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CFEL – building 99, seminar room III, ground floor

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Multiple conformational states of a protein in solution elucidated using X-ray laser scattering

Measurements of protein structure in non-crystalline solutions using azimuthal angular correlations of X-ray scattering data were proposed many years ago, but sufficient X-ray fluences to produce useable data were not available at the time.

Here we present data collected using x-ray Free Electron Laser (XFEL) scattering on the Galpha_i protein which is an important component of signaling pathways based on G-protein coupled receptors. Analysis of the data based on an ensemble of simulated model structures elucidates a range of conformational states of the protein with occupancies depending on solution conditions.

The simulated ensemble of model structures is derived to cover a broad range of conformations that covers the previously observed existence of multiple states with varying distances between the Ras and Helical domains of the GDP-bound Galpha_i, including both closed and open states.

The XFEL-scattering-determined occupancies of the ensemble of simulated states were used to measure the inter-residue distances found in double electron-electron resonance (DEER) data. We show that these XFEL-derived distances are consistent with those found from the DEER measurements.