

Computational design of artificial metallo-haloalkane dehalogenase

ABSTRACT

Haloalkane dehalogenases (HLDs) can catalyze conversion of some toxic haloalkanes to corresponding harmless alcohols. The limiting factors of native HLDs are their slow product releasing step, low activity against non-natural substrates and synthetic substrates. By creating an artificial metallo-HLD might provide solutions for these problems as metalloenzymes can provide certain advantages like high turnover rate, better stabilization of substrate-enzyme docking and broader substrate specificity. Metallo-HLDs are expected to carry out hydrolysis of haloalkane in 1 step catalysis and with higher K_M . Nowadays, computational studies have been improved and commonly used by researchers to validate some structural designs before engineer the proteins in the lab. Computational studies using molecular dynamic simulation software and online molecular tools had largely increase the rate of success in protein engineering. In this work, through the computational design starting from template and metal binding site selection, *in silico* mutation, *in silico* metal docking, several validation of metal binding site and *in silico* docking of substrates had successful created 2 model of metallo-HLDs. These computational approaches had been validated using native metalloenzyme and functional artificial metalloenzyme as positive controls.

Keyword: Metallo-haloalkane dehalogenase; Artificial metalloenzyme; Haloalkane dehalogenase; Computational design; Molecular dynamic simulation