

Poster Presentation

MS22.P14

Current status of protein micro-crystallography at SPring-8

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Protein micro-crystallography is one of the most advanced technologies for protein structure analysis. In order to realize this, an undulator beamline, named BL32XU, was constructed at SPring-8. The beamline can provide beam with size of 0.9 x 0.9 μm and photon flux of 6E10 photons/s. The beam size can be easily changed by users from 1 to 10 μm square with the same flux density. Through three years user operation, we have established several key systems for efficient protein micro-crystallography. One of them is the software for precise positioning of micro-crystals in 'raster scan'. SHIKA is a program with GUI which searches diffraction spots in a plenty of low dose diffraction images obtained in raster scan. Finally, it generates 2D map of crystal positions based on the number of spots or spot intensities. Parameters and thresholds in peak search have been empirically optimized for LCP crystals and it provides robust results. Another system is for the data collection strategy. Almost all successful data collections were conducted via 'helical data collection' on BL32XU using the line-focused beam. The GUI software, named KUMA, enables estimation of an accumulated dose and suggests suitable experimental conditions for helical data collection. The system is proven to be useful for experimental phasing using tiny LCP crystals of membrane proteins[1-3]. Based on them, the rapid and automatic data collection system using protein micro-crystals is under development. The new CCD detector, Rayonix MX225HS, was installed for faster data acquisition in 10 Hz with the pixel size of 78 μm square. The new SHIKA using GPUs is under development for faster and more accurate crystal alignment. Following this step, KUMA system can suggest experimental conditions for each crystal found on the loop. We also report about the effects of higher dose rate in protein crystallography up to the order of 100 MGy/s. This work was supported by Platform for Drug Discovery, Informatics, and Structural Life Science from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

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Keywords: micro crystal, protein crystallography, micro focus beamline