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Supplementary data

Application of copper (I) selective ligands for PET imaging of reactive oxygen species through metabolic trapping

Tetsuro Tada ^a, Yuki Mizuno ^{b, c, *}, Yuki Shibata ^b, Hironobu Yasui ^{d, e}, Yuji Kuge ^{b, c}

a. Graduate School of Biomedical Science and Engineering, Hokkaido University, Hokkaido 060-0815, Japan

b. Central Institute of Isotope Science, Hokkaido University, Hokkaido 060-0815, Japan

c. Global Center for Biomedical Science and Engineering, Hokkaido University, Hokkaido 060-0815, Japan

d. Faculty of Veterinary Medicine, Hokkaido University, Hokkaido 060-0818, JAPAN

e. One Health Research Center, Hokkaido University, Hokkaido 060-0818, JAPAN

ESI-MS of [^{nat}Cu][Cu^I(BCA)₂]³⁻ and [^{nat}Cu][Cu^I(BCS)₂]³⁻ (Figures S1 and S2)

HPLC chromatograms of BCA, BCS, [^{nat/64}Cu][Cu^I(BCA)₂]³⁻, and [^{nat/64}Cu][Cu^I(BCS)₂]³⁻ (Figures S3-S8)

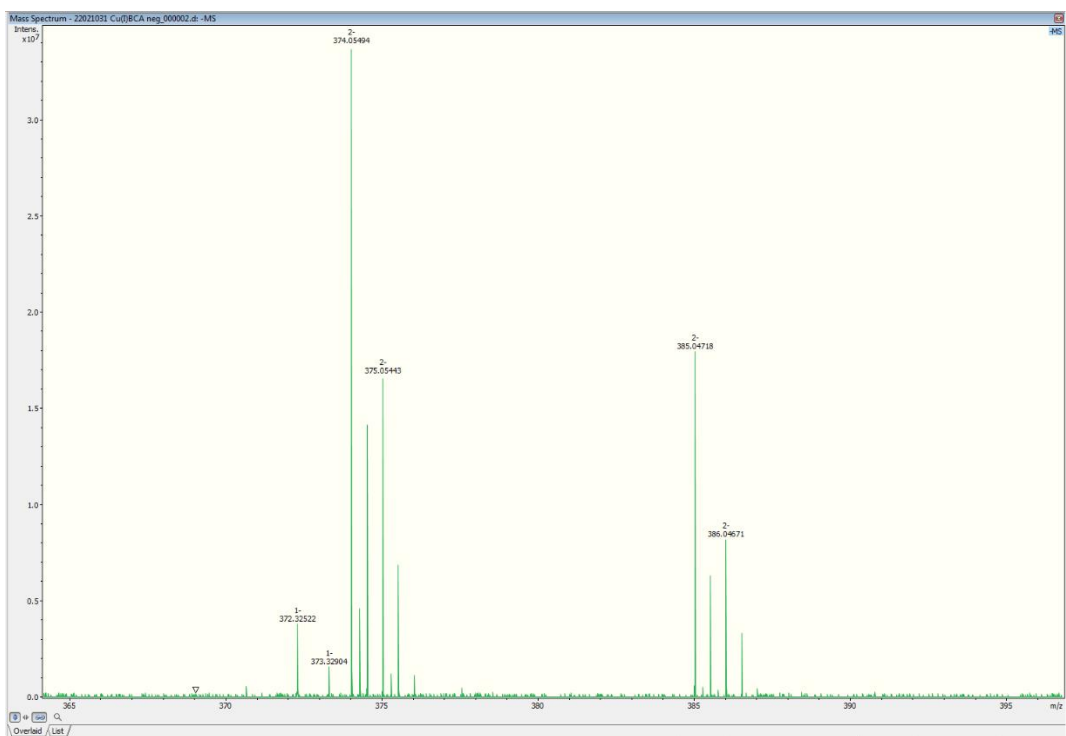
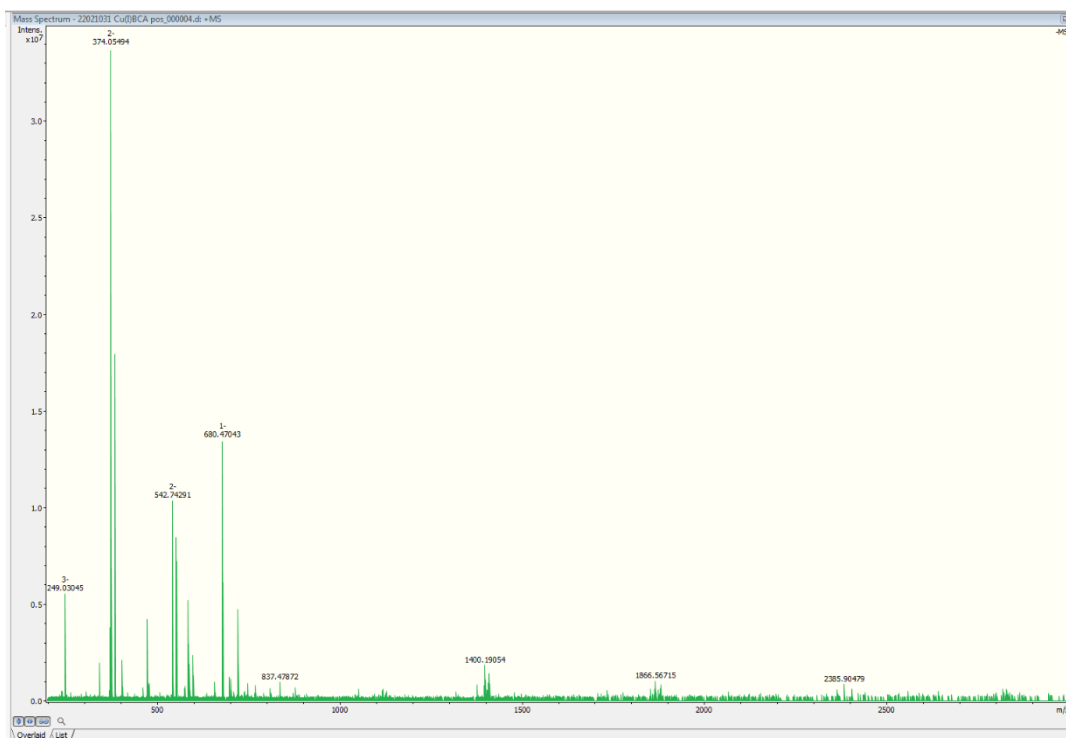


