Supplementary Material

Structure and mechanism of Cu- and Ni-substituted analogs of metallo-β-lactamase L1

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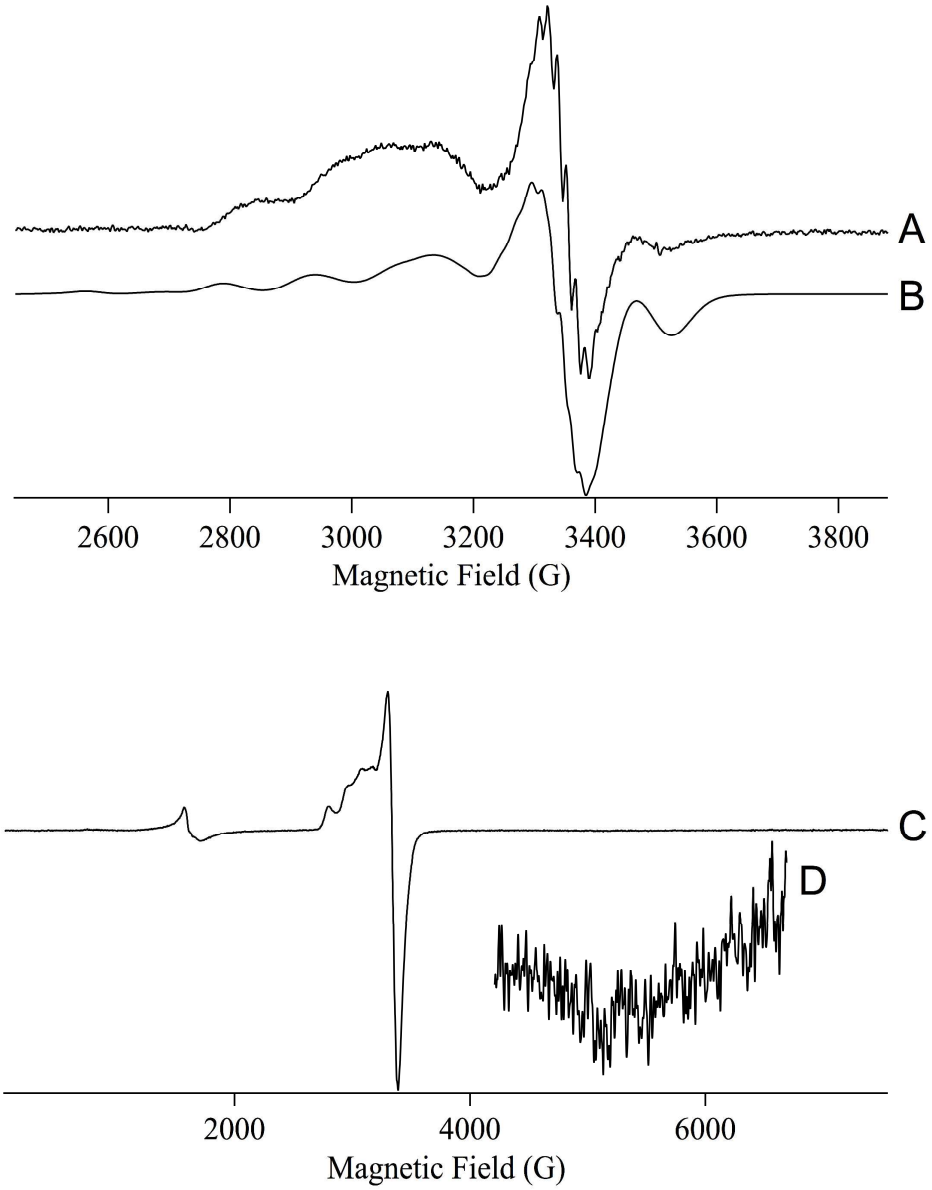

Figure S1. EPR spectra of Cu-L1. (A) difference spectrum generated by subtraction of the spectrum from Cu-L1 recorded at 0.1 mW, 10 K, from that recorded at 2 mW, 10 K. (B) Computer simulation assuming two Cu(II) ions with $g_{\parallel} = 2.284$, $A_{\parallel}(Cu) = 15.5 \times 10^{-3}$ cm^{-1}, $g_{\perp} = 2.055$, $A_{\perp}$ (Cu) = 1.10×10^{-3} cm^{-1}, and a Cu-Cu distance of 5 Å. The contribution of ^{14}N

superhyperfine was neglected in the simulation. (C) Experimental spectrum of Cu-L1 recorded at 2 mW, 10 K. (D) Expanded view of high-field region.