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Automation for BioSAXS experiments at BM29 of the ESRF

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Small Angle X-ray Scattering (SAXS) experiments of macromolecules (proteins, nucleic acids, ...) in solution can provide a wealth of information concerning structure, dynamics and therefore function. However, correct interpretation of results depends critically on data quality. To achieve this, well defined acquisition protocols and immediate feedback are essential. At beamline BM29 at ESRF, BioSAXS data are acquired in a temperature controlled flow through capillary. Samples and buffers can be loaded into the capillary via a robotic liquid handling sample changer (SC) [1] or by connecting the capillary to the outlet of a size exclusion chromatography (SEC) setup [2]. Samples loaded by the SC can be passed through the beam to avoid unwanted effects caused by radiation damage. All recorded data are immediately analyzed to give user-oriented feedback on estimated molecular weight, size, possible radiation damage and inter-particle effects, quality of background correction, etc. Subsequent downstream analysis, also carried out automatically, results in the calculation of molecular envelopes for solution structures. The information management system ISPyBB (Information System for Protein crystallography Beamlines and BioSAXS) logs and presents all information on data acquisition and analysis and allows users to easily compare the results of different data acquisitions and to decide whether further measurements or changes of acquisition parameters are necessary. The combination of these tools allows non-expert users to carry out BioSAXS experiments autonomously, thereby making the technique accessible to a broader community.

[1] P. Pernot, A. Round, R. Barrett, et al., *J. Synch. Rad.* 20, 2013, 660-664, [2] A. Round, E. Brown, R. Marcellin et al., *Acta Cryst. D*69, 2013, 2072–2080



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