

High-throughput BioSAXS at ESRF BM29

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BioSAXS, the collection and interpretation of small angle X-ray scattering data of biological macromolecules such as proteins or nucleic acids in solution, provides a wealth of information on their shape and structure. ESRF BM29 is a SAXS beamline dedicated to the structural biology community, routinely offering two experimental modes: i) Automated measurement of individual concentrations using a sample changer and ii) online size exclusion chromatography (SEC-SAXS). In both modes, data reduction, primary analysis and basic modelling are fully automated, providing even non-expert users with rapid feedback on their experiments.

To allow even more automated screening of conditions, we recently developed a SAXS-compatible droplet microfluidics setup that allows automated variation of buffer parameters, in nanoliter-sized micro-reactors. First proof-of-principle experiments on the structure factor of lysozyme and crystallisation of glucose isomerase proofed the usefulness of this approach [1].

To facilitate the collection of high quality SAXS data on dynamic systems, we extended the SEC-SAXS principle to gradient elution chromatography techniques, such as ion exchange chromatography (IEC) or nickel affinity chromatography. Although the uncertainty in the background correction increases to a certain extent, these techniques allow the preparation of monodisperse states at comparatively high macromolecular concentrations. Both techniques have been successfully applied to user projects [2].

These developments are accompanied by the development of ExiSAXS, an improved version of the user interface for ISPyB database. This is a joint development among several sites in Europe.

[1] N.V. Pham, et al. (2017) *Analytical Chemistry* 89 (4), 2282-2287.

[2] S. Hutin, et al. (2016), *Acta Cryst.* D72, 1090-1099.

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