

Storing and sharing X-ray scattering data on the NIH Figshare instance

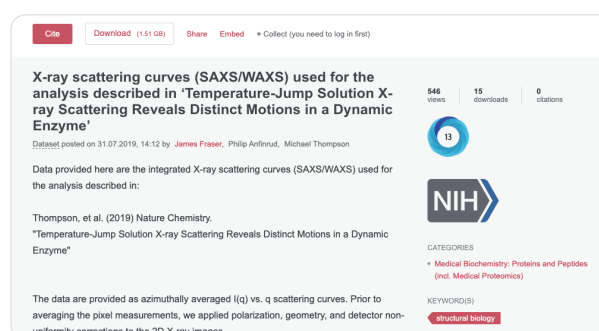
The NIH Figshare instance¹ published its first dataset titled *X-ray scattering curves (SAXS/WAXS) used for the analysis described in 'Temperature-Jump Solution X-ray Scattering Reveals Distinct Motions in a Dynamic Enzyme'*². The data was collected and uploaded by Professor James Fraser at the University of California, San Francisco (UCSF) and Michael Thompson, a postdoctoral fellow in the Fraser Lab³.

The dataset combines temperature conformations using an infrared laser with x-ray measurements of protein structure in order to study molecular motions that are related to the function of the molecules.

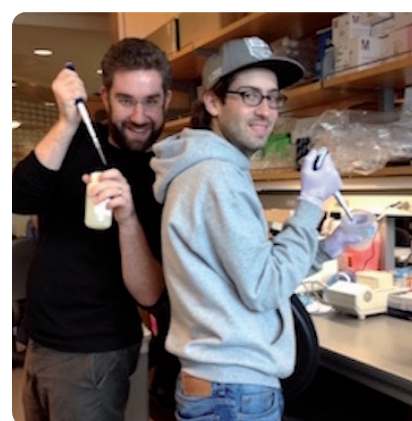
Their collaborators in Philip Anfinrud's group at the NIH designed instrumentation that can quickly collect this information, resulting in terabytes of data. "It's a very large package to upload to any of the other databases that collect and make x-ray scattering data available to the public," said Michael. "Figshare was one of the only resources that was able to handle that volume of data in a flexible format."

Existing databases for small angle scattering experiments specialize in taking data from single experiments and lack the infrastructure to support programmatic bulk uploads. Uploading this data to one of those databases would have resulted in hundreds of hours of metadata paperwork. "We created about 12 metadata files with descriptions of the experiments and it took about five minutes to upload them to the NIH Figshare instance," said Michael.

The authors will continue to use the NIH Figshare instance to store and share x-ray scattering data.



Fraser, James; Anfinrud, Philip; Thompson, Michael (2019): X-ray scattering curves (SAXS/WAXS) used for the analysis described in 'Temperature-Jump Solution X-ray Scattering Reveals Distinct Motions in a Dynamic Enzyme'. figshare. Dataset. <https://doi.org/10.35092/yhjc.9177143>



James Fraser (left) and Michael Thompson (right).
<https://fraserlab.com/members/>

References:

1. <https://nih.figshare.com/>
2. <https://doi.org/10.35092/yhjc.9177143.v1>
3. <https://fraserlab.com/>