Development of automated high-throughput MX beamline at SPring-8

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Macromolecular crystallography (MX) has progressed through the development of brilliant micro-focus beamlines, rapid-readout detectors, and smart crystal handling apparatus.

At the micro-focus beamline BL32XU at SPring-8, we have been developing an automatic data collection system named ZOO [1, 2] so that all users can easily collect large amounts of data from high-difficulty samples. Data quality can be adequately controlled by strategies with automated crystal selection and radiation damage control. The ZOO system has enhanced experimental efficiency and data quality accelerated the accumulation of better data sets within the limited beam time and accelerated the high-resolution structural analysis of challenging samples.

The ZOO system is also capable of collecting a few hundred full data sets within a day. The capability also benefits high-throughput data collections of fragment-based drug design (FBDD) by examining a large number of crystals in a complex with ligands. For this purpose, the beamline BL45XU was rebuilt to a fully automated high-throughput MX beamline dedicated to the ZOO system and the high-speed crystal handling system SPACE-II [3]. The expansion of developed technologies among SPring-8 beamlines eventually benefits all users. Due to the COVID-19 from 2020, many users could not visit the SPring-8 site, and more than 90% of the beamtime is now used for fully automated data collection at the BL45XU.

Simultaneously with the beamline development, we are establishing the automated structure analysis pipeline NABE system and the ligand screening pipeline using an acoustic liquid handler ECHO for more efficient data collection and structure analysis.

We will present the current status and the prospects of the high-throughput MX at SPring-8.

References
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