Figure S1. ESI-MS of $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCA})_2]^{3-}$. Calculated for $\text{C}_{40}\text{H}_{21}\text{CuN}_4\text{O}_8$, 374.04; found 374.05 $[\text{M} - 3\text{H}]^{2-}$.

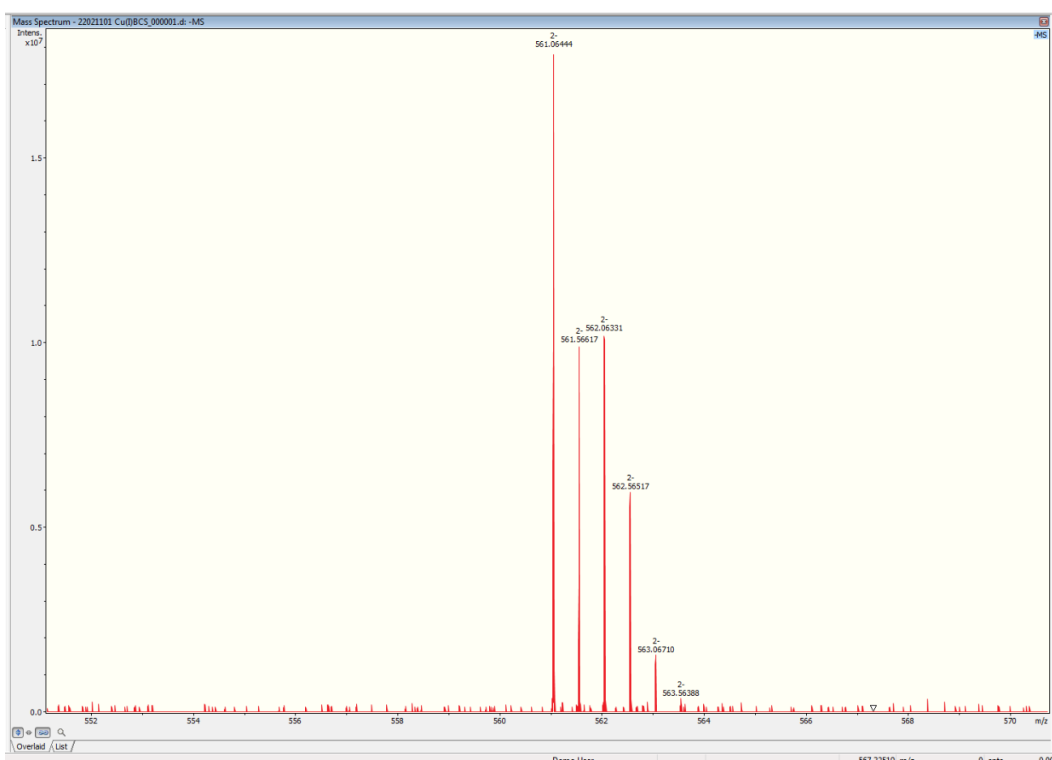
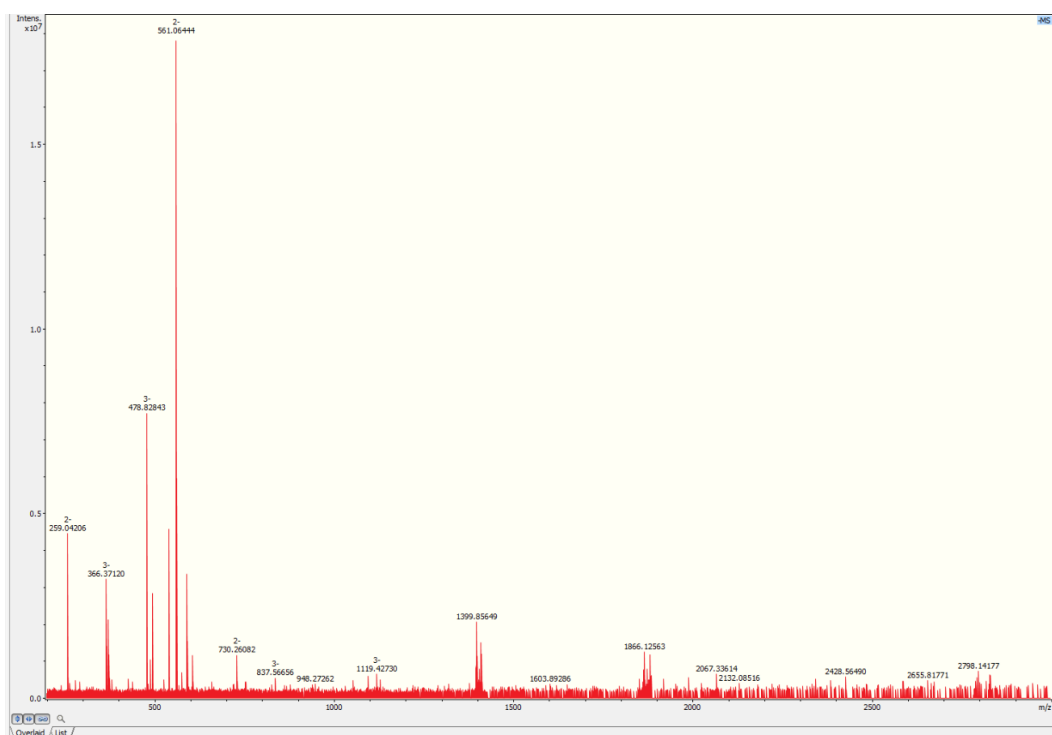


Figure S2. ESI-MS of $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCS})_2]^{3-}$. Calculated for $\text{C}_{52}\text{H}_{36}\text{CuN}_4\text{NaO}_{12}\text{S}_4$, 561.02; found 561.06 $[\text{M} - 3\text{Na}]^{2-}$.

