The atsas software suite for small angle scattering from macromolecular solutions

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The ATSAS software suite for the analysis of small angle scattering of biological macromolecules in solution is a comprehensive cross-platform package with applications for all stages of the Small Angle X-ray and Neutron Scattering workflow, from primary data processing to ab-initio and rigid body modelling (Franke, et. al., J Appl Cryst, 2017). It includes applications to integrate information from X-ray crystallography, nuclear magnetic resonance spectroscopy, electron microscopy and atomistic homology modelling to construct hybrid models based on the scattering data.

Here an overview of well-established ATSAS applications and more recent developments will be provided. This includes, but is not limited to: CRYSOL/CRSYON to calculate SAXS and SANS patterns from atomistic models and to fit them to experimental data; DAMIN/DAMMIF for ab-initio bead modelling, with the recent addition of DAMMIX, a tool to restore the shape of an unknown component in evolving systems ab initio, e.g. during fibril formation (Konarev & Svergun, IUCrJ, 2018); SASREF for rigid-body modelling; and EOM to approximate ensembles.

Further, a new application will be introduced: IMGSIM simulates realistic 2D scattering images from a 1D input file, e.g. calculated from an atomic model by CRYSOL. Based on the input data, IMGSIM generates random scattering events onto a virtual detector plane, taking into account the detector distance, dimensions and pixel size, incoming virtual photon/neutron flux and wavelength, as well as the sample concentration (for zero concentration, a flat background is generated). The resulting 2D images can be readily radially averaged by existing tools and the variation in the simulated data exhibits the expected statistical properties (normal distribution, statistically independent). With initial input on absolute scale, $[cm^{-1}]/c[mg/ml]$, the simulated data frames may be scaled to absolute scale by DATABSOLUTE, and the final I(0) after subtraction of the background will be proportional to the molecular weight of the input model. The angular range and spacing, as well as perceived noisiness depends on the input parameters and may be set to mimic the experimental data obtained at existing instruments. Thus, the simulated data may directly be used to validate existing data processing and modelling procedures, as well as for development of new methods.

ATSAS is freely available for academic users to download at https://www.embl-hamburg.de/biosaxs/software.html.

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