High-Throughput Solution SAXS: low-cost portable instrumentation

G. Lotze[1], N. Terrill[2], K. Inoue[2] and A. Squires[1]*

[1]Department of Chemistry, University of Reading, RG6 6AD, UK

[2]Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, OX11 0DE, UK

Outline

We have designed and built a low-cost instrument for automated solution SAXS of biological molecules, which has the following features:

1) Small sample volumes – droplets with a volume down to 30 uL (for 1.5mm path length) or 1 uL (0.5mm path length) can be analysed,

2) Sample and buffer flow through the same capillary kept in the same position in the beam, to allow accurate background subtraction,

3) Sample flows (slowly) during data acquisition to minimise beam damage,

4) Data acquisition is automated by monitoring beam flux. The computer detects when a new sample or buffer droplet is in the beam, and begins acquisition. When acquisition is complete, a signal is sent to the pump to move the next droplet more rapidly into position, ready for the next data acquisition.

Our instrument is relatively low cost, and portable. We set it up on P03 at PETRA (Figure 1), and arranged an interface between the flow control instrument and the beamline computer. Now that the software to allow this interface has been written, the setup process would take approximately half a day.

Figure 1: flow-through small-volume SAXS cell on P03 in PETRA

Results

We show proof-of-concept data from a dilution series of ovalbumin (Figure 2) using 6 uL sample volumes. The data show good scaling with concentration, and allow an estimate of the (infinite dilution limit) value of radius of gyration, R_G, of 2.749nm ± 0.004nm. This is in reasonably good agreement with a literature value of 2.8nm [1] (given that buffer conditions were slightly different).

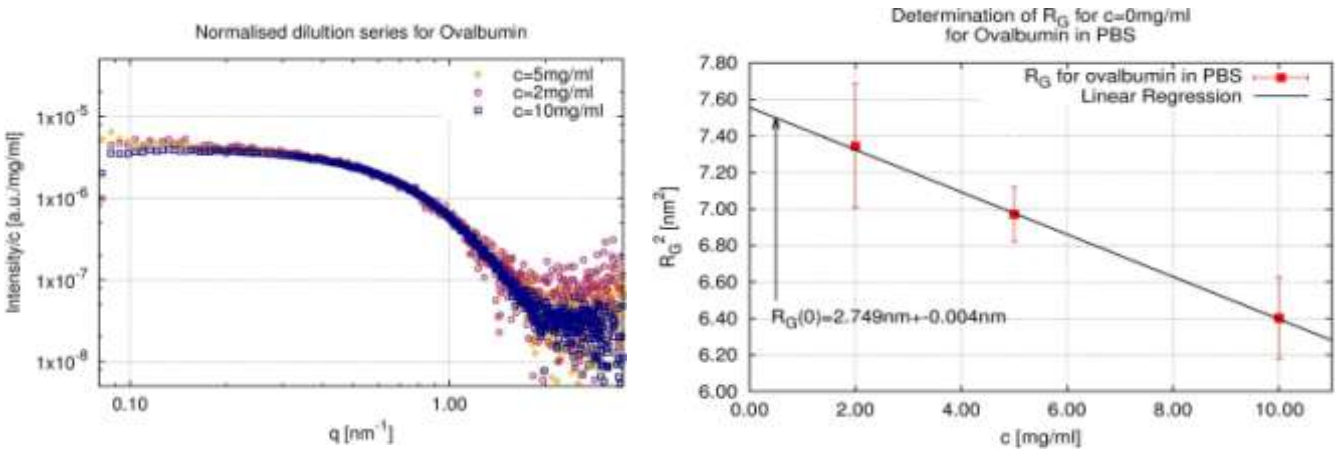

Figure 2 (Left): data from automated background-corrected dilution series of ovalbumin, scaled for concentration; (Right): determination of extrapolated radius of gyration from dilution series

Conclusions and future improvement

In the future, automated data reduction would allow data analysis *in situ* to optimise conditions (flow rate, exposure time) for signal/noise vs beam damage. Nonetheless, this represents a successful first attempt to set up versatile instrumentation for solution SAXS. It is particularly suitable for SAXS beamlines that are used with many different sample environments and not exclusively for solution SAXS, because the low cost and ease of setup make this instrument more appropriate than larger more expensive automated "robots".

References

[1] Luca Ianeselli *et al*, J. Phys. Chem. B **114**, 3776–3783 (2010)