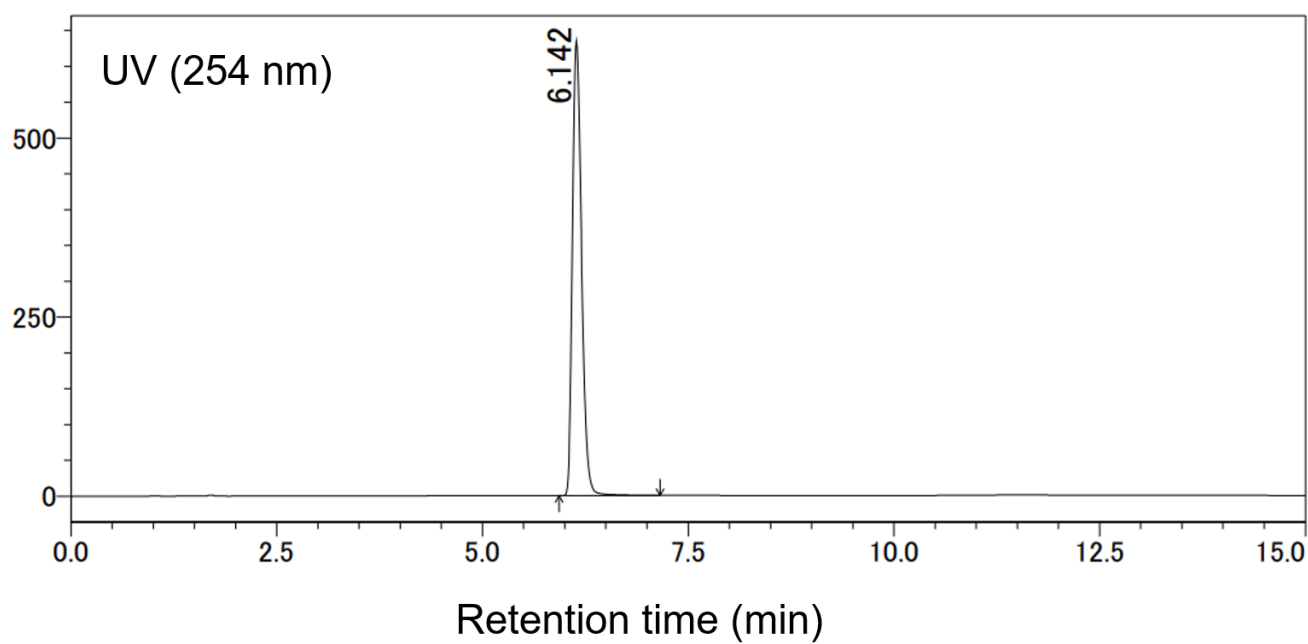


Figure S3. HPLC analysis of BCA (2 nmol).

