Electronic Supplementary Material (ESI) for Metallomics.

Supplementary information

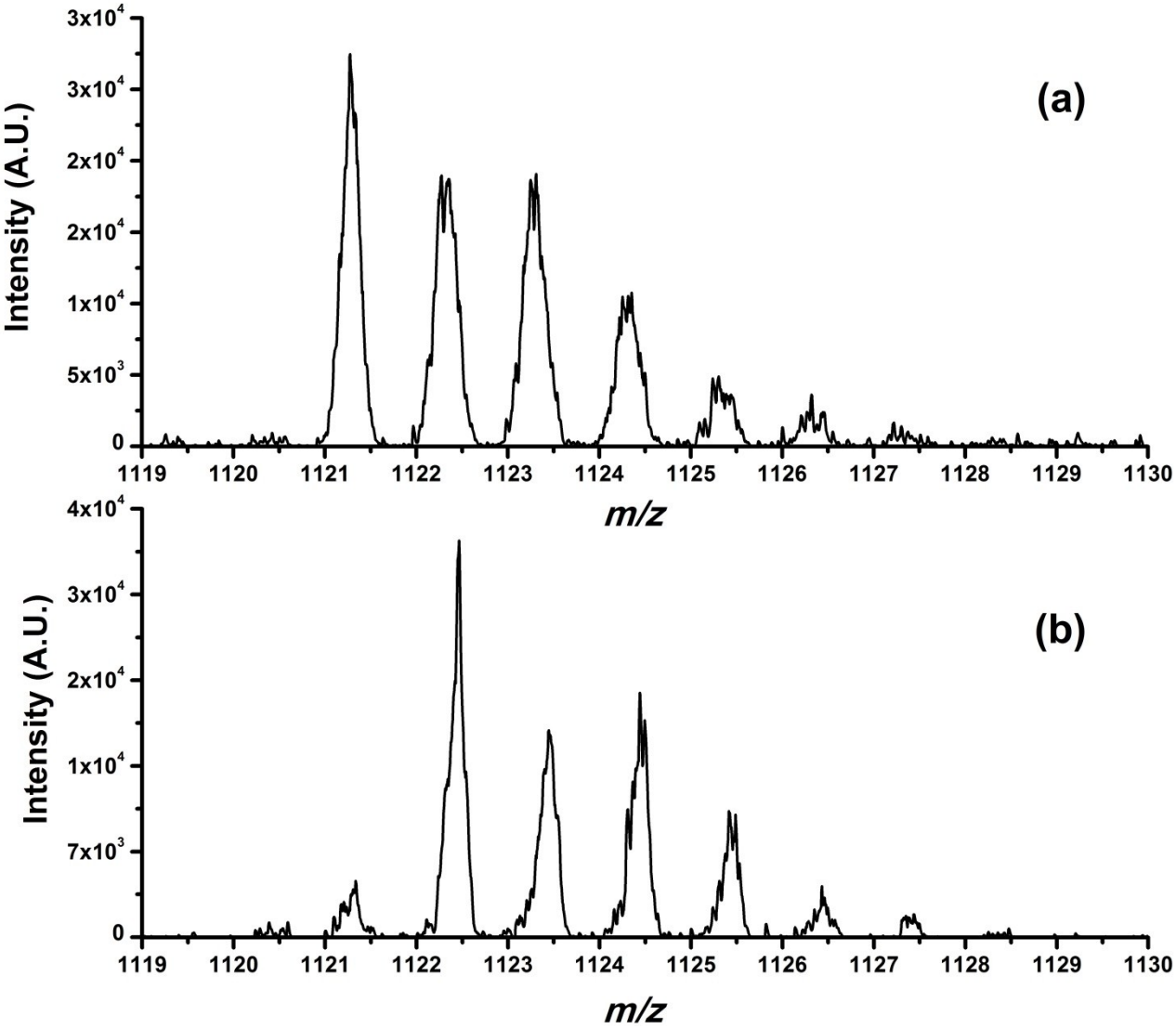

Figure 1S: +veESI mass spectrum of BK 1μM and $CuSO_4$ 1μM in water acquired in the Zoom Scan mode. Spray voltage was 0.8 kV in (a) and 4.3 kV in (b).

