Structural and Physical Properties of Salen-type Copper (II) Complexes in Lysozyme for Oxygen Reduction

Kumpei Kashiwagi^a, Sayantan Pradhan^b*, Tomoyuki Haraguchi^a, Takashiro Akitsu^{a*}

a Department of Chemistry, Tokyo University of Science, Tokyo, Japan

b Department of Chemistry, Jadavpur University, Kolkata, India

*E-mail: sayan23us@gmail.com (Sayantan Pradhan), akitsu2@rs. tus.ac.jp (Takashiro Akitsu).



Abstract: Artificial metalloenzymes (ArM) have emerged as a promising strategy to emulate the catalytic efficiency of natural metalloenzymes in new to nature reactions. ArM consisting of lysozyme derived from hen egg white lysozyme (HEWL) and several chiral salen type Cu(II) complexes was prepared in this study. Twenty types of salen-type metal complexes were obtained from crystal database and then were virtually screened with help of molecular docking procedure. Docking results verified that the Cu(II) complexes interacts with lysozyme by hydrogen and hydrophobic bonds. Four Cu(II) complexes with best docking score were synthesized. It was confirmed by the CV curve that there is an electrochemical difference between lysozyme simple substance and complex to attempt to reduce oxygen.

Keywords: Artificial metalloprotein, salen type Cu (II) complexes, DFT, Docking.