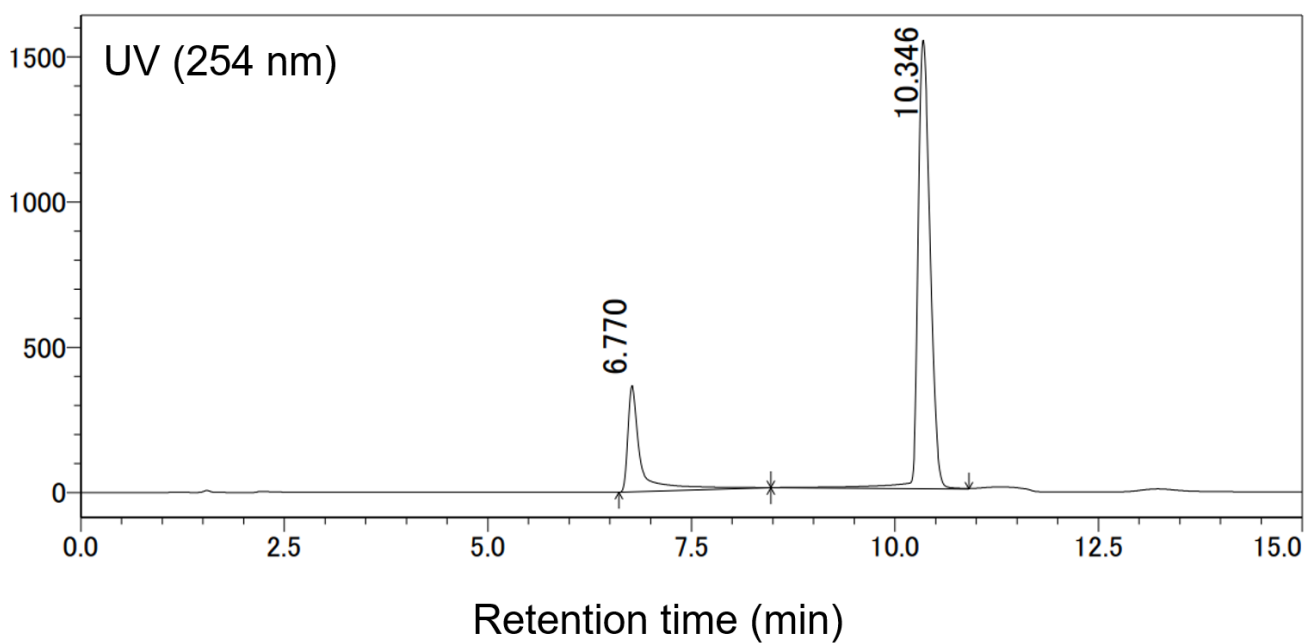


Figure S4. HPLC analysis of $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCA})_2]^{3-}$ (10 nmol).