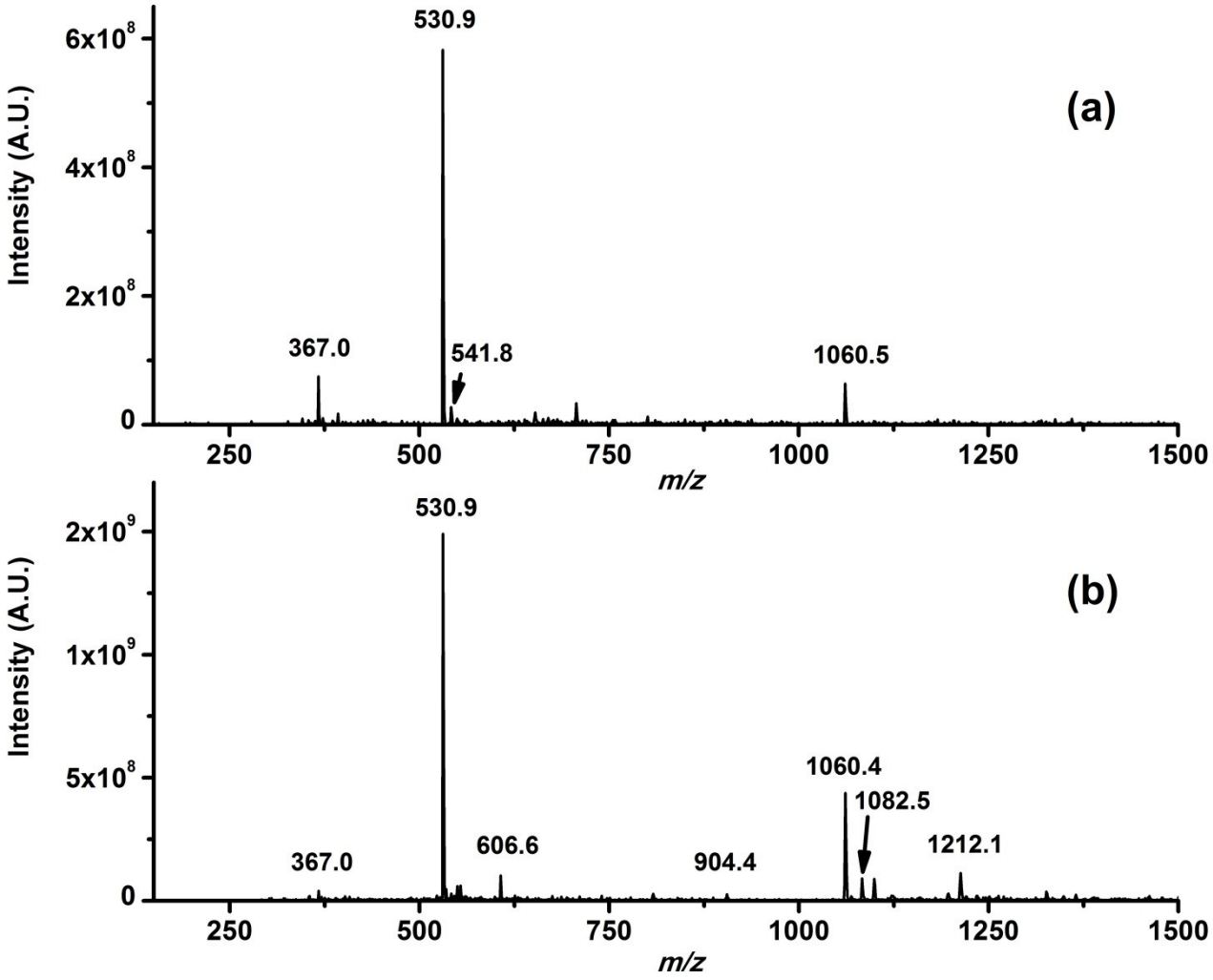

Figure 2S: +ve ESI mass spectrum of BK 1μM (a) and 30μM (b) in water. Mass range is m/z 200-1500, discussion is in the text.

