Invited Lecture

Mapping the reaction coordinates of proteins using time-resolved and multi-temperature X-ray crystallography

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Enzymes catalyse biochemical reactions through precise positioning of substrates, cofactors, and amino acids to modulate the transition-state free energy. However, the role of conformational dynamics remains poorly understood due to poor experimental access. I will describe ligand-, temperature-, and electric-field-based perturbations during X-ray diffraction experiments that make it possible to map the correlated motions of an enzyme in atomic and temporal detail. The resulting analysis shows how an enzyme can rapidly switch conformation between two catalytic steps in response to completion of the first step.