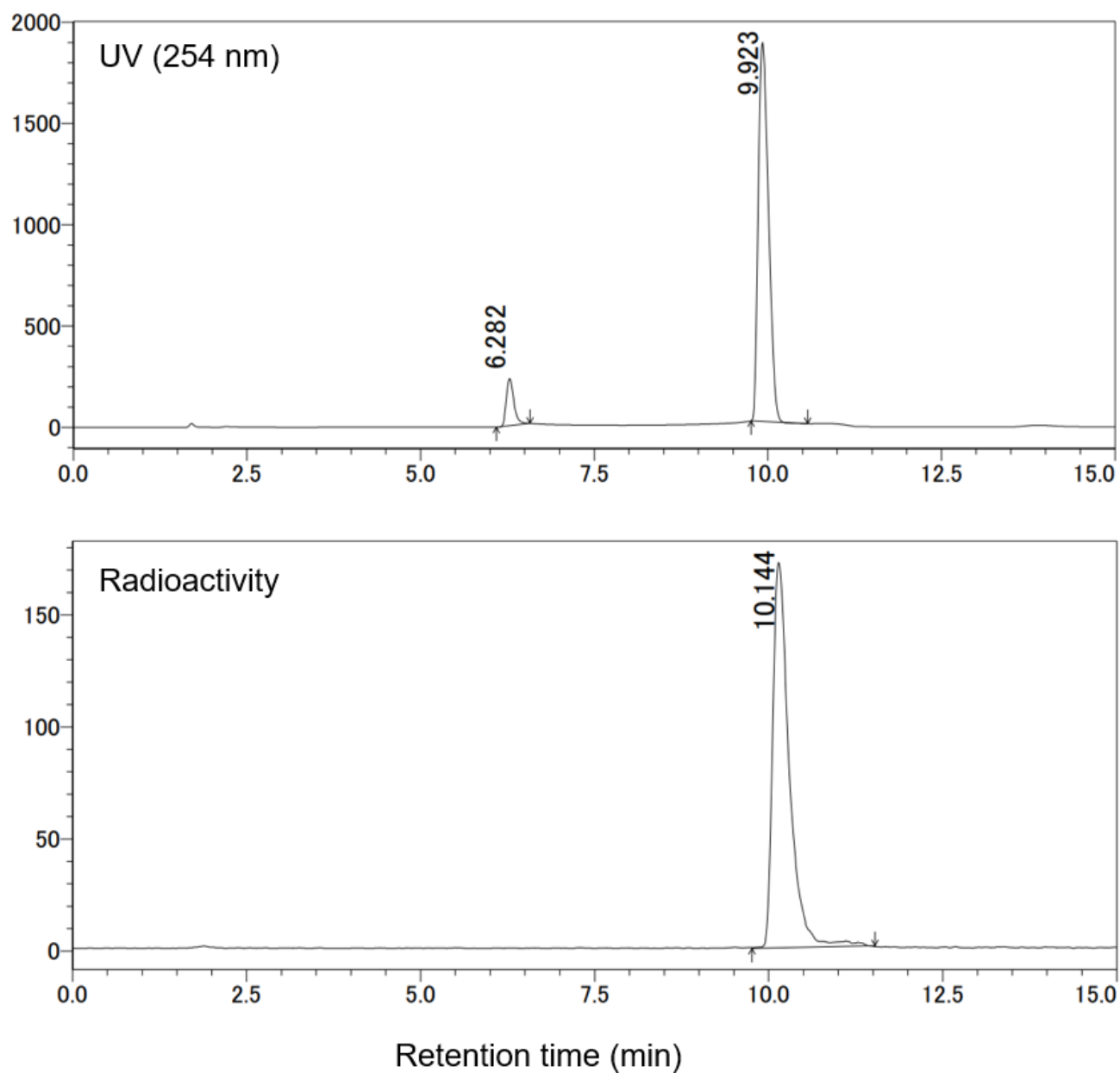


Figure S5. HPLC analysis of a ^{64}Cu -labeling reaction solution of BCA. $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCA})_2]^{3-}$ (10 nmol) was co-injected as a standard.

