SAngler, New Software for Analysis of Small-Angle X-Ray Scattering Data

We newly developed and released the software SAngler to analyze the data measured by Small-Angle X-ray Scattering (SAXS). This GUI software runs under Windows 7, 8.1 and 10 32/64 bit, and can handle SAXS data not only for essential processes such as azimuthal averaging but also for typical analyses like the Guinier approximation. Users can freely download it with the Japanese or English manual from the website, http://pfwww.kek.jp/saxs/SAngler.html

SAXS is widely used for structural analysis of hard and soft materials including biological molecules at spatial resolutions ranging from ~nm to ~µm. X-ray scattering intensities in recent SAXS experiments are generally acquired as two-dimensional image data, and the intensities are converted into one-dimensional data by azimuthal averaging against the beam center. An imaging plate and a CCD have been used as a SAXS detector for many years at the SAXS beamlines of the Photon Factory. However, all of them were recently replaced with new hybrid pixel detectors (PILATUS3 2M and 1M, Dectris). Therefore, we newly developed GUI software, SAngler [1], in order to analyze the image data measured with those new detectors. It was created using Microsoft Visual Studio Express 2013 for Windows in C# language. It is able to perform various basic processing, for example, making mask files, calibrating camera distance and beam center, azimuthal averaging to convert 2D image data into 1D text data, and subtracting the background intensities. It also has a function for making various plots, for example, the log plot of the scattering intensity, Guinier plot [2] and Kratky plot [3], in order to assist the analysis of biological SAXS (BioSAXS). This software is compatible with the 64- and 32-bit versions of Windows 7, 8.1 and 10. The imaging plate detector, R-AXIS (Rigaku), can also be used with SAngler.

Figure 1 shows the data processing and analysis using SAngler. **Figure 1A** displays the Mask tab for making masks. PILATUS has not only gaps between the detector modules which appear in the shape of a lattice but also a lot of dead pixels in the modules. Since the intensities of the gap region and the dead pixels are outputted as negative values, SAngler can automatically choose and mask from the program menu. As for the shadow of a direct beam stopper, users are able to mask it by drawing a round and/or polygon shape. In order to refine the camera distance and the beam center position, calibration is performed from the Calibration tab of SAngler, using the Debye-Scherrer ring pattern of silver behenate for which the lattice spacing is 58.38 Å
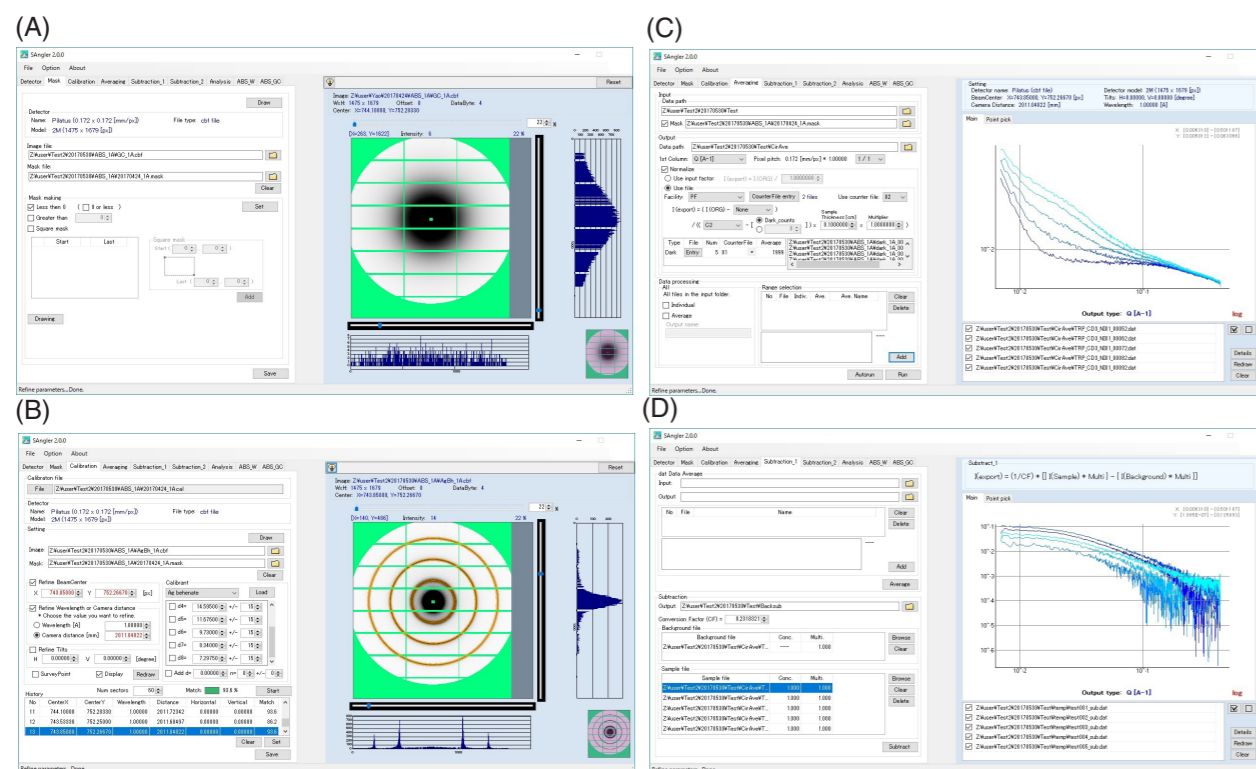
(**Fig. 1B**). The orange-colored ring displays the prediction based on the present parameters, and the character color after refining the values changes to red. Since the mask pattern and the calibrated parameters are saved to respective files, users can carry out data processing under the same conditions at any time using these files. From the Averaging tab (**Fig. 1C**), the scattering intensities recorded on a 2D image are azimuthally averaged to convert 2D data to 1D data using the results of the calibration. **Figure 1D** shows the scattering intensities after subtraction of the background intensities from the sample intensities.

