

Molecular Dynamics Studies of Ni(II)-containing Methyl Coenzyme M Reductase

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Ni(II)-containing coenzyme F430 catalyzes the final step of methanogenic process by producing methane gas and a heterodisulfide(CoM-S-S-HTP) compound. Methyl CoM reductase system consists of $\alpha_2\beta_2\gamma_2$ dimer (MW=300,000 dalton) with two catalytic active sites. F430, Methylated Coenzyme M, a reducing agent HS-HTP are major novel enzymes involved in methane production via activated square pyramidal organic-nickel complex. For the detail molecular dynamic studies of the F430-dependent methyl reductase system, the catalytic processes were divided into three substeps including a initial state, an activated complex formation via the change oxidoreduction state of Ni(II)-containing corphinoid, and the termination of catalytic process. The detail conformational changes monitored in molecular dynamic computations and NMR observations for F430 are discussed to assess the mechanistic pathway in detail.