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Fully autonomous end-to-end protein to structure pipelines: the CrystalDirect harvester on MASSIF-1

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Abstract

Recent advances in automation and method development at synchrotron facilities increased the interest in developing 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].

The combination of the CrystalDirect harvester with the automation on MASSIF-1 beamline will help to respond to multiple technical and experimental challenges [3,4,5]. The CrystalDirect harvester gives access to a fully automated protein crystallography workflow, integrating protein crystallization, sample harvesting and cryocooling into an automated process [3,6,7], while the automation of MASSIF-1 allows large amounts of high-quality data to be efficiently collected [1,2].

To date, room temperature (RT) data collection and dehydration experiments require a large number of manual steps and the experimental set-up is time-consuming; the automation of this process will render those experiments more reliable and reproducible, and facilitate their access to non-expert users [8,9,10,11].

The beamline commissioning is currently ongoing, with the main goal to develop different approaches for data collection that are both target-based and automated, and the initial focus on defining pipelines for room temperature data collection and dehydration experiments.

The CrystalDirect harvester has been installed in the beamline environment and the software integration, that permit the communication of the harvester with different software interfaces (CRIMS, MXCuBE3, and ISPyB), has enabled multiple and sequential crystal harvesting, sample mounting, and data collection to be executed in automated mode. The proper operation of each pipeline has been validated, showing the potential to develop multiple data collection approaches at both cryogenic and room temperature. Initial results indicate the possibility to collect complete datasets from single crystals at room temperature; the optimization of the automated data collection pipeline for different protein target is currently ongoing.

The beamline upgrade will, therefore, open new experimental opportunities and help respond to the dynamic change of scientific needs, such as the increased interest in structural data at physiological temperatures [10,11,12].

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