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# Fingerprinting redox/ligand states and driving catalysis in protein single crystals

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Single crystal spectroscopic analysis may be used to gain a complete and accurate identification of the redox and ligation states of metal (redox) centres in protein crystals [1,2]. Combining this approach with controlled X-ray radiolysis can allow the generation and characterisation of functional species and intermediates [3].

Cytochrome c'(CYTcp) is a haem protein with the remarkable ability to discriminate between NO and CO by binding them to opposite faces of the haem while excluding O2 [4]. The binding of NO to CYTcp provides a model for the activation of soluble guanylate cyclase. We will describe the use of UV-visible absorption and resonance Raman spectroscopies to monitor radiolysis and 'fingerprint'key redox and ligand states in crystals of native and mutant CYTcp, from which high resolution crystal structures have been determined. We will also describe the radiolysis-driven conversion of substrate-to-product in crystals of copper nitrite reductase.

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4. Hough M. A. et al, (2011) J. Mol. Biol. 405, 395-409.

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