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Turning Up the Heat on Dynamic Proteins with Temperature-Jump X-ray Crystallography

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Protein dynamics are critical for function, but it remains challenging to understand, in atomic detail, how a molecule's biological activity is enabled by the physical coupling of its conformational fluctuations across varied length and time scales. Time-dependent X-ray crystallographic measurements of molecular structure can overcome some of the limitations of traditional structural biology and yield deep insight into protein conformational landscapes, but it remains challenging to initiate synchronous conformational changes in crystallized macromolecules, which is a requirement for such experiments. I will describe how observations from multi-temperature structural measurements motivated the development of temperature-jump (T-jump) crystallography, and summarize the results of our early T-jump experiments on the model enzyme lysozyme. I will also discuss ongoing efforts to democratize these experiments and apply them to increasingly complex biological systems, including the metalloenzyme soybean lipoxygenase, whose catalytic mechanism involves a rate-limiting hydrogen tunneling step that is coupled to motion of the protein scaffold.

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