ATSAS 2.1 - A Program Suite for Small-angle Scattering Data Analysis

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A new release 2.1 of the program package ATSAS for small-angle scattering data analysis is presented. The package allows one to perform a complete analysis of the scattering data covering major steps from data reduction to automated 3D modelling. ATSAS is primarily oriented towards macromolecular solutions but can also be used for other types of systems. Its main components are:

1) Primary data processing and reduction package PRIMUS [1], which also computes overall structural parameters and characteristic functions and permits to invoke major data analysis programs from a single graphical user interface.

2) An *ab initio* three-dimensional modelling suite including e.g. programs DAMMIN and GASBOR bead and dummy residues modelling [2,3].

3) A rigid body modelling suite (programs MASSHA [4], GLOBSYMM, SASREF etc) to characterize macromolecular complexes in terms of the structure of sugbunits.

4) A suite for quantitative analysis of interacting systems and mixtures (programs PEAK, SVDPLOT, MIXTURE etc [1]).

[1] Konarev P.V., et.al., *J. Appl. Cryst*., 2003, **36**, 1277. [2] Svergun D.I., *Biophys. J*., 1999, **76**, 2879. [3] Svergun D.I., et.al., *Biophys. J.*, 2001, **80**, 2946. [4] Konarev P.V., et.al., *J.Appl. Cryst.,* 2001, **34**, 527.

Keywords: small-angle scattering, data processing software, macromolecules