Atomic Resolution Structures of Resting State, Substrate- and Product-Complexed Cu Nitrite Reductase Provide Insight into Catalytic Mechanism

Svetlana V. Antonyuk¹, Richard W. Strange¹, Gary Sawers², Robert R. Eady¹ & S. Samar Hasnain¹

¹Molecular Biophysics Group, CCLRC Daresbury Laboratory, Warrington, WA4 4AD, UK; ²Department of Molecular Microbiology, John Innes Centre, Norwich, NR4 7UH, UK

Cu-containing nitrite reductases catalyse the reduction of nitrite to nitric oxide, a key step in denitrification that results in the loss of terrestrial nitrogen to the atmosphere, are found in a wide variety of denitrifying bacteria and fungi of different physiology from a range of soil and aquatic ecosystems. Structural analysis of potential intermediates in the catalytic cycle is an important goal in understanding enzyme mechanism. Using ‘crystal harvesting’ and substrate-soaking techniques we have determined atomic or near atomic resolution structures of four forms of the Cu-nitrite reductase. These structures provide, for the first time, incisive insights into the initial binding of substrate, its repositioning prior to catalysis, bond breakage (O-NO) and the formation of the product.