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MS38-O5 Crystallisation in-situ - and much more - at the ESRF BioSAXS BM29 beamline

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BioSAXS, or macromolecular solution scattering, plays an ever-increasing role in structural evaluation in biology since the introduction of dedicated synchrotron beamlines. A number of robots have been developed to offer high throughput and automation. The combination of SAXS with size exclusion chromatography (SEC), where the eluted sample is exposed to X-rays immediately after separation, is also explored. The ESRF BioSAXS beamline BM29 provides routinely two experimental modes: i) STATIC mode using a sample changer and ii) HPLC mode with SEC on line. Automatic switching between these two modes is done by remote control allowing optimal use of available beamtime. Dedicated beamline control and data acquisition software allows sample-changer control and real-time data display (two-dimensional and one-dimensional). It is connected to a data processing pipeline, providing automatic data processing up to *ab initio* models for both modes. Data collection parameters and results are logged and stored in the modified ISPyB database (a laboratory information management system that combines sample tracking and experiment reporting).

Recently, within a Long Term Project cooperation, droplet microfluidics devices were introduced to the beamline. The figure shows the current set-up on the beamline with the inset photograph of droplet generation in the microfluidics chip. The droplets (containing buffer, protein in solution and crystallisation agent) are driven by an oil phase and exposed to X-rays in a fused silica capillary of 300 µm diameter in vacuum. The capillary is connected directly to the exit of the microfluidic chip and sealed into BM29 standard sample holder. Thanks to an external trigger signal, data are recorded only when droplets cross the X-ray beam to avoid radiation damage of oil and total reflection on droplet walls. With help of such a device crystallisation studies in situ of *glucose isomerase* were carried out.

In the presentation, an overview of macromolecules in solution experiments and possibilities at BM29 will be given, together with the description of latest results with digital microfluidic devices.

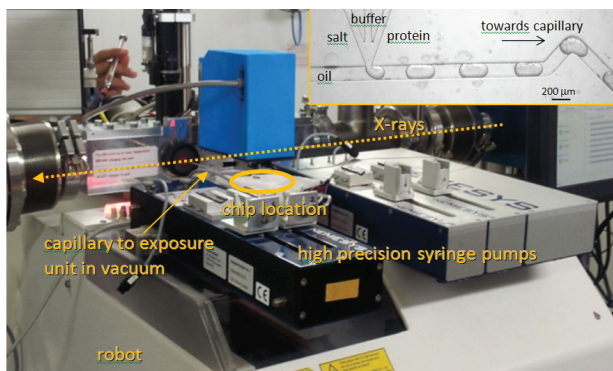


Figure 1. Photograph of microfluidics set-up at BM29 beamline. Inset represents a screen snapshot of droplet generation during crystallisation experiment. Small black dots appearing in droplets on right side are first crystals.

Keywords: small angle X-ray scattering, microfluidics, proteins in solution