Supporting Information for

Copper binding modulates the platination of human copper chaperone Atox1 by antitumor trans-platinum complexes

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Fig. S1 Plots of the concentration of unreacted trans-EE versus time for the reactions between Atox1 and trans-EE in the absence (black square and line) and presence (red circle and line) of copper.
Fig. S2 Selected ESI-MS spectra of platinated peptides from trypsin digestion of Atox1. Protein samples were treated with trans-EE for 4 h prior to the trypsin digestion. (A) apo-Atox1; (B) Cu\textsuperscript{1}-Atox1. The isotopic distributions of the e1 peak (the most abundant isotopomer at m/z 743.70, [P2+Pt(Ime)\textsubscript{2}+H\textsuperscript{3+}]) and e2 peak (the most abundant isotopomer at m/z 746.63, [P1+Pt(Ime)+H\textsuperscript{3+}]) are well consistent with the simulated patterns (C) and (D). P1 and P2 represent the peptides H\textsuperscript{4}EFSVDMTC\textsuperscript{12}GGC\textsuperscript{15}AEAVSR\textsuperscript{21} and V\textsuperscript{40}CIESEHSMDTLATLK\textsuperscript{56}, respectively.

Fig. S3 ESI-MS/MS spectra of the triply charged ion e2 at m/z 746.63 from trypsin digestion of (A) Atox1 and (C) Cu\textsuperscript{1}-Atox1 treated with trans-EE for 4 h. Fragmentation schemes based on the spectra (A) and (C) are shown in (B) and (D), respectively. The precursor ion is denoted in #. P1 represents the peptide H\textsuperscript{4}EFSVDMTC\textsuperscript{12}GGC\textsuperscript{15}AEAVSR\textsuperscript{21}.
Fig. S4 Platinum complexes induced protein aggregation monitored by tricine-SDS-PAGE. The protein samples were incubated with equimolar platinum complexes at 25 °C for different time before loading to the gel. Incubation time of the samples is 10 min, 30 min, 1 h, 2 h, 4 h, 8 h, 12 h and 24 h from left to right. (A) cisplatin + apo-Atox1. (B) cisplatin + CuI-Atox1. (C) trans-EE + apo-Atox1. (D) trans-EE + CuI-Atox1. (E) trans-PtTz + apo-Atox1. (F) trans-PtTz + CuI-Atox1.