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RIKEN Structural Genomics II

1. Introduction

RIKEN Structural Genomics Beamline II consists of SPring-8 standard bending magnet beamline components and an end station dedicated to high-throughput protein crystallography [1]. Asymmetric diffraction crystals have been adopted for the double-crystal monochromator (asymmetric angle of 6.33°) to increase the total photon flux of the monochromatic beam. Also, optional focusing with capillary lens optics (Hamamatsu J12432) upstream of the sample can be selected by the user to enhance the flux density of the incident X-ray beam at the sample [2].

Diffraction data can be automatically collected from a vast amount of cryo-cooled protein crystals through the user interface BSS with the high-framerate CCD detector MX225HS (RAYONIX), utilizing the twin-armed auto-sample exchanger SPACE installed at the end station [3,4]. Two types of remote access for users are supported: mail-in data collection in which a web database system, D-Cha, supports sample and experimental information input/output on a web browser [5] and the remote control of beamline equipment via a dedicated interface program, SP8Remote, which allows users to directly log in to the beamline control system under a restricted safety interlock system [6]. Currently, 20% of the total beam time is assigned to public users and 10% is assigned to Basis for Supporting Innovative Drug Discovery and Life Science Research by AMED (BINDS) project users.

2. Recent activities

The development of new sample-handling devices and further improvement of data collection throughput are being continuously conducted to contribute to research projects such as ligand screening for drug discovery. To improve the throughput of X-ray crystallography, including the sample preparation process, a new microfluidic device that allows the injection of crystal suspensions and the trapping crystals aligned in pit patterns inside the fluidic channel without handling the crystals one by one is being developed. By replacing the content buffer with a ligand solution, ligand–protein complex crystals are formed. The device is made of transparent material (PDMS) and is easily mounted on the goniometer to collect diffraction data at room temperature. We have confirmed that ligand screening by room-temperature crystallography with merged diffraction datasets with multiple crystals is possible by this method [7]. Aiming at the application to larger scale ligand screening, we are optimizing the design of the device to increase the efficiency of crystal trapping. This fiscal year, integration of the multiple channels into a device, which allows 32 compound conditions equipped on a holder of a compatible size with the SBS crystallization plate was developed (Fig. 1). Notably, sample injection and replacement are automated with a commercially available autopipetting robot, ASSIST PLUS (INTEGRA Biosciences). The upgrading of beamline equipment, such as a goniometer for a crystallization plate and a control

system for efficient data collection from the microfluidics, was conducted.

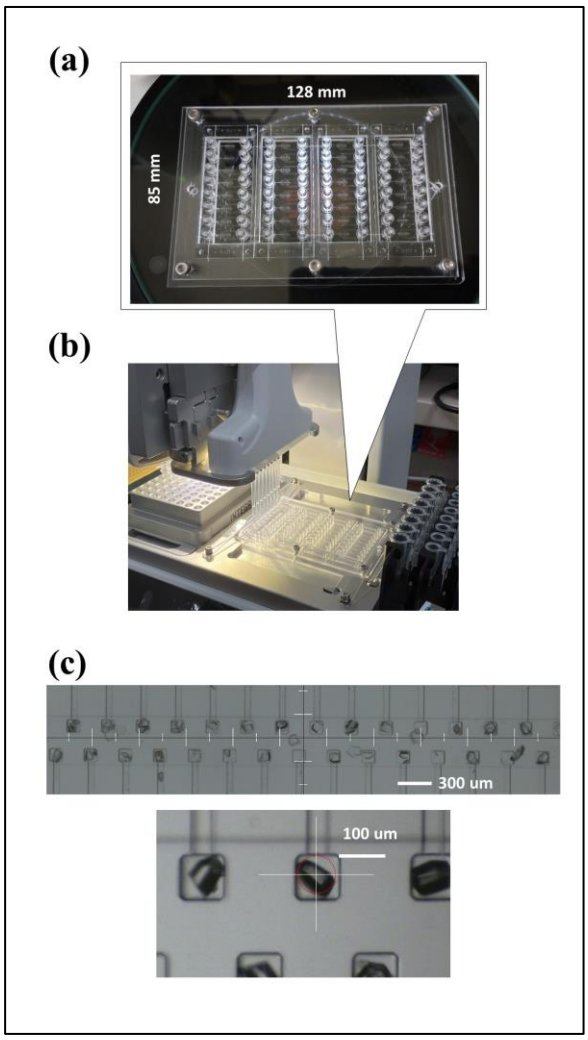

Fig. 1. Development of the new microfluidic device. (a) 32-ch integrated microfluidic device fixed on a holder designed to be of a compatible size with a SBS crystallization plate. (b) Multichannel autopipetting robot system for automation of sample loading. (c) Photographs of magnified channels and pits in which lysozyme crystals are trapped.

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