Impacts of Crystallization on Protein Structural Dynamics

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Spiraling Into Gallstone Disease: A Physicist's Spin (abstract)

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Scientists have been fascinated for decades with the ability of nature to form self-assembled structures of various configurations. One such configuration is a spiral or a helix. The (double) helical geometrical configuration is a well-known secondary structure of DNA; however, DNA is not the only biological system possessing this shape. Spirals have been found in a variety of biological and synthetic systems, one of which is bile in the gallbladder. In this system, helical ribbons appear as metastable intermediates in the process of cholesterol crystallization that leads to the formation of gallstones. The bile system is particularly interesting and unique due to the richness in variety of the helical structures formed. Understanding the mechanisms for nature's self-assembly of helical ribbons is crucial in both the prevention of gallstone disease and in developing potential technological and medical applications. We describe a model bile system, composed of three major components of native bile in water: a phospholipid, a fatty acid, and a sterol. This system behaves similarly to the native bile in terms of the kinetics of the formation and evolution of intermediate metastables, including helical ribbons. We further describe our experimental findings and phenomenological model explaining the geometrical shape, elastic properties, and behavior of helical ribbons in model bile systems. We also propose possible applications of these structures as drug delivery vehicles, metallization templates, and antifouling devices.

Impacts of Crystallization on Protein Structural Dynamics (abstract)

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X-ray crystallographic technique is a powerful technique for structural determination of steady state proteins. Now this technique has been further developed to determine the structures of transient states of proteins during their functional processes. Can a protein function in the crystalline state? It is often assumed but untested that the functionally important structural dynamics of a protein are preserved in the crystalline state. This lack of test is largely due to the fact that major structural determination techniques, x-ray crystallography and nuclear magnetic resonance (NMR) spectroscopy, can only be applied to either crystalline state or solution state, not both. Here we report our direct study on the impacts of protein crystallization on the structural dynamics of a blue light photoreceptor protein using time-resolved Fourier transform infrared (FTIR) difference spectroscopic techniques. We found that proteins in crystalline state experience suppressed conformational changes, accelerated kinetics, and altered proton transfer pathway upon light activation. Furthermore, we show that crystallization salt itself has profound impacts on structural dynamics and proton transfer pathway. These results strongly demonstrate that it is necessary and crucial to test and determine whether transient/cold-trapped x-ray crystallography can resolve the protein structures of intermediate states that reflect the natural protein structural dynamics.