

Australia's contribution to an International Project to Generate a Consensus Standard Set of SAS Data to Benchmark Methods for SAS profile Prediction

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The small-angle scattering (SAS) facilities and personnel at ANSTO's Centre for Neutron Scattering and Synchrotron are part of an international project aimed at generating a set of SAS data sets from well-characterized biomolecules that can be used to benchmark different approaches to predicting SAS profiles from atomic coordinates (project description can be found at <https://sas.wwpdb.org/?q=node/25>). This project emerged from the deliberations of the International Union of Crystallography Commission (IUCr) on Small Angle Scattering (CSAS) and the Small-Angle Scattering validation task force (SASvtf) of the world-wide Protein Data Bank (wwPDB) that led to the 2017 publication guidelines for structural modelling of small-angle scattering data from biomolecules in solution (<https://scripts.iucr.org/cgi-bin/paper?jc5010>). The current project involves the efforts of 37 researchers with participants from 11 X-ray and 3 neutron scattering centres across Asia, Europe and North America.

The specific objectives of the project are to measure SAS data at each of the participating facilities for 5 standard proteins with known structures using a common batch for each protein and appropriate standard buffer(s). The data sets are to be compared for consistency and then an agreed set will be made available to the research community. The data, measurement protocols and sources of material will be made available via a publicly accessible Website(s). A "Multi-SAXS Hub" web site is under development (Emre Brookes, University of Texas Health Science Center at San Antonio) to provide a single point from which different methods for scattering profile prediction can be accessed.

Data have been acquired for the 5 selected proteins (RNase A, Lysozyme, Xylanase, Urate Oxidase, Glucose Isomerase) at a number of the participating facilities. We will present here the results obtained from the Australia Center for Neutron Scattering and Synchrotron, highlighting what is learned by having X-ray and neutron scattering data on each protein, as well as lessons learned to date from participating in this international project.

Speakers Gender

Male

Travel Funding

No

Level of Expertise

Expert

Do you wish to take part in the poster slam

No

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