

Preparation of protein sample and data acquisition All examples of data in this manuscript are based on a deletion construct of the D5 protein from vaccinia virus (VACV). The sequences of D5R are from the VACV strain Copenhagen (GenBank accession number M35027.1). D5 391-785 was cloned into the pProEx Htb plasmid (Invitrogen), fused to an N-terminal TEV(tobacco etch virus) protease-cleavable hexahistidine tag. The protein was expressed in BL21* and purified over a HIS-select column (Sigma); lysis buffer: 50 mM Tris pH 8.5, 150 mM NaCl, 5 mM MgCl₂; complete protease inhibitor cocktail (Roche), DNaseA, 10 mM beta-Mercaptoethanol; binding buffer: 50 mM Tris pH 8.5, 150 mM NaCl, 10 mM beta-Mercaptoethanol; high salt wash buffer: 50 mM Tris pH 8.5, 1 M NaCl, 10 mM beta-Mercaptoethanol; elution buffer: 50 mM Tris pH 8.5, 150 mM NaCl, 200 mM imidazole, 10 mM beta-Mercaptoethanol. The buffer of the eluates was exchanged to a binding buffer on a PD10 column and the protein was TEV-digested over night at RT. After a second Ni-column, the sample was injected into a Superdex 200 GL 10/300 column (GE Healthcare), equilibrated with gel filtration buffer (20 mM Tris pH 8.5, 150 mM NaCl, 1 mM dithiothreitol, DTT). Eluted peaks were analysed by SDS-PAGE, stained with InstantBlue (Expedeon). In SC mode a dilution series of five different concentrations was prepared (see table 1). For size exclusion, 50 μ l of sample at 20 mg/ml on a Superdex 200 5/150 GL column (GE healthcare) were injected.

Software distribution and licensing

All pieces of software developed for online data analysis at the bioSAXS beamline

are open source. Nevertheless they rely on the ATLAS package which, although free for academic use, is neither open source, nor redistributable.

EDNA is licensed under LGPL for the kernel part (the pipeline engine) and GPL for the bioSAXS part. The source code is now hosted on a public repository at:
<https://github.com/edna-site>.

EDNA is a server tool for online data analysis and the developers are aware of the difficulty to install and configure it properly. EDNA controls ATLAS modules by executing external programs in pipe mode, avoiding any licensing issues.

The azimuthal integration is performed via pyFAI (Kieffer & Karkoulis, 2013), the Python library for fast azimuthal integration, which can be GPU-accelerated (Ashiotis *et al.*, 2015). Diffraction images are read by the FabIO library (Knudsen *et al.*, 2013). Both libraries are licensed under GPL and hosted under the following web pages:
<http://github.com/pyFAI> and <https://fable.sf.net>

Some ATLAS parts have been re-implemented directly in EDNA to offer a better integration into the processing pipelines (by avoiding the forking of many sub-processes): *dataver*, *datop*, ... *Supycomb* is available as part of the FREESAS package which re-implements the *supcomb* algorithms, featuring a MIT license scheme. FreeSAS can be downloaded from <https://github.com/kif/freesas> but waiving any numerical equivalence to the reference implementation. Finally the other tools of the Python scientific stack (NumPy, SciPy, Matplotlib) are subjected to the BSD license conditions.