Poster Presentation

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ATSAS 2.8 software for small-angle scattering from macromolecular solutions

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ATSAS is a comprehensive cross-platform software suite for the analysis of small angle scattering data of biological macromolecules in solution. It contains applications for primary data processing, ab initio bead modelling and model validation, and methods for the analysis of flexibility and mixtures. In addition, it includes programs to integrate information from X-ray crystallography, Nuclear Magnetic Resonance spectroscopy or atomistic homology modelling to construct hybrid models based on the scattering data. Here we summarize the developments made during recent years for the 2.5-2.8 ATSAS release series and highlight the latest developments. These include, but are not limited to: AMBIMETER, an assessment of the reconstruction ambiguity of experimental data; DATCLASS, a multi-class shape classification of experimental data; SASRES, which provides the resolution estimate of ab initio model reconstructions; SECPLOT, a convenient graphical user interface to analyse the in-line size exclusion chromatography data; SHANUM, to evaluate the useful angular range in the measured data; SREFLEX, to refine available high resolution models using normal mode analysis; SUPALM for a rapid superposition of low and high resolution models; and SASPy, an ATSAS plugin for interactive modelling in PyMOL. All these features and other improvements are included in the ATSAS release 2.8 and are freely available for academic users from the URL https://www.embl-hamburg.de/biosaxs/software.html. Additionally, the ATSAS-online interface, which allows users to submit jobs to our computational cluster for major ATSAS programs is available at the URL https://www.embl-hamburg.de/biosaxs/atsas-online/.

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