MS82.O05

Evaluation of pKa of Amino Acid Residue in Proteins by Neutron Crystallography

N. Niimura[1]

[1]*Ibaraki University, Frontier Research Center for Applied Atomic Sciences*

The pKa values of isolated amino acids in solution are tabulated in standard textbooks. However, the protonation state of a given amino-acid side chain in a protein cannot be estimated from standard pKa values measured from isolated amino acids in solution, because inside a protein it may vary significantly depending on the local environment. The electrically charged states of the amino-acid residues are very important in understanding the physiological function of the protein, the interaction between ligands and proteins, molecular recognition, structural stability, and so on. Neutron Protein Crystallography (NPC) is the unique method to provide the definite protonation states of the amino acid residue in proteins because neutron can identify not only hydrogen atoms but also protons. (N.Niimura & R. Bau: Acta Cryst. A64, 12 (2008); N.Niimura & A. Podjarny: IUCr Monographs on Crystallography 25 (2011)) Biological mechanism such as enzymatic reactions is well understood by studying protonation states of the catalytic polar amino acid residues, which can be identified by NPC. It is proposed that the protonation states should be systematically discussed from the view point of the pKa values of the amino acid residues in proteins. Several examples of the protonation states of the catalytic residues determined by NPC, such as serine proteases (trypsin, elastase, thrombin, & acromabacter), insulin, hen egg white lysozyme, RNase A, and HIV-1 protease will be introduced and discussed on the basis of the pKa values.

Keywords: Neutron Protein Ceystallography, pKa, Polar Amino Acid Residues