Getting correlated SAXS data to the outside world with SIMPLE SAXS

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A significant gap that needs to be filled is the availability of Small Angle X-ray Scattering (SAXS) data to users, SAXS software developers, and reviewers. When SIBYLS beamline staff introduced BioISIS, (www.bioisis.net) a repository of SAXS data that predated the SASBDB (www.sasbdb.org), many programmers could grab the data and develop software. We introduce a hybrid data delivery, data repository, and data analysis web interface in our SIMPLE SAXS platform (https://simplescattering.com/). SIMPLE SAXS is differentiated from SASBDB in that SASBDB presents isolated SAXS results and structures. High throughput SAXS (1) is often used to compare and contrast constructs, conditions, and formulations. SEC-SAXS results are a series of scattering curves from the purification profile of a sample. Both are correlated sets of data that are not easily ported to the SASDB. We envision SIMPLE SAXS as a tool to communicate these correlated sets between beamline scientists who collected the data and the sample supplier. We will connect our automated analysis tools, like SAXS Similarity (2), FoXS, BILBOMD (3,4) to be applied to the deposited data. Later the data entry, with modified permissions and annotations provided by the sample supplier, can be released to the public through the web.

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