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Hydrogen bonding network running through protein kinase investigated by neutron crystallography

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Casein kinase II (CK2), is a serine / threonine kinase ubiquitously distributed among eukaryotic cells, is known to be involved in the cell cycle and cell survival and proliferation. CK2 is one of the drug target proteins, because the relationship between CK2 over-expression and carcinogenesis and cancer metastasis has been pointed out. We aimed to elucidate the hydrogen bonding network involved in the catalytic reaction of CK2 and to obtain the knowledge of conformation of the hydrogen atom and hydration structure effective for the development of inhibitors. In this study, we prepared large crystals for neutron diffraction experiments of wild type CK2 α (catalytic subunit). The large crystal of about 2 mm³ was obtained by the macro seeding method. After the dialysis of the obtained crystal against deuterium solvent, a neutron diffraction data were collected at FRMII BioDIFF(100 K) to resolution of 1.90 Å. Then, X-ray diffraction experiment at PF BL-5A was collected using the same crystal to resolution 1.10 Å for the joint refinement. As a result of neutron crystallography, an interesting hydrogen bonding network running through CK2 α was found. This discovery can be expected to contribute to the development of an anticancer drug with a new inhibitory mechanism.

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