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Validation of biological small-angle scattering data and models in SASBDB

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Small angle scattering (SAS) of X-rays and neutrons is actively used to study the global shapes of proteins, nucleic acids, macromolecular complexes and assemblies in solution. Due to recent advances in instrumentation and computational methods, the quantity of experimental scattering data and subsequent publications is increasing dramatically. Small Angle Scattering Biological Data Bank (SASBDB, www.sasbdb.org, [1]) is a curated repository that makes the experimental SAS data and derived models underlying scientific publications discoverable, accessible and citable. SASBDB allows investigators to locate and freely access:

• experimental scattering data presented in various ways (logarithmic plot, Guinier plot, dimensionless Kratky plot, derived pair distance distribution function);
• overall parameters derived from the data (radius of gyration, maximum intra-particle distance, molecular weight, excluded volume);
• associated models of various types (high resolution models from PDB, hybrid models, ab initio models, mixtures) along with scattering patterns computed from them and fitted to SAS data;
• technical details about the experiment;
• a priori information about the sample (sequence, expected oligomeric state etc.).

The information contained in SASBDB is available via a Web interface and the REST API in a number of formats including XML, JSON and sasCIF, an extension of core Crystallographic Information File for SAS [2].

When the number of entries in SASBDB reached a few hundreds it became obvious that the quality of the data and of the biomacromolecular structures deposited in SASBDB needs to be assessed critically using community-accepted validation methods. We propose a number of formal criteria for evaluating the quality of the experimental data, accuracy of data processing, reliability of the models and the extent to which a given model fits SAS data. Our goal is to collect feedback from the SAS community and ultimately obtain agreement for the approaches to SAS data validation and model validation with the perspective of incorporating into the wwPDB validation reports and setting up publication standard for journals. The development of SASBDB is correlated with the activities and recommendations of the SAS and validation Task Forces of the wwPDB.

[1] Valentini et al. (2015) Nucleic Acids Res. 43(D1), D357-D363.
[2] Kachala et al. (2016) J. Appl. Cryst. 49, 302-310.

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