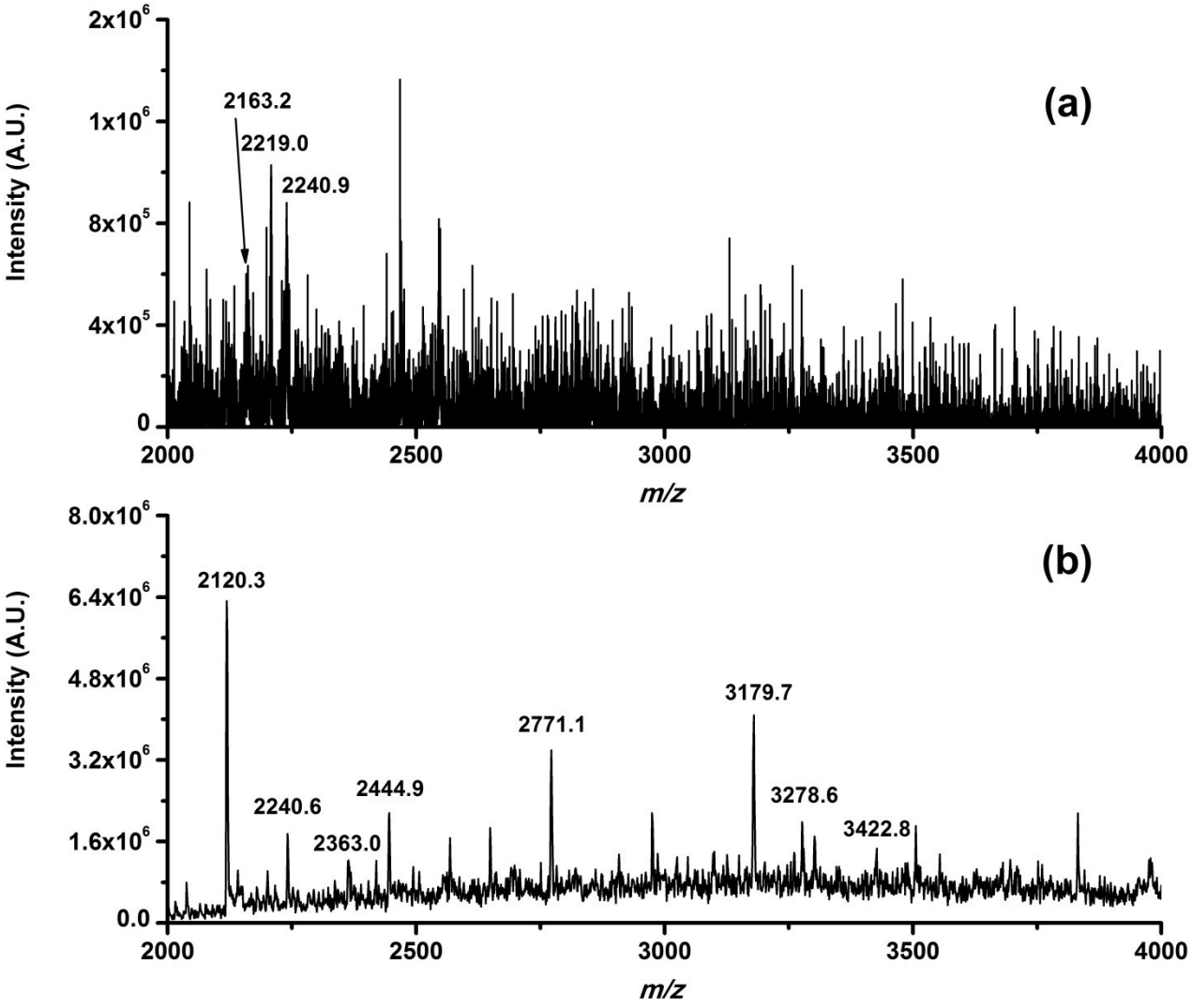

Figure 3S: +ve ESI mass spectrum of BK 1μM (a) and 30μM (b) in water. Mass range is *m/z* 2000-4000, assignment is reported in Table 1. Peaks that are not listed in the latter refers to multi-sodiated species.

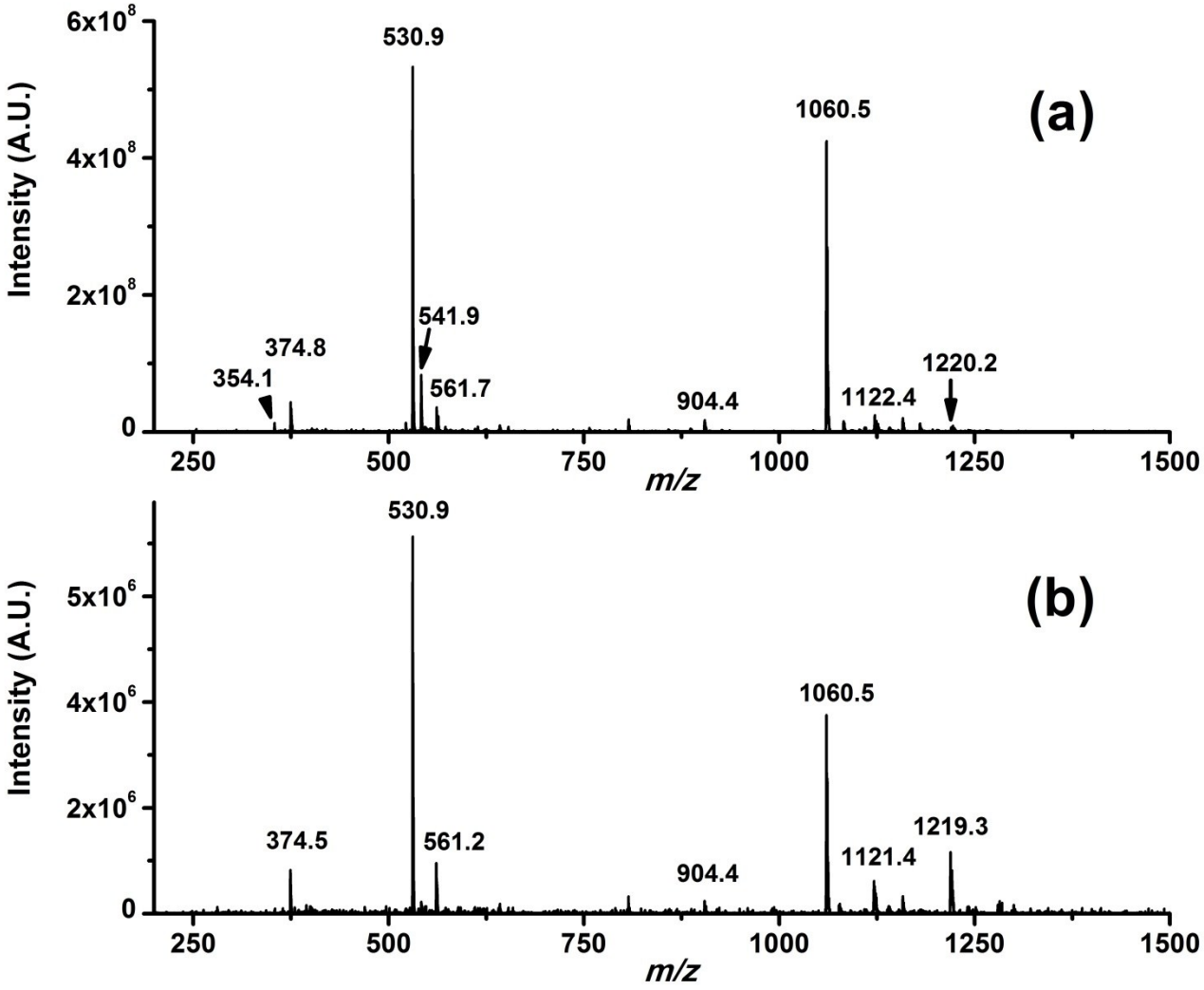

Figure 4S: +ve ESI mass spectrum of BK 30μM with $ZnSO_4$ 50μM (a) and $CuSO_4$ 50μM (b) in water, *m/*z range 200-1500. Assignment is in Table 1.

