

BL32XU

RIKEN Targeted Proteins

1. Introduction

BL32XU is the RIKEN targeted protein beamline dedicated to high-resolution diffraction data collection from protein microcrystals. Since FY2015, we have been developing a fully automated data-collection system, ZOO, dedicated to protein crystallography at BL32XU [1]. ZOO covers all existing experimental schemes in goniometer-based cryo-crystallography data collection from protein crystals. Furthermore, it has achieved unattended data collection. Hence, remote users can acquire high-resolution datasets using SPring-8 by sending crystal samples. BL32XU has supported numerous structure determinations of challenging proteins, such as membrane proteins, as part of the Basis for Supporting Innovative Drug Discovery and Life Science Research (BINDS) program since FY2017.

2. Recent activities

In the beamlines in FY2021, it has been noted that the rise of cryoEM is causing a downward trend in the number of users performing crystallographic structure analysis. It can be said that the balance of the contribution of crystallographic structure analysis is gradually changing owing to the efficiency of the structural analysis of protein molecules by cryoEM and the signs of this change are becoming visible in the form of user operation. However, from the previous year, 60% of the machine time was provided to the BINDS project and 20% to shared users of the ZOO automated measurement system. Automated measurements consumed more than 95% of the project machine

time.

In automated data collection with ZOO, the user specifies the main experimental parameters. The experimenter describes the experimental conditions in a spreadsheet and sends it to the facility along with the sample. The spreadsheets prepared by beamline users need to be reviewed by the beamline staff, especially if the experimental conditions are set up strangely. The SPring-8 Structural Biology Beamline has started to develop a database to store necessary experimental information from wet experiments to diffraction experiments, cryoEM experiments, and analysis. As a first step, this fiscal year, a database of experimental conditions to be input into ZOO was created, and the database was edited via a web browser and then implemented so that the beamline could perform automatic measurements using ZOO based on the stored experimental conditions. This prototyping consists of a database using MongoDB, an API server using Javascript (Node.js) to reference the database, and a web client (React). The experimental information can be registered in the database by uploading spreadsheets from the experimenter onto the web client, which can then be edited by the client. The beamline proceeds with the experiment while retrieving the registered information from the database as needed. Since the prototyping was successful, a full-scale, secure system has been constructed. In the future, we aim to open the web client to users to realize easy registration of experimental information and to automate the review of experimental conditions by creating a detailed flowchart, thereby building a

system that minimizes the interaction between staff and users.

In user experiments, we have continued to contribute to many structure analysis projects since last year by conducting regular crystal structure analysis and crystal structure analysis using sub-micron crystals^[1-9].

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