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Fully autonomous end-to-end protein to structure pipelines at MASSIF-1 using the CrystalDirect harvester

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Recent advances in automation and method development at synchrotron facilities has allowed the development of different data collection pipelines and plate-to-beam applications to respond to modern structural biology projects and to improve the efficiency for high throughput applications [1, 2]. This dynamic change in scientific needs, as well as the increased interest in structural data at physiological temperatures [2, 3], has driven us to expand the beamline experimental capabilities.
The main goal of this upgrade is to develop different approaches for data collection that are both automated and target-based, with the initial focus on defining pipelines for challenging experiments, such as room temperature data collection and dehydration. To date, these require a large number of manual steps and the experimental set-up is time-consuming [2, 3, 4]. Through the automation of this process, made possible by combining the already available resources on-site, we intend to render those experiments more reliable, reproducible, and accessible to non-expert users. The CrystalDirect harvester gives access to a fully automated protein crystallography workflow, integrating protein crystallization, sample harvesting and cryocooling into an automated process [5, 6], while the automation of MASSIF-1 allows large amounts of high-quality data to be efficiently collected [1]. Combining the CrystalDirect harvester and MASSIF-1, we are aiming to help to respond to multiple technical and experimental challenges [2, 3].
The commissioning phase is currently ongoing. The integration of the CrystalDirect harvester in the beamline environment enables multiple and sequential crystal harvesting, sample mounting, and data collection to be executed in automated mode, with no user intervention. The operation of each pipeline has been validated, showing the potential to develop different data collection pipelines at both cryogenic and room temperatures. Preliminary results indicate the possibility to collect complete datasets from single crystals at room temperature and the optimization of this pipeline, using different protein targets is ongoing. The upgrade will allow full automation of the entire spectrum of crystallography experiments, including the most complex room temperature experiments from gene to structure.

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