MIROAS Crystal Structure Analysis of Aleuria Aurantia Lectin with the Automatic Diffractometer

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A lectin (AAL) from fruiting bodies of aleuria aurantia shows sugar-binding specificity for L-fucose. AAL is composed of two identical non-glycosylated subunits of 312 amino acids each. Although we tried to prepare heavy atom derivatives for native AAL crystal using many chemical compounds at many conditions, no suitable derivative could be obtained. Contrary, we have succeeded recently to prepare cocrystals of AAL and mercury ion (AAL-Hg), which is similar in size and shape to the native AAL crystals. Furthermore, a gold derivative can fortunately be obtained for the AAL-Hg cocrystal. Since the Bio-Crystallography beamline (BL41XU) was constructed for crystal structure analysis of biological macromolecules on the multiple isomorphous replacement method with optimized anomalous scattering (MIROAS), the phase determination of the AAL-Hg cocrystal using only one heavy atom derivative is a preferable target to demonstrate abilities of the MIROAS technique on BL41XU.

In order to realize the MIROAS phase determination, free alteration of X-ray energy including automatic adjustment of speciment-detector distance is very much convenient for users. We constructed a data base for precise setting parameters of all beamline components for twelve points of X-ray energy between 7 keV and 37.6keV. Another data base for the setting parameters of automatic diffractometer was also prepared for the twelve points of X-ray energy. Using these data bases, automatic settings of the beamline was realized for every X-ray energies selected freely by users.

After the development of the automatic beamline setting technique mentioned above, MAD experiments were tried for the gold derivative of AAL-Hg cocrystal at three energy values around gold L3 absorption edge. The data collection was successfully completed, and an initial structure model of AAL is at present to be constructed.