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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 an 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 for public users and 10% is assigned for BINDS (Basis for Supporting Innovative Drug Discovery and Life Science Research by AMED) project users.

2. Recent activities

In FY2020, further improvement of throughput and the development of new devices were continuously conducted to contribute to research projects such as ligand screening for drug discovery. An automatic structure analysis script named

IMAPROC, which sequentially invokes DIMPLE in the CCP4 suite while monitoring the result of data processing with KAMO [7], has been developed and implemented to the mail-in data collection system. The captured image of the resulting difference Fourier density blob is shown on D-Cha with a web browser (Fig. 1). In addition, to improve the throughput of room-temperature crystallography, the development of a micro-fluidic chip device that allows *in situ* ligand soaking and data collection is in progress. Moreover, the development of a new web database system to cover the entire data flow, including, for example, crystallization and data analysis, is a work in process.

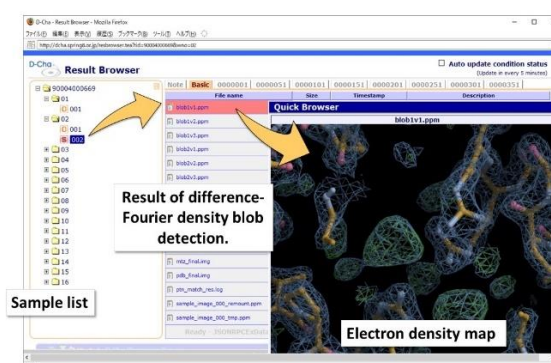


Fig. 1. Result browser of D-Cha. An image of the electron density blob corresponding to a ligand candidate output from DIMPLE invoked by IMAPROC is shown.

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References:

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