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Unravelling Protein Dynamics: Advancing Structural Biology with Time-Resolved Crystallography

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Proteins are dynamic molecular machines, and their ability to function depends not only on their 3-dimensional structure but also on subtle motions, cooperativity, and long-range communication between distant sites. However, capturing these processes at high resolution is often compounded with substantial experimental challenges [1,2]. To address this, we develop and apply advanced crystallographic methods, which we use at synchrotrons and free electron laser sources [3]. These include ultra-high-resolution crystallography, novel cryo-trapping methods (Spitrobot [4,5], microED), as well as time-resolved, multi-temperature, and multi-dimensional X-ray diffraction [6,7]. These approaches enable the direct observation of protein motions, enzymatic reaction and ligand binding events as they occur. By revealing phenomena like 'molecular breathing' during catalysis, half-the-sites reactivity without significant conformational change, and meta-stable intermediates during drug binding or substrate catalysis, they have provided unique insight into the function and dynamics of proteins. In addition to these insights, our methods enable to map cooperativity and allosteric networks inside enzyme complexes, bridging the gap between dynamic functional behaviour and static structural snapshots. Furthermore, we combine this insight with biochemical results and integrate them with insight from other biophysical methods, such as NMR-spectroscopy or MD-simulations. By resolving these dynamic processes, structural biology is advancing from static models towards a mechanistic understanding of protein function at atomic detail, offering a framework to interpret enzyme activity and regulation and develop focused therapeutic strategies.

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