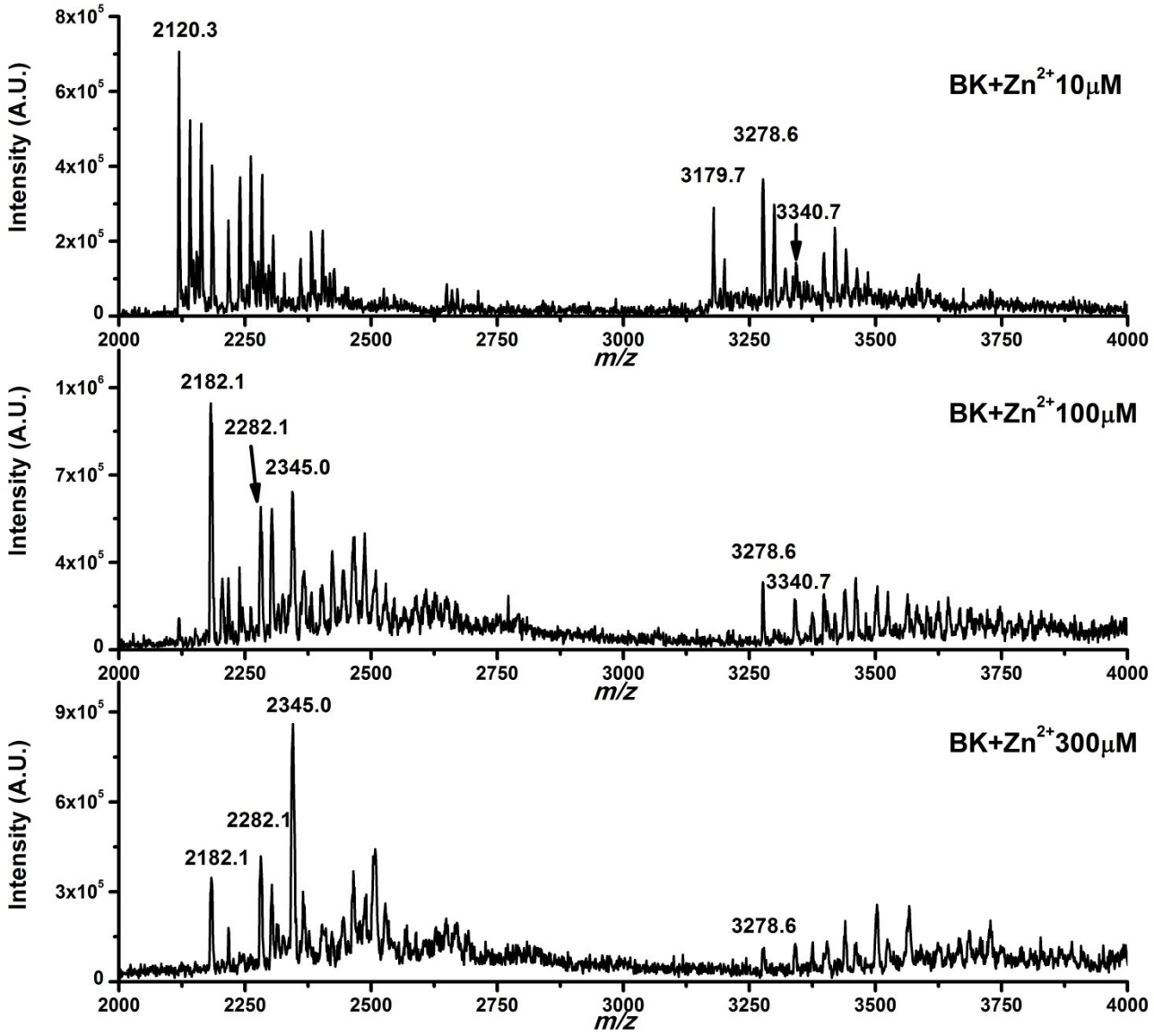

Figure 5S: +ve ESI mass spectrum of BK 30μM with $ZnSO_4$ in water at the indicated concentrations, *m/z* range 2000-4000. Assignment is in Table 1.

