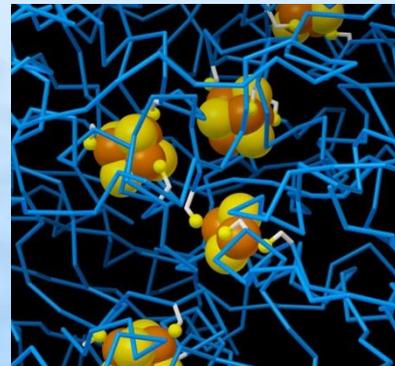
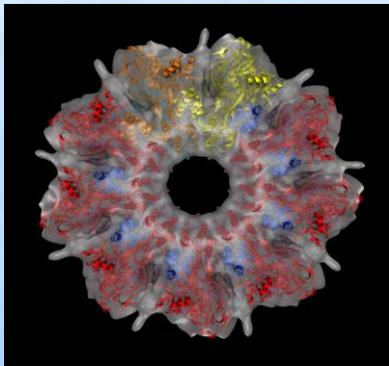
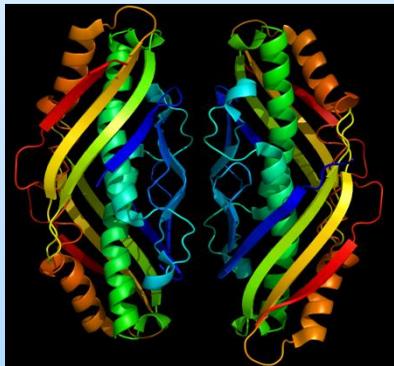


Structural Molecular Biology Resource at the Stanford Synchrotron Radiation Lightsource



The SSRL Structural Molecular Biology program operates as an integrated Resource with three primary core areas of technological R&D and scientific focus: macromolecular crystallography (MC), small angle x-ray scattering/diffraction (SAXS), and x-ray spectroscopy (XAS/XES) including x-ray microXAS imaging. Technological foci include development and enhancement of beam lines, specialized instrumentation, detectors, methods, and techniques, taking maximum advantage of the high x-ray brightness of SSRL's storage ring (SPEAR3). This is coupled with vigorous R&D in enhanced data collection, data management and data analysis to provide remote-access and "user-friendly, real-time and on-line" data interpretation. The innovations are guided by close coupling to scientific projects aimed at solving forefront problems in SMB. Significant synergy between the core areas enable addressing increasingly complex and challenging problems. The SMB program seeks to sustain and enhance the user community through excellent support, training and dissemination.

The SMB program is supported by the DOE Office of Biology and Environmental Research and the NIH National Institute of General Medical Sciences.



<https://www-ssrl.slac.stanford.edu/smb/index.html>

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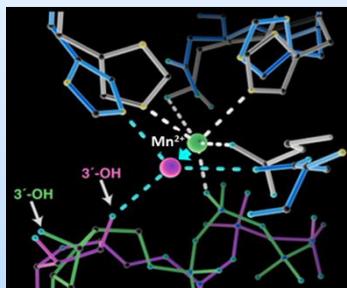
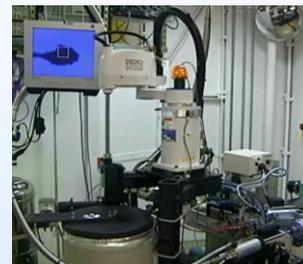




Macromolecular Crystallography

three-dimensional structural information at the atomic level

The SMB Resource provides four stations dedicated to macromolecular crystallography (MC) that enable studies on the most challenging problems in structural biology. These include undulator station BL12-2 optimized for micro-beam experiments, BL9-2, BL7-1 and BL14-1 optimized for high-throughput screening, and MAD or SAD data collection.



All MC stations are fully **remote access** (run the experiment from your home institution) with standard experiments fully automated, using a user friendly interface (*Blu-Ice*) and the SAM robot for crystal mounting and screening. Diffraction images are automatically analyzed, indexed and scored. BL12-2 and BL9-2 have high-speed Pilatus detectors for fast shutterless data collection and low-dose crystal searches.

