

BL26B2

RIKEN Structural Genomics II

1. Introduction

BL26B2 is the RIKEN Structural Genomics Beamline II. It consists of SPring-8 standard bending-magnet beamline components and an end-station dedicated to high-throughput protein crystallography^[1]. Users can collect diffraction data from a vast amount of cryo-cooled protein crystals in an automated manner using the auto-sample exchanger SPACE and user interface BSS^[2, 3]. Two types of remote access for users are available. One is mail-in data collection in which a web database system D-Cha supports sample and experimental information input/output on a web browser^[4]. The other is remote control of beamline equipment via a dedicated interface program, SP8Remote, which allows users to directly login into the beamline control system under the districted safety interlock system^[5]. 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

In FY2019, further improvements for the

throughput and development of new devices contributed to various research projects such as ligand screening for drug discovery. Upstream of the sample position, a capillary lens optics (focus size of 0.08 mm, Hamamatsu J12432) was installed to enhance the flux density of the incident X-ray beam. Hence, the throughput of data collection for smaller crystal samples was improved. Combining this with asymmetric diffraction crystals for the monochromator has increased the photon flux to 2×10^{11} photons/s at 12.4 keV (Fig. 1)^[6]. In addition, to automate crystal centering, a program, DeepCentering, was developed based on the deep-learning algorithm^[7]. DeepCentering was implemented to the automated data collection system for the mail-in data collection described above.

In addition to improving the throughput of room-temperature crystallography, the development of a microfluidic-chip device for *in situ* ligand soaking and data collection is underway. Additionally, efforts to implement data processing and a structure analysis pipeline as well as to develop a new web database system to cover all the data flow, including crystallization and data analysis, are underway.

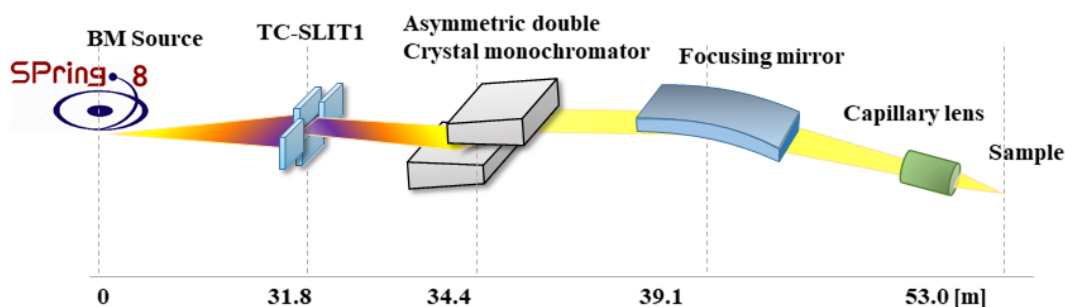


Fig. 1 Schematic of BL26B2 optics design.

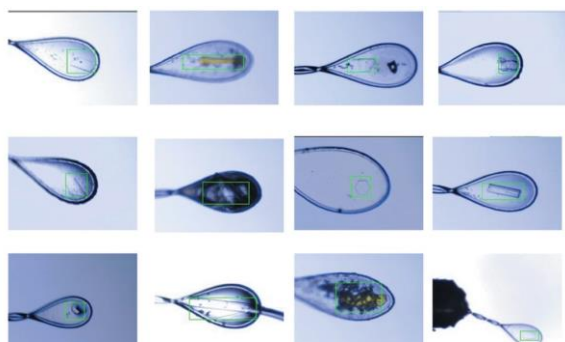


Fig. 2. Result of automated crystal detection by the DeepCentering program.

Go Ueno

SR Life Science Instrumentation Team, Life Science Research Infrastructure Group, Advanced Photon Technology Division, RIKEN SPring-8 Center

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