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JINXED: Just in Time Crystallization for Easy Structure Determination of Biological Macromolecules

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Macromolecular crystallography is a well-established method in structural biology and after focusing on static structures, the method is now developing towards the investigation of structural dynamics, e.g. by looking at protein-ligand or enzyme-substrate interactions. In time-resolved serial crystallography and room-temperature data collection, the reaction is triggered within the crystals –either optically or chemically. For the latter, the use of micron-sized crystals is necessary to ensure short diffusion times and quick saturation within each crystal. However, certain crystal morphologies e.g. small solvent channels can prevent sufficient ligand diffusion. Presented here is a method combining protein crystallization and data collection in a novel one-step-process to overcome the aforementioned challenges. We successfully performed corresponding experiments as a proof-of-principle using hen egg-white lysozyme with crystallization times of a few seconds. This method called JINXED (Just in time crystallization for easy structure determination) promises to result in high-quality data due to the avoidance of crystal handling and could enable time-resolved experiments regardless of crystal morphology by adding potential ligands to the crystallization buffer, simulating co-crystallization approaches. In combination with upcoming automated data processing, this method may offer the possibility to combine high-throughput ligand screenings and detailed dynamical investigations with a high level of automation.

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