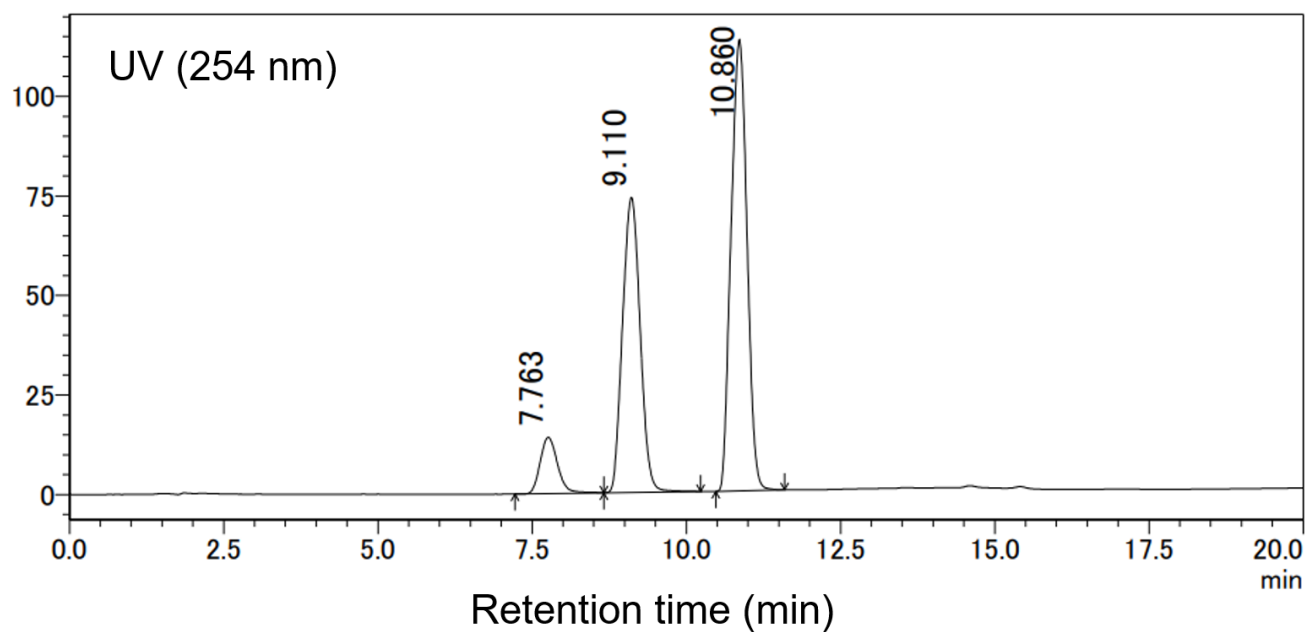


Figure S6. HPLC analysis of BCS (2 nmol).

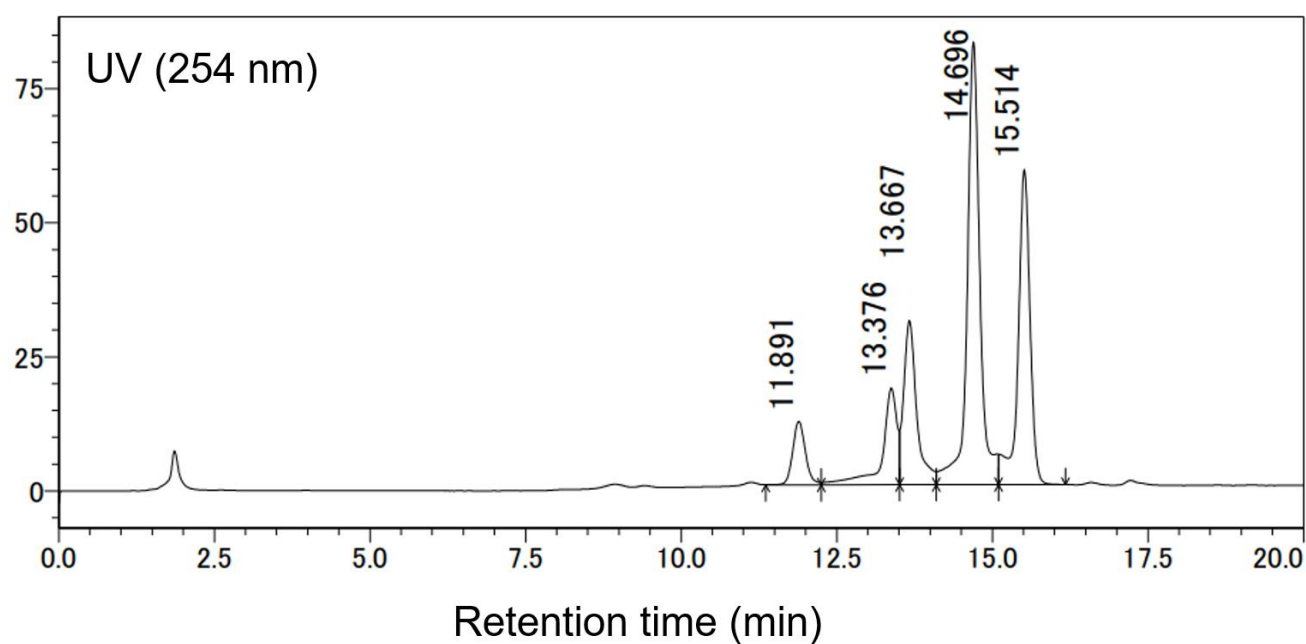


Figure S7. HPLC analysis of $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCS})_2]^{3-}$ (1 nmol).

