Supporting Information

for

Conserved Residue Modulates Copper Binding Properties through Structural Dynamics in Human Copper Chaperone Atox1

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Figure S1. Copper titration of the K60A mutant. (A) An overlay of ¹H-¹⁵N HSQC spectra of K60A mutant in the presence of 0 (black), 0.2 (red), 0.4 (green), 0.6 (blue) 0.8 (yellow) and 1 (magenta) equivalent of copper.



Figure S2. Copper transfer from Atox1 to MNK4. Panels show an overlay of ${}^{1}\text{H}{-}{}^{15}\text{N}$ HSQC spectra of Cu-Atox1 (A) or Cu-K60A (B) in the presence of 0 (cyan), 0.25 (red), 0.5 (green), 0.75 (blue) and 1 (magenta) equivalent of unlabeled apo-MNK4. Panels also show an overlay of ${}^{1}\text{H}{-}{}^{15}\text{N}$ HSQC spectra of apo-Atox1 (black) and Cu-Atox1 (red) in the presence of 1 equivalent of unlabeled apo-MNK4. (C) the wild-type Atox1; (D) the K60A mutant.



Figure S3. Copper transfer from wild-type Atox1 or K60A mutant to MNK4. Panels show an overlay of selected regions of ¹H-¹⁵N HSQC spectra of Cu-Atox1 (A) and Cu-K60A (B) in the presence of 0 (cyan), 0.25 (red), 0.5 (green), 0.75 (blue) and 1 (magenta) equivalent of unlabeled apo-MNK4.