

BIOISIS.net Data Deposit Ready Form

A successful deposit contains, at a minimum, the following:

- **General Details**
- one or more **DataSet** containers
- descriptive **Supporting Figure**
- user chosen **BIOISIS ID** (BID, must be at least 6 characters, number or letters only)

Data Deposit form Preparation List

Items

General Details (required)

1	Title	The Title is a concise statement, often related to a publication title. For example, if samples are long chain waxes, a suitable title could be <i>"Melting studies of polyacrylate esters in paraffin"</i> .
2	Abstract	The Abstract should expand on the title and provide context for the SAS experiment. Abstract can be derived from publication abstract, but in general, the abstract should indicate to the reader why the experiment was performed and provide a conclusion. In some cases, deposits may not be affiliated with a publication such as a calibration measurement set.
3	Publication DOI	DOI could be for bioRxiv or other pre-print server. We can update to peer-review publication DOI later. If no DOI, leave blank
4	Contributors	Names of those that deserve credit for the SAS measurement

DataSet (required, one or more)

1	Title	DataSet Title simply describes contents of the dataset, e.g., <i>"Batch mode measurement of paraffin waxes"</i> or <i>"Concentration series of BSA in PBS"</i>
2	Description	DataSet Description provides details regarding sample names, concentration and temperature, molecular masses. If columns were used, the name of the column and flow rate need to be specified. The description should as detailed as possible. If SEC-SAXS, what volume and concentration were injected? If batch, what were the concentrations used? This information will be tagged to the uploaded data files so there should be a reasonable correspondence between filenames and the information in this description.
3	Source	Choices are : <i>home, synchrotron, spallation, reactor</i>
4	Instrument	<i>"B21 Diamond Light Source"</i> or instrument e.g., <i>"SAXSLab XEUSS"</i>
5	Background/buffer	Describe the Background , if buffer all details should be included e.g., <i>10 mM TRIS pH 8.0 with 5 mM DTT and 1% sucrose</i> . If background is water, specify water.
6	Sample Composition	Choose one or more : <i>protein, RNA, DNA, lipids, carbohydrate, glycosylated, detergent, surfactant, peptide, peptide-conjugate, gel, polymer, diblock copolymer, other</i>

Supporting Figure (required)

Data Deposit form Preparation List		
1	Figure	Supporting Figure is a png file the best captures or illustrates the SAS experiment. Could be an image of a molecular structure, <i>ab initio</i> model, cartoon of the experiment.
Supporting Files (optional, one or more)		
1	Description	<p>Detailed description of the contents of the archive file. This could be an archive of the directory that contained all the modelling such as outputs from DENSS, BILBOMD, mutli-FOXS. If SAS data was used for molecular dynamics simulations, the archive could be the CNS scripts and outputs. Please include the PDB files used for the modelling in the archive file. Description must be written before uploading file.</p> <p>If SAS data was analysed using form factors via SASFIT, SASVIEW, IGOR, etc. The archive file should contain outputs and constraints used in the analysis. Please specify type of form factor such as cylinder, core-shell, sphere, etc and include the fit files.</p>
2	File	ZIP file (must be .zip).