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Ab Initio MO Studies of the Weak Interaction in Cu-Histamine-Tyrosine Complex as an Model of Pseudoazurin M16Y Mutant

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Noncovalent weak interactions play important roles in biological systems. Hydrogen bonding and aromatic ring stacking interactions are well established weak interaction in the structure and function of proteins and nucleic acids. Recently, the biological significance of a weak interaction between metal ion coordinated imidazole ring and the phenyl ring of a phenylalanine residue has been found in plastocyanin from fern plant. We reported the spectroscopic and electrochemical studies of the M16F mutant of a blue copper protein, pseudoazurin to investigate the effects of the aromatic ring stacking interaction. The Met16 mutants of pseudoazurin variant, in which several alkyl and aromatic groups are introduced in the vicinity of the His81 imidazole ligand, have been constructed and characterized in order to probe more detailed roles of the stacking interaction on the structure and function of blue copper active site.

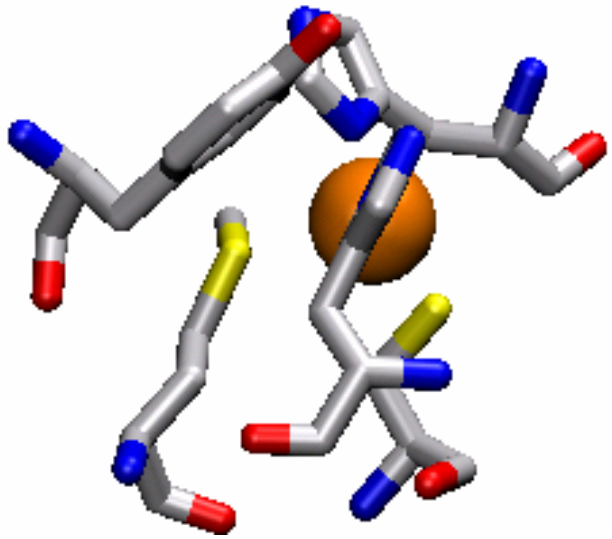

Figure 1.Model system of M16Y

The aromatic ring stacking interaction of a ternary Cu-histamine-tyrosine complex as an model of wild type pseudoazurin M16Y and its mutant was investigated by ab initio MO method with LANL2DZ basis set to elucidate the detailed effect of the interaction between imidazole of histamine and the phenol moiety of tyrosine.According to the coordination on Cu, the p- p interaction between imidazole of histamine and the phenol moiety of tyrosine is enhanced by hyperconjugation.