

S30-4 Collaborative use of neutron and X-ray for determination of drug target proteins

○Ryota KUROKI¹

¹QuBS, JAEA

Crystallography enables us to obtain accurate atomic positions within proteins. High resolution X-ray crystallography provides information for most of the atoms comprising a protein, with the exception of hydrogens. Neutron diffraction data can provide information of the location of hydrogen atoms to the structural information determined by X-ray crystallography. Here, we show the recent result of the structural determination of drug-target proteins, porcine pancreatic elastase and human immuno-deficiency virus type-1 protease by both X-ray and neutron diffraction. The structure of porcine pancreatic elastase with its potent inhibitor was determined to 0.94Å resolution by X-ray diffraction and 1.75 Å resolution by neutron diffraction. The structure of HIV-PR with its potent inhibitor was also determined to 0.93 Å resolution by X-ray diffraction and 2.3 Å resolution by neutron diffraction. The ionization state and the location of hydrogen atoms of the catalytic residue in these enzymes were determined by neutron diffraction. Furthermore, collaborative use of both X-ray and neutron to identify the location of ambiguous hydrogen atoms will be shown.