

## Methods for Quaternary and Domain Structure Analysis by Small Angle Scattering

Maxim Petoukhov<sup>a,b</sup>, Dmitri Svergun<sup>a,b</sup>, <sup>a</sup>European Molecular Biology Laboratory Hamburg Outstation. <sup>b</sup>Institute of Crystallography RAS, Moscow, Russia. E-mail: petoukhov@embl-hamburg.de

During the last decade, small-angle scattering (SAS) has become an increasingly important tool for the study of biological macromolecules. The method allows one to study native particles, from individual proteins to large macromolecular complexes, in solution under nearly physiological conditions. SAS not only provides low resolution models of particle shapes but in many cases answers important functional questions, in particular, by the analysis of structural changes in response to variations in external conditions.

Recently developed data analysis methods are presented, which significantly improve resolution and reliability of structural models deduced from SAS data for biomacromolecular solutions. These methods include: *ab initio* low resolution structure analysis [1,2]; addition of missing fragments to high resolution protein models [3]; rigid body modelling of protein complexes [4,5], determination of three-dimensional domain structure of proteins based on multiple scattering data sets from deletion mutants [6]. The efficiency of the methods is illustrated by results from recent experimental projects.

[1] Svergun D.I., et al., *Biophys. J.*, 2001, **80**, 2946-53. [2] Petoukhov M.V., Svergun D.I., *J. Appl. Crystallogr.*, 2003, **36**, 540-4. [3] Petoukhov M.V., et al., *Biophys. J.*, 2002, **83**, 3113-25. [4] Petoukhov M.V., et al., *J. Biol. Chem.*, 2003, **278**, 29933-9. [5] Rosano C., et al., *BBRC*, 2004, **320**, 176-82. [6] Mórquez J.A., et al., *EMBO J.*, 2003, **22**, 4616-24.

**Keywords: small-angle scattering, biomacromolecular structures, computational modelling methods**