A theoretical study of glucose oxidase using canonical molecular orbital calculation

Toshiyuki Hirano, Fumitoshi Sato

Institute of Industrial Science, The University of Tokyo, 153-8505, Japan

Glucose oxidase (GOD; EC 1.1.3.4) is an enzyme which catalyzes the oxidation of beta-D-glucose to D-glucono-1,5-lactone, and has been widely used in some glucose meters [1]. In order to understand the reaction mechanism and interaction of residues, there is a compelling need for revelations from electronic structure of the GOD. In this report, we show the computational procedure of the canonical molecular orbitals (CMO) for the GOD protein, and the electronic structure around the active site, the flavin adenine dinucleotide (FAD).

The computation model of the GOD was formed on the basis of the experimental structure data (PDB accession code 3QVP). The prepared whole model is shown in Fig. 1. For examination of interactions of the FAD with residues, the partial calculation models were also constructed by changing the range threshold 200, 300, 400 pm from the FAD. The B3LYP density functional calculations were carried out by using the program, ProteinDF [2]. The MOs spreading from the FAD to surrounding residues were obtained by the CMO calculation. Details will be reported at the conference.

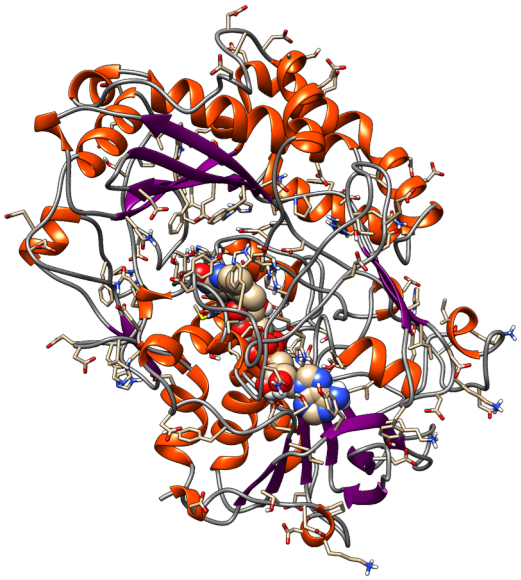

Fig. 1. The structure of the computaional model, GOD (581 A.A.)

[1] S. B. Bankar, M. V. Bule, R. S. Singhal, L. Ananthanarayan, *Biotech. Adv.*, **27**, 489 (2009).

[2] TH and FS, *Phys. Chem. Chem. Phys.*, **16**, 14496 (2014).