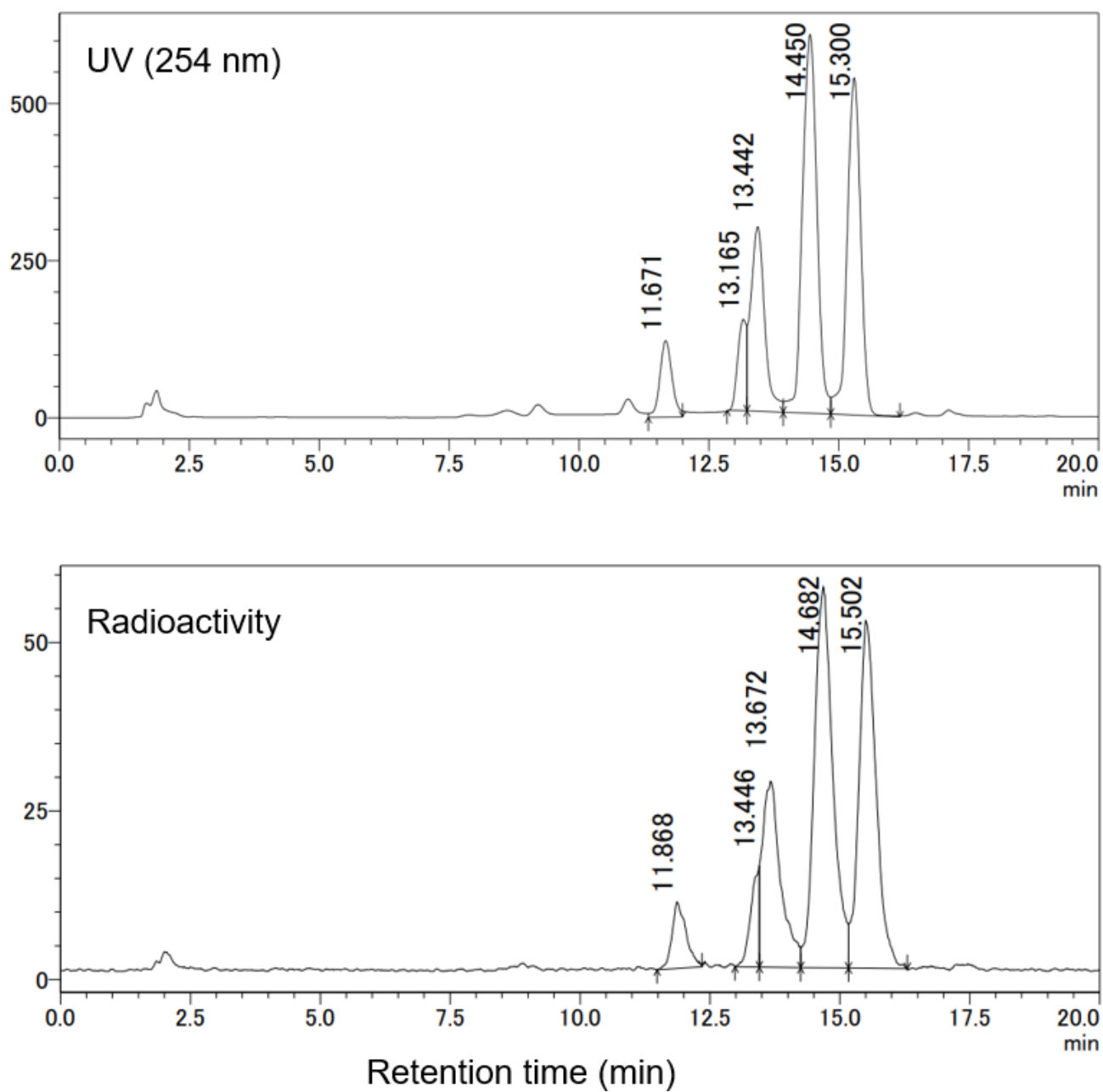


Figure S8. HPLC analysis of a ^{64}Cu -labeling reaction solution of BCS. $[\text{natCu}][\text{Cu}^{\text{I}}(\text{BCS})_2]^{3-}$ (10 nmol) was co-injected as a standard.