IN-SILICO BASED REDESIGN OF CO-DEHYDROGENASE CATALYZING THE OXIDATION OF TOXIC WASTE CO GAS FOR IMPROVED O_2 RESISTANCE AND MEDIATOR AFFINITY

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Carbon monoxide (CO) harmful to most creatures, is largely discharged by industrial processes in steel mill and thermal power plant. Conversion of toxic waste CO gas to safe gas or more valuable chemicals will be a great worth at this point. Interestingly, carbons and high potential electrons from CO-oxidation can be resourced as essential core parts for the chemical products by using CO-dehydrogenase (CODH) and artificial mediator. For industrial application of the enzymatic CO-oxidation, however, key issues remain that most CODHs show oxygen (O_2) sensitivity and low-affinity for artificial mediator. Because steel mill waste gas such as blast furnace gas (BFG) commonly contains a little O_2 and higher affinity is required to achieve higher reaction rate.

In this research, *in-silico* based approach was used to redesign *Carboxydothermus hydrogenoformans* CODH (*Ch*CODH) II, capable of increasing O_2 resistance and affinity to ethyl viologen (EV) mediator. *Ch*CODHs belong to a group of Ni-Fe containing CODH. Among five known *Ch*CODHs (*Ch*CODH I-V), *Ch*CODH II shows the highest activity toward CO but more O_2 sensitive than *Ch*CODH IV. The artificial mediator of EV functions as an electron acceptor for *Ch*CODH II but the affinity of *Ch*CODH II to EV mediator is known poor. As our result, more than 10 folds increase of O_2 resistance was achieved for the redesigned *Ch*CODH II enzyme, which will be definitely a working horse in the conversion of waste CO gas into value-added chemicals.