Visualizing the gas channel of a monofunctional carbon monoxide dehydrogenase

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Carbon monoxide dehydrogenase (CODH) plays an important role in the processing of the one-carbon gases carbon monoxide and carbon dioxide. In CODH enzymes, these gases are channeled to and from the Ni-Fe-S active sites using hydrophobic cavities. In this work, we investigate these gas channels in a monofunctional CODH from Desulfovibrio vulgaris, which is unusual among CODHs for its oxygen-tolerance. By pressurizing D. vulgaris CODH protein crystals with xenon and solving the structure to 2.10 Å resolution, we identify 12 xenon sites per CODH monomer, thereby elucidating hydrophobic gas channels. We find that D. vulgaris CODH has one gas channel that has not been experimentally validated previously in a CODH, and a second channel that is shared with Moorella thermoacetica carbon monoxide dehydrogenase/acetyl-CoA synthase (CODH/ACS). This experimental visualization of D. vulgaris CODH gas channels lays groundwork for further exploration of factors contributing to oxygen-tolerance in this CODH, as well as study of channels in other CODHs.