Electronic Supplementary Material (ESI) for Metallomics

Supporting Information

for

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

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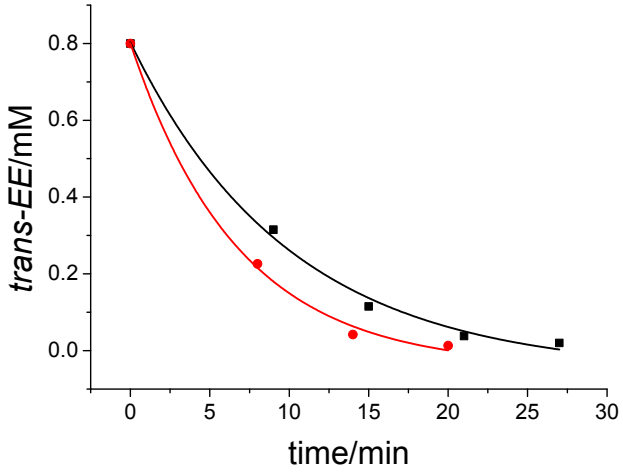

Fig. S1 Plots of the concentration of unreacted *trans-EE versus* time for the reactions between Atox1 and *trans-EE* in the absence (black square and line) and presence (red circle and line) of copper.

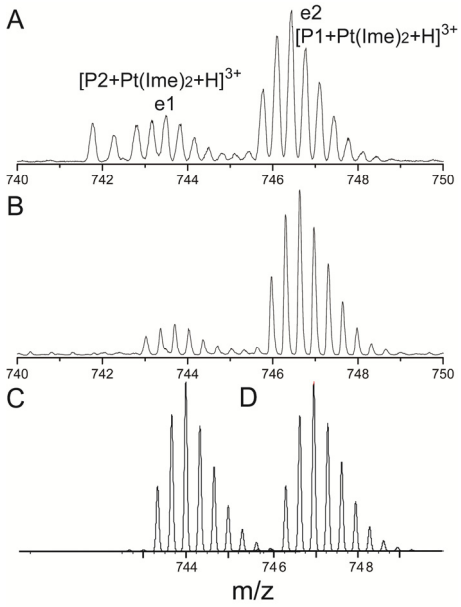

Fig. S2 Selected ESI-MS spectra of platinated peptides from trypsin digestion of Atox1. Protein samples were treated with *trans-EE* for 4 h prior to the trypsin digestion. (A) apo-Atox1; (B) Cu^{I}-Atox1. The isotopic distributions of the e1 peak (the most abundant isotopomer at *m/z* 743.70, $[P2+Pt(Ime)_2+H]^{3+}$) and e2 peak (the most abundant isotopomer at *m/z* 746.63, $[P1+Pt(Ime)_2+H]^{3+}$) are well consistent with the simulated patterns (C) and (D). P1 and P2 represent the peptides $H^{4}EFSVDMTC^{12}GGC^{15}AEAVSR^{21}$ and $V^{40}CIESEHSMDTLLATLK^{56}$, respectively.