The serial data outputted from SAXS with inline size-exclusion chromatography (SEC-SAXS) is processed and analyzed using SAngler. **Figure 2** shows the Guinier plot for the serial data measured by SEC-SAXS. Since SAngler links to the program package ATSAS [4], Guinier approximations for such multiple scattering data were automatically performed by using either our developed algorithm or AUTORG of ATSAS. The forward scattering intensity, I(0), and the radius of gyration, Rg, which were acquired as a result of the Guinier analysis, can be outputted to the table file to be used for the subsequent analysis.

Figure 2: Guinier plot for multiple data measured by SEC-SAXS experiment.

REFERENCES
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BEAMLINES
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Figure 1: User interface of SAngler. **(A)** Mask file making. **(B)** Calibration of the camera distance and the beam center position. 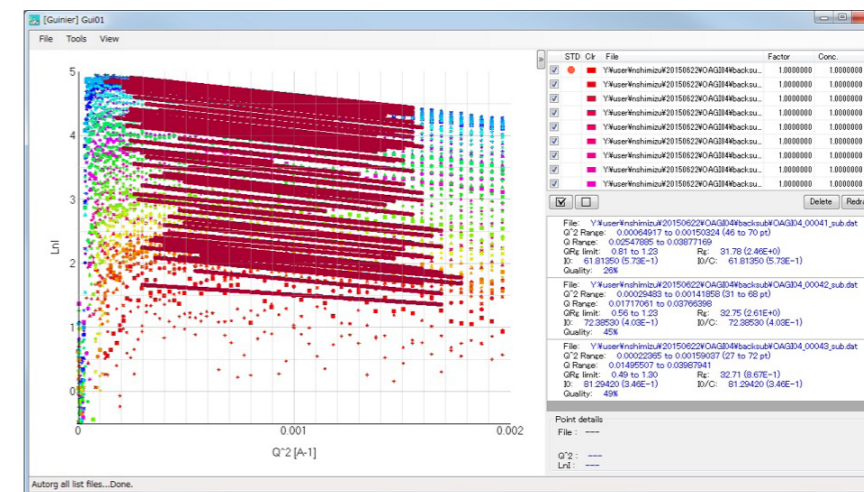**(C)** Azimuthal average. **(D)** Background subtraction.