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Electrostatically Gated Enzyme Dynamics During Catalysis

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Abstract: Enzyme catalysis is essential for life and is a central phenomenon in biochemistry. The advent of time-resolved serial crystallography, initially enabled by X-ray free electron lasers (XFELs) and now expanding to synchrotron X-ray sources, allows enzyme catalysis to be observed catalysis in real time, in near-physiological conditions, and at atomic resolution. I will describe our work using mix-and-inject serial crystallography (MISC) to observe catalysis by isocyanide hydratase (ICH). MISC allowed us to observe formation of an unusual thioimidate intermediate and to watch ICH's conformational dynamics respond to changes in active site ionization during catalysis. We also used an engineered ICH mutant to enrich for rare conformations during catalysis, permitting a clearer view of later steps in the reaction. ICH exemplifies a class of enzymes whose non-equilibrium dynamics are gated by changes in active site electrostatics, which is a potentially common enzymological phenomenon.

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