Remote Experiments and Automation for biological SAXS at SSRL BL4-2

Thomas Weiss¹, Tsutomu Matsui², Ivan Rajkovic³, Ping Liu⁴

¹Stanford University / SLAC, ²Stanford University SSRL, ³Stanford University SSRL, ⁴Stanford University SSRL

weiss@slac.stanford.edu

The biological small-angle x-ray scattering station BL4-2 at the Stanford Synchrotron Radiation Lightsource (SSRL) provides state-of-the-art experimental facilities for studies focused on structural biology and biophysics of non-crystalline matter. Highly optimized sample environments for a variety experiments ranging from static and fast time-resolved solution scattering to lipid and fiber diffraction are available for experiments. Over the past few years significant progress has been made in developing new and refining the existing sample handling methods to enable high quality and truly remote controlled SAXS experiments. Since samples for biological SAXS experiments are typically non-frozen, fragile and only have a very limited lifetime, sample handling and manipulation at the beam line is often an integral part of the SAXS experiment. To perform a realistic SAXS experiment remotely some of these capabilities need to be available to the remote experimenter. At the BL4-2 we have recently successfully implemented instrumental capabilities towards this goal. For example, in the case of solution scattering our high throughput Autosampler has been enhanced to enable remote pipetting and mixing of samples on the tray just before the SAXS measurement if required. It can also and can run through several 96-well plates of samples without further intervention. A size-exclusion chromatography (SEC) option can be remotely selected to switch between regular solution SAXS and SEC-SAXS experiments. Our regular SEC-SAXS data collection setup is highly optimized for minimizing sample dilution during the chromatography as well as for preserving the full chromatographic resolution before the SAXS data collection. For more viscous samples typically measured in single pre-filled capillaries a high-capacity cassette system was developed allowing for shipment and save handling of the capillaries at the beamline. The cassettes are robotically mounted at the beamline and the samples can be aligned for the X-ray measurement using a remotely accessible sample microscope integrated into the BluIce interface. The whole experiment can thus be run fully remotely.