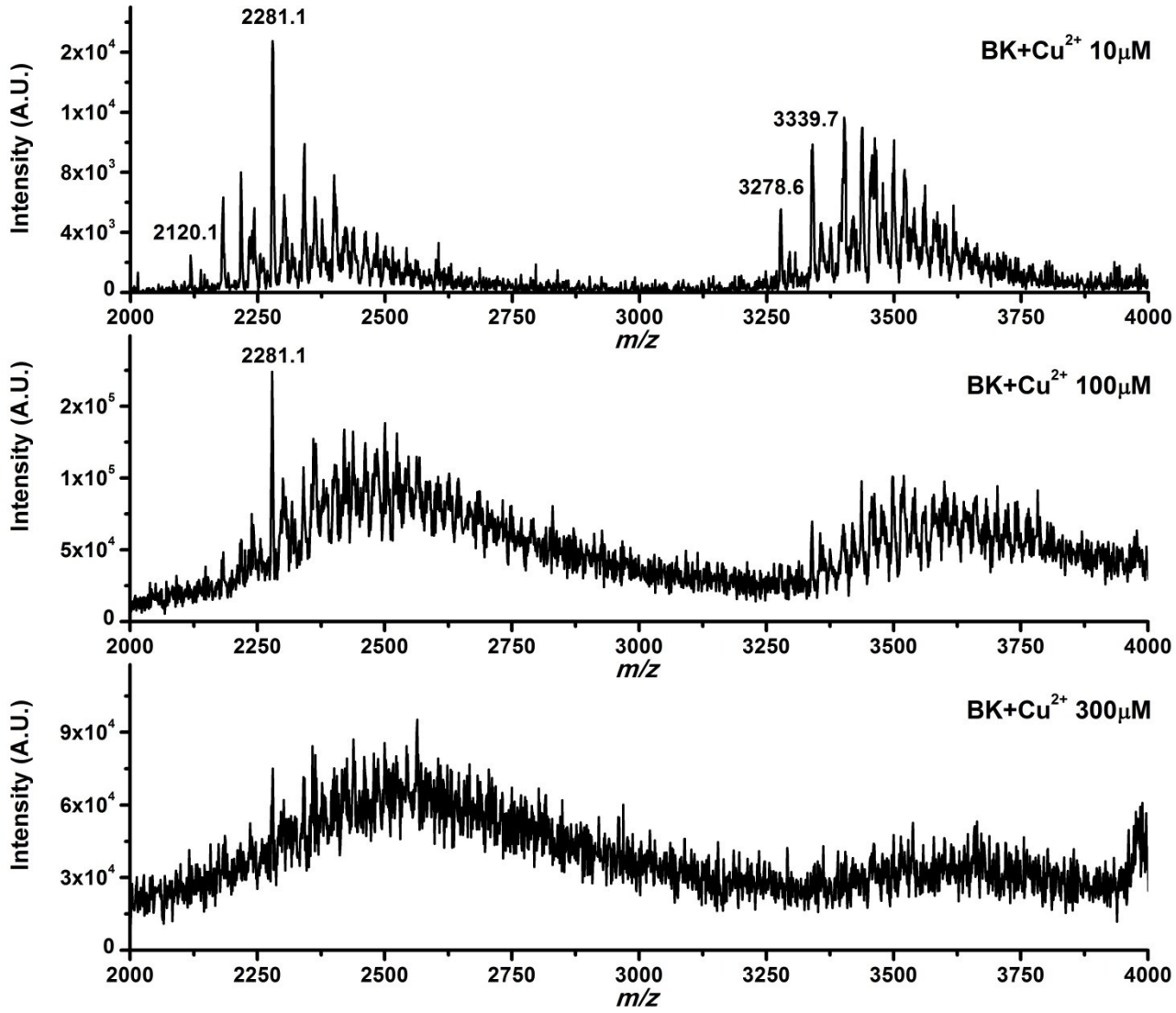

Figure 6S: +ve ESI mass spectrum of BK 30μM with $CuSO_4$ in water at the indicated concentrations, m/z range 2000-4000. Assignment is in Table 1.

