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Protein Dynamics in Real-Time: Insights from 2D-IR with site-specific resolution and time-resolved serial crystallography

Observing protein dynamics with highest spatial and temporal resolution is key to understand the structure-dynamics relationship relevant for biological function. For 2D-IR spectroscopy, the use of vibrational reporter groups has enabled detailed studies with high local resolution. This approach can provide access to protein-ligand interactions or processes like allosteric communication.
However, while 2D-IR is an extremely powerful method to investigate biomolecules in solution, it doesn't provide the full atomically resolved protein dynamics and has limitations due to the incorporation of vibrational reporter groups. Latest developments in time-resolved serial crystallography (TR-SX) overcome these limitations and now can give access to fully resolved dynamic structures at room-temperature.

I will briefly review the concept of site-specific labels in 2D-IR and in a second part highlight developments in serial crystallography, both on the topic of allosteric regulation without large conformational changes. Both methods, 2D-IR and TR-SX are highly complementary and a stronger integration between both could lead to new experiments and more detailed understanding of protein dynamics.

In the final part of my talk I'll introduce how we expand the concept of site-specific vibrational reporters to another important class of biological macromolecules and their building blocks, as we start to investigate labelled carbohydrates for applications in biomolecular recognition.