HEAVY-METAL BINDING AFFINITY IN METALLOPROTEINS: A COMPUTATIONAL APPROACH

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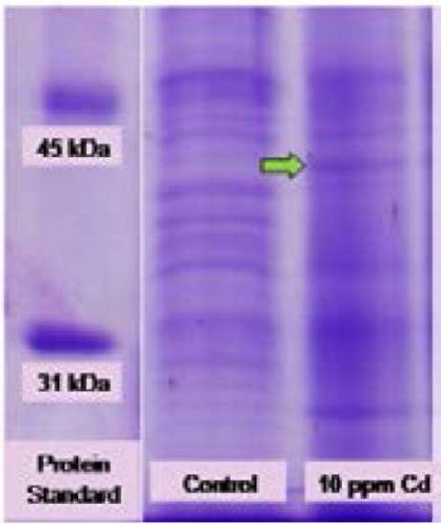
Introduction. The use of biological organisms for removal of heavy-metal *in situ* brings down the production cost due to the lesser pre-treatment steps in the removal process. Initial assessments of the heavy-metal binding bacteria from wastewaters, indicates that *Bacillus and Chryseomonas sp.* exhibited positive growth response behavior when exposed to lead and cadmium [1]. This incorporation of the heavy-metal species leads to the increase in the molecular mass of the protein as shown in the SDS-PAGE result (Figure 1). In this research, two metal-binding proteins of *B. subtilis* 1C7I and 1P3J were analyzed and optimized using DFT method to look into the possibility of replacement of heavy metals (Cd, Cr, Hg, and Pb) in its metal active sites.



Figurel. Protein Profile of *Chryseomonas sp.* in 10% SDS-PAGE.

Materials and methods. X-ray structures of 1C7I and 1P3J proteins were recovered from protein data bank (www.rcsb.org). Metal binding sites were optimized using density functional theory with B3LYP/LANL2DZ theoretical methodology without symmetry constraints. Frequency calculations were done using the same theoretical methodology to make sure the structures are stable. Excited-state energies were calculated using time-dependent DFT in water with conductor-like polarized continuum model framework.

Results and discussion. The electronic structures of the Ca-binding site of 1C7I protein and Mg- and Zn-binding sites of 1P3J protein from *B. subtilis* were fully optimized using DFT methodology. Figure 2 represents the most stable conformation of the Ca-binding site of 1C7I protein. Replacement of heavy metals in the metal binding sites indicated that Cd, Cr, and Hg forms thermodynamically stable structures compared to its original geometries. The changes of the metal species can be monitored by the changes in the absorption spectra.

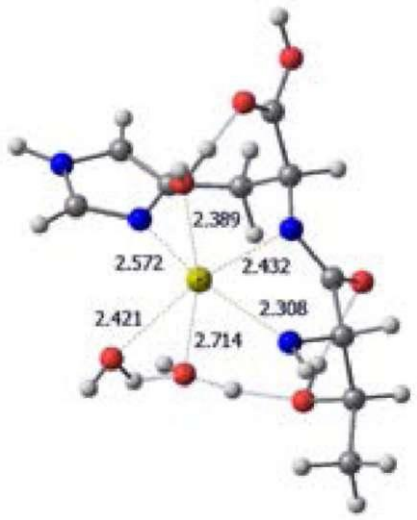


Figure 2. Ground-state geometry of Ca-binding site of 1C71 protein.

Conclusions. The results show that heavy metal substitution in metal binding sites of protein can form stable conformations suggesting the heavy-metal binding to these proteins. This study also presented the relative affinity of the heavy-metals to the metal-binding sites.

Acknowledgments. The author would like to thank Prof. Dong Hee Kim, Molecular Structural Laboratory, Department of Chemistry, Kunsan National University, Gunsan, Jeonbuk, Republic of Korea for the use of the computational facilities.

Reference

1. M.P. Balanay, M.S. Mahinay, A.B. Balala, A.P. Rivera, A.C. Daquinag. *Kimika.* 22 (2006) 87.