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Publication guidelines for biomolecular small-angle scattering: a community driven effort

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On behalf of our colleagues in this broad community effort, we wish to present an update of the preliminary publication guidelines published five years ago (Jacques et al. 2012) addressing information that should be made available regarding sample quality, data acquisition and reduction, presentation of scattering data and validation, and modelling for biomolecular small-angle scattering (SAS) experiments. The objective of the preliminary guidelines, developed in consultation with the SAS and Journals Commissions of the IUCr and other experts in the field, was to provide a reporting framework so that "readers can independently assess the quality of the data and the basis for any interpretations presented" concerning the results of SAS experiments aimed at obtaining structural information for a biomolecule in solution including the generation or testing of 3D models. These guidelines are now used by many authors and are endorsed by the IUCr Journals (<http://journals.iucr.org/services/sas/>). Since these preliminary publications appeared, the world-wide Protein Data Bank (wwPDB) established the Small-Angle Scattering validation task force (SASvtf) that has made recommendations regarding the archiving and validation of SAS data and models (Trehwella et al. 2013). Further, the wwPDB Integrative/Hybrid methods (IHM) validation task force has been formed to address the complex issues concerning the archiving and validation of models of biomolecular complexes and assemblies that depend upon disparate, often data representing different information at different scales and from multiple techniques (Sali et al. 2015). There also have been substantial advances in instrumentation, in particular the growth of SAS measurement with in-line purification and characterization capabilities and analysis tools for SAS. A manuscript updating the publication guidelines is in preparation in consultation with the members of the wwPDB SASvtf, IUCr Commission of Small-Angle Scattering (CSAS) and other experts in the field to be submitted after the 24th IUCr Congress in Hyderabad where there will also be an open meeting of the CSAS that will provide an opportunity for input into this international effort to strengthen the role of SAS in structural biology.

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