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The ANSTO contribution to a project to provide experimental standards for SAS profile prediction

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The program CRYSOL1, was the first method developed to rapidly calculate small-angle scattering (SAS) profiles from atomic coordinates of biomolecules. It was a major breakthrough, providing the missing link between high-resolution structures and solution SAS data. The importance of this breakthrough is evident in the fact that decades later, alternate methods continue to be published with various claims of improvement.

To date, each of the alternate methods published have been validated using different data sets and models. A consensus set of high quality data would be of considerable value in benchmarking the different approaches. In order to evaluate different approaches to including the hydration layer contribution to the SAS profile, it is desirable to have data obtained using X-rays (SAXS) and neutrons (SANS), the latter in H2O and D2O, as the hydration layer contribution differs significantly for each of these measurements.

To develop a consensus set of high quality data, an international project involving the efforts of 37 researchers from 11 different X-ray and 3 different neutron scattering facilities across Asia, Europe and North America was undertaken. Here, we report on the contribution of ANSTO to this international project.

1Svergun (1995) J. Appl. Cryst. 28:768

Speakers Gender

Male

Level of Expertise

Experienced Research

Do you wish to take part in the poster slam

No

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