Anomalies in Vibrational Dynamics of Proteins: A Consequence of Fractal-Like Structure

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Proteins have been shown to exhibit strange/anomalous dynamics displaying non-Debye density of vibrational states, anomalous spread of vibrational energy, large conformational changes, non-exponential decay of correlations and non-exponential unfolding times. The anomalous behavior may, in principle, stem from various factors affecting the energy landscape under which a protein vibrates. Investigating the origins of such unconventional dynamics, we focus on the structure-dynamics interplay and introduce a stochastic approach to the vibrational dynamics of proteins. We use diffusion, a method sensitive to the structural features of the protein fold and them alone, in order to probe protein structure. Conducting a large scale study of diffusion on over 500 PDB structures we find it to be anomalous, an indication of a fractal-like structure. Taking advantage of known and newly derived relations between vibrational dynamics and diffusion, we demonstrate the equivalence of our findings to the existence of structurally originated anomalies in the vibrational dynamics of proteins. We conclude that these anomalies are a direct result of the fractal-like structure of proteins. The duality between diffusion and vibrational dynamics allows us to make, single molecule level, experimentally testable predictions. The time dependent vibrational mean square displacement of an amino acid is predicted to be subdiffusive. The thermal variance in the instantaneous distance between amino acids is shown to grow as a power law of the equilibrium distance. Mean first passage time analysis is offered as a practical tool that may aid in the identification of amino acid pairs involved in large conformational changes.