A single-crystal **UV-Vis microspectrophotometry** capability at BL9-2 enables spectroscopic monitoring of x-ray dose effects on the metal center of metalloenzymes. The system is compatible with the SAM robot and fully remote accessible.



MC staff provide strong training programs for new and experienced users.

A next-generation **microfocus station**, BL12-1 is becoming available in 2020. A **broad bandpass** capability providing exceptionally bright microbeams and a high-speed Eiger16M detector (**133 Hz**) will support crystal injectors and other emerging techniques. Similarities in instrumentation, existing and new sample delivery systems, and software environments form the foundation of a synergistic relationship between SSRL's BL12-1 and a Macromolecular Femtosecond crystallography instrument (MFX) at LCLS, through a gateway approach.

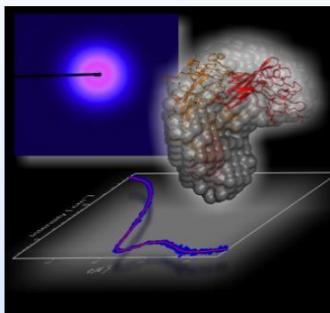
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Small Angle X-ray Scattering

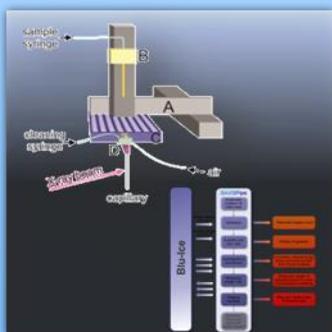
solution conformation of macromolecules



Small angle x-ray scattering (SAXS) from solutions of macromolecules and their complexes provides 3D structural information at nanometer resolution, enabling interpretation of atomic-resolution structures in a physiological context, providing a structural tool for studying molecular interactions, complex structures as well as domain folding properties and structural flexibilities in **solution**.

The SMB Resource's SAXS BL4-2 is dedicated to non-crystalline x-ray scattering and diffraction studies in biology.

The beam line features state-of-the-art large area silicon pixel array and gap-free CCD detectors with high photon detection efficiency, a widely reconfigurable SAXS camera, a variety of sample handling devices for automated high throughput and chromatography-coupled solution scattering (SEC-SAXS), **time-resolved** scattering in the millisecond time regime, as well as lipid and fiber diffraction studies.



User friendly software with an intuitive graphical interface (*Blu-Ice*) is used to control all aspects of the instruments and sample handling.

Fully automated solution scattering data collection, with a robotic sample changer and integrated software pipeline for data reduction and analysis, providing real-time data processing and analysis, make the data collection at the beam line highly efficient.

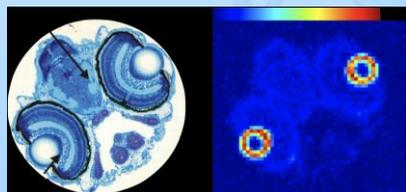
<https://www-ssrl.slac.stanford.edu/~saxs>

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X-ray Spectroscopy & Imaging

electronic & geometric structure of metal sites

The SMB Resource has developed one of the largest dedicated bioXAS activities in the world with optimized beam lines, specialized instrumentation, including high-performance detector arrays, data collection software, and data analysis capabilities, for enabling biological applications.



The Resource provides two beam lines for solution XAS on **metals** and access to beam lines for studies of **ligands** such as sulfur, chlorine and phosphorous. Integrated facilities for microXAS **imaging** and tomography (sub- μm to mm spatial resolution, over a wide energy range) are provided, as is a facility for XES/HERFD based spectroscopies.

The Resource supports studies of ultra-dilute **metalloprotein solutions** at liq-He temperatures. Specialized instrumentation enable simultaneous single-crystal XAS and crystallography. Anaerobic sample handling facilities are available. Studies of freeze trapped samples and *in-situ* bio-catalysis provide paths to pursue the structure-function paradigm.



The SMB Resource offers robust training programs for the novice and experienced user community, focusing on the experimental and theoretical aspects of data measurement, analysis and structural understanding.

<https://www-ssrl.slac.stanford.edu/smb/programs/xas/home.html>

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