

# Title

A Bio-Inspired Catalyst for Carbon Dioxide Reduction based on the  $(\beta\alpha)_8$  Protein Structure

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## Abstract

Efficient storage of solar energy is critical for the next generation of solar energy conversion systems. Herein is described a bio-inspired catalytic module, using the robust  $(\beta\alpha)_8$  TIM barrel fold of the EutB subunit of ethanolamine-ammonia lyase (EAL), for high specificity recognition and light-driven reduction of  $\text{CO}_2$  to energy rich biofuels, such as formate. In vivo, EAL catalyzes the deamination of ethanolamine via a free radical mechanism, by using an adenosylcobalamin (AdoCbl) cofactor. Our aim is to use the reducing power of Co(I) in cobalamin to drive the reduction of  $\text{CO}_2$ . To this end, molecular biology techniques have been used to isolate the EutB and EutC subunits of EAL and to attach histidine tags to these subunits, for high throughput protein production and purification. The binding of AdoCbl and other cobalamins to EutB was probed by using measurements of the endogenous tryptophan fluorescence quenching. Using a Hill model, the Hill constant ( $K_H$ ) and coefficient ( $n_H$ ) for AdoCbl-EutB binding were found to be  $40 \mu\text{M}$  and 0.7, respectively. Cyano-Cbl displays comparable binding parameters ( $70 \mu\text{M}$ , 1.0). The results show that Cbl in the Co(III) state binds to the isolated EutB subunit, and suggest that Co(II) and Co(I) states will also be bound. Rational active site modifications of EutB will be made to facilitate specific  $\text{CO}_2$  binding to Co(I) in the  $\eta^1\text{-C}$  mode, and to introduce a proton delivery network. The catalytic site design is informed by  $\text{CO}_2$  binding strategies used by natural proteins. The results will give insight into the challenging task of rational enzyme design, and also have implications for carbon neutral energy storage.