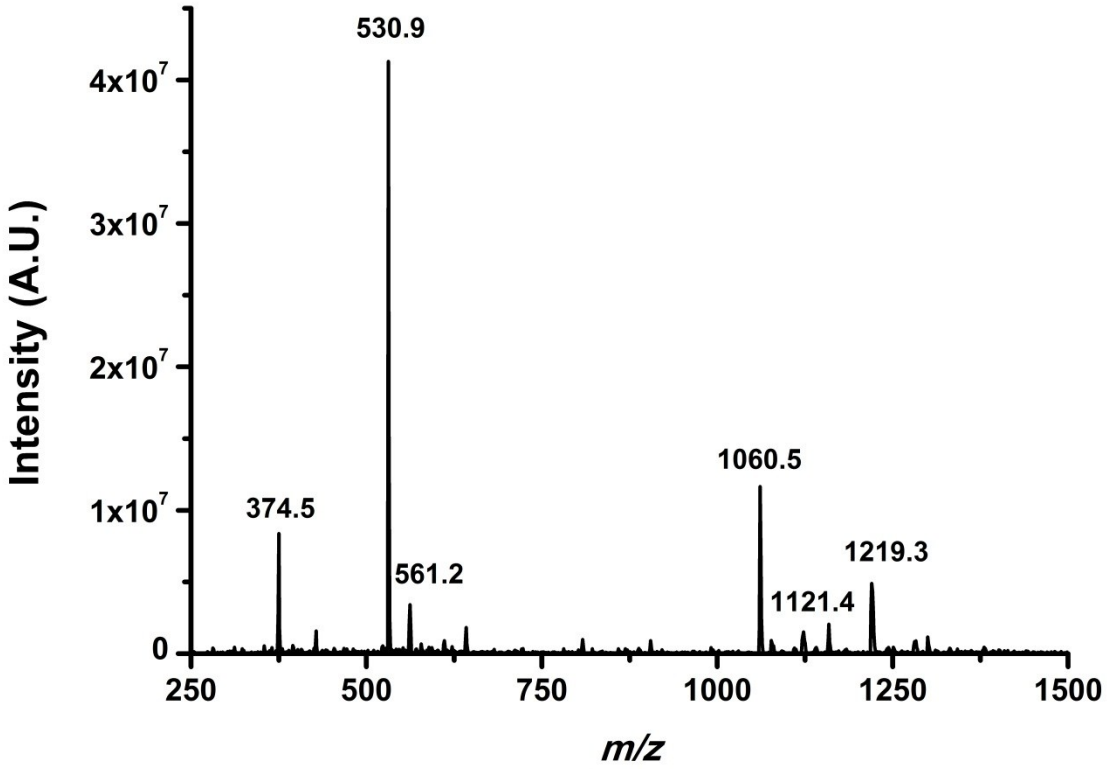

Figure 7S: +ve ESI mass spectrum of BK 30μM with $CuSO_4$ 300μM in water, *m/z* range 250-1500. Assignment is in Table 1.

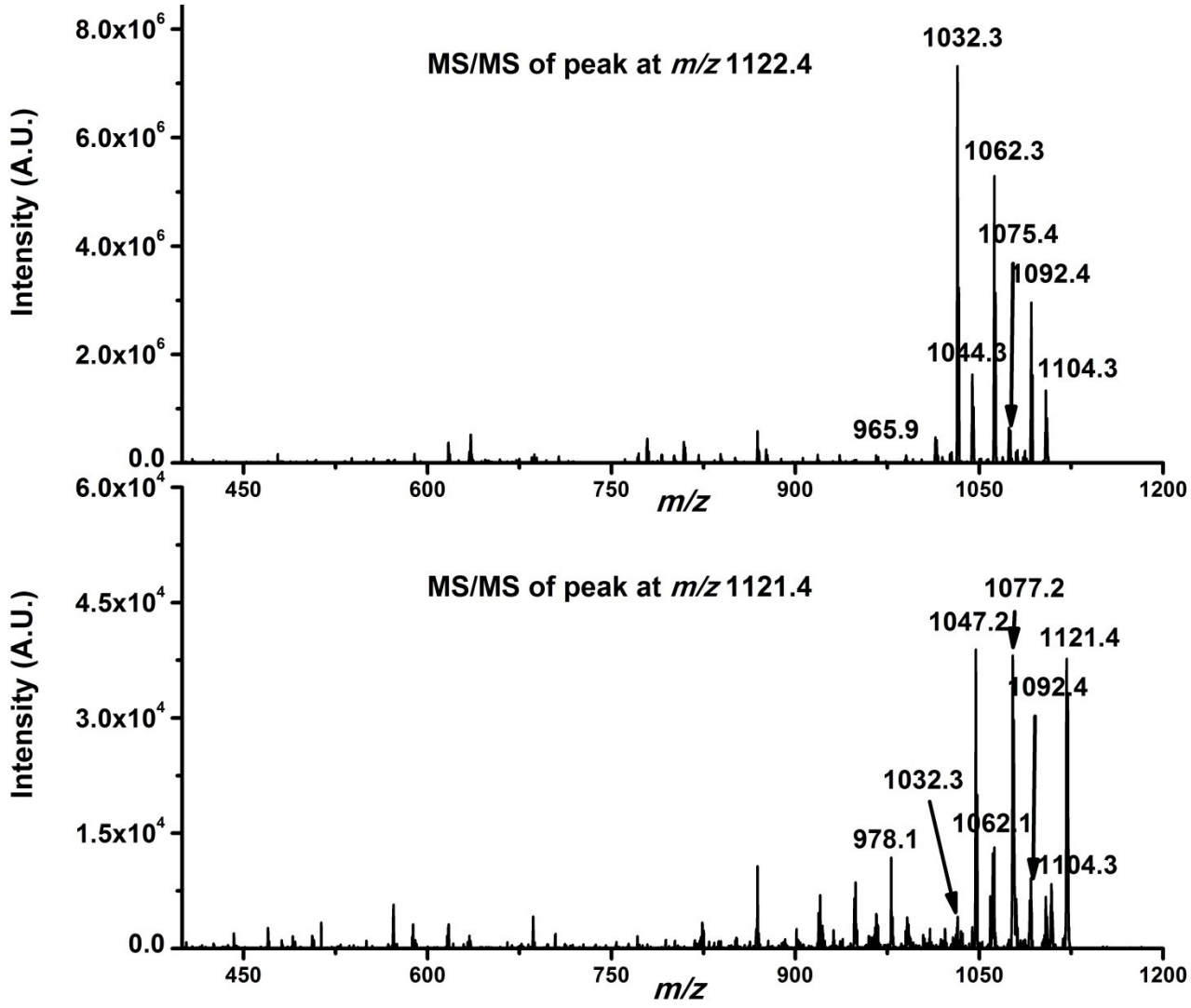

Figure 8S: MS/MS experiments for the BK-Zn (upper part) and BK-Cu (bottom part) molecular peaks. Differences in the spectra are interpreted as different coordination features of the two metal complexes, discussion is in the text.

