Contribution ID: **63** Type: **not specified**

Importance of Validation in SAXS/SANS

The biomolecular SAS community of users has grown sharply since the 1990's with increased ease of access and innovation in instrumentation and analysis tools. With this growth, SAS methods have become attractive to main-stream structural biologists who traditionally have relied almost exclusively on high-resolution, data-rich techniques. Key to this development have been the modelling tools for calculating SAS profiles from atomic coordinates that bridge the gap between high resolution structure and solution scattering. At the same time, there have been important community efforts (reviewed in [1]) to develop and agree standards for data quality, model validation, publication, and data sharing with the aim of ensuring transparency and completeness in reporting so that the broader structural biology community can be confident in assessing and using the results of biomolecular SAS experiments. The biomolecular SAS community now has a set of comprehensive guidelines for publication of biomolecular SAS [2] with standard reporting templates [3]. In a major new development, we also now have a core consensus set of SAXS and SANS profiles on five proteins against which existing and new methods for SAS profile calculation from atomic coordinates can be benchmarked [4]. This consensus data set was derived from 171 SAXS and 76 SANS profiles collected on 12 small-angle X-ray scattering (SAXS) and four small-angle neutron scattering (SANS) instruments across the Americas, Europe and Asia and provided an important quantitative assessment of SAS data reproducibility. The value of adherence to the 2017 guidelines for publication of biomolecular SAS and 3D modelling was well demonstrated in this study. Further, while calculation of SAS profiles from atomic coordinates for a current set of popular methods show good general agreement with the consensus profiles, there are residual differences that offer the opportunity for evaluating, comparing and potentially improving any one approach to theoretical SAS profile prediction.

References

[1] Trewhella, J. (2022) Methods in Enzymology 678, 1-22
[2] Trewhella, J., Duff, A. P., Durand, D., et al. (2017) Acta Cryst. D 73, 710-728.
[3] Trewhella, J., Jeffries, C. M., & Whitten, A.E. (2023) Acta Cryst. D 79, 122-132
[4] Trewhella, J., Vachette, P., Bierma, J., et al., (2022) Acta Cryst. D 78, 1315-1336

Primary author: Prof. TREWHELLA, Jill (The University of Sydney)

Presenter: Prof. TREWHELLA, Jill (The University of Sydney)