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Preparation for X-ray crystal structure analysis of weakly binding Schiff base metal complexes and Lysozyme

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As a preparatory step for direct observation by X-ray crystallography of optical switching of azo-containing Schiff base copper complex and lysozyme complex system, fluorescence observation of crystallization / bonding behavior of Schiff base zinc complex and lysozyme complex system / preliminary The measurement was carried out, and it was confirmed that the complex was weakly bound to the lysozyme crystal and was not retained under a certain condition.

1 Introduction

Disrupting protein conformation is useful information for the treatment of proteins in unreported diseases. Previously, we found that hybrid of Human Serum Albumin with a Schiff base Zn(II) complex could by damaged easily by irradiation of infrared free electron laser (IR-FEL) for 30 min, which was associated with disruption of conformation of the secondary structure of protein [1].

Herein, to investigate the effect of a complex and its intermolecular interaction with a lysozyme, we performed (transient) fluorescence spectroscopy for quenching and life-time of excited state and preliminary X-ray crystallography for proof of equilibrium state of docking to a surface of lysozyme similar to previous study [2].

2 Experiment

Dipeptide Schiff base Zn(II) complexes (ZnGlyGlyH and ZnGlyGlyPh) [1] were prepared and characterized previously. Commercially available chicken egg white lysozyme was used. After adjusting phosphate buffer solutions of ZnGlyGlyH or ZnGlyGlyPh and Lysozyme , we measured conventional and transient fluorescence spectra and grew single crystals. X-ray crystallography was carried out at KEK-PF BL-5A.

3 Results and Discussion

Docking simulation showed that the Zn(II) complex was spatially stacked on the concave molecular surface of lysozyme . This played an important role in disrupting conformation of lysozyme . The extinction and lifetime of the excited state of Lysozyme also supported intermolecular features by the computational investigation. The variable temperature fluorescence spectra also indicated their equilibrium thermodynamically. In addition, we attempted to prepare a single crystal of Lysozyme containing the Zn(II) complex (Fig. 1). Although color changed from colorless to yellow appeared, electron density of the Zn(II) complex could not be observed by X-ray crystal structure analysis (Fig. 2). This also suggested weak bonding of the Zn(II) complex to molecular surface of lysozyme .

References

[1] Y. Onami *et al*., *Int. J. Mol. Sci.* **20**, 2846 (2019).
[2] T. Akitsu and M. Unno *et al.*, *Key Engineering Materials* **888**, 105 (2021).

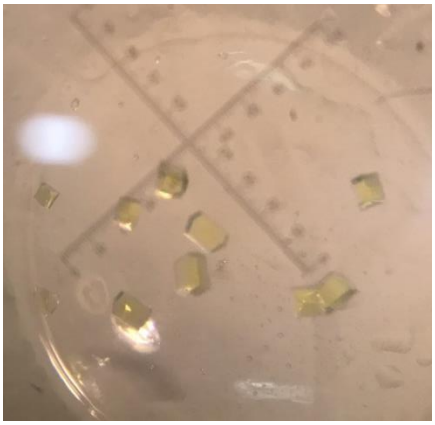

Fig. 1: Pale yellow single crystals of lysozyme containing a Zn(II) complex.

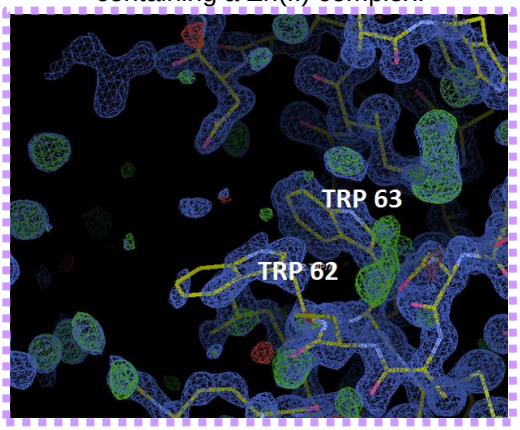

Fig. 2: Electron density of crystals of lysozyme without a Zn(II) complex.

Research Achievements

1. We obtained pale yellow single crystals of lysozyme containing a Zn(II) complex.

2. We could have confirmed that electron density suggested weak bonding of the Zn(II) complex to molecular surface of lysozyme under a certain condition.

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