Automated systems for X-ray crystallography at Photon Factory

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X-ray crystallography has been the most widely utilized method for 3D structure determination of biological macromolecules at atomic resolution. Since modern biology is studied at the molecular level, the 3D structures of biological macromolecules provide critical information for rational biological studies. X-ray crystallography is therefore becoming an essential tool for molecular and cellular biology and is increasingly being adopted by non-crystallographers. To facilitate this movement, the Structural Biology Research Center (SBRC) in KEK has developed several robotics and automation systems for crystallization, data collection, and structure determination. For the initial crystallization screening, we have developed protein crystallization system (PXS) that can automatically perform initial crystallization screenings in a sitting drop setting. The PXS possesses an automated image acquisition function for crystallization droplets. The obtained images can be checked from outside the KEK campus via a VPN connection. Moreover, the crystallization plate can be directly mounted to a specific goniometer at BL-17A for in situ data collection. Our protein crystallography beamlines, BL-1A, 5A, 17A, AR-NW12A, and AR-NE3A, are highly automated by the PReMo program. Once a cassette containing protein crystals is set to the system, a robot can mount a crystal to the goniometer in a beamline; do the centering of the crystal and start data collection. Beginning in May 2018, we will provide a fully automated data collection service for users. In this service, the obtained diffraction data sets will be automatically processed by a data-processing routine in PReMo. The processed data can then further be analyzed with PReMo for structural determination using the SAD method. Although at present the structure determination following the data processing must be performed manually, we are developing a new routine for automated structure determination. It is of note that all these automated functions are based on a database system in PReMo, and thus data from crystallization to structure determination can be treated in an integrated manner. Our service is expected to provide the basis of an intelligent system for crystallography.

Recent Publications


Biography
Toshiya Senda has completed his PhD from Nagaoka University of Technology, Niigata, Japan in 1995. He was a Research Associate in Nagaoka University of Technology during 1995-2001 and a Senior Researcher in Institute of Advanced Industrial Science and Technology during 2001-2012. Now, he is the Director/Professor of Structural Biology Research Center of High Energy Accelerator Research Organization (KEK) in Japan. He was awarded the CrSJ (Crystallographic Society of Japan) award in 2014.