

MS41 Automation in data collection and processing

MS41-05

MASSIF-1, the macromolecular beamline dedicated to automation

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Abstract

From the beginning back in 2014, Massif-1 [1] at ESRF has been designed to be fully automated from crystal mounting up to data collection and processing [2]. To profit from the Extremely Brilliant Source project and the drastic increase of performance of the storage ring, the beamline entered in a depth refurbishment and upgrade of the entire experimental hutch in august 2020. It is now equipped with a micro-diffractometer with kappa option (MD2S) and fitted with an ESRF-FlexHCD sample changer taking up to 368 samples in Unipuck (Figure 1). The CrystalDirect harvester for automatic harvesting of crystals is also installed since May 2021.

With the experience gleaned from more than 70,000 crystals collected since the kick-off [3], we manage to specify experimental roadmaps conforming to the user requirements. Our aim is to design the best data collection protocol allowing the best quality of the final data set and helping the scientist in solving their biological questions in an automated manner. The workflows in charge of the setting up the experiment, is also the decision maker and according to the previous results will follow the best data collection strategy taking advantage of the beamline setup. As examples: we strengthen the quality of the services by adapting the beam diameter to match the best diffracting volume with the help of DOZOR software; we collect two different kappa orientation with low symmetry space groups; we constantly check the state of the beam and the hardware and report any misbehaviour and correct suitably and more will be revealed during the presentation. The automation has been further pushed in data processing and data solving. The data sets collected on the beamline are screened for anomalous signal and/or molecular replacement and small molecule fitting.

References

[1] Journal of synchrotron Radiation. Volume 22 Part 6 November 2015, 1540-1547. [2] Acta Cryst. (2015). D71, 1757-1767. [3] IUCR Journal. Volume 6 Part 5 September 2019, 822-831

MASSIF-1 Experimental Hutch