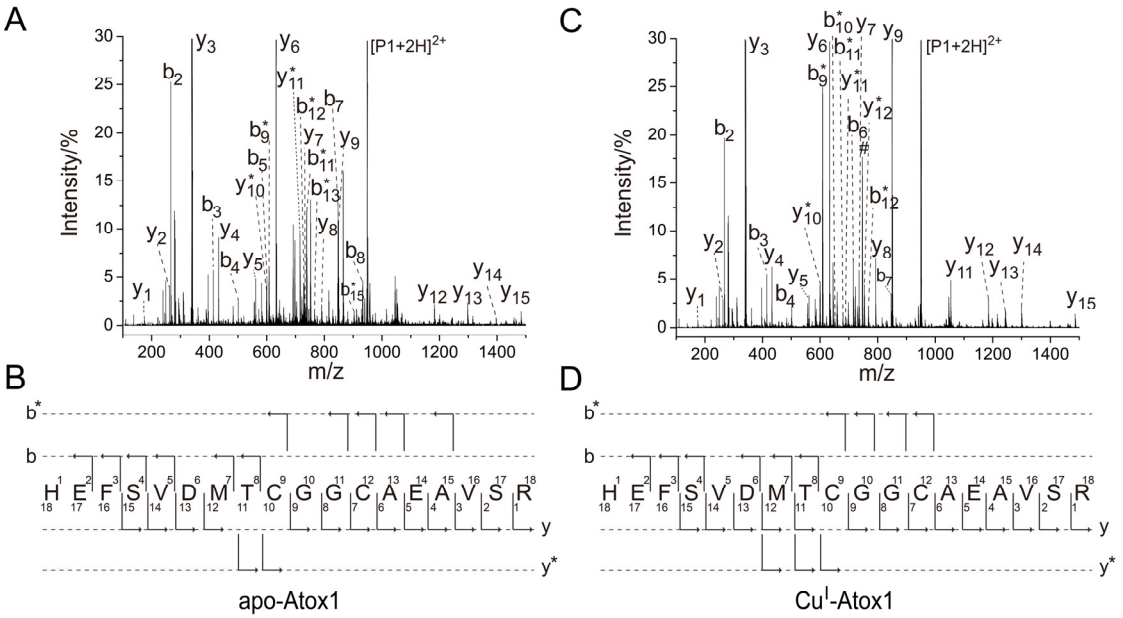

Fig. S3 ESI-MS/MS spectra of the triply charged ion e2 at *m/z* 746.63 from trypsin digestion of (A) Atox1 and (C) Cu^{I}-Atox1 treated with *trans-EE* for 4 h. Fragmentation schemes based on the spectra (A) and (C) are shown in (B) and (D), respectively. The precursor ion is denoted in #. P1 represents the peptide $H^{4}EFSVDMTC^{12}GGC^{15}AEAVSR^{21}$.

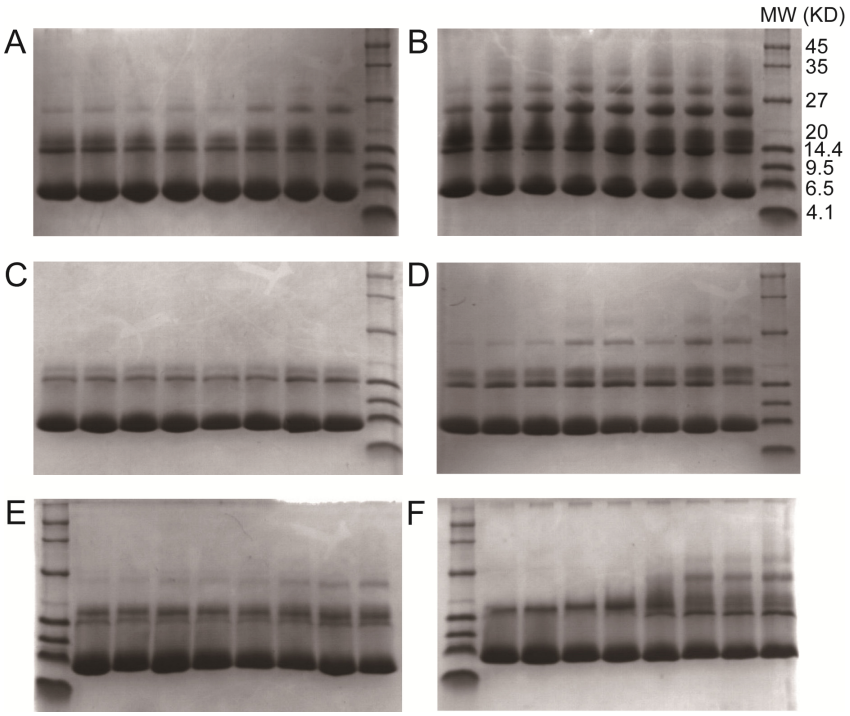

Fig. S4 Platinum complexes induced protein aggregation monitored by tricine-SDS-PAGE. The protein samples were incubated with equimolar platinum complexes at 25 °C for different time before loading to the gel. Incubation time of the samples is 10 min, 30 min, 1 h, 2 h, 4 h, 8 h, 12 h and 24 h from left to right. (A) cisplatin + apo-Atox1. (B) cisplatin + Cu^{I}-Atox1. (C) *trans-EE* + apo-Atox1. (D) *trans-EE* + Cu^{I}-Atox1. (E) *trans*-PtTz + apo-Atox1. (F) *trans*-PtTz + Cu^{I}-Atox1.