

Examining Bioethanol-Producing Ultrastructures with Electron Microscopy and Molecular Dynamics

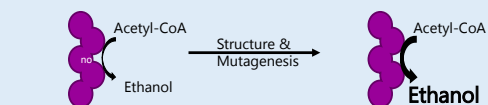
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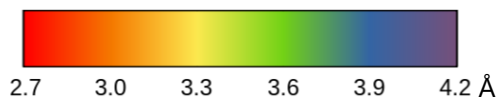
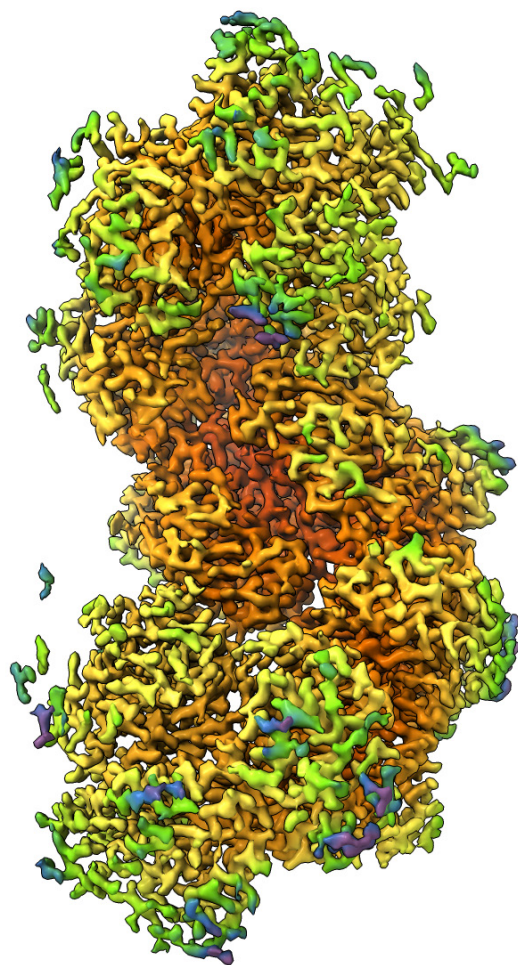
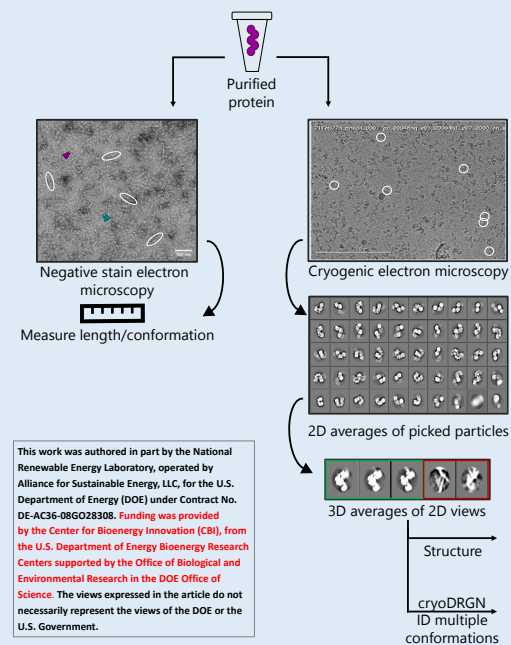
Mutagenesis of the AdhE spiroosome to improve ethanol production is confounded by native ultrastructure flexibility of conformation

Background

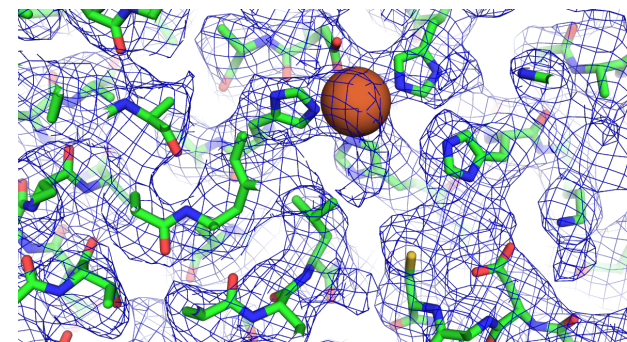
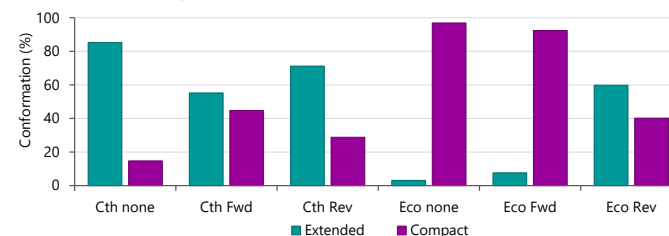
AdhE makes ethanol and other long chain alcohols in consolidated bioprocessing organisms like *Clostridium thermocellum*. *C. thermocellum* is an ideal microbe because it effectively degrades cellulose, so we only need to amplify its biosynthesis of ethanol. Our aim is to improve alcohol production and tolerance by determining the *C. thermocellum* AdhE atomic structure in multiple conformations to understand its chemical mechanism and guide mutagenesis.



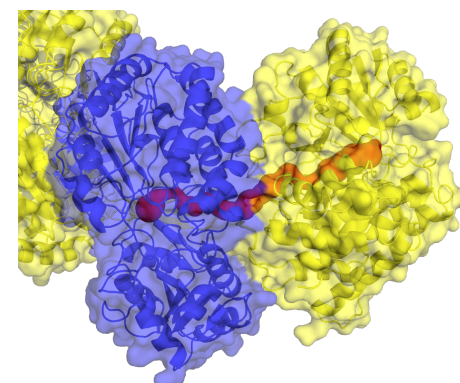
Graphical Methods



Spiroosome Conformation Prevalence



Density of the iron-coordinated active site of the alcohol dehydrogenase domain



Enclosed channel between the aldehyde dehydrogenase and alcohol dehydrogenase domains of two AdhE molecules



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