MS84 THEORETICAL METHODS FOR ANALYSES OF DATA FROM SOLUTIONS
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Analysis of Small-angle Scattering Data from Block Copolymer Micelles using Models Based on Monte Carlo Simulations
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Numerous studies of block copolymer micelles formed in selective solvent by scattering methods have been published in the literature. In order to extract information on the structure of the micellar core and corona, modelling is required. Recently, there has been a large progress in the model expressions available for the analysis of such scattering data. The expressions are based on results from Monte Carlo simulations on models with a compact core and a corona of interacting, self-avoiding chains. During the simulations, both scattering form factors and the real-space structure are sampled, so that various semi-empirical expressions can be tested. When established, these expressions can be used in the analysis of experimental scattering data. An overview of the developments is given and the application to micelles of the diblock copolymer Brij700 (C_{18} EO_{100}) in water (D_2O) solution is presented. The micelles consist of a hydrophobic core surrounded by a corona of PEO chains in contact with the solvent. SAXS and SANS experiments are combined to provide complementary information. Both the effect of concentration and temperature are investigated, where the latter parameter induces a change of solvent quality for the PEO chains.
Keywords: small-angle scattering, polymer, theory

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Theoretical Treatment and Practical Aspects of Systems with Preferred Orientation
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While scattering data generated from solution is usually isotropic, an anisotropic shape of the structural unit in a sufficiently dense system can lead to preferred orientation which poses interesting problems both theoretically and practically.

Straightforward treatments of preferred orientation based on truncated expansions into spherical harmonics are known to converge poorly unless both the orientation distribution and the intensity distribution of the structural unit are sufficiently broad.

Therefore, we consider the problem of preferred orientation on the level of the integral transformation relating the intensity distribution of the structural unit to that of the preferentially oriented ensemble. Under the assumptions of cylindrical symmetry of both the structural unit and the ensemble and of statistical independence of orientation and position of the structural units, the treatment can be kept exact without approximation.

The state of the literature on this topic will be briefly reviewed. We will focus on orientation distribution functions for which all or most of the involved integrations can be solved analytically. Practical applications of these techniques to both small-angle and wide-angle scattering from various systems of interest will be discussed, many of which leading to rather compact fully analytic closed-form expressions for the resulting intensity distributions that previously were only treated numerically.
Keywords: preferred orientation, anisotropy, applied mathematics

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Structural Biology Studies coupling SAXS with Crystallography and NMR
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Major cellular functions are performed by complexes involving multiple partners and modular proteins in which well-characterized domains are linked by fragments of unknown conformation. Such particles do not crystallize easily and their structural study requires complementary approaches. We present here two examples of systems studied by a combination of SAXS with high resolution (MX and NMR) approaches.

The interaction of the C-terminal domain of ribosomal protein L20 with its rRNA binding site was studied by NMR and SAXS. Scattering data show the existence of a dimer of the RNA/L20C complex in solution. Using the complex structure in the 50S context, NMR and SAXS data, a low resolution model is obtained [1].

$P47^{PHOX}$ is a soluble member of the NADPH oxidase complex of neutrophils. This modular protein comprises a PX domain and two SH3 domains together with fragments of unknown structure. Phosphorylation of Serine residues in the C-terminal part is the first step in the activation of the complex. A combination of rigid-body and *ab initio* modelling was used to model the conformation of the whole protein from the solution scattering pattern.

[1] Raibaud S., Vachette P., Guillier M., Allemand F., Chiaruttini C., Dardel F., *J. Biol. Chem*., 2003, 36522.
Keywords: SAXS, biological macromolecules, conformation

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Methods for Quaternary and Domain Structure Analysis by Small Angle Scattering
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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] Mõrquez J.A., et al., *EMBO J.*,2003, **22**, 4616-24.
Keywords: small-angle scattering, biomacromolecular structures, computational modelling methods