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Modelling of a Biocatalytic Unit for Efficient CO2 Conversion to Formate Based on Enzyme Crystal

Global warming and climate change are directly related to increased atmospheric CO2 levels, which are currently higher than ever and continue to growth. Current strategies for CO2 reduction are mainly emission mitigation strategies, so that the rate of increase of global CO2 emissions from fossil resource utilization has slowed recently. However, utilizing CO2 as a carbon source for production of high-in-demand chemicals could represent a win-win strategy by both replenishing fossil-fuel processes and simultaneously assisting in mitigating CO2 accumulation and climate change. In the field of enzymatic reactions, formate dehydrogenase (FDH), that catalyses the interconversion between CO2 and formic acid through an oxidoreductive process, could represent a suitable biomimetic catalyst for effective and sustainable CO2 fixation and direct conversion into formate. The overall goal is to develop a new bio-enabled material capable of effective conversion of CO2 to alternative fuels and chemicals, where the complex chemical processes carried out in bacteria or living cells are reproduced by a biomimetic artificial system composed of individual enzymes in their active form, closely packed to reach the highest possible density and embedded into bacterial-like coats able to preserve the enzymes in working conditions. The crystallographic structures derived from different organisms with similar sequence, but essentially different characteristics, were examined; the most significant difference concerns the presence (metal-dependent) or absence (metal-independent) of metal in the cavity. Among the metal-containing FDHs, five were found to be unaffected by the presence of oxygen. Among them, that with pdb entry 8J83 is the only one characterized structurally by crystallography and has an alpha domain containing the active site and a beta domain, which serves for NAD docking and is called a diaphorase unit.[1] The metal ion, W, in the active site is coordinated by six ligands in a trigonal prismatic geometry. The rectangular base of the prism is formed by the two dithiolene groups of the bis-MGD (metal-binding pterin guanine dinucleotide cofactor). The other two sites are ligated by the cysteine sulfur and oxygen (Figure 1). A series of alpha domain variants was analysed to select that exhibiting the best compatibility with the beta domain of the 8j83 protein and then, exploiting the system for in silico study of the catalytic process for CO2 conversion into formate.

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