Computing the Redox Potential of the Copper-N_2S_2 Site in Methanobactin Using Quantum Mechanical/Molecular Mechanical Simulations

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The metal complexing polypeptide, Methanobactin, is found in the methane fixing bacteria *Methylosinus trichosporium.* Secreted by the bacteria into their environment, Methanobactin binds to Cu(II) and spontaneously reduces it to Cu(I), facilitating the bacteria's metal uptake. Previous research has been performed to establish the structure of the enzyme that exhibits copper center with N_2S_2 donor set. Yet, there is still a lack of understanding of the source of the electrons involved in the reduction. In the present study, efforts have been made to establish a procedure for properly modeling the Methanobactin system by standardizing calculations with Methanobactin analogs with known redox potentials. These studies include density functional theory based calculations on several copper containing small molecules in nitrogen-sulfur donor environments. Calculations are then extended to the Methanobactin system using quantum mechanical/molecular mechanical (QM/MM) setup. Results of the study provide an insight into the change of geometry of the redox center and the energetics of the electron transfer process.