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Original article

Exploring particulate methane monooxygenase (pMMO) proteins using experimentation and computational molecular docking

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ABSTRACT

Researchers had difficulty studying pure full-length pMMO due to the solubility problem and loss of enzymatic activity after its elimination from the native membrane. To study pMMO, we performed several bioinformatics tools to analyze the entire structure of it available in the PDB database. We also carried out molecular docking studies to prove that quinone and duroquinone can bind to several sites of eight pMMO proteins. However, some sites in the orientation are not required by the catalysis process. Furthermore, molecular docking was done for predicting the binding affinity of P450 with target enzymes. Interestingly, our analysis illustrated that pMMO can produce methanol in the presence of quinone and duroquinone and the absence of Cu. Moreover, pmoB1 can interact with P450. Consequently, our findings highlight, for the first time, the significance of studying the membrane of pMMO to provide valuable insights into its functions.

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1. Introduction

Sustainable energy is arguably a very important challenge to society. (Hanson and Hanson 1996, Park et al., 2002). Methanol production is a standard outlet for natural gas. The production of methanol from methane has been receiving much attention for a long time and is still ongoing by various methods (Fig. 1). Effective production of methanol from methanotrophs requires inhibition of methanol dehydrogenase (MDH) (EC 1.1.1.244) to stop further methanol oxidation. The oxidation of methanol is required to generate reduction equivalents. Thus, inhibiting MDH needs the addition

of an external reducing counterpart to drive methane oxidation. Generally, most studies focus on utilizing methane monooxygenase (MMO) (EC 1.14.13.25), but other choices include the use of ammonia-oxidizing bacteria (Ge et al., 2014). The toxicity of methanol to methanotrophic bacteria is a likely challenge that is often discussed for commercialization.

Methanotrophic bacteria use methane and convert it to methanol in the first step of their metabolic pathway; Methane is known as a considerable greenhouse gas (Hanson and Hanson 1996). Methanotrophs are gram-negative bacteria belonging to the phyla Proteobacteria and Verrucomicrobia, they are divided into three groups, Type I (also known as Gammaproteobacteria), Type II (Alphaproteobacteria) methanotrophs, and Verrucomicrobia. The methanotrophs convert methane to methanol, which is present in particulate or soluble form, and the MDHs catalyzed methanol to formaldehyde. After two more oxidation steps, the final intermediate products are used for carbon assimilation (Guerrero-Cruz et al., 2021). As the most important methane sinks in nature, these methanotroph bacteria are hopeful biological tools for bio-fuel production as well as methane remediation (Fei et al., 2014, Kalyuzhnaya et al., 2015, Lawton and Rosenzweig 2016). These

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