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Recent activity of neutron diffractometers for biological crystallography at JAEA

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Hydrogen atoms and hydration water molecules in proteins are indispensable components for many biochemical processes, and are important to the understanding of protein-protein and protein-nucleic acid molecular recognition interactions. The locations of protein atoms are usually predicted by theoretical approaches, but it is still very difficult to determine the ionization status of catalytic residues, hydration structure, and the characteristics of hydrogen-bonding interactions (particularly for low-barrier hydrogen-bonds). Neutron diffraction is a powerful probe to directly observe hydrogen atoms located in proteins.

By the use of single-crystal neutron diffractometers for biological macromolecules (BIX-3 and 4) at JAEA, a total 16 neutron diffraction data sets for proteins and DNA oligomers have been collected. Since X-ray diffraction can be used to reveal the locations of electrons, bond distances are sometimes different from those obtained by neutron diffraction. Careful comparison of the location of the hydrogen atoms is necessary; thus, we attempted to determine the structure of a protein using both X-ray and neutron diffraction. Three data sets involving 1) X-ray diffraction data at 100 K, 2) X-ray diffraction at room temperature, and 3) neutron diffraction data at room temperature (using exactly the same crystal used for X-ray data collection at room temperature) were obtained. In addition, we installed cryogenic systems to both BIX-3 and 4 diffractometers. A cryogenic system enables us to collect higher resolution data because temperature factors of atoms in a biomolecule decrease at 100K in comparison to room temperature. Here, we report the recent activities for developments of the neutron diffractometers and the structure analyses of enzyme-inhibitor complex.

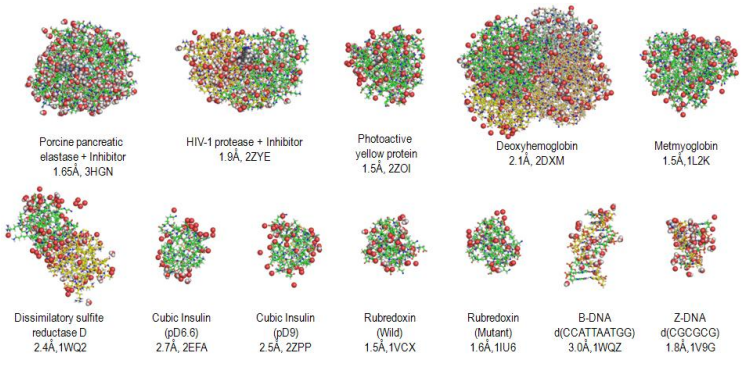

Figure 1. Structures of bimolecules determined using BIX-3 and 4 in JAEA

Reference

[1] Adachi, M., et al., *Proc. Nati. Acad. Sci. USA* 106, 2009, 4641.

[2] Tamada, T., et al., *J. Am. Chem. Soc.* 131, 2009, 11033.