



Contribution ID: 148

Type: Poster

Metadata collection and creation of sample identifier in the Bio-SAXS use case based on the concept of the Small Angle Scattering Biological Data Base

To support the principles of FAIR data, the Small Angle Scattering Biological Data Base (SASBDB) serves as a platform to make biological SAXS and SANS data more accessible and findable [1]. Within the SASBDB framework, experimental data can be deposited alongside relevant experimental conditions, sample details, and instrument characteristics, ensuring comprehensive documentation for future reuse [2].

Using SASBDB as a benchmark, we identified essential metadata and information required to properly deposit entries in such a database. While some beamlines are already designed to save important metadata during data collection, many smaller or laboratory X-ray sources lack automated metadata recording, resulting in raw detector images being stored without crucial sample or instrument information. To address this challenge, we introduce a standardized metadata catalogue related to BioSAXS experiments, along with a method for sample identification using the generation of an International Generic Sample Number (IGSN). We present a use case specific workflow scheme that includes the creation of a Nexus file as an additional step that incorporates metadata and IGSN information in a standardized format.

[1] E. Valentini et al. Nucleic Acids Research, 2015, Vol. 43, Database issue D357–D363

[2] A. Kikhney et al. Protein Science, 2019, Vol. 29, Issue 1

Primary authors: DARGASZ, Michelle; HÖVELMANN, Svenja (Kiel University)

Co-authors: MURPHY, Bridget; GUTT, Christian (Universität Siegen)

Presenters: DARGASZ, Michelle; HÖVELMANN, Svenja (Kiel University)

Session Classification: Poster