

SASBDB and DARA as biological solution scattering teaching tools

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Small angle X-ray and neutron scattering (SAXS and SANS) are important research tools which address increasingly complicated questions in structural biology. SAXS and SANS are used not only complementary to other techniques but also used as primary methods allowing us to investigate the structures and structural changes of biological molecules.

The Small Angle Scattering Biological Data Bank (SASBDB, www.sasbdb.org) is a curated repository of freely accessible and fully searchable small angle scattering experimental data, which are deposited together with the relevant experimental conditions, sample details, instrument characteristic and derived models [1]. Most of the entries are published data and models from the studies where SAXS was employed for the structural analysis of macromolecular solutions. There are also "benchmark" experimental data available from a set of well-characterised commercially available proteins. The high resolution structures of the benchmark set are available, and these data are used to test computational approaches and in numerous tutorials.

DARA is a web-server (dara.embl-hamburg.de) that queries over 150 000 scattering profiles pre-computed from the high resolution models of macromolecules and biological assemblies in the Protein Data Bank, to rapidly find nearest neighbours of a given (experimental or computed) SAXS profile [2]. Identification of the best scattering equivalents provides a straightforward and automated way of structural assessment of macromolecules based on the SAXS data. DARA output includes a list of PDB IDs with pre-computed overall parameters which are routinely used in SAXS data analysis: radius of gyration, maximum intra-particle distance, molecular weight and excluded volume. DARA is a perfect tool to demonstrate not only the power of SAXS but also the inherent ambiguity of SAXS data interpretation in terms of three-dimensional models. For each DARA search a list of neighbours is provided, which may contain false positives illustrating possible ambiguity of the SAXS-based interpretation and its resolution limits. Both SASBDB and DARA are freely accessible and can be useful educational tools for SAS tutorials and workshops.

[1] Valentini et al. (2015) *Nucleic Acids Res.* 43(D1), D357-D363.

[2] Kikhney et al. (2016) *Bioinformatics* 32(4), 616-618.

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