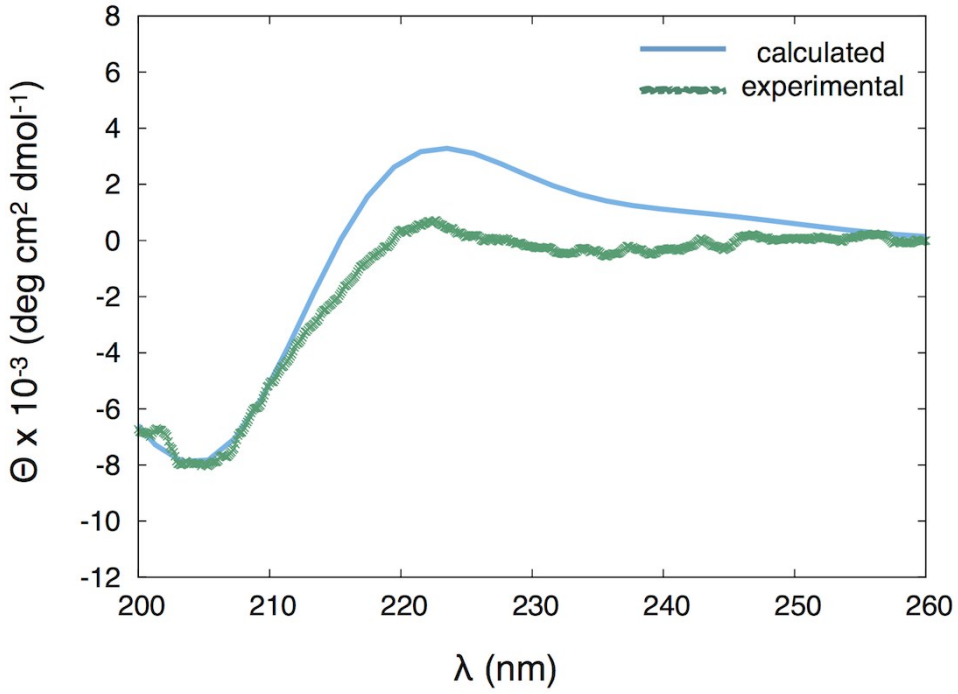

Figure 9S: Experimental and calculated CD spectra of BK. The spectrum was calculated as the average CD spectra of the two main clusters derived from Parallel Tempering simulations.

