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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 monochromator (asymmetric angle of 6.33°) to increase the total photon flux, and optional capillary lens optics (Hamamatsu J12432) can also 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 with the twin-armed auto-sample exchanger SPACE and the user interface BSS [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 districted safety interlock system [6]. Currently, 20% of the total beam time is assigned to public users and 10% is assigned to BINDS (Basis for Supporting Innovative Drug Discovery and Life Science Research by AMED) project users.

2. Recent activities

The development of new devices and further improvement of throughput were 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 crystal one by one is being developed. By replacing the content with a ligand solution, ligand–protein complex crystals are formed. The device is made of transparent material (PDMS) and is readily mounted on the goniometer to collect diffraction data at room temperature. We have demonstrated the feasibility of the ligand screening experiment using trypsin crystals with a single-channel test device (Fig. 1) [7]. Now, to use the device for large-scale ligand screening, we are currently updating the design of the device to increase the efficiency of crystal trapping, integrating multiple channels into the device, and automating the sample injection. Moreover, the development of a new web database

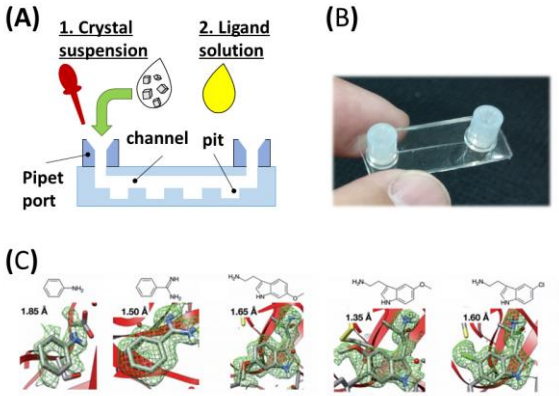

Fig. 1. Development of new microfluidics. (A) Schematic view of the device. (B) One-dimensional prototype device. (C) Ligand structures of trypsin were analyzed with the test device.

system to cover the entire data flow, including, for example, crystallization and data analysis, is a work in process.

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