high fluctuations of structural regions can be grouped depending on the level of fluctuations in each region. To verify our hypothesis, we analyzed the pattern of fluctuations for chymotrypsin inhibitor-2 (CI2) by unstructuring (melting) of sub-regions. Our approach introduces a new concept for classifying building blocks of proteins based on thermal fluctuations.