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Small-Angle Scattering Validation Task Force Members
Wayne A. Hendrickson, Columbia University
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Transmitted: by email

Dear Colleagues

I am contacting you to request feedback on membership of our task force and to propose a virtual meeting of the Small-Angle Scattering validation task force (SASvtf) with the following agenda:

1. review progress to date on the implementation of our recommendations as outlined in our 2013 report in Structure and plan next steps; and
2. consider in detail the fourth recommendation from the SASvtf; that is “criteria need to be agreed upon for the assessment of the quality of deposited data and the accuracy of SAS-derived models, and the extent to which a given model fits the SAS data.”

With respect to item 2, in our 2013 report (Trehella et al, 2013, attached) we expanded upon preliminary guidelines (Jacques et al., 2012, attached) that addressed **sample quality, data acquisition and reduction, presentation of scattering data and validation, and modelling** for biomolecular SAS. These preliminary guidelines were developed in consultation with the IUCr SAS Commission and other experts in the field and formally adopted by the IUCr Journals. They have subsequently been used by a growing cohort of SAS researchers.

I am in the process of drafting an update of the preliminary publication guidelines to a v1.0 that would incorporate the additional points made in from our 2013 report, as well as input from the IUCr SAS Commission and other experts in the field. I propose to circulate this draft to the SASvtf for comment. At our virtual meeting we would review the comments and agree a final set of guidelines, including specific, implementable recommendations for both data and model validation, which we would formally recommend as the SASvtf.

I plan to present the revised, updated publication guidelines at the IUCr Congress in Hyderabad in August during an open meeting of the IUCr SAS Commission that I have



called for as Chair of the SAS Commission. Subsequently we will submit the paper for publication describing the revised guidelines and the basis for recommended adjustments.

As we embark on this next phase of work, I propose expanding the SAS expertise on our task force and would be happy to entertain any and all suggestions for additions. I would like to suggest that we recruit from among Masaaki Sugiyama (Kyoto), Patrice Vachette (Saclay Paris), Frank Gabel (Institut de Biologie Structurale, Grenoble), Lois Pollack (Cornell), and Dina Schneidman (Hebrew University) each of whom is publishing high quality work using SAS. With these additions, we can diversify and strengthen our expertise with respect to SANS, combined SANS/NMR, SAXS on large virus particles and RNA.

Please let me know your thoughts on membership and I will be asking the RSCB PDB to assist in setting up the virtual meeting in early May at a time that best suits all participants.

Yours sincerely,

Jill Trewhella, PhD

cc John L. Markley, BMRB
Haruki Nakamura, PDBj
Sameer Valenkar, PDBe
Stephen K. Burley, PDB RSCB
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