

Automation of high-throughput MX beamline at SPring-8

Macromolecular crystallography (MX) has advanced as an essential structural analysis technique for modern life science research and drug discovery research with the development of excellent microfocus beamlines, fast readout detectors, and smart crystal handling equipment.

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 diffraction data from high-difficulty samples. In addition, strategies with automated crystal positioning and radiation damage estimation can control data quality. As a result, the ZOO system has enhanced experimental efficiency and data quality, accelerated the accumulation of better data sets within the limited beam time, and opened the high-resolution structural analysis of challenging targets.

The ZOO system can also collect a few hundred complete data sets within a day. The capability also benefits high-throughput data collection of fragment-based drug design (FBDD) by examining many crystals in a complex with ligands. For this purpose, the beamline BL45XU was rebuilt to a fully automated high-throughput MX beamline with 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. However, due to 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 established 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.

[1] Yamashita K., Hirata K., Yamamoto M. (2018) *Acta Cryst.* **D74**, 441-449

[2] Hirata K., Yamashita K. et al. and Yamamoto M. (2019) *Acta Cryst.* **D75**, 138-150

[3] Murakami H. et al. and Kumasaka T. (2020) *Acta Cryst.* **D76**, 155-165

emphasized text

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