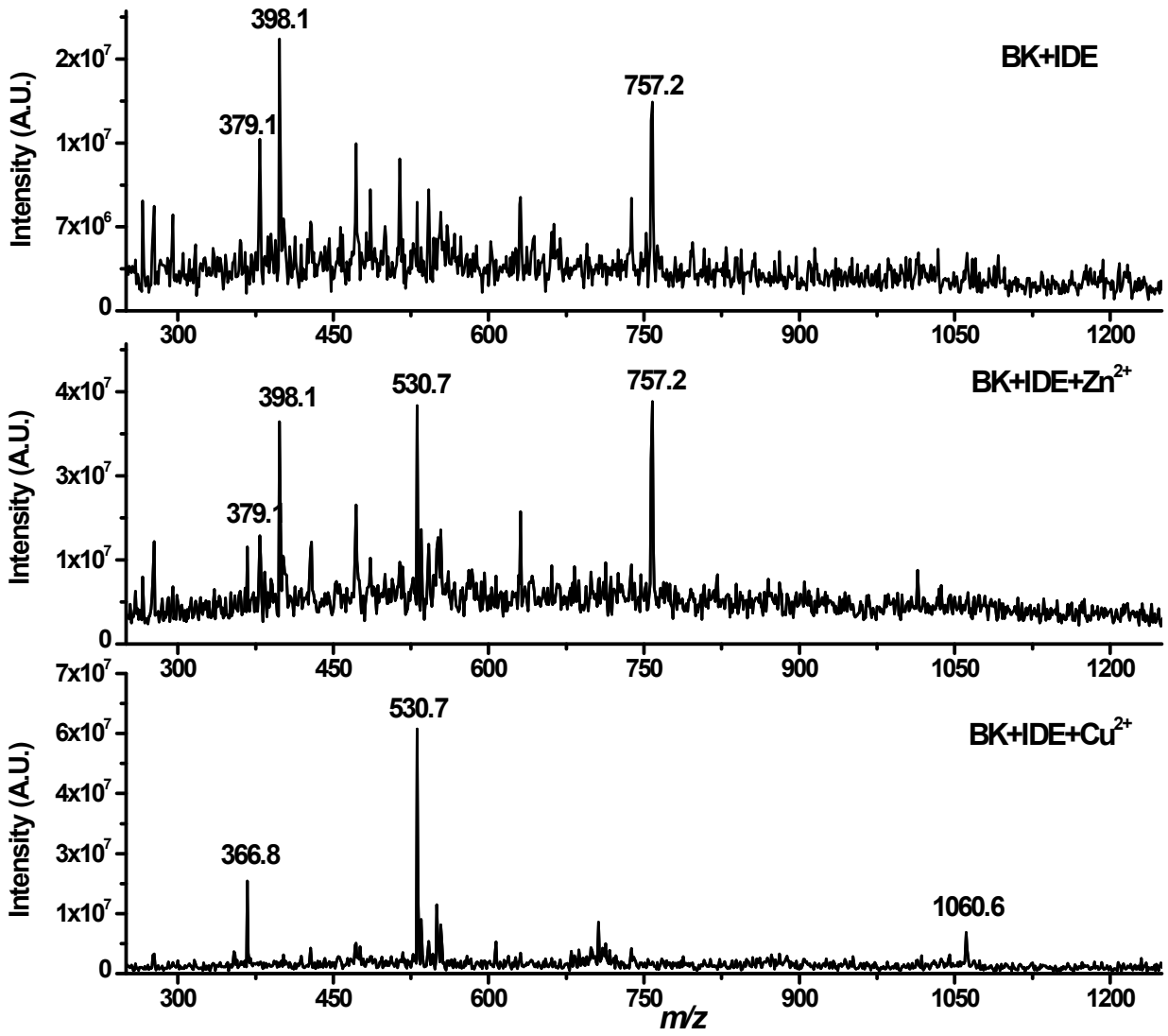

Figure 10S: BK fragmentation patterns after enzymatic digestion of IDE in the presence and in the absence of the indicated metal ions. The main fragment at *m/z* 757.2 has been assigned to the HArgProProGlyPheSerProOH fragment (confirmed by MS/MS experiments and in accordance with Ref. 10 of the manuscript). The main cleavage site of IDE on BK is therefore between Pro7 and Phe8.

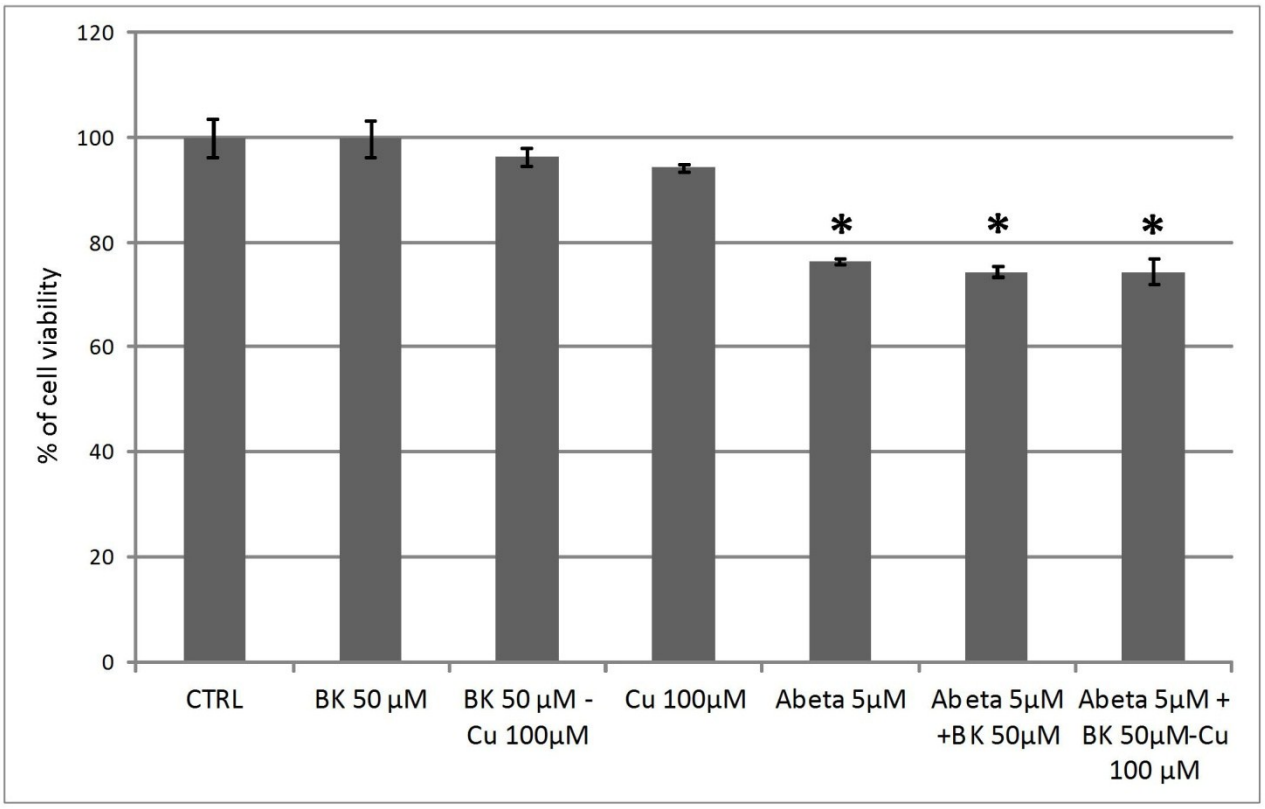

Figure 11S: Dose response experiment to test the cell viability after treatment with Aβ(1-42), BK, BK-Cu(II) and Cu(II). Neuroblastoma SH-SY5Y cells were incubated for 48hrs and then cell viability was measured using MTT assay. Aβ toxicity was not affected by treatment in the presence of BK. Results are presented as the means ± SEM, the experiments were performed 3 times in triplicate. Asterisks (*) represent the correlation significant at the $p \leq 0.05$ level w.r.t. control, One-way Anova.