Test for the Routine Structure Analysis of Biological Macromolecules at the Bio-Crystallography Beamline

Nobuo Kamiya[1](0000315)※, Yoshiaki Kawano[1](0000083), Masahide Kawamoto[1](0001325), Yoshikazu Tomisugi[2](0003015), Yoji Yagi[2](0003013), Akitake Akita3(0001335), Yuichi Ishida[3](0003471), Michiaki Tanaka[3](0003611), Kazuhiko Kakoi[4](0003353), Junichi Saito[5](0003196), Diane H. Peapus[5](0003195), Yukio Morimoto[2](0003007), Kensaku Hamada[4](0001241), Kunio Miki[5](0003192)

[1]The Institute of Phisical and Chemical Research (RIKEN), 323-3 Mihara, Mikazuki-cho, Sayo-gun, Hyogo 679-5143, Japan. [2]Faculty of Science, Himeji Institute of Technology, Kamigori, Hyogo 678-12, Japan, [3]Department of Biotechnology, Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464, Japan, [4]Shimane University, Nishikawatsu 1060, Matsue 690, Japan, [5]Department of Chemistry, Graduate School of Science, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan.

The Bio-Crystallography beamline was constructed for crystal structure analysis of biological macromolecules on the multiple isomorphous replacement method with optimized anomalous scattering (MIR-OAS). An on-line imaging plate (IP) diffractometer was installed in the experimental hutch. Automatic X-ray exposures on sample crystals, required for the MIR-OAS routine structure analysis, were successful on the Weissenberg and oscillation photograph techniques. All of diffraction patterns were very fine, and we could observe higher resolution spots compared with the experiments at second-generation SR facilities. This may depend on the highly brilliant beam from the undulator light source.

Since the on-line IP readout mechanism of the diffractometer was still under construction, all of our test data were digitized with a RIGAKU IP dram scanner. Several data sets were collected for each of hen egg white lysozyme (HEWL) and *Aleuria Aurantia* Lectin ($P6_122$, a=83.4 A, c=253.7 A) at room temperature and trypsin crystals at cryo-temperature. The reflection integrations were carried out by a newly developed software system; AUTO (Dr. Higashi, RIGAKU Co. Ltd). Rmerge values were reduced to less than 5% at 2.0 A resolution for all data sets. The MIR-OAS software dedicated for immediate checking of data quality was installed and opened for users.

Since the high flux X-ray beam was available at the Bio-Crystallography beamline, X-ray damage on sample crystals was the most serious problem. Except the tough crystals such as HEWL and AAL, the cryo-cooling may be indispensable for almost of all biological macromolecule crystals.