

Cadmium binding to antioxidant enzymes: in silico study

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Abstract. Cadmium (Cd) is a heavy metal that can be used for industry. Cd is toxic and can damage the kidneys, neurotoxic, glucose metabolism disorders and others. The reaction of Cd with protein causes oxidative stress, which is an imbalance of oxidants and antioxidant enzymes. Antioxidant enzymes include Superoxide dismutase (SOD), Catalase (CAT), and Glutathione reductase (GSR). There are not many studies that explain the interactions between Cd and antioxidant enzymes. For this reason, this research was carried out using in silico. The structure of the enzymes was obtained from the RCSB Protein Data Bank (<http://www.rcsb.org>) with the following code SOD (PDB ID 1E9Q), CAT (PDB ID 3RGP), and GSR (PDB ID 1GRT). Cd interactions with these enzymes were used by MIB: Metal Ion-Binding site prediction and docking server (<http://bioinfo.cmu.edu.tw/MIB/>). The interactions between Cd and amino acids of targeted protein were visualized on UCSF Chimera 1.14. The results of the study identified amino acid residues involved in the mechanism of binding of Cd with antioxidant enzymes. SOD binding sites with Cd were GLU-121 and SER-142; CAT binding sites were amino acid residues of HIS-230, ASP-228, HIS-181, HIS-109 and ASP-178; GSR binding sites were